



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 5Z20 / pdb_00005z20
Title : The ternary structure of D-lactate dehydrogenase from *Pseudomonas aeruginosa* with NADH and oxamate
Authors : Furukawa, N.; Miyanaga, A.; Nakajima, M.; Taguchi, H.
Deposited on : 2017-12-28
Resolution : 2.20 Å(reported)

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

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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

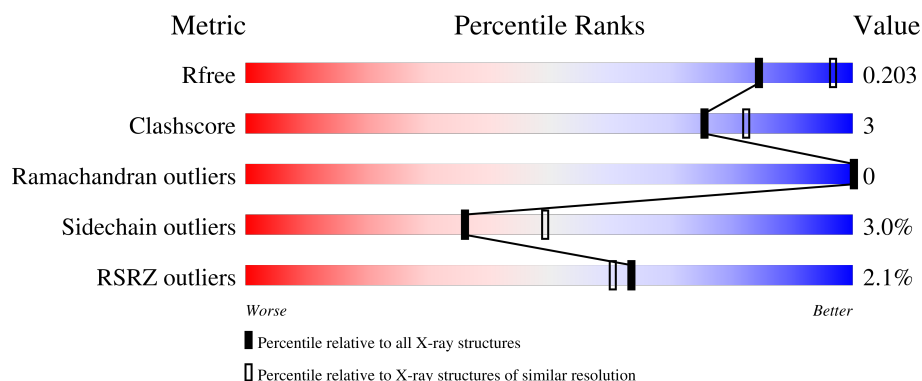
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	345	% 87% 7% . .
1	B	345	3% 86% 9% . .
1	C	345	% 86% 9% . .
1	D	345	% 90% . . 5%
1	E	345	% 86% 8% . .

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Mol	Chain	Length	Quality of chain
1	F	345	5% 86% 10% . .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16588 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 D-lactate dehydrogenase (Fermentative).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2534	1597	461	469	7			
1	B	334	Total	C	N	O	S	0	0	0
			2570	1620	470	473	7			
1	C	330	Total	C	N	O	S	0	0	0
			2534	1597	461	469	7			
1	D	329	Total	C	N	O	S	0	1	0
			2536	1598	462	469	7			
1	E	330	Total	C	N	O	S	0	1	0
			2542	1601	463	471	7			
1	F	336	Total	C	N	O	S	0	1	0
			2598	1636	478	477	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q9I530
A	-14	ASN	-	expression tag	UNP Q9I530
A	-13	HIS	-	expression tag	UNP Q9I530
A	-12	LYS	-	expression tag	UNP Q9I530
A	-11	VAL	-	expression tag	UNP Q9I530
A	-10	HIS	-	expression tag	UNP Q9I530
A	-9	HIS	-	expression tag	UNP Q9I530
A	-8	HIS	-	expression tag	UNP Q9I530
A	-7	HIS	-	expression tag	UNP Q9I530
A	-6	HIS	-	expression tag	UNP Q9I530
A	-5	HIS	-	expression tag	UNP Q9I530
A	-4	ILE	-	expression tag	UNP Q9I530
A	-3	GLU	-	expression tag	UNP Q9I530
A	-2	GLY	-	expression tag	UNP Q9I530
A	-1	ARG	-	expression tag	UNP Q9I530
A	0	HIS	-	expression tag	UNP Q9I530
B	-15	MET	-	expression tag	UNP Q9I530

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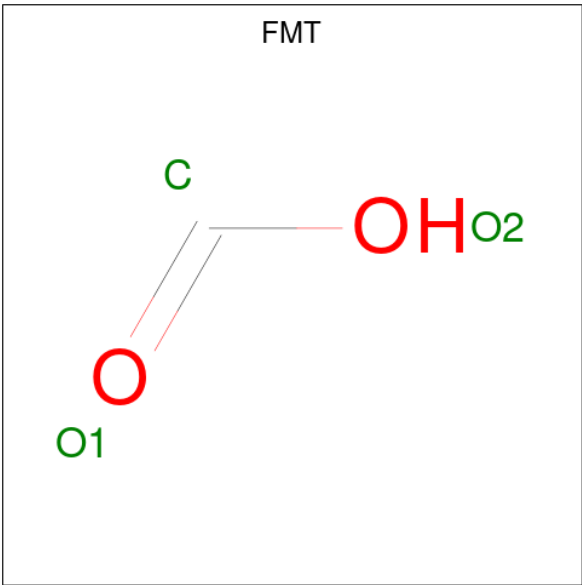
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B	-14	ASN	-	expression tag	UNP Q9I530
B	-13	HIS	-	expression tag	UNP Q9I530
B	-12	LYS	-	expression tag	UNP Q9I530
B	-11	VAL	-	expression tag	UNP Q9I530
B	-10	HIS	-	expression tag	UNP Q9I530
B	-9	HIS	-	expression tag	UNP Q9I530
B	-8	HIS	-	expression tag	UNP Q9I530
B	-7	HIS	-	expression tag	UNP Q9I530
B	-6	HIS	-	expression tag	UNP Q9I530
B	-5	HIS	-	expression tag	UNP Q9I530
B	-4	ILE	-	expression tag	UNP Q9I530
B	-3	GLU	-	expression tag	UNP Q9I530
B	-2	GLY	-	expression tag	UNP Q9I530
B	-1	ARG	-	expression tag	UNP Q9I530
B	0	HIS	-	expression tag	UNP Q9I530
C	-15	MET	-	expression tag	UNP Q9I530
C	-14	ASN	-	expression tag	UNP Q9I530
C	-13	HIS	-	expression tag	UNP Q9I530
C	-12	LYS	-	expression tag	UNP Q9I530
C	-11	VAL	-	expression tag	UNP Q9I530
C	-10	HIS	-	expression tag	UNP Q9I530
C	-9	HIS	-	expression tag	UNP Q9I530
C	-8	HIS	-	expression tag	UNP Q9I530
C	-7	HIS	-	expression tag	UNP Q9I530
C	-6	HIS	-	expression tag	UNP Q9I530
C	-5	HIS	-	expression tag	UNP Q9I530
C	-4	ILE	-	expression tag	UNP Q9I530
C	-3	GLU	-	expression tag	UNP Q9I530
C	-2	GLY	-	expression tag	UNP Q9I530
C	-1	ARG	-	expression tag	UNP Q9I530
C	0	HIS	-	expression tag	UNP Q9I530
D	-15	MET	-	expression tag	UNP Q9I530
D	-14	ASN	-	expression tag	UNP Q9I530
D	-13	HIS	-	expression tag	UNP Q9I530
D	-12	LYS	-	expression tag	UNP Q9I530
D	-11	VAL	-	expression tag	UNP Q9I530
D	-10	HIS	-	expression tag	UNP Q9I530
D	-9	HIS	-	expression tag	UNP Q9I530
D	-8	HIS	-	expression tag	UNP Q9I530
D	-7	HIS	-	expression tag	UNP Q9I530
D	-6	HIS	-	expression tag	UNP Q9I530
D	-5	HIS	-	expression tag	UNP Q9I530

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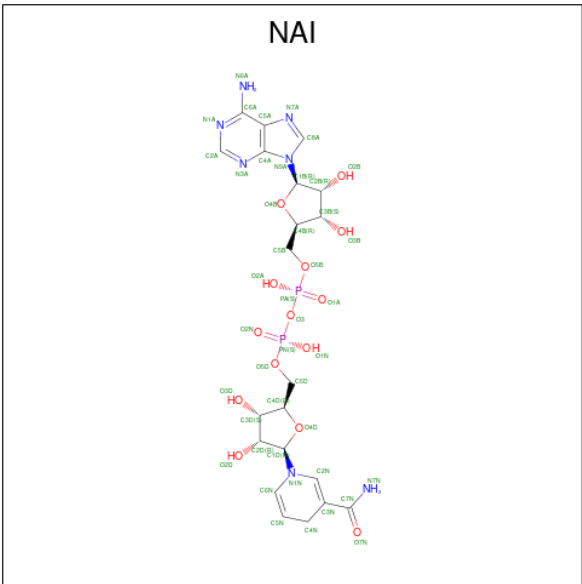
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ILE	-	expression tag	UNP Q9I530
D	-3	GLU	-	expression tag	UNP Q9I530
D	-2	GLY	-	expression tag	UNP Q9I530
D	-1	ARG	-	expression tag	UNP Q9I530
D	0	HIS	-	expression tag	UNP Q9I530
E	-15	MET	-	expression tag	UNP Q9I530
E	-14	ASN	-	expression tag	UNP Q9I530
E	-13	HIS	-	expression tag	UNP Q9I530
E	-12	LYS	-	expression tag	UNP Q9I530
E	-11	VAL	-	expression tag	UNP Q9I530
E	-10	HIS	-	expression tag	UNP Q9I530
E	-9	HIS	-	expression tag	UNP Q9I530
E	-8	HIS	-	expression tag	UNP Q9I530
E	-7	HIS	-	expression tag	UNP Q9I530
E	-6	HIS	-	expression tag	UNP Q9I530
E	-5	HIS	-	expression tag	UNP Q9I530
E	-4	ILE	-	expression tag	UNP Q9I530
E	-3	GLU	-	expression tag	UNP Q9I530
E	-2	GLY	-	expression tag	UNP Q9I530
E	-1	ARG	-	expression tag	UNP Q9I530
E	0	HIS	-	expression tag	UNP Q9I530
F	-15	MET	-	expression tag	UNP Q9I530
F	-14	ASN	-	expression tag	UNP Q9I530
F	-13	HIS	-	expression tag	UNP Q9I530
F	-12	LYS	-	expression tag	UNP Q9I530
F	-11	VAL	-	expression tag	UNP Q9I530
F	-10	HIS	-	expression tag	UNP Q9I530
F	-9	HIS	-	expression tag	UNP Q9I530
F	-8	HIS	-	expression tag	UNP Q9I530
F	-7	HIS	-	expression tag	UNP Q9I530
F	-6	HIS	-	expression tag	UNP Q9I530
F	-5	HIS	-	expression tag	UNP Q9I530
F	-4	ILE	-	expression tag	UNP Q9I530
F	-3	GLU	-	expression tag	UNP Q9I530
F	-2	GLY	-	expression tag	UNP Q9I530
F	-1	ARG	-	expression tag	UNP Q9I530
F	0	HIS	-	expression tag	UNP Q9I530

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



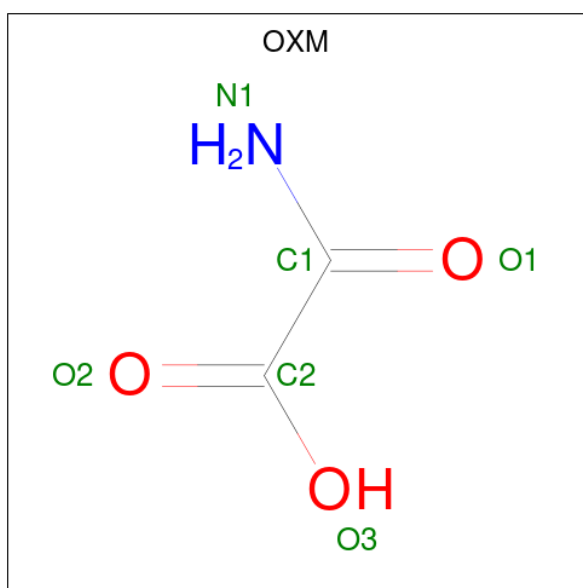
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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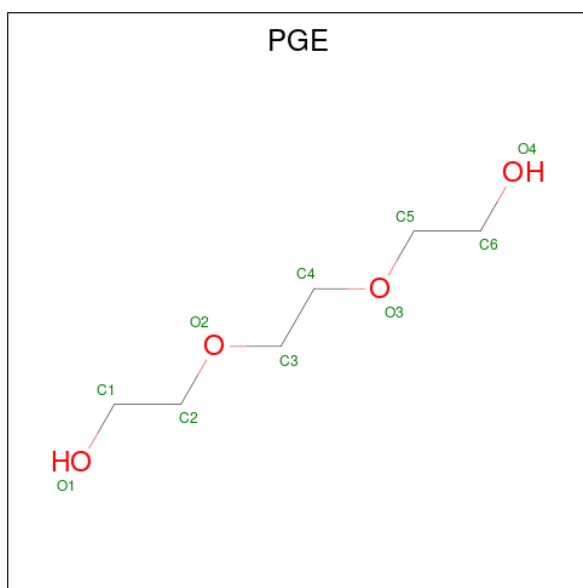
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



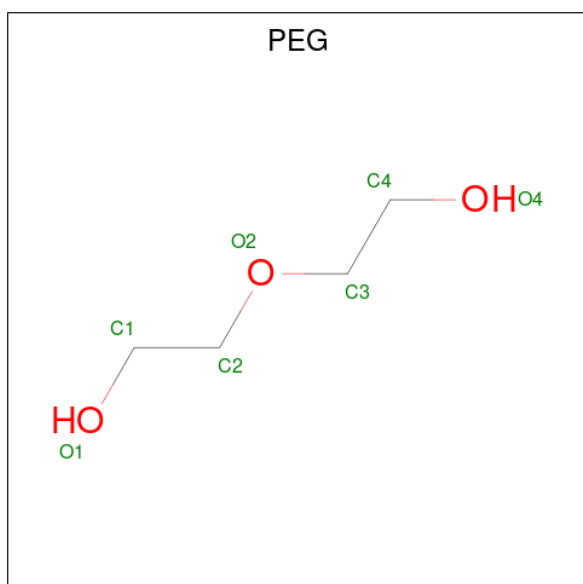
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	2	1	3		
4	B	1	Total	C	N	O	0	0
			6	2	1	3		
4	C	1	Total	C	N	O	0	0
			6	2	1	3		
4	D	1	Total	C	N	O	0	0
			6	2	1	3		
4	E	1	Total	C	N	O	0	0
			6	2	1	3		
4	F	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



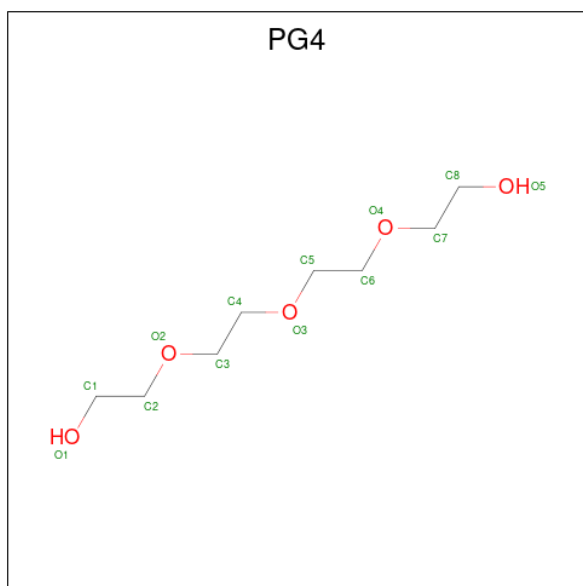
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			13	8	5		

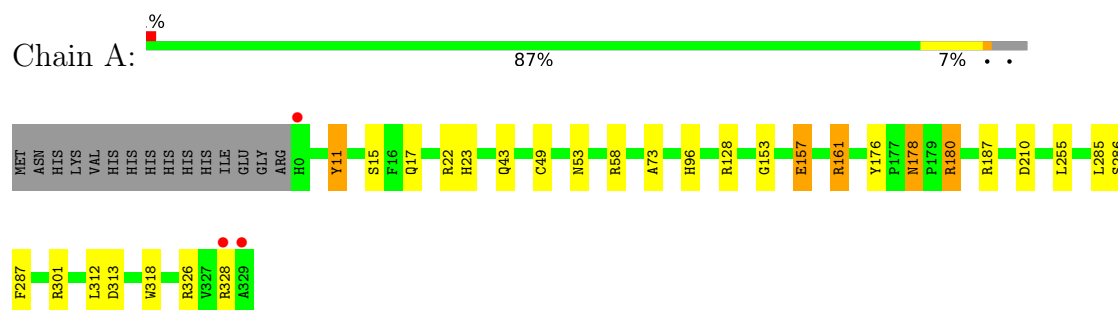
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	218	Total	O	0	0
			218	218		
8	B	144	Total	O	0	0
			144	144		
8	C	160	Total	O	0	0
			160	160		
8	D	157	Total	O	0	0
			157	157		
8	E	130	Total	O	0	0
			130	130		
8	F	99	Total	O	0	0
			99	99		

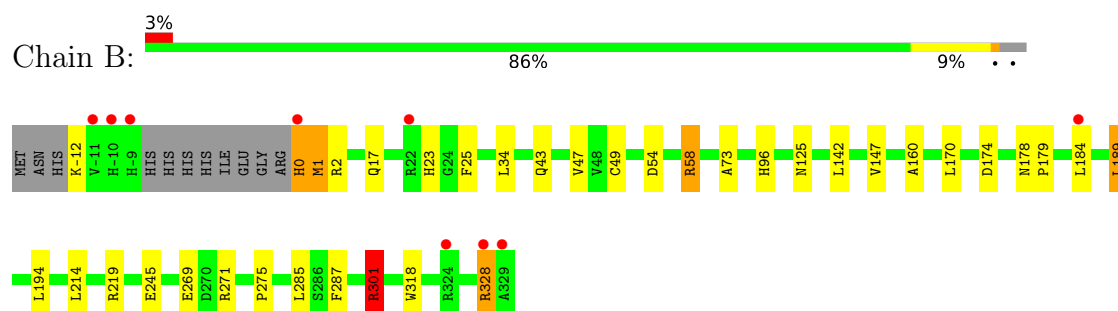
3 Residue-property plots [i](#)

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.

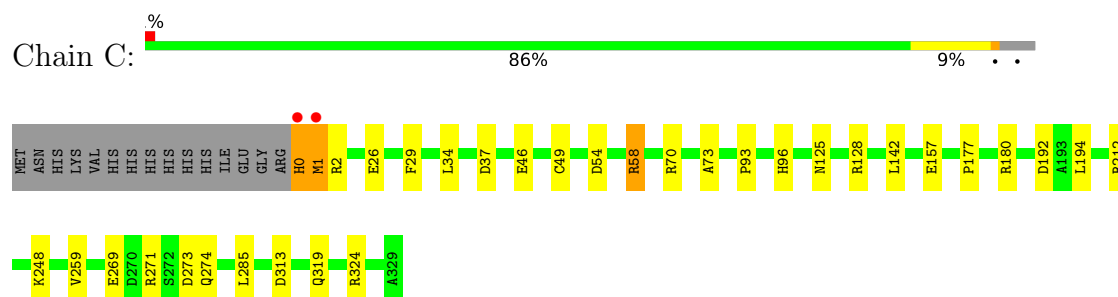
- Molecule 1: D-lactate dehydrogenase (Fermentative)



- Molecule 1: D-lactate dehydrogenase (Fermentative)

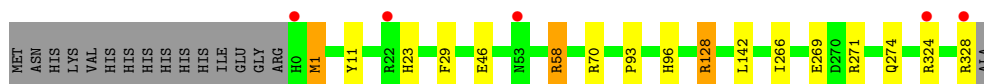


- Molecule 1: D-lactate dehydrogenase (Fermentative)

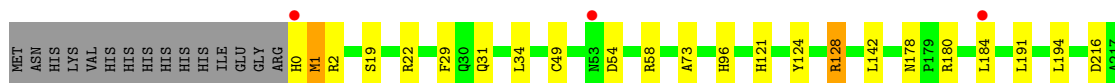
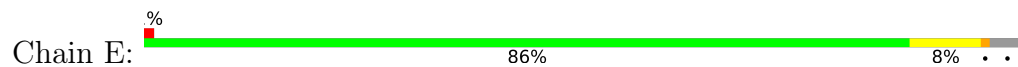


- Molecule 1: D-lactate dehydrogenase (Fermentative)

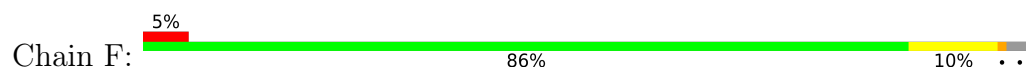




- Molecule 1: D-lactate dehydrogenase (Fermentative)



- Molecule 1: D-lactate dehydrogenase (Fermentative)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.69Å 155.69Å 230.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.40 – 2.20 37.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.40-2.20) 98.8 (37.40-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.171 , 0.199 0.179 , 0.203	Depositor DCC
R_{free} test set	8194 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16588	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: PEG, NAI, FMT, PGE, OXM, PG4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.43	17/2586 (0.7%)	1.05	4/3514 (0.1%)
1	B	1.34	13/2623 (0.5%)	1.00	1/3562 (0.0%)
1	C	1.30	11/2586 (0.4%)	0.99	2/3514 (0.1%)
1	D	1.30	9/2588 (0.3%)	0.99	1/3518 (0.0%)
1	E	1.27	9/2594 (0.3%)	0.97	2/3525 (0.1%)
1	F	1.23	9/2653 (0.3%)	0.97	1/3603 (0.0%)
All	All	1.31	68/15630 (0.4%)	1.00	11/21236 (0.1%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	121	HIS	CG-ND1	-7.69	1.29	1.38
1	A	176	TYR	C-O	-7.62	1.15	1.24
1	A	58	ARG	C-O	-7.60	1.17	1.24
1	A	285	LEU	C-O	-7.37	1.14	1.24
1	E	58	ARG	C-O	-6.89	1.17	1.24
1	A	96	HIS	CG-ND1	-6.86	1.30	1.38
1	C	248	LYS	C-O	-6.70	1.16	1.24
1	C	58	ARG	C-O	-6.41	1.18	1.24
1	A	286	SER	C-O	-6.40	1.15	1.24
1	B	287	PHE	CA-C	6.40	1.61	1.53
1	B	23	HIS	CG-ND1	-6.36	1.31	1.38
1	D	23	HIS	CD2-NE2	-6.21	1.31	1.37
1	C	125	ASN	C-O	-6.20	1.16	1.24
1	B	301	ARG	C-O	-6.18	1.16	1.24
1	B	96	HIS	CG-ND1	-6.18	1.31	1.38
1	C	274	GLN	C-O	-6.12	1.17	1.24
1	B	58	ARG	C-O	-6.11	1.18	1.24
1	E	274	GLN	C-O	-6.10	1.17	1.24
1	F	58	ARG	C-O	-6.10	1.18	1.24
1	D	96	HIS	CG-ND1	-6.03	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLU	C-O	-6.00	1.16	1.24
1	A	326	ARG	C-O	-5.99	1.16	1.23
1	B	245	GLU	N-CA	5.97	1.53	1.46
1	C	128	ARG	C-O	-5.92	1.16	1.24
1	B	23	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	17	GLN	C-O	-5.90	1.16	1.24
1	A	96	HIS	CD2-NE2	-5.83	1.31	1.37
1	C	96	HIS	CG-ND1	-5.81	1.31	1.38
1	F	318	TRP	NE1-CE2	-5.80	1.31	1.37
1	D	128	ARG	C-O	-5.78	1.16	1.24
1	E	29	PHE	C-O	-5.78	1.17	1.24
1	F	274	GLN	C-O	-5.76	1.18	1.24
1	C	285	LEU	C-O	-5.75	1.16	1.24
1	F	96	HIS	CG-ND1	-5.75	1.31	1.38
1	A	178	ASN	C-O	-5.71	1.18	1.25
1	F	103	HIS	CG-ND1	-5.71	1.31	1.38
1	A	53	ASN	C-O	-5.71	1.16	1.24
1	B	147	VAL	N-CA	-5.70	1.39	1.46
1	A	187	ARG	N-CA	-5.61	1.39	1.46
1	C	273	ASP	C-O	-5.59	1.16	1.24
1	D	23	HIS	CG-ND1	-5.59	1.32	1.38
1	D	96	HIS	CD2-NE2	-5.57	1.31	1.37
1	D	58	ARG	C-O	-5.55	1.19	1.24
1	A	318	TRP	NE1-CE2	-5.50	1.31	1.37
1	B	275	PRO	N-CA	-5.46	1.40	1.47
1	A	161	ARG	C-O	-5.42	1.17	1.24
1	A	255	LEU	N-CA	-5.40	1.39	1.46
1	C	177	PRO	C-O	-5.34	1.17	1.23
1	D	29	PHE	C-O	-5.34	1.17	1.24
1	B	96	HIS	CD2-NE2	-5.30	1.32	1.37
1	D	11	TYR	C-O	-5.28	1.17	1.24
1	B	125	ASN	CA-C	-5.27	1.45	1.52
1	E	270	ASP	C-O	-5.21	1.17	1.23
1	E	121	HIS	CD2-NE2	-5.20	1.32	1.37
1	D	274	GLN	C-O	-5.18	1.18	1.24
1	C	259	VAL	N-CA	-5.17	1.40	1.46
1	E	96	HIS	CG-ND1	-5.17	1.32	1.38
1	B	318	TRP	NE1-CE2	-5.14	1.31	1.37
1	E	249	SER	C-O	-5.13	1.17	1.24
1	F	21	HIS	CG-ND1	-5.12	1.32	1.38
1	A	11	TYR	C-O	-5.08	1.17	1.24
1	C	29	PHE	C-O	-5.07	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LEU	C-O	-5.04	1.17	1.24
1	E	31	GLN	C-O	-5.03	1.17	1.24
1	F	177	PRO	C-O	-5.03	1.17	1.23
1	A	328	ARG	N-CA	5.02	1.52	1.46
1	F	-6	HIS	CG-ND1	-5.02	1.32	1.38
1	F	-9	HIS	CG-ND1	-5.01	1.32	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	266	ILE	N-CA-CB	-7.30	105.65	111.64
1	B	1	MET	N-CA-C	6.41	118.73	108.41
1	A	176	TYR	N-CA-C	5.98	118.97	109.40
1	C	37	ASP	N-CA-C	5.53	119.28	112.54
1	C	96	HIS	N-CA-C	5.50	116.33	108.74
1	A	287	PHE	CA-C-N	5.49	125.10	119.56
1	A	287	PHE	C-N-CA	5.49	125.10	119.56
1	A	96	HIS	N-CA-C	5.32	116.35	108.86
1	E	96	HIS	N-CA-C	5.07	115.73	108.74
1	F	327	VAL	CB-CA-C	-5.02	103.17	110.81
1	D	266	ILE	N-CA-C	5.01	116.33	112.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2534	0	2497	9	0
1	B	2570	0	2535	19	0
1	C	2534	0	2497	16	0
1	D	2536	0	2497	4	0
1	E	2542	0	2502	22	0
1	F	2598	0	2554	17	0
2	A	3	0	1	0	0
2	D	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	27	2	0
3	B	44	0	27	2	0
3	C	44	0	27	1	0
3	D	44	0	27	1	0
3	E	44	0	27	1	0
3	F	44	0	27	1	0
4	A	6	0	2	1	0
4	B	6	0	2	1	0
4	C	6	0	2	1	0
4	D	6	0	2	1	0
4	E	6	0	2	1	0
4	F	6	0	2	1	0
5	A	10	0	14	0	0
5	C	10	0	14	1	0
5	D	10	0	14	0	0
5	F	10	0	14	0	0
6	A	7	0	10	0	0
7	E	13	0	18	0	0
8	A	218	0	0	1	0
8	B	144	0	0	1	0
8	C	160	0	0	5	0
8	D	157	0	0	1	0
8	E	130	0	0	3	0
8	F	99	0	0	2	0
All	All	16588	0	15342	94	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 3.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HE1	1:E:318:TRP:HZ3	1.21	1.03
1:E:1:MET:HE1	1:E:318:TRP:CZ3	2.04	0.92
1:B:328:ARG:HH11	1:B:328:ARG:HG3	1.36	0.90
1:D:1:MET:HE1	1:D:46:GLU:OE1	1.72	0.89
1:E:328:ARG:HH11	1:E:328:ARG:CB	1.89	0.86
1:B:184:LEU:O	1:B:184:LEU:HD13	1.79	0.82
1:E:1:MET:CE	1:E:318:TRP:HZ3	1.96	0.78
1:C:313:ASP:HB3	1:C:324:ARG:HH21	1.51	0.74
1:B:1:MET:HE1	1:B:47:VAL:HG23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE2	8:C:652:HOH:O	1.89	0.71
1:C:192:ASP:HB2	8:C:651:HOH:O	1.91	0.70
1:E:328:ARG:HH11	1:E:328:ARG:HB3	1.56	0.70
1:F:179:PRO:HA	1:F:182:GLN:OE1	1.92	0.68
3:C:401:NAI:H42N	4:C:402:OXM:C1	2.24	0.68
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.07	0.67
1:E:328:ARG:HH11	1:E:328:ARG:CG	2.07	0.66
3:B:401:NAI:H42N	4:B:402:OXM:C1	2.26	0.66
1:E:19:SER:OG	1:E:22:ARG:NH1	2.29	0.66
1:C:313:ASP:HB3	1:C:324:ARG:NH2	2.11	0.65
1:F:58:ARG:HD2	1:F:62:GLU:OE2	1.97	0.64
1:B:269:GLU:OE2	1:B:271:ARG:NH2	2.31	0.63
3:A:402:NAI:H42N	4:A:403:OXM:C1	2.29	0.62
1:D:58:ARG:NH1	8:D:501:HOH:O	2.23	0.61
3:D:402:NAI:H42N	4:D:403:OXM:C1	2.31	0.61
1:C:0:HIS:HB2	1:C:26:GLU:HB2	1.83	0.61
1:A:210:ASP:HB3	8:A:609:HOH:O	2.01	0.59
3:E:401:NAI:H42N	4:E:402:OXM:C1	2.33	0.58
1:F:19:SER:OG	1:F:309:ASP:OD1	2.21	0.58
5:C:403:PGE:H6	8:C:637:HOH:O	2.02	0.58
1:B:301:ARG:NH2	8:B:502:HOH:O	2.36	0.57
1:F:21:HIS:CE1	1:F:22:ARG:HG3	2.41	0.56
1:B:1:MET:HE1	1:B:47:VAL:CG2	2.35	0.56
1:C:157:GLU:OE2	1:C:180:ARG:HD2	2.06	0.56
1:F:322:THR:HG23	1:F:322:THR:O	2.05	0.55
1:A:161:ARG:HD3	1:A:161:ARG:C	2.33	0.54
1:B:1:MET:HG2	1:B:25:PHE:CD1	2.43	0.53
1:C:269:GLU:OE2	1:C:271:ARG:NH2	2.41	0.53
1:B:189:LEU:HD13	1:B:194:LEU:HB2	1.91	0.53
1:F:124:TYR:OH	1:F:128:ARG:NE	2.43	0.52
1:E:328:ARG:HB3	1:E:328:ARG:NH1	2.25	0.52
1:E:124:TYR:CZ	1:E:128:ARG:CD	2.92	0.51
1:E:326:ARG:NH1	1:E:328:ARG:NH2	2.59	0.51
1:E:1:MET:HG3	1:E:2:ARG:N	2.26	0.50
1:C:212:ARG:HD2	8:C:581:HOH:O	2.11	0.50
1:F:178:ASN:OD1	1:F:180:ARG:HG3	2.12	0.50
1:F:124:TYR:CZ	1:F:128:ARG:NE	2.81	0.49
3:F:401:NAI:H42N	4:F:402:OXM:C1	2.42	0.49
1:E:124:TYR:CZ	1:E:128:ARG:HD2	2.47	0.49
1:B:178:ASN:HB2	1:B:179:PRO:HD2	1.95	0.49
1:E:178:ASN:OD1	1:E:180:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TYR:O	1:A:15:SER:HB2	2.13	0.48
1:F:19:SER:HB3	1:F:312:LEU:HD12	1.94	0.48
1:F:157:GLU:OE2	1:F:180:ARG:CZ	2.62	0.48
1:E:328:ARG:CG	1:E:328:ARG:NH1	2.73	0.47
1:F:157:GLU:OE2	1:F:180:ARG:NE	2.48	0.47
1:A:161:ARG:HD3	1:A:161:ARG:O	2.14	0.47
1:B:174:ASP:OD2	3:B:401:NAI:H1B	2.15	0.47
1:A:23:HIS:HE1	1:A:313:ASP:OD1	1.98	0.47
1:B:160:ALA:O	1:B:170:LEU:HD11	2.14	0.47
1:D:269:GLU:OE1	1:D:271:ARG:NH2	2.41	0.47
1:E:218:GLN:HG2	8:E:564:HOH:O	2.13	0.47
1:B:189:LEU:CD1	1:B:194:LEU:HB2	2.45	0.46
1:B:1:MET:HE3	1:B:2:ARG:N	2.30	0.45
1:E:191:LEU:HD23	1:E:219:ARG:NH1	2.32	0.45
1:B:214:LEU:O	1:B:219:ARG:HD2	2.17	0.45
1:A:22:ARG:HA	1:A:312:LEU:HD13	1.99	0.45
1:E:268:PHE:N	8:E:515:HOH:O	2.49	0.45
1:F:194:LEU:C	1:F:194:LEU:HD23	2.42	0.45
1:B:184:LEU:HD13	1:B:184:LEU:C	2.39	0.44
1:C:1:MET:CE	8:C:652:HOH:O	2.57	0.44
1:F:103:HIS:HB2	8:F:522:HOH:O	2.17	0.44
1:C:269:GLU:CD	1:C:271:ARG:HH21	2.25	0.44
1:B:0:HIS:HB3	1:B:1:MET:H	1.58	0.44
1:C:0:HIS:O	1:C:0:HIS:ND1	2.51	0.43
1:E:216:ASP:HB2	8:E:522:HOH:O	2.18	0.43
1:E:34:LEU:HB3	1:E:54:ASP:HB3	2.00	0.43
1:A:49:CYS:HA	1:A:73:ALA:O	2.19	0.42
1:C:49:CYS:HA	1:C:73:ALA:O	2.19	0.42
1:E:326:ARG:NH1	1:E:328:ARG:CZ	2.82	0.42
1:B:49:CYS:HA	1:B:73:ALA:O	2.19	0.42
1:C:34:LEU:HB3	1:C:54:ASP:HB3	2.01	0.42
1:C:1:MET:HE1	1:C:46:GLU:OE2	2.19	0.42
1:D:70:ARG:O	1:D:93:PRO:HD2	2.19	0.42
1:A:178:ASN:OD1	1:A:180:ARG:HB2	2.19	0.42
1:F:70:ARG:O	1:F:93:PRO:HD2	2.20	0.42
1:C:194:LEU:C	1:C:194:LEU:HD23	2.45	0.41
1:A:153:GLY:HA3	3:A:402:NAI:O5B	2.20	0.41
1:F:49:CYS:HA	1:F:73:ALA:O	2.20	0.41
1:F:1:MET:HB3	1:F:25:PHE:CD1	2.56	0.41
1:E:49:CYS:HA	1:E:73:ALA:O	2.21	0.41
1:E:194:LEU:C	1:E:194:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HB3	1:B:54:ASP:HB3	2.03	0.41
1:C:70:ARG:O	1:C:93:PRO:HD2	2.21	0.41
1:F:218:GLN:HB2	8:F:511:HOH:O	2.21	0.41

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	328/345 (95%)	321 (98%)	7 (2%)	0	100	100
1	B	330/345 (96%)	320 (97%)	10 (3%)	0	100	100
1	C	328/345 (95%)	321 (98%)	7 (2%)	0	100	100
1	D	328/345 (95%)	319 (97%)	9 (3%)	0	100	100
1	E	329/345 (95%)	321 (98%)	8 (2%)	0	100	100
1	F	333/345 (96%)	324 (97%)	9 (3%)	0	100	100
All	All	1976/2070 (96%)	1926 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/271 (95%)	252 (98%)	5 (2%)	50	66
1	B	261/271 (96%)	252 (97%)	9 (3%)	32	44
1	C	257/271 (95%)	251 (98%)	6 (2%)	44	59
1	D	258/271 (95%)	253 (98%)	5 (2%)	50	66
1	E	258/271 (95%)	249 (96%)	9 (4%)	32	43
1	F	264/271 (97%)	252 (96%)	12 (4%)	24	33
All	All	1555/1626 (96%)	1509 (97%)	46 (3%)	36	49

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	128	ARG
1	A	157	GLU
1	A	180	ARG
1	A	301	ARG
1	B	-12	LYS
1	B	0	HIS
1	B	17	GLN
1	B	43	GLN
1	B	58	ARG
1	B	142	LEU
1	B	189	LEU
1	B	301	ARG
1	B	328	ARG
1	C	0	HIS
1	C	1	MET
1	C	2	ARG
1	C	58	ARG
1	C	142	LEU
1	C	319	GLN
1	D	1	MET
1	D	128	ARG
1	D	142	LEU
1	D	324	ARG
1	D	328	ARG
1	E	0	HIS
1	E	1	MET
1	E	128	ARG
1	E	142	LEU
1	E	184	LEU

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Mol	Chain	Res	Type
1	E	218	GLN
1	E	301	ARG
1	E	326	ARG
1	E	328	ARG
1	F	-11	VAL
1	F	1	MET
1	F	19	SER
1	F	30	GLN
1	F	43	GLN
1	F	58	ARG
1	F	84	LEU
1	F	88	GLU
1	F	142	LEU
1	F	274	GLN
1	F	301	ARG
1	F	324	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	143	HIS
1	A	296	GLN
1	B	125	ASN
1	C	43	GLN
1	C	143	HIS
1	D	143	HIS
1	D	296	GLN
1	E	21	HIS
1	E	143	HIS
1	E	218	GLN
1	E	296	GLN
1	F	31	GLN
1	F	143	HIS
1	F	296	GLN

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 ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAI	D	402	-	47,48,48	2.21	17 (36%)	64,73,73	1.64	11 (17%)
4	OXM	B	402	-	5,5,5	3.58	1 (20%)	2,6,6	0.67	0
4	OXM	E	402	-	5,5,5	3.55	1 (20%)	2,6,6	0.64	0
4	OXM	C	402	-	5,5,5	3.58	1 (20%)	2,6,6	0.67	0
5	PGE	C	403	-	9,9,9	0.40	0	8,8,8	0.64	0
3	NAI	F	401	-	47,48,48	1.98	11 (23%)	64,73,73	1.90	14 (21%)
5	PGE	D	404	-	9,9,9	0.34	0	8,8,8	0.56	0
4	OXM	A	403	-	5,5,5	3.54	1 (20%)	2,6,6	0.64	0
3	NAI	E	401	-	47,48,48	2.21	14 (29%)	64,73,73	1.72	9 (14%)
5	PGE	F	403	-	9,9,9	0.45	0	8,8,8	0.29	0
2	FMT	A	401	-	2,2,2	1.20	0	1,1,1	0.92	0
3	NAI	C	401	-	47,48,48	2.26	16 (34%)	64,73,73	1.86	14 (21%)
4	OXM	F	402	-	5,5,5	3.56	1 (20%)	2,6,6	0.65	0
5	PGE	A	404	-	9,9,9	0.35	0	8,8,8	0.30	0
6	PEG	A	405	-	6,6,6	0.44	0	5,5,5	0.31	0
3	NAI	B	401	-	47,48,48	2.12	13 (27%)	64,73,73	1.82	14 (21%)
3	NAI	A	402	-	47,48,48	2.35	14 (29%)	64,73,73	1.82	14 (21%)
7	PG4	E	403	-	12,12,12	0.45	0	11,11,11	0.27	0
4	OXM	D	403	-	5,5,5	3.53	1 (20%)	2,6,6	0.64	0
2	FMT	D	401	-	2,2,2	0.71	0	1,1,1	1.48	0

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	OXM	A	403	-	-	1/4/4/4	-
3	NAI	E	401	-	-	3/29/72/72	0/5/5/5
5	PGE	F	403	-	-	1/7/7/7	-
4	OXM	C	402	-	-	1/4/4/4	-
3	NAI	B	401	-	-	5/29/72/72	0/5/5/5
5	PGE	C	403	-	-	4/7/7/7	-
3	NAI	C	401	-	-	3/29/72/72	0/5/5/5
3	NAI	A	402	-	-	2/29/72/72	0/5/5/5
3	NAI	D	402	-	-	2/29/72/72	0/5/5/5
4	OXM	B	402	-	-	1/4/4/4	-
4	OXM	F	402	-	-	1/4/4/4	-
3	NAI	F	401	-	-	4/29/72/72	0/5/5/5
5	PGE	A	404	-	-	4/7/7/7	-
6	PEG	A	405	-	-	1/4/4/4	-
7	PG4	E	403	-	-	4/10/10/10	-
4	OXM	E	402	-	-	0/4/4/4	-
5	PGE	D	404	-	-	6/7/7/7	-
4	OXM	D	403	-	-	0/4/4/4	-

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	OXM	C1-C2	-7.66	1.46	1.55
4	B	402	OXM	C1-C2	-7.65	1.46	1.55
4	F	402	OXM	C1-C2	-7.60	1.46	1.55
4	E	402	OXM	C1-C2	-7.56	1.46	1.55
4	A	403	OXM	C1-C2	-7.56	1.46	1.55
4	D	403	OXM	C1-C2	-7.52	1.46	1.55
3	E	401	NAI	C4N-C3N	-6.46	1.37	1.50
3	D	402	NAI	C4N-C3N	-6.37	1.37	1.50
3	F	401	NAI	C4N-C3N	-6.31	1.38	1.50
3	A	402	NAI	C4N-C3N	-6.25	1.38	1.50
3	C	401	NAI	C4N-C3N	-5.98	1.38	1.50
3	B	401	NAI	C4N-C3N	-5.65	1.39	1.50
3	A	402	NAI	C5A-N7A	-5.14	1.29	1.39
3	D	402	NAI	C5A-N7A	-4.96	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAI	C5A-N7A	-4.89	1.30	1.39
3	C	401	NAI	C5A-N7A	-4.83	1.30	1.39
3	E	401	NAI	C5A-N7A	-4.64	1.30	1.39
3	A	402	NAI	C4N-C5N	-4.63	1.37	1.49
3	F	401	NAI	C5A-N7A	-4.59	1.30	1.39
3	B	401	NAI	C4N-C5N	-4.48	1.37	1.49
3	D	402	NAI	C4N-C5N	-4.38	1.37	1.49
3	F	401	NAI	C4N-C5N	-4.36	1.37	1.49
3	E	401	NAI	C4N-C5N	-4.34	1.37	1.49
3	C	401	NAI	C4N-C5N	-4.31	1.37	1.49
3	A	402	NAI	PN-O3	-4.29	1.54	1.59
3	D	402	NAI	C4A-N9A	-4.24	1.28	1.37
3	A	402	NAI	PA-O3	-4.21	1.55	1.59
3	C	401	NAI	C4A-N9A	-4.02	1.29	1.37
3	C	401	NAI	PA-O3	-4.00	1.55	1.59
3	E	401	NAI	C8A-N9A	-3.97	1.30	1.37
3	E	401	NAI	C4A-N9A	-3.93	1.29	1.37
3	C	401	NAI	C8A-N9A	-3.92	1.30	1.37
3	E	401	NAI	PN-O3	-3.92	1.55	1.59
3	A	402	NAI	C4A-N9A	-3.91	1.29	1.37
3	B	401	NAI	C4A-N9A	-3.70	1.30	1.37
3	F	401	NAI	C4A-N9A	-3.67	1.30	1.37
3	D	402	NAI	PA-O3	-3.60	1.55	1.59
3	C	401	NAI	PN-O1N	-3.57	1.38	1.55
3	A	402	NAI	PA-O2A	-3.42	1.39	1.55
3	A	402	NAI	C8A-N9A	-3.36	1.31	1.37
3	C	401	NAI	PA-O2A	-3.35	1.39	1.55
3	A	402	NAI	PN-O1N	-3.35	1.39	1.55
3	F	401	NAI	C8A-N9A	-3.31	1.31	1.37
3	E	401	NAI	PN-O1N	-3.31	1.40	1.55
3	D	402	NAI	PN-O3	-3.11	1.56	1.59
3	B	401	NAI	O7N-C7N	-3.10	1.17	1.24
3	A	402	NAI	PA-O1A	-3.09	1.40	1.50
3	D	402	NAI	PN-O1N	-3.06	1.41	1.55
3	A	402	NAI	O7N-C7N	-3.03	1.17	1.24
3	B	401	NAI	PN-O1N	-2.99	1.41	1.55
3	D	402	NAI	O7N-C7N	-2.96	1.17	1.24
3	B	401	NAI	C5A-C4A	2.92	1.44	1.39
3	D	402	NAI	PA-O1A	-2.86	1.40	1.50
3	D	402	NAI	C8A-N9A	-2.86	1.32	1.37
3	B	401	NAI	PA-O1A	-2.82	1.41	1.50
3	B	401	NAI	C8A-N9A	-2.76	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAI	PA-O1A	-2.72	1.41	1.50
3	B	401	NAI	PN-O3	-2.70	1.56	1.59
3	E	401	NAI	PA-O2A	-2.66	1.43	1.55
3	C	401	NAI	C6N-N1N	-2.64	1.30	1.37
3	B	401	NAI	PA-O3	-2.64	1.56	1.59
3	E	401	NAI	PA-O1A	-2.63	1.41	1.50
3	B	401	NAI	PN-O2N	-2.59	1.41	1.50
3	C	401	NAI	PN-O2N	-2.53	1.42	1.50
3	E	401	NAI	PA-O3	-2.45	1.56	1.59
3	E	401	NAI	PN-O2N	-2.44	1.42	1.50
3	B	401	NAI	PA-O2A	-2.42	1.44	1.55
3	D	402	NAI	PA-O2A	-2.40	1.44	1.55
3	F	401	NAI	C5A-C4A	2.39	1.43	1.39
3	F	401	NAI	C6N-N1N	-2.37	1.31	1.37
3	C	401	NAI	C5A-C4A	2.32	1.43	1.39
3	D	402	NAI	C6N-N1N	-2.32	1.31	1.37
3	E	401	NAI	C5A-C4A	2.31	1.43	1.39
3	D	402	NAI	C5A-C4A	2.31	1.43	1.39
3	F	401	NAI	O4B-C4B	-2.27	1.39	1.45
3	C	401	NAI	O4B-C4B	-2.27	1.39	1.45
3	D	402	NAI	PN-O2N	-2.25	1.43	1.50
3	C	401	NAI	PN-O3	-2.24	1.57	1.59
3	F	401	NAI	O7N-C7N	-2.20	1.19	1.24
3	A	402	NAI	C6A-N6A	-2.20	1.28	1.34
3	D	402	NAI	C2A-N3A	-2.19	1.30	1.33
3	E	401	NAI	C6N-N1N	-2.19	1.31	1.37
3	E	401	NAI	O4B-C4B	-2.18	1.40	1.45
3	F	401	NAI	PN-O1N	-2.15	1.45	1.55
3	D	402	NAI	C2A-N1A	-2.11	1.30	1.33
3	D	402	NAI	O4B-C4B	-2.10	1.40	1.45
3	C	401	NAI	O7N-C7N	-2.10	1.19	1.24
3	C	401	NAI	O4D-C4D	-2.09	1.40	1.45
3	F	401	NAI	PA-O2A	-2.06	1.45	1.55
3	A	402	NAI	PN-O2N	-2.04	1.43	1.50
3	A	402	NAI	O4D-C4D	-2.02	1.40	1.45

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	NAI	C5A-C4A-N3A	-6.87	117.26	126.72
3	C	401	NAI	C5A-C4A-N3A	-6.37	117.94	126.72
3	E	401	NAI	C5A-C4A-N3A	-6.31	118.03	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAI	C5A-C4A-N3A	-6.26	118.10	126.72
3	A	402	NAI	C5A-C4A-N3A	-5.83	118.68	126.72
3	B	401	NAI	N3A-C4A-N9A	5.45	136.43	127.17
3	D	402	NAI	C5A-C4A-N3A	-5.32	119.39	126.72
3	A	402	NAI	N3A-C4A-N9A	5.23	136.06	127.17
3	E	401	NAI	N3A-C4A-N9A	4.79	135.31	127.17
3	C	401	NAI	N3A-C4A-N9A	4.70	135.16	127.17
3	F	401	NAI	N3A-C4A-N9A	4.65	135.07	127.17
3	C	401	NAI	C4A-C5A-N7A	-4.54	105.39	110.58
3	F	401	NAI	C4A-C5A-N7A	-4.46	105.48	110.58
3	A	402	NAI	O4B-C1B-N9A	4.35	116.45	108.09
3	A	402	NAI	C2A-N3A-C4A	4.24	122.19	111.83
3	F	401	NAI	C2A-N3A-C4A	4.23	122.17	111.83
3	C	401	NAI	C2A-N3A-C4A	4.02	121.66	111.83
3	A	402	NAI	N3A-C2A-N1A	-4.00	122.53	128.58
3	E	401	NAI	C2A-N3A-C4A	3.93	121.44	111.83
3	E	401	NAI	C4A-C5A-N7A	-3.90	106.12	110.58
3	D	402	NAI	N3A-C4A-N9A	3.85	133.71	127.17
3	D	402	NAI	C2A-N3A-C4A	3.81	121.13	111.83
3	B	401	NAI	C2A-N3A-C4A	3.76	121.02	111.83
3	C	401	NAI	O4B-C1B-N9A	3.65	115.09	108.09
3	D	402	NAI	N3A-C2A-N1A	-3.57	123.18	128.58
3	F	401	NAI	O4B-C1B-N9A	3.49	114.80	108.09
3	B	401	NAI	O4B-C1B-N9A	3.47	114.76	108.09
3	D	402	NAI	C3D-C2D-C1D	3.42	107.94	101.46
3	D	402	NAI	O4B-C1B-N9A	3.41	114.64	108.09
3	E	401	NAI	N3A-C2A-N1A	-3.36	123.49	128.58
3	C	401	NAI	C5A-N7A-C8A	3.34	108.70	103.45
3	C	401	NAI	C6N-N1N-C2N	3.25	122.80	119.32
3	F	401	NAI	C5A-N7A-C8A	3.22	108.52	103.45
3	E	401	NAI	O4B-C1B-N9A	3.22	114.27	108.09
3	F	401	NAI	O1N-PN-O3	3.13	115.73	107.27
3	C	401	NAI	O4D-C1D-N1N	3.07	113.94	108.08
3	B	401	NAI	C3N-C7N-N7N	3.07	123.12	117.67
3	F	401	NAI	C3D-C2D-C1D	3.05	107.24	101.46
3	F	401	NAI	O7N-C7N-N7N	-2.93	116.33	122.89
3	F	401	NAI	N3A-C2A-N1A	-2.88	124.22	128.58
3	B	401	NAI	C4A-C5A-N7A	-2.88	107.29	110.58
3	B	401	NAI	O7N-C7N-N7N	-2.86	116.49	122.89
3	A	402	NAI	C4A-N9A-C8A	2.82	108.70	105.74
3	D	402	NAI	C4A-C5A-N7A	-2.81	107.37	110.58
3	A	402	NAI	C3N-C7N-N7N	2.80	122.65	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAI	C6A-C5A-N7A	2.79	137.48	132.09
3	C	401	NAI	N3A-C2A-N1A	-2.74	124.44	128.58
3	E	401	NAI	C5A-N7A-C8A	2.72	107.73	103.45
3	B	401	NAI	O3-PA-O1A	-2.60	102.88	110.70
3	A	402	NAI	C5A-N7A-C8A	2.59	107.52	103.45
3	A	402	NAI	C4A-C5A-N7A	-2.57	107.64	110.58
3	B	401	NAI	N3A-C2A-N1A	-2.56	124.70	128.58
3	B	401	NAI	C5A-N7A-C8A	2.54	107.44	103.45
3	E	401	NAI	C6A-C5A-N7A	2.48	136.87	132.09
3	F	401	NAI	O2A-PA-O1A	2.39	123.58	112.44
3	B	401	NAI	O2A-PA-O3	2.35	113.63	107.27
3	D	402	NAI	C3N-C7N-N7N	2.33	121.81	117.67
3	F	401	NAI	N9A-C8A-N7A	-2.33	110.63	113.94
3	A	402	NAI	C6A-C5A-N7A	2.33	136.58	132.09
3	C	401	NAI	C3N-C7N-N7N	2.31	121.76	117.67
3	E	401	NAI	C4A-N9A-C8A	2.30	108.15	105.74
3	F	401	NAI	C6A-C5A-N7A	2.29	136.51	132.09
3	D	402	NAI	C6A-C5A-N7A	2.29	136.50	132.09
3	C	401	NAI	C4A-N9A-C8A	2.27	108.12	105.74
3	D	402	NAI	C2A-N1A-C6A	2.27	122.46	118.73
3	A	402	NAI	C3D-C2D-C1D	2.20	105.62	101.46
3	D	402	NAI	O2A-PA-O1A	2.19	122.65	112.44
3	B	401	NAI	C3D-C2D-C1D	2.18	105.59	101.46
3	A	402	NAI	O7N-C7N-N7N	-2.18	118.02	122.89
3	F	401	NAI	O4B-C1B-C2B	-2.17	101.96	106.62
3	C	401	NAI	N9A-C8A-N7A	-2.16	110.87	113.94
3	A	402	NAI	C5A-C6A-N6A	-2.16	117.95	123.29
3	A	402	NAI	N9A-C8A-N7A	-2.15	110.89	113.94
3	C	401	NAI	O7N-C7N-N7N	-2.13	118.12	122.89
3	B	401	NAI	O4D-C1D-N1N	2.08	112.04	108.08
3	B	401	NAI	O4B-C4B-C3B	2.07	109.27	105.15

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	OXM	O1-C1-C2-O3
4	B	402	OXM	O1-C1-C2-O3
4	C	402	OXM	O1-C1-C2-O3
4	F	402	OXM	O1-C1-C2-O3
5	D	404	PGE	O2-C3-C4-O3
5	A	404	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	C	403	PGE	O3-C5-C6-O4
7	E	403	PG4	O2-C3-C4-O3
5	A	404	PGE	O1-C1-C2-O2
5	C	403	PGE	O1-C1-C2-O2
5	A	404	PGE	O3-C5-C6-O4
5	C	403	PGE	O2-C3-C4-O3
3	B	401	NAI	O4D-C4D-C5D-O5D
3	F	401	NAI	O4D-C4D-C5D-O5D
7	E	403	PG4	O3-C5-C6-O4
7	E	403	PG4	C4-C3-O2-C2
5	A	404	PGE	C3-C4-O3-C5
7	E	403	PG4	C3-C4-O3-C5
3	F	401	NAI	C3D-C4D-C5D-O5D
5	D	404	PGE	C6-C5-O3-C4
5	D	404	PGE	O1-C1-C2-O2
3	B	401	NAI	C3D-C4D-C5D-O5D
3	B	401	NAI	C2B-C1B-N9A-C8A
3	F	401	NAI	C2B-C1B-N9A-C8A
3	D	402	NAI	O4D-C1D-N1N-C2N
5	D	404	PGE	C1-C2-O2-C3
3	E	401	NAI	O4D-C1D-N1N-C2N
5	D	404	PGE	O3-C5-C6-O4
3	A	402	NAI	O4D-C1D-N1N-C2N
3	F	401	NAI	O4D-C1D-N1N-C2N
3	A	402	NAI	O4D-C4D-C5D-O5D
3	B	401	NAI	O4D-C1D-N1N-C2N
3	C	401	NAI	O4D-C1D-N1N-C2N
3	C	401	NAI	C2B-C1B-N9A-C8A
3	E	401	NAI	C2B-C1B-N9A-C8A
3	E	401	NAI	O4B-C4B-C5B-O5B
5	D	404	PGE	C4-C3-O2-C2
3	D	402	NAI	C2B-C1B-N9A-C8A
5	C	403	PGE	C6-C5-O3-C4
6	A	405	PEG	C4-C3-O2-C2
5	F	403	PGE	O3-C5-C6-O4
3	B	401	NAI	C2D-C1D-N1N-C2N
3	C	401	NAI	O4B-C4B-C5B-O5B

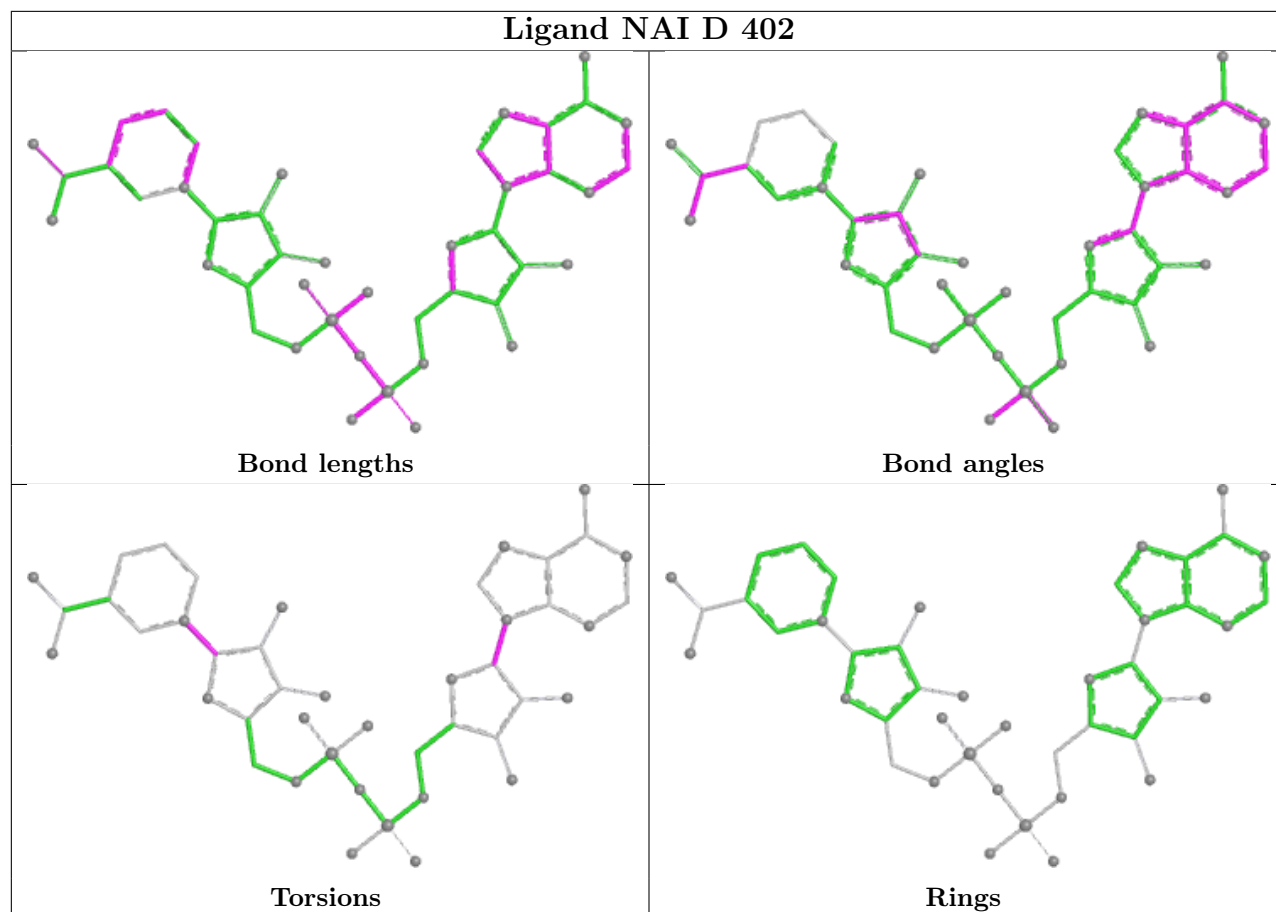
There are no ring outliers.

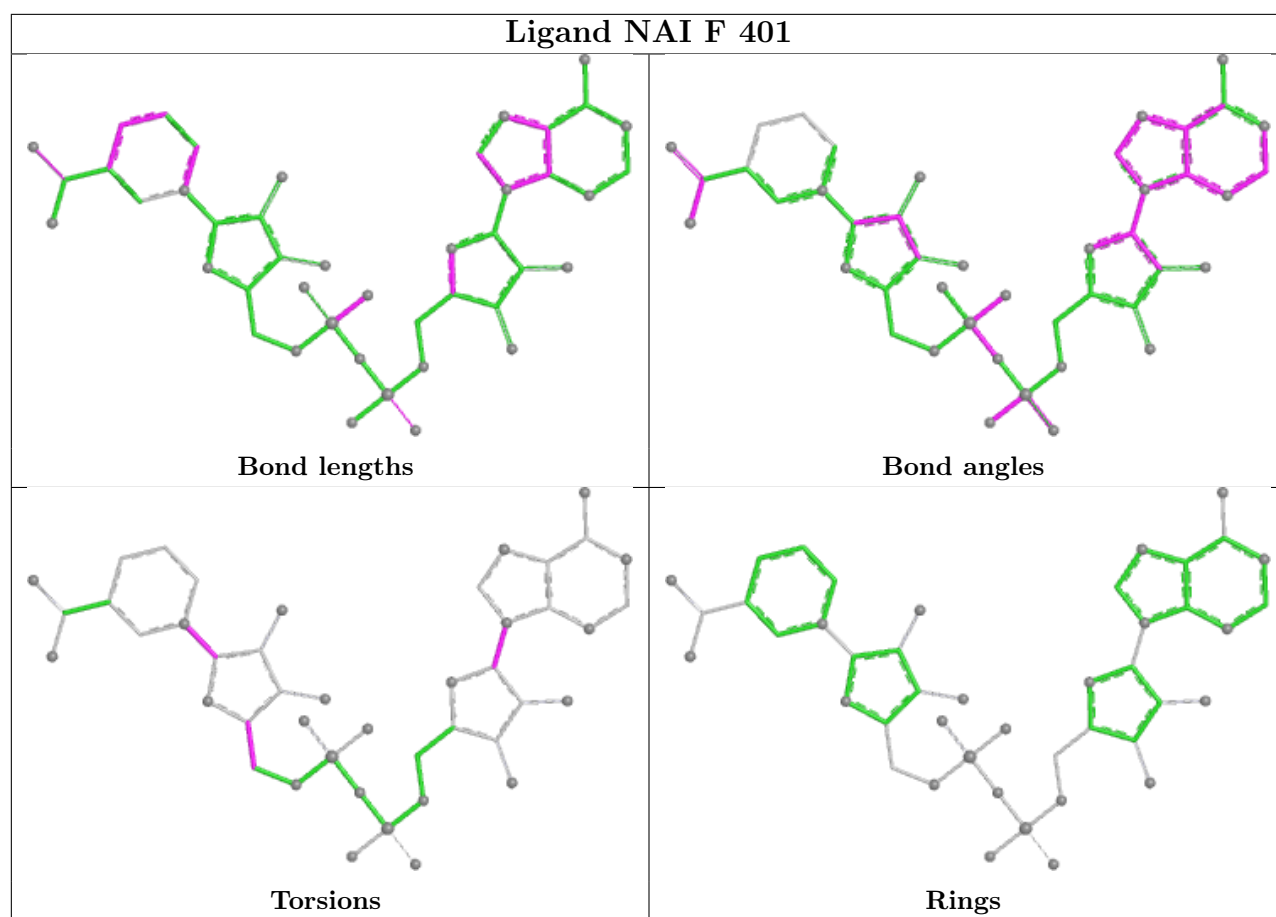
13 monomers are involved in 9 short contacts:

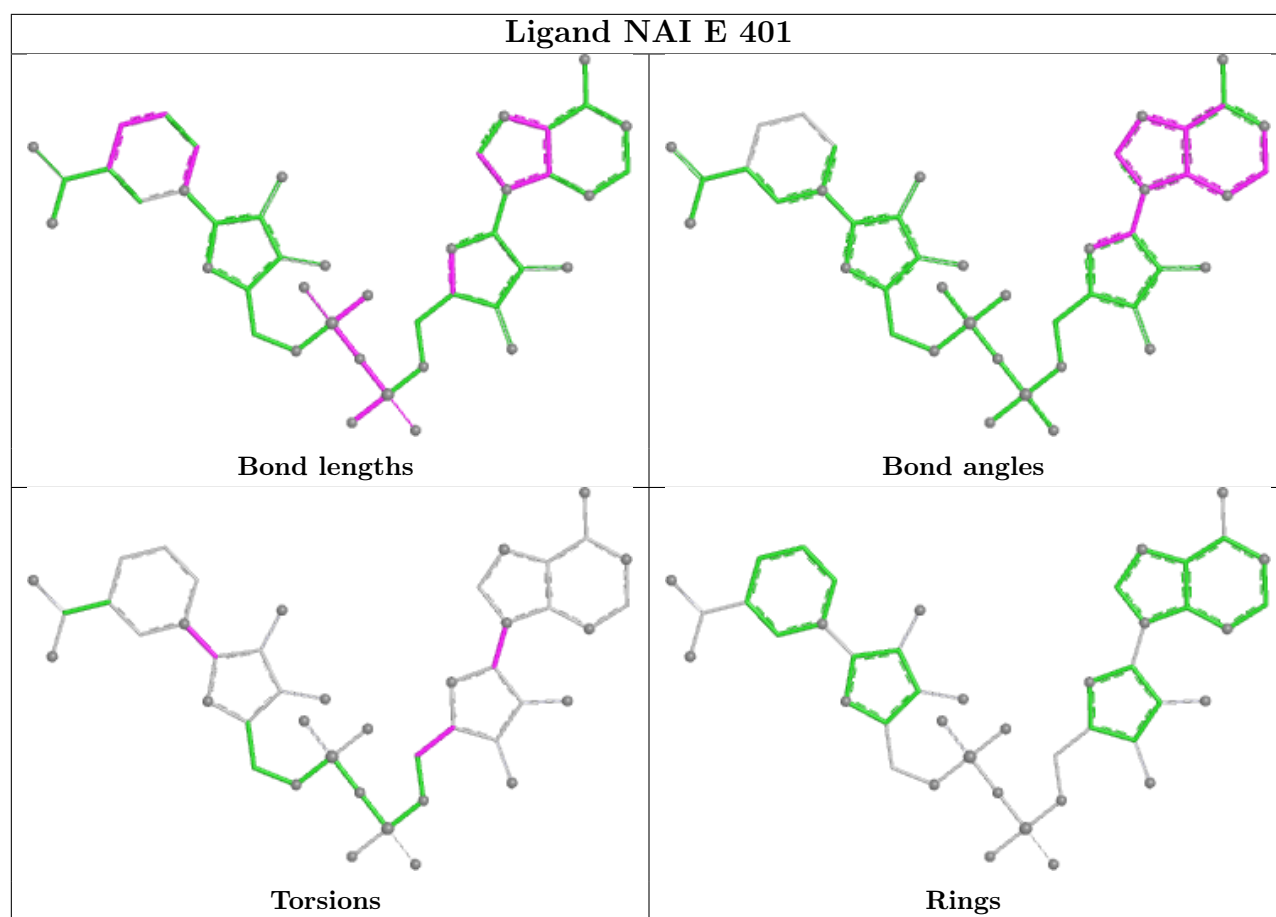
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	NAI	1	0
4	B	402	OXM	1	0
4	E	402	OXM	1	0
4	C	402	OXM	1	0
5	C	403	PGE	1	0
3	F	401	NAI	1	0
4	A	403	OXM	1	0
3	E	401	NAI	1	0
3	C	401	NAI	1	0
4	F	402	OXM	1	0
3	B	401	NAI	2	0
3	A	402	NAI	2	0
4	D	403	OXM	1	0

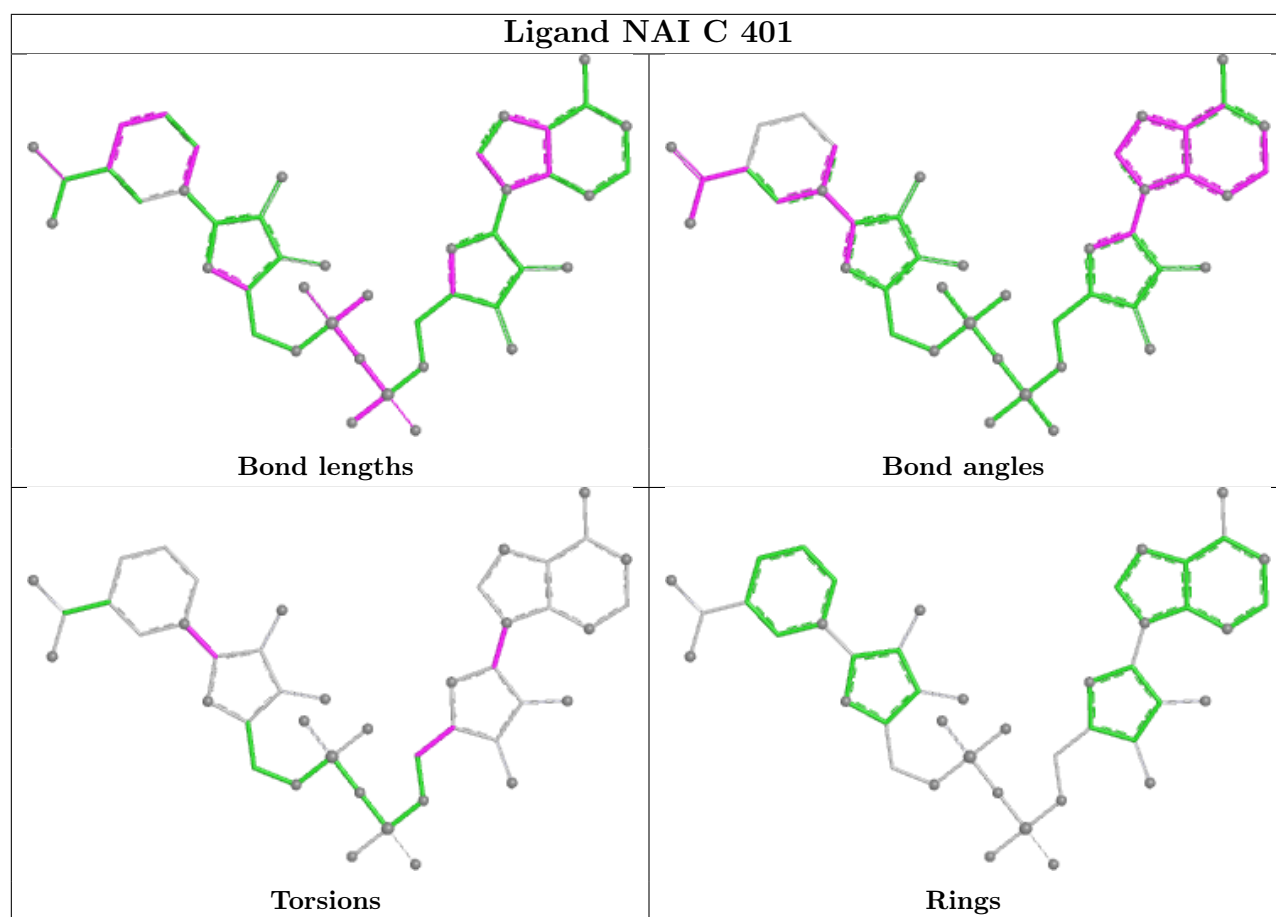
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

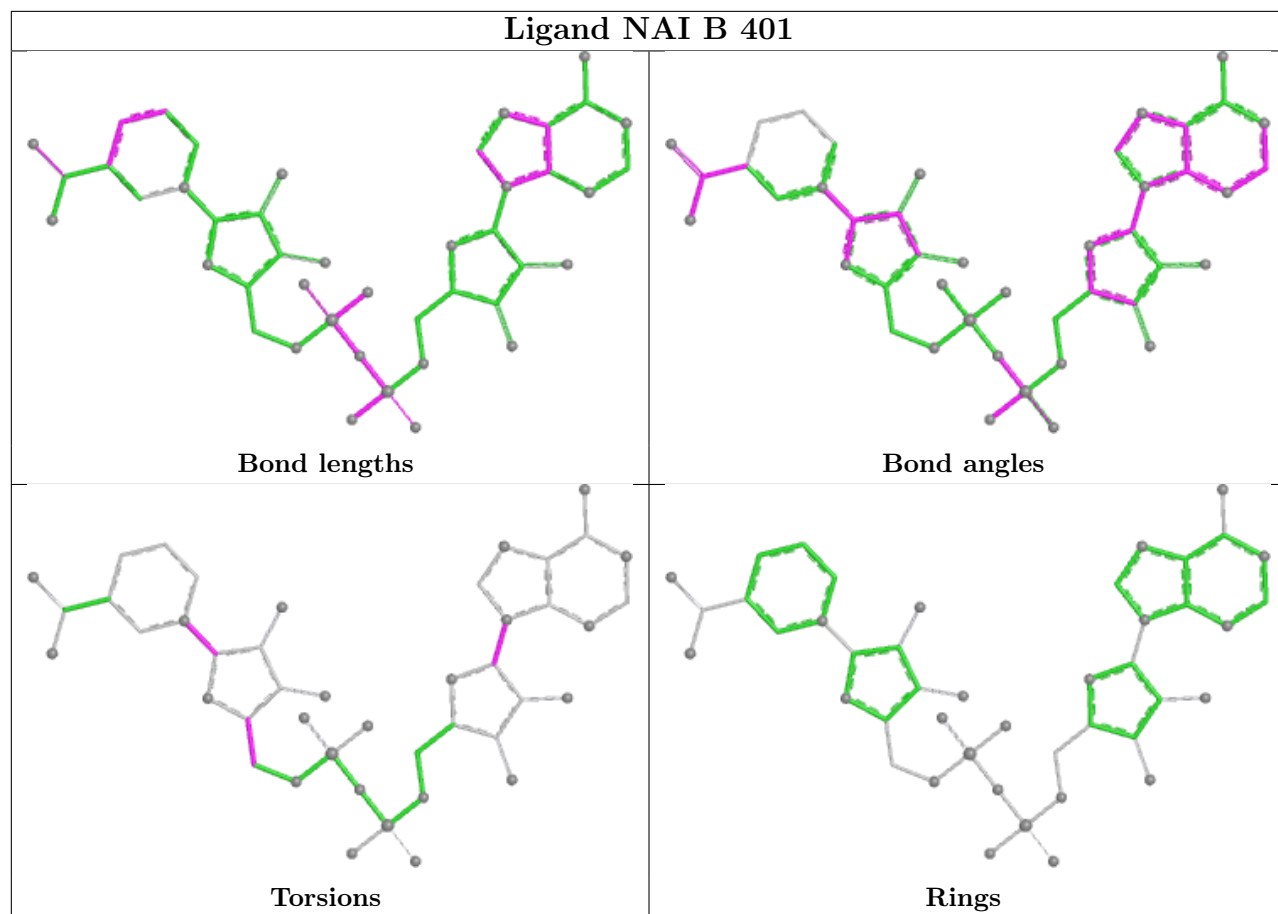
Ligand NAI D 402

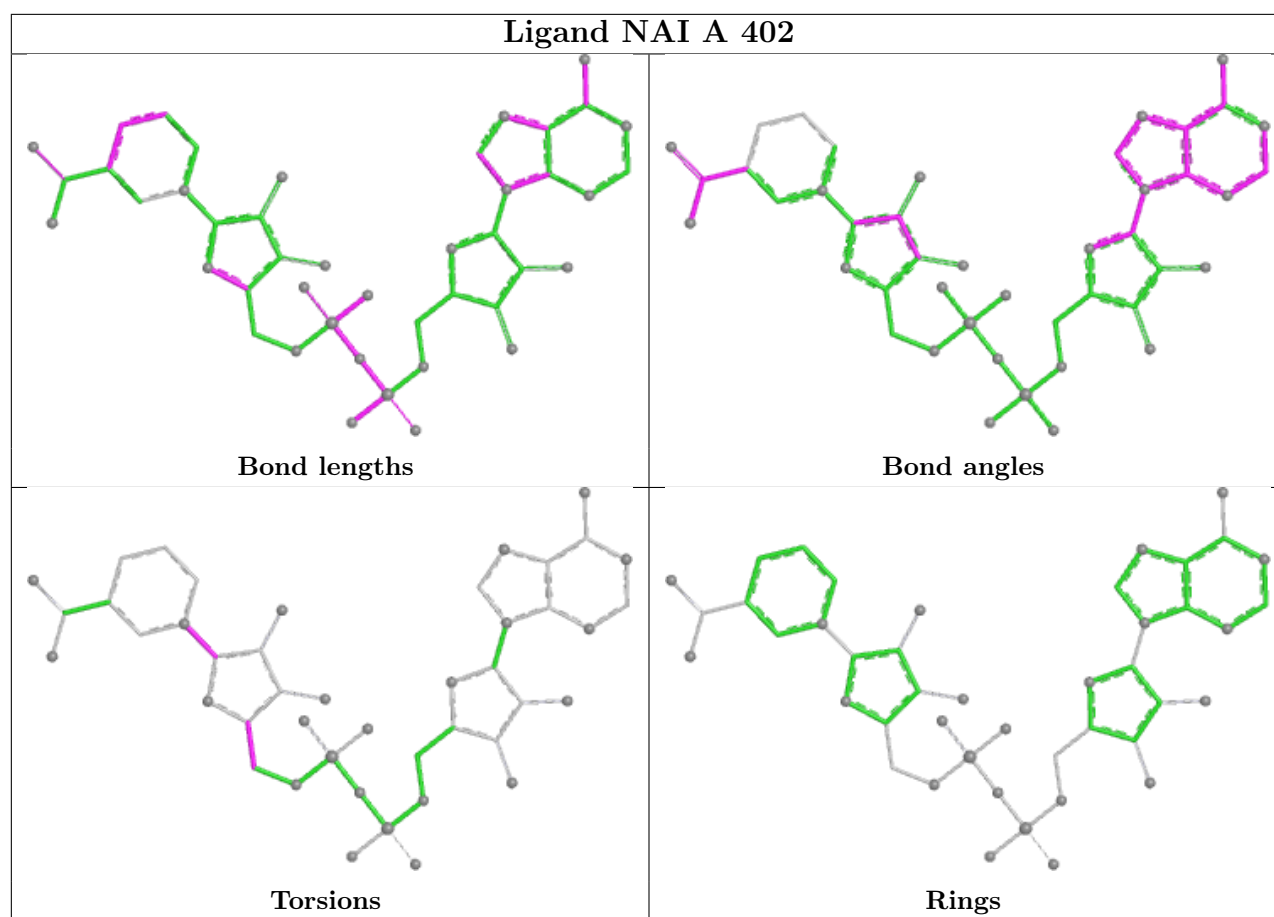












5.7 Other polymers [i](#)

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	330/345 (95%)	-0.55	3 (0%) 81 79	16, 23, 43, 77	0
1	B	334/345 (96%)	-0.32	9 (2%) 56 53	17, 28, 52, 95	0
1	C	330/345 (95%)	-0.34	2 (0%) 85 83	18, 28, 49, 97	0
1	D	329/345 (95%)	-0.33	5 (1%) 72 69	11, 29, 49, 80	2 (0%)
1	E	330/345 (95%)	-0.23	5 (1%) 72 69	12, 32, 52, 83	1 (0%)
1	F	336/345 (97%)	0.13	18 (5%) 31 28	14, 36, 66, 90	1 (0%)
All	All	1989/2070 (96%)	-0.27	42 (2%) 63 60	11, 30, 53, 97	4 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	HIS	5.8
1	B	-11	VAL	5.7
1	C	0	HIS	5.5
1	F	322	THR	5.5
1	B	0	HIS	4.4
1	D	328	ARG	4.4
1	E	329	ALA	4.1
1	A	0	HIS	4.1
1	E	0	HIS	4.0
1	F	178	ASN	3.9
1	F	179	PRO	3.8
1	F	1	MET	3.6
1	F	-6	HIS	3.4
1	B	-10	HIS	3.4
1	F	180	ARG	3.1
1	F	320	ASP	3.0
1	E	328	ARG	2.9
1	B	-9	HIS	2.8
1	F	321	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.7
1	F	-9	HIS	2.7
1	F	323	PRO	2.7
1	F	-11	VAL	2.7
1	E	184	LEU	2.7
1	D	22	ARG	2.6
1	B	324	ARG	2.5
1	D	324	ARG	2.5
1	F	88	GLU	2.4
1	D	53[A]	ASN	2.4
1	B	184	LEU	2.4
1	B	22	ARG	2.4
1	F	176	TYR	2.3
1	A	329	ALA	2.3
1	F	-10	HIS	2.3
1	F	182	GLN	2.3
1	B	328	ARG	2.2
1	F	326	ARG	2.2
1	A	328	ARG	2.2
1	F	-8	HIS	2.2
1	B	329	ALA	2.1
1	F	328	ARG	2.1
1	E	53[A]	ASN	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.

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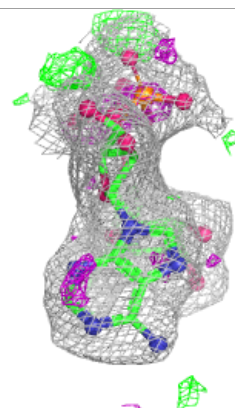
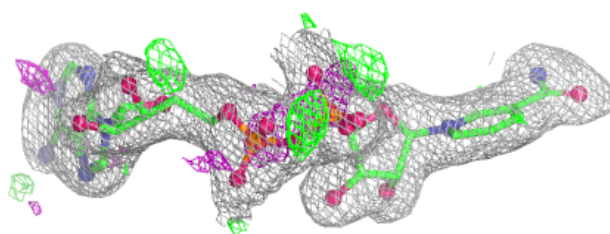
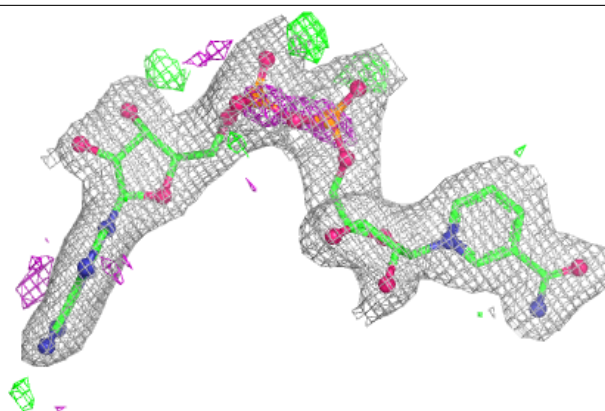
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PGE	F	403	10/10	0.80	0.21	48,50,54,57	10
5	PGE	D	404	10/10	0.81	0.21	48,52,55,59	10
2	FMT	D	401	3/3	0.81	0.17	40,40,40,40	0
7	PG4	E	403	13/13	0.83	0.20	35,38,41,42	13
5	PGE	C	403	10/10	0.84	0.18	50,59,63,66	0
6	PEG	A	405	7/7	0.86	0.19	35,41,44,48	7
5	PGE	A	404	10/10	0.87	0.16	30,43,44,44	10
2	FMT	A	401	3/3	0.88	0.10	37,37,41,43	0
3	NAI	F	401	44/44	0.95	0.08	26,33,41,51	0
4	OXM	E	402	6/6	0.97	0.06	19,23,24,27	0
4	OXM	F	402	6/6	0.97	0.07	19,26,28,28	0
3	NAI	C	401	44/44	0.97	0.06	18,23,28,32	0
3	NAI	D	402	44/44	0.97	0.06	17,24,28,28	0
3	NAI	E	401	44/44	0.97	0.06	19,27,33,35	0
3	NAI	B	401	44/44	0.97	0.07	18,24,30,34	0
4	OXM	A	403	6/6	0.97	0.06	16,20,23,24	0
4	OXM	D	403	6/6	0.97	0.05	17,22,24,29	0
3	NAI	A	402	44/44	0.98	0.05	13,17,21,23	0
4	OXM	B	402	6/6	0.98	0.06	17,23,24,27	0
4	OXM	C	402	6/6	0.98	0.06	17,19,25,27	0

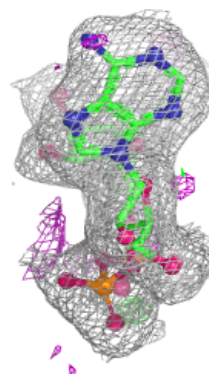
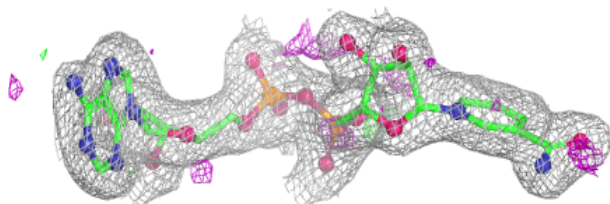
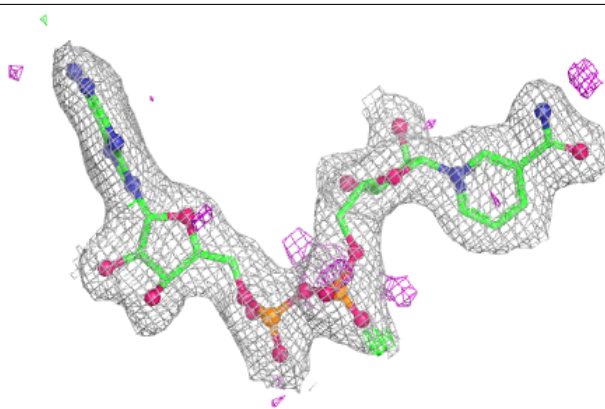
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI F 401:

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

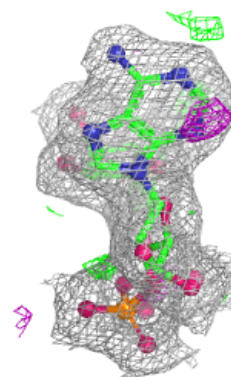
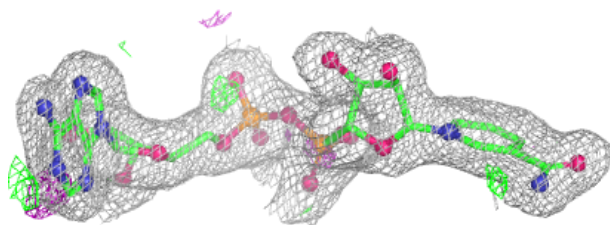
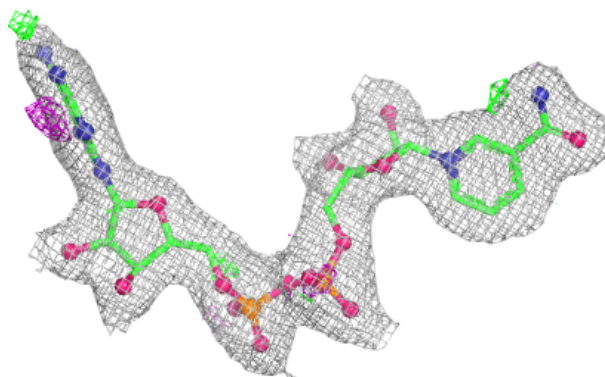
**Electron density around NAI C 401:**

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

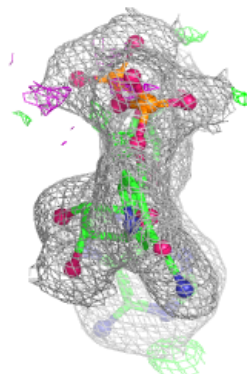
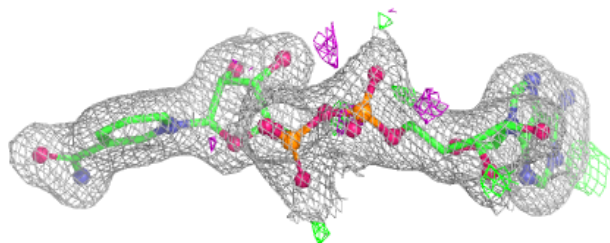
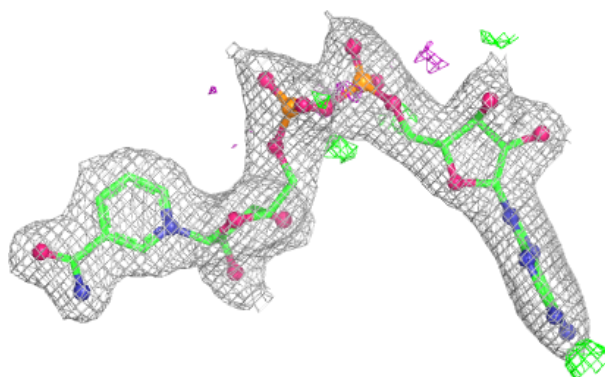


Electron density around NAI D 402:

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

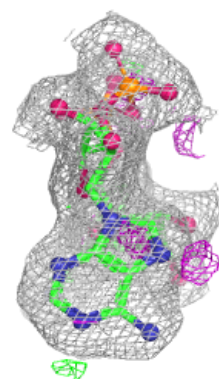
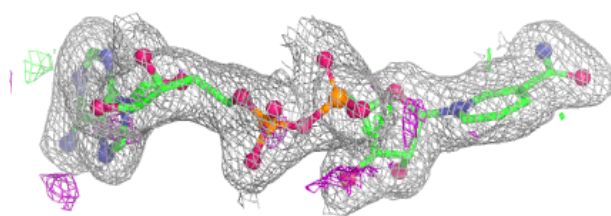
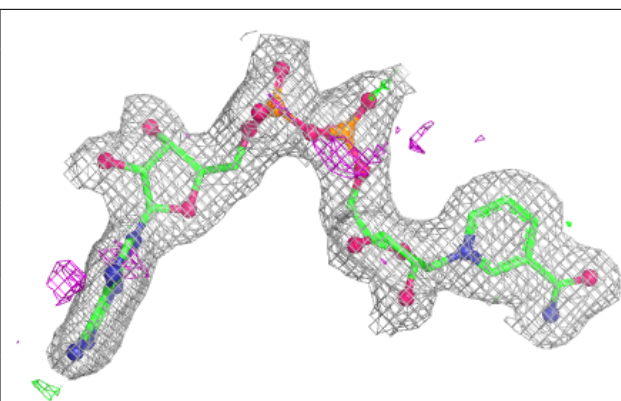
**Electron density around NAI E 401:**

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

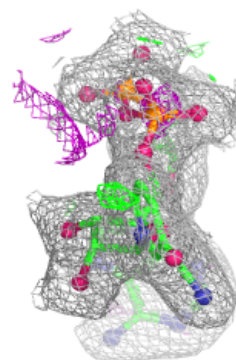
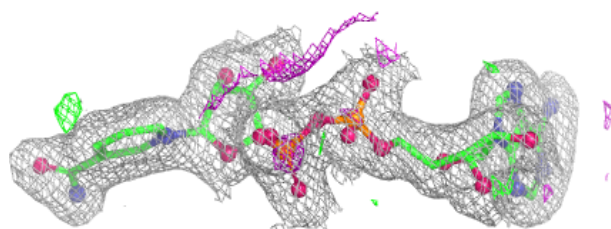
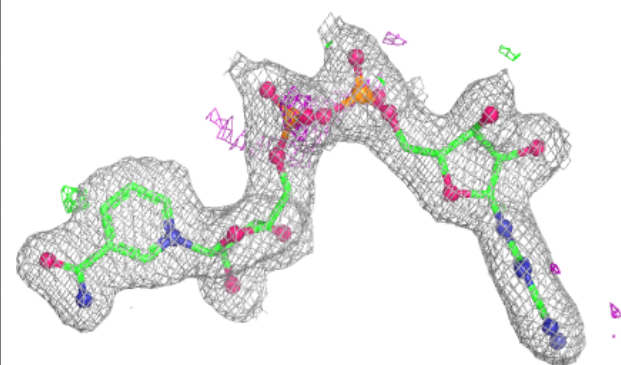


Electron density around NAI B 401:

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

**Electron density around NAI A 402:**

$2mF_o-DF_c$ (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.