Worldwide PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 05:20 am BST

PDB ID	:	5VOH
Title	:	Crystal structure of engineered water-forming NADPH oxidase (TPNOX) bound to NADPH. The G159A, D177A, A178R, M179S, P184R mutant of LbNOX.
Authors	:	Cracan, V.; Grabarek, Z.
Deposited on	:	2017-05-02
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
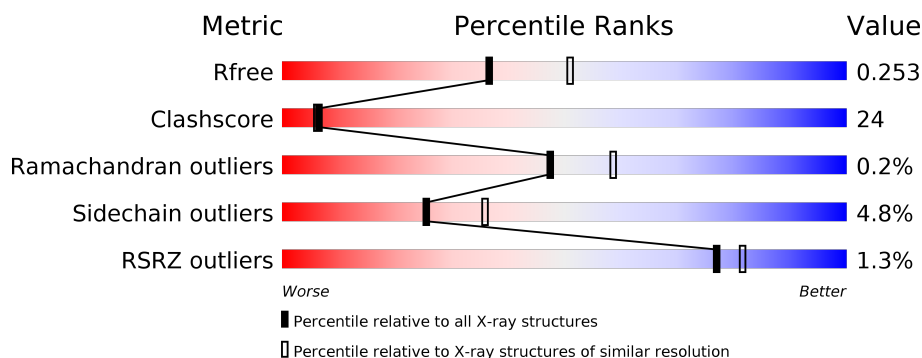
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	518	% 50% 35% · 14%
1	B	518	% 53% 32% · 14%
1	C	518	2% 49% 35% · 13%
1	D	518	% 46% 39% · 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSO	C	42	-	-	X	-
6	CL	A	506	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14726 atoms, of which 272 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 NADH oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total 3427	C 2155	N 577	O 678	S 17	0	0	0
1	B	448	Total 3427	C 2155	N 577	O 678	S 17	0	0	0
1	C	449	Total 3435	C 2159	N 579	O 680	S 17	0	0	0
1	D	450	Total 3441	C 2162	N 580	O 682	S 17	0	0	0

There are 292 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-49	MET	-	initiating methionine	UNP M5B0V2
A	-48	HIS	-	expression tag	UNP M5B0V2
A	-47	HIS	-	expression tag	UNP M5B0V2
A	-46	HIS	-	expression tag	UNP M5B0V2
A	-45	HIS	-	expression tag	UNP M5B0V2
A	-44	HIS	-	expression tag	UNP M5B0V2
A	-43	HIS	-	expression tag	UNP M5B0V2
A	-42	SER	-	expression tag	UNP M5B0V2
A	-41	SER	-	expression tag	UNP M5B0V2
A	-40	GLY	-	expression tag	UNP M5B0V2
A	-39	LEU	-	expression tag	UNP M5B0V2
A	-38	VAL	-	expression tag	UNP M5B0V2
A	-37	PRO	-	expression tag	UNP M5B0V2
A	-36	ARG	-	expression tag	UNP M5B0V2
A	-35	GLY	-	expression tag	UNP M5B0V2
A	-34	SER	-	expression tag	UNP M5B0V2
A	-33	GLY	-	expression tag	UNP M5B0V2
A	-32	MET	-	expression tag	UNP M5B0V2
A	-31	LYS	-	expression tag	UNP M5B0V2
A	-30	GLU	-	expression tag	UNP M5B0V2
A	-29	THR	-	expression tag	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	ALA	-	expression tag	UNP M5B0V2
A	-27	ALA	-	expression tag	UNP M5B0V2
A	-26	ALA	-	expression tag	UNP M5B0V2
A	-25	LYS	-	expression tag	UNP M5B0V2
A	-24	PHE	-	expression tag	UNP M5B0V2
A	-23	GLU	-	expression tag	UNP M5B0V2
A	-22	ARG	-	expression tag	UNP M5B0V2
A	-21	GLN	-	expression tag	UNP M5B0V2
A	-20	HIS	-	expression tag	UNP M5B0V2
A	-19	MET	-	expression tag	UNP M5B0V2
A	-18	ASP	-	expression tag	UNP M5B0V2
A	-17	SER	-	expression tag	UNP M5B0V2
A	-16	PRO	-	expression tag	UNP M5B0V2
A	-15	ASP	-	expression tag	UNP M5B0V2
A	-14	LEU	-	expression tag	UNP M5B0V2
A	-13	GLY	-	expression tag	UNP M5B0V2
A	-12	THR	-	expression tag	UNP M5B0V2
A	-11	ASP	-	expression tag	UNP M5B0V2
A	-10	ASP	-	expression tag	UNP M5B0V2
A	-9	ASP	-	expression tag	UNP M5B0V2
A	-8	ASP	-	expression tag	UNP M5B0V2
A	-7	LYS	-	expression tag	UNP M5B0V2
A	-6	ALA	-	expression tag	UNP M5B0V2
A	-5	MET	-	expression tag	UNP M5B0V2
A	-4	ALA	-	expression tag	UNP M5B0V2
A	-3	ASP	-	expression tag	UNP M5B0V2
A	-2	ILE	-	expression tag	UNP M5B0V2
A	-1	GLY	-	expression tag	UNP M5B0V2
A	0	SER	-	expression tag	UNP M5B0V2
A	159	ALA	GLY	engineered mutation	UNP M5B0V2
A	177	ALA	ASP	engineered mutation	UNP M5B0V2
A	178	ARG	ALA	engineered mutation	UNP M5B0V2
A	179	SER	MET	engineered mutation	UNP M5B0V2
A	184	ARG	PRO	engineered mutation	UNP M5B0V2
A	451	GLY	-	expression tag	UNP M5B0V2
A	452	GLY	-	expression tag	UNP M5B0V2
A	453	SER	-	expression tag	UNP M5B0V2
A	454	GLY	-	expression tag	UNP M5B0V2
A	455	GLY	-	expression tag	UNP M5B0V2
A	456	SER	-	expression tag	UNP M5B0V2
A	457	GLY	-	expression tag	UNP M5B0V2
A	458	GLY	-	expression tag	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	459	SER	-	expression tag	UNP M5B0V2
A	460	MET	-	expression tag	UNP M5B0V2
A	461	ASP	-	expression tag	UNP M5B0V2
A	462	TYR	-	expression tag	UNP M5B0V2
A	463	LYS	-	expression tag	UNP M5B0V2
A	464	ASP	-	expression tag	UNP M5B0V2
A	465	ASP	-	expression tag	UNP M5B0V2
A	466	ASP	-	expression tag	UNP M5B0V2
A	467	ASP	-	expression tag	UNP M5B0V2
A	468	LYS	-	expression tag	UNP M5B0V2
B	-49	MET	-	initiating methionine	UNP M5B0V2
B	-48	HIS	-	expression tag	UNP M5B0V2
B	-47	HIS	-	expression tag	UNP M5B0V2
B	-46	HIS	-	expression tag	UNP M5B0V2
B	-45	HIS	-	expression tag	UNP M5B0V2
B	-44	HIS	-	expression tag	UNP M5B0V2
B	-43	HIS	-	expression tag	UNP M5B0V2
B	-42	SER	-	expression tag	UNP M5B0V2
B	-41	SER	-	expression tag	UNP M5B0V2
B	-40	GLY	-	expression tag	UNP M5B0V2
B	-39	LEU	-	expression tag	UNP M5B0V2
B	-38	VAL	-	expression tag	UNP M5B0V2
B	-37	PRO	-	expression tag	UNP M5B0V2
B	-36	ARG	-	expression tag	UNP M5B0V2
B	-35	GLY	-	expression tag	UNP M5B0V2
B	-34	SER	-	expression tag	UNP M5B0V2
B	-33	GLY	-	expression tag	UNP M5B0V2
B	-32	MET	-	expression tag	UNP M5B0V2
B	-31	LYS	-	expression tag	UNP M5B0V2
B	-30	GLU	-	expression tag	UNP M5B0V2
B	-29	THR	-	expression tag	UNP M5B0V2
B	-28	ALA	-	expression tag	UNP M5B0V2
B	-27	ALA	-	expression tag	UNP M5B0V2
B	-26	ALA	-	expression tag	UNP M5B0V2
B	-25	LYS	-	expression tag	UNP M5B0V2
B	-24	PHE	-	expression tag	UNP M5B0V2
B	-23	GLU	-	expression tag	UNP M5B0V2
B	-22	ARG	-	expression tag	UNP M5B0V2
B	-21	GLN	-	expression tag	UNP M5B0V2
B	-20	HIS	-	expression tag	UNP M5B0V2
B	-19	MET	-	expression tag	UNP M5B0V2
B	-18	ASP	-	expression tag	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP M5B0V2
B	-16	PRO	-	expression tag	UNP M5B0V2
B	-15	ASP	-	expression tag	UNP M5B0V2
B	-14	LEU	-	expression tag	UNP M5B0V2
B	-13	GLY	-	expression tag	UNP M5B0V2
B	-12	THR	-	expression tag	UNP M5B0V2
B	-11	ASP	-	expression tag	UNP M5B0V2
B	-10	ASP	-	expression tag	UNP M5B0V2
B	-9	ASP	-	expression tag	UNP M5B0V2
B	-8	ASP	-	expression tag	UNP M5B0V2
B	-7	LYS	-	expression tag	UNP M5B0V2
B	-6	ALA	-	expression tag	UNP M5B0V2
B	-5	MET	-	expression tag	UNP M5B0V2
B	-4	ALA	-	expression tag	UNP M5B0V2
B	-3	ASP	-	expression tag	UNP M5B0V2
B	-2	ILE	-	expression tag	UNP M5B0V2
B	-1	GLY	-	expression tag	UNP M5B0V2
B	0	SER	-	expression tag	UNP M5B0V2
B	159	ALA	GLY	engineered mutation	UNP M5B0V2
B	177	ALA	ASP	engineered mutation	UNP M5B0V2
B	178	ARG	ALA	engineered mutation	UNP M5B0V2
B	179	SER	MET	engineered mutation	UNP M5B0V2
B	184	ARG	PRO	engineered mutation	UNP M5B0V2
B	451	GLY	-	expression tag	UNP M5B0V2
B	452	GLY	-	expression tag	UNP M5B0V2
B	453	SER	-	expression tag	UNP M5B0V2
B	454	GLY	-	expression tag	UNP M5B0V2
B	455	GLY	-	expression tag	UNP M5B0V2
B	456	SER	-	expression tag	UNP M5B0V2
B	457	GLY	-	expression tag	UNP M5B0V2
B	458	GLY	-	expression tag	UNP M5B0V2
B	459	SER	-	expression tag	UNP M5B0V2
B	460	MET	-	expression tag	UNP M5B0V2
B	461	ASP	-	expression tag	UNP M5B0V2
B	462	TYR	-	expression tag	UNP M5B0V2
B	463	LYS	-	expression tag	UNP M5B0V2
B	464	ASP	-	expression tag	UNP M5B0V2
B	465	ASP	-	expression tag	UNP M5B0V2
B	466	ASP	-	expression tag	UNP M5B0V2
B	467	ASP	-	expression tag	UNP M5B0V2
B	468	LYS	-	expression tag	UNP M5B0V2
C	-49	MET	-	initiating methionine	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-48	HIS	-	expression tag	UNP M5B0V2
C	-47	HIS	-	expression tag	UNP M5B0V2
C	-46	HIS	-	expression tag	UNP M5B0V2
C	-45	HIS	-	expression tag	UNP M5B0V2
C	-44	HIS	-	expression tag	UNP M5B0V2
C	-43	HIS	-	expression tag	UNP M5B0V2
C	-42	SER	-	expression tag	UNP M5B0V2
C	-41	SER	-	expression tag	UNP M5B0V2
C	-40	GLY	-	expression tag	UNP M5B0V2
C	-39	LEU	-	expression tag	UNP M5B0V2
C	-38	VAL	-	expression tag	UNP M5B0V2
C	-37	PRO	-	expression tag	UNP M5B0V2
C	-36	ARG	-	expression tag	UNP M5B0V2
C	-35	GLY	-	expression tag	UNP M5B0V2
C	-34	SER	-	expression tag	UNP M5B0V2
C	-33	GLY	-	expression tag	UNP M5B0V2
C	-32	MET	-	expression tag	UNP M5B0V2
C	-31	LYS	-	expression tag	UNP M5B0V2
C	-30	GLU	-	expression tag	UNP M5B0V2
C	-29	THR	-	expression tag	UNP M5B0V2
C	-28	ALA	-	expression tag	UNP M5B0V2
C	-27	ALA	-	expression tag	UNP M5B0V2
C	-26	ALA	-	expression tag	UNP M5B0V2
C	-25	LYS	-	expression tag	UNP M5B0V2
C	-24	PHE	-	expression tag	UNP M5B0V2
C	-23	GLU	-	expression tag	UNP M5B0V2
C	-22	ARG	-	expression tag	UNP M5B0V2
C	-21	GLN	-	expression tag	UNP M5B0V2
C	-20	HIS	-	expression tag	UNP M5B0V2
C	-19	MET	-	expression tag	UNP M5B0V2
C	-18	ASP	-	expression tag	UNP M5B0V2
C	-17	SER	-	expression tag	UNP M5B0V2
C	-16	PRO	-	expression tag	UNP M5B0V2
C	-15	ASP	-	expression tag	UNP M5B0V2
C	-14	LEU	-	expression tag	UNP M5B0V2
C	-13	GLY	-	expression tag	UNP M5B0V2
C	-12	THR	-	expression tag	UNP M5B0V2
C	-11	ASP	-	expression tag	UNP M5B0V2
C	-10	ASP	-	expression tag	UNP M5B0V2
C	-9	ASP	-	expression tag	UNP M5B0V2
C	-8	ASP	-	expression tag	UNP M5B0V2
C	-7	LYS	-	expression tag	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP M5B0V2
C	-5	MET	-	expression tag	UNP M5B0V2
C	-4	ALA	-	expression tag	UNP M5B0V2
C	-3	ASP	-	expression tag	UNP M5B0V2
C	-2	ILE	-	expression tag	UNP M5B0V2
C	-1	GLY	-	expression tag	UNP M5B0V2
C	0	SER	-	expression tag	UNP M5B0V2
C	159	ALA	GLY	engineered mutation	UNP M5B0V2
C	177	ALA	ASP	engineered mutation	UNP M5B0V2
C	178	ARG	ALA	engineered mutation	UNP M5B0V2
C	179	SER	MET	engineered mutation	UNP M5B0V2
C	184	ARG	PRO	engineered mutation	UNP M5B0V2
C	451	GLY	-	expression tag	UNP M5B0V2
C	452	GLY	-	expression tag	UNP M5B0V2
C	453	SER	-	expression tag	UNP M5B0V2
C	454	GLY	-	expression tag	UNP M5B0V2
C	455	GLY	-	expression tag	UNP M5B0V2
C	456	SER	-	expression tag	UNP M5B0V2
C	457	GLY	-	expression tag	UNP M5B0V2
C	458	GLY	-	expression tag	UNP M5B0V2
C	459	SER	-	expression tag	UNP M5B0V2
C	460	MET	-	expression tag	UNP M5B0V2
C	461	ASP	-	expression tag	UNP M5B0V2
C	462	TYR	-	expression tag	UNP M5B0V2
C	463	LYS	-	expression tag	UNP M5B0V2
C	464	ASP	-	expression tag	UNP M5B0V2
C	465	ASP	-	expression tag	UNP M5B0V2
C	466	ASP	-	expression tag	UNP M5B0V2
C	467	ASP	-	expression tag	UNP M5B0V2
C	468	LYS	-	expression tag	UNP M5B0V2
D	-49	MET	-	initiating methionine	UNP M5B0V2
D	-48	HIS	-	expression tag	UNP M5B0V2
D	-47	HIS	-	expression tag	UNP M5B0V2
D	-46	HIS	-	expression tag	UNP M5B0V2
D	-45	HIS	-	expression tag	UNP M5B0V2
D	-44	HIS	-	expression tag	UNP M5B0V2
D	-43	HIS	-	expression tag	UNP M5B0V2
D	-42	SER	-	expression tag	UNP M5B0V2
D	-41	SER	-	expression tag	UNP M5B0V2
D	-40	GLY	-	expression tag	UNP M5B0V2
D	-39	LEU	-	expression tag	UNP M5B0V2
D	-38	VAL	-	expression tag	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-37	PRO	-	expression tag	UNP M5B0V2
D	-36	ARG	-	expression tag	UNP M5B0V2
D	-35	GLY	-	expression tag	UNP M5B0V2
D	-34	SER	-	expression tag	UNP M5B0V2
D	-33	GLY	-	expression tag	UNP M5B0V2
D	-32	MET	-	expression tag	UNP M5B0V2
D	-31	LYS	-	expression tag	UNP M5B0V2
D	-30	GLU	-	expression tag	UNP M5B0V2
D	-29	THR	-	expression tag	UNP M5B0V2
D	-28	ALA	-	expression tag	UNP M5B0V2
D	-27	ALA	-	expression tag	UNP M5B0V2
D	-26	ALA	-	expression tag	UNP M5B0V2
D	-25	LYS	-	expression tag	UNP M5B0V2
D	-24	PHE	-	expression tag	UNP M5B0V2
D	-23	GLU	-	expression tag	UNP M5B0V2
D	-22	ARG	-	expression tag	UNP M5B0V2
D	-21	GLN	-	expression tag	UNP M5B0V2
D	-20	HIS	-	expression tag	UNP M5B0V2
D	-19	MET	-	expression tag	UNP M5B0V2
D	-18	ASP	-	expression tag	UNP M5B0V2
D	-17	SER	-	expression tag	UNP M5B0V2
D	-16	PRO	-	expression tag	UNP M5B0V2
D	-15	ASP	-	expression tag	UNP M5B0V2
D	-14	LEU	-	expression tag	UNP M5B0V2
D	-13	GLY	-	expression tag	UNP M5B0V2
D	-12	THR	-	expression tag	UNP M5B0V2
D	-11	ASP	-	expression tag	UNP M5B0V2
D	-10	ASP	-	expression tag	UNP M5B0V2
D	-9	ASP	-	expression tag	UNP M5B0V2
D	-8	ASP	-	expression tag	UNP M5B0V2
D	-7	LYS	-	expression tag	UNP M5B0V2
D	-6	ALA	-	expression tag	UNP M5B0V2
D	-5	MET	-	expression tag	UNP M5B0V2
D	-4	ALA	-	expression tag	UNP M5B0V2
D	-3	ASP	-	expression tag	UNP M5B0V2
D	-2	ILE	-	expression tag	UNP M5B0V2
D	-1	GLY	-	expression tag	UNP M5B0V2
D	0	SER	-	expression tag	UNP M5B0V2
D	159	ALA	GLY	engineered mutation	UNP M5B0V2
D	177	ALA	ASP	engineered mutation	UNP M5B0V2
D	178	ARG	ALA	engineered mutation	UNP M5B0V2
D	179	SER	MET	engineered mutation	UNP M5B0V2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	184	ARG	PRO	engineered mutation	UNP M5B0V2
D	451	GLY	-	expression tag	UNP M5B0V2
D	452	GLY	-	expression tag	UNP M5B0V2
D	453	SER	-	expression tag	UNP M5B0V2
D	454	GLY	-	expression tag	UNP M5B0V2
D	455	GLY	-	expression tag	UNP M5B0V2
D	456	SER	-	expression tag	UNP M5B0V2
D	457	GLY	-	expression tag	UNP M5B0V2
D	458	GLY	-	expression tag	UNP M5B0V2
D	459	SER	-	expression tag	UNP M5B0V2
D	460	MET	-	expression tag	UNP M5B0V2
D	461	ASP	-	expression tag	UNP M5B0V2
D	462	TYR	-	expression tag	UNP M5B0V2
D	463	LYS	-	expression tag	UNP M5B0V2
D	464	ASP	-	expression tag	UNP M5B0V2
D	465	ASP	-	expression tag	UNP M5B0V2
D	466	ASP	-	expression tag	UNP M5B0V2
D	467	ASP	-	expression tag	UNP M5B0V2
D	468	LYS	-	expression tag	UNP M5B0V2

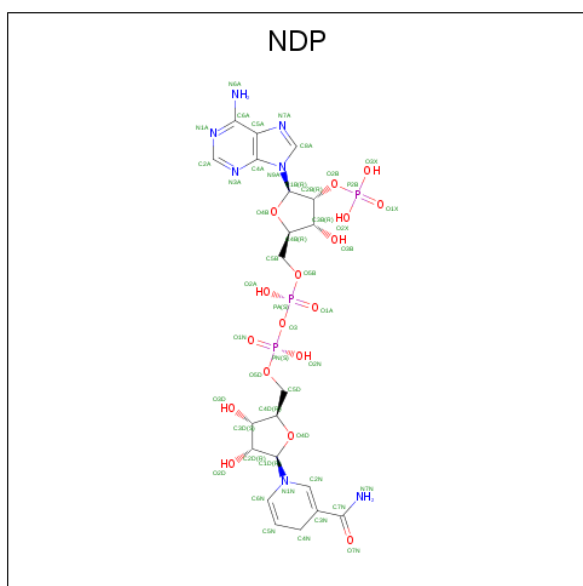- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
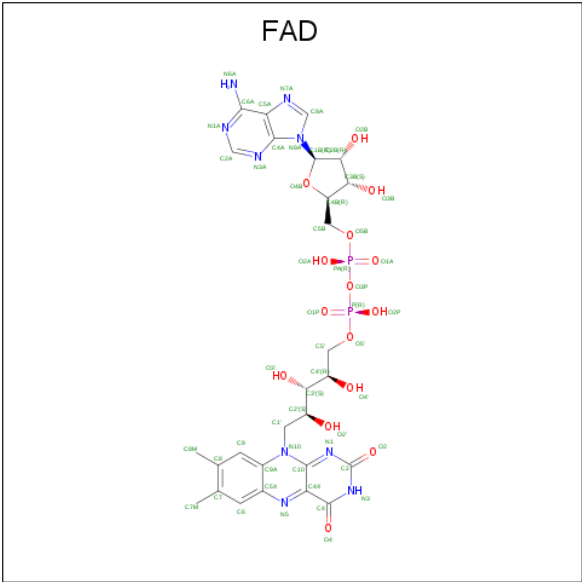
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	83	27	30	9	15	2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	B	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	C	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	D	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Full wwPDB X-ray Structure Validation Report

EDO

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	A	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0
4	D	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cl 1	0	0
6	D	1	Total 1	Cl 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	80	Total 80	O 80	0	0
7	B	77	Total 77	O 77	0	0
7	C	55	Total 55	O 55	0	0
7	D	69	Total 69	O 69	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: NADH oxidase

- Molecule 1: NADH oxidase

• Molecule 1: NADH oxidase

Chain C:

• Molecule 1: NADH oxidase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.26Å 96.53Å 119.06Å 90.00° 116.76° 90.00°	Depositor
Resolution (Å)	47.89 – 2.30 47.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.89-2.30) 93.8 (47.89-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.58 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.192 , 0.255 0.190 , 0.253	Depositor DCC
R_{free} test set	2010 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 20.9	EDS
L-test for twinning[2]	$<\vert L\vert>\ = 0.45,\ <L^2>\ = 0.28$	Xtriage
Estimated twinning fraction	0.367 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.370 for h,-k,-h-l	Depositor
Outliers	5 of 96155 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14726	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6216e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<\vert L\vert>$, $<L^2>$ 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: CSO, CL, EDO, SO4, NDP, FAD

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	0.25	0/3481	0.42	0/4736
1	B	0.24	0/3481	0.43	0/4736
1	C	0.24	0/3489	0.43	0/4747
1	D	0.24	0/3495	0.43	0/4755
All	All	0.24	0/13946	0.43	0/18974

There are no bond length outliers.

There are no bond angle outliers.

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	3427	0	3391	164	0
1	B	3427	0	3391	168	0
1	C	3435	0	3397	175	0
1	D	3441	0	3402	175	0
2	A	53	30	31	6	0
2	B	53	30	31	4	0
2	C	53	30	31	11	0
2	D	53	30	31	7	0
3	A	48	26	26	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	26	26	10	0
3	C	48	26	26	9	0
3	D	48	26	26	10	0
4	A	8	12	12	3	0
4	B	8	12	12	0	0
4	C	8	12	12	0	0
4	D	8	12	12	0	0
5	A	5	0	0	0	0
6	A	1	0	0	2	0
6	D	1	0	0	0	0
7	A	80	0	0	4	0
7	B	77	0	0	6	0
7	C	55	0	0	3	0
7	D	69	0	0	4	0
All	All	14454	272	13857	668	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 24.

All (668) 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:120:ILE:HG12	1:A:121:PRO:HD2	1.48	0.94
1:A:121:PRO:HG2	1:A:214:SER:HB3	1.53	0.90
1:B:445:ALA:HA	1:B:448:VAL:HG12	1.55	0.89
1:C:79:VAL:HA	1:C:91:VAL:HG12	1.53	0.89
1:A:155:ALA:HB1	1:A:182:VAL:HA	1.53	0.89
1:C:130:LEU:HD21	1:C:238:LEU:HD12	1.56	0.87
1:B:41:SER:OG	7:B:601:HOH:O	1.92	0.87
1:B:185:LYS:HD2	1:B:185:LYS:H	1.40	0.87
1:D:152:VAL:HG11	1:D:159:ALA:HA	1.56	0.87
1:D:178:ARG:NE	3:D:502:NDP:O3X	2.09	0.85
1:A:153:ILE:HG22	1:A:240:ILE:HD11	1.61	0.81
1:C:197:GLN:NE2	1:C:201:ASP:OD1	2.14	0.81
1:C:445:ALA:HA	1:C:448:VAL:HG22	1.63	0.80
1:D:158:ILE:H	1:D:158:ILE:HD12	1.47	0.80
1:A:120:ILE:HG22	1:A:123:ILE:HB	1.62	0.79
1:D:117:VAL:HG12	1:D:123:ILE:HD11	1.64	0.79
1:D:157:TYR:HD1	1:D:327:LEU:HD13	1.48	0.79
1:D:79:VAL:HA	1:D:91:VAL:HG12	1.63	0.79
1:D:117:VAL:CG1	1:D:123:ILE:HD11	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:HG2	1:A:214:SER:CB	2.12	0.79
1:B:82:ILE:O	1:B:252:LYS:NZ	2.15	0.79
1:B:183:MET:HA	1:B:185:LYS:HE2	1.65	0.78
1:B:155:ALA:HB2	1:B:177:ALA:HB1	1.64	0.78
1:A:155:ALA:O	1:A:183:MET:N	2.16	0.78
1:B:67:GLN:HG3	1:B:73:VAL:HG23	1.65	0.78
1:D:354:VAL:CG1	1:D:443:LYS:HE2	2.13	0.78
1:D:19:ILE:HD13	1:D:311:LEU:HD22	1.65	0.78
1:D:42:CSO:HB2	2:D:501:FAD:N5	1.99	0.77
1:B:123:ILE:HD12	1:B:215:PHE:HE2	1.50	0.77
1:C:118:PRO:HD3	1:C:240:ILE:HD11	1.67	0.77
1:A:20:LEU:HD11	1:A:71:ALA:HB2	1.68	0.76
1:D:243:ARG:NH1	7:D:602:HOH:O	2.19	0.76
1:A:195:ILE:HD11	1:A:334:ILE:HD13	1.68	0.76
1:C:32:GLU:OE2	2:C:501:FAD:O2B	2.04	0.75
1:D:148:LYS:NZ	1:D:170:GLY:O	2.18	0.75
1:B:63:PRO:HB3	1:B:73:VAL:HG11	1.69	0.75
1:B:264:ASP:OD2	1:B:268:ARG:NH2	2.20	0.75
1:D:363:GLU:N	1:D:363:GLU:OE1	2.19	0.75
1:D:186:TYR:OH	3:D:502:NDP:O2A	2.04	0.74
1:B:334:ILE:HG13	1:B:390:MET:HG3	1.69	0.74
1:C:107:LEU:HD21	1:C:109:MET:HE2	1.69	0.74
1:A:157:TYR:HB3	3:A:502:NDP:H42N	1.70	0.74
1:B:157:TYR:HD1	1:B:183:MET:HE1	1.52	0.74
1:A:295:PRO:HG2	3:A:502:NDP:O3D	1.87	0.74
1:D:157:TYR:HE1	1:D:327:LEU:HD22	1.53	0.73
1:D:354:VAL:HG13	1:D:443:LYS:HE2	1.70	0.73
1:C:345:LYS:NZ	1:C:351:ALA:O	2.20	0.73
1:B:120:ILE:HG22	1:B:123:ILE:HB	1.69	0.73
1:B:310:ASN:OD1	1:B:315:THR:N	2.18	0.73
1:D:353:GLN:OE1	1:D:374:SER:OG	2.05	0.73
1:D:126:ASP:O	1:D:129:LYS:NZ	2.21	0.73
1:C:41:SER:HA	1:C:44:ILE:HG13	1.71	0.73
1:B:1:MET:HE3	1:B:26:ALA:HB2	1.71	0.72
1:D:29:THR:HA	1:D:72:ASN:HB3	1.71	0.72
1:A:240:ILE:HG23	3:A:502:NDP:N7A	2.05	0.72
1:B:127:ARG:NH1	1:B:221:GLY:HA2	2.04	0.72
1:D:42:CSO:HB2	2:D:501:FAD:C4X	2.20	0.72
1:D:158:ILE:HD13	3:D:502:NDP:PN	2.28	0.71
1:D:295:PRO:HG2	3:D:502:NDP:O3D	1.90	0.71
1:A:397:GLN:HB2	1:B:397:GLN:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PHE:HZ	2:B:501:FAD:HM81	1.56	0.71
1:C:157:TYR:HB3	3:C:502:NDP:H42N	1.71	0.71
1:C:242:PHE:HZ	2:C:501:FAD:HM81	1.55	0.71
1:C:295:PRO:HG2	3:C:502:NDP:O3D	1.91	0.70
1:A:47:TYR:O	1:A:50:GLY:N	2.16	0.70
1:C:127:ARG:NH1	1:C:221:GLY:HA2	2.06	0.70
1:C:152:VAL:HG11	1:C:159:ALA:HA	1.73	0.70
1:D:327:LEU:HD11	1:D:329:LEU:HD11	1.72	0.70
1:D:158:ILE:HD11	3:D:502:NDP:C6N	2.22	0.70
1:A:132:LYS:HD2	1:A:242:PHE:HE1	1.57	0.70
1:C:82:ILE:HG21	1:C:107:LEU:HD13	1.74	0.70
1:B:443:LYS:O	1:B:446:GLN:HG2	1.91	0.70
1:B:42:CSO:O	7:B:602:HOH:O	2.09	0.69
1:A:335:VAL:HG11	1:A:396:SER:HA	1.73	0.69
1:B:150:ILE:HD12	1:B:235:LEU:HD23	1.73	0.69
1:A:213:GLU:HB2	1:A:225:LYS:HD3	1.75	0.69
1:B:2:LYS:HE3	1:B:27:GLU:HG3	1.75	0.69
1:C:193:ASP:OD1	7:C:601:HOH:O	2.11	0.69
1:D:266:TYR:HB3	1:D:310:ASN:HD22	1.58	0.69
1:D:158:ILE:HD11	3:D:502:NDP:H6N	1.76	0.68
1:B:156:GLY:HA3	3:B:502:NDP:O5B	1.92	0.68
1:D:196:GLU:O	1:D:200:ARG:HG3	1.93	0.68
1:B:341:LEU:HD22	1:B:353:GLN:HG2	1.76	0.67
1:A:354:VAL:HG11	1:A:440:ALA:HA	1.77	0.67
1:A:82:ILE:HG13	1:A:248:LEU:HD22	1.75	0.67
1:D:197:GLN:OE1	7:D:601:HOH:O	2.13	0.66
1:B:157:TYR:HB3	3:B:502:NDP:H42N	1.77	0.66
1:C:42:CSO:HB2	2:C:501:FAD:C4X	2.25	0.66
1:D:242:PHE:HZ	2:D:501:FAD:HM81	1.60	0.66
1:C:247:ASP:OD1	1:C:247:ASP:N	2.27	0.66
1:B:158:ILE:HG12	3:B:502:NDP:H5N	1.78	0.66
1:A:129:LYS:HG3	1:A:235:LEU:HD11	1.76	0.66
1:B:176:ILE:HA	1:B:207:ALA:HB3	1.78	0.66
1:A:129:LYS:CG	1:A:235:LEU:HD11	2.25	0.65
1:B:2:LYS:CE	1:B:27:GLU:HG3	2.26	0.65
1:D:122:GLY:O	1:D:215:PHE:HB2	1.96	0.65
1:D:158:ILE:N	1:D:158:ILE:HD12	2.10	0.65
1:A:63:PRO:HB3	1:A:73:VAL:HG11	1.79	0.64
1:C:350:ASN:ND2	1:C:380:ASP:OD2	2.30	0.64
1:B:218:SER:HB3	1:B:221:GLY:O	1.97	0.64
1:B:83:ASP:OD2	1:B:86:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB2	1:A:177:ALA:CB	2.28	0.64
1:B:1:MET:CE	1:B:26:ALA:HB2	2.27	0.64
1:C:106:LYS:HD3	1:C:273:ASP:HB3	1.79	0.64
1:A:38:SER:OG	1:A:61:SER:HB3	1.98	0.64
1:D:120:ILE:HD13	1:D:215:PHE:CE1	2.33	0.64
1:D:191:PHE:CD2	1:D:390:MET:HE3	2.32	0.64
1:A:184:ARG:HH22	1:C:184:ARG:HH22	1.46	0.64
1:D:122:GLY:HA3	1:D:215:PHE:O	1.98	0.64
1:B:299:ASN:OD1	7:B:603:HOH:O	2.15	0.63
1:B:116:ILE:HB	1:B:240:ILE:HG13	1.81	0.63
1:D:33:ARG:HG3	2:D:501:FAD:C2A	2.29	0.63
1:A:265:ASP:HB3	1:A:317:LYS:CG	2.29	0.62
1:B:185:LYS:CD	1:B:185:LYS:H	2.06	0.62
1:C:74:GLN:HG3	1:C:77:HIS:NE2	2.13	0.62
1:B:152:VAL:HG12	1:B:175:LEU:HG	1.82	0.62
1:B:160:ALA:HB3	1:B:183:MET:HE3	1.82	0.62
1:B:185:LYS:HE3	3:B:502:NDP:O3B	1.98	0.62
1:B:67:GLN:HG3	1:B:73:VAL:CG2	2.28	0.62
1:C:136:HIS:O	1:C:140:LEU:HG	1.99	0.62
1:A:360:TYR:HB3	1:A:371:VAL:HG21	1.81	0.62
1:A:418:VAL:N	1:B:319:MET:HE1	2.14	0.62
1:D:87:LYS:HE2	1:D:104:TYR:O	2.00	0.62
1:D:47:TYR:CE2	1:D:55:PRO:HB3	2.35	0.62
1:B:11:ALA:HB2	1:B:300:ALA:HB1	1.82	0.62
1:C:64:GLU:O	1:C:68:LYS:HG3	2.00	0.62
1:B:126:ASP:OD1	1:B:126:ASP:N	2.33	0.61
1:A:49:GLY:O	7:A:601:HOH:O	2.16	0.61
1:A:157:TYR:HB3	3:A:502:NDP:C4N	2.30	0.61
1:A:42:CSO:HB2	2:A:501:FAD:C4X	2.31	0.61
1:C:38:SER:HB2	1:C:60:TYR:CZ	2.36	0.60
1:C:358:ASP:O	1:C:371:VAL:HG12	2.01	0.60
1:D:354:VAL:HG12	1:D:443:LYS:HE2	1.83	0.60
1:C:80:LEU:HD21	1:C:92:GLU:OE1	2.01	0.60
1:C:130:LEU:O	1:C:136:HIS:HB3	2.02	0.60
1:C:413:ASP:HA	1:C:441:GLN:HE21	1.66	0.60
1:B:123:ILE:HD12	1:B:215:PHE:CE2	2.35	0.60
1:C:148:LYS:HG3	1:C:172:ASP:OD2	2.02	0.60
1:C:215:PHE:HB3	1:C:222:LEU:HD11	1.83	0.60
1:C:413:ASP:HA	1:C:441:GLN:NE2	2.16	0.60
1:D:301:VAL:O	1:D:305:ILE:HG13	2.02	0.60
1:C:187:PHE:CZ	1:C:334:ILE:HG22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:PHE:CG	1:D:429:PRO:HA	2.37	0.59
1:A:271:ASN:HB3	1:A:274:ILE:HD12	1.83	0.59
1:D:157:TYR:CD1	1:D:327:LEU:HD13	2.35	0.59
1:C:283:VAL:HG12	1:C:303:GLN:NE2	2.17	0.59
1:C:42:CSO:OD	2:C:501:FAD:O2'	2.20	0.59
1:C:341:LEU:HD22	1:C:353:GLN:HG2	1.85	0.59
1:D:134:TRP:O	1:D:138:GLN:HG3	2.01	0.59
1:B:152:VAL:CG1	1:B:159:ALA:HB1	2.32	0.59
1:B:335:VAL:HG11	1:B:396:SER:HA	1.83	0.59
1:D:440:ALA:O	1:D:444:VAL:HG13	2.02	0.59
1:A:428:ARG:HB3	1:A:429:PRO:HD2	1.85	0.59
1:B:3:VAL:HA	1:B:106:LYS:O	2.02	0.59
1:D:360:TYR:O	1:D:427:ASP:HA	2.03	0.59
1:C:428:ARG:HB3	1:C:429:PRO:HD2	1.85	0.59
1:A:334:ILE:HG12	1:A:390:MET:HG3	1.84	0.59
1:A:67:GLN:HG3	1:A:71:ALA:O	2.03	0.58
1:B:65:GLU:O	1:B:69:LEU:HG	2.02	0.58
1:A:126:ASP:N	1:A:126:ASP:OD1	2.33	0.58
1:C:149:ARG:HG2	1:C:172:ASP:HB2	1.86	0.58
1:A:315:THR:HG22	1:A:316:VAL:HG23	1.85	0.58
1:A:360:TYR:HB3	1:A:371:VAL:CG2	2.33	0.58
1:D:47:TYR:CZ	1:D:55:PRO:HB3	2.38	0.58
1:A:188:ASP:OD2	1:A:353:GLN:NE2	2.36	0.58
1:B:157:TYR:HB3	3:B:502:NDP:C4N	2.34	0.58
1:A:84:PRO:O	1:A:87:LYS:N	2.36	0.58
1:A:8:CYS:HB2	1:A:30:VAL:HG21	1.86	0.58
1:A:42:CSO:HB2	2:A:501:FAD:N5	2.19	0.58
1:C:288:THR:O	1:C:290:GLN:HG2	2.03	0.58
1:B:124:ASP:N	1:B:124:ASP:OD1	2.26	0.58
1:B:178:ARG:H	3:B:502:NDP:C2A	2.16	0.57
1:C:130:LEU:CD2	1:C:238:LEU:HD12	2.31	0.57
1:C:444:VAL:O	1:C:448:VAL:HG13	2.03	0.57
1:D:130:LEU:HD21	1:D:238:LEU:HD12	1.84	0.57
1:A:126:ASP:O	1:A:129:LYS:HE3	2.04	0.57
1:D:12:GLY:O	1:D:16:ILE:HG13	2.03	0.57
1:A:2:LYS:N	1:A:105:ASP:OD2	2.30	0.57
1:C:177:ALA:HA	3:C:502:NDP:H2A	1.85	0.57
1:B:217:ASP:HA	1:B:222:LEU:HD12	1.84	0.57
1:B:83:ASP:O	1:B:87:LYS:N	2.37	0.57
1:B:157:TYR:HB3	3:B:502:NDP:C5N	2.34	0.57
1:D:19:ILE:CD1	1:D:311:LEU:HD22	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:PHE:O	7:B:604:HOH:O	2.18	0.57
1:D:27:GLU:HA	1:D:27:GLU:OE1	2.05	0.57
1:C:118:PRO:C	1:C:119:LYS:HE2	2.25	0.57
1:C:150:ILE:HD12	1:C:166:TYR:CD1	2.40	0.57
1:D:79:VAL:HG13	1:D:89:VAL:CG2	2.35	0.57
1:A:382:HIS:ND1	1:A:413:ASP:OD2	2.32	0.56
1:C:326:GLY:HA3	1:C:335:VAL:HG12	1.87	0.56
1:D:125:SER:OG	1:D:127:ARG:HG3	2.04	0.56
1:B:157:TYR:CD1	1:B:183:MET:HE1	2.38	0.56
1:C:5:VAL:HG22	1:C:108:VAL:HG21	1.87	0.56
1:B:223:THR:HA	1:B:232:GLU:HA	1.87	0.56
1:C:82:ILE:CG1	1:C:89:VAL:HG12	2.36	0.56
1:D:46:LEU:HD22	1:D:51:LYS:HE3	1.87	0.56
1:C:400:ASN:O	1:C:404:VAL:HG23	2.05	0.56
1:B:155:ALA:HB2	1:B:177:ALA:CB	2.34	0.56
1:B:41:SER:O	2:B:501:FAD:HM72	2.06	0.56
1:C:122:GLY:HA3	1:C:215:PHE:O	2.05	0.56
1:D:0:SER:O	1:D:2:LYS:HE3	2.06	0.56
1:D:284:HIS:CE1	1:D:289:HIS:HA	2.41	0.56
1:D:118:PRO:HD3	1:D:240:ILE:HD11	1.88	0.56
1:B:183:MET:CA	1:B:185:LYS:HE2	2.35	0.55
1:B:295:PRO:HG2	3:B:502:NDP:O3D	2.06	0.55
1:A:113:SER:O	1:A:132:LYS:HE2	2.05	0.55
1:B:187:PHE:CE1	1:B:334:ILE:HG22	2.40	0.55
1:A:33:ARG:O	1:A:76:ASN:HA	2.06	0.55
1:A:213:GLU:N	1:A:225:LYS:O	2.39	0.55
1:D:265:ASP:HB3	1:D:317:LYS:HG3	1.87	0.55
1:D:352:GLU:OE1	1:D:379:PRO:HB3	2.05	0.55
1:A:265:ASP:HB3	1:A:317:LYS:HG3	1.88	0.55
1:A:64:GLU:N	1:A:64:GLU:OE1	2.32	0.55
1:C:192:THR:O	1:C:196:GLU:HG3	2.06	0.55
1:D:118:PRO:O	1:D:123:ILE:HD12	2.07	0.55
1:D:29:THR:CA	1:D:72:ASN:HB3	2.37	0.55
1:B:116:ILE:O	1:B:240:ILE:HD11	2.06	0.55
1:B:198:ASP:O	1:B:201:ASP:HB2	2.06	0.55
1:B:65:GLU:HA	1:B:68:LYS:HE2	1.89	0.55
1:C:313:LYS:HB2	1:C:314:PRO:HD2	1.88	0.55
1:C:80:LEU:N	1:C:90:THR:O	2.37	0.55
1:C:113:SER:HB3	1:C:279:ASP:HB3	1.88	0.55
1:A:153:ILE:HD12	1:A:153:ILE:N	2.22	0.54
1:A:167:SER:OG	1:A:330:TYR:OH	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ILE:HG21	1:B:323:SER:OG	2.07	0.54
1:B:322:GLN:NE2	1:B:403:SER:OG	2.29	0.54
1:C:124:ASP:N	1:C:124:ASP:OD1	2.35	0.54
1:B:428:ARG:HB3	1:B:429:PRO:HD2	1.88	0.54
1:D:120:ILE:CG1	1:D:121:PRO:HD2	2.37	0.54
1:D:4:THR:HA	1:D:29:THR:O	2.08	0.54
1:B:120:ILE:HG21	1:B:215:PHE:CE2	2.43	0.54
1:D:423:GLN:OE1	1:D:425:ASN:ND2	2.26	0.54
1:B:382:HIS:HB3	1:B:412:ILE:HG12	1.88	0.54
1:A:322:GLN:HG2	1:A:406:ILE:HB	1.89	0.54
1:A:93:ASP:OD1	1:A:95:THR:HG22	2.08	0.54
1:B:114:TRP:CD2	1:B:115:PRO:HD2	2.42	0.54
1:D:130:LEU:HD23	1:D:238:LEU:HB2	1.89	0.54
1:A:179:SER:HB3	3:A:502:NDP:O2X	2.07	0.54
1:A:44:ILE:O	1:A:48:LEU:HG	2.07	0.54
1:A:120:ILE:HG12	1:A:121:PRO:CD	2.32	0.54
1:C:3:VAL:HG21	1:C:311:LEU:HD21	1.89	0.54
1:D:228:LYS:O	1:D:229:ASN:HB2	2.06	0.54
1:B:158:ILE:HG13	3:B:502:NDP:O2N	2.08	0.54
1:C:87:LYS:HE2	1:C:104:TYR:O	2.07	0.54
1:A:51:LYS:N	7:A:612:HOH:O	2.41	0.54
1:C:268:ARG:HG2	1:C:275:PHE:CE2	2.43	0.54
1:C:423:GLN:HG3	1:D:326:GLY:O	2.07	0.54
1:D:114:TRP:CD2	1:D:115:PRO:HD2	2.43	0.54
1:A:419:ASP:OD1	7:A:602:HOH:O	2.18	0.54
1:D:192:THR:O	1:D:196:GLU:HG3	2.08	0.54
1:A:160:ALA:O	1:A:199:TYR:OH	2.26	0.53
1:B:294:ILE:O	1:B:299:ASN:ND2	2.40	0.53
1:B:79:VAL:HG22	1:B:91:VAL:HG23	1.90	0.53
1:C:15:ALA:O	1:C:19:ILE:HG13	2.07	0.53
1:C:89:VAL:O	1:C:101:THR:HA	2.08	0.53
1:D:191:PHE:O	1:D:195:ILE:HG13	2.08	0.53
1:C:128:VAL:HG22	1:C:222:LEU:HD21	1.90	0.53
1:D:341:LEU:HD22	1:D:353:GLN:HB3	1.89	0.53
1:D:5:VAL:HB	1:D:30:VAL:HG23	1.90	0.53
1:C:4:THR:HA	1:C:29:THR:O	2.08	0.53
1:C:215:PHE:CE2	1:C:224:ILE:HG12	2.44	0.53
1:D:151:THR:O	1:D:236:ALA:HA	2.08	0.53
1:D:37:ILE:HG12	1:D:63:PRO:HD3	1.90	0.53
1:C:360:TYR:O	1:C:427:ASP:HA	2.08	0.53
1:D:9:THR:HG22	1:D:10:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:HG11	1:B:159:ALA:HB1	1.91	0.53
1:D:157:TYR:CE1	1:D:327:LEU:HD22	2.38	0.53
1:C:19:ILE:HG12	1:C:308:GLY:HA2	1.91	0.53
1:C:42:CSO:HA	2:C:501:FAD:N5	2.24	0.53
1:A:32:GLU:HB3	1:A:75:MET:HE1	1.91	0.53
1:C:335:VAL:HG23	1:C:399:ALA:HB2	1.91	0.53
1:A:114:TRP:CD2	1:A:115:PRO:HD2	2.44	0.53
1:D:120:ILE:HD11	1:D:212:VAL:HG12	1.91	0.52
1:C:5:VAL:HG22	1:C:108:VAL:CG2	2.39	0.52
1:D:157:TYR:O	1:D:161:GLU:HG3	2.10	0.52
1:D:256:ALA:HB1	1:D:257:PRO:HD2	1.91	0.52
1:B:215:PHE:HB3	1:B:222:LEU:HD21	1.91	0.52
1:B:106:LYS:NZ	1:B:273:ASP:HA	2.25	0.52
1:B:333:THR:O	1:B:390:MET:HA	2.08	0.52
1:C:208:LEU:O	1:C:210:GLU:HG3	2.09	0.52
1:C:32:GLU:HG3	1:C:34:ASN:H	1.75	0.52
1:C:82:ILE:HG12	1:C:89:VAL:HG12	1.91	0.52
1:C:158:ILE:HD12	3:C:502:NDP:O1N	2.09	0.52
1:D:120:ILE:CD1	1:D:212:VAL:HG12	2.40	0.52
1:D:158:ILE:HG13	3:D:502:NDP:H5N	1.91	0.52
1:B:285:TYR:O	1:B:289:HIS:N	2.42	0.52
1:B:47:TYR:CE2	1:B:141:ILE:HG13	2.45	0.52
1:C:352:GLU:OE2	1:C:379:PRO:HG3	2.10	0.52
1:C:38:SER:HB2	1:C:60:TYR:CE2	2.44	0.52
1:D:309:LYS:HD2	1:D:316:VAL:HG21	1.92	0.52
1:B:132:LYS:HG2	1:B:132:LYS:O	2.08	0.52
1:B:1:MET:O	1:B:27:GLU:N	2.33	0.52
1:C:341:LEU:HD22	1:C:353:GLN:CG	2.39	0.52
1:D:158:ILE:H	1:D:158:ILE:CD1	2.20	0.52
1:A:127:ARG:HD3	1:A:222:LEU:HB2	1.91	0.52
1:A:127:ARG:O	1:A:235:LEU:HD12	2.10	0.52
1:C:445:ALA:O	1:C:448:VAL:HG22	2.10	0.52
1:A:153:ILE:HD11	1:A:236:ALA:HB1	1.91	0.52
1:B:266:TYR:CD2	1:B:314:PRO:HB3	2.45	0.52
1:B:321:THR:HB	7:B:654:HOH:O	2.09	0.52
1:C:12:GLY:O	1:C:16:ILE:HG13	2.10	0.52
1:D:120:ILE:HG21	1:D:215:PHE:HE1	1.73	0.52
1:C:335:VAL:CG2	1:C:399:ALA:HB2	2.40	0.51
1:C:445:ALA:CA	1:C:448:VAL:HG22	2.35	0.51
1:D:187:PHE:CE1	1:D:336:SER:HB3	2.44	0.51
1:A:4:THR:HB	1:A:107:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:HB3	1:A:317:LYS:HG2	1.92	0.51
1:A:83:ASP:O	1:A:87:LYS:N	2.43	0.51
1:B:133:ASN:HB3	1:B:136:HIS:H	1.74	0.51
1:D:327:LEU:HG	1:D:329:LEU:HG	1.93	0.51
1:A:240:ILE:HD12	3:A:502:NDP:C5A	2.41	0.51
1:C:141:ILE:HD12	1:C:141:ILE:H	1.75	0.51
1:C:244:PRO:HG3	1:C:293:TYR:CE1	2.46	0.51
1:D:89:VAL:O	1:D:101:THR:HA	2.10	0.51
1:C:445:ALA:HA	1:C:448:VAL:CG2	2.36	0.51
1:D:37:ILE:HD11	1:D:62:SER:C	2.31	0.51
1:B:157:TYR:CE1	1:B:327:LEU:HD22	2.46	0.51
1:B:79:VAL:HA	1:B:91:VAL:HA	1.92	0.51
1:C:46:LEU:HD13	1:D:365:MET:SD	2.51	0.51
1:D:164:GLU:HG2	1:D:330:TYR:CE1	2.46	0.51
1:D:361:ARG:NH2	1:D:367:SER:OG	2.43	0.51
1:D:38:SER:HB2	1:D:60:TYR:CZ	2.46	0.51
1:A:115:PRO:HD3	1:A:132:LYS:HD2	1.93	0.51
1:C:47:TYR:CE2	1:C:141:ILE:HD11	2.46	0.51
1:A:46:LEU:HD23	1:A:51:LYS:HD2	1.93	0.51
1:D:222:LEU:O	1:D:232:GLU:HG3	2.11	0.51
1:D:250:LYS:O	1:D:252:LYS:HG3	2.11	0.51
1:C:210:GLU:HG2	1:C:228:LYS:HD2	1.93	0.50
1:C:80:LEU:HD11	1:C:92:GLU:HB3	1.92	0.50
1:A:12:GLY:O	1:A:16:ILE:HG13	2.12	0.50
1:D:154:GLY:HA3	1:D:239:CYS:O	2.11	0.50
1:D:64:GLU:N	1:D:64:GLU:OE2	2.30	0.50
1:C:82:ILE:HG21	1:C:107:LEU:CD1	2.39	0.50
1:D:244:PRO:HG3	1:D:293:TYR:CE1	2.46	0.50
1:C:130:LEU:CD2	1:C:238:LEU:HB2	2.41	0.50
1:A:121:PRO:HG2	1:A:214:SER:HB2	1.94	0.50
1:B:113:SER:HB3	1:B:279:ASP:HB3	1.94	0.50
1:B:216:THR:C	1:B:222:LEU:HD12	2.32	0.50
1:A:319:MET:CE	1:B:417:MET:HB2	2.41	0.50
1:C:188:ASP:HB3	7:C:618:HOH:O	2.12	0.50
1:D:187:PHE:CZ	1:D:334:ILE:HG22	2.46	0.50
1:D:242:PHE:CZ	2:D:501:FAD:HM81	2.46	0.50
1:C:212:VAL:HG12	1:C:213:GLU:N	2.27	0.50
1:C:215:PHE:CD2	1:C:224:ILE:HG12	2.46	0.50
1:A:152:VAL:HG11	1:A:159:ALA:HA	1.93	0.50
1:A:178:ARG:H	3:A:502:NDP:C2A	2.25	0.50
1:C:127:ARG:HH11	1:C:221:GLY:HA2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:VAL:HA	1:C:108:VAL:HG23	1.93	0.50
1:D:120:ILE:HG13	1:D:121:PRO:HD2	1.93	0.50
1:D:428:ARG:HB3	1:D:429:PRO:HD2	1.94	0.50
1:A:18:GLN:O	1:A:22:GLU:HG2	2.12	0.49
1:C:79:VAL:CA	1:C:91:VAL:HG12	2.35	0.49
1:A:256:ALA:HB2	1:A:262:ILE:HD11	1.93	0.49
6:A:506:CL:CL	1:C:184:ARG:NH2	2.82	0.49
1:C:39:PHE:HB2	1:C:59:PHE:CE2	2.47	0.49
1:D:119:LYS:O	1:D:119:LYS:HG3	2.11	0.49
1:D:256:ALA:HB1	1:D:257:PRO:CD	2.42	0.49
1:D:318:TYR:CE2	1:D:320:GLY:HA2	2.46	0.49
1:D:38:SER:O	1:D:59:PHE:HA	2.12	0.49
1:A:283:VAL:CG2	1:A:294:ILE:HD12	2.42	0.49
1:C:315:THR:HG22	1:C:316:VAL:HG23	1.94	0.49
1:C:74:GLN:HG3	1:C:77:HIS:CE1	2.47	0.49
1:C:92:GLU:HB2	1:C:99:GLN:HG2	1.93	0.49
1:D:3:VAL:HG21	1:D:311:LEU:HD21	1.93	0.49
1:A:132:LYS:HA	2:A:501:FAD:HM82	1.93	0.49
1:C:120:ILE:O	1:C:123:ILE:HG12	2.12	0.49
1:C:271:ASN:HB3	1:C:274:ILE:HB	1.94	0.49
1:A:319:MET:HE3	7:A:640:HOH:O	2.13	0.49
1:B:334:ILE:N	1:B:334:ILE:HD12	2.28	0.49
1:D:116:ILE:O	1:D:240:ILE:HD11	2.12	0.49
1:C:212:VAL:HA	1:C:226:THR:HA	1.95	0.49
1:D:285:TYR:O	1:D:289:HIS:N	2.43	0.49
1:B:44:ILE:O	1:B:48:LEU:HG	2.13	0.49
1:B:434:ASN:O	1:B:438:GLN:HG3	2.13	0.48
1:D:35:ASP:OD1	1:D:36:VAL:HG13	2.13	0.48
1:D:65:GLU:O	1:D:68:LYS:HB3	2.13	0.48
1:D:80:LEU:HD11	1:D:92:GLU:HG2	1.94	0.48
1:B:108:VAL:HG12	1:B:110:THR:HG23	1.95	0.48
1:C:448:VAL:O	1:C:449:ASN:HB3	2.12	0.48
1:D:294:ILE:O	1:D:299:ASN:ND2	2.46	0.48
4:A:504:EDO:H22	1:B:429:PRO:HG2	1.95	0.48
1:A:132:LYS:HD2	1:A:242:PHE:CE1	2.44	0.48
1:A:33:ARG:HG3	2:A:501:FAD:C2A	2.43	0.48
1:B:127:ARG:HH12	1:B:221:GLY:HA2	1.74	0.48
1:D:111:SER:O	2:D:501:FAD:H8A	2.13	0.48
1:D:157:TYR:HB3	3:D:502:NDP:H42N	1.95	0.48
1:B:266:TYR:CG	1:B:314:PRO:HB3	2.49	0.48
1:B:445:ALA:HA	1:B:448:VAL:CG1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:O	1:B:76:ASN:HA	2.14	0.48
1:C:249:LEU:HB3	1:C:253:VAL:HG22	1.94	0.48
1:D:3:VAL:HB	1:D:28:VAL:HG22	1.95	0.48
1:B:4:THR:HG21	1:B:89:VAL:HG21	1.95	0.48
1:D:229:ASN:ND2	1:D:230:SER:H	2.12	0.48
1:A:184:ARG:NH2	6:A:506:CL:CL	2.83	0.48
1:B:310:ASN:OD1	1:B:316:VAL:N	2.45	0.48
1:C:322:GLN:HG3	1:C:406:ILE:HG21	1.95	0.48
1:D:350:ASN:HD21	1:D:379:PRO:HG2	1.79	0.48
1:C:157:TYR:HB3	3:C:502:NDP:C4N	2.41	0.48
1:C:441:GLN:O	1:C:444:VAL:HG22	2.14	0.48
1:C:82:ILE:HG23	1:C:89:VAL:HG12	1.94	0.48
1:A:319:MET:HB3	1:A:407:GLN:HE22	1.78	0.47
1:A:92:GLU:OE2	1:A:97:HIS:HA	2.14	0.47
1:A:1:MET:HE3	1:A:26:ALA:HB2	1.96	0.47
1:A:199:TYR:HD1	1:A:204:VAL:HG21	1.79	0.47
1:C:162:LEU:HD12	1:C:239:CYS:SG	2.54	0.47
1:C:29:THR:HA	1:C:72:ASN:O	2.14	0.47
1:C:79:VAL:HG22	1:C:91:VAL:HG12	1.96	0.47
1:A:65:GLU:O	1:A:69:LEU:HD23	2.13	0.47
1:B:119:LYS:O	1:B:120:ILE:HD12	2.14	0.47
1:C:128:VAL:HG22	1:C:222:LEU:CD2	2.44	0.47
1:D:421:LEU:C	1:D:421:LEU:HD12	2.35	0.47
1:A:1:MET:O	1:A:27:GLU:N	2.40	0.47
1:A:327:LEU:HD23	1:A:327:LEU:N	2.30	0.47
1:B:155:ALA:O	1:B:183:MET:N	2.35	0.47
1:C:42:CSO:HB2	2:C:501:FAD:C4	2.44	0.47
1:C:42:CSO:HA	2:C:501:FAD:C5X	2.44	0.47
1:C:93:ASP:OD1	1:C:95:THR:HG22	2.15	0.47
1:C:441:GLN:HA	1:C:444:VAL:HG22	1.97	0.47
1:D:85:ASP:N	1:D:85:ASP:OD1	2.46	0.47
1:A:119:LYS:HD2	1:A:119:LYS:H	1.80	0.47
1:B:275:PHE:CZ	1:B:311:LEU:HA	2.50	0.47
1:B:363:GLU:OE2	1:B:428:ARG:NH2	2.33	0.47
1:C:156:GLY:HA3	3:C:502:NDP:O5B	2.14	0.47
1:A:158:ILE:HD12	3:A:502:NDP:O1N	2.15	0.47
1:A:417:MET:C	1:B:319:MET:HE1	2.34	0.47
1:B:224:ILE:N	1:B:231:TYR:O	2.26	0.47
1:A:157:TYR:HB3	3:A:502:NDP:C5N	2.45	0.47
1:C:5:VAL:HA	1:C:108:VAL:CG2	2.45	0.47
1:A:355:ILE:CD1	1:A:374:SER:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLY:C	1:C:177:ALA:HB2	2.35	0.47
1:C:79:VAL:HG22	1:C:91:VAL:CG1	2.44	0.47
1:B:22:GLU:OE1	1:B:309:LYS:NZ	2.42	0.47
1:C:285:TYR:O	1:C:289:HIS:N	2.47	0.47
1:D:18:GLN:O	1:D:22:GLU:HG2	2.15	0.47
1:B:240:ILE:HG12	7:B:620:HOH:O	2.14	0.46
1:D:142:GLU:OE2	1:D:145:LYS:NZ	2.27	0.46
1:D:211:THR:O	1:D:213:GLU:HG3	2.14	0.46
1:D:132:LYS:HA	2:D:501:FAD:HM82	1.97	0.46
1:A:422:PHE:CG	1:A:429:PRO:HA	2.50	0.46
1:C:301:VAL:O	1:C:305:ILE:HG13	2.15	0.46
1:A:418:VAL:HA	1:B:319:MET:CE	2.45	0.46
1:B:341:LEU:HD22	1:B:353:GLN:CG	2.43	0.46
1:A:12:GLY:HA2	1:A:110:THR:HG21	1.98	0.46
1:B:106:LYS:HZ2	1:B:273:ASP:HA	1.80	0.46
1:C:141:ILE:HD12	1:C:141:ILE:N	2.31	0.46
1:D:326:GLY:HA3	1:D:335:VAL:HG12	1.96	0.46
1:A:159:ALA:HB2	1:A:239:CYS:HB2	1.96	0.46
1:A:19:ILE:CG1	1:A:308:GLY:HA2	2.46	0.46
1:C:107:LEU:HD21	1:C:109:MET:CE	2.42	0.46
1:D:209:GLY:O	1:D:228:LYS:NZ	2.49	0.46
1:C:9:THR:O	1:C:38:SER:HA	2.15	0.46
1:A:240:ILE:O	1:A:240:ILE:HG22	2.16	0.46
1:A:14:PHE:CE1	1:A:301:VAL:HG12	2.51	0.46
1:B:178:ARG:H	3:B:502:NDP:H2A	1.80	0.46
1:B:54:ASP:OD1	1:B:56:GLN:HB2	2.16	0.46
1:C:44:ILE:O	1:C:47:TYR:HB3	2.16	0.46
1:A:176:ILE:HG12	1:A:207:ALA:HB3	1.98	0.46
1:A:269:SER:OG	1:A:274:ILE:HB	2.16	0.46
1:B:160:ALA:HB3	1:B:183:MET:CE	2.44	0.46
1:D:261:ILE:HG13	1:D:280:SER:O	2.16	0.46
1:C:400:ASN:HB3	1:D:420:MET:HG2	1.97	0.46
1:A:283:VAL:HG21	1:A:294:ILE:HD12	1.98	0.46
1:B:141:ILE:HG22	1:B:142:GLU:OE1	2.15	0.46
1:B:48:LEU:HD13	1:B:166:TYR:OH	2.16	0.46
1:C:426:PHE:CZ	1:D:333:THR:HG23	2.50	0.46
1:D:216:THR:OG1	1:D:223:THR:HB	2.15	0.46
1:C:271:ASN:OD1	1:C:274:ILE:HG13	2.16	0.45
1:D:350:ASN:ND2	1:D:379:PRO:HG2	2.32	0.45
1:B:19:ILE:CD1	1:B:311:LEU:HD22	2.47	0.45
1:D:108:VAL:HG12	1:D:110:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HG21	1:A:131:CYS:SG	2.56	0.45
1:B:218:SER:OG	1:B:219:ALA:N	2.50	0.45
1:B:150:ILE:HD13	1:B:235:LEU:HB3	1.98	0.45
1:B:176:ILE:HG12	1:B:207:ALA:HB3	1.98	0.45
1:C:41:SER:HA	1:C:44:ILE:CG1	2.43	0.45
1:D:357:GLU:OE2	7:D:603:HOH:O	2.21	0.45
1:B:152:VAL:HG13	1:B:159:ALA:HB1	1.98	0.45
1:B:224:ILE:O	1:B:230:SER:HA	2.16	0.45
1:C:371:VAL:HG13	1:C:371:VAL:O	2.16	0.45
1:A:319:MET:HB3	1:A:407:GLN:NE2	2.31	0.45
1:B:157:TYR:HA	1:B:183:MET:HE2	1.98	0.45
1:C:80:LEU:HD11	1:C:92:GLU:CB	2.47	0.45
1:B:126:ASP:O	1:B:129:LYS:HE3	2.17	0.45
1:B:444:VAL:HG23	1:B:445:ALA:N	2.32	0.45
1:D:88:THR:HG22	1:D:103:SER:HA	1.99	0.45
1:B:160:ALA:CB	1:B:183:MET:HE3	2.46	0.45
1:B:217:ASP:CA	1:B:222:LEU:HD12	2.46	0.45
1:B:22:GLU:OE1	1:B:309:LYS:HD3	2.17	0.45
1:A:213:GLU:HG3	1:A:225:LYS:HE2	1.99	0.45
1:A:428:ARG:HB3	1:A:429:PRO:CD	2.47	0.45
1:A:80:LEU:HD11	1:A:92:GLU:HB2	1.99	0.45
1:D:296:LEU:HD23	3:D:502:NDP:H1D	1.99	0.45
1:B:267:MET:HE2	1:B:267:MET:HA	1.98	0.44
1:B:354:VAL:HG11	1:B:440:ALA:HA	1.98	0.44
1:C:51:LYS:O	1:D:366:PRO:HD3	2.17	0.44
1:A:112:GLY:HA3	2:A:501:FAD:C5B	2.46	0.44
1:A:120:ILE:HD11	1:A:212:VAL:O	2.16	0.44
1:A:218:SER:HB3	1:A:221:GLY:O	2.17	0.44
1:A:253:VAL:HA	1:A:270:SER:OG	2.17	0.44
1:B:361:ARG:HB2	1:B:362:PRO:CD	2.47	0.44
1:D:99:GLN:O	1:D:100:THR:HG23	2.17	0.44
1:D:268:ARG:HD2	1:D:272:PRO:HA	1.97	0.44
1:B:331:ASP:O	1:B:392:LYS:HG3	2.17	0.44
1:C:127:ARG:HG3	1:C:217:ASP:OD2	2.17	0.44
1:D:351:ALA:O	1:D:352:GLU:HG3	2.18	0.44
1:A:178:ARG:HD3	3:A:502:NDP:C6A	2.46	0.44
1:B:371:VAL:HG22	1:B:391:SER:CB	2.47	0.44
1:C:428:ARG:HB3	1:C:429:PRO:CD	2.47	0.44
1:C:5:VAL:HG13	1:C:108:VAL:HG23	2.00	0.44
1:D:352:GLU:OE2	1:D:379:PRO:HG3	2.17	0.44
1:A:278:GLY:HA3	2:A:501:FAD:O2P	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:HA	1:A:71:ALA:O	2.18	0.44
1:B:118:PRO:HG2	1:B:123:ILE:HD13	2.00	0.44
1:C:114:TRP:CD2	1:C:115:PRO:HD2	2.52	0.44
1:C:119:LYS:HE2	1:C:119:LYS:N	2.32	0.44
1:C:163:ALA:O	1:C:167:SER:HB3	2.17	0.44
1:A:112:GLY:HA2	1:A:279:ASP:HB2	1.99	0.44
1:B:1:MET:HB3	1:B:1:MET:HE3	1.78	0.44
1:B:210:GLU:HG2	1:B:228:LYS:CE	2.48	0.44
1:C:67:GLN:HG3	1:C:71:ALA:O	2.17	0.44
1:D:63:PRO:HB3	1:D:73:VAL:HG11	1.99	0.44
2:B:501:FAD:O4'	2:B:501:FAD:O2A	2.27	0.44
1:B:382:HIS:O	1:B:411:THR:HB	2.18	0.44
1:C:32:GLU:CD	2:C:501:FAD:HO2A	2.11	0.44
1:D:294:ILE:O	1:D:294:ILE:HG22	2.17	0.44
1:D:360:TYR:HB3	1:D:371:VAL:CG2	2.48	0.44
1:A:328:ALA:O	1:A:329:LEU:HD23	2.18	0.43
1:B:181:ARG:NH1	1:B:184:ARG:HA	2.34	0.43
1:D:176:ILE:HA	1:D:207:ALA:O	2.19	0.43
1:A:361:ARG:HB2	1:A:362:PRO:CD	2.48	0.43
1:B:68:LYS:HB3	1:B:68:LYS:HE2	1.66	0.43
1:C:178:ARG:NE	3:C:502:NDP:O3X	2.42	0.43
1:C:386:GLY:HA2	1:C:406:ILE:HD11	2.00	0.43
1:C:93:ASP:CG	1:C:95:THR:HG22	2.39	0.43
1:A:140:LEU:CD2	1:A:235:LEU:HD21	2.48	0.43
1:D:343:ALA:O	1:D:347:GLN:HG3	2.19	0.43
1:D:191:PHE:CG	1:D:390:MET:HE3	2.54	0.43
1:A:158:ILE:HG12	3:A:502:NDP:H5N	2.01	0.43
1:A:372:LEU:HB2	4:A:503:EDO:H21	2.01	0.43
1:B:14:PHE:CE1	1:B:301:VAL:HG12	2.53	0.43
1:C:353:GLN:HA	1:C:375:LEU:O	2.18	0.43
1:D:87:LYS:NZ	1:D:105:ASP:HA	2.34	0.43
1:A:345:LYS:HE3	1:A:351:ALA:O	2.19	0.43
1:D:335:VAL:HG11	1:D:396:SER:HA	2.01	0.43
1:D:443:LYS:O	1:D:446:GLN:HG3	2.19	0.43
1:A:15:ALA:HA	1:A:304:GLY:O	2.19	0.43
1:B:242:PHE:CZ	2:B:501:FAD:HM81	2.45	0.43
1:C:355:ILE:N	1:C:355:ILE:HD12	2.34	0.43
1:A:181:ARG:NH1	1:A:192:THR:HG21	2.33	0.43
1:A:327:LEU:HD11	1:A:329:LEU:HD11	2.00	0.43
1:A:195:ILE:CD1	1:A:334:ILE:HD13	2.46	0.43
1:A:83:ASP:HB3	1:A:88:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLY:O	1:B:16:ILE:HG13	2.19	0.43
1:B:91:VAL:HG22	1:B:92:GLU:H	1.83	0.43
1:D:127:ARG:HG3	1:D:222:LEU:HD13	2.01	0.43
1:D:362:PRO:HB2	1:D:364:PHE:CE2	2.54	0.43
1:A:445:ALA:O	1:A:448:VAL:HG12	2.19	0.42
1:B:428:ARG:HB3	1:B:429:PRO:CD	2.49	0.42
1:C:151:THR:HA	1:C:174:THR:O	2.18	0.42
1:D:185:LYS:HB2	1:D:185:LYS:NZ	2.33	0.42
1:D:378:ASP:O	1:D:382:HIS:HA	2.19	0.42
1:D:331:ASP:O	1:D:392:LYS:HG2	2.19	0.42
1:B:178:ARG:HA	1:B:210:GLU:O	2.19	0.42
1:B:30:VAL:HG13	1:B:73:VAL:HA	2.00	0.42
1:C:397:GLN:HB2	1:D:397:GLN:HB2	2.00	0.42
1:D:41:SER:HB2	1:D:132:LYS:O	2.19	0.42
1:D:121:PRO:HG2	1:D:214:SER:HB3	2.00	0.42
1:A:421:LEU:C	1:A:421:LEU:HD12	2.40	0.42
1:A:42:CSO:SG	1:B:422:PHE:HE2	2.43	0.42
1:A:415:LEU:HD23	1:A:437:ALA:HB2	2.01	0.42
1:A:179:SER:HB3	3:A:502:NDP:P2B	2.59	0.42
1:B:151:THR:O	1:B:236:ALA:HA	2.19	0.42
1:C:112:GLY:HA2	1:C:279:ASP:HB2	2.00	0.42
1:C:389:LEU:HB3	1:C:395:VAL:HG21	2.00	0.42
1:D:39:PHE:HB2	1:D:59:PHE:CE2	2.55	0.42
1:D:73:VAL:HG13	1:D:75:MET:HE3	2.01	0.42
1:A:19:ILE:HG12	1:A:308:GLY:HA2	2.01	0.42
1:C:35:ASP:HB3	7:C:615:HOH:O	2.18	0.42
1:A:188:ASP:OD1	1:A:340:THR:HB	2.19	0.42
1:A:319:MET:HE1	1:B:417:MET:HB2	2.01	0.42
1:B:422:PHE:CG	1:B:429:PRO:HA	2.54	0.42
1:C:149:ARG:HH12	1:C:232:GLU:HG2	1.84	0.42
1:D:114:TRP:CG	1:D:115:PRO:HD2	2.54	0.42
1:A:155:ALA:HB2	1:A:177:ALA:HB1	1.98	0.42
1:A:212:VAL:HA	1:A:226:THR:HG22	2.02	0.42
1:B:415:LEU:HD23	1:B:437:ALA:HB2	2.01	0.42
1:D:192:THR:HA	1:D:195:ILE:HD12	2.00	0.42
1:D:215:PHE:HB3	1:D:222:LEU:HD11	2.01	0.42
1:B:378:ASP:HB3	1:B:381:THR:OG1	2.19	0.42
1:B:120:ILE:HG21	1:B:215:PHE:CD2	2.55	0.42
1:B:322:GLN:HG3	1:B:406:ILE:HG21	2.00	0.42
1:C:243:ARG:C	1:C:243:ARG:HD2	2.40	0.42
1:A:149:ARG:HB2	1:A:234:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HB3	1:A:173:VAL:HG21	2.01	0.42
1:A:181:ARG:HH21	1:A:184:ARG:NH2	2.17	0.42
1:A:156:GLY:HA3	3:A:502:NDP:O5B	2.20	0.42
1:B:327:LEU:N	1:B:327:LEU:HD23	2.35	0.42
1:D:121:PRO:HG2	1:D:214:SER:CB	2.50	0.42
1:D:218:SER:O	1:D:221:GLY:N	2.50	0.42
1:A:357:GLU:HA	1:A:371:VAL:O	2.20	0.41
1:B:335:VAL:HB	1:B:399:ALA:HB2	2.02	0.41
1:C:421:LEU:C	1:C:421:LEU:HD12	2.40	0.41
1:A:325:SER:HA	1:B:421:LEU:HB2	2.02	0.41
1:A:213:GLU:CB	1:A:225:LYS:HD3	2.48	0.41
1:A:123:ILE:HD11	1:A:238:LEU:HD11	2.01	0.41
1:B:183:MET:HA	1:B:185:LYS:CE	2.42	0.41
1:C:108:VAL:HG23	1:C:108:VAL:O	2.20	0.41
1:C:212:VAL:HG13	1:C:224:ILE:HG23	2.03	0.41
1:D:16:ILE:HD11	1:D:30:VAL:HG21	2.02	0.41
1:C:250:LYS:HD2	1:C:251:GLY:N	2.34	0.41
1:A:197:GLN:NE2	1:A:201:ASP:OD1	2.46	0.41
1:C:33:ARG:HG3	2:C:501:FAD:C2A	2.51	0.41
1:A:215:PHE:HD2	1:A:224:ILE:HG12	1.86	0.41
1:A:47:TYR:CE2	1:A:141:ILE:HG13	2.56	0.41
1:B:224:ILE:O	1:B:231:TYR:N	2.45	0.41
1:C:158:ILE:HG12	3:C:502:NDP:H5N	2.03	0.41
1:D:120:ILE:HD11	1:D:214:SER:N	2.35	0.41
1:A:129:LYS:HG2	1:A:235:LEU:HD11	1.99	0.41
1:B:138:GLN:O	1:B:142:GLU:HG2	2.21	0.41
1:B:18:GLN:NE2	1:B:309:LYS:HE2	2.35	0.41
1:C:123:ILE:HA	1:C:123:ILE:HD13	1.95	0.41
1:D:156:GLY:HA3	3:D:502:NDP:O2N	2.20	0.41
1:D:427:ASP:HB2	7:D:642:HOH:O	2.18	0.41
1:A:178:ARG:HA	1:A:210:GLU:O	2.21	0.41
1:A:113:SER:HB3	1:A:279:ASP:HB3	2.03	0.41
1:A:7:GLY:O	1:A:110:THR:OG1	2.36	0.41
1:C:240:ILE:HB	3:C:502:NDP:N7A	2.36	0.41
1:D:81:ALA:HA	1:D:248:LEU:HD22	2.02	0.41
1:A:151:THR:HA	1:A:174:THR:O	2.21	0.41
1:A:178:ARG:HG2	3:A:502:NDP:N3A	2.36	0.41
1:C:120:ILE:HG23	1:C:213:GLU:O	2.21	0.41
1:D:73:VAL:HG13	1:D:75:MET:CE	2.49	0.41
1:A:158:ILE:HG13	3:A:502:NDP:PN	2.60	0.41
1:B:266:TYR:CZ	1:B:314:PRO:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:CG	1:C:230:SER:H	2.24	0.41
1:C:440:ALA:O	1:C:444:VAL:HG13	2.20	0.41
1:D:267:MET:HE2	1:D:267:MET:HA	2.02	0.41
1:A:332:ARG:NH1	4:A:503:EDO:O1	2.53	0.41
1:B:157:TYR:O	1:B:161:GLU:HG3	2.21	0.41
1:B:371:VAL:HA	1:B:391:SER:HB2	2.02	0.41
1:C:106:LYS:HD3	1:C:273:ASP:CB	2.49	0.41
1:C:191:PHE:HB3	1:C:390:MET:HE3	2.03	0.41
1:C:87:LYS:HB3	1:C:87:LYS:HE2	1.90	0.41
1:D:393:TYR:O	1:D:395:VAL:HG13	2.21	0.41
1:B:134:TRP:O	1:B:138:GLN:HG3	2.21	0.40
1:C:329:LEU:HB2	1:C:334:ILE:HD11	2.03	0.40
1:A:121:PRO:CG	1:A:214:SER:HB3	2.37	0.40
1:A:288:THR:HG22	1:A:349:LEU:HD11	2.03	0.40
1:C:42:CSO:HD	2:C:501:FAD:HO2'	1.52	0.40
1:C:65:GLU:O	1:C:69:LEU:HD22	2.21	0.40
1:D:127:ARG:NH1	1:D:221:GLY:HA2	2.37	0.40
1:A:175:LEU:HD23	1:A:175:LEU:C	2.42	0.40
1:B:267:MET:CE	1:B:267:MET:HA	2.50	0.40
1:B:441:GLN:O	1:B:444:VAL:HG22	2.21	0.40
1:C:353:GLN:CD	1:C:355:ILE:HD11	2.41	0.40
1:D:213:GLU:OE2	1:D:227:ASP:HB3	2.22	0.40
1:D:371:VAL:HG22	1:D:391:SER:HB2	2.02	0.40
1:D:88:THR:HA	1:D:102:GLU:O	2.20	0.40
1:A:162:LEU:HD13	1:A:237:ILE:HG21	2.03	0.40
1:A:334:ILE:HG23	1:A:390:MET:HE2	2.02	0.40
1:B:443:LYS:HG3	1:B:446:GLN:OE1	2.22	0.40
1:C:166:TYR:O	1:C:171:HIS:HB2	2.21	0.40
1:C:294:ILE:HG22	1:C:294:ILE:O	2.21	0.40
1:D:0:SER:C	1:D:2:LYS:HE3	2.41	0.40
1:B:20:LEU:HD13	1:B:69:LEU:HB2	2.03	0.40
1:C:267:MET:HE2	1:C:303:GLN:HB3	2.03	0.40
1:C:42:CSO:HB2	2:C:501:FAD:N5	2.36	0.40
1:D:174:THR:OG1	1:D:205:GLN:HB3	2.20	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	445/518 (86%)	408 (92%)	36 (8%)	1 (0%)	47	58
1	B	445/518 (86%)	417 (94%)	28 (6%)	0	100	100
1	C	446/518 (86%)	416 (93%)	28 (6%)	2 (0%)	34	42
1	D	447/518 (86%)	413 (92%)	33 (7%)	1 (0%)	47	58
All	All	1783/2072 (86%)	1654 (93%)	125 (7%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	394	ASP
1	D	394	ASP
1	C	227	ASP
1	A	84	PRO

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	373/426 (88%)	355 (95%)	18 (5%)	25	36
1	B	373/426 (88%)	356 (95%)	17 (5%)	27	38
1	C	374/426 (88%)	353 (94%)	21 (6%)	21	29
1	D	375/426 (88%)	359 (96%)	16 (4%)	29	40
All	All	1495/1704 (88%)	1423 (95%)	72 (5%)	25	36

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	46	LEU
1	A	91	VAL
1	A	95	THR
1	A	107	LEU
1	A	126	ASP
1	A	141	ILE
1	A	142	GLU
1	A	143	ASP
1	A	145	LYS
1	A	146	GLU
1	A	157	TYR
1	A	184	ARG
1	A	190	ASP
1	A	205	GLN
1	A	230	SER
1	A	313	LYS
1	A	446	GLN
1	B	35	ASP
1	B	85	ASP
1	B	120	ILE
1	B	124	ASP
1	B	126	ASP
1	B	143	ASP
1	B	157	TYR
1	B	184	ARG
1	B	185	LYS
1	B	190	ASP
1	B	212	VAL
1	B	217	ASP
1	B	239	CYS
1	B	262	ILE
1	B	273	ASP
1	B	294	ILE
1	B	446	GLN
1	C	69	LEU
1	C	74	GLN
1	C	92	GLU
1	C	124	ASP
1	C	146	GLU
1	C	157	TYR
1	C	164	GLU

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Mol	Chain	Res	Type
1	C	167	SER
1	C	184	ARG
1	C	195	ILE
1	C	198	ASP
1	C	216	THR
1	C	232	GLU
1	C	247	ASP
1	C	250	LYS
1	C	254	ASP
1	C	327	LEU
1	C	352	GLU
1	C	353	GLN
1	C	354	VAL
1	C	432	TYR
1	D	85	ASP
1	D	92	GLU
1	D	119	LYS
1	D	124	ASP
1	D	127	ARG
1	D	141	ILE
1	D	185	LYS
1	D	223	THR
1	D	226	THR
1	D	283	VAL
1	D	290	GLN
1	D	327	LEU
1	D	354	VAL
1	D	432	TYR
1	D	444	VAL
1	D	446	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	284	HIS
1	A	408	ASN
1	A	446	GLN
1	B	74	GLN
1	B	410	ASN
1	B	425	ASN
1	C	74	GLN

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Mol	Chain	Res	Type
1	C	350	ASN
1	C	353	GLN
1	D	23	HIS
1	D	229	ASN
1	D	350	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	CSO	C	42	1	3,6,7	0.66	0	0,6,8	0.00	-
1	CSO	D	42	1	3,6,7	0.68	0	0,6,8	0.00	-
1	CSO	A	42	1	3,6,7	0.68	0	0,6,8	0.00	-
1	CSO	B	42	1	3,6,7	0.94	0	0,6,8	0.00	-

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
1	CSO	C	42	1	-	1/1/5/7	-
1	CSO	D	42	1	-	1/1/5/7	-
1	CSO	A	42	1	-	1/1/5/7	-
1	CSO	B	42	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	42	CSO	N-CA-CB-SG
1	D	42	CSO	N-CA-CB-SG
1	A	42	CSO	N-CA-CB-SG
1	B	42	CSO	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	42	CSO	7	0
1	D	42	CSO	2	0
1	A	42	CSO	3	0
1	B	42	CSO	1	0

5.5　Carbohydrates (i)

There are no carbohydrates in this entry.

5.6　Ligand geometry (i)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	EDO	D	504	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.32	0
3	NDP	C	502	-	45,52,52	0.99	2 (4%)	53,80,80	1.26	4 (7%)
3	NDP	D	502	-	45,52,52	1.00	2 (4%)	53,80,80	1.32	5 (9%)
4	EDO	D	503	-	3,3,3	0.45	0	2,2,2	0.34	0
2	FAD	B	501	-	51,58,58	4.31	20 (39%)	60,89,89	2.46	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FAD	A	501	-	51,58,58	4.31	21 (41%)	60,89,89	2.45	15 (25%)
2	FAD	D	501	-	51,58,58	4.30	21 (41%)	60,89,89	2.49	16 (26%)
2	FAD	C	501	-	51,58,58	4.30	20 (39%)	60,89,89	2.48	15 (25%)
4	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.32	0
3	NDP	B	502	-	45,52,52	1.01	2 (4%)	53,80,80	1.23	4 (7%)
4	EDO	C	504	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	C	503	-	3,3,3	0.47	0	2,2,2	0.33	0
5	SO4	A	505	-	4,4,4	0.32	0	6,6,6	0.05	0
4	EDO	A	504	-	3,3,3	0.45	0	2,2,2	0.33	0
3	NDP	A	502	-	45,52,52	1.00	3 (6%)	53,80,80	1.23	4 (7%)

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	EDO	D	504	-	-	0/1/1/1	-
4	EDO	B	503	-	-	1/1/1/1	-
3	NDP	C	502	-	-	5/30/77/77	0/5/5/5
3	NDP	D	502	-	-	6/30/77/77	0/5/5/5
4	EDO	D	503	-	-	0/1/1/1	-
2	FAD	B	501	-	-	5/30/50/50	0/6/6/6
2	FAD	A	501	-	-	2/30/50/50	0/6/6/6
2	FAD	D	501	-	-	4/30/50/50	0/6/6/6
2	FAD	C	501	-	-	1/30/50/50	0/6/6/6
4	EDO	B	504	-	-	0/1/1/1	-
3	NDP	B	502	-	-	6/30/77/77	0/5/5/5
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
3	NDP	A	502	-	-	6/30/77/77	0/5/5/5

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C2B-C1B	-16.15	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C2B-C1B	-16.07	1.29	1.53
2	D	501	FAD	C2B-C1B	-16.06	1.29	1.53
2	C	501	FAD	C2B-C1B	-16.05	1.29	1.53
2	D	501	FAD	O4B-C1B	14.13	1.60	1.41
2	B	501	FAD	O4B-C1B	14.04	1.60	1.41
2	A	501	FAD	O4B-C1B	14.02	1.60	1.41
2	C	501	FAD	O4B-C1B	14.00	1.60	1.41
2	B	501	FAD	C5X-N5	8.23	1.49	1.35
2	C	501	FAD	C5X-N5	8.18	1.48	1.35
2	A	501	FAD	C5X-N5	8.17	1.48	1.35
2	D	501	FAD	C5X-N5	8.10	1.48	1.35
2	A	501	FAD	C10-N1	7.91	1.43	1.33
2	C	501	FAD	C10-N1	7.90	1.43	1.33
2	B	501	FAD	C10-N1	7.87	1.43	1.33
2	D	501	FAD	C10-N1	7.85	1.43	1.33
2	C	501	FAD	O4B-C4B	-7.14	1.29	1.45
2	D	501	FAD	O4B-C4B	-7.10	1.29	1.45
2	A	501	FAD	O4B-C4B	-7.07	1.29	1.45
2	B	501	FAD	O4B-C4B	-7.01	1.29	1.45
2	B	501	FAD	C4X-N5	6.76	1.43	1.33
2	C	501	FAD	C4X-N5	6.71	1.42	1.33
2	D	501	FAD	C4X-N5	6.69	1.42	1.33
2	A	501	FAD	C4X-N5	6.65	1.42	1.33
2	B	501	FAD	C4-N3	5.89	1.43	1.33
2	D	501	FAD	C4-N3	5.83	1.43	1.33
2	A	501	FAD	C4-N3	5.80	1.43	1.33
2	C	501	FAD	C9A-N10	5.79	1.46	1.38
2	C	501	FAD	C4-N3	5.77	1.43	1.33
2	D	501	FAD	C9A-N10	5.76	1.46	1.38
2	A	501	FAD	C9A-N10	5.73	1.46	1.38
2	B	501	FAD	C9A-N10	5.69	1.46	1.38
2	A	501	FAD	C4-C4X	4.87	1.49	1.41
2	D	501	FAD	C4-C4X	4.83	1.49	1.41
2	C	501	FAD	C4-C4X	4.83	1.49	1.41
2	B	501	FAD	C4-C4X	4.81	1.49	1.41
2	A	501	FAD	C4X-C10	4.68	1.43	1.38
2	C	501	FAD	C4X-C10	4.62	1.43	1.38
2	B	501	FAD	C4X-C10	4.56	1.43	1.38
2	D	501	FAD	C4X-C10	4.43	1.43	1.38
2	C	501	FAD	C2-N1	4.43	1.46	1.38
2	A	501	FAD	C2-N1	4.42	1.46	1.38
2	D	501	FAD	C2-N1	4.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	O2B-C2B	4.38	1.53	1.43
2	C	501	FAD	O2B-C2B	4.36	1.53	1.43
2	A	501	FAD	O2B-C2B	4.36	1.53	1.43
2	B	501	FAD	O2B-C2B	4.35	1.53	1.43
2	B	501	FAD	C2-N1	4.35	1.46	1.38
2	C	501	FAD	C2-N3	4.21	1.46	1.38
2	B	501	FAD	C2-N3	4.17	1.46	1.38
2	D	501	FAD	C2-N3	4.17	1.46	1.38
2	A	501	FAD	C2-N3	4.15	1.46	1.38
2	B	501	FAD	O4-C4	-3.68	1.15	1.24
2	A	501	FAD	O4-C4	-3.67	1.15	1.24
2	C	501	FAD	O4-C4	-3.66	1.15	1.24
2	D	501	FAD	O4-C4	-3.65	1.15	1.24
3	B	502	NDP	C6N-C5N	3.56	1.39	1.33
3	A	502	NDP	C6N-C5N	3.53	1.39	1.33
3	D	502	NDP	C6N-C5N	3.44	1.39	1.33
3	C	502	NDP	C6N-C5N	3.44	1.39	1.33
2	B	501	FAD	C6A-N6A	3.30	1.46	1.34
2	A	501	FAD	C6A-N6A	3.29	1.46	1.34
2	C	501	FAD	C6A-N6A	3.29	1.46	1.34
2	D	501	FAD	C6A-N6A	3.28	1.46	1.34
2	C	501	FAD	C2A-N3A	3.25	1.37	1.32
2	B	501	FAD	C2A-N3A	3.24	1.37	1.32
2	A	501	FAD	C2A-N3A	3.22	1.37	1.32
2	D	501	FAD	C2A-N3A	3.21	1.37	1.32
2	D	501	FAD	C8M-C8	3.17	1.57	1.51
2	B	501	FAD	C8M-C8	3.17	1.57	1.51
2	C	501	FAD	C8M-C8	3.16	1.57	1.51
2	A	501	FAD	C8M-C8	3.09	1.57	1.51
2	D	501	FAD	C7M-C7	2.82	1.56	1.51
2	A	501	FAD	C7M-C7	2.77	1.56	1.51
2	B	501	FAD	C7M-C7	2.77	1.56	1.51
2	C	501	FAD	C7M-C7	2.76	1.56	1.51
2	B	501	FAD	O4'-C4'	-2.75	1.37	1.43
2	C	501	FAD	O4'-C4'	-2.75	1.37	1.43
2	D	501	FAD	O4'-C4'	-2.74	1.37	1.43
2	A	501	FAD	O4'-C4'	-2.74	1.37	1.43
3	D	502	NDP	C5A-C4A	2.38	1.47	1.40
3	B	502	NDP	C5A-C4A	2.37	1.47	1.40
3	C	502	NDP	C5A-C4A	2.34	1.47	1.40
3	A	502	NDP	C5A-C4A	2.34	1.47	1.40
2	B	501	FAD	C5'-C4'	2.31	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C5'-C4'	2.31	1.55	1.51
2	C	501	FAD	C5'-C4'	2.19	1.54	1.51
2	D	501	FAD	C5'-C4'	2.07	1.54	1.51
2	A	501	FAD	C2A-N1A	2.06	1.37	1.33
3	A	502	NDP	C2A-N3A	2.03	1.35	1.32
2	D	501	FAD	C2A-N1A	2.01	1.37	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C5A-C6A-N6A	8.71	133.59	120.35
2	B	501	FAD	C5A-C6A-N6A	8.67	133.53	120.35
2	D	501	FAD	C5A-C6A-N6A	8.64	133.48	120.35
2	A	501	FAD	C5A-C6A-N6A	8.45	133.19	120.35
2	D	501	FAD	C7M-C7-C8	7.50	136.11	120.74
2	A	501	FAD	C7M-C7-C8	7.46	136.03	120.74
2	C	501	FAD	C7M-C7-C8	7.38	135.86	120.74
2	B	501	FAD	C7M-C7-C8	7.37	135.84	120.74
2	D	501	FAD	C7M-C7-C6	-6.79	104.10	120.34
2	A	501	FAD	C7M-C7-C6	-6.74	104.22	120.34
2	B	501	FAD	C7M-C7-C6	-6.70	104.31	120.34
2	C	501	FAD	C7M-C7-C6	-6.67	104.39	120.34
2	C	501	FAD	N6A-C6A-N1A	-5.81	106.51	118.57
2	B	501	FAD	N6A-C6A-N1A	-5.80	106.53	118.57
2	D	501	FAD	N6A-C6A-N1A	-5.75	106.64	118.57
2	A	501	FAD	N6A-C6A-N1A	-5.65	106.84	118.57
2	C	501	FAD	N3A-C2A-N1A	-5.49	120.09	128.68
2	A	501	FAD	N3A-C2A-N1A	-5.46	120.14	128.68
2	B	501	FAD	N3A-C2A-N1A	-5.42	120.20	128.68
2	D	501	FAD	N3A-C2A-N1A	-5.39	120.25	128.68
2	D	501	FAD	C4-N3-C2	5.38	119.69	115.14
2	B	501	FAD	C4-N3-C2	5.33	119.64	115.14
2	A	501	FAD	C4-N3-C2	5.30	119.62	115.14
2	C	501	FAD	C4-N3-C2	5.26	119.58	115.14
3	D	502	NDP	PN-O3-PA	-3.91	119.40	132.83
3	D	502	NDP	N3A-C2A-N1A	-3.76	122.80	128.68
3	C	502	NDP	N3A-C2A-N1A	-3.60	123.04	128.68
3	B	502	NDP	N3A-C2A-N1A	-3.57	123.09	128.68
2	B	501	FAD	C1'-N10-C9A	3.52	121.06	118.29
2	D	501	FAD	C4X-N5-C5X	3.50	120.27	116.77
2	A	501	FAD	C1'-N10-C9A	3.45	121.01	118.29
2	C	501	FAD	C1'-N10-C9A	3.45	121.01	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	NDP	N3A-C2A-N1A	-3.40	123.36	128.68
2	B	501	FAD	C5X-C9A-N10	3.39	120.17	117.72
2	C	501	FAD	C5X-C9A-N10	3.39	120.17	117.72
3	C	502	NDP	PN-O3-PA	-3.37	121.28	132.83
3	B	502	NDP	PN-O3-PA	-3.35	121.32	132.83
2	D	501	FAD	C5X-C9A-N10	3.35	120.14	117.72
2	C	501	FAD	C4X-N5-C5X	3.31	120.08	116.77
3	A	502	NDP	PN-O3-PA	-3.29	121.53	132.83
2	A	501	FAD	C5X-C9A-N10	3.28	120.09	117.72
2	D	501	FAD	C1'-N10-C9A	3.27	120.87	118.29
2	B	501	FAD	C4X-N5-C5X	3.22	119.99	116.77
2	D	501	FAD	C3B-C2B-C1B	3.17	105.76	100.98
2	A	501	FAD	C4X-N5-C5X	3.16	119.93	116.77
2	A	501	FAD	C8M-C8-C7	-3.16	114.26	120.74
2	C	501	FAD	C3B-C2B-C1B	3.14	105.70	100.98
2	C	501	FAD	C8M-C8-C7	-3.08	114.42	120.74
2	D	501	FAD	C8M-C8-C7	-3.07	114.44	120.74
2	B	501	FAD	C8M-C8-C7	-2.93	114.72	120.74
3	D	502	NDP	C4A-C5A-N7A	-2.87	106.41	109.40
2	A	501	FAD	P-O3P-PA	-2.77	123.31	132.83
3	C	502	NDP	C3D-C2D-C1D	2.69	106.54	101.43
2	C	501	FAD	P-O3P-PA	-2.69	123.60	132.83
3	C	502	NDP	C4A-C5A-N7A	-2.67	106.62	109.40
2	B	501	FAD	P-O3P-PA	-2.66	123.68	132.83
2	D	501	FAD	C4X-C4-N3	-2.66	119.80	123.43
2	A	501	FAD	C4X-C4-N3	-2.65	119.80	123.43
2	D	501	FAD	P-O3P-PA	-2.64	123.76	132.83
2	B	501	FAD	C4X-C4-N3	-2.59	119.89	123.43
2	C	501	FAD	C4X-C4-N3	-2.58	119.90	123.43
3	A	502	NDP	C4A-C5A-N7A	-2.58	106.72	109.40
3	B	502	NDP	C4A-C5A-N7A	-2.55	106.74	109.40
3	B	502	NDP	C3D-C2D-C1D	2.54	106.25	101.43
3	A	502	NDP	C3D-C2D-C1D	2.46	106.10	101.43
2	A	501	FAD	C3B-C2B-C1B	2.19	104.28	100.98
2	A	501	FAD	C8M-C8-C9	2.17	125.54	120.34
2	D	501	FAD	C4'-C3'-C2'	-2.14	108.91	113.36
2	C	501	FAD	C8M-C8-C9	2.13	125.45	120.34
3	D	502	NDP	O4D-C1D-N1N	2.13	112.22	108.06
2	B	501	FAD	C3B-C2B-C1B	2.12	104.17	100.98
2	D	501	FAD	C8M-C8-C9	2.11	125.40	120.34
2	D	501	FAD	C10-C4X-N5	-2.04	119.85	121.26
2	B	501	FAD	C10-C4X-N5	-2.03	119.85	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	FAD	C10-C4X-N5	-2.02	119.86	121.26
3	D	502	NDP	C2A-N1A-C6A	2.02	122.22	118.75
2	A	501	FAD	C10-C4X-N5	-2.02	119.86	121.26
2	B	501	FAD	C8M-C8-C9	2.02	125.18	120.34

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	NDP	O4B-C4B-C5B-O5B
3	C	502	NDP	O4D-C1D-N1N-C2N
3	B	502	NDP	O4D-C1D-N1N-C2N
3	A	502	NDP	O4B-C4B-C5B-O5B
3	A	502	NDP	C2B-O2B-P2B-O3X
3	A	502	NDP	O4D-C1D-N1N-C2N
3	D	502	NDP	O4D-C1D-N1N-C2N
3	D	502	NDP	O4B-C4B-C5B-O5B
3	B	502	NDP	O4B-C4B-C5B-O5B
3	B	502	NDP	C3B-C4B-C5B-O5B
2	B	501	FAD	C2'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-O4'
3	C	502	NDP	C3B-C4B-C5B-O5B
2	B	501	FAD	C2'-C3'-C4'-C5'
3	A	502	NDP	C3B-C4B-C5B-O5B
2	B	501	FAD	O3'-C3'-C4'-C5'
3	D	502	NDP	C3B-C4B-C5B-O5B
3	C	502	NDP	PA-O3-PN-O1N
3	D	502	NDP	PN-O3-PA-O5B
2	A	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5'-O5'-P-O3P
3	B	502	NDP	C2B-O2B-P2B-O3X
2	D	501	FAD	O4B-C4B-C5B-O5B
3	D	502	NDP	PA-O3-PN-O2N
3	A	502	NDP	PA-O3-PN-O2N
4	C	504	EDO	O1-C1-C2-O2
3	C	502	NDP	PA-O3-PN-O2N
3	D	502	NDP	PA-O3-PN-O1N
3	A	502	NDP	PA-O3-PN-O1N
4	A	504	EDO	O1-C1-C2-O2
4	B	503	EDO	O1-C1-C2-O2
2	D	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	502	NDP	C5B-O5B-PA-O3
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	C5'-O5'-P-O2P
3	B	502	NDP	C5B-O5B-PA-O1A
2	A	501	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

10 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	NDP	9	0
3	D	502	NDP	10	0
2	B	501	FAD	4	0
2	A	501	FAD	6	0
2	D	501	FAD	7	0
2	C	501	FAD	11	0
3	B	502	NDP	10	0
4	A	503	EDO	2	0
4	A	504	EDO	1	0
3	A	502	NDP	15	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 NDP C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP D 502

Bond lengths

Bond angles
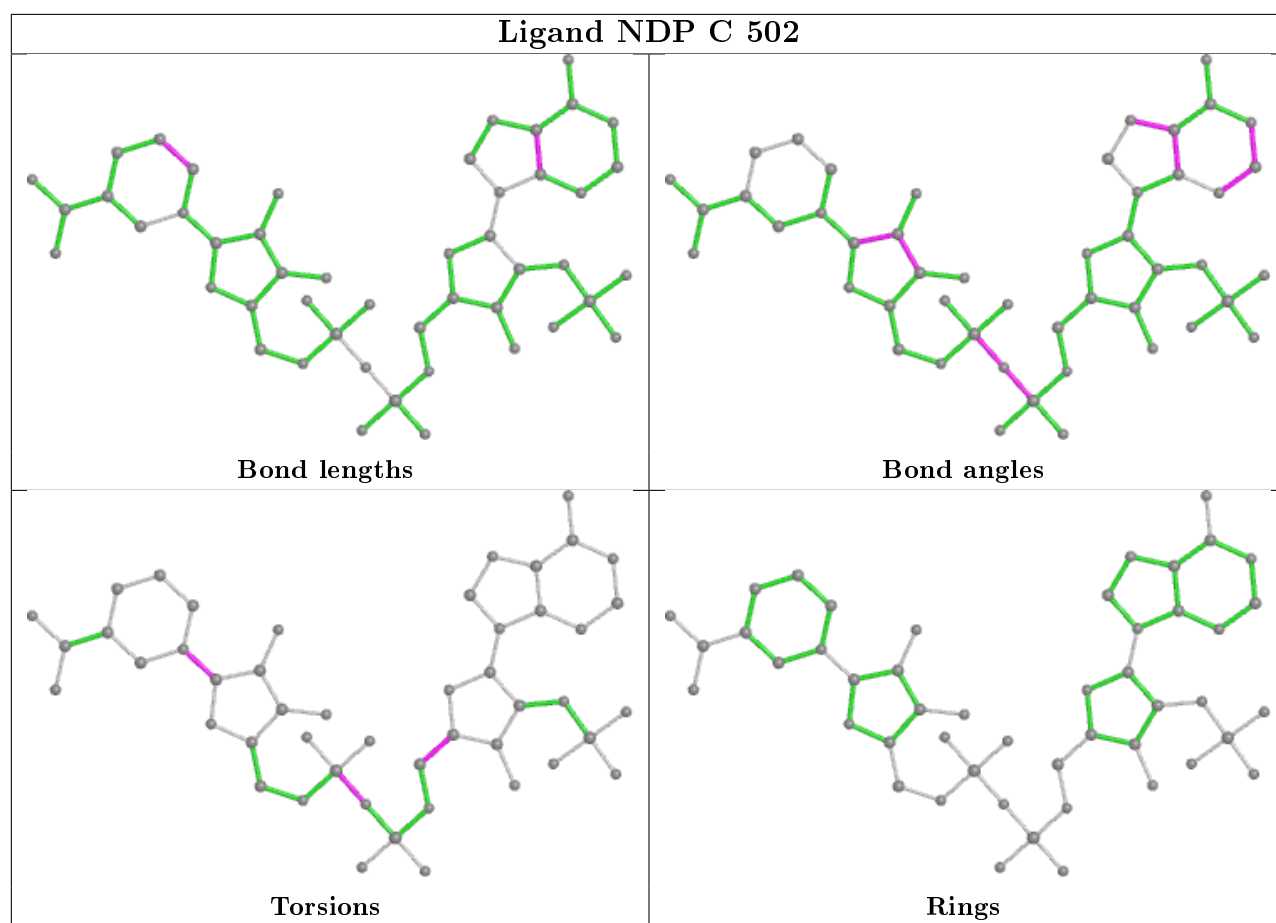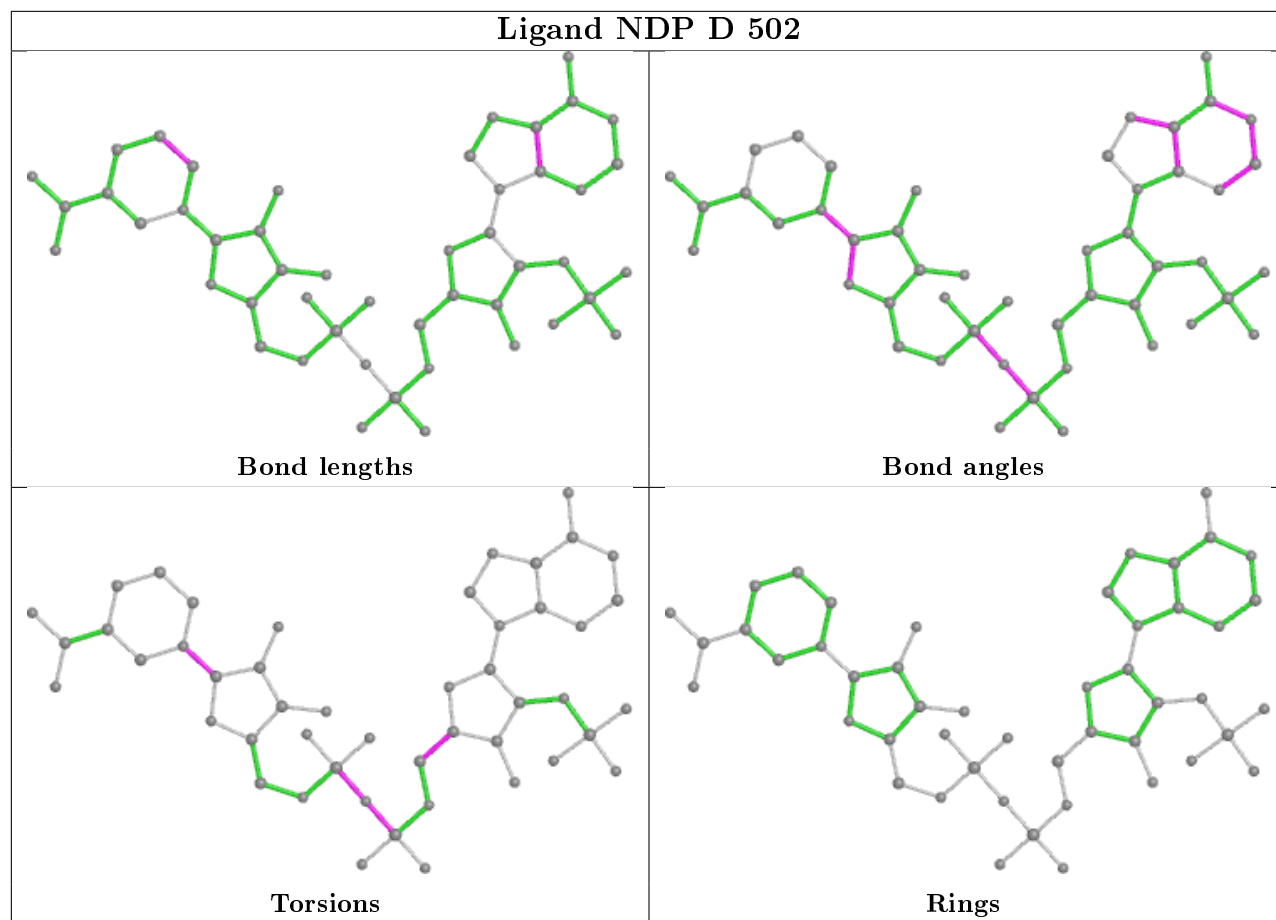
Torsions

Rings

Ligand FAD B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 502

Bond lengths
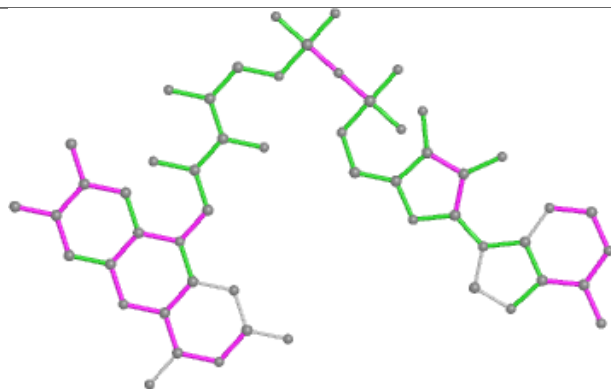
Bond angles
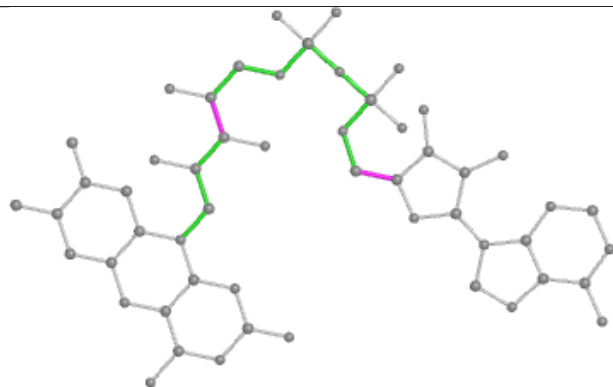
Torsions

Rings
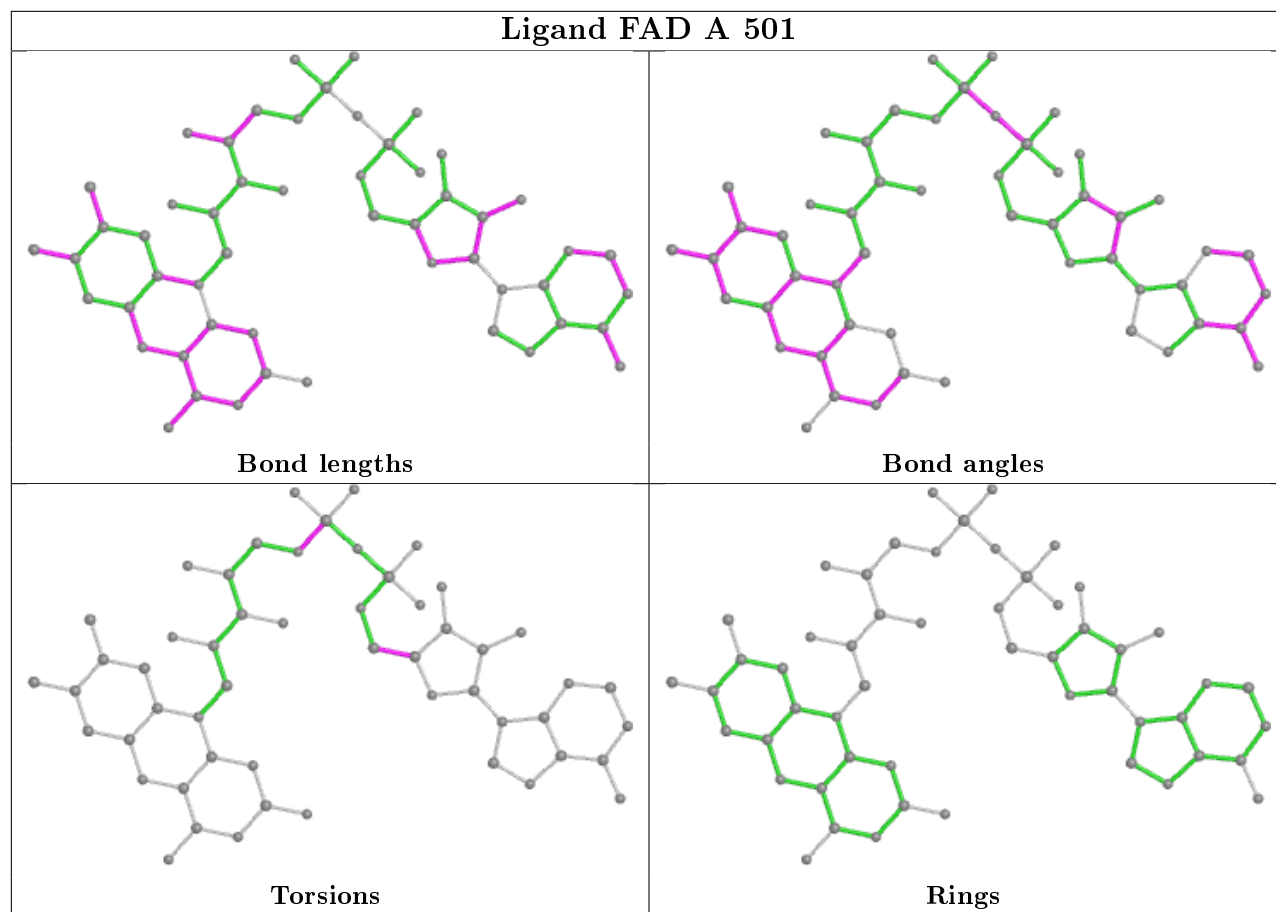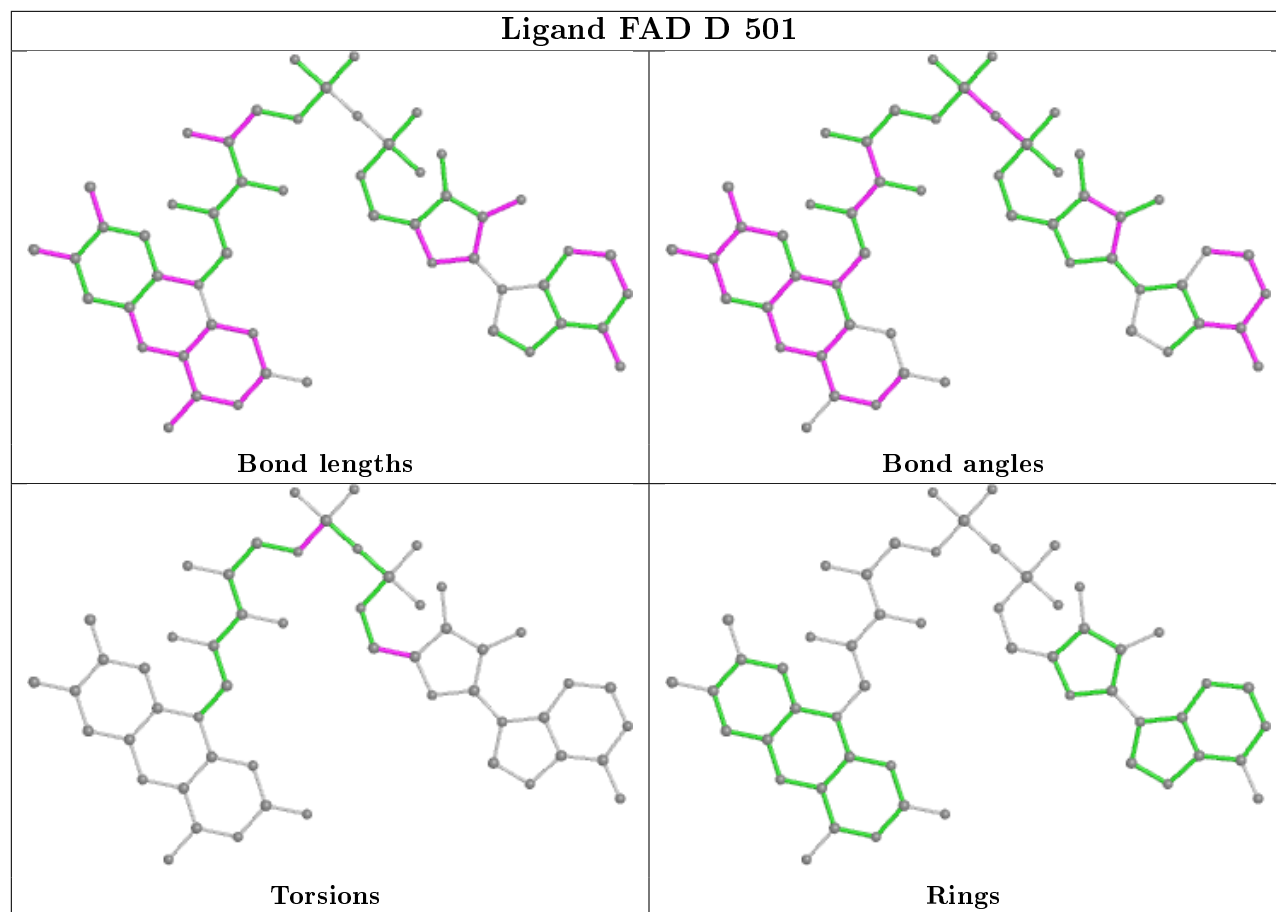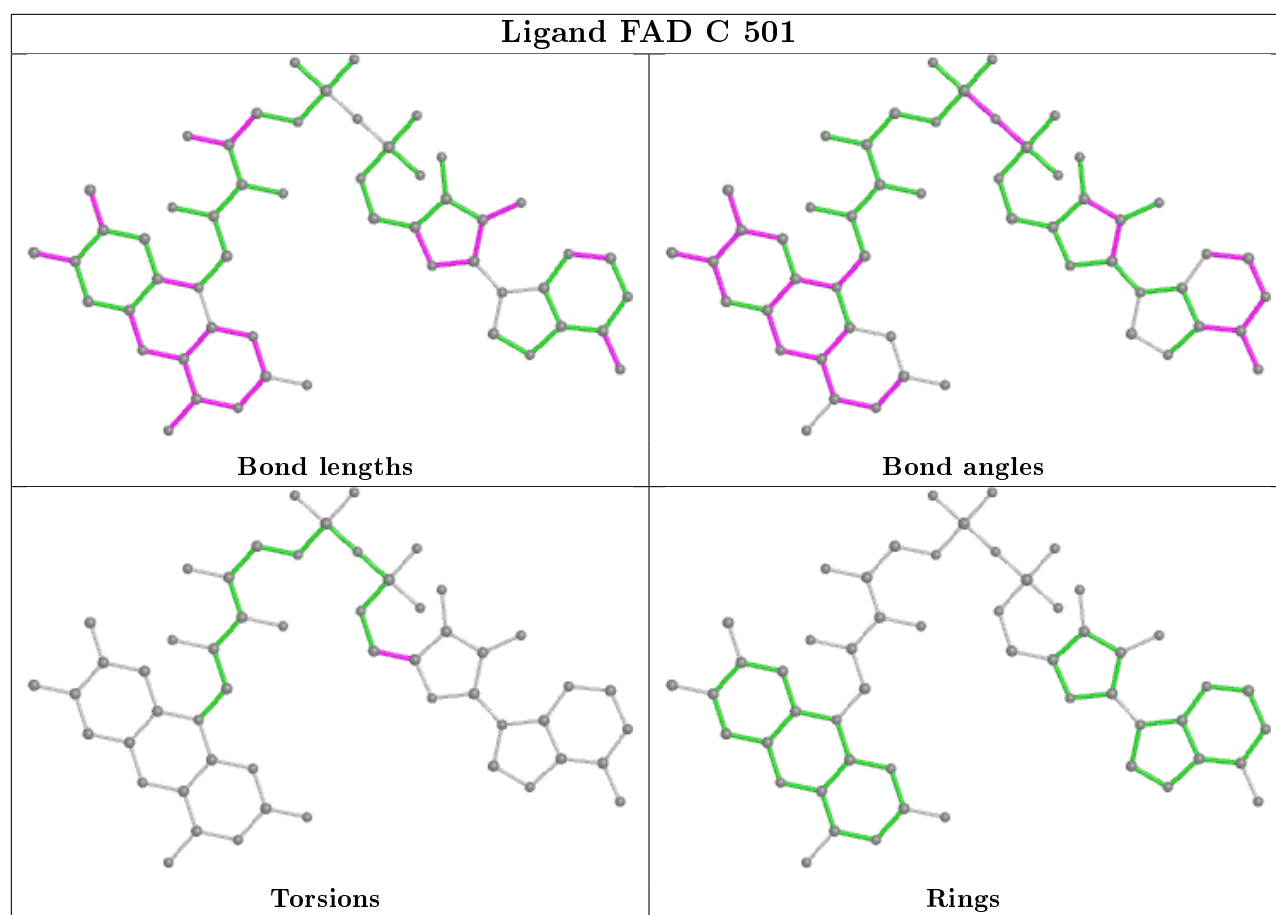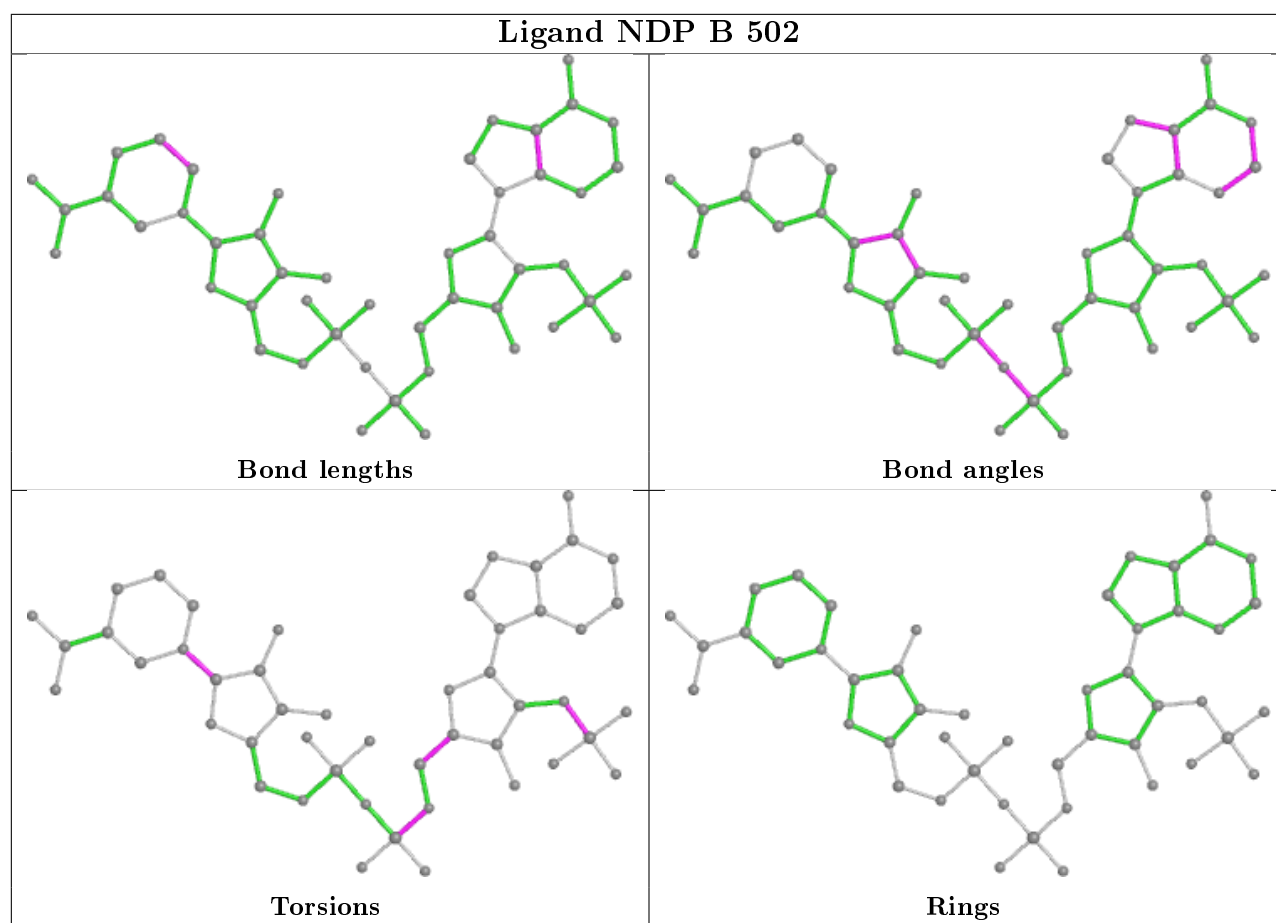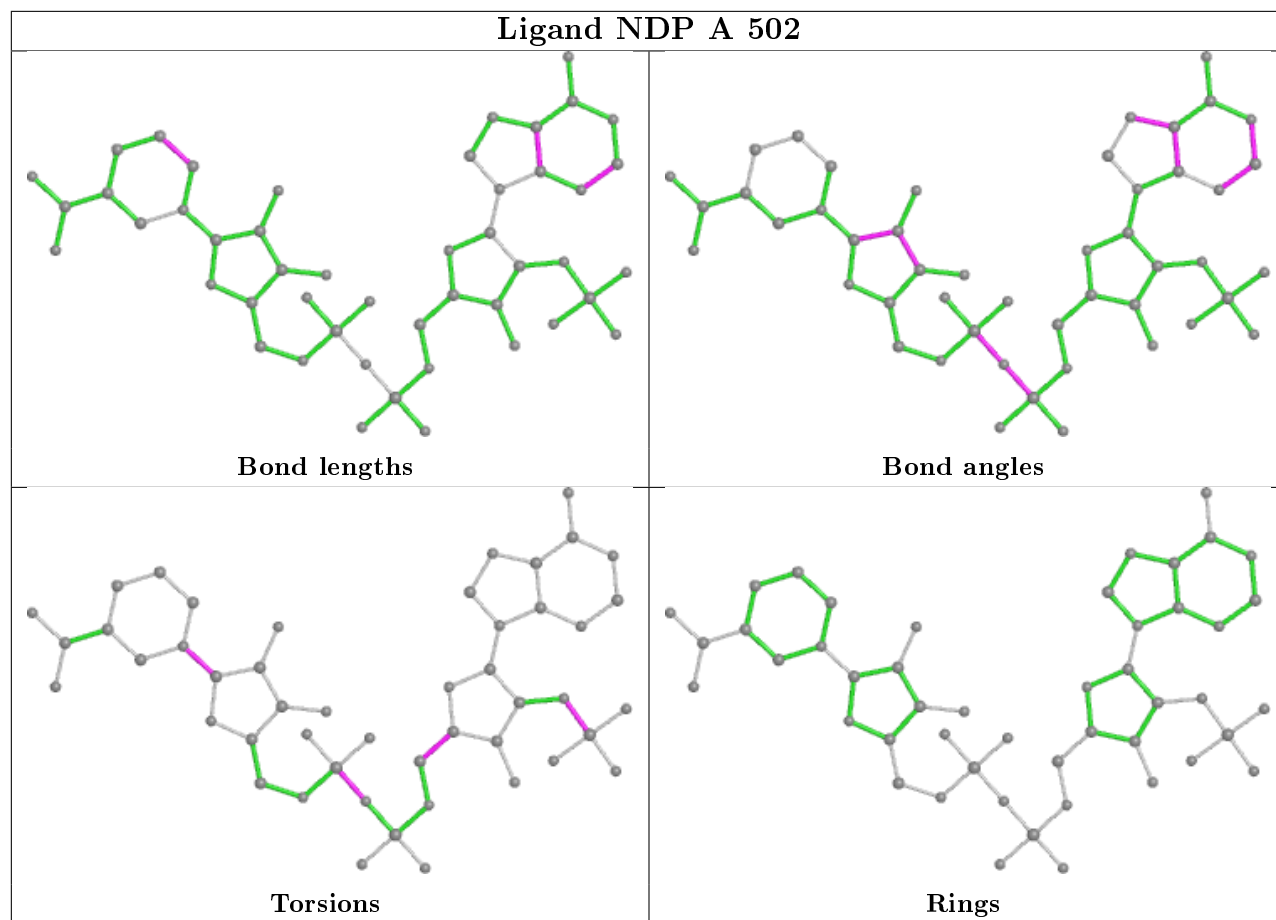
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	447/518 (86%)	0.05	3 (0%)	87	91	23, 37, 52, 68	0
1	B	447/518 (86%)	0.11	6 (1%)	77	81	21, 37, 51, 65	0
1	C	448/518 (86%)	0.17	8 (1%)	68	74	24, 40, 55, 67	0
1	D	449/518 (86%)	0.13	6 (1%)	77	81	25, 37, 52, 67	0
All	All	1791/2072 (86%)	0.12	23 (1%)	77	81	21, 38, 53, 68	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	THR	3.9
1	D	449	ASN	3.8
1	D	47	TYR	3.1
1	C	449	ASN	3.0
1	B	118	PRO	2.9
1	A	146	GLU	2.7
1	C	116	ILE	2.6
1	A	147	ALA	2.6
1	D	25	ASP	2.5
1	B	446	GLN	2.5
1	C	446	GLN	2.5
1	A	117	VAL	2.5
1	B	157	TYR	2.5
1	C	124	ASP	2.5
1	D	446	GLN	2.4
1	D	448	VAL	2.3
1	D	447	SER	2.3
1	C	216	THR	2.2
1	C	117	VAL	2.2
1	C	348	GLY	2.1
1	B	120	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	243	ARG	2.1
1	C	31	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	B	42	7/8	0.81	0.12	28,39,40,50	0
1	CSO	A	42	7/8	0.89	0.13	28,36,39,44	0
1	CSO	C	42	7/8	0.92	0.15	37,43,44,45	0
1	CSO	D	42	7/8	0.93	0.14	29,37,41,45	0

6.3 Carbohydrates (i)

There are no carbohydrates 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	NDP	C	502	48/48	0.76	0.34	44,67,87,94	0
4	EDO	C	503	4/4	0.80	0.15	36,44,51,53	0
3	NDP	A	502	48/48	0.81	0.31	35,61,86,94	0
3	NDP	D	502	48/48	0.81	0.27	36,66,90,95	0
3	NDP	B	502	48/48	0.82	0.32	39,62,82,86	0
6	CL	D	505	1/1	0.89	0.20	76,76,76,76	0
4	EDO	B	503	4/4	0.90	0.18	28,35,42,50	0
4	EDO	A	504	4/4	0.91	0.15	28,44,49,53	0
4	EDO	B	504	4/4	0.91	0.18	32,39,42,42	0
6	CL	A	506	1/1	0.92	0.11	45,45,45,45	0
5	SO4	A	505	5/5	0.92	0.13	48,51,57,57	0
4	EDO	D	504	4/4	0.93	0.21	37,45,56,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	EDO	A	503	4/4	0.93	0.21	35,42,43,43	0
4	EDO	C	504	4/4	0.94	0.15	28,37,40,45	0
2	FAD	C	501	53/53	0.95	0.13	31,42,51,58	0
4	EDO	D	503	4/4	0.95	0.09	34,41,46,47	0
2	FAD	B	501	53/53	0.95	0.12	28,39,50,53	0
2	FAD	A	501	53/53	0.95	0.12	25,36,45,48	0
2	FAD	D	501	53/53	0.95	0.12	26,38,47,50	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.
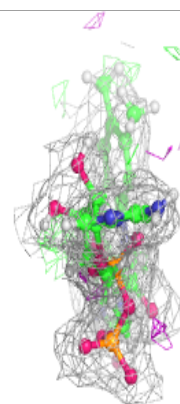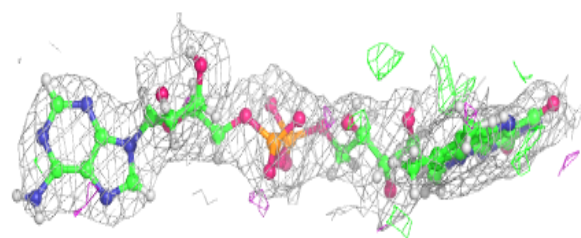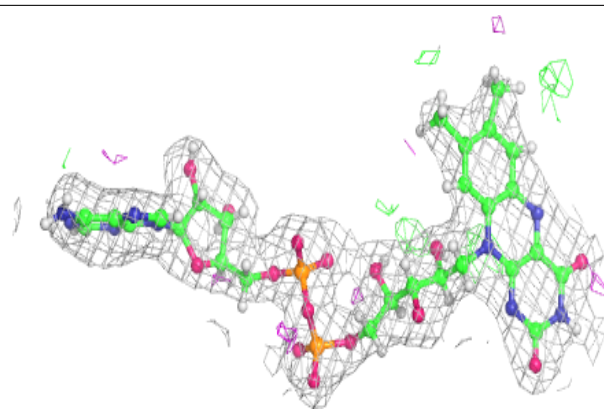

Electron density around NDP C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
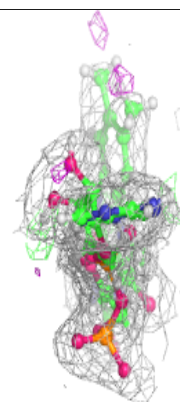mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)
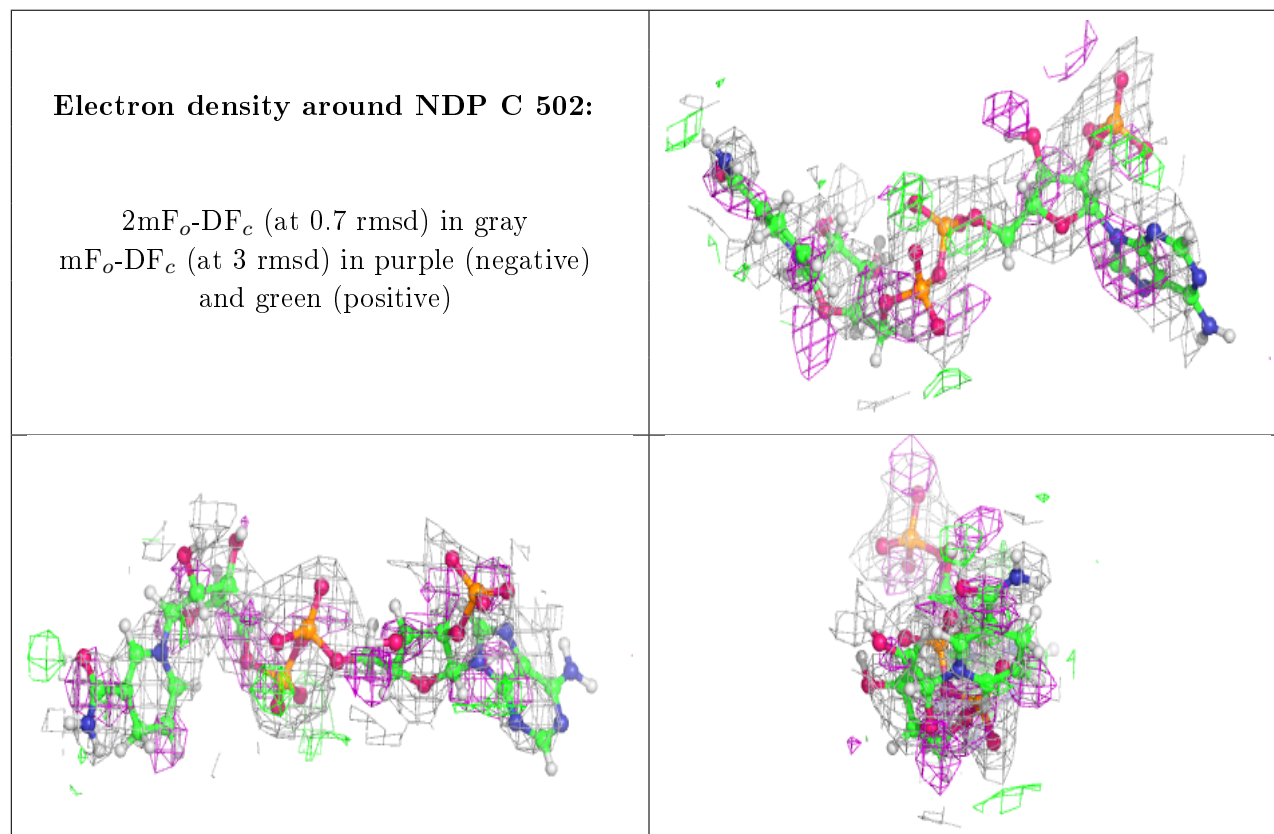
Electron density around NDP A 502:

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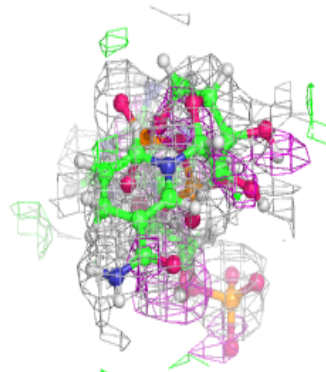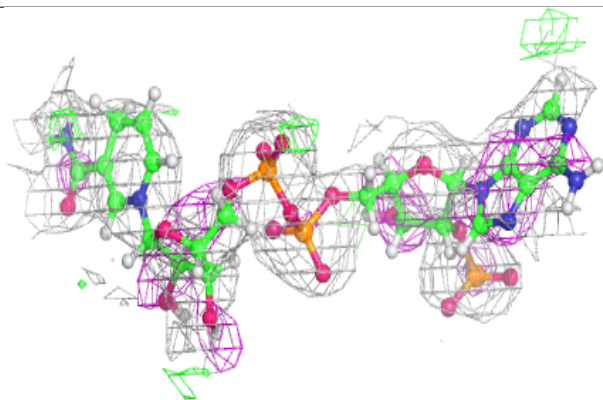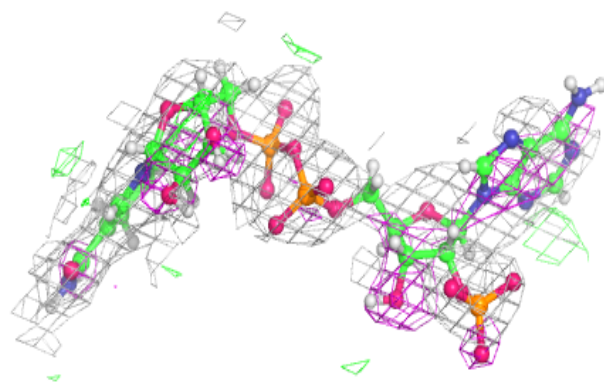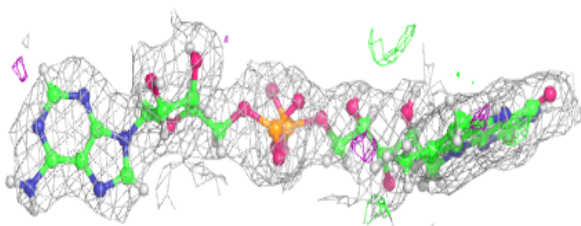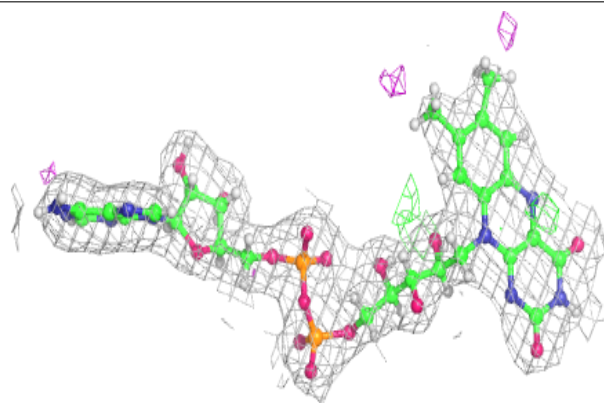

Electron density around NDP D 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
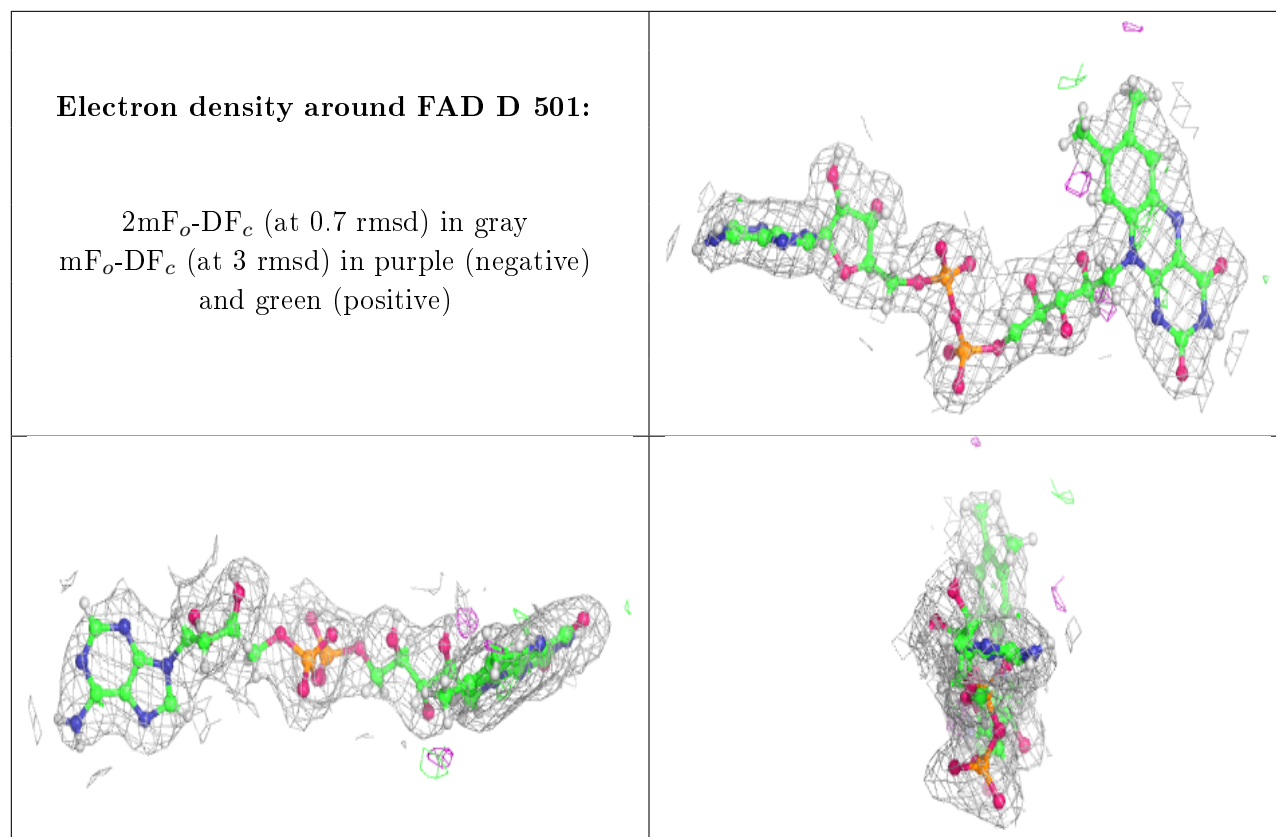mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
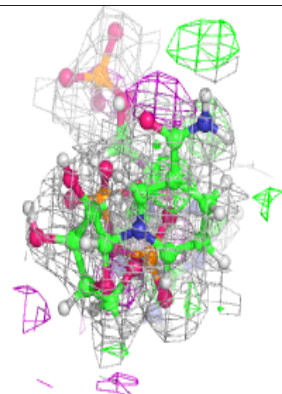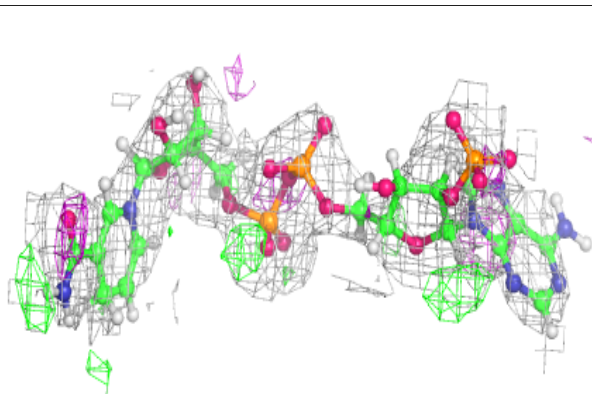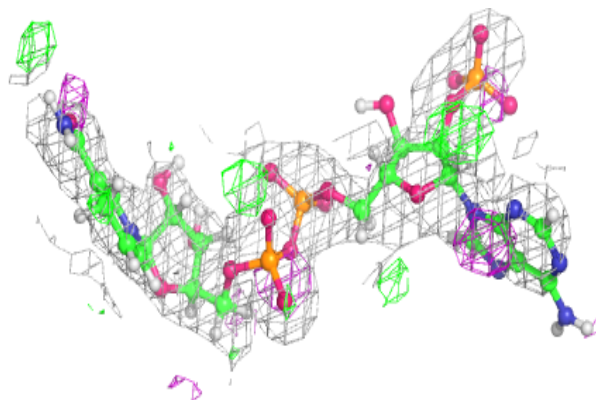
Electron density around NDP B 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
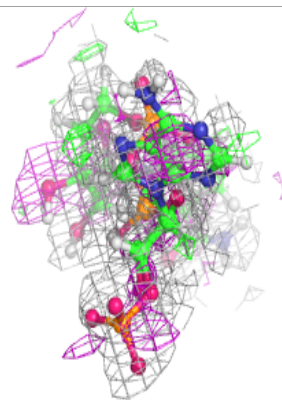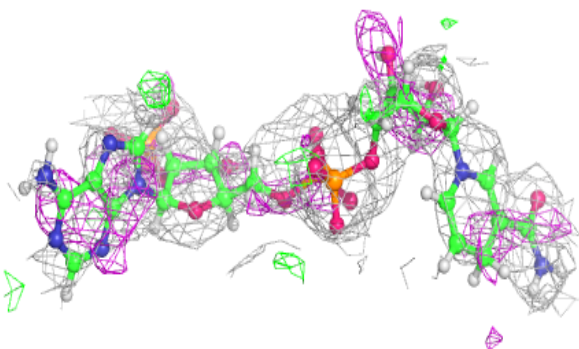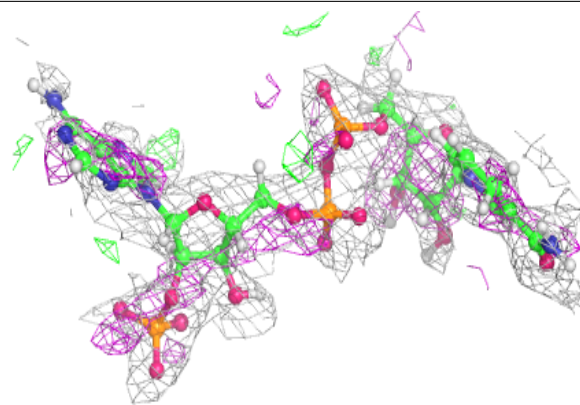
Electron density around FAD C 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
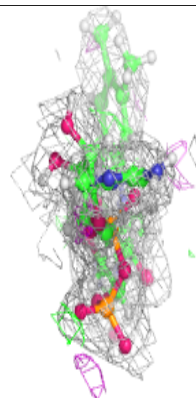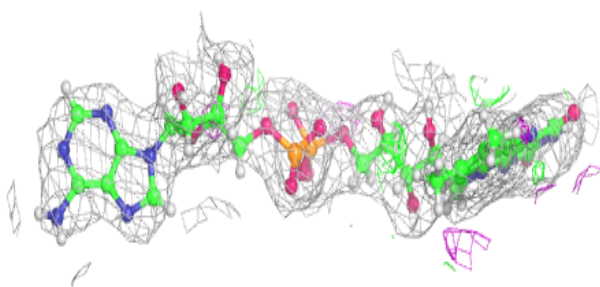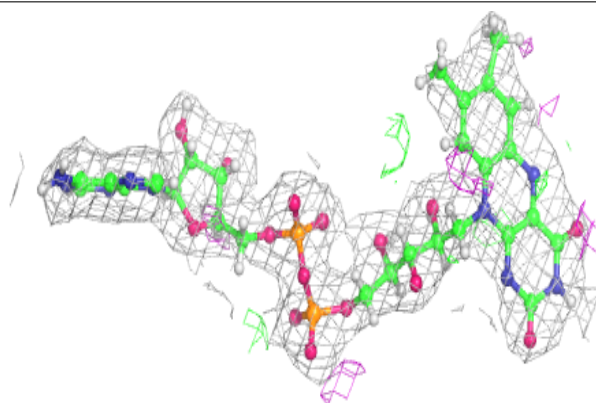
Electron density around FAD B 501:

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

Electron density around FAD A 501:

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

Electron density around FAD D 501:

$2mF_o$-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.