



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:20 PM UTC

PDB ID : 4CV1 / pdb_00004cv1
Title : Crystal structure of S. aureus FabI in complex with NADPH and CG400549
Authors : Schiebel, J.; Chang, A.; Shah, S.; Tonge, P.J.; Kisker, C.
Deposited on : 2014-03-22
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

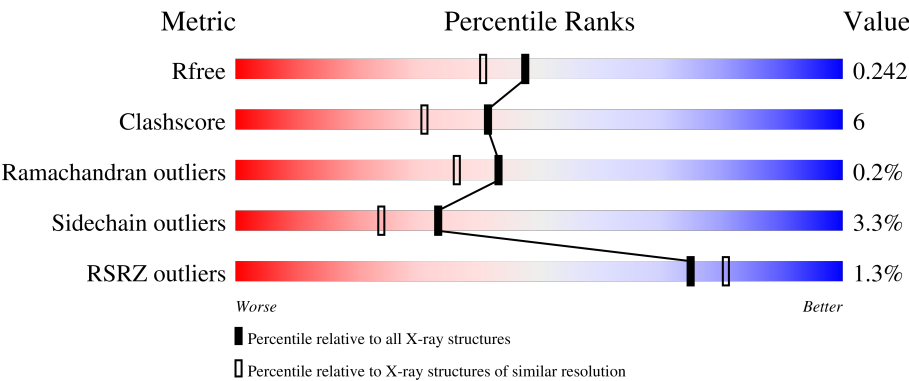
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	282	0.2% 81% 12% 7%
1	B	282	2% 79% 11% 9%
1	C	282	0.2% 78% 13% 7%
1	D	282	78% 11% 9%
1	E	282	3% 78% 11% 9%

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Mol	Chain	Length	Quality of chain
1	F	282	% 85%7%• 7%
1	G	282	% 75%15%• 9%
1	H	282	78%13%• 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17795 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	7	0
			2060	1301	353	401	5			
1	B	256	Total	C	N	O	S	0	13	0
			2057	1299	352	401	5			
1	C	262	Total	C	N	O	S	0	4	0
			2047	1295	350	397	5			
1	D	256	Total	C	N	O	S	0	6	0
			2007	1269	344	389	5			
1	E	256	Total	C	N	O	S	0	13	0
			2063	1303	357	398	5			
1	F	262	Total	C	N	O	S	0	2	0
			2028	1282	347	394	5			
1	G	257	Total	C	N	O	S	0	5	0
			2007	1264	347	390	6			
1	H	263	Total	C	N	O	S	0	3	0
			2047	1294	353	395	5			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q7A6D8
A	-24	LYS	-	expression tag	UNP Q7A6D8
A	-23	HIS	-	expression tag	UNP Q7A6D8
A	-22	HIS	-	expression tag	UNP Q7A6D8
A	-21	HIS	-	expression tag	UNP Q7A6D8
A	-20	HIS	-	expression tag	UNP Q7A6D8
A	-19	HIS	-	expression tag	UNP Q7A6D8
A	-18	HIS	-	expression tag	UNP Q7A6D8
A	-17	PRO	-	expression tag	UNP Q7A6D8
A	-16	MET	-	expression tag	UNP Q7A6D8
A	-15	SER	-	expression tag	UNP Q7A6D8
A	-14	ASP	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	TYR	-	expression tag	UNP Q7A6D8
A	-12	ASP	-	expression tag	UNP Q7A6D8
A	-11	ILE	-	expression tag	UNP Q7A6D8
A	-10	PRO	-	expression tag	UNP Q7A6D8
A	-9	THR	-	expression tag	UNP Q7A6D8
A	-8	THR	-	expression tag	UNP Q7A6D8
A	-7	GLU	-	expression tag	UNP Q7A6D8
A	-6	ASN	-	expression tag	UNP Q7A6D8
A	-5	LEU	-	expression tag	UNP Q7A6D8
A	-4	TYR	-	expression tag	UNP Q7A6D8
A	-3	PHE	-	expression tag	UNP Q7A6D8
A	-2	GLN	-	expression tag	UNP Q7A6D8
A	-1	GLY	-	expression tag	UNP Q7A6D8
A	0	ALA	-	expression tag	UNP Q7A6D8
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
B	-25	MET	-	expression tag	UNP Q7A6D8
B	-24	LYS	-	expression tag	UNP Q7A6D8
B	-23	HIS	-	expression tag	UNP Q7A6D8
B	-22	HIS	-	expression tag	UNP Q7A6D8
B	-21	HIS	-	expression tag	UNP Q7A6D8
B	-20	HIS	-	expression tag	UNP Q7A6D8
B	-19	HIS	-	expression tag	UNP Q7A6D8
B	-18	HIS	-	expression tag	UNP Q7A6D8
B	-17	PRO	-	expression tag	UNP Q7A6D8
B	-16	MET	-	expression tag	UNP Q7A6D8
B	-15	SER	-	expression tag	UNP Q7A6D8
B	-14	ASP	-	expression tag	UNP Q7A6D8
B	-13	TYR	-	expression tag	UNP Q7A6D8
B	-12	ASP	-	expression tag	UNP Q7A6D8
B	-11	ILE	-	expression tag	UNP Q7A6D8
B	-10	PRO	-	expression tag	UNP Q7A6D8
B	-9	THR	-	expression tag	UNP Q7A6D8
B	-8	THR	-	expression tag	UNP Q7A6D8
B	-7	GLU	-	expression tag	UNP Q7A6D8
B	-6	ASN	-	expression tag	UNP Q7A6D8
B	-5	LEU	-	expression tag	UNP Q7A6D8
B	-4	TYR	-	expression tag	UNP Q7A6D8
B	-3	PHE	-	expression tag	UNP Q7A6D8
B	-2	GLN	-	expression tag	UNP Q7A6D8
B	-1	GLY	-	expression tag	UNP Q7A6D8
B	0	ALA	-	expression tag	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	MET	-	expression tag	UNP Q7A6D8
C	-24	LYS	-	expression tag	UNP Q7A6D8
C	-23	HIS	-	expression tag	UNP Q7A6D8
C	-22	HIS	-	expression tag	UNP Q7A6D8
C	-21	HIS	-	expression tag	UNP Q7A6D8
C	-20	HIS	-	expression tag	UNP Q7A6D8
C	-19	HIS	-	expression tag	UNP Q7A6D8
C	-18	HIS	-	expression tag	UNP Q7A6D8
C	-17	PRO	-	expression tag	UNP Q7A6D8
C	-16	MET	-	expression tag	UNP Q7A6D8
C	-15	SER	-	expression tag	UNP Q7A6D8
C	-14	ASP	-	expression tag	UNP Q7A6D8
C	-13	TYR	-	expression tag	UNP Q7A6D8
C	-12	ASP	-	expression tag	UNP Q7A6D8
C	-11	ILE	-	expression tag	UNP Q7A6D8
C	-10	PRO	-	expression tag	UNP Q7A6D8
C	-9	THR	-	expression tag	UNP Q7A6D8
C	-8	THR	-	expression tag	UNP Q7A6D8
C	-7	GLU	-	expression tag	UNP Q7A6D8
C	-6	ASN	-	expression tag	UNP Q7A6D8
C	-5	LEU	-	expression tag	UNP Q7A6D8
C	-4	TYR	-	expression tag	UNP Q7A6D8
C	-3	PHE	-	expression tag	UNP Q7A6D8
C	-2	GLN	-	expression tag	UNP Q7A6D8
C	-1	GLY	-	expression tag	UNP Q7A6D8
C	0	ALA	-	expression tag	UNP Q7A6D8
C	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	-25	MET	-	expression tag	UNP Q7A6D8
D	-24	LYS	-	expression tag	UNP Q7A6D8
D	-23	HIS	-	expression tag	UNP Q7A6D8
D	-22	HIS	-	expression tag	UNP Q7A6D8
D	-21	HIS	-	expression tag	UNP Q7A6D8
D	-20	HIS	-	expression tag	UNP Q7A6D8
D	-19	HIS	-	expression tag	UNP Q7A6D8
D	-18	HIS	-	expression tag	UNP Q7A6D8
D	-17	PRO	-	expression tag	UNP Q7A6D8
D	-16	MET	-	expression tag	UNP Q7A6D8
D	-15	SER	-	expression tag	UNP Q7A6D8
D	-14	ASP	-	expression tag	UNP Q7A6D8
D	-13	TYR	-	expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	-	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
E	-25	MET	-	expression tag	UNP Q7A6D8
E	-24	LYS	-	expression tag	UNP Q7A6D8
E	-23	HIS	-	expression tag	UNP Q7A6D8
E	-22	HIS	-	expression tag	UNP Q7A6D8
E	-21	HIS	-	expression tag	UNP Q7A6D8
E	-20	HIS	-	expression tag	UNP Q7A6D8
E	-19	HIS	-	expression tag	UNP Q7A6D8
E	-18	HIS	-	expression tag	UNP Q7A6D8
E	-17	PRO	-	expression tag	UNP Q7A6D8
E	-16	MET	-	expression tag	UNP Q7A6D8
E	-15	SER	-	expression tag	UNP Q7A6D8
E	-14	ASP	-	expression tag	UNP Q7A6D8
E	-13	TYR	-	expression tag	UNP Q7A6D8
E	-12	ASP	-	expression tag	UNP Q7A6D8
E	-11	ILE	-	expression tag	UNP Q7A6D8
E	-10	PRO	-	expression tag	UNP Q7A6D8
E	-9	THR	-	expression tag	UNP Q7A6D8
E	-8	THR	-	expression tag	UNP Q7A6D8
E	-7	GLU	-	expression tag	UNP Q7A6D8
E	-6	ASN	-	expression tag	UNP Q7A6D8
E	-5	LEU	-	expression tag	UNP Q7A6D8
E	-4	TYR	-	expression tag	UNP Q7A6D8
E	-3	PHE	-	expression tag	UNP Q7A6D8
E	-2	GLN	-	expression tag	UNP Q7A6D8
E	-1	GLY	-	expression tag	UNP Q7A6D8
E	0	ALA	-	expression tag	UNP Q7A6D8
E	2	VAL	LEU	engineered mutation	UNP Q7A6D8
F	-25	MET	-	expression tag	UNP Q7A6D8
F	-24	LYS	-	expression tag	UNP Q7A6D8
F	-23	HIS	-	expression tag	UNP Q7A6D8

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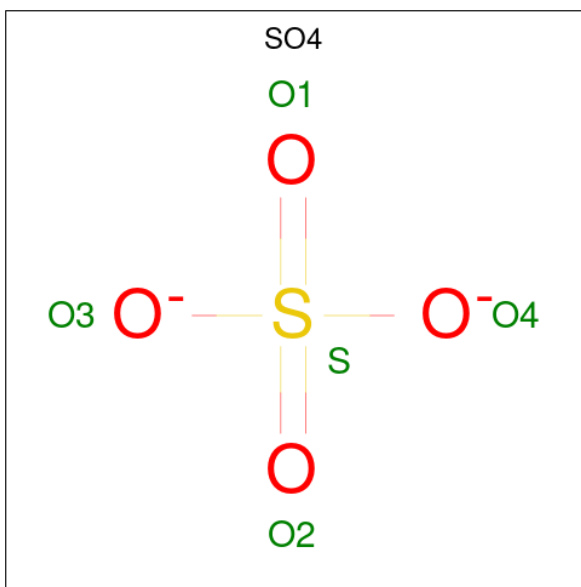
Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	UNP Q7A6D8
F	-15	SER	-	expression tag	UNP Q7A6D8
F	-14	ASP	-	expression tag	UNP Q7A6D8
F	-13	TYR	-	expression tag	UNP Q7A6D8
F	-12	ASP	-	expression tag	UNP Q7A6D8
F	-11	ILE	-	expression tag	UNP Q7A6D8
F	-10	PRO	-	expression tag	UNP Q7A6D8
F	-9	THR	-	expression tag	UNP Q7A6D8
F	-8	THR	-	expression tag	UNP Q7A6D8
F	-7	GLU	-	expression tag	UNP Q7A6D8
F	-6	ASN	-	expression tag	UNP Q7A6D8
F	-5	LEU	-	expression tag	UNP Q7A6D8
F	-4	TYR	-	expression tag	UNP Q7A6D8
F	-3	PHE	-	expression tag	UNP Q7A6D8
F	-2	GLN	-	expression tag	UNP Q7A6D8
F	-1	GLY	-	expression tag	UNP Q7A6D8
F	0	ALA	-	expression tag	UNP Q7A6D8
F	2	VAL	LEU	engineered mutation	UNP Q7A6D8
G	-25	MET	-	expression tag	UNP Q7A6D8
G	-24	LYS	-	expression tag	UNP Q7A6D8
G	-23	HIS	-	expression tag	UNP Q7A6D8
G	-22	HIS	-	expression tag	UNP Q7A6D8
G	-21	HIS	-	expression tag	UNP Q7A6D8
G	-20	HIS	-	expression tag	UNP Q7A6D8
G	-19	HIS	-	expression tag	UNP Q7A6D8
G	-18	HIS	-	expression tag	UNP Q7A6D8
G	-17	PRO	-	expression tag	UNP Q7A6D8
G	-16	MET	-	expression tag	UNP Q7A6D8
G	-15	SER	-	expression tag	UNP Q7A6D8
G	-14	ASP	-	expression tag	UNP Q7A6D8
G	-13	TYR	-	expression tag	UNP Q7A6D8
G	-12	ASP	-	expression tag	UNP Q7A6D8
G	-11	ILE	-	expression tag	UNP Q7A6D8
G	-10	PRO	-	expression tag	UNP Q7A6D8
G	-9	THR	-	expression tag	UNP Q7A6D8
G	-8	THR	-	expression tag	UNP Q7A6D8

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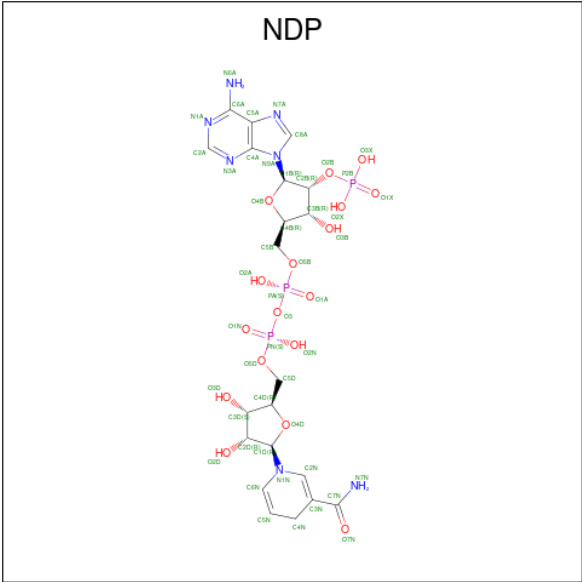
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
G	0	ALA	-	expression tag	UNP Q7A6D8
G	2	VAL	LEU	engineered mutation	UNP Q7A6D8
H	-25	MET	-	expression tag	UNP Q7A6D8
H	-24	LYS	-	expression tag	UNP Q7A6D8
H	-23	HIS	-	expression tag	UNP Q7A6D8
H	-22	HIS	-	expression tag	UNP Q7A6D8
H	-21	HIS	-	expression tag	UNP Q7A6D8
H	-20	HIS	-	expression tag	UNP Q7A6D8
H	-19	HIS	-	expression tag	UNP Q7A6D8
H	-18	HIS	-	expression tag	UNP Q7A6D8
H	-17	PRO	-	expression tag	UNP Q7A6D8
H	-16	MET	-	expression tag	UNP Q7A6D8
H	-15	SER	-	expression tag	UNP Q7A6D8
H	-14	ASP	-	expression tag	UNP Q7A6D8
H	-13	TYR	-	expression tag	UNP Q7A6D8
H	-12	ASP	-	expression tag	UNP Q7A6D8
H	-11	ILE	-	expression tag	UNP Q7A6D8
H	-10	PRO	-	expression tag	UNP Q7A6D8
H	-9	THR	-	expression tag	UNP Q7A6D8
H	-8	THR	-	expression tag	UNP Q7A6D8
H	-7	GLU	-	expression tag	UNP Q7A6D8
H	-6	ASN	-	expression tag	UNP Q7A6D8
H	-5	LEU	-	expression tag	UNP Q7A6D8
H	-4	TYR	-	expression tag	UNP Q7A6D8
H	-3	PHE	-	expression tag	UNP Q7A6D8
H	-2	GLN	-	expression tag	UNP Q7A6D8
H	-1	GLY	-	expression tag	UNP Q7A6D8
H	0	ALA	-	expression tag	UNP Q7A6D8
H	2	VAL	LEU	engineered mutation	UNP Q7A6D8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



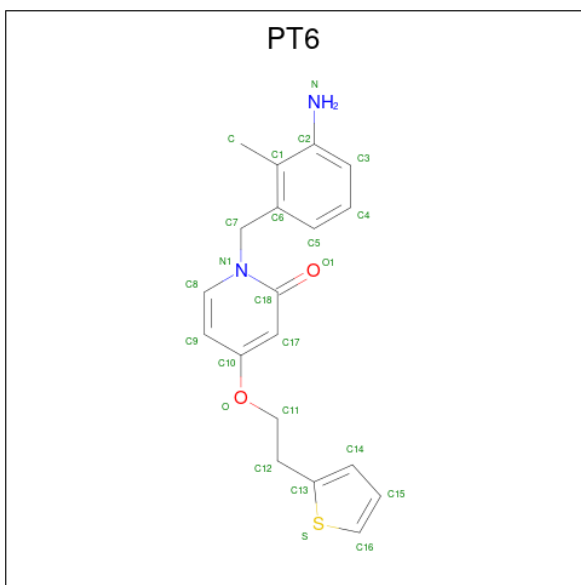
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



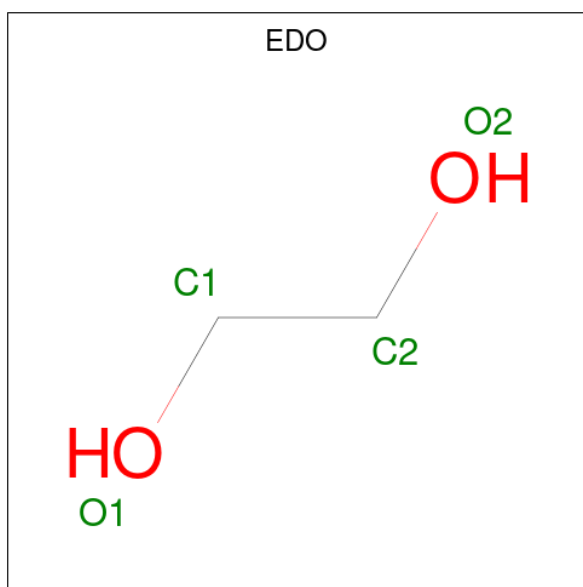
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G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

- Molecule 4 is 1-(3-amino-2-methylbenzyl)-4-[2-(thiophen-2-yl)ethoxy]pyridin-2(1H)-one (CCD ID: PT6) (formula: C₁₉H₂₀N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	C	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	E	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	F	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	G	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	H	1	Total	C	N	O	S	0	0
			24	19	2	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	134	Total O 134 134	0	0

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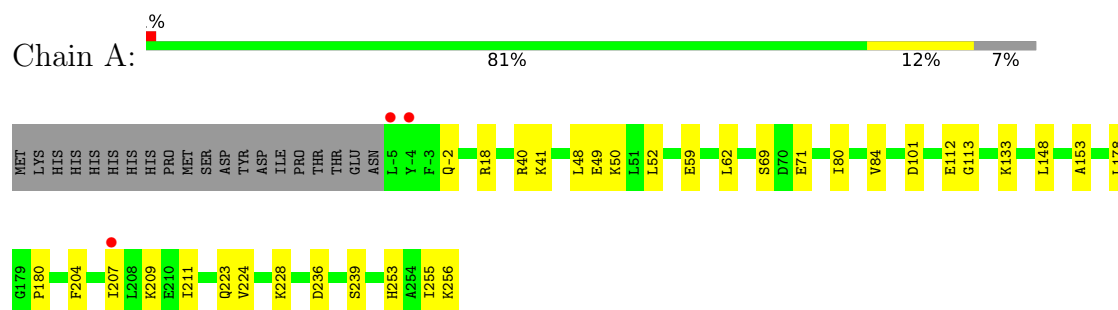
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	110	Total 110	O 110	0	0
7	C	106	Total 106	O 106	0	0
7	D	87	Total 87	O 87	0	0
7	E	138	Total 138	O 138	0	0
7	F	112	Total 112	O 112	0	0
7	G	82	Total 82	O 82	0	0
7	H	80	Total 80	O 80	0	0

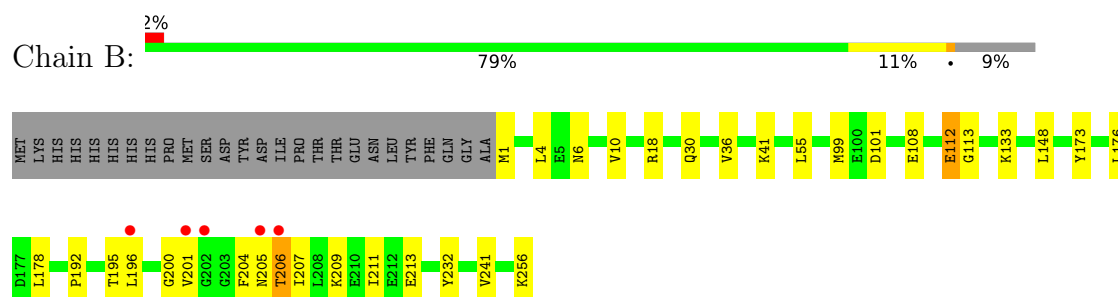
3 Residue-property plots [i](#)

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.

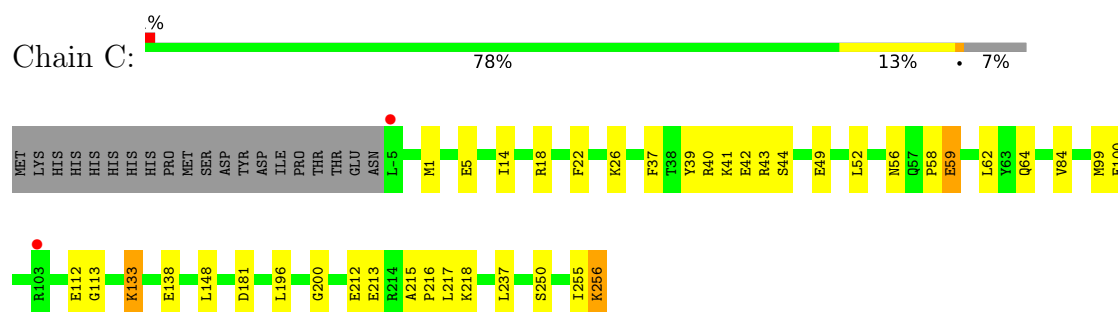
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



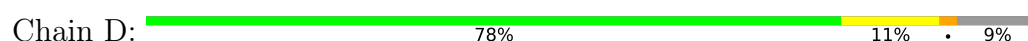
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

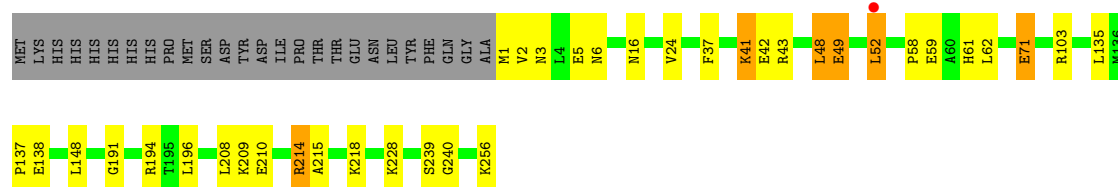


• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

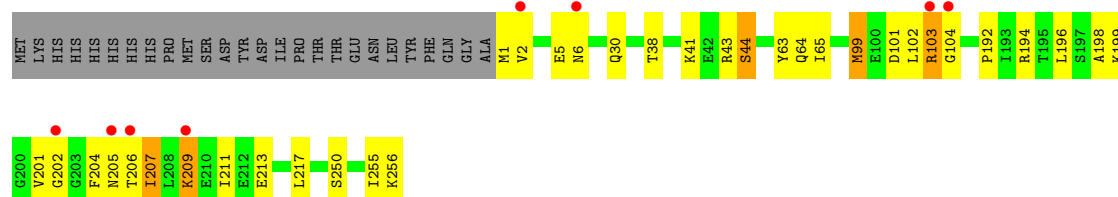
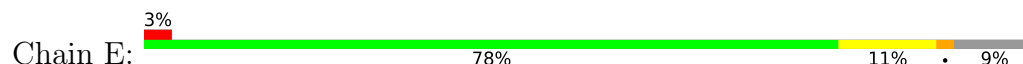


• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

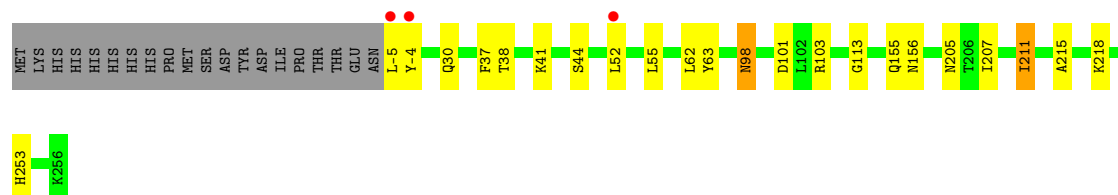
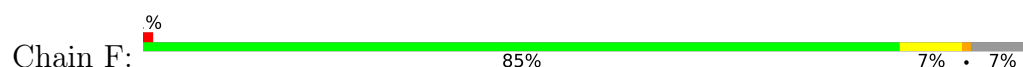




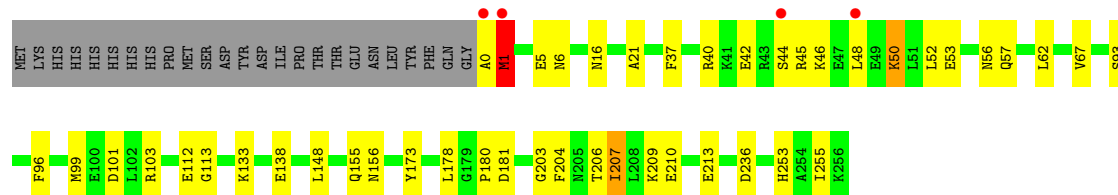
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



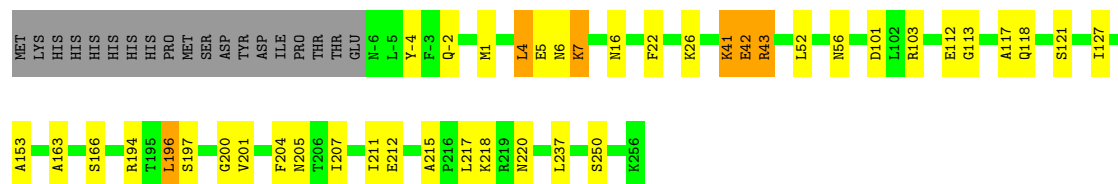
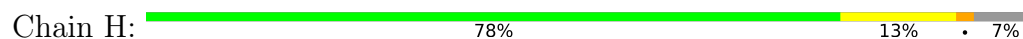
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.90Å 108.47Å 296.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 1.95 47.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.56-1.95) 99.9 (47.56-1.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.168 , 0.231 0.182 , 0.242	Depositor DCC
R_{free} test set	7320 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17795	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NDP, CL, EDO, PT6

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	0.70	0/2104	1.00	0/2834
1	B	0.66	0/2094	1.02	2/2821 (0.1%)
1	C	0.65	0/2084	1.01	1/2803 (0.0%)
1	D	0.68	0/2052	1.07	7/2763 (0.3%)
1	E	0.68	0/2097	1.01	3/2823 (0.1%)
1	F	0.69	0/2063	1.01	2/2780 (0.1%)
1	G	0.63	0/2040	0.99	1/2747 (0.0%)
1	H	0.64	0/2085	1.02	3/2808 (0.1%)
All	All	0.67	0/16619	1.02	19/22379 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	2
All	All	0	3

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	VAL	N-CA-C	8.98	121.52	112.90
1	D	2	VAL	N-CA-C	7.42	120.02	112.90
1	D	239	SER	CA-C-N	-6.44	111.21	122.09
1	D	239	SER	C-N-CA	-6.44	111.21	122.09
1	E	104	GLY	N-CA-C	-5.91	101.34	112.10
1	H	-4	TYR	N-CA-C	-5.90	106.13	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	GLU	N-CA-C	5.52	116.84	108.07
1	F	205	ASN	N-CA-C	5.52	117.30	111.28
1	D	214	ARG	N-CA-C	5.52	121.03	113.97
1	F	211	ILE	N-CA-C	-5.50	105.36	110.53
1	H	163	ALA	N-CA-C	5.47	117.24	111.28
1	H	56	ASN	CB-CA-C	-5.44	104.47	111.22
1	E	2	VAL	CB-CA-C	-5.41	104.50	111.20
1	D	24	VAL	N-CA-C	5.28	115.49	110.42
1	D	2	VAL	CB-CA-C	-5.28	104.66	111.20
1	B	241	VAL	N-CA-C	5.25	115.41	107.80
1	B	176	LEU	N-CA-C	5.18	117.01	111.36
1	D	240	GLY	N-CA-C	5.11	122.14	115.40
1	G	57	GLN	N-CA-C	5.00	115.73	109.57

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200[A]	GLY	Peptide
1	E	103[A]	ARG	Peptide
1	E	103[B]	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2060	0	2078	28	0
1	B	2057	0	2079	28	0
1	C	2047	0	2071	34	0
1	D	2007	0	2044	29	0
1	E	2063	0	2095	41	0
1	F	2028	0	2045	15	0
1	G	2007	0	2028	38	0
1	H	2047	0	2072	26	0
2	A	10	0	0	1	0
2	B	5	0	0	0	0
2	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	5	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	0	0
3	C	48	0	26	1	0
3	D	48	0	26	0	0
3	E	48	0	26	1	0
3	F	48	0	26	0	0
3	G	48	0	26	2	0
3	H	48	0	26	2	0
4	A	24	0	20	0	0
4	B	24	0	20	0	0
4	C	24	0	20	0	0
4	D	24	0	20	0	0
4	E	24	0	20	0	0
4	F	24	0	20	0	0
4	G	24	0	20	0	0
4	H	24	0	20	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
5	E	4	0	6	2	0
5	G	8	0	12	3	0
5	H	4	0	6	0	0
6	F	1	0	0	0	0
7	A	134	0	0	6	0
7	B	110	0	0	4	0
7	C	106	0	0	3	0
7	D	87	0	0	2	0
7	E	138	0	0	5	0
7	F	112	0	0	2	0
7	G	82	0	0	4	0
7	H	80	0	0	4	0
All	All	17795	0	16922	215	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 6.

All (215) 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:A:40:ARG:HH11	1:A:41:LYS:HD2	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ASP:OD1	7:E:2062:HOH:O	1.86	0.93
1:G:112[A]:GLU:HG3	7:G:2046:HOH:O	1.71	0.89
1:E:207[B]:ILE:O	1:E:211:ILE:HG12	1.73	0.88
1:C:215:ALA:O	1:C:218[A]:LYS:HD3	1.73	0.88
7:E:2121:HOH:O	1:G:210:GLU:HG3	1.75	0.85
1:B:99:MET:HE1	1:B:201[B]:VAL:HG22	1.57	0.84
1:D:49:GLU:HA	1:D:52:LEU:CD1	2.07	0.84
1:B:30:GLN:HE22	1:F:-4:TYR:H	1.26	0.84
1:B:209[B]:LYS:O	1:B:213:GLU:HG3	1.78	0.84
1:E:256:LYS:HG2	1:G:148:LEU:HD21	1.61	0.82
1:C:1:MET:HE2	1:C:237:LEU:HD21	1.63	0.81
1:B:204[A]:PHE:O	1:B:207[A]:ILE:HG22	1.81	0.81
1:G:0:ALA:O	1:G:1[A]:MET:HB3	1.83	0.77
1:H:205:ASN:O	7:H:2068:HOH:O	2.01	0.77
1:A:40:ARG:NH1	1:A:41:LYS:HD2	1.99	0.76
1:A:256:LYS:HG2	1:C:148:LEU:HD21	1.67	0.76
1:E:204[A]:PHE:O	1:E:207[A]:ILE:HG23	1.86	0.75
1:A:255:ILE:O	1:C:256[B]:LYS:HE2	1.87	0.74
1:B:6:ASN:HB2	7:B:2004:HOH:O	1.88	0.74
1:A:101:ASP:OD2	1:A:113:GLY:HA3	1.88	0.74
1:H:43:ARG:HG2	7:H:2015:HOH:O	1.88	0.73
1:B:204[A]:PHE:HA	1:B:207[A]:ILE:HG22	1.69	0.72
1:A:180:PRO:HG3	1:D:218[B]:LYS:HD2	1.70	0.72
1:G:0:ALA:O	1:G:1[B]:MET:HB2	1.89	0.71
1:B:206[A]:THR:HG22	7:B:2087:HOH:O	1.92	0.70
1:G:0:ALA:O	1:G:1[A]:MET:CB	2.40	0.69
1:C:18:ARG:HD2	7:C:2018:HOH:O	1.92	0.69
1:H:204:PHE:O	1:H:207:ILE:HG22	1.93	0.68
1:D:5:GLU:O	1:D:6:ASN:HB2	1.93	0.68
1:E:99:MET:HE1	1:E:201[B]:VAL:HB	1.76	0.68
1:C:18:ARG:HG2	7:C:2021:HOH:O	1.93	0.68
1:E:256:LYS:HG2	1:G:148:LEU:CD2	2.24	0.67
1:G:112[B]:GLU:HG2	1:G:113:GLY:N	2.07	0.67
1:C:213:GLU:O	1:C:218[A]:LYS:HE3	1.95	0.67
1:C:49:GLU:HG2	1:C:62:LEU:HD11	1.77	0.67
1:D:41:LYS:HG3	1:D:43:ARG:HG3	1.75	0.66
1:E:1:MET:N	7:E:2002:HOH:O	2.29	0.66
1:A:41:LYS:NZ	7:A:2022:HOH:O	2.27	0.65
1:A:256:LYS:HG2	1:C:148:LEU:CD2	2.25	0.65
1:D:49:GLU:HA	1:D:52:LEU:HD12	1.79	0.64
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ILE:O	1:F:211:ILE:HD13	1.98	0.63
1:C:49:GLU:HG2	1:C:62:LEU:CD1	2.29	0.63
1:B:204[A]:PHE:C	1:B:207[A]:ILE:HG22	2.23	0.63
1:B:204[A]:PHE:CA	1:B:207[A]:ILE:HG22	2.29	0.62
1:E:205[B]:ASN:O	1:E:206[B]:THR:C	2.41	0.61
1:D:16:ASN:ND2	1:D:196[B]:LEU:HD22	2.15	0.61
1:D:41:LYS:HE2	1:D:43:ARG:NE	2.16	0.61
1:H:22:PHE:CE2	1:H:26:LYS:HE3	2.35	0.61
1:B:204[A]:PHE:O	1:B:207[A]:ILE:CG2	2.48	0.60
1:E:194:ARG:HH11	1:E:194:ARG:HG2	1.64	0.60
1:H:5:GLU:O	1:H:6:ASN:HB2	2.00	0.60
1:A:253:HIS:HD2	7:A:2131:HOH:O	1.84	0.60
1:H:103:ARG:NH2	1:H:200:GLY:O	2.34	0.60
1:D:41:LYS:HB3	7:D:2016:HOH:O	2.01	0.60
1:G:204:PHE:O	1:G:207:ILE:HG22	2.01	0.60
1:G:209:LYS:O	1:G:213:GLU:HG3	2.02	0.60
1:D:59:GLU:HG3	1:D:61:HIS:NE2	2.17	0.60
1:D:71:GLU:H	1:D:71:GLU:CD	2.10	0.59
1:F:37:PHE:HB2	1:F:62:LEU:HD23	1.84	0.59
1:H:201:VAL:O	7:H:3135:HOH:O	2.16	0.59
1:A:148:LEU:HD21	1:C:256[A]:LYS:HD2	1.85	0.59
1:C:56:ASN:ND2	1:F:30:GLN:OE1	2.36	0.59
1:F:253:HIS:HD2	7:F:2031:HOH:O	1.86	0.59
1:E:204[A]:PHE:HA	1:E:207[A]:ILE:CG2	2.33	0.58
1:E:43:ARG:HD3	5:E:1261:EDO:H12	1.85	0.58
1:B:148:LEU:CD2	1:D:256:LYS:HG2	2.33	0.58
1:B:204[A]:PHE:HA	1:B:207[A]:ILE:CG2	2.32	0.58
1:C:58:PRO:O	1:C:59:GLU:HB3	2.03	0.58
1:E:201[B]:VAL:HG13	1:E:204[B]:PHE:HB2	1.86	0.58
1:E:41:LYS:HD2	1:E:43:ARG:CZ	2.34	0.58
1:H:112:GLU:CD	1:H:112:GLU:H	2.12	0.58
1:B:30:GLN:NE2	1:F:-4:TYR:H	1.97	0.57
1:E:103[A]:ARG:HG2	1:E:103[A]:ARG:HH11	1.69	0.57
1:G:5:GLU:O	1:G:6:ASN:HB2	2.05	0.57
1:B:112[A]:GLU:CD	1:B:112[A]:GLU:H	2.12	0.57
1:A:256:LYS:HD2	1:C:256[B]:LYS:HE3	1.86	0.57
1:D:48:LEU:O	1:D:52:LEU:HD12	2.05	0.57
1:C:41:LYS:HD2	1:C:43:ARG:NH2	2.19	0.57
1:G:1[A]:MET:HE1	1:G:236:ASP:H	1.71	0.56
1:D:49:GLU:HA	1:D:52:LEU:HD11	1.85	0.56
1:D:37:PHE:HB2	1:D:62:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:MET:HE2	1:C:200:GLY:O	2.06	0.55
1:A:112[A]:GLU:HG2	7:A:2067:HOH:O	2.07	0.55
1:D:16:ASN:HD22	1:D:196[B]:LEU:HD22	1.72	0.55
1:H:207:ILE:O	1:H:211:ILE:HG12	2.07	0.55
1:G:96:PHE:HD1	7:G:2032:HOH:O	1.88	0.55
1:F:98:ASN:ND2	7:F:2040:HOH:O	2.40	0.55
1:G:37:PHE:HB2	1:G:62:LEU:HD23	1.89	0.55
1:G:101:ASP:OD2	1:G:113:GLY:HA3	2.07	0.54
1:H:41:LYS:HE3	3:H:1258:NDP:O2X	2.07	0.54
1:C:42[A]:GLU:OE1	1:C:64:GLN:NE2	2.40	0.54
1:G:99:MET:O	1:G:103[A]:ARG:HG3	2.08	0.54
1:F:218:LYS:HD3	1:G:180:PRO:HG3	1.90	0.53
1:G:0:ALA:O	1:G:1[B]:MET:CB	2.54	0.53
1:A:255:ILE:O	1:C:256[B]:LYS:CE	2.56	0.53
1:E:43:ARG:CD	5:E:1261:EDO:H12	2.39	0.53
1:F:101:ASP:OD2	1:F:113:GLY:HA3	2.09	0.53
1:H:118:GLN:HE22	1:H:166:SER:CB	2.21	0.53
1:A:207:ILE:O	1:A:211:ILE:HG12	2.08	0.53
1:A:239[B]:SER:O	7:A:2124:HOH:O	2.19	0.53
1:C:5:GLU:OE2	1:G:1[B]:MET:HA	2.10	0.52
1:E:41:LYS:HG2	7:E:2022:HOH:O	2.10	0.52
1:D:210:GLU:HG2	1:D:214:ARG:HD2	1.91	0.52
1:B:232:TYR:HA	1:C:1:MET:HE1	1.91	0.52
1:E:198:ALA:O	1:E:201[B]:VAL:HG12	2.09	0.52
1:E:256:LYS:HE2	1:G:255:ILE:O	2.10	0.52
1:G:50:LYS:O	1:G:53:GLU:HG3	2.10	0.52
1:D:215:ALA:O	1:D:218[A]:LYS:HD2	2.10	0.52
1:H:101:ASP:OD2	1:H:113:GLY:HA3	2.10	0.52
1:A:133:LYS:HD2	1:A:178:LEU:HD22	1.92	0.50
1:E:5:GLU:O	1:E:6:ASN:HB2	2.11	0.50
1:H:212:GLU:HG3	1:H:220:ASN:ND2	2.26	0.50
1:H:-2:GLN:H	1:H:-2:GLN:CD	2.19	0.50
1:A:256:LYS:HE2	1:C:255:ILE:O	2.12	0.50
1:D:16:ASN:HD21	1:D:196[A]:LEU:HB2	1.77	0.50
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.46	0.50
1:G:155:GLN:O	1:G:156:ASN:HB2	2.12	0.50
1:G:253:HIS:HD2	7:G:2016:HOH:O	1.93	0.50
1:C:112[B]:GLU:HG2	1:C:113:GLY:N	2.27	0.49
1:B:192:PRO:HG2	1:B:207[B]:ILE:CG2	2.42	0.49
1:E:194:ARG:HG2	1:E:194:ARG:NH1	2.27	0.49
1:B:205[A]:ASN:HB3	7:B:2087:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ASN:HD21	1:D:196[B]:LEU:CB	2.26	0.49
1:C:37:PHE:HB2	1:C:62:LEU:HD23	1.94	0.49
1:C:49:GLU:CG	1:C:62:LEU:CD1	2.89	0.49
1:G:206:THR:HG23	5:G:1257:EDO:H11	1.95	0.48
1:E:205[B]:ASN:O	1:E:207[B]:ILE:N	2.46	0.48
1:C:37:PHE:CD2	1:C:52:LEU:HD21	2.49	0.48
1:C:52:LEU:HD22	1:C:62:LEU:HD21	1.96	0.48
1:E:103[A]:ARG:HG2	1:E:103[A]:ARG:NH1	2.29	0.48
1:H:4:LEU:O	1:H:7:LYS:HB2	2.14	0.48
1:A:18[A]:ARG:NE	1:A:223:GLN:HE22	2.12	0.47
1:G:67:VAL:HG22	3:G:1259:NDP:N1A	2.29	0.47
1:E:38:THR:HG21	1:E:65:ILE:HD12	1.96	0.47
1:B:207[B]:ILE:O	1:B:211:ILE:HG12	2.15	0.47
1:H:117:ALA:O	1:H:121:SER:HB2	2.15	0.47
1:A:18[A]:ARG:CZ	1:A:223:GLN:HE22	2.27	0.47
1:E:41:LYS:O	1:E:44:SER:HB2	2.14	0.47
1:F:41:LYS:HE2	1:F:44:SER:OG	2.14	0.47
1:H:5:GLU:O	1:H:6:ASN:CB	2.61	0.47
1:A:224:VAL:O	1:A:228:LYS:HG3	2.15	0.47
1:E:41:LYS:HE2	3:E:1259:NDP:O2X	2.15	0.47
1:D:16:ASN:HD21	1:D:196[B]:LEU:HB2	1.79	0.47
1:E:196:LEU:HB3	7:E:2010:HOH:O	2.14	0.46
1:G:203:GLY:O	1:G:207:ILE:HB	2.14	0.46
1:F:-5:LEU:HD22	1:G:56:ASN:ND2	2.30	0.46
1:B:112[A]:GLU:HG2	7:B:2050:HOH:O	2.14	0.46
1:G:133:LYS:HE3	1:G:181:ASP:OD2	2.15	0.46
1:H:16:ASN:HD21	1:H:196:LEU:HB2	1.81	0.46
1:E:99:MET:CE	1:E:201[B]:VAL:HB	2.44	0.46
1:H:42:GLU:HB2	7:H:2015:HOH:O	2.15	0.46
1:D:3:ASN:OD1	1:D:5:GLU:HB2	2.16	0.46
1:G:21:ALA:HB2	1:G:93:SER:CB	2.46	0.46
7:A:2073:HOH:O	1:B:108:GLU:OE2	2.21	0.46
1:A:69:SER:OG	2:A:1259:SO4:O1	2.33	0.46
1:E:196:LEU:HD13	1:E:199[B]:LYS:NZ	2.31	0.46
1:F:38:THR:HA	1:F:63:TYR:O	2.15	0.46
1:E:103[B]:ARG:CZ	1:E:202[B]:GLY:CA	2.95	0.45
1:G:42:GLU:O	1:G:45:ARG:N	2.48	0.45
1:E:217:LEU:HD12	1:E:250:SER:HA	1.99	0.45
1:D:135:LEU:C	1:D:137:PRO:HD3	2.41	0.45
1:H:1:MET:HE2	1:H:237:LEU:HD21	2.00	0.45
1:H:215:ALA:O	1:H:218[A]:LYS:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:LEU:HD13	1:E:199[B]:LYS:HZ2	1.81	0.44
1:G:1[A]:MET:CE	1:G:236:ASP:H	2.30	0.44
1:A:236:ASP:OD2	1:D:228:LYS:NZ	2.50	0.44
1:B:133:LYS:HD2	1:B:178:LEU:HD22	1.98	0.44
1:E:41:LYS:HD2	1:E:43:ARG:NH2	2.32	0.44
1:G:0:ALA:HB2	5:G:1358:EDO:H22	2.00	0.44
1:G:133:LYS:HD2	1:G:178:LEU:HD22	2.00	0.44
1:F:155:GLN:O	1:F:156:ASN:HB2	2.18	0.44
1:B:101:ASP:OD2	1:B:113:GLY:HA3	2.17	0.44
1:C:22:PHE:O	1:C:26:LYS:HG3	2.18	0.43
1:E:201[B]:VAL:HG13	1:E:201[B]:VAL:O	2.18	0.43
1:A:253:HIS:CD2	7:A:2131:HOH:O	2.65	0.43
1:B:10:VAL:HG22	1:B:36:VAL:HB	2.01	0.43
1:F:41:LYS:HG2	1:F:44:SER:OG	2.18	0.43
1:F:215:ALA:O	1:F:218:LYS:HD2	2.18	0.43
1:D:191:GLY:HA3	7:D:2082:HOH:O	2.18	0.43
1:E:103[B]:ARG:CZ	1:E:202[B]:GLY:HA2	2.48	0.43
1:H:7:LYS:HA	1:H:7:LYS:HD3	1.75	0.43
1:H:112:GLU:CD	1:H:112:GLU:N	2.77	0.43
1:C:217:LEU:HD12	1:C:250:SER:HA	2.00	0.43
1:D:137:PRO:HB2	1:D:138:GLU:OE1	2.19	0.43
1:G:40:ARG:HB3	3:G:1259:NDP:O2X	2.19	0.42
1:E:38:THR:HA	1:E:63:TYR:O	2.20	0.42
1:D:210:GLU:OE2	1:D:214:ARG:NH1	2.45	0.42
1:C:1:MET:CE	1:C:237:LEU:HD21	2.43	0.42
1:E:207[B]:ILE:HD12	1:E:211:ILE:HD11	2.02	0.42
1:G:16:ASN:C	1:G:16:ASN:OD1	2.61	0.42
1:C:39:TYR:HA	7:C:2015:HOH:O	2.20	0.42
1:G:206:THR:H	5:G:1257:EDO:H11	1.85	0.41
1:A:204:PHE:O	1:A:207:ILE:HG22	2.20	0.41
1:E:209[A]:LYS:O	1:E:213:GLU:HG3	2.20	0.41
1:H:197:SER:HB3	3:H:1258:NDP:O1A	2.21	0.41
1:A:153:ALA:HA	1:B:173:TYR:CZ	2.56	0.41
1:C:133:LYS:HE2	1:C:181:ASP:OD2	2.20	0.41
1:A:48:LEU:HD11	1:A:52:LEU:HD11	2.02	0.41
1:A:49:GLU:HG2	1:A:62:LEU:HD11	2.03	0.41
1:A:80:ILE:O	1:A:84:VAL:HG22	2.21	0.41
1:C:212:GLU:O	1:C:218[B]:LYS:HD2	2.19	0.41
1:G:253:HIS:CD2	7:G:2016:HOH:O	2.70	0.41
1:C:14:ILE:HD12	1:C:37:PHE:CD1	2.56	0.41
1:H:217:LEU:HB2	1:H:250:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HD3	3:C:1258:NDP:C5A	2.51	0.41
1:D:194:ARG:NH1	1:D:208:LEU:HD13	2.36	0.41
1:B:256:LYS:HE3	1:D:148:LEU:HD21	2.02	0.40
1:B:18:ARG:O	1:B:195:THR:HG22	2.21	0.40
1:E:192:PRO:HG3	1:E:207[B]:ILE:HG23	2.03	0.40
1:E:204[A]:PHE:HA	1:E:207[A]:ILE:HG22	2.03	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	267/282 (95%)	256 (96%)	10 (4%)	1 (0%)	30	21
1	B	267/282 (95%)	259 (97%)	8 (3%)	0	100	100
1	C	263/282 (93%)	257 (98%)	6 (2%)	0	100	100
1	D	260/282 (92%)	248 (95%)	11 (4%)	1 (0%)	30	21
1	E	267/282 (95%)	250 (94%)	17 (6%)	0	100	100
1	F	262/282 (93%)	253 (97%)	9 (3%)	0	100	100
1	G	260/282 (92%)	250 (96%)	8 (3%)	2 (1%)	16	8
1	H	264/282 (94%)	252 (96%)	11 (4%)	1 (0%)	30	21
All	All	2110/2256 (94%)	2025 (96%)	80 (4%)	5 (0%)	43	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	1[A]	MET
1	G	1[B]	MET
1	H	42	GLU
1	D	58	PRO

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Mol	Chain	Res	Type
1	A	-2	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/234 (94%)	215 (98%)	5 (2%)	44	38
1	B	220/234 (94%)	211 (96%)	9 (4%)	27	17
1	C	218/234 (93%)	209 (96%)	9 (4%)	27	17
1	D	216/234 (92%)	206 (95%)	10 (5%)	24	13
1	E	220/234 (94%)	210 (96%)	10 (4%)	24	14
1	F	216/234 (92%)	212 (98%)	4 (2%)	50	45
1	G	214/234 (92%)	205 (96%)	9 (4%)	26	16
1	H	218/234 (93%)	210 (96%)	8 (4%)	30	20
All	All	1742/1872 (93%)	1678 (96%)	64 (4%)	33	20

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	59[A]	GLU
1	A	59[B]	GLU
1	A	71	GLU
1	A	209	LYS
1	B	1	MET
1	B	4	LEU
1	B	41	LYS
1	B	55	LEU
1	B	112[A]	GLU
1	B	112[B]	GLU
1	B	196	LEU
1	B	206[A]	THR
1	B	206[B]	THR

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Mol	Chain	Res	Type
1	C	44	SER
1	C	84	VAL
1	C	100	GLU
1	C	133	LYS
1	C	138	GLU
1	C	196	LEU
1	C	216	PRO
1	C	256[A]	LYS
1	C	256[B]	LYS
1	D	1	MET
1	D	41	LYS
1	D	42	GLU
1	D	48	LEU
1	D	49	GLU
1	D	52	LEU
1	D	71	GLU
1	D	103[A]	ARG
1	D	103[B]	ARG
1	D	209	LYS
1	E	30	GLN
1	E	44	SER
1	E	64	GLN
1	E	99	MET
1	E	102	LEU
1	E	207[A]	ILE
1	E	207[B]	ILE
1	E	209[A]	LYS
1	E	209[B]	LYS
1	E	255	ILE
1	F	52	LEU
1	F	55	LEU
1	F	98	ASN
1	F	103	ARG
1	G	1[A]	MET
1	G	1[B]	MET
1	G	44	SER
1	G	46	LYS
1	G	48	LEU
1	G	50	LYS
1	G	52	LEU
1	G	138	GLU
1	G	207	ILE

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Mol	Chain	Res	Type
1	H	4	LEU
1	H	7	LYS
1	H	41	LYS
1	H	43	ARG
1	H	52	LEU
1	H	127	ILE
1	H	194	ARG
1	H	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	64	GLN
1	A	98	ASN
1	A	253	HIS
1	B	30	GLN
1	B	61	HIS
1	B	68	GLN
1	B	86	ASN
1	B	170	ASN
1	C	-2	GLN
1	C	30	GLN
1	C	56	ASN
1	C	64	GLN
1	C	98	ASN
1	C	220	ASN
1	C	253	HIS
1	D	16	ASN
1	D	56	ASN
1	D	155	GLN
1	D	253	HIS
1	E	75	ASN
1	F	-2	GLN
1	F	56	ASN
1	F	98	ASN
1	F	130	HIS
1	F	253	HIS
1	G	56	ASN
1	G	253	HIS
1	H	64	GLN
1	H	118	GLN

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Mol	Chain	Res	Type
1	H	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 for Mogul analysis.

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	$\# Z > 2$
4	PT6	D	1258	-	26,26,26	0.40	0	29,35,35	0.60	1 (3%)
4	PT6	H	1259	-	26,26,26	0.46	0	29,35,35	0.57	0
4	PT6	C	1259	-	26,26,26	0.34	0	29,35,35	0.54	0
3	NDP	F	1258	-	51,52,52	0.73	2 (3%)	71,80,80	1.14	5 (7%)
5	EDO	H	1257	-	3,3,3	0.48	0	2,2,2	0.46	0
2	SO4	B	1257	-	4,4,4	0.18	0	6,6,6	0.26	0
5	EDO	C	1270	-	3,3,3	0.50	0	2,2,2	0.42	0
5	EDO	G	1257	-	3,3,3	0.43	0	2,2,2	0.78	0
3	NDP	E	1259	-	51,52,52	0.66	2 (3%)	71,80,80	1.30	9 (12%)
2	SO4	E	1257	-	4,4,4	0.26	0	6,6,6	0.22	0
3	NDP	H	1258	-	51,52,52	0.78	2 (3%)	71,80,80	1.43	8 (11%)
5	EDO	G	1358	-	3,3,3	0.43	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PT6	B	1260	-	26,26,26	0.47	0	29,35,35	0.49	0
5	EDO	E	1261	-	3,3,3	0.42	0	2,2,2	0.75	0
2	SO4	A	1259	-	4,4,4	0.25	0	6,6,6	0.64	0
3	NDP	C	1258	-	51,52,52	0.60	1 (1%)	71,80,80	1.46	9 (12%)
2	SO4	A	1257	-	4,4,4	0.27	0	6,6,6	0.20	0
4	PT6	A	1261	-	26,26,26	0.62	1 (3%)	29,35,35	0.72	0
4	PT6	G	1260	-	26,26,26	0.47	0	29,35,35	0.51	0
3	NDP	B	1259	-	51,52,52	0.90	3 (5%)	71,80,80	1.12	7 (9%)
4	PT6	F	1259	-	26,26,26	0.38	0	29,35,35	0.56	0
4	PT6	E	1260	-	26,26,26	0.53	0	29,35,35	0.74	0
5	EDO	B	1258	-	3,3,3	0.43	0	2,2,2	0.42	0
3	NDP	D	1257	-	51,52,52	0.67	1 (1%)	71,80,80	1.29	5 (7%)
2	SO4	H	1358	-	4,4,4	0.33	0	6,6,6	0.19	0
3	NDP	A	1260	-	51,52,52	0.70	2 (3%)	71,80,80	1.12	4 (5%)
5	EDO	A	1270	-	3,3,3	0.36	0	2,2,2	0.79	0
3	NDP	G	1259	-	51,52,52	0.85	2 (3%)	71,80,80	1.34	10 (14%)

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
4	PT6	D	1258	-	-	2/10/10/10	0/3/3/3
4	PT6	H	1259	-	-	1/10/10/10	0/3/3/3
4	PT6	C	1259	-	-	1/10/10/10	0/3/3/3
3	NDP	F	1258	-	-	4/34/77/77	0/5/5/5
5	EDO	H	1257	-	-	0/1/1/1	-
5	EDO	C	1270	-	-	0/1/1/1	-
5	EDO	G	1257	-	-	1/1/1/1	-
3	NDP	E	1259	-	-	9/34/77/77	0/5/5/5
3	NDP	H	1258	-	-	9/34/77/77	0/5/5/5
5	EDO	G	1358	-	-	1/1/1/1	-
4	PT6	B	1260	-	-	2/10/10/10	0/3/3/3
5	EDO	E	1261	-	-	1/1/1/1	-
3	NDP	C	1258	-	-	10/34/77/77	0/5/5/5
4	PT6	A	1261	-	-	0/10/10/10	0/3/3/3
4	PT6	G	1260	-	-	1/10/10/10	0/3/3/3
3	NDP	B	1259	-	-	6/34/77/77	0/5/5/5
4	PT6	F	1259	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PT6	E	1260	-	-	0/10/10/10	0/3/3/3
5	EDO	B	1258	-	-	1/1/1/1	-
3	NDP	D	1257	-	-	10/34/77/77	0/5/5/5
3	NDP	A	1260	-	-	9/34/77/77	0/5/5/5
5	EDO	A	1270	-	-	0/1/1/1	-
3	NDP	G	1259	-	-	8/34/77/77	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1259	NDP	PN-O3	4.82	1.64	1.59
3	H	1258	NDP	PN-O3	4.06	1.63	1.59
3	G	1259	NDP	PN-O3	3.94	1.63	1.59
3	A	1260	NDP	PN-O3	3.60	1.63	1.59
3	D	1257	NDP	C6N-N1N	3.50	1.45	1.37
3	G	1259	NDP	C6N-N1N	3.38	1.45	1.37
3	F	1258	NDP	PN-O3	3.14	1.62	1.59
3	F	1258	NDP	C7N-C3N	2.61	1.54	1.48
3	B	1259	NDP	P2B-O2B	2.57	1.64	1.59
3	H	1258	NDP	C6N-N1N	2.48	1.43	1.37
3	E	1259	NDP	C6N-N1N	2.46	1.43	1.37
4	A	1261	PT6	C2-C1	2.41	1.47	1.40
3	E	1259	NDP	PN-O3	2.32	1.62	1.59
3	C	1258	NDP	C6N-N1N	2.27	1.42	1.37
3	A	1260	NDP	C6N-N1N	2.21	1.42	1.37
3	B	1259	NDP	C6N-N1N	2.19	1.42	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1258	NDP	O3-PA-O1A	-7.82	87.19	110.70
3	H	1258	NDP	O3-PA-O1A	-5.53	94.05	110.70
3	D	1257	NDP	O3-PA-O1A	-5.45	94.29	110.70
3	H	1258	NDP	O2N-PN-O3	-4.91	94.01	107.27
3	E	1259	NDP	O3-PA-O1A	-4.82	96.21	110.70
3	D	1257	NDP	O2N-PN-O3	-4.64	94.74	107.27
3	G	1259	NDP	O3-PA-O1A	-4.56	96.99	110.70
3	A	1260	NDP	O3-PA-O1A	-4.31	97.74	110.70
3	B	1259	NDP	O3-PA-O1A	-3.73	99.49	110.70
3	F	1258	NDP	O3-PA-O1A	-3.72	99.51	110.70
3	E	1259	NDP	O7N-C7N-C3N	-3.67	113.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1258	NDP	O2X-P2B-O2B	-3.50	92.22	105.85
3	G	1259	NDP	O2A-PA-O1A	3.33	127.95	112.44
3	D	1257	NDP	O7N-C7N-C3N	-3.12	115.01	120.90
3	E	1259	NDP	O2N-PN-O3	-3.04	99.05	107.27
3	H	1258	NDP	O7N-C7N-C3N	-2.97	115.31	120.90
3	G	1259	NDP	O7N-C7N-C3N	-2.96	115.32	120.90
3	D	1257	NDP	C2D-C1D-N1N	2.92	120.50	113.31
3	A	1260	NDP	O2N-PN-O3	-2.91	99.41	107.27
3	F	1258	NDP	O2X-P2B-O2B	-2.90	94.54	105.85
3	C	1258	NDP	O2A-PA-O1A	2.89	125.88	112.44
3	F	1258	NDP	O4B-C1B-C2B	-2.87	101.64	106.59
3	G	1259	NDP	O4B-C1B-C2B	-2.85	101.68	106.59
3	E	1259	NDP	O4B-C1B-C2B	-2.82	101.73	106.59
3	G	1259	NDP	C3N-C2N-N1N	-2.72	119.21	123.20
3	B	1259	NDP	O7N-C7N-C3N	-2.71	115.79	120.90
3	E	1259	NDP	O2A-PA-O1A	2.69	124.98	112.44
3	G	1259	NDP	O2N-PN-O1N	2.64	124.71	112.44
3	E	1259	NDP	C3N-C7N-N7N	2.58	122.26	117.67
3	H	1258	NDP	O4B-C1B-C2B	-2.57	102.16	106.59
3	G	1259	NDP	O3-PN-O1N	-2.56	103.00	110.70
3	H	1258	NDP	O2A-PA-O3	2.54	114.12	107.27
3	C	1258	NDP	O2N-PN-O3	-2.52	100.46	107.27
3	A	1260	NDP	O4B-C1B-C2B	-2.52	102.25	106.59
3	H	1258	NDP	O2N-PN-O1N	2.52	124.16	112.44
3	C	1258	NDP	C3N-C7N-N7N	2.49	122.09	117.67
3	C	1258	NDP	O7N-C7N-C3N	-2.48	116.22	120.90
3	C	1258	NDP	O2N-PN-O1N	2.46	123.89	112.44
3	B	1259	NDP	C3N-C7N-N7N	2.43	121.98	117.67
3	D	1257	NDP	C3N-C7N-N7N	2.41	121.95	117.67
3	G	1259	NDP	O2N-PN-O3	-2.37	100.87	107.27
3	E	1259	NDP	O2N-PN-O1N	2.34	123.35	112.44
3	C	1258	NDP	O2X-P2B-O2B	-2.33	96.78	105.85
3	C	1258	NDP	O4B-C1B-N9A	2.31	112.52	108.09
3	B	1259	NDP	O2N-PN-O3	-2.31	101.04	107.27
3	F	1258	NDP	O2N-PN-O1N	2.28	123.07	112.44
3	G	1259	NDP	C2D-C1D-N1N	2.24	118.82	113.31
3	A	1260	NDP	O2N-PN-O1N	2.23	122.83	112.44
3	F	1258	NDP	C3B-C2B-C1B	-2.23	98.54	102.81
3	H	1258	NDP	C3N-C2N-N1N	-2.21	119.96	123.20
3	C	1258	NDP	C2D-C1D-N1N	2.17	118.64	113.31
3	B	1259	NDP	O4B-C1B-C2B	-2.14	102.90	106.59
3	E	1259	NDP	O2X-P2B-O1X	2.11	119.07	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1259	NDP	O2N-PN-O1N	2.06	122.02	112.44
3	G	1259	NDP	O2X-P2B-O2B	-2.04	97.89	105.85
3	E	1259	NDP	O2X-P2B-O2B	-2.03	97.93	105.85
3	B	1259	NDP	O3-PN-O1N	-2.03	104.60	110.70
4	D	1258	PT6	C1-C2-N	2.01	122.86	120.32

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1260	NDP	C5D-O5D-PN-O3
3	A	1260	NDP	C5D-O5D-PN-O1N
3	B	1259	NDP	PN-O3-PA-O5B
3	B	1259	NDP	C5D-O5D-PN-O3
3	B	1259	NDP	C5D-O5D-PN-O1N
3	C	1258	NDP	C5D-O5D-PN-O3
3	C	1258	NDP	C5D-O5D-PN-O1N
3	D	1257	NDP	C5D-O5D-PN-O3
3	D	1257	NDP	C5D-O5D-PN-O1N
3	E	1259	NDP	C5D-O5D-PN-O3
3	E	1259	NDP	C5D-O5D-PN-O1N
3	F	1258	NDP	C5D-O5D-PN-O3
3	F	1258	NDP	C5D-O5D-PN-O1N
3	G	1259	NDP	C5D-O5D-PN-O3
3	G	1259	NDP	C5D-O5D-PN-O1N
3	H	1258	NDP	C5B-O5B-PA-O1A
3	H	1258	NDP	C5D-O5D-PN-O3
3	H	1258	NDP	C5D-O5D-PN-O1N
3	D	1257	NDP	C1B-C2B-O2B-P2B
3	E	1259	NDP	C1B-C2B-O2B-P2B
3	D	1257	NDP	C3B-C2B-O2B-P2B
3	E	1259	NDP	C3B-C2B-O2B-P2B
4	C	1259	PT6	O-C11-C12-C13
4	G	1260	PT6	O-C11-C12-C13
3	D	1257	NDP	PN-O3-PA-O5B
3	E	1259	NDP	PN-O3-PA-O5B
3	G	1259	NDP	PN-O3-PA-O5B
3	H	1258	NDP	PN-O3-PA-O5B
3	A	1260	NDP	C5D-O5D-PN-O2N
3	B	1259	NDP	C5D-O5D-PN-O2N
3	C	1258	NDP	C5B-O5B-PA-O3
3	C	1258	NDP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	D	1257	NDP	C5D-O5D-PN-O2N
3	E	1259	NDP	C5D-O5D-PN-O2N
3	F	1258	NDP	C5D-O5D-PN-O2N
3	G	1259	NDP	C5D-O5D-PN-O2N
3	A	1260	NDP	C1B-C2B-O2B-P2B
4	B	1260	PT6	C11-C12-C13-S
4	D	1258	PT6	C11-C12-C13-C14
3	H	1258	NDP	O4B-C4B-C5B-O5B
3	G	1259	NDP	PN-O3-PA-O1A
5	E	1261	EDO	O1-C1-C2-O2
3	G	1259	NDP	O4D-C1D-N1N-C6N
4	D	1258	PT6	C11-C12-C13-S
3	C	1258	NDP	C1B-C2B-O2B-P2B
4	B	1260	PT6	O-C11-C12-C13
4	H	1259	PT6	O-C11-C12-C13
3	C	1258	NDP	O4D-C1D-N1N-C6N
3	F	1258	NDP	O4D-C1D-N1N-C6N
3	B	1259	NDP	O4D-C1D-N1N-C6N
3	E	1259	NDP	O4D-C1D-N1N-C6N
3	E	1259	NDP	C2D-C1D-N1N-C6N
3	H	1258	NDP	C1B-C2B-O2B-P2B
3	A	1260	NDP	O4D-C1D-N1N-C6N
3	D	1257	NDP	O4D-C1D-N1N-C6N
3	H	1258	NDP	O4D-C1D-N1N-C6N
3	G	1259	NDP	C2D-C1D-N1N-C6N
3	A	1260	NDP	C2B-O2B-P2B-O1X
3	D	1257	NDP	C2B-O2B-P2B-O1X
3	C	1258	NDP	PA-O3-PN-O1N
3	C	1258	NDP	PA-O3-PN-O2N
3	A	1260	NDP	C2D-C1D-N1N-C6N
3	C	1258	NDP	C2D-C1D-N1N-C6N
3	A	1260	NDP	C3B-C2B-O2B-P2B
5	G	1358	EDO	O1-C1-C2-O2
5	G	1257	EDO	O1-C1-C2-O2
3	D	1257	NDP	C2D-C1D-N1N-C6N
3	H	1258	NDP	C2D-C1D-N1N-C6N
3	A	1260	NDP	O4B-C4B-C5B-O5B
3	E	1259	NDP	C2B-O2B-P2B-O3X
5	B	1258	EDO	O1-C1-C2-O2
3	B	1259	NDP	O4B-C4B-C5B-O5B
3	C	1258	NDP	C3B-C2B-O2B-P2B
3	H	1258	NDP	C3B-C2B-O2B-P2B

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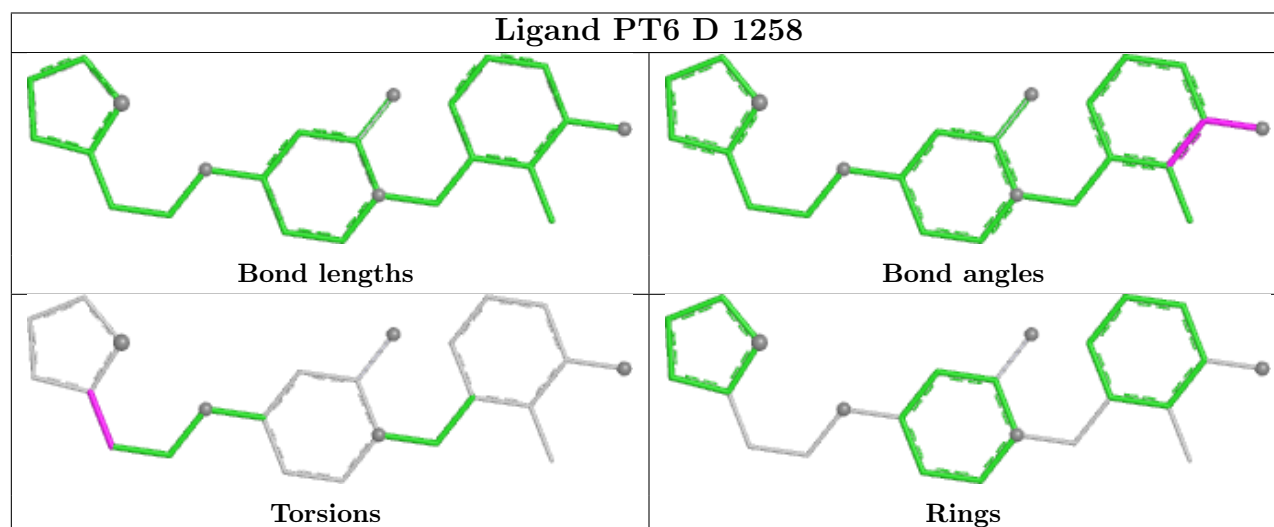
Mol	Chain	Res	Type	Atoms
3	D	1257	NDP	C2N-C3N-C7N-O7N
3	G	1259	NDP	O4B-C4B-C5B-O5B

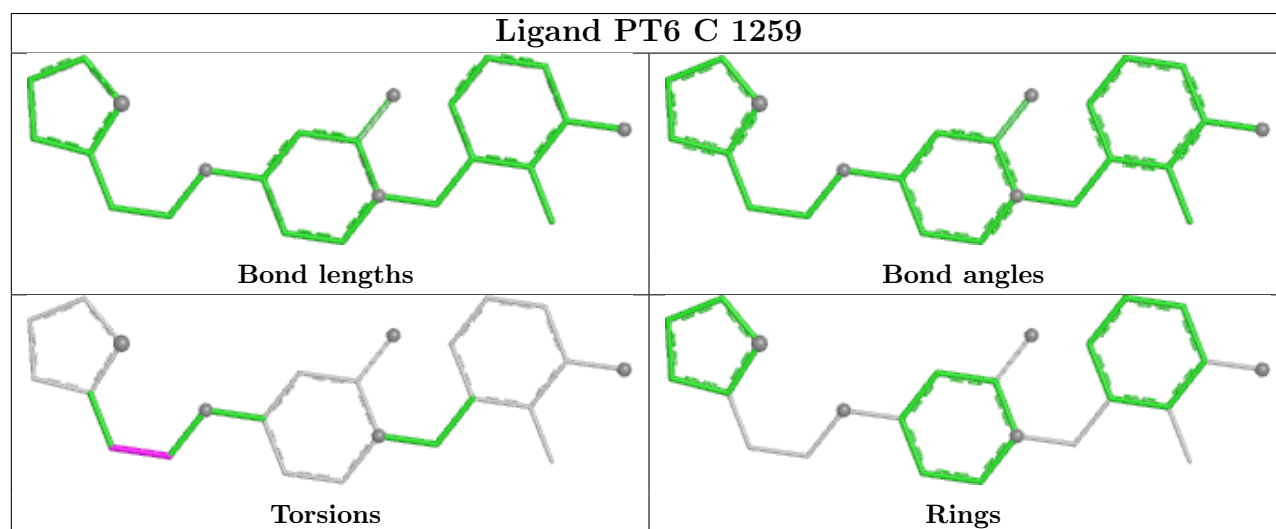
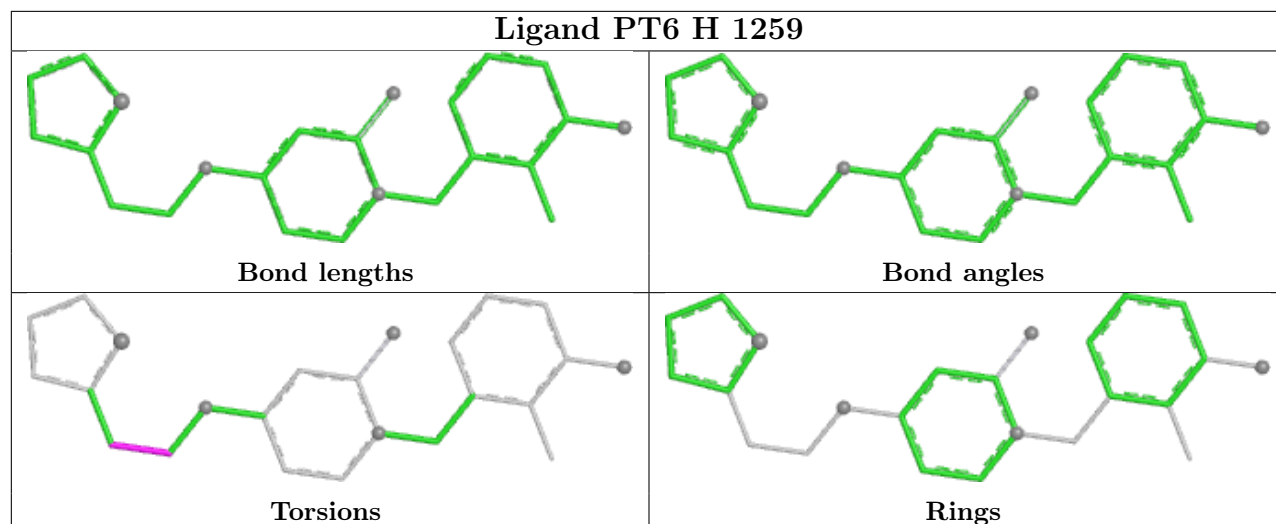
There are no ring outliers.

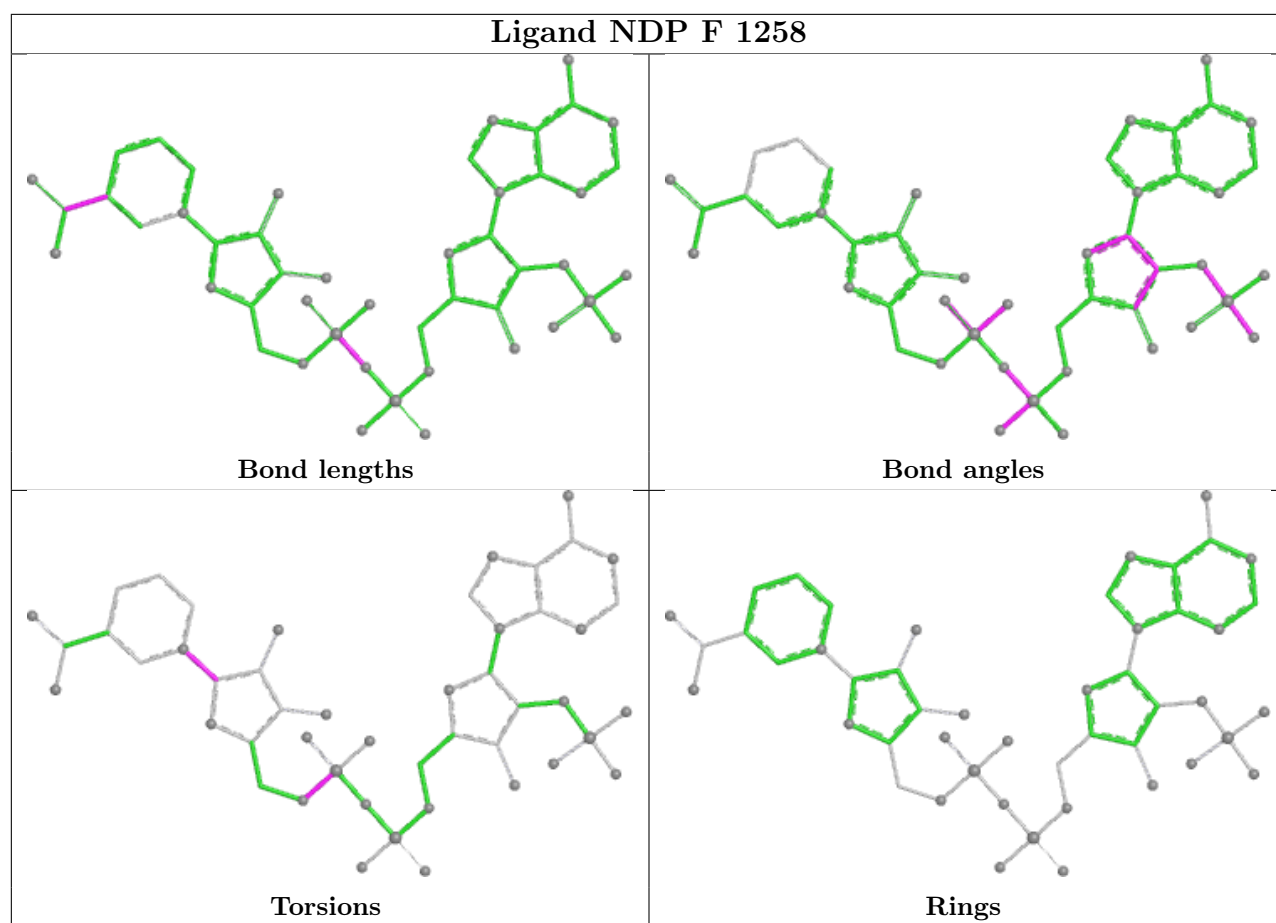
8 monomers are involved in 12 short contacts:

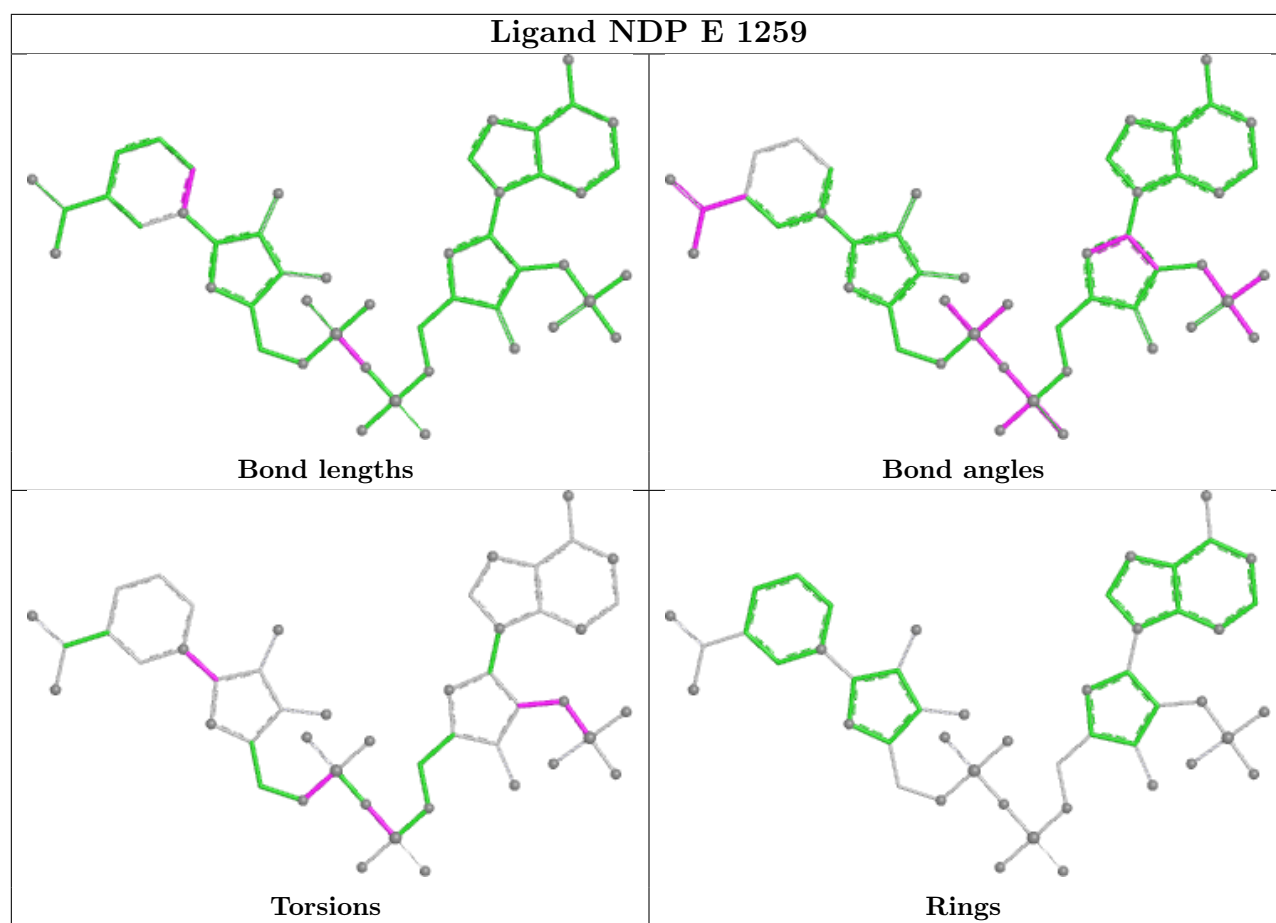
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1257	EDO	2	0
3	E	1259	NDP	1	0
3	H	1258	NDP	2	0
5	G	1358	EDO	1	0
5	E	1261	EDO	2	0
2	A	1259	SO4	1	0
3	C	1258	NDP	1	0
3	G	1259	NDP	2	0

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

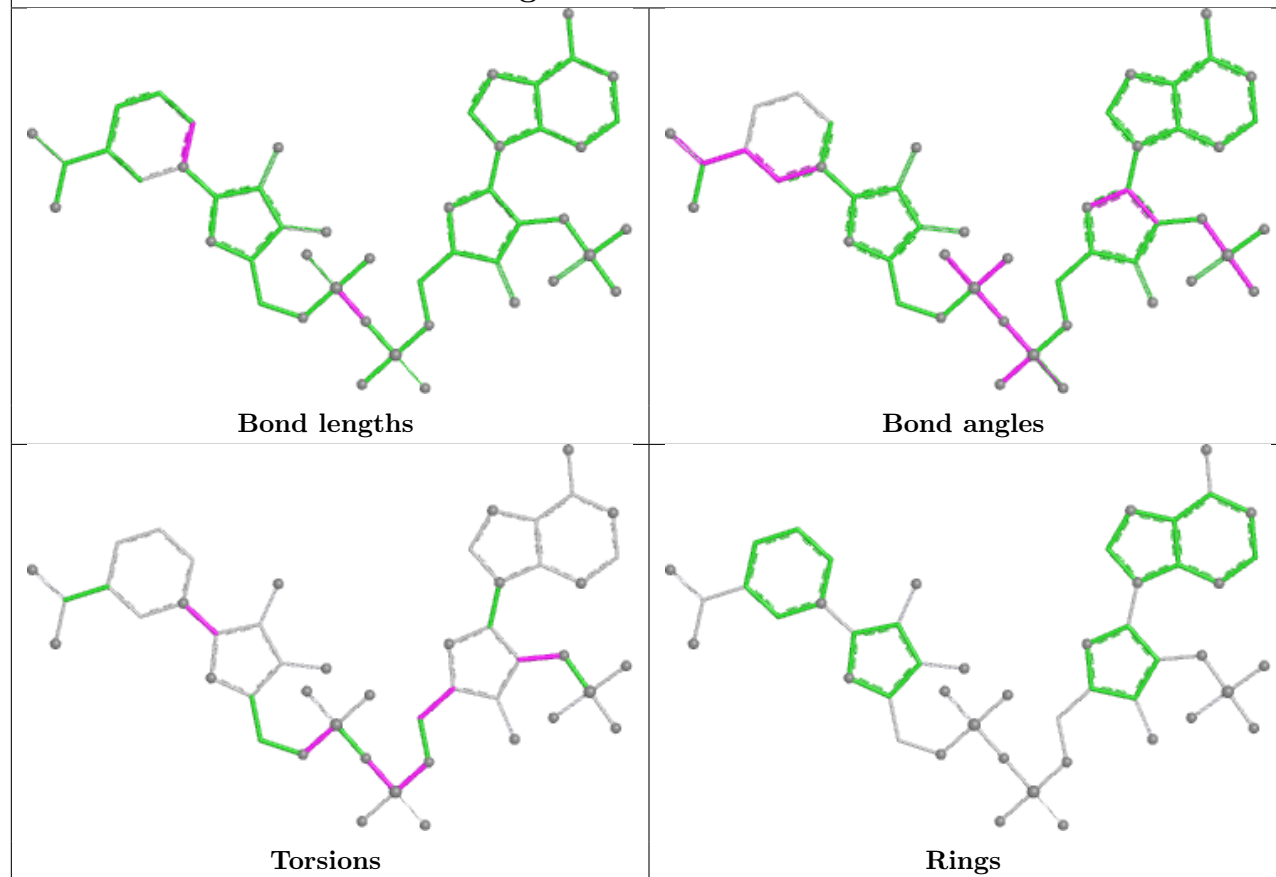




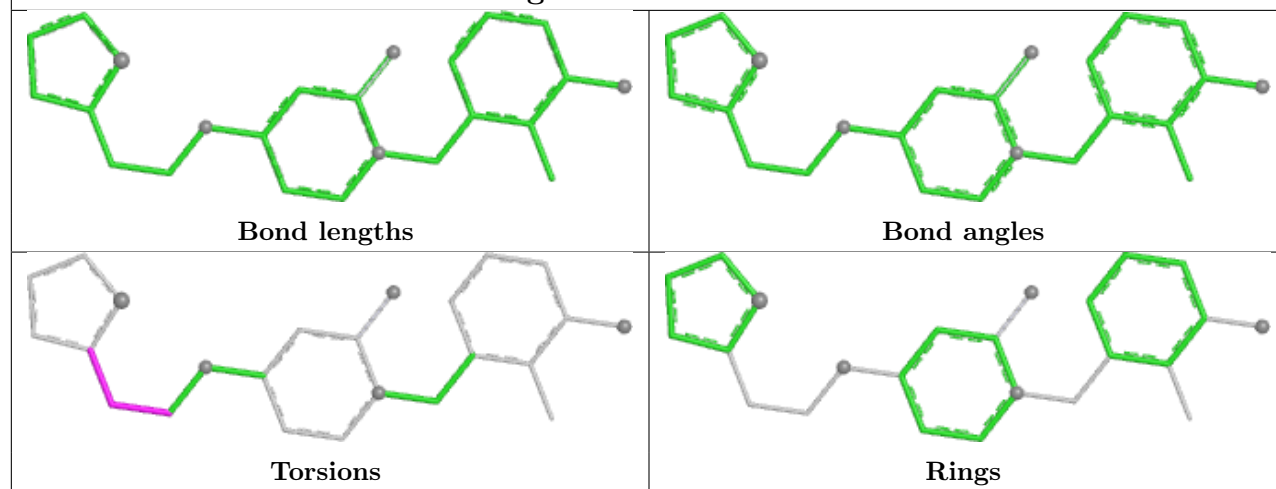




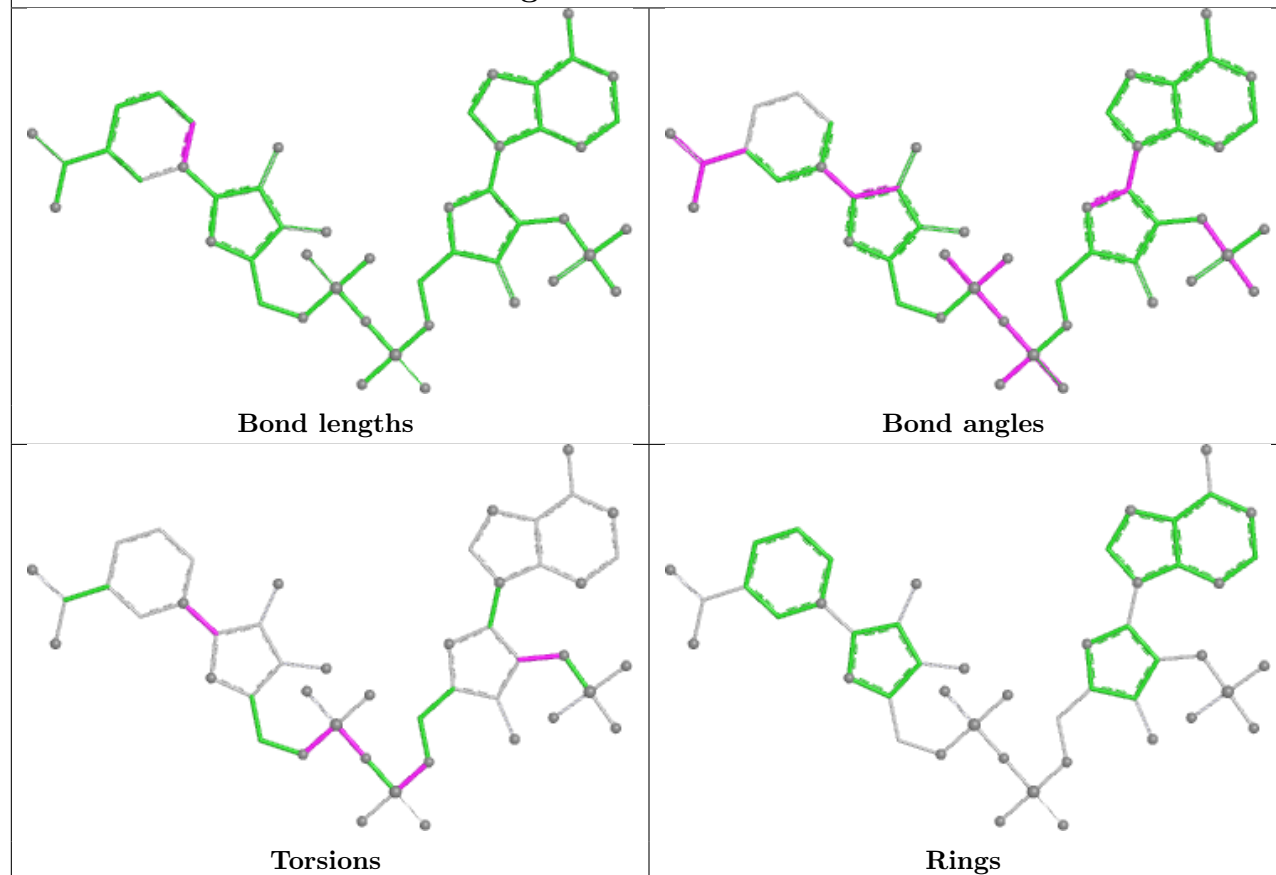
Ligand NDP H 1258



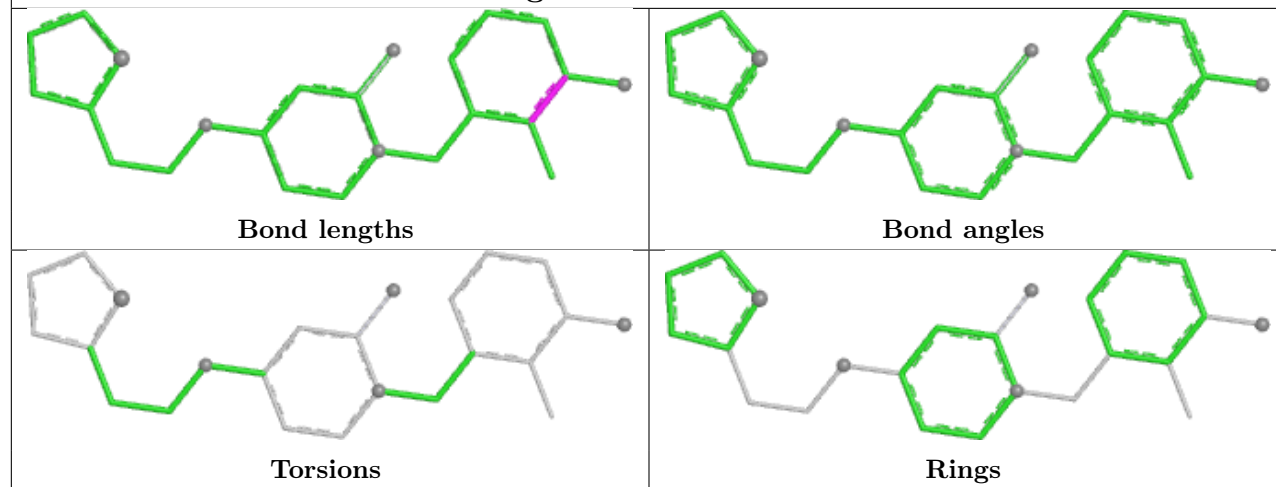
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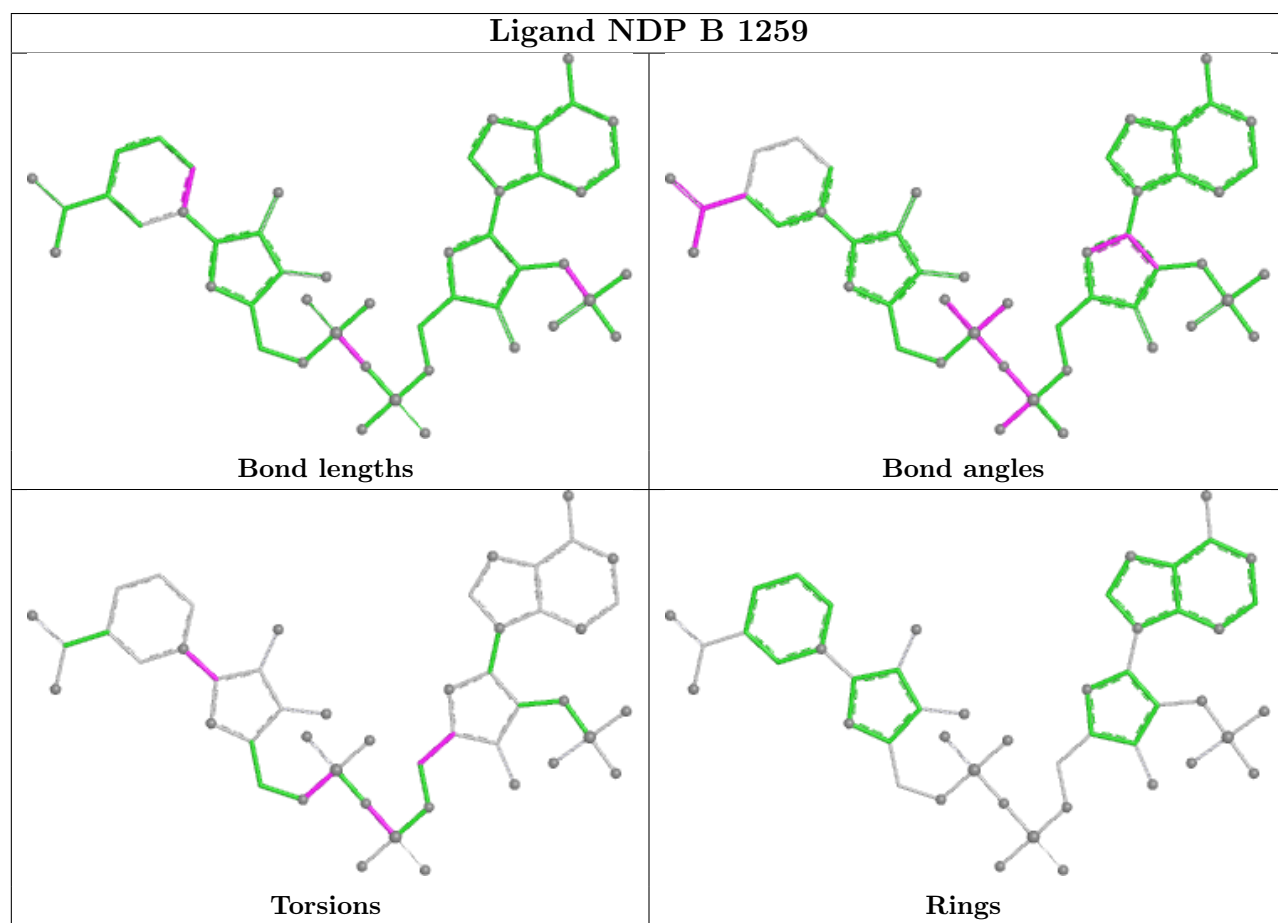
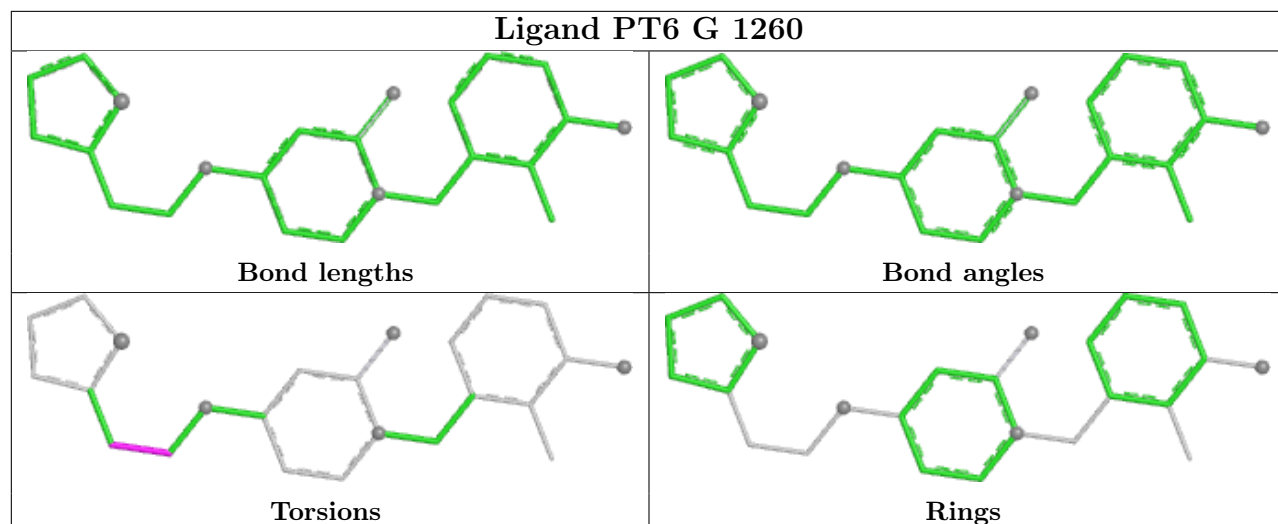


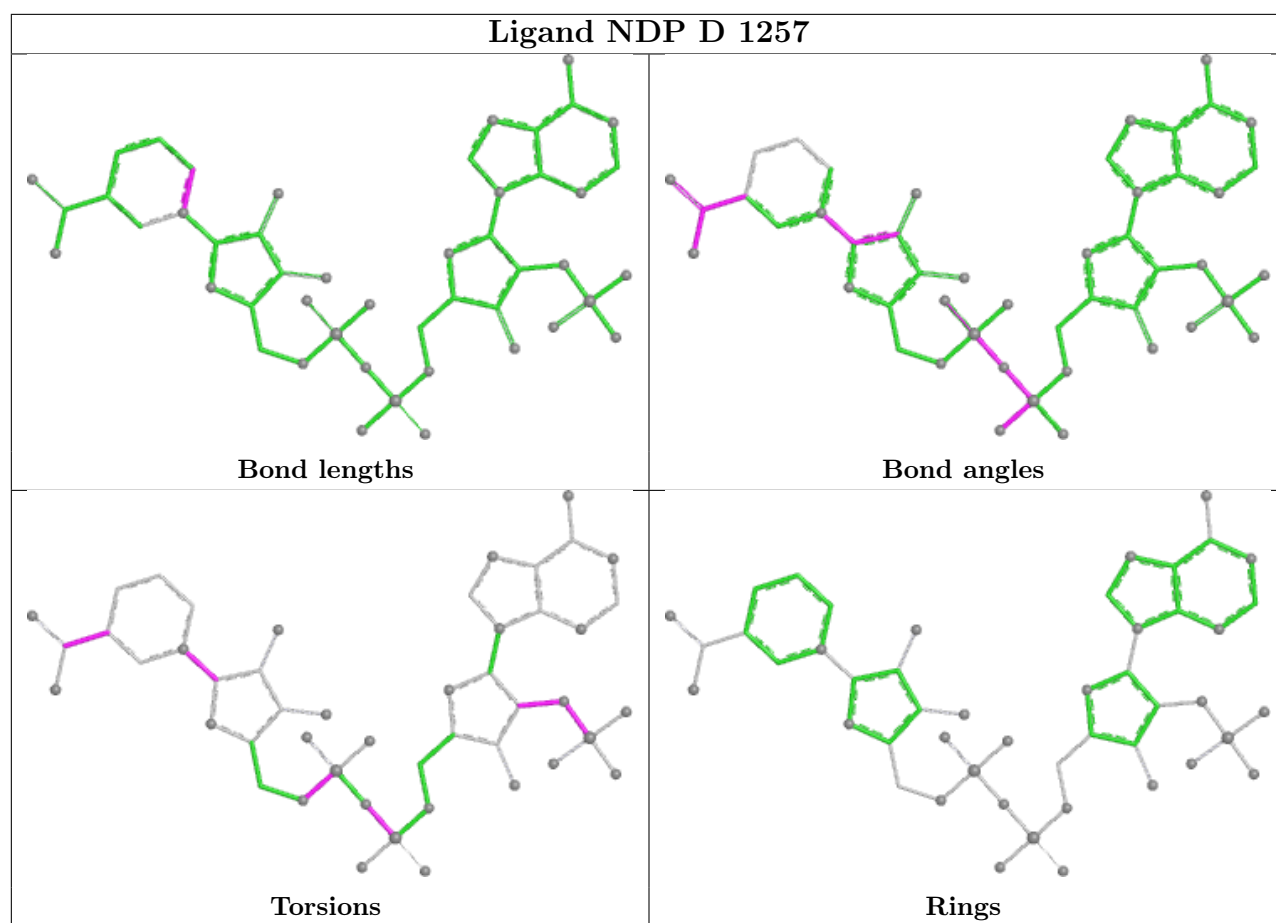
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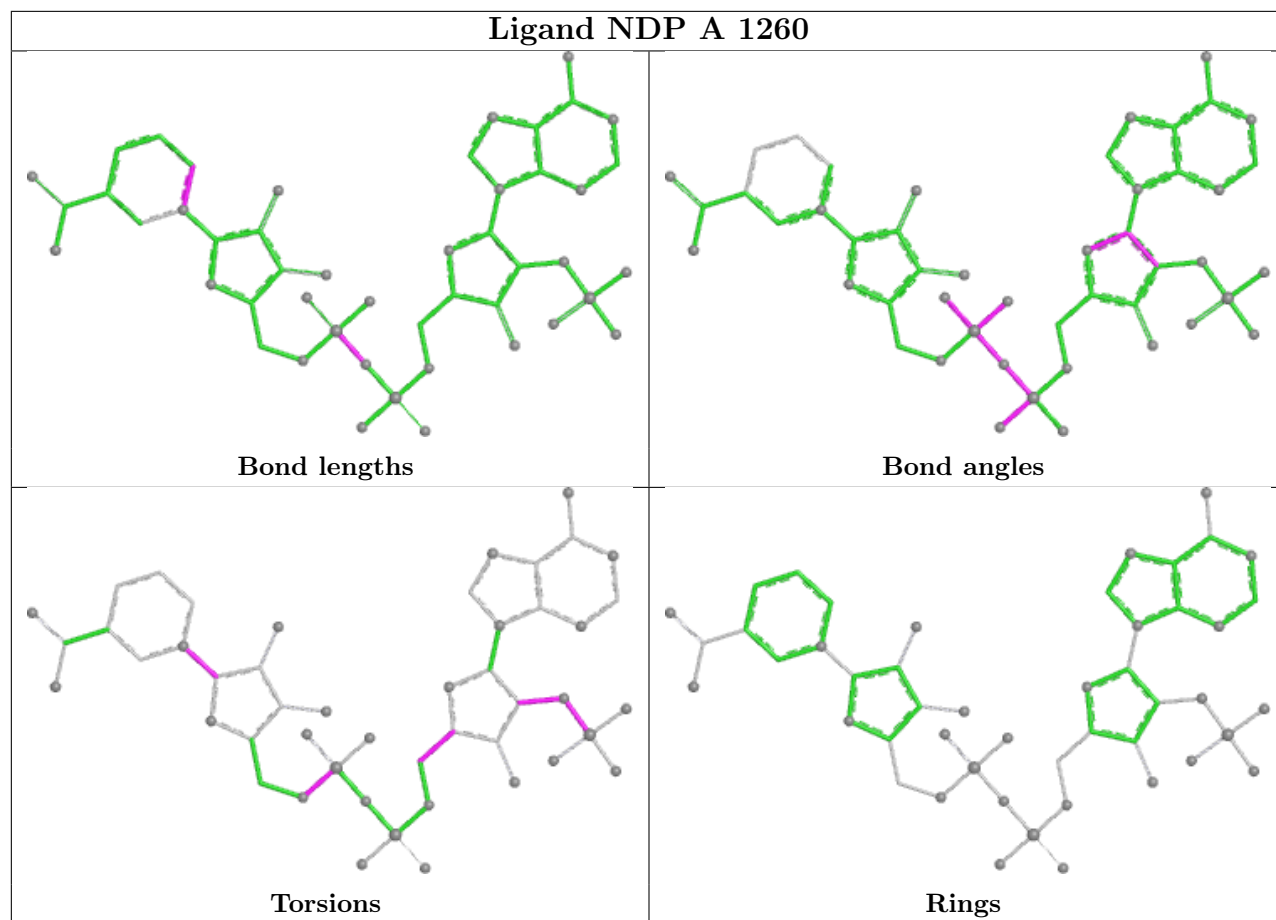


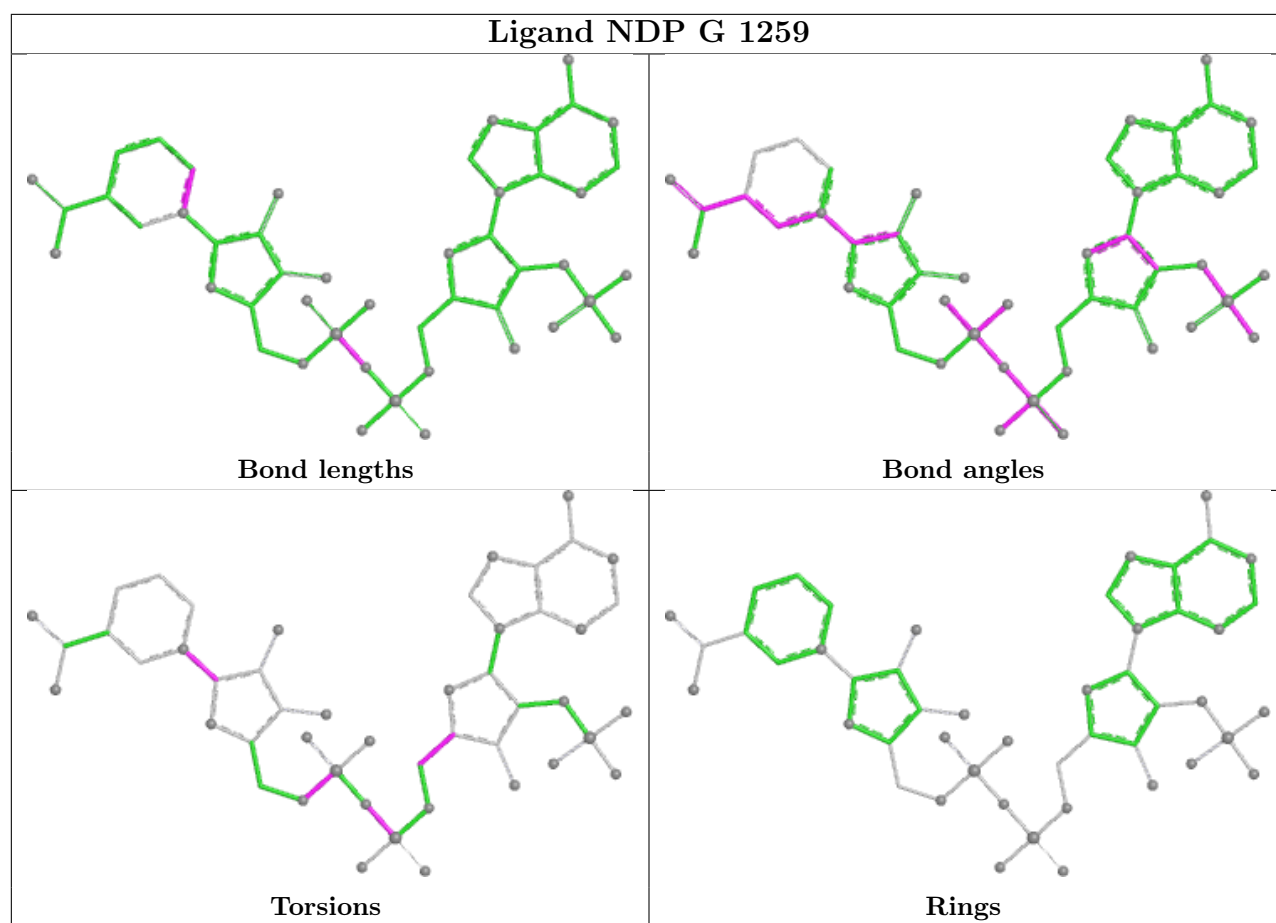
Ligand PT6 A 1261











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	262/282 (92%)	-0.34	3 (1%) 78 83	9, 25, 50, 62	7 (2%)
1	B	256/282 (90%)	-0.30	5 (1%) 65 72	14, 24, 46, 57	13 (5%)
1	C	262/282 (92%)	-0.24	2 (0%) 82 86	13, 27, 50, 62	4 (1%)
1	D	256/282 (90%)	-0.26	1 (0%) 88 91	14, 26, 52, 67	6 (2%)
1	E	256/282 (90%)	-0.26	8 (3%) 51 58	13, 24, 51, 64	13 (5%)
1	F	262/282 (92%)	-0.35	3 (1%) 78 83	13, 26, 49, 59	2 (0%)
1	G	257/282 (91%)	-0.17	4 (1%) 70 77	10, 29, 56, 79	5 (1%)
1	H	263/282 (93%)	-0.15	0 100 100	15, 29, 57, 78	3 (1%)
All	All	2074/2256 (91%)	-0.26	26 (1%) 75 81	9, 26, 51, 79	53 (2%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	206[A]	THR	5.1
1	C	-5	LEU	4.9
1	E	103[A]	ARG	4.1
1	E	205[A]	ASN	3.7
1	B	205[A]	ASN	3.6
1	B	206[A]	THR	3.3
1	B	202[A]	GLY	3.0
1	E	104	GLY	3.0
1	C	103	ARG	2.9
1	A	-5	LEU	2.8
1	G	44	SER	2.7
1	B	196	LEU	2.5
1	A	-4	TYR	2.4
1	F	-5	LEU	2.4
1	A	207	ILE	2.4
1	D	52	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	209[A]	LYS	2.3
1	G	0	ALA	2.3
1	G	1[A]	MET	2.3
1	F	52	LEU	2.2
1	E	202[A]	GLY	2.1
1	G	48	LEU	2.1
1	B	201[A]	VAL	2.1
1	E	6	ASN	2.1
1	F	-4	TYR	2.0
1	E	2	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	E	1261	4/4	0.77	0.15	61,62,64,64	0
5	EDO	G	1257	4/4	0.79	0.13	43,44,45,46	0
5	EDO	A	1270	4/4	0.81	0.16	49,49,51,53	0
2	SO4	H	1358	5/5	0.83	0.10	52,52,55,57	0
5	EDO	H	1257	4/4	0.88	0.12	40,42,44,45	0
5	EDO	G	1358	4/4	0.89	0.12	45,47,51,56	0
2	SO4	B	1257	5/5	0.90	0.09	33,34,36,36	5
2	SO4	A	1259	5/5	0.91	0.09	51,51,54,54	0
2	SO4	A	1257	5/5	0.91	0.09	47,50,53,54	0
5	EDO	B	1258	4/4	0.91	0.12	43,45,51,52	0
5	EDO	C	1270	4/4	0.91	0.10	36,37,39,40	0
2	SO4	E	1257	5/5	0.92	0.08	45,45,45,46	5
3	NDP	G	1259	48/48	0.95	0.07	20,28,47,56	0

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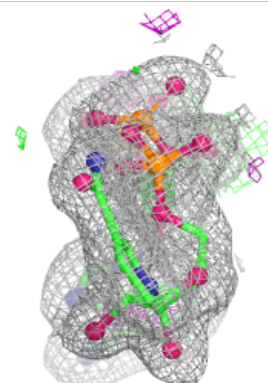
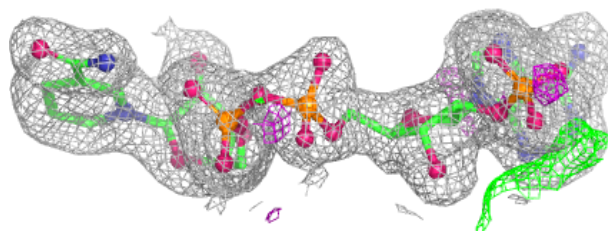
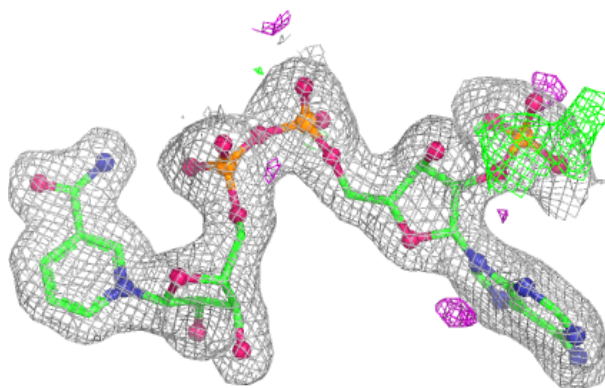
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	F	1357	1/1	0.95	0.13	60,60,60,60	0
3	NDP	C	1258	48/48	0.96	0.06	21,27,42,47	0
3	NDP	H	1258	48/48	0.96	0.07	22,31,46,54	0
4	PT6	A	1261	24/24	0.96	0.06	23,26,29,30	0
4	PT6	H	1259	24/24	0.96	0.07	23,28,31,33	0
4	PT6	F	1259	24/24	0.97	0.06	17,22,26,29	0
4	PT6	G	1260	24/24	0.97	0.06	21,28,34,35	0
3	NDP	E	1259	48/48	0.97	0.05	18,25,43,44	0
3	NDP	F	1258	48/48	0.97	0.05	19,27,44,50	0
3	NDP	B	1259	48/48	0.97	0.06	17,26,38,40	0
3	NDP	A	1260	48/48	0.97	0.06	20,27,43,48	0
3	NDP	D	1257	48/48	0.97	0.06	17,26,41,50	0
4	PT6	B	1260	24/24	0.97	0.06	18,23,27,31	0
4	PT6	C	1259	24/24	0.97	0.06	21,29,31,32	0
4	PT6	D	1258	24/24	0.97	0.05	19,25,29,32	0
4	PT6	E	1260	24/24	0.97	0.05	20,24,27,30	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.

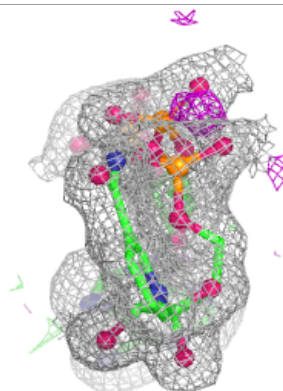
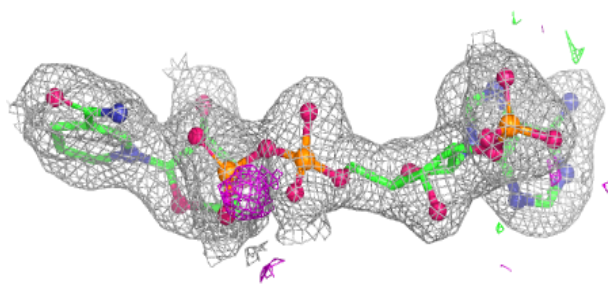
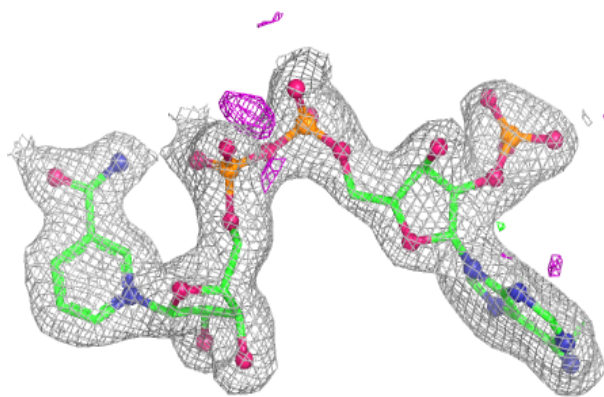
Electron density around NDP G 1259:

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

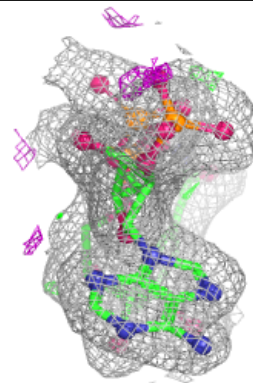
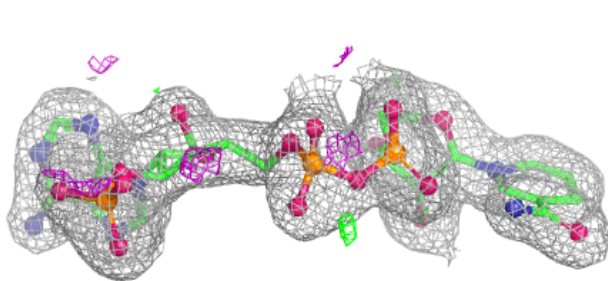
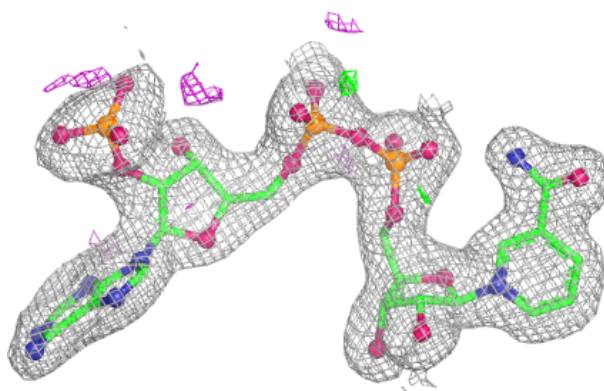


Electron density around NDP C 1258:

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

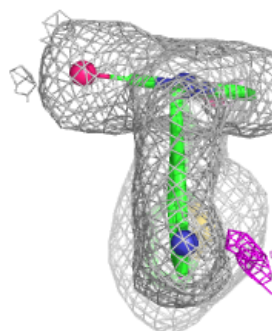
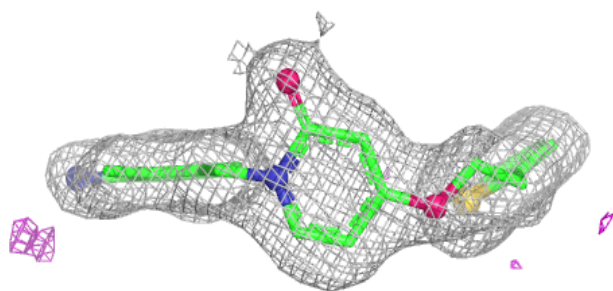
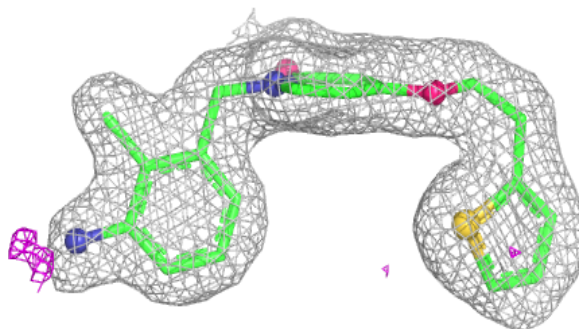
**Electron density around NDP H 1258:**

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

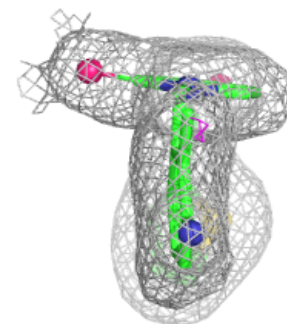
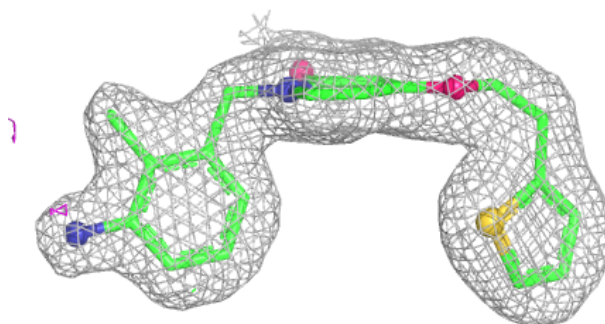


Electron density around PT6 A 1261:

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

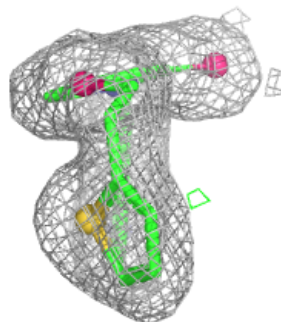
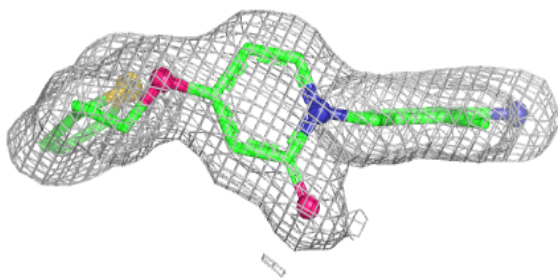
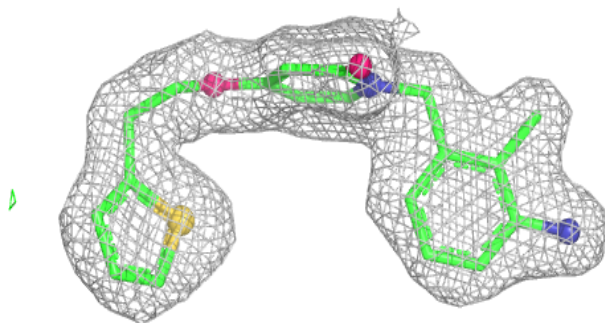
**Electron density around PT6 H 1259:**

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

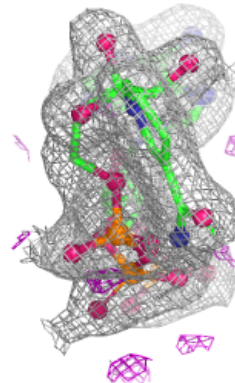
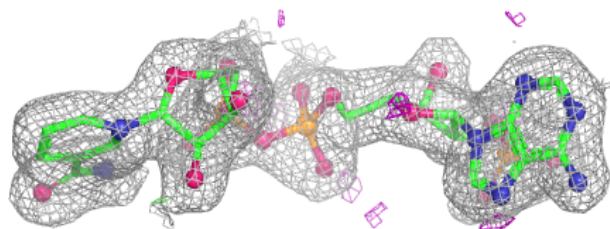
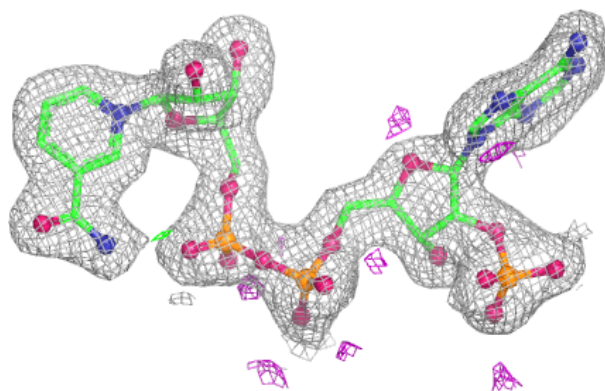


Electron density around PT6 G 1260:

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

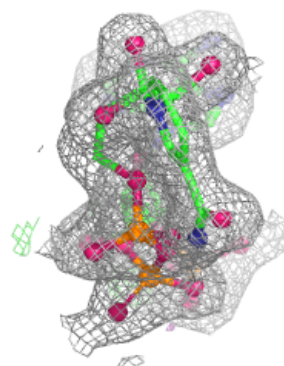
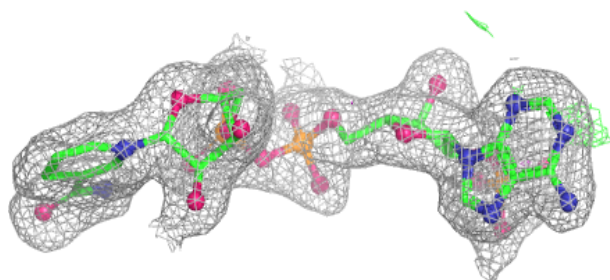
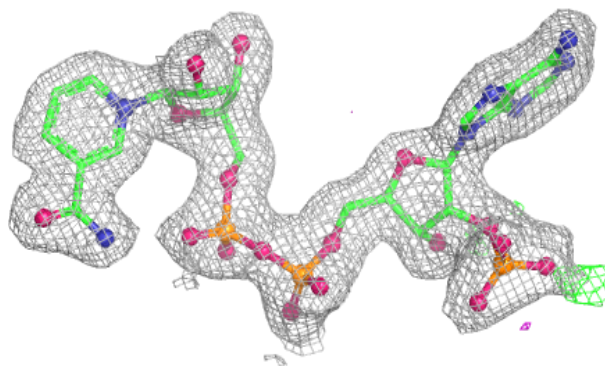
**Electron density around NDP E 1259:**

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

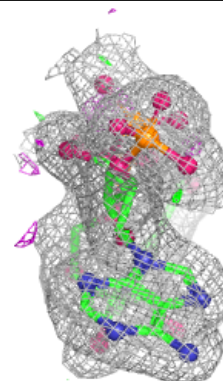
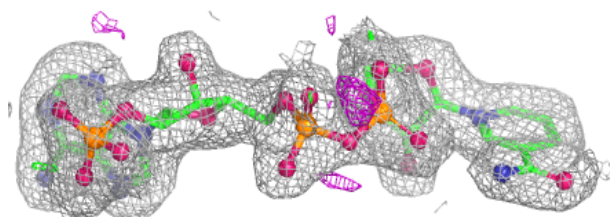
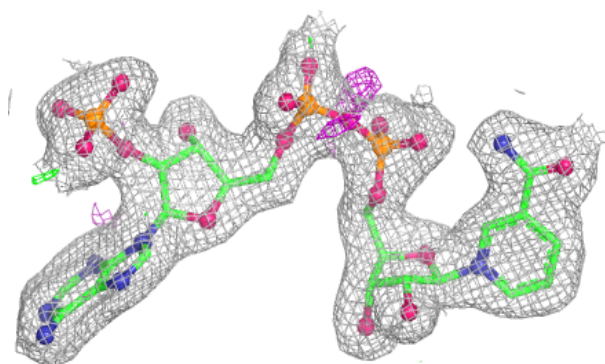


Electron density around NDP F 1258:

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

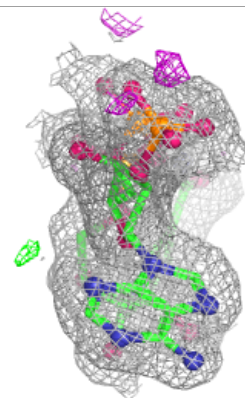
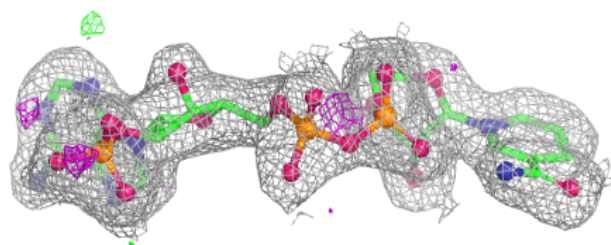
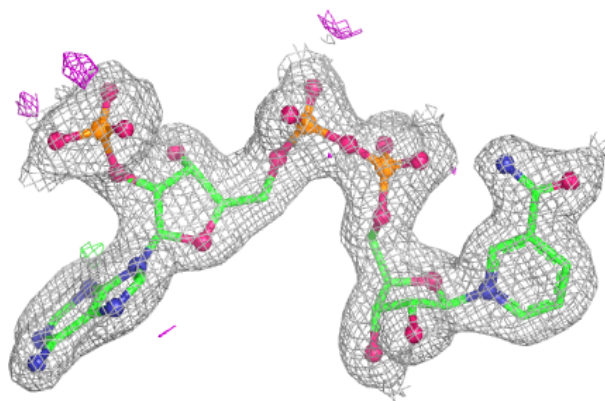
**Electron density around NDP B 1259:**

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

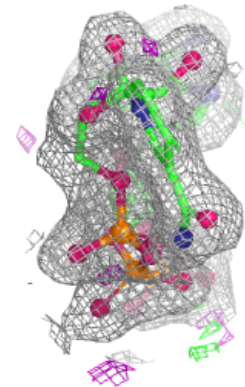
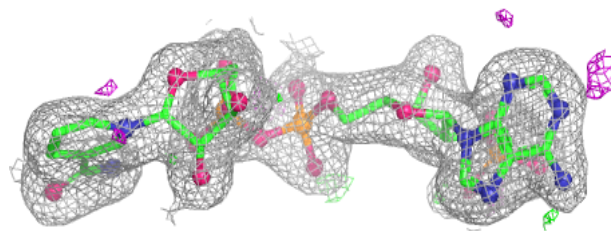
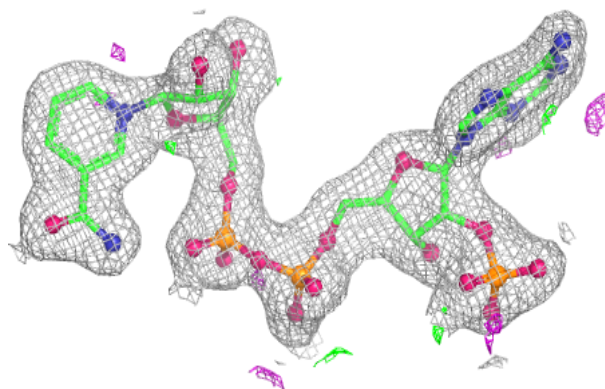


Electron density around NDP A 1260:

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

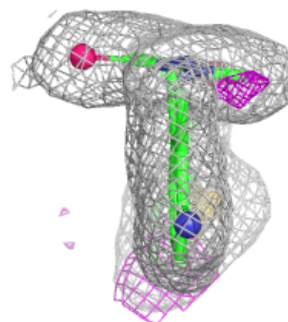
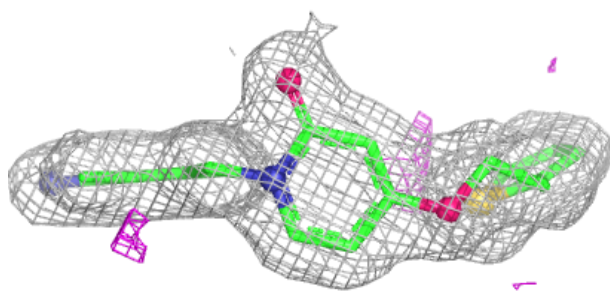
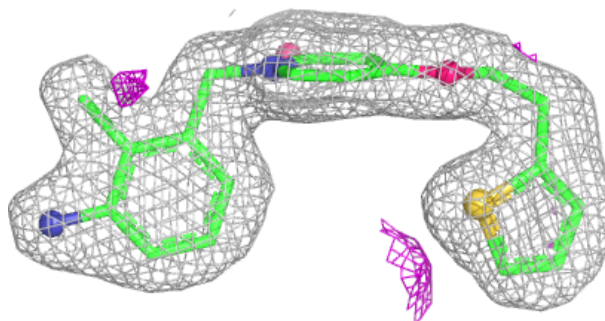
**Electron density around NDP D 1257:**

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

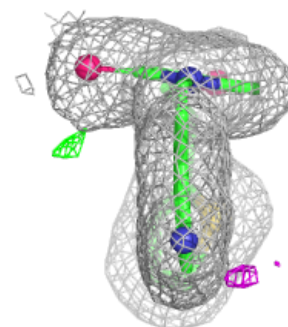
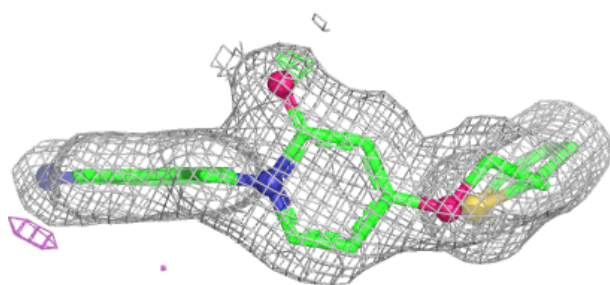
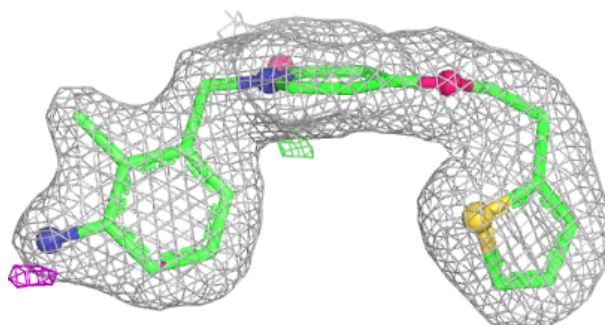


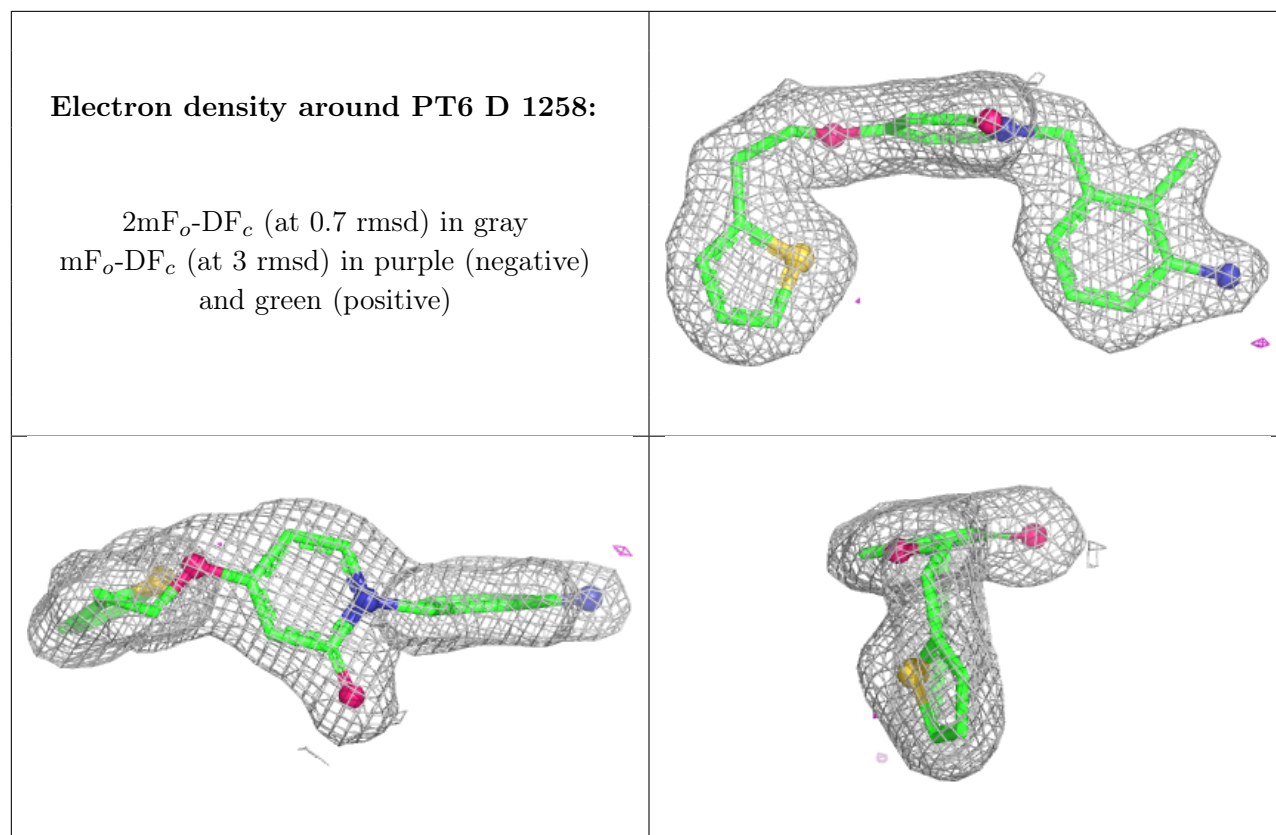
Electron density around PT6 B 1260:

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

**Electron density around PT6 C 1259:**

$2mF_o-DF_c$ (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.