Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 11:55 AM EDT

PDB ID	:	4B4O
Title	:	Crystal Structure of human epimerase family protein SDR39U1 (isoform2) with NADPH
Authors	:	Vollmar, M.; Muniz, J.R.C.; Shafqat, N.; Picaud, S.; Krojer, T.; Chaikuad, A.; Pike, A.C.W.; Yue, W.W.; Filippakopoulos, P.; Kavanagh, K.L.; von Delft, F.; Weigelt, J.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.; Oppermann, U.
Deposited on	:	2012-07-31
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

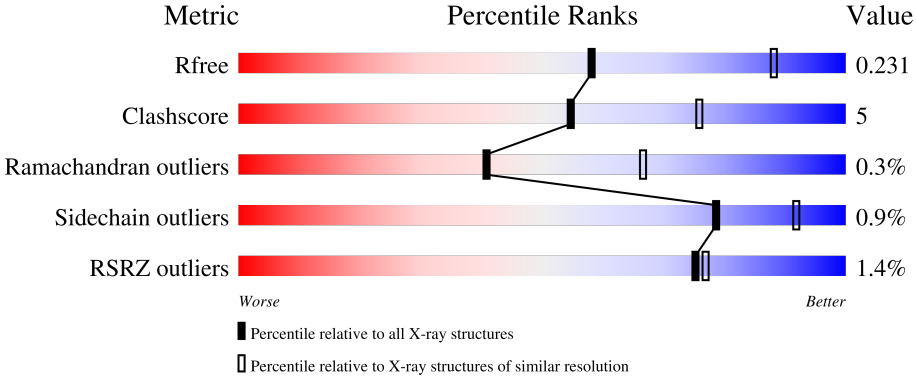
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	298	2%, 87%, 11%
1	B	298	84%, 15%
1	C	298	%, 87%, 11%
1	D	298	%, 88%, 10%
1	E	298	3%, 87%, 11%

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Mol	Chain	Length	Quality of chain
1	F	298	% 91% 7% •
1	G	298	% 86% 12% ••
1	H	298	% 88% 10% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18478 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 EPIMERASE FAMILY PROTEIN SDR39U1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	295	2192	1402	385	400	1	4	0	2	0
1	B	295	2190	1401	388	396	1	4	0	0	0
1	C	295	2176	1391	380	400	1	4	0	1	0
1	D	295	2181	1392	384	400	1	4	0	0	0
1	E	295	2185	1398	389	393	1	4	0	1	0
1	F	295	2179	1392	381	401	1	4	0	1	0
1	G	294	2171	1389	384	393	1	4	0	1	0
1	H	295	2148	1379	375	389	1	4	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ALA	-	expression tag	UNP Q9NRG7
A	293	GLU	-	expression tag	UNP Q9NRG7
A	294	ASN	-	expression tag	UNP Q9NRG7
A	295	LEU	-	expression tag	UNP Q9NRG7
A	296	TYR	-	expression tag	UNP Q9NRG7
A	297	PHE	-	expression tag	UNP Q9NRG7
A	298	GLN	-	expression tag	UNP Q9NRG7
A	79	LEU	ILE	engineered mutation	UNP Q9NRG7
A	232	PHE	LEU	engineered mutation	UNP Q9NRG7
A	270	ARG	GLN	engineered mutation	UNP Q9NRG7
B	292	ALA	-	expression tag	UNP Q9NRG7
B	293	GLU	-	expression tag	UNP Q9NRG7
B	294	ASN	-	expression tag	UNP Q9NRG7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	295	LEU	-	expression tag	UNP Q9NRG7
B	296	TYR	-	expression tag	UNP Q9NRG7
B	297	PHE	-	expression tag	UNP Q9NRG7
B	298	GLN	-	expression tag	UNP Q9NRG7
B	79	LEU	ILE	engineered mutation	UNP Q9NRG7
B	232	PHE	LEU	engineered mutation	UNP Q9NRG7
B	270	ARG	GLN	engineered mutation	UNP Q9NRG7
C	292	ALA	-	expression tag	UNP Q9NRG7
C	293	GLU	-	expression tag	UNP Q9NRG7
C	294	ASN	-	expression tag	UNP Q9NRG7
C	295	LEU	-	expression tag	UNP Q9NRG7
C	296	TYR	-	expression tag	UNP Q9NRG7
C	297	PHE	-	expression tag	UNP Q9NRG7
C	298	GLN	-	expression tag	UNP Q9NRG7
C	79	LEU	ILE	engineered mutation	UNP Q9NRG7
C	232	PHE	LEU	engineered mutation	UNP Q9NRG7
C	270	ARG	GLN	engineered mutation	UNP Q9NRG7
D	292	ALA	-	expression tag	UNP Q9NRG7
D	293	GLU	-	expression tag	UNP Q9NRG7
D	294	ASN	-	expression tag	UNP Q9NRG7
D	295	LEU	-	expression tag	UNP Q9NRG7
D	296	TYR	-	expression tag	UNP Q9NRG7
D	297	PHE	-	expression tag	UNP Q9NRG7
D	298	GLN	-	expression tag	UNP Q9NRG7
D	79	LEU	ILE	engineered mutation	UNP Q9NRG7
D	232	PHE	LEU	engineered mutation	UNP Q9NRG7
D	270	ARG	GLN	engineered mutation	UNP Q9NRG7
E	292	ALA	-	expression tag	UNP Q9NRG7
E	293	GLU	-	expression tag	UNP Q9NRG7
E	294	ASN	-	expression tag	UNP Q9NRG7
E	295	LEU	-	expression tag	UNP Q9NRG7
E	296	TYR	-	expression tag	UNP Q9NRG7
E	297	PHE	-	expression tag	UNP Q9NRG7
E	298	GLN	-	expression tag	UNP Q9NRG7
E	79	LEU	ILE	engineered mutation	UNP Q9NRG7
E	232	PHE	LEU	engineered mutation	UNP Q9NRG7
E	270	ARG	GLN	engineered mutation	UNP Q9NRG7
F	292	ALA	-	expression tag	UNP Q9NRG7
F	293	GLU	-	expression tag	UNP Q9NRG7
F	294	ASN	-	expression tag	UNP Q9NRG7
F	295	LEU	-	expression tag	UNP Q9NRG7
F	296	TYR	-	expression tag	UNP Q9NRG7

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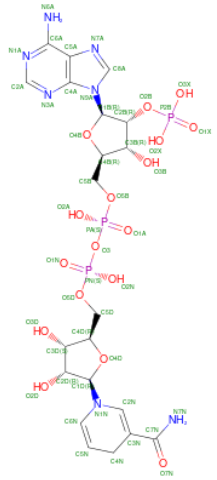
Chain	Residue	Modelled	Actual	Comment	Reference
F	297	PHE	-	expression tag	UNP Q9NRG7
F	298	GLN	-	expression tag	UNP Q9NRG7
F	79	LEU	ILE	engineered mutation	UNP Q9NRG7
F	232	PHE	LEU	engineered mutation	UNP Q9NRG7
F	270	ARG	GLN	engineered mutation	UNP Q9NRG7
G	292	ALA	-	expression tag	UNP Q9NRG7
G	293	GLU	-	expression tag	UNP Q9NRG7
G	294	ASN	-	expression tag	UNP Q9NRG7
G	295	LEU	-	expression tag	UNP Q9NRG7
G	296	TYR	-	expression tag	UNP Q9NRG7
G	297	PHE	-	expression tag	UNP Q9NRG7
G	298	GLN	-	expression tag	UNP Q9NRG7
G	79	LEU	ILE	engineered mutation	UNP Q9NRG7
G	232	PHE	LEU	engineered mutation	UNP Q9NRG7
G	270	ARG	GLN	engineered mutation	UNP Q9NRG7
H	292	ALA	-	expression tag	UNP Q9NRG7
H	293	GLU	-	expression tag	UNP Q9NRG7
H	294	ASN	-	expression tag	UNP Q9NRG7
H	295	LEU	-	expression tag	UNP Q9NRG7
H	296	TYR	-	expression tag	UNP Q9NRG7
H	297	PHE	-	expression tag	UNP Q9NRG7
H	298	GLN	-	expression tag	UNP Q9NRG7
H	79	LEU	ILE	engineered mutation	UNP Q9NRG7
H	232	PHE	LEU	engineered mutation	UNP Q9NRG7
H	270	ARG	GLN	engineered mutation	UNP Q9NRG7

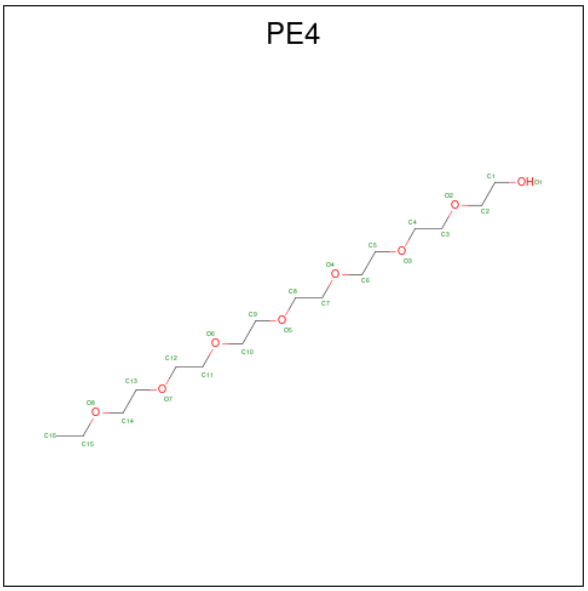
- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

NDP



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

- Molecule 3 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	19	12	7	0	0
3	B	1	19	12	7	0	0
3	C	1	19	12	7	0	0
3	D	1	19	12	7	0	0
3	E	1	19	12	7	0	0
3	F	1	19	12	7	0	0
3	G	1	19	12	7	0	0
3	H	1	19	12	7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	89	89	89	0	0
4	B	83	83	83	0	0
4	C	74	74	74	0	0
4	D	66	66	66	0	0

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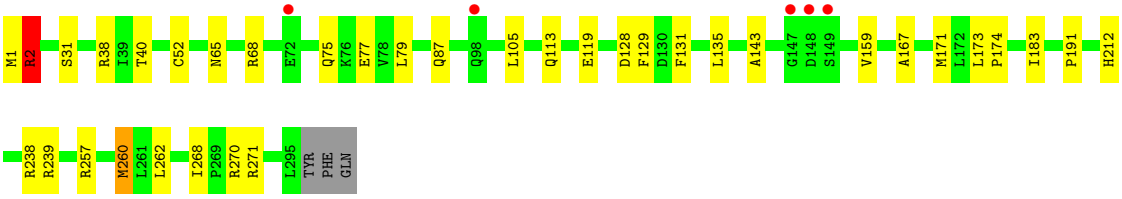
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	46	46	46	0	0
			Total	O		
4	F	52	52	52	0	0
			Total	O		
4	G	60	60	60	0	0
			Total	O		
4	H	50	50	50	0	0

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.

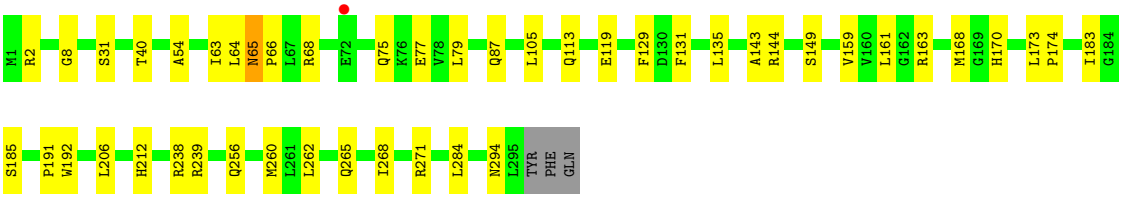
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1

Chain A:



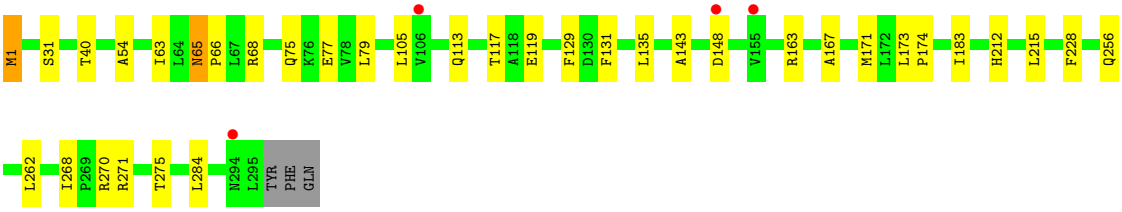
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1

Chain B:



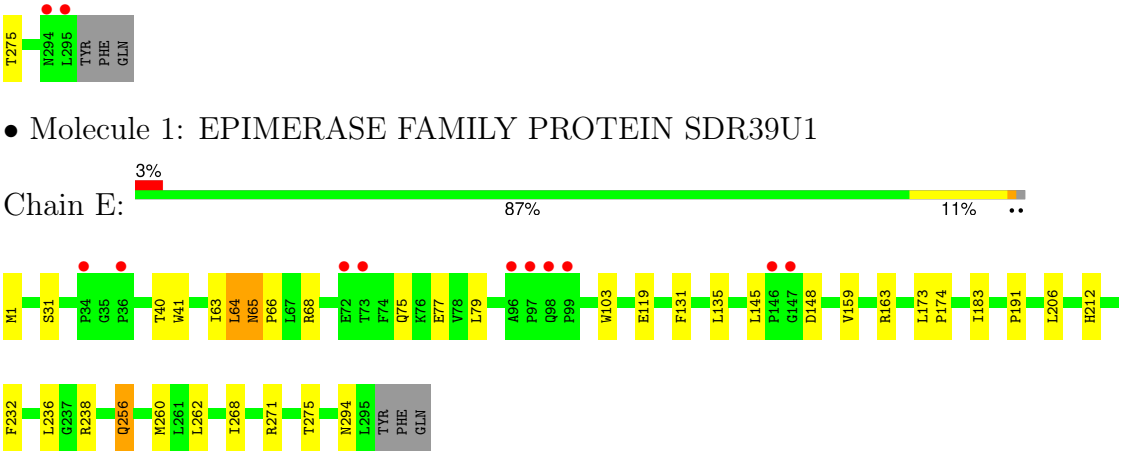
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1

Chain C:



• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1

Chain D:


T275
N294
L295
TYR
PHE
GLN
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1
Chain E:
3%
87%
11%
M1 S31 P34 G35 P36 T40 W41 I63 L64 N65 P66 L67 R68 E72 T73 F74 Q75 K76 E77 V78 L79 A96 P97 Q98 P99 W103 E119 F131 L135 L145 P146 G147 D148 V159 R163 L173 P174 I183 P191 L206 H212
F232 L236 G237 R238 Q256 M260 L261 L262 I268 R271 T275 N294 L295 TYR PHE GLN
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1
Chain F:
%
91%
7%
M1 H25 S31 T40 S47 I63 L64 N65 E72 Q75 K76 E77 V78 L79 L105 Q113 F129 D130 F131 L135 A143 R151 L173 P174 H212 Q256 R270 R271 E293 N294 L295 TYR PHE GLN
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1
Chain G:
%
86%
12%
M1 H25 S31 T40 W41 I63 L64 N65 P66 L67 R68 E72 T73 F74 Q75 K76 E77 V78 L79 T85 W103 V104 L105 Q113 E119 P125 F129 D130 F131 F132 L135 A143 G147 D148 V159 A167 M171 L172 L173 P174 E207
H212 Q256 M260 Q265 I268 P269 R270 R271 T275 N294 LEU TYR PHE GLN
• Molecule 1: EPIMERASE FAMILY PROTEIN SDR39U1
Chain H:
%
88%
10%
M1 I12 H25 S31 T40 I63 L64 N65 P66 L67 R68 M71 E72 Q75 K76 E77 V78 L79 P97 W103 Q113 E119 F129 D130 F131 L135 A167 M171 L172 L173 P174 I183 N209 H212 F232 L236 Q256 L262
I268 R271 N294 L295 TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.82Å 83.36Å 105.19Å 89.93° 76.73° 71.52°	Depositor
Resolution (Å)	102.07 – 2.70 29.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (102.07-2.70) 98.3 (29.76-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.60 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.198 , 0.231 0.200 , 0.231	Depositor DCC
R_{free} test set	3466 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18478	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP, PE4

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	0.64	0/2247	0.77	4/3058 (0.1%)
1	B	0.67	1/2239 (0.0%)	0.74	1/3047 (0.0%)
1	C	0.62	0/2227	0.74	4/3033 (0.1%)
1	D	0.64	1/2229 (0.0%)	0.72	2/3034 (0.1%)
1	E	0.63	2/2237 (0.1%)	0.70	1/3045 (0.0%)
1	F	0.64	0/2230	0.71	1/3037 (0.0%)
1	G	0.65	1/2222 (0.0%)	0.72	2/3024 (0.1%)
1	H	0.62	1/2197 (0.0%)	0.71	0/2997
All	All	0.64	6/17828 (0.0%)	0.73	15/24275 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	103	TRP	CD2-CE2	6.04	1.48	1.41
1	E	41	TRP	CD2-CE2	5.33	1.47	1.41
1	D	103	TRP	CD2-CE2	5.16	1.47	1.41
1	B	149	SER	CA-CB	5.14	1.60	1.52
1	H	103	TRP	CD2-CE2	5.05	1.47	1.41
1	G	103	TRP	CD2-CE2	5.05	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	D	270	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	G	270[A]	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	G	270[B]	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	F	270	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	270	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	238	ARG	CG-CD-NE	-6.82	97.49	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	1	MSE	CG-SE-CE	-6.26	85.13	98.90
1	D	88	LEU	CB-CG-CD2	-6.04	100.74	111.00
1	E	238	ARG	CG-CD-NE	-5.33	100.60	111.80
1	B	238	ARG	CG-CD-NE	-5.17	100.93	111.80
1	C	148	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	260	MSE	CG-SE-CE	-5.15	87.58	98.90
1	C	215	LEU	CB-CG-CD1	-5.13	102.28	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2173	20	0
1	B	2190	0	2177	33	0
1	C	2176	0	2143	25	0
1	D	2181	0	2161	18	0
1	E	2185	0	2164	24	0
1	F	2179	0	2147	16	0
1	G	2171	0	2158	29	0
1	H	2148	0	2098	20	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	2	0
2	E	48	0	26	0	0
2	F	48	0	26	2	0
2	G	48	0	26	3	0
2	H	48	0	26	2	0
3	A	19	0	25	0	0
3	B	19	0	25	1	0
3	C	19	0	25	2	0
3	D	19	0	25	3	0
3	E	19	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	19	0	25	3	0
3	G	19	0	25	6	0
3	H	19	0	25	2	0
4	A	89	0	0	2	0
4	B	83	0	0	7	0
4	C	74	0	0	1	0
4	D	66	0	0	1	0
4	E	46	0	0	4	0
4	F	52	0	0	1	0
4	G	60	0	0	2	0
4	H	50	0	0	0	0
All	All	18478	0	17629	186	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 5.

All (186) 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:E:163:ARG:HD3	1:E:294:ASN:O	1.70	0.91
1:D:63:ILE:HD12	3:D:1296:PE4:H21	1.52	0.88
1:A:270:ARG:HD3	1:D:148:ASP:O	1.74	0.86
1:E:260:MSE:HE3	3:E:1296:PE4:O3	1.82	0.79
1:B:163:ARG:CD	1:B:294:ASN:O	2.34	0.75
1:B:8:GLY:O	4:B:2003:HOH:O	2.05	0.74
1:E:163:ARG:CD	1:E:294:ASN:O	2.35	0.73
1:H:12:ILE:HD12	2:H:999:NDP:H51N	1.71	0.73
1:B:163:ARG:HD2	1:B:294:ASN:O	1.90	0.72
1:A:239:ARG:NH2	4:A:2041:HOH:O	2.23	0.71
1:H:63:ILE:HD12	3:H:1296:PE4:H21	1.73	0.71
1:C:79:LEU:HD12	1:C:135:LEU:CD1	2.24	0.68
1:E:163:ARG:O	4:E:2020:HOH:O	2.11	0.68
1:G:1:MSE:HE3	1:G:25:HIS:CE1	2.29	0.67
1:D:1:MSE:HE2	1:D:25:HIS:CE1	2.29	0.67
1:G:63:ILE:HD12	3:G:1295:PE4:C2	2.25	0.65
1:A:257:ARG:HA	1:A:260:MSE:HE2	1.79	0.65
1:B:163:ARG:HD3	1:B:294:ASN:O	1.96	0.65
1:B:64:LEU:HD13	1:B:260:MSE:CE	2.27	0.64
1:G:63:ILE:HD12	3:G:1295:PE4:H21	1.78	0.63
1:F:212:HIS:O	1:F:271:ARG:NH2	2.30	0.63
1:G:212:HIS:O	1:G:271:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MSE:HE2	1:F:25:HIS:CE1	2.32	0.63
1:H:212:HIS:O	1:H:271:ARG:NH2	2.32	0.62
1:D:212:HIS:O	1:D:271:ARG:NH2	2.32	0.62
1:C:212:HIS:O	1:C:271:ARG:NH2	2.33	0.62
1:B:144:ARG:HD3	4:B:2034:HOH:O	1.98	0.62
1:G:132:PHE:CE2	1:G:260:MSE:HE2	2.35	0.62
1:C:167:ALA:HB1	1:C:171:MSE:HE2	1.81	0.62
1:B:212:HIS:O	1:B:271:ARG:NH2	2.32	0.62
1:G:132:PHE:CZ	1:G:260:MSE:HE2	2.34	0.62
1:A:212:HIS:O	1:A:271:ARG:NH2	2.33	0.61
1:E:212:HIS:O	1:E:271:ARG:NH2	2.34	0.60
2:G:999:NDP:H41N	3:G:1295:PE4:H31	1.83	0.60
1:B:64:LEU:HD13	1:B:260:MSE:HE1	1.82	0.60
1:B:163:ARG:O	4:B:2040:HOH:O	2.17	0.60
1:E:145:LEU:O	4:E:2016:HOH:O	2.16	0.59
1:F:212:HIS:CE1	1:G:125:PRO:HD3	2.36	0.59
1:B:159:VAL:HG23	1:B:191:PRO:O	2.03	0.58
1:H:119:GLU:CD	1:H:268:ILE:HD11	2.25	0.57
1:H:12:ILE:HD12	2:H:999:NDP:C5D	2.34	0.56
1:B:79:LEU:HD12	1:B:135:LEU:HD13	1.88	0.56
1:B:163:ARG:NH1	4:B:2041:HOH:O	2.38	0.56
1:D:63:ILE:HD12	3:D:1296:PE4:C2	2.28	0.56
1:A:159:VAL:HG23	1:A:191:PRO:O	2.06	0.56
1:E:63:ILE:HD12	3:E:1296:PE4:H21	1.88	0.56
1:D:79:LEU:HD12	1:D:135:LEU:CD1	2.37	0.55
1:B:63:ILE:HD12	3:B:1296:PE4:H21	1.88	0.55
1:A:167:ALA:HB1	1:A:171:MSE:HE2	1.88	0.55
1:G:167:ALA:HB1	1:G:171:MSE:HE2	1.89	0.55
1:G:79:LEU:HD12	1:G:135:LEU:CD1	2.36	0.54
1:F:79:LEU:HD12	1:F:135:LEU:CD1	2.37	0.54
1:H:183:ILE:HG22	1:H:262:LEU:HD23	1.90	0.54
1:F:212:HIS:CG	1:G:125:PRO:HB3	2.43	0.53
1:G:1:MSE:HE1	1:G:207:GLU:HG2	1.90	0.53
1:D:119:GLU:CD	1:D:268:ILE:HD11	2.30	0.52
1:B:119:GLU:CD	1:B:268:ILE:HD11	2.30	0.52
1:G:79:LEU:HD12	1:G:135:LEU:HD12	1.91	0.52
1:H:63:ILE:HD12	3:H:1296:PE4:C2	2.39	0.51
1:D:79:LEU:HD12	1:D:135:LEU:HD12	1.93	0.51
1:E:1:MSE:HE1	1:E:206:LEU:O	2.10	0.51
1:G:63:ILE:HD12	3:G:1295:PE4:H22	1.92	0.51
1:G:105:LEU:HD22	1:G:143:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:LEU:HD12	1:H:135:LEU:CD1	2.41	0.50
1:A:2:ARG:HG2	1:A:52:CYS:HA	1.94	0.50
1:A:183:ILE:HG22	1:A:262:LEU:HD23	1.93	0.50
2:F:999:NDP:C6N	3:F:1296:PE4:H11	2.42	0.50
1:C:1:MSE:CE	1:C:54:ALA:HB2	2.42	0.49
1:A:119:GLU:CD	1:A:268:ILE:HD11	2.32	0.49
1:B:183:ILE:HG22	1:B:262:LEU:HD23	1.93	0.49
1:B:105:LEU:HD22	1:B:143:ALA:HB2	1.94	0.49
1:B:170:HIS:ND1	4:B:2044:HOH:O	2.01	0.49
1:H:79:LEU:HD12	1:H:135:LEU:HD12	1.94	0.49
1:C:79:LEU:HD12	1:C:135:LEU:HD12	1.95	0.48
1:F:63:ILE:HD12	3:F:1296:PE4:C2	2.44	0.48
1:C:1:MSE:HE2	1:C:54:ALA:HB2	1.95	0.48
2:D:999:NDP:O2D	3:D:1296:PE4:H22	2.13	0.48
1:B:2:ARG:HH11	1:B:2:ARG:HG2	1.79	0.48
1:G:74:PHE:O	1:G:78:VAL:HG23	2.14	0.48
1:E:119:GLU:CD	1:E:268:ILE:HD11	2.34	0.48
1:B:79:LEU:HD12	1:B:135:LEU:CD1	2.43	0.47
1:C:79:LEU:HD12	1:C:135:LEU:HD13	1.96	0.47
1:C:63:ILE:HD12	3:C:1296:PE4:C2	2.44	0.47
2:D:999:NDP:H1B	4:D:2008:HOH:O	2.13	0.47
2:G:999:NDP:H1B	4:G:2008:HOH:O	2.14	0.47
1:A:105:LEU:HD22	1:A:143:ALA:HB2	1.95	0.47
1:C:163:ARG:O	4:C:2044:HOH:O	2.20	0.47
1:H:173:LEU:HB3	1:H:174:PRO:HD3	1.97	0.47
1:E:31:SER:O	1:E:40:THR:HA	2.15	0.47
1:B:239:ARG:NH2	4:B:2046:HOH:O	2.48	0.47
2:G:999:NDP:C5N	3:G:1295:PE4:H12	2.45	0.46
1:F:63:ILE:HD12	3:F:1296:PE4:H21	1.97	0.46
1:F:79:LEU:HD12	1:F:135:LEU:HD12	1.97	0.46
1:G:68:ARG:NH1	1:G:77:GLU:OE1	2.40	0.46
1:C:79:LEU:CD1	1:C:135:LEU:HD13	2.46	0.46
1:H:31:SER:O	1:H:40:THR:HA	2.16	0.46
1:H:232:PHE:CE1	1:H:236:LEU:HD11	2.51	0.46
1:A:31:SER:O	1:A:40:THR:HA	2.15	0.46
1:B:31:SER:O	1:B:40:THR:HA	2.15	0.46
1:C:105:LEU:HD22	1:C:143:ALA:HB2	1.97	0.46
1:D:161:LEU:HD22	1:D:168:MSE:HE2	1.98	0.46
1:B:173:LEU:HB3	1:B:174:PRO:HD3	1.98	0.46
1:A:79:LEU:HD12	1:A:135:LEU:HD12	1.98	0.45
1:B:161:LEU:HD22	1:B:168:MSE:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ILE:HG22	1:D:262:LEU:HD23	1.98	0.45
1:G:132:PHE:CZ	1:G:260:MSE:CE	2.99	0.45
1:G:159:VAL:HG22	3:G:1295:PE4:H52	1.98	0.45
1:G:119:GLU:CD	1:G:268:ILE:HD11	2.37	0.45
1:C:75:GLN:HG2	1:C:131:PHE:CE2	2.52	0.45
1:C:79:LEU:CD1	1:C:135:LEU:CD1	2.93	0.45
1:E:173:LEU:HB3	1:E:174:PRO:HD3	1.99	0.45
1:D:173:LEU:HB3	1:D:174:PRO:HD3	1.99	0.45
1:E:79:LEU:HD12	1:E:135:LEU:HD12	1.98	0.45
1:G:265:GLN:NE2	4:G:2056:HOH:O	2.49	0.45
1:E:64:LEU:HD12	1:E:64:LEU:HA	1.67	0.45
1:H:167:ALA:HB1	1:H:171:MSE:HE2	1.98	0.45
1:C:31:SER:O	1:C:40:THR:HA	2.17	0.44
1:F:31:SER:O	1:F:40:THR:HA	2.17	0.44
1:G:31:SER:O	1:G:40:THR:HA	2.17	0.44
1:A:38:ARG:NE	4:A:2007:HOH:O	2.25	0.44
1:D:31:SER:O	1:D:40:THR:HA	2.18	0.44
1:G:75:GLN:HG2	1:G:131:PHE:CE1	2.52	0.44
1:C:1:MSE:HE2	1:C:54:ALA:CB	2.48	0.44
1:E:260:MSE:HE3	3:E:1296:PE4:C4	2.47	0.44
1:C:113:GLN:HA	1:C:129:PHE:CZ	2.53	0.44
1:E:183:ILE:HG22	1:E:262:LEU:HD23	2.00	0.44
1:A:68:ARG:NH1	1:A:77[A]:GLU:OE1	2.40	0.44
1:A:173:LEU:HB3	1:A:174:PRO:HD3	2.00	0.44
1:F:77[B]:GLU:HA	1:F:77[B]:GLU:OE1	2.16	0.44
1:B:54:ALA:HB1	1:B:206:LEU:HD22	2.00	0.43
1:E:131:PHE:HB2	1:E:256:GLN:HE21	1.83	0.43
1:B:265:GLN:NE2	4:B:2072:HOH:O	2.51	0.43
1:E:148:ASP:CB	4:E:2017:HOH:O	2.66	0.43
1:A:260:MSE:HE3	1:A:260:MSE:HB2	1.72	0.43
1:G:271:ARG:O	1:G:275:THR:HG23	2.18	0.43
1:H:113:GLN:HA	1:H:129:PHE:CZ	2.53	0.43
1:C:173:LEU:HB3	1:C:174:PRO:HD3	2.00	0.43
1:F:173:LEU:HB3	1:F:174:PRO:HD3	2.00	0.43
1:G:131:PHE:HB2	1:G:256:GLN:HE21	1.83	0.43
1:B:185:SER:HB3	1:F:47:SER:HB2	2.00	0.43
1:D:113:GLN:HA	1:D:129:PHE:CZ	2.53	0.43
1:E:65:ASN:HA	1:E:66:PRO:HD2	1.92	0.43
1:G:105:LEU:HD22	1:G:143:ALA:CB	2.48	0.43
1:B:113:GLN:HA	1:B:129:PHE:CZ	2.54	0.43
1:D:75:GLN:HG2	1:D:131:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ARG:NH1	1:E:77:GLU:OE1	2.40	0.43
1:E:79:LEU:HD12	1:E:135:LEU:CD1	2.49	0.43
1:A:113:GLN:HA	1:A:129:PHE:CZ	2.54	0.43
1:A:128:ASP:OD2	1:B:212:HIS:CE1	2.72	0.43
1:F:113:GLN:HA	1:F:129:PHE:CZ	2.54	0.43
1:A:75:GLN:HG2	1:A:131:PHE:CE1	2.54	0.42
1:G:173:LEU:HB3	1:G:174:PRO:HD3	2.00	0.42
1:B:65:ASN:HA	1:B:66:PRO:HD2	1.89	0.42
1:D:65:ASN:HA	1:D:66:PRO:HD2	1.90	0.42
1:G:113:GLN:HA	1:G:129:PHE:CZ	2.55	0.42
1:C:183:ILE:HG22	1:C:262:LEU:HD23	2.00	0.42
1:G:65:ASN:HA	1:G:66:PRO:HD2	1.89	0.42
1:B:64:LEU:CD1	1:B:260:MSE:CE	2.97	0.42
1:B:75:GLN:HG2	1:B:131:PHE:CE1	2.55	0.42
1:E:75:GLN:HG2	1:E:131:PHE:CE1	2.55	0.42
1:F:105:LEU:HD22	1:F:143:ALA:HB2	2.00	0.42
1:D:74:PHE:O	1:D:78:VAL:HG23	2.20	0.42
1:G:41:TRP:CH2	1:G:85:THR:HB	2.55	0.42
1:C:117:THR:HG22	1:H:97:PRO:HB3	2.02	0.41
1:E:159:VAL:HG23	1:E:191:PRO:O	2.19	0.41
1:E:271:ARG:O	1:E:275:THR:HG23	2.20	0.41
1:F:75:GLN:HG2	1:F:131:PHE:CE2	2.55	0.41
4:E:2017:HOH:O	1:H:209:ASN:ND2	2.50	0.41
1:F:151:ARG:HG3	1:F:212:HIS:CE1	2.56	0.41
1:H:1:MSE:HE2	1:H:25:HIS:CE1	2.55	0.41
1:C:119:GLU:CD	1:C:268:ILE:HD11	2.41	0.41
1:C:228:PHE:HA	1:C:284:LEU:HD21	2.03	0.41
1:C:63:ILE:HD12	3:C:1296:PE4:H21	2.02	0.41
1:D:41:TRP:CH2	1:D:85:THR:HB	2.56	0.41
1:D:271:ARG:O	1:D:275:THR:HG23	2.20	0.41
1:H:65:ASN:HA	1:H:66:PRO:HD2	1.91	0.41
1:E:232:PHE:CE1	1:E:236:LEU:HD11	2.56	0.41
1:A:257:ARG:HG2	1:A:260:MSE:HE1	2.02	0.40
1:B:192:TRP:CE2	1:B:284:LEU:HD13	2.57	0.40
1:H:75:GLN:HG2	1:H:131:PHE:CE1	2.56	0.40
1:C:65:ASN:HA	1:C:66:PRO:HD2	1.92	0.40
1:C:68:ARG:NH1	1:C:77:GLU:OE1	2.40	0.40
1:C:271:ARG:O	1:C:275:THR:HG23	2.21	0.40
2:F:999:NDP:H8A	4:F:2051:HOH:O	2.21	0.40
1:H:68:ARG:NH1	1:H:77:GLU:OE1	2.41	0.40
1:B:68:ARG:NH1	1:B:77:GLU:OE1	2.41	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	295/298 (99%)	289 (98%)	5 (2%)	1 (0%)	41	66
1	B	293/298 (98%)	288 (98%)	4 (1%)	1 (0%)	41	66
1	C	294/298 (99%)	289 (98%)	4 (1%)	1 (0%)	41	66
1	D	293/298 (98%)	289 (99%)	3 (1%)	1 (0%)	41	66
1	E	294/298 (99%)	289 (98%)	4 (1%)	1 (0%)	41	66
1	F	294/298 (99%)	288 (98%)	5 (2%)	1 (0%)	41	66
1	G	293/298 (98%)	289 (99%)	3 (1%)	1 (0%)	41	66
1	H	293/298 (98%)	286 (98%)	6 (2%)	1 (0%)	41	66
All	All	2349/2384 (98%)	2307 (98%)	34 (1%)	8 (0%)	41	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	B	65	ASN
1	F	65	ASN
1	G	65	ASN
1	C	65	ASN
1	D	65	ASN
1	E	65	ASN
1	H	65	ASN

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	218/224 (97%)	215 (99%)	3 (1%)	67	86
1	B	217/224 (97%)	215 (99%)	2 (1%)	78	92
1	C	214/224 (96%)	213 (100%)	1 (0%)	88	96
1	D	217/224 (97%)	215 (99%)	2 (1%)	78	92
1	E	214/224 (96%)	212 (99%)	2 (1%)	78	92
1	F	215/224 (96%)	213 (99%)	2 (1%)	78	92
1	G	214/224 (96%)	213 (100%)	1 (0%)	88	96
1	H	206/224 (92%)	204 (99%)	2 (1%)	76	91
All	All	1715/1792 (96%)	1700 (99%)	15 (1%)	78	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	ARG
1	A	87	GLN
1	B	87	GLN
1	B	256	GLN
1	C	256	GLN
1	D	1	MSE
1	D	256	GLN
1	E	64	LEU
1	E	256	GLN
1	F	1	MSE
1	F	256	GLN
1	G	256	GLN
1	H	1	MSE
1	H	256	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	HIS

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)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PE4	D	1296	-	18,18,23	1.77	3 (16%)	17,17,22	0.92	0
2	NDP	E	999	-	47,52,52	1.22	4 (8%)	61,80,80	1.45	13 (21%)
3	PE4	A	1296	-	18,18,23	1.68	4 (22%)	17,17,22	0.96	1 (5%)
2	NDP	G	999	-	47,52,52	1.19	4 (8%)	61,80,80	1.34	8 (13%)
3	PE4	B	1296	-	18,18,23	1.97	11 (61%)	17,17,22	0.96	1 (5%)
3	PE4	C	1296	-	18,18,23	1.91	6 (33%)	17,17,22	0.96	0
2	NDP	C	999	-	47,52,52	1.43	6 (12%)	61,80,80	1.37	6 (9%)
2	NDP	H	999	-	47,52,52	1.34	5 (10%)	61,80,80	1.59	13 (21%)
3	PE4	F	1296	-	18,18,23	1.96	8 (44%)	17,17,22	1.44	3 (17%)
2	NDP	D	999	-	47,52,52	1.31	5 (10%)	61,80,80	1.25	6 (9%)
2	NDP	F	999	-	47,52,52	1.42	7 (14%)	61,80,80	1.24	6 (9%)
2	NDP	B	999	-	47,52,52	1.28	6 (12%)	61,80,80	1.42	10 (16%)
2	NDP	A	999	-	47,52,52	1.28	5 (10%)	61,80,80	1.47	10 (16%)
3	PE4	E	1296	-	18,18,23	1.57	3 (16%)	17,17,22	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PE4	H	1296	-	18,18,23	1.85	5 (27%)	17,17,22	0.89	0
3	PE4	G	1295	-	18,18,23	1.60	2 (11%)	17,17,22	0.95	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PE4	D	1296	-	-	9/16/16/21	-
2	NDP	E	999	-	-	4/30/77/77	0/5/5/5
3	PE4	A	1296	-	-	9/16/16/21	-
2	NDP	G	999	-	-	1/30/77/77	0/5/5/5
3	PE4	B	1296	-	-	8/16/16/21	-
3	PE4	C	1296	-	-	9/16/16/21	-
2	NDP	C	999	-	-	4/30/77/77	0/5/5/5
2	NDP	H	999	-	-	2/30/77/77	0/5/5/5
3	PE4	F	1296	-	-	7/16/16/21	-
2	NDP	D	999	-	-	3/30/77/77	0/5/5/5
2	NDP	F	999	-	-	2/30/77/77	0/5/5/5
2	NDP	B	999	-	-	2/30/77/77	0/5/5/5
2	NDP	A	999	-	-	2/30/77/77	0/5/5/5
3	PE4	E	1296	-	-	12/16/16/21	-
3	PE4	H	1296	-	-	6/16/16/21	-
3	PE4	G	1295	-	-	13/16/16/21	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	999	NDP	PA-O3	4.51	1.64	1.59
2	F	999	NDP	PA-O3	4.50	1.64	1.59
2	D	999	NDP	PA-O3	4.14	1.64	1.59
2	E	999	NDP	P2B-O2B	4.12	1.66	1.59
2	H	999	NDP	PN-O3	4.01	1.63	1.59
2	C	999	NDP	C2A-N3A	3.95	1.38	1.32
2	A	999	NDP	P2B-O2B	3.75	1.66	1.59
2	C	999	NDP	PA-O3	3.70	1.63	1.59
2	B	999	NDP	PN-O3	3.60	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	999	NDP	O4B-C1B	3.60	1.45	1.40
2	C	999	NDP	O4B-C1B	3.45	1.45	1.40
2	F	999	NDP	P2B-O2B	3.40	1.65	1.59
2	F	999	NDP	C2A-N3A	3.39	1.37	1.32
2	C	999	NDP	P2B-O2B	3.38	1.65	1.59
2	G	999	NDP	P2B-O2B	3.33	1.65	1.59
2	D	999	NDP	PN-O3	3.27	1.63	1.59
2	C	999	NDP	PN-O3	3.17	1.62	1.59
2	A	999	NDP	C8A-N7A	3.15	1.40	1.34
3	H	1296	PE4	O3-C4	3.12	1.55	1.42
2	E	999	NDP	O4B-C1B	3.07	1.44	1.40
2	G	999	NDP	C2A-N3A	3.05	1.36	1.32
2	B	999	NDP	O4B-C1B	3.02	1.44	1.40
3	C	1296	PE4	O3-C4	2.94	1.54	1.42
3	B	1296	PE4	O3-C4	2.90	1.54	1.42
2	A	999	NDP	C4A-N3A	-2.81	1.31	1.35
2	H	999	NDP	C8A-N7A	2.79	1.39	1.34
3	C	1296	PE4	O5-C9	2.77	1.54	1.42
2	B	999	NDP	PA-O3	2.76	1.62	1.59
2	F	999	NDP	PN-O3	2.67	1.62	1.59
3	F	1296	PE4	C6-C5	2.66	1.62	1.49
3	C	1296	PE4	C4-C3	2.63	1.62	1.49
3	F	1296	PE4	O4-C6	2.61	1.53	1.42
2	F	999	NDP	O4B-C1B	2.60	1.44	1.40
2	B	999	NDP	P2B-O2B	2.60	1.64	1.59
2	A	999	NDP	PA-O3	2.59	1.62	1.59
2	E	999	NDP	PA-O3	2.57	1.62	1.59
3	D	1296	PE4	O5-C8	2.56	1.53	1.42
3	F	1296	PE4	O3-C4	2.55	1.53	1.42
2	F	999	NDP	C6N-C5N	2.48	1.40	1.33
3	E	1296	PE4	C8-C7	2.47	1.61	1.49
3	D	1296	PE4	O3-C4	2.46	1.52	1.42
2	F	999	NDP	P2B-O1X	2.44	1.58	1.50
2	G	999	NDP	PN-O3	2.43	1.62	1.59
3	B	1296	PE4	O4-C6	2.41	1.52	1.42
2	H	999	NDP	O4B-C1B	2.41	1.44	1.40
3	H	1296	PE4	C4-C3	2.39	1.61	1.49
3	G	1295	PE4	C6-C5	2.34	1.60	1.49
3	C	1296	PE4	C10-C9	2.34	1.60	1.49
2	B	999	NDP	C2A-N3A	2.30	1.35	1.32
3	D	1296	PE4	O6-C10	2.30	1.52	1.42
3	B	1296	PE4	C6-C5	2.28	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1296	PE4	C4-C3	2.28	1.60	1.49
2	C	999	NDP	C6N-C5N	2.27	1.40	1.33
2	D	999	NDP	P2B-O2B	2.25	1.63	1.59
3	F	1296	PE4	O5-C8	2.24	1.51	1.42
3	B	1296	PE4	C4-C3	2.23	1.60	1.49
3	A	1296	PE4	O5-C8	2.21	1.51	1.42
3	C	1296	PE4	C6-C5	2.20	1.60	1.49
2	G	999	NDP	O4B-C1B	2.19	1.43	1.40
3	H	1296	PE4	C2-C1	2.18	1.61	1.49
3	C	1296	PE4	O5-C8	2.17	1.51	1.42
3	G	1295	PE4	C8-C7	2.16	1.59	1.49
3	B	1296	PE4	C8-C7	2.14	1.59	1.49
3	B	1296	PE4	C10-C9	2.14	1.59	1.49
3	H	1296	PE4	C6-C5	2.14	1.59	1.49
2	A	999	NDP	C2A-N3A	2.11	1.35	1.32
3	B	1296	PE4	C2-C1	2.10	1.60	1.49
3	F	1296	PE4	C2-C1	2.09	1.60	1.49
3	A	1296	PE4	O3-C4	2.08	1.51	1.42
3	F	1296	PE4	O5-C9	2.08	1.51	1.42
3	A	1296	PE4	O7-C12	2.08	1.52	1.42
2	D	999	NDP	C2A-N3A	2.07	1.35	1.32
3	B	1296	PE4	O6-C10	2.07	1.51	1.42
3	H	1296	PE4	C11-C12	2.07	1.60	1.49
3	A	1296	PE4	C2-C1	2.06	1.60	1.49
3	E	1296	PE4	O3-C4	2.05	1.50	1.42
3	F	1296	PE4	O7-C12	2.04	1.52	1.42
3	B	1296	PE4	O3-C5	2.03	1.50	1.42
3	B	1296	PE4	C11-C12	2.02	1.60	1.49
2	B	999	NDP	C6N-C5N	2.02	1.39	1.33
3	B	1296	PE4	O5-C8	2.01	1.50	1.42
2	H	999	NDP	C1B-N9A	-2.01	1.45	1.49
2	E	999	NDP	C2N-C3N	2.00	1.40	1.35
3	E	1296	PE4	C2-C1	2.00	1.60	1.49

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	999	NDP	C1B-N9A-C4A	-5.03	117.80	126.64
2	C	999	NDP	N3A-C2A-N1A	-4.92	122.00	128.67
2	A	999	NDP	C1B-N9A-C4A	-4.48	118.78	126.64
2	H	999	NDP	N3A-C2A-N1A	-4.42	122.68	128.67
2	G	999	NDP	O3-PA-O1A	-4.15	98.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1296	PE4	C11-O6-C10	3.95	130.54	113.26
2	D	999	NDP	N3A-C2A-N1A	-3.88	123.41	128.67
2	F	999	NDP	O4B-C1B-N9A	-3.80	103.71	108.75
2	E	999	NDP	N3A-C2A-N1A	-3.57	123.82	128.67
2	F	999	NDP	N3A-C2A-N1A	-3.50	123.93	128.67
2	H	999	NDP	C6N-N1N-C2N	3.31	122.86	119.32
2	C	999	NDP	O4D-C1D-N1N	3.22	114.23	108.08
2	B	999	NDP	O3-PA-O1A	-3.22	101.02	110.70
2	B	999	NDP	C2B-C1B-N9A	-3.20	105.46	112.56
2	G	999	NDP	N3A-C2A-N1A	-3.15	124.40	128.67
2	B	999	NDP	N6A-C6A-N1A	3.12	125.00	118.33
2	B	999	NDP	N3A-C2A-N1A	-3.07	124.51	128.67
2	B	999	NDP	O2A-PA-O1A	3.06	126.67	112.44
2	A	999	NDP	O3-PA-O1A	-3.02	101.62	110.70
2	E	999	NDP	O2A-PA-O3	2.93	115.19	107.27
2	A	999	NDP	C2B-C1B-N9A	-2.90	106.11	112.56
2	A	999	NDP	N3A-C2A-N1A	-2.88	124.76	128.67
2	C	999	NDP	C4A-C5A-N7A	-2.86	106.31	109.34
2	D	999	NDP	O2N-PN-O3	2.86	114.99	107.27
2	H	999	NDP	O4B-C1B-N9A	-2.81	105.02	108.75
2	G	999	NDP	C3N-C2N-N1N	-2.81	119.08	123.20
2	H	999	NDP	C5A-C6A-N6A	-2.80	116.04	120.31
2	E	999	NDP	C1B-N9A-C4A	-2.80	121.73	126.64
2	E	999	NDP	C4B-O4B-C1B	-2.76	107.39	109.92
2	D	999	NDP	O3-PA-O1A	-2.75	102.42	110.70
2	E	999	NDP	O2N-PN-O1N	2.70	125.02	112.44
2	G	999	NDP	C1D-N1N-C6N	-2.70	115.07	120.77
2	E	999	NDP	O4B-C1B-C2B	2.68	111.18	106.61
2	A	999	NDP	O3X-P2B-O2X	2.64	117.70	107.80
2	C	999	NDP	O2N-PN-O3	2.59	114.28	107.27
2	E	999	NDP	C2B-C1B-N9A	-2.54	106.91	112.56
2	G	999	NDP	O2A-PA-O1A	2.53	124.21	112.44
2	E	999	NDP	O2B-P2B-O1X	-2.53	100.33	109.33
2	G	999	NDP	C6N-N1N-C2N	2.42	121.91	119.32
2	A	999	NDP	C4A-C5A-N7A	-2.41	106.79	109.34
2	A	999	NDP	O3X-P2B-O2B	-2.40	96.51	105.85
2	H	999	NDP	O4B-C1B-C2B	2.39	110.69	106.61
2	A	999	NDP	O4B-C1B-C2B	2.35	110.61	106.61
2	H	999	NDP	N6A-C6A-N1A	2.33	123.31	118.33
2	G	999	NDP	N6A-C6A-N1A	2.32	123.28	118.33
2	A	999	NDP	O2A-PA-O3	2.31	113.51	107.27
2	E	999	NDP	O2A-PA-O1A	2.29	123.11	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	999	NDP	O2B-P2B-O1X	-2.29	101.17	109.33
2	D	999	NDP	C6N-N1N-C2N	2.28	121.76	119.32
2	F	999	NDP	O2A-PA-O3	2.27	113.42	107.27
2	A	999	NDP	C6N-N1N-C2N	2.26	121.74	119.32
2	B	999	NDP	C1B-N9A-C4A	-2.26	122.68	126.64
2	H	999	NDP	C3N-C2N-N1N	-2.25	119.89	123.20
2	F	999	NDP	P2B-O2B-C2B	-2.24	117.44	123.43
2	E	999	NDP	C3N-C2N-N1N	-2.22	119.95	123.20
2	F	999	NDP	N6A-C6A-N1A	2.22	123.07	118.33
2	G	999	NDP	O4B-C1B-N9A	-2.22	105.81	108.75
2	E	999	NDP	O4D-C1D-N1N	2.20	112.28	108.08
2	E	999	NDP	O4B-C4B-C3B	2.19	109.50	105.15
2	H	999	NDP	C6A-C5A-C4A	-2.17	113.67	117.90
2	B	999	NDP	O4D-C1D-N1N	2.15	112.19	108.08
3	A	1296	PE4	C9-O5-C8	2.15	122.67	113.26
3	B	1296	PE4	O5-C8-C7	2.14	120.13	110.35
2	B	999	NDP	C3N-C2N-N1N	-2.14	120.06	123.20
2	E	999	NDP	C6N-N1N-C2N	2.14	121.61	119.32
2	D	999	NDP	C4A-C5A-N7A	-2.13	107.09	109.34
2	B	999	NDP	C5A-C6A-N6A	-2.12	117.09	120.31
3	F	1296	PE4	O4-C6-C5	2.09	119.86	110.35
2	B	999	NDP	C6N-N1N-C2N	2.08	121.54	119.32
3	G	1295	PE4	C7-O4-C6	2.08	122.35	113.26
2	H	999	NDP	O2B-C2B-C1B	-2.08	102.75	110.05
2	H	999	NDP	C4B-O4B-C1B	-2.07	108.03	109.92
3	F	1296	PE4	O5-C8-C7	2.06	119.73	110.35
2	F	999	NDP	C6N-N1N-C2N	2.05	121.51	119.32
2	D	999	NDP	O2A-PA-O1A	2.04	121.95	112.44
2	C	999	NDP	C6N-N1N-C2N	2.02	121.48	119.32
2	H	999	NDP	O2A-PA-O1A	2.00	121.76	112.44
2	C	999	NDP	C3N-C2N-N1N	-2.00	120.26	123.20

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	999	NDP	C5B-O5B-PA-O1A
3	E	1296	PE4	C1-C2-O2-C3
3	A	1296	PE4	C1-C2-O2-C3
3	A	1296	PE4	O3-C5-C6-O4
3	E	1296	PE4	O3-C5-C6-O4
3	G	1295	PE4	O6-C10-C9-O5

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Mol	Chain	Res	Type	Atoms
3	H	1296	PE4	O6-C10-C9-O5
3	B	1296	PE4	O6-C10-C9-O5
3	E	1296	PE4	O2-C3-C4-O3
3	G	1295	PE4	O3-C5-C6-O4
3	B	1296	PE4	O2-C3-C4-O3
3	E	1296	PE4	O6-C10-C9-O5
3	D	1296	PE4	C1-C2-O2-C3
3	C	1296	PE4	O3-C5-C6-O4
3	F	1296	PE4	O6-C10-C9-O5
3	A	1296	PE4	C10-C9-O5-C8
3	D	1296	PE4	O1-C1-C2-O2
3	G	1295	PE4	O2-C3-C4-O3
3	E	1296	PE4	C10-C9-O5-C8
3	C	1296	PE4	O6-C11-C12-O7
3	G	1295	PE4	O1-C1-C2-O2
3	H	1296	PE4	O3-C5-C6-O4
3	C	1296	PE4	O6-C10-C9-O5
3	B	1296	PE4	C1-C2-O2-C3
3	A	1296	PE4	O4-C7-C8-O5
3	B	1296	PE4	O6-C11-C12-O7
3	C	1296	PE4	O1-C1-C2-O2
3	F	1296	PE4	O6-C11-C12-O7
3	H	1296	PE4	O6-C11-C12-O7
3	D	1296	PE4	O3-C5-C6-O4
3	E	1296	PE4	C8-C7-O4-C6
3	D	1296	PE4	C9-C10-O6-C11
3	C	1296	PE4	C1-C2-O2-C3
3	B	1296	PE4	C5-C6-O4-C7
3	E	1296	PE4	O4-C7-C8-O5
3	C	1296	PE4	C5-C6-O4-C7
3	D	1296	PE4	C10-C9-O5-C8
3	C	1296	PE4	C8-C7-O4-C6
3	D	1296	PE4	C4-C3-O2-C2
3	A	1296	PE4	C12-C11-O6-C10
3	G	1295	PE4	C4-C3-O2-C2
3	G	1295	PE4	C1-C2-O2-C3
3	G	1295	PE4	C9-C10-O6-C11
3	G	1295	PE4	C3-C4-O3-C5
3	G	1295	PE4	C5-C6-O4-C7
3	G	1295	PE4	C7-C8-O5-C9
3	F	1296	PE4	C8-C7-O4-C6
3	F	1296	PE4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	C	1296	PE4	C7-C8-O5-C9
3	E	1296	PE4	C5-C6-O4-C7
3	D	1296	PE4	C3-C4-O3-C5
3	B	1296	PE4	C8-C7-O4-C6
2	D	999	NDP	O4D-C1D-N1N-C6N
2	G	999	NDP	O4D-C1D-N1N-C6N
3	F	1296	PE4	C7-C8-O5-C9
3	H	1296	PE4	O2-C3-C4-O3
3	G	1295	PE4	C8-C7-O4-C6
2	C	999	NDP	O4B-C4B-C5B-O5B
3	F	1296	PE4	O2-C3-C4-O3
3	E	1296	PE4	C3-C4-O3-C5
2	C	999	NDP	O4D-C1D-N1N-C6N
2	E	999	NDP	O4D-C1D-N1N-C6N
2	F	999	NDP	O4D-C1D-N1N-C6N
3	G	1295	PE4	O4-C7-C8-O5
2	A	999	NDP	O4D-C1D-N1N-C6N
3	A	1296	PE4	O6-C10-C9-O5
2	B	999	NDP	O4D-C1D-N1N-C6N
3	F	1296	PE4	C5-C6-O4-C7
3	E	1296	PE4	O6-C11-C12-O7
3	B	1296	PE4	C7-C8-O5-C9
2	A	999	NDP	O4D-C4D-C5D-O5D
2	D	999	NDP	C2N-C3N-C7N-N7N
2	H	999	NDP	O4D-C1D-N1N-C6N
3	E	1296	PE4	C7-C8-O5-C9
3	B	1296	PE4	C6-C5-O3-C4
3	E	1296	PE4	C6-C5-O3-C4
3	A	1296	PE4	C7-C8-O5-C9
3	H	1296	PE4	O1-C1-C2-O2
3	G	1295	PE4	C6-C5-O3-C4
2	E	999	NDP	O4B-C4B-C5B-O5B
2	E	999	NDP	PN-O3-PA-O2A
3	H	1296	PE4	O4-C7-C8-O5
3	A	1296	PE4	C8-C7-O4-C6
3	D	1296	PE4	O2-C3-C4-O3
3	C	1296	PE4	O2-C3-C4-O3
2	B	999	NDP	O4B-C4B-C5B-O5B
2	C	999	NDP	C3B-C4B-C5B-O5B
2	H	999	NDP	O4B-C4B-C5B-O5B
2	E	999	NDP	O4D-C4D-C5D-O5D
2	F	999	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
3	A	1296	PE4	O2-C3-C4-O3
3	D	1296	PE4	O6-C10-C9-O5
2	D	999	NDP	O4D-C4D-C5D-O5D

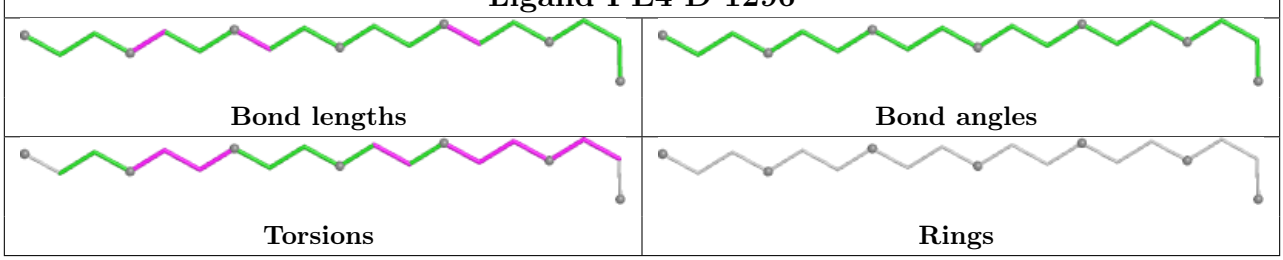
There are no ring outliers.

11 monomers are involved in 25 short contacts:

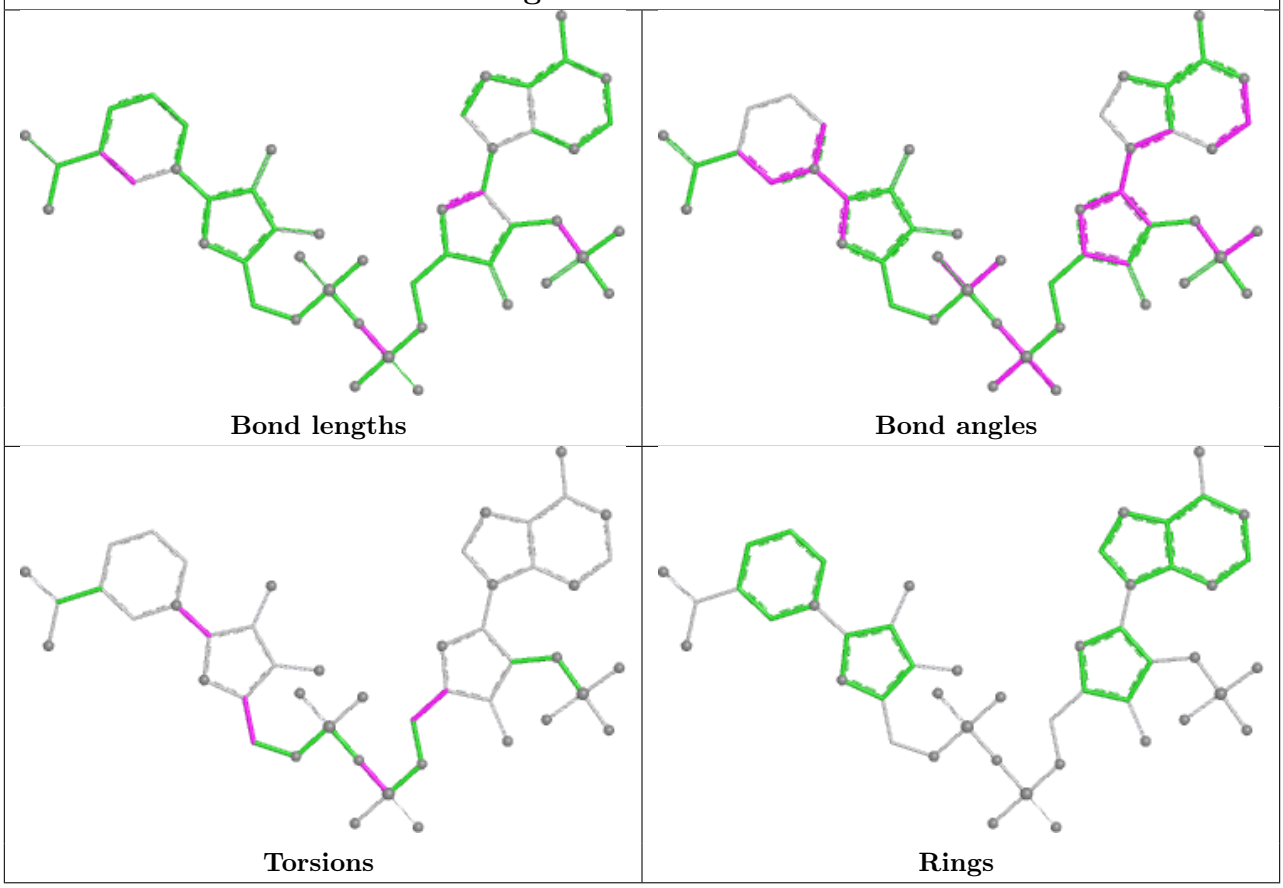
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1296	PE4	3	0
2	G	999	NDP	3	0
3	B	1296	PE4	1	0
3	C	1296	PE4	2	0
2	H	999	NDP	2	0
3	F	1296	PE4	3	0
2	D	999	NDP	2	0
2	F	999	NDP	2	0
3	E	1296	PE4	3	0
3	H	1296	PE4	2	0
3	G	1295	PE4	6	0

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 then 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.

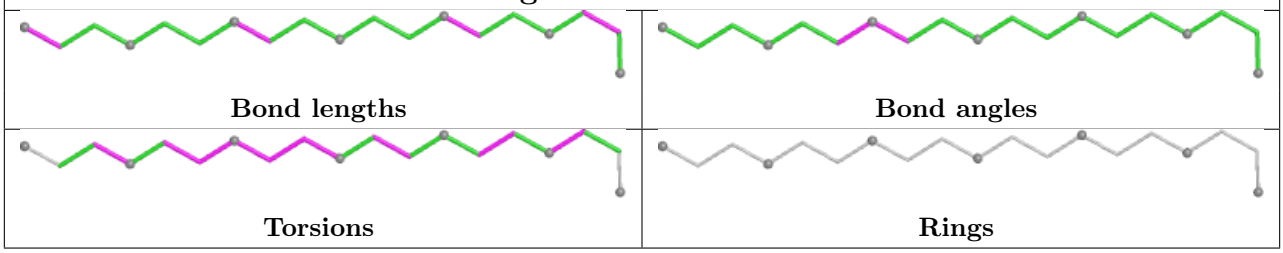
Ligand PE4 D 1296



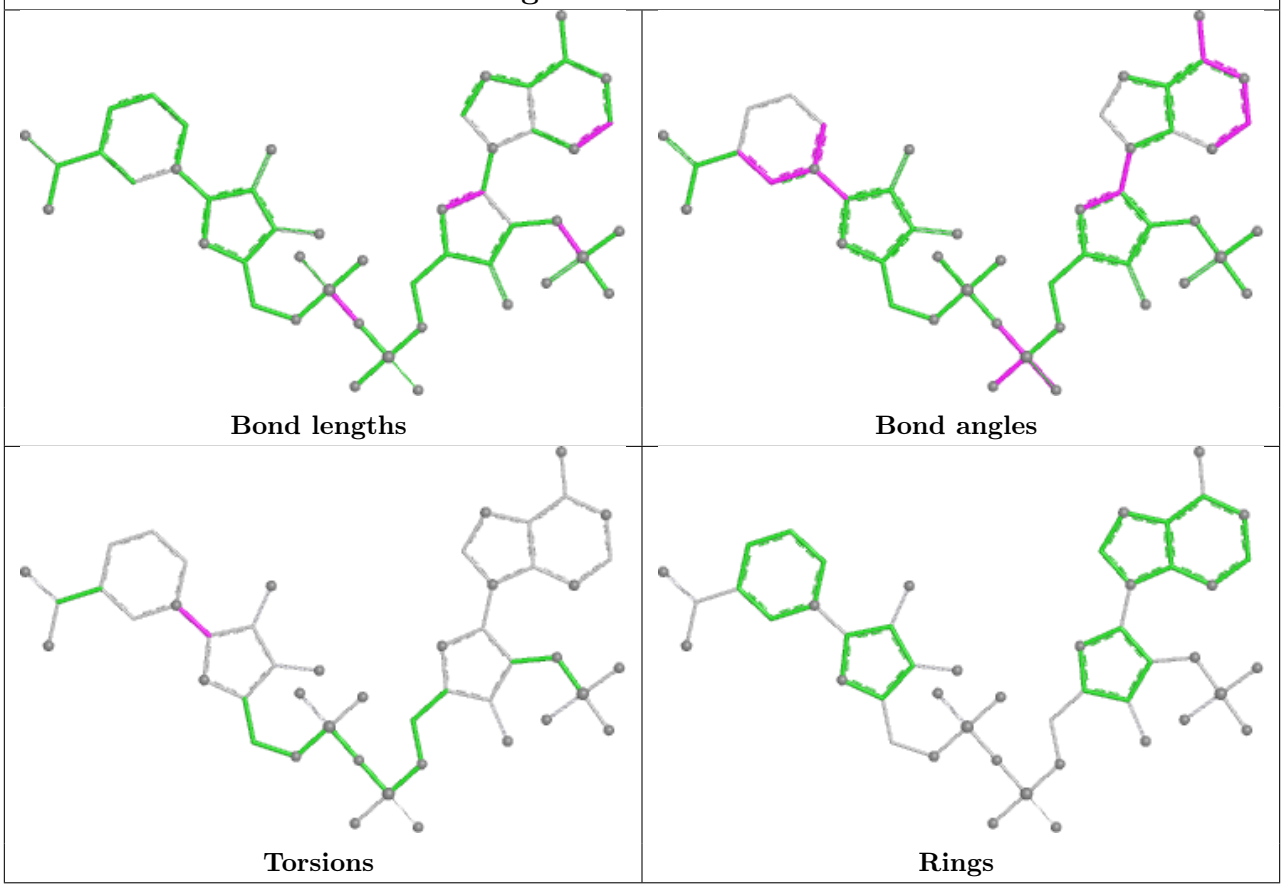
Ligand NDP E 999



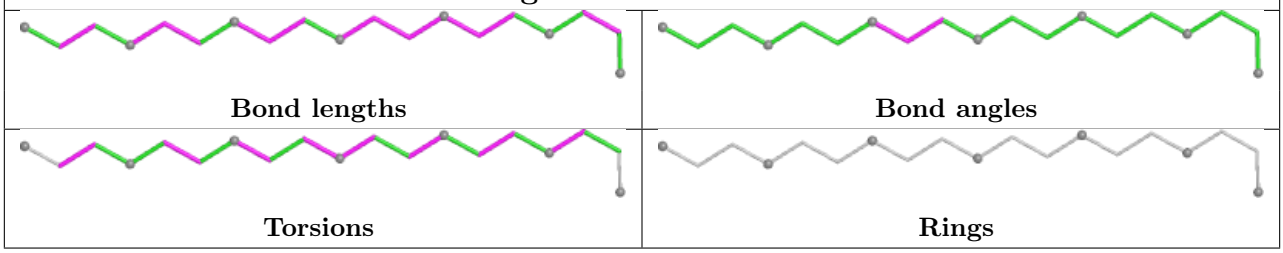
Ligand PE4 A 1296



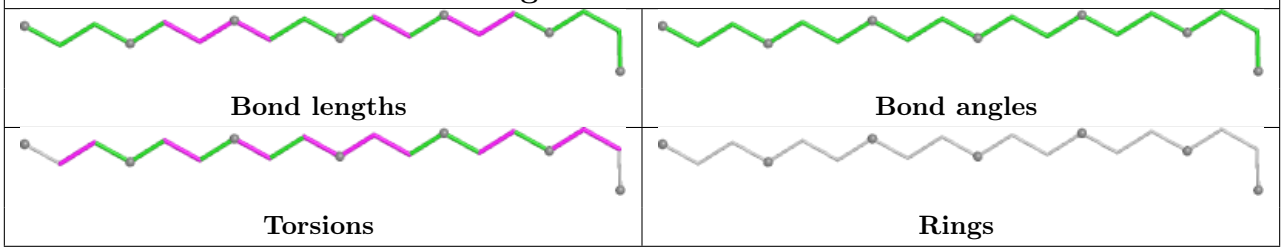
Ligand NDP G 999



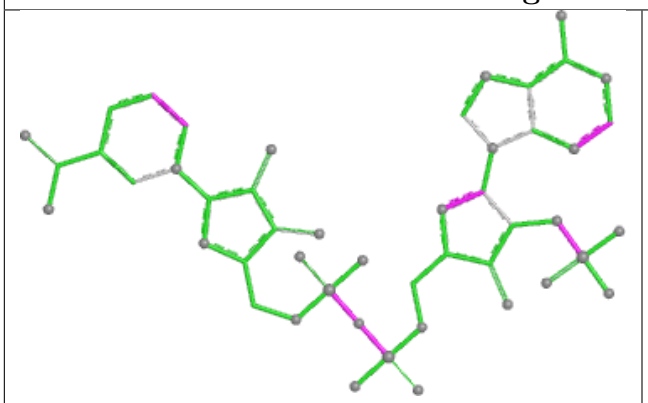
Ligand PE4 B 1296



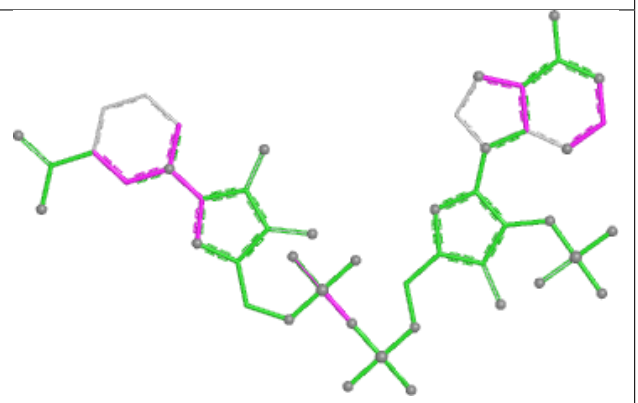
Ligand PE4 C 1296



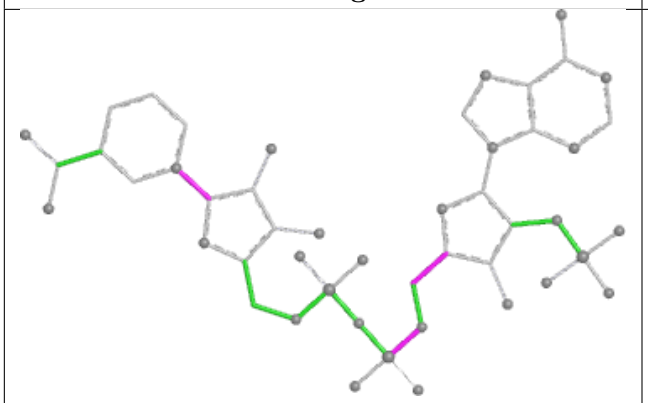
Ligand NDP C 999



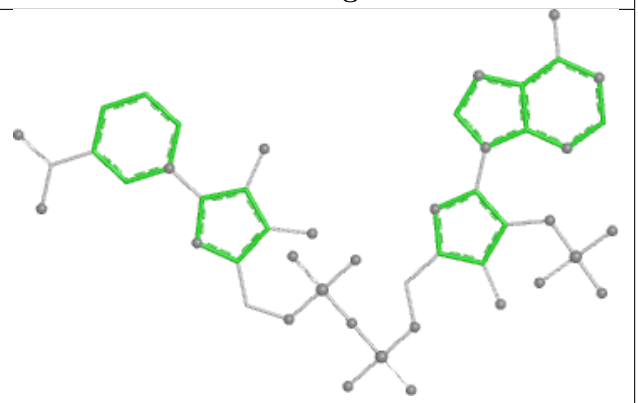
Bond lengths



Bond angles

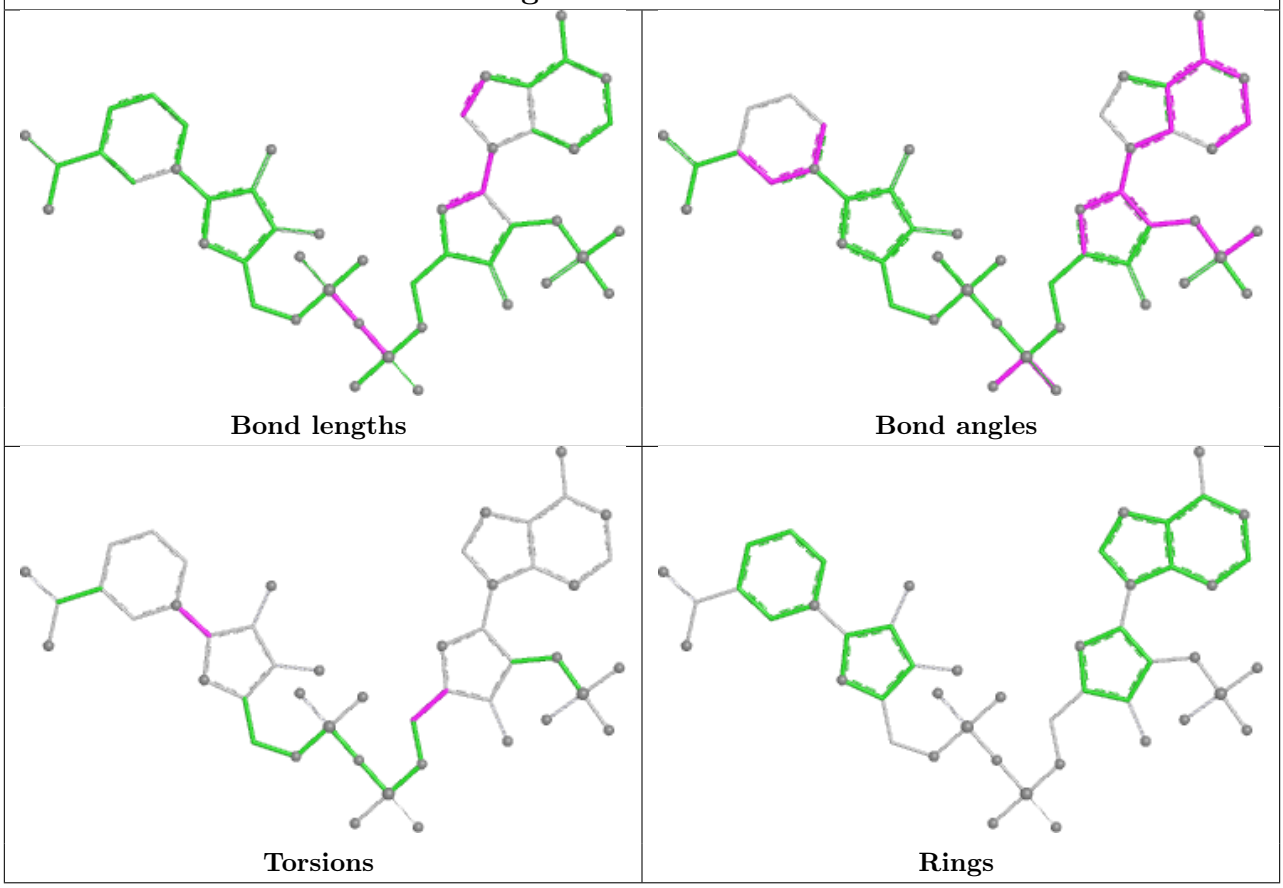


Torsions

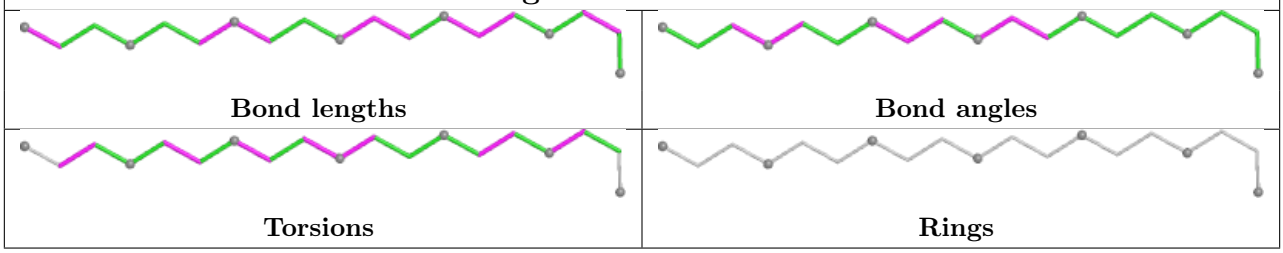


Rings

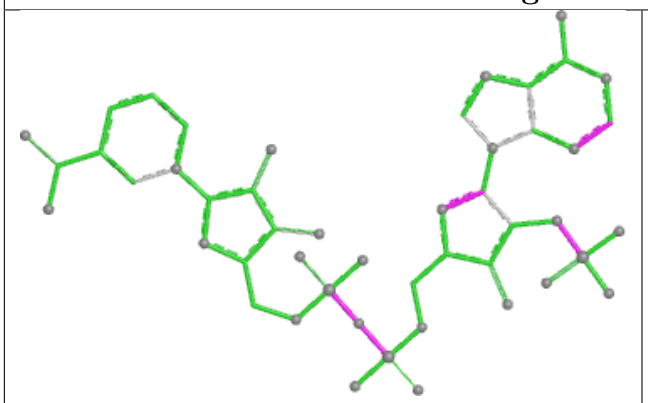
Ligand NDP H 999



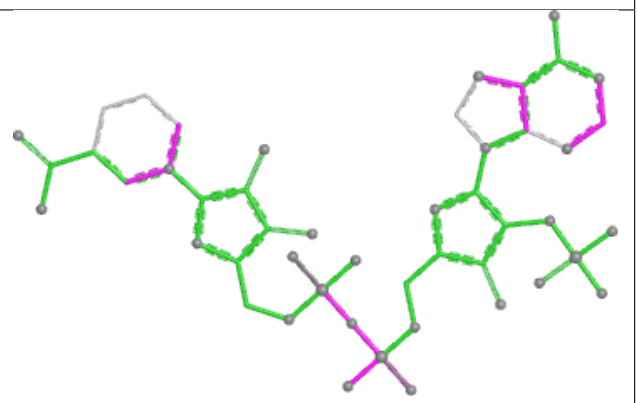
Ligand PE4 F 1296



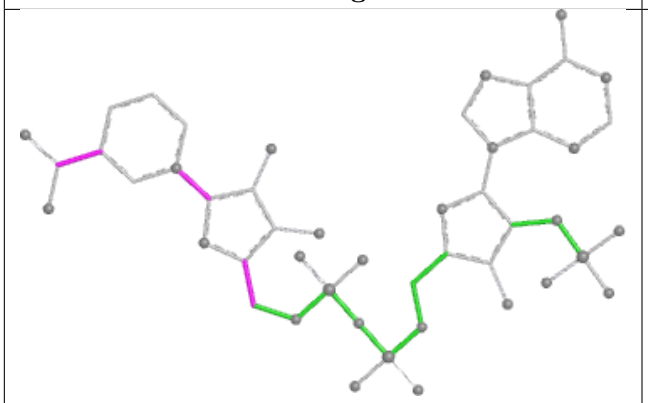
Ligand NDP D 999



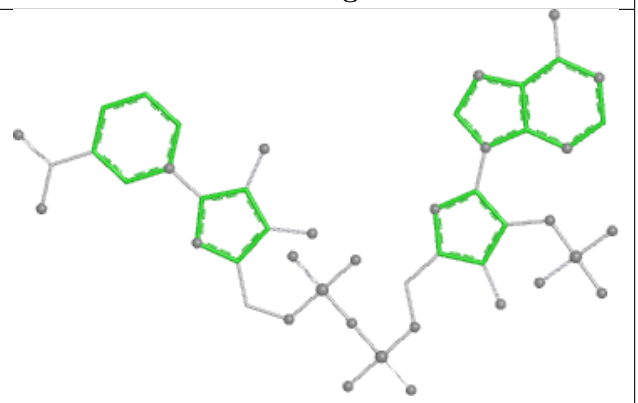
Bond lengths



Bond angles

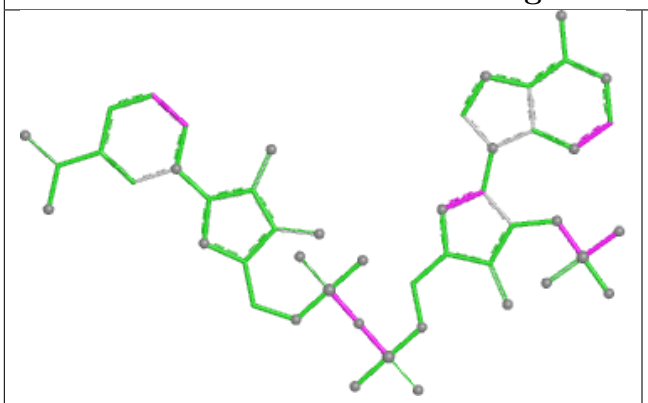


Torsions

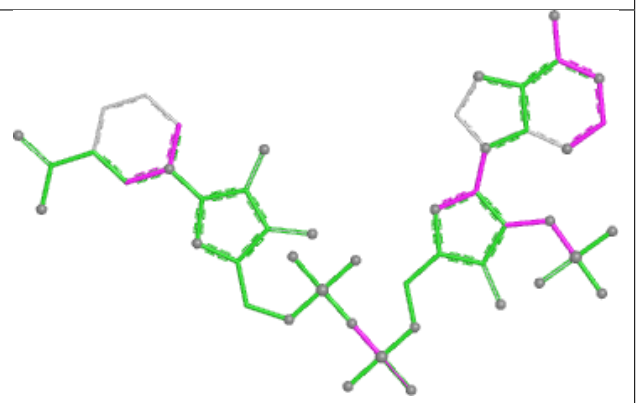


Rings

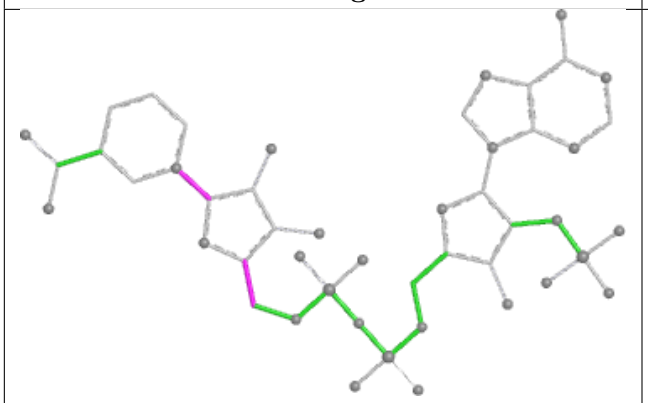
Ligand NDP F 999



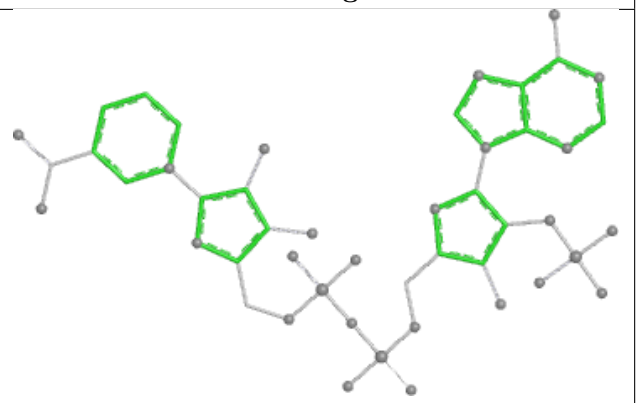
Bond lengths



Bond angles

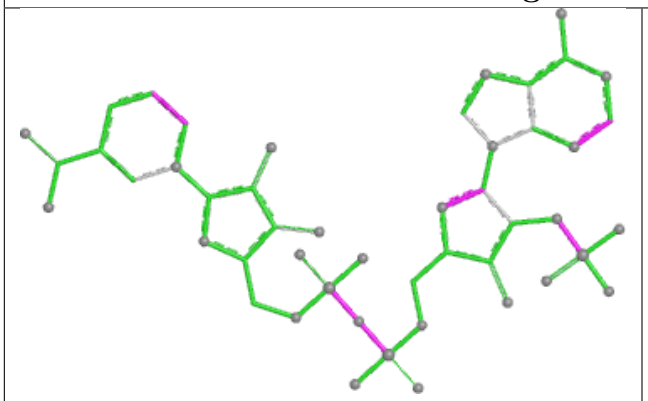


Torsions

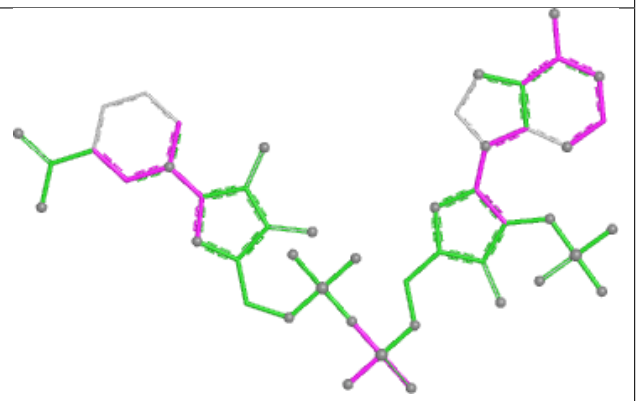


Rings

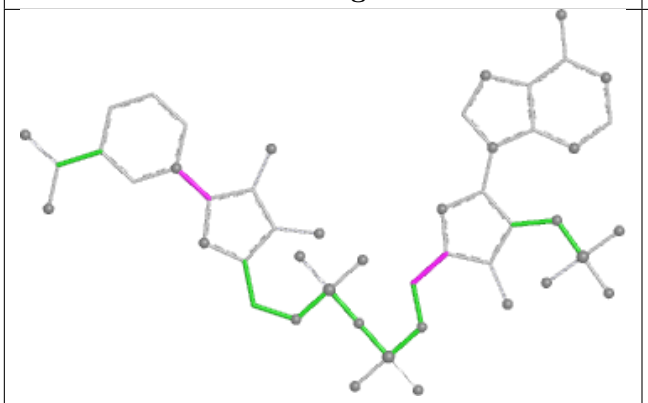
Ligand NDP B 999



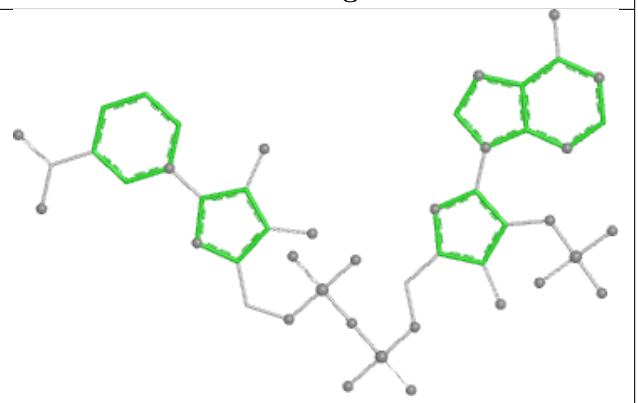
Bond lengths



Bond angles

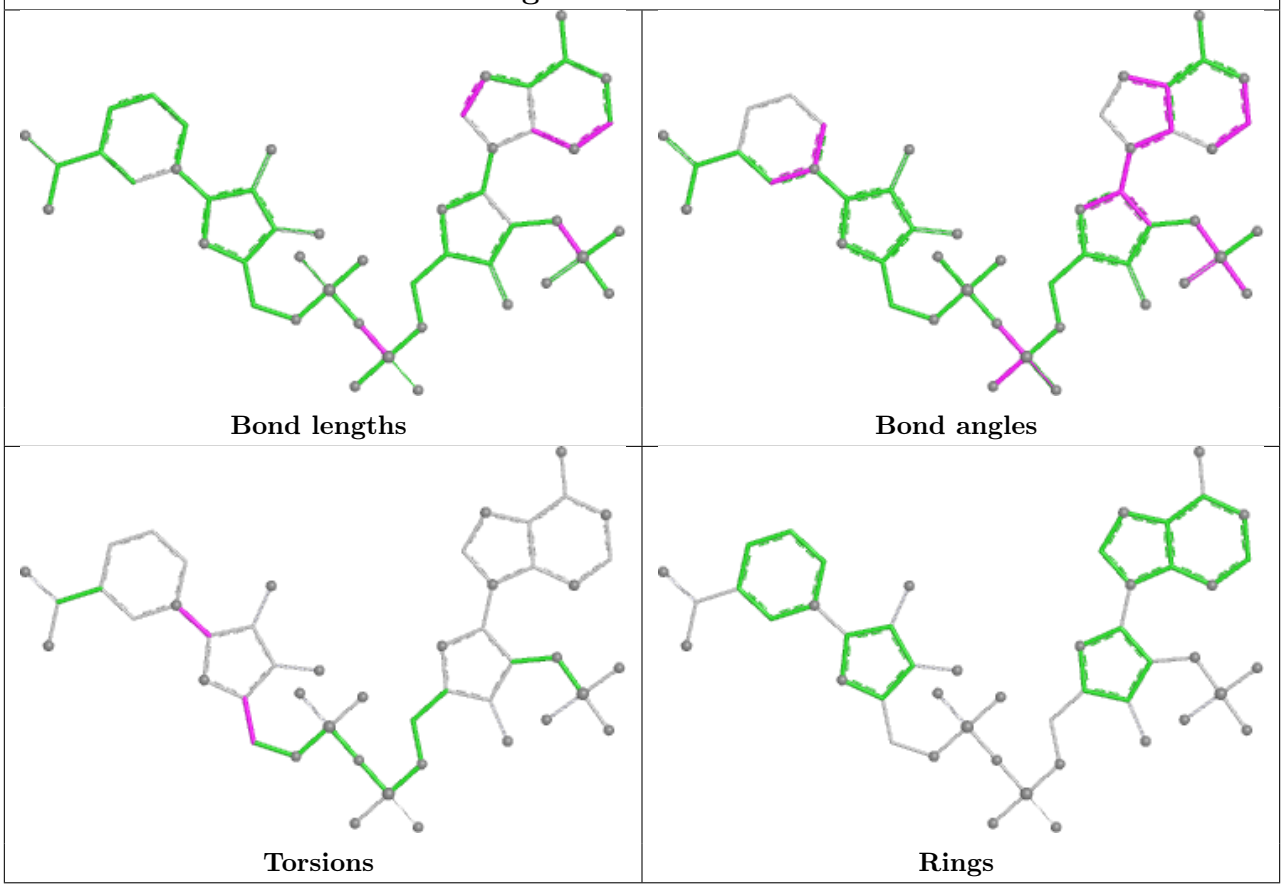


Torsions

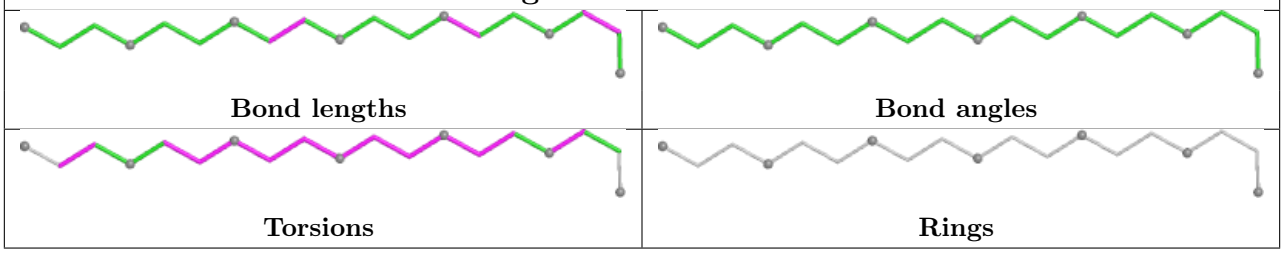


Rings

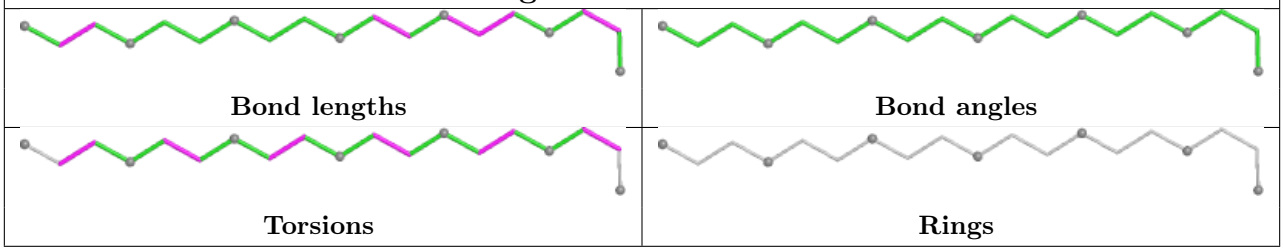
Ligand NDP A 999



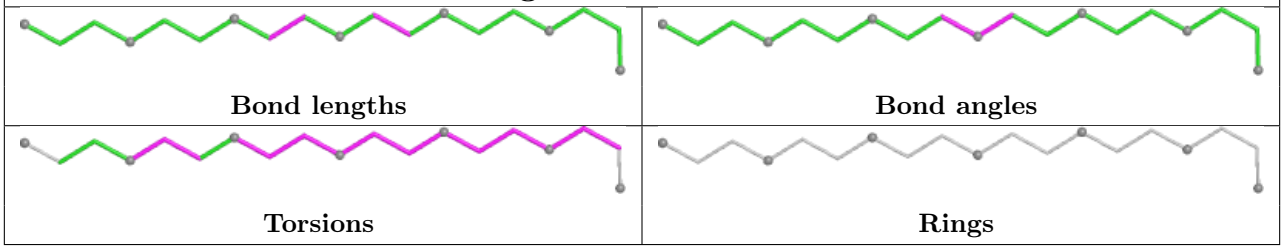
Ligand PE4 E 1296



Ligand PE4 H 1296



Ligand PE4 G 1295



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	291/298 (97%)	-0.26	5 (1%)	70	72	12, 20, 38, 48	0
1	B	291/298 (97%)	-0.29	1 (0%)	94	95	12, 20, 33, 40	0
1	C	291/298 (97%)	-0.17	4 (1%)	75	77	13, 21, 33, 43	0
1	D	291/298 (97%)	-0.18	3 (1%)	82	83	2, 22, 31, 44	0
1	E	291/298 (97%)	-0.09	10 (3%)	45	45	13, 25, 46, 58	0
1	F	291/298 (97%)	-0.21	4 (1%)	75	77	14, 22, 34, 47	0
1	G	290/298 (97%)	-0.28	3 (1%)	82	83	13, 20, 30, 38	0
1	H	291/298 (97%)	-0.20	3 (1%)	82	83	14, 26, 41, 47	0
All	All	2327/2384 (97%)	-0.21	33 (1%)	75	77	2, 22, 38, 58	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	294	ASN	3.0
1	E	99	PRO	2.9
1	A	98	GLN	2.8
1	H	72	GLU	2.8
1	B	72	GLU	2.8
1	H	71	ASN	2.6
1	C	106	VAL	2.5
1	F	72	GLU	2.5
1	D	294	ASN	2.5
1	E	72	GLU	2.5
1	C	294	ASN	2.4
1	E	34	PRO	2.4
1	A	149	SER	2.4
1	C	148	ASP	2.3
1	A	72	GLU	2.3
1	E	147	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	295	LEU	2.2
1	H	294	ASN	2.2
1	E	36	PRO	2.2
1	E	96	ALA	2.2
1	E	146	PRO	2.2
1	A	148	ASP	2.1
1	D	98	GLN	2.1
1	D	295	LEU	2.1
1	G	148	ASP	2.1
1	C	155	VAL	2.1
1	F	293	GLU	2.1
1	E	73	THR	2.1
1	G	72	GLU	2.1
1	A	147	GLY	2.1
1	G	147	GLY	2.0
1	E	97	PRO	2.0
1	E	98	GLN	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	PE4	F	1296	19/24	0.86	0.26	2,2,3,3	19
3	PE4	H	1296	19/24	0.87	0.25	3,4,5,5	19
3	PE4	C	1296	19/24	0.88	0.26	2,2,2,2	19
3	PE4	B	1296	19/24	0.89	0.22	2,2,2,2	19
3	PE4	D	1296	19/24	0.89	0.23	2,2,2,2	19
3	PE4	G	1295	19/24	0.90	0.20	2,2,2,2	19

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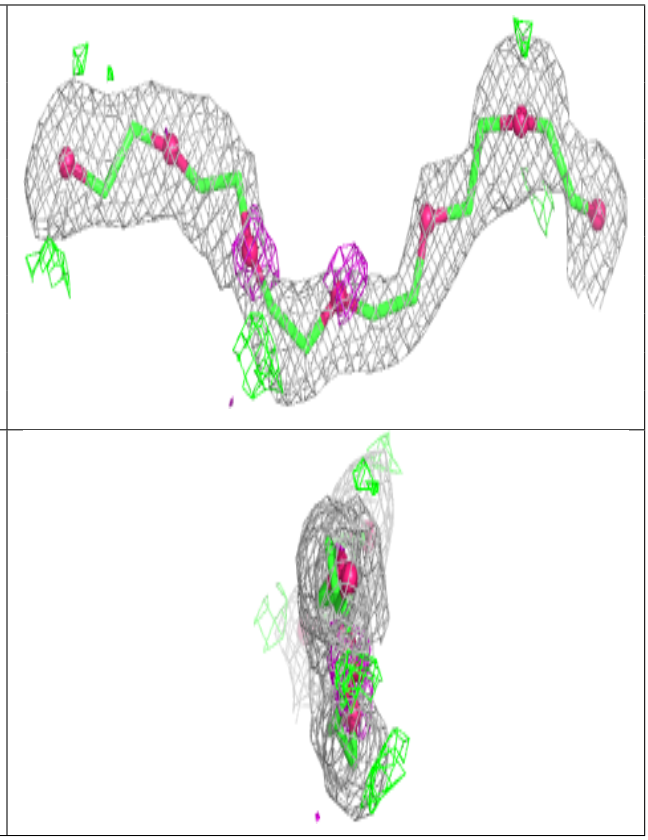
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PE4	A	1296	19/24	0.92	0.18	2,2,2,2	19
3	PE4	E	1296	19/24	0.93	0.17	2,2,2,3	19
2	NDP	E	999	48/48	0.96	0.12	2,2,2,2	0
2	NDP	F	999	48/48	0.96	0.11	2,2,2,2	0
2	NDP	G	999	48/48	0.96	0.11	2,2,2,2	0
2	NDP	H	999	48/48	0.96	0.13	2,2,2,2	0
2	NDP	C	999	48/48	0.96	0.11	2,2,2,2	0
2	NDP	D	999	48/48	0.96	0.12	2,2,2,2	0
2	NDP	A	999	48/48	0.97	0.11	2,2,2,2	0
2	NDP	B	999	48/48	0.97	0.11	2,2,2,2	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.

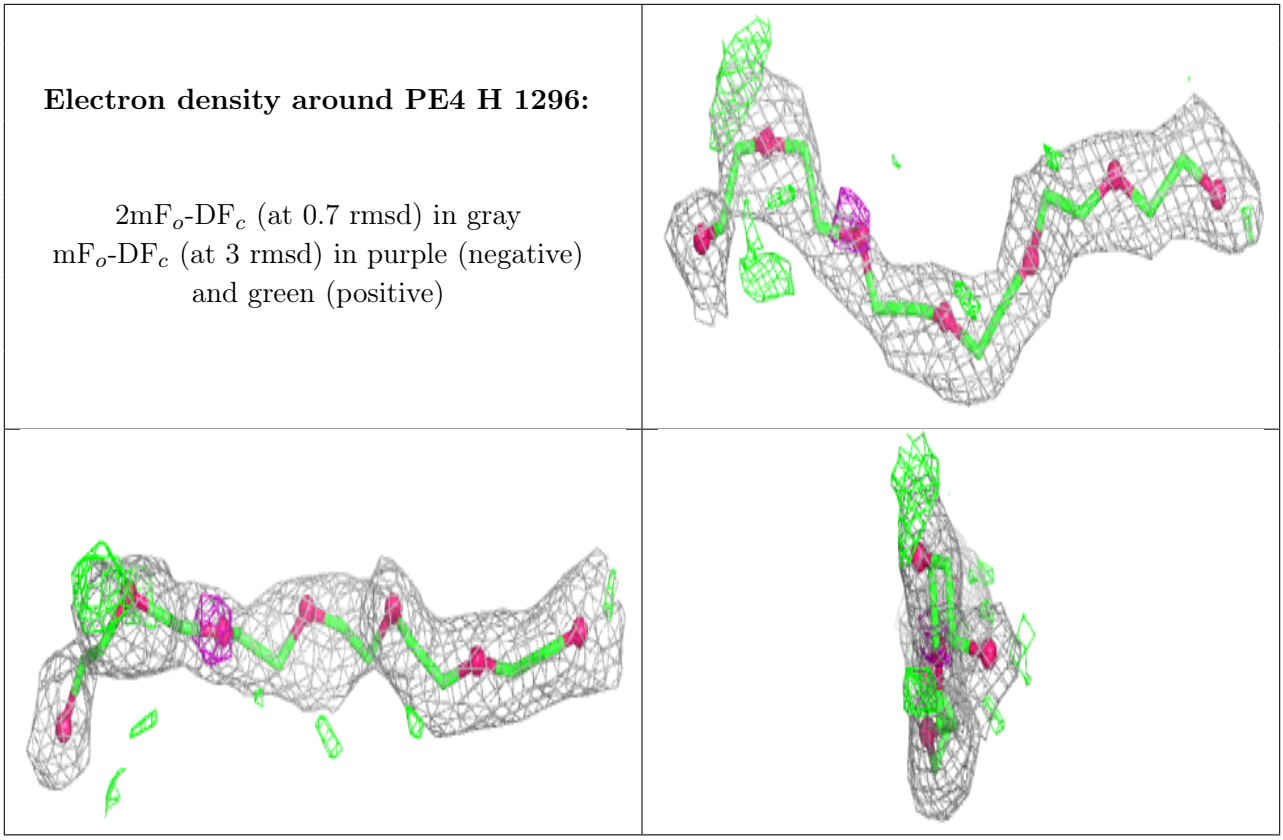
Electron density around PE4 F 1296:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



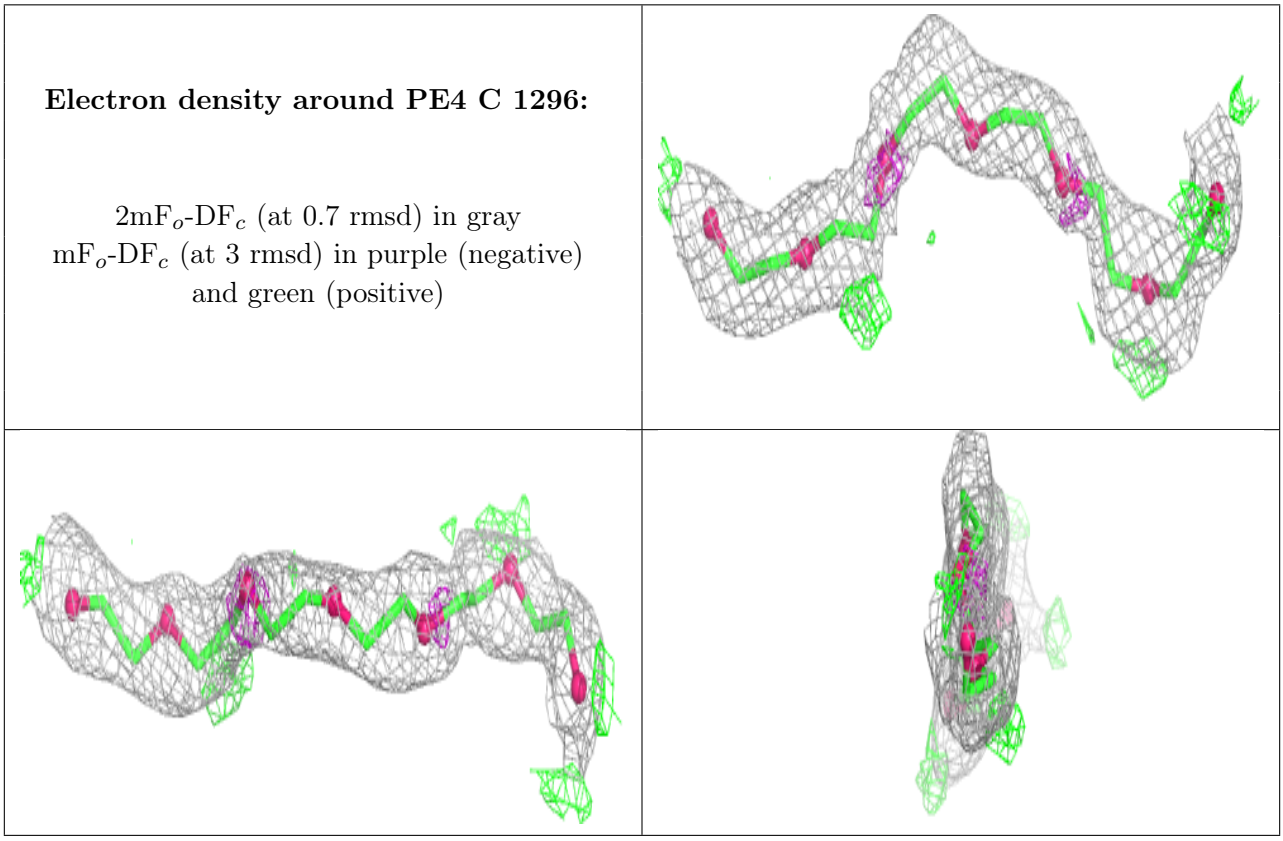
Electron density around PE4 H 1296:

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



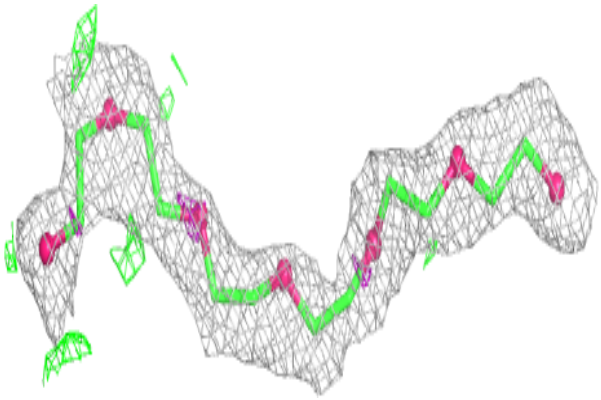
Electron density around PE4 C 1296:

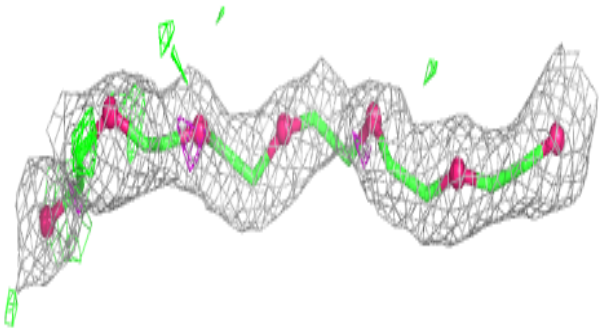
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

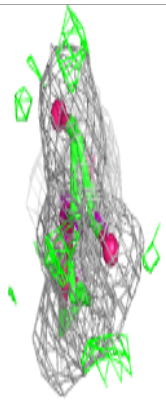


Electron density around PE4 B 1296:

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

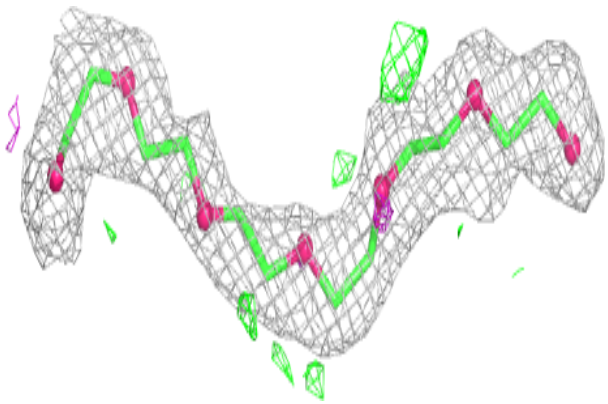


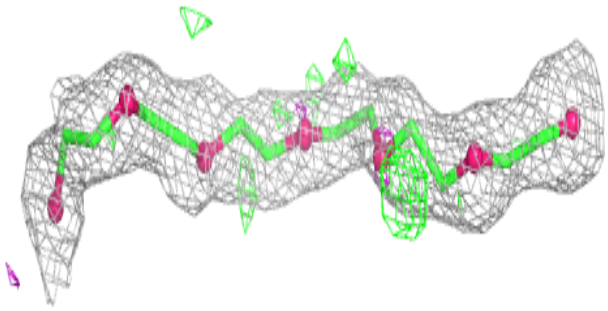


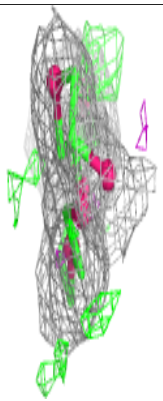


Electron density around PE4 D 1296:

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

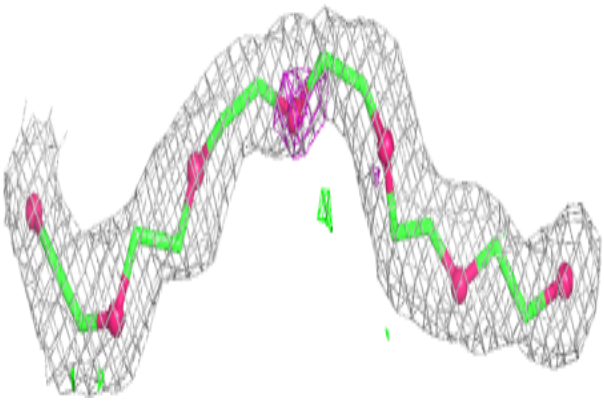


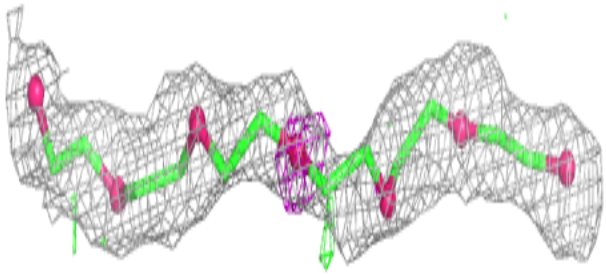


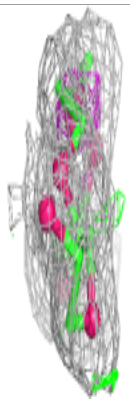


Electron density around PE4 G 1295:

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

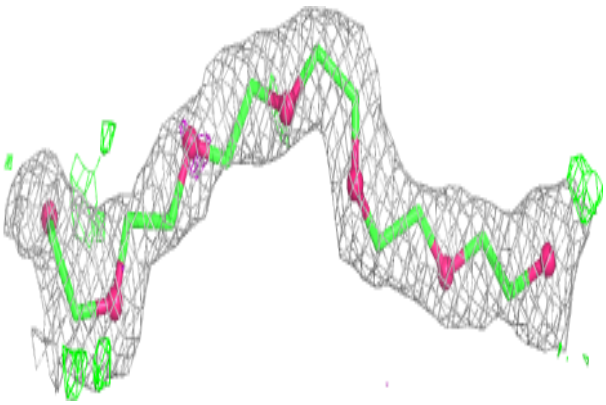


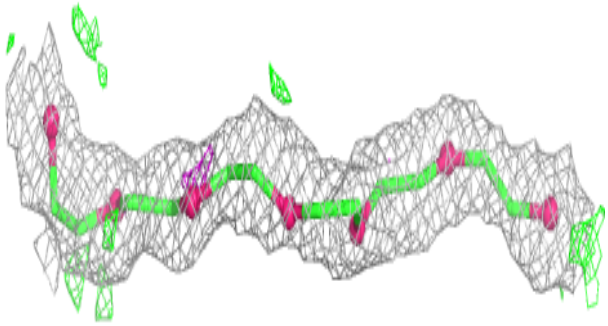


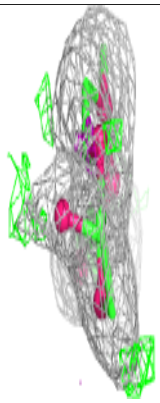


Electron density around PE4 A 1296:

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

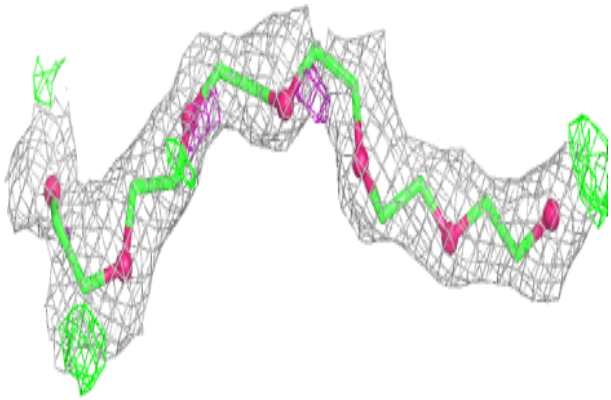


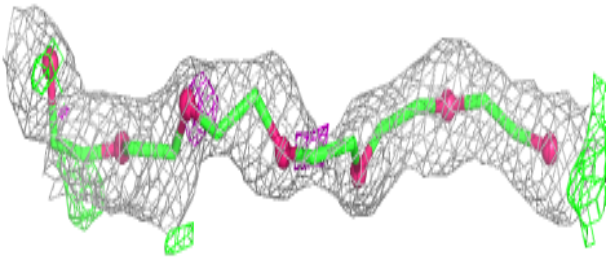


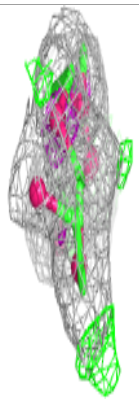


Electron density around PE4 E 1296:

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

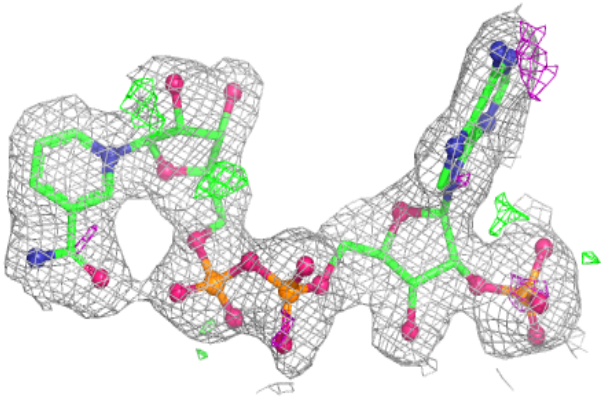


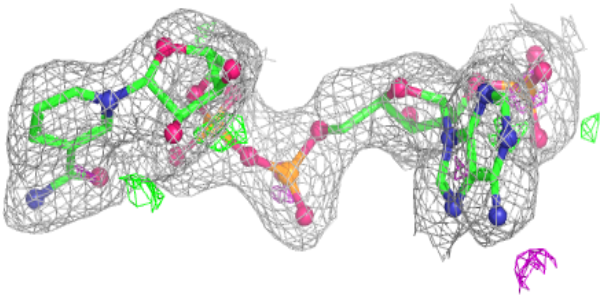


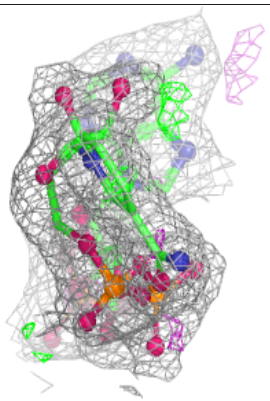


Electron density around NDP E 999:

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

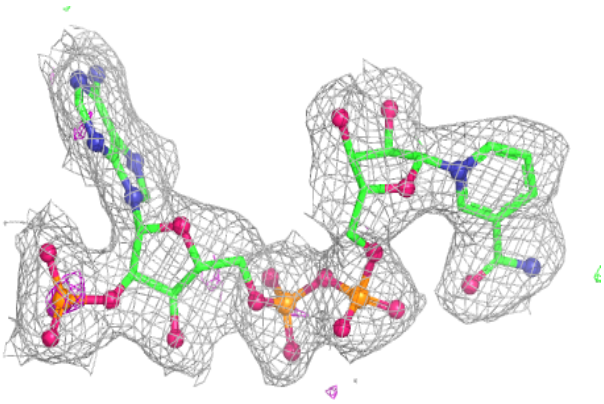


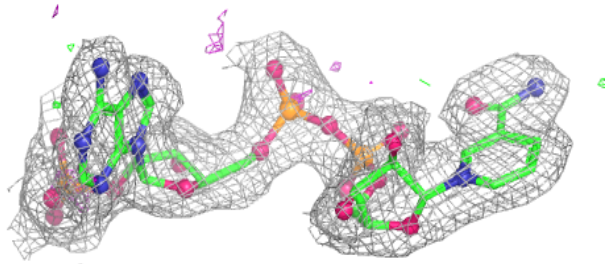


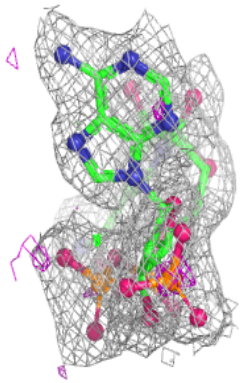


Electron density around NDP F 999:

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

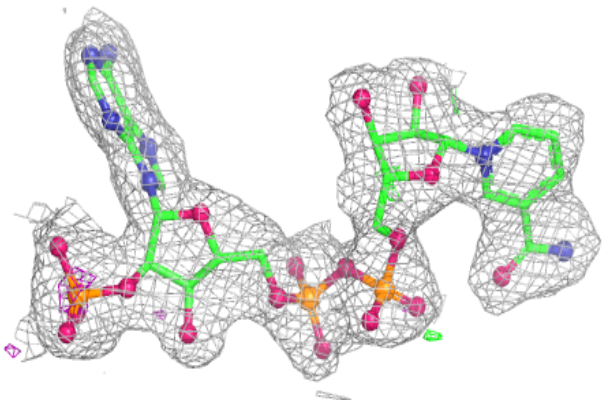


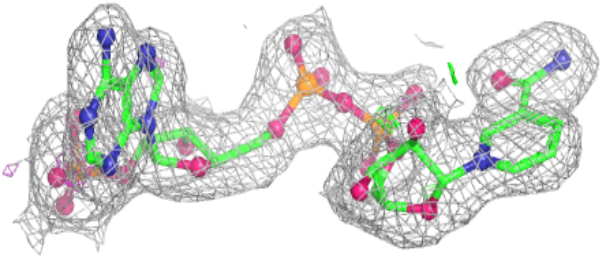


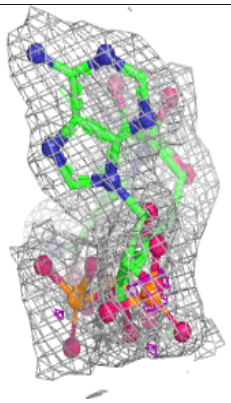


Electron density around NDP G 999:

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

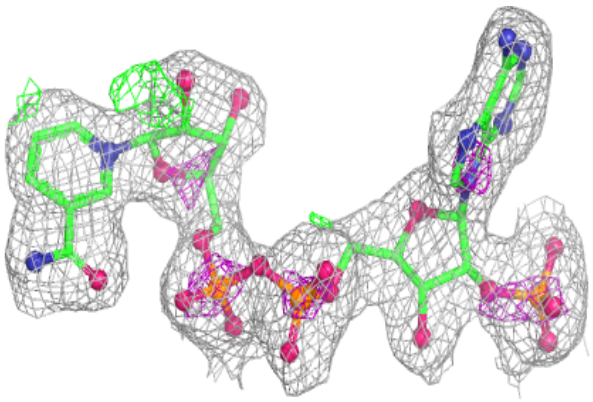


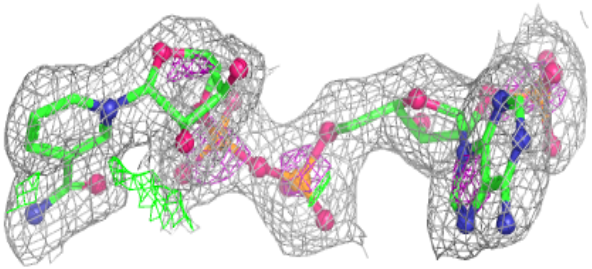


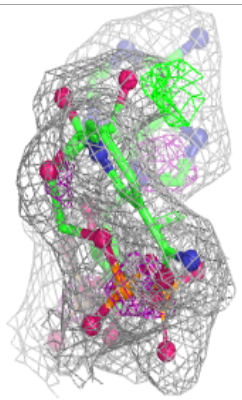


Electron density around NDP H 999:

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

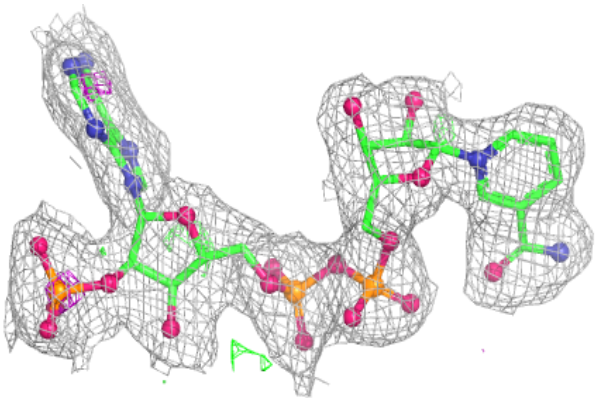


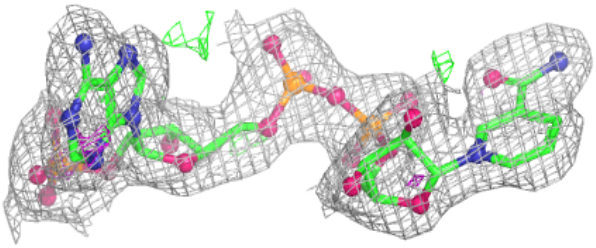


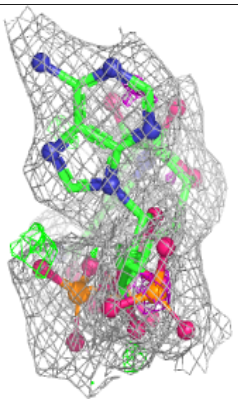


Electron density around NDP C 999:

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

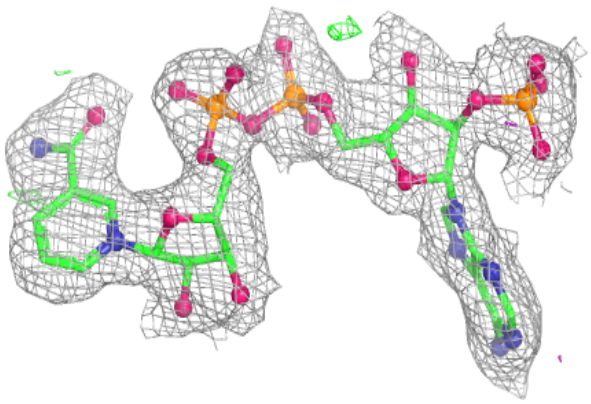


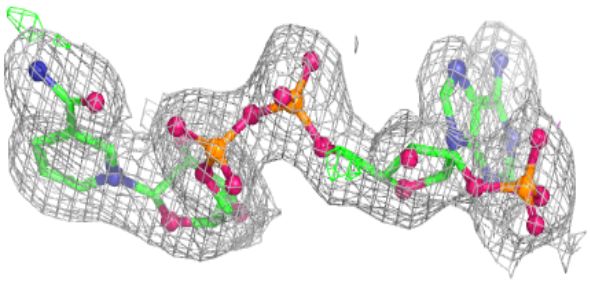


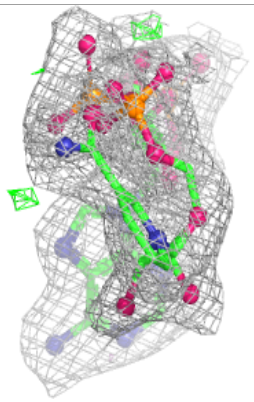


Electron density around NDP D 999:

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

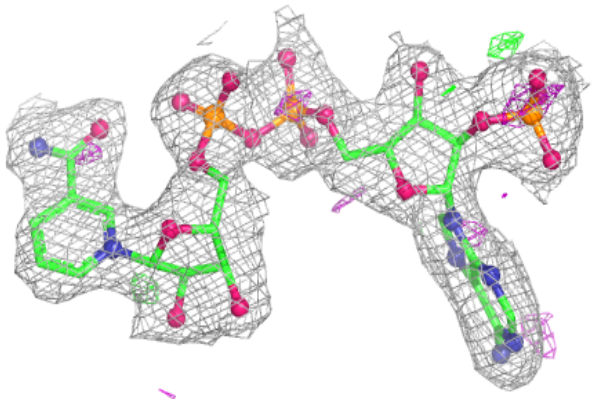


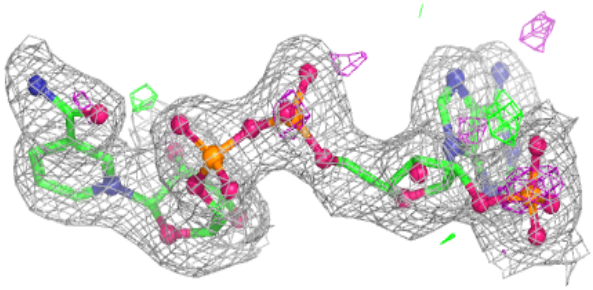


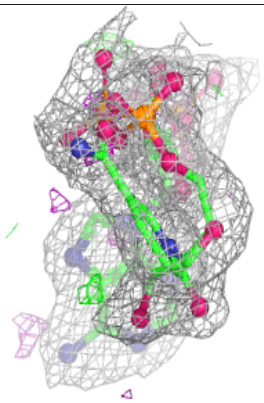


Electron density around NDP A 999:

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

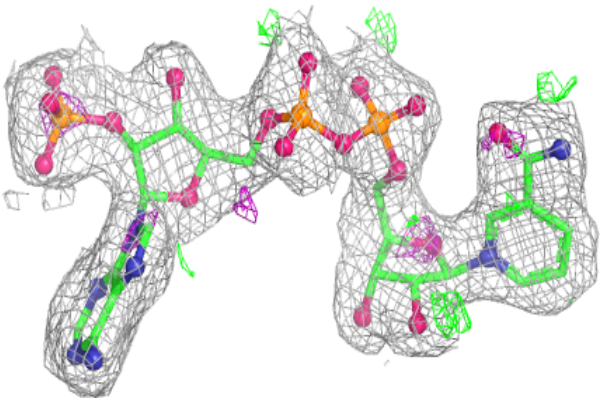


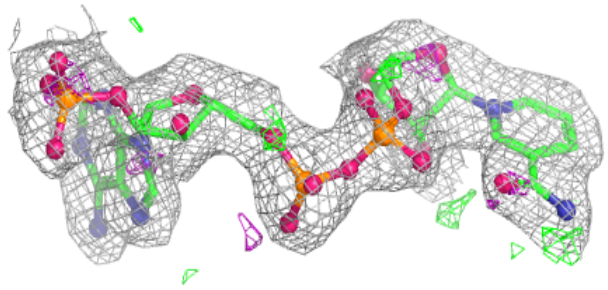


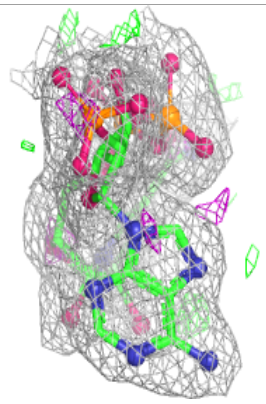


Electron density around NDP B 999:

$2mF_o$-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.