



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:56 PM UTC

PDB ID : 6VO6 / pdb_00006vo6
Title : Crystal Structure of Cj1427, an Essential NAD-dependent Dehydrogenase from *Campylobacter jejuni*, in the Presence of NADH and GDP
Authors : Anderson, T.K.; Spencer, K.D.; Thoden, J.B.; Huddleston, J.P.; Raushel, F.M.; Holden, H.M.
Deposited on : 2020-01-30
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

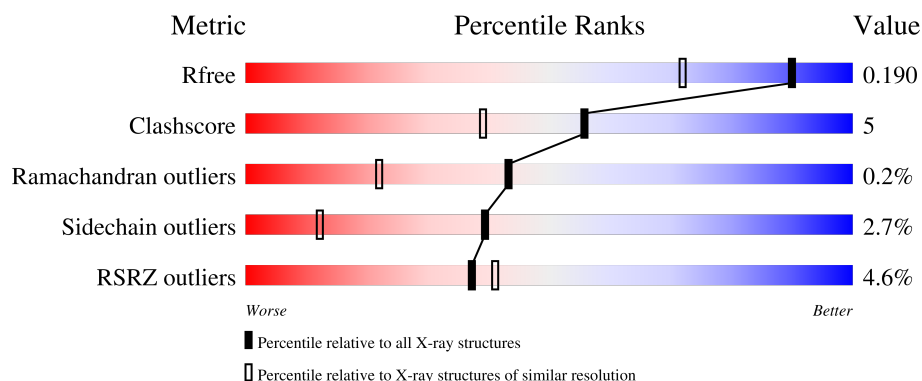
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	321	2% 87% 8% ...
1	B	321	3% 88% 7% ...
1	C	321	11% 81% 9% 7%
1	D	321	2% 89% 7% ...

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11506 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 Putative sugar-nucleotide epimerase/dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	4	0
			2472	1587	416	453	16			
1	B	310	Total	C	N	O	S	0	10	0
			2532	1624	429	464	15			
1	C	297	Total	C	N	O	S	0	4	0
			2397	1540	407	435	15			
1	D	311	Total	C	N	O	S	0	2	0
			2497	1603	421	458	15			

There are 32 discrepancies between the modelled and reference sequences:

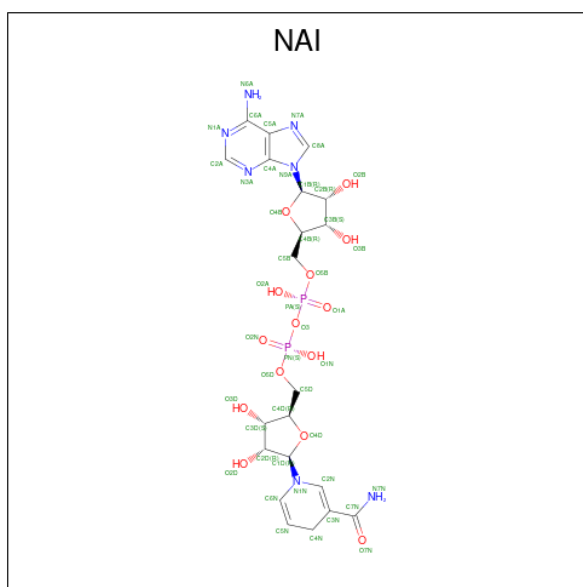
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	LEU	-	expression tag	UNP Q0P8I7
A	315	GLU	-	expression tag	UNP Q0P8I7
A	316	HIS	-	expression tag	UNP Q0P8I7
A	317	HIS	-	expression tag	UNP Q0P8I7
A	318	HIS	-	expression tag	UNP Q0P8I7
A	319	HIS	-	expression tag	UNP Q0P8I7
A	320	HIS	-	expression tag	UNP Q0P8I7
A	321	HIS	-	expression tag	UNP Q0P8I7
B	314	LEU	-	expression tag	UNP Q0P8I7
B	315	GLU	-	expression tag	UNP Q0P8I7
B	316	HIS	-	expression tag	UNP Q0P8I7
B	317	HIS	-	expression tag	UNP Q0P8I7
B	318	HIS	-	expression tag	UNP Q0P8I7
B	319	HIS	-	expression tag	UNP Q0P8I7
B	320	HIS	-	expression tag	UNP Q0P8I7
B	321	HIS	-	expression tag	UNP Q0P8I7
C	314	LEU	-	expression tag	UNP Q0P8I7
C	315	GLU	-	expression tag	UNP Q0P8I7
C	316	HIS	-	expression tag	UNP Q0P8I7
C	317	HIS	-	expression tag	UNP Q0P8I7
C	318	HIS	-	expression tag	UNP Q0P8I7

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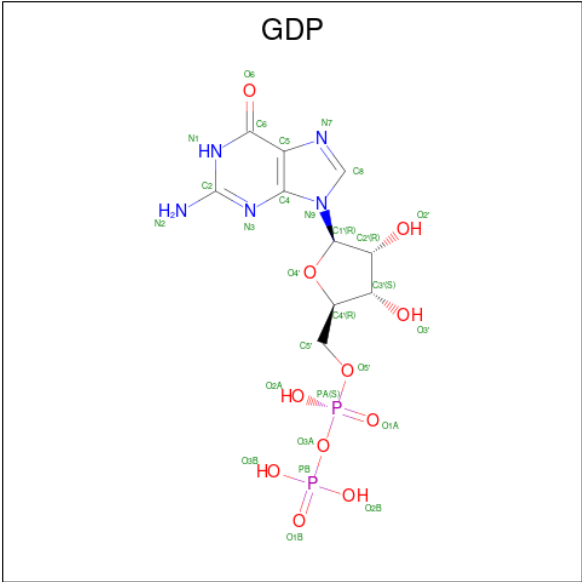
Chain	Residue	Modelled	Actual	Comment	Reference
C	319	HIS	-	expression tag	UNP Q0P8I7
C	320	HIS	-	expression tag	UNP Q0P8I7
C	321	HIS	-	expression tag	UNP Q0P8I7
D	314	LEU	-	expression tag	UNP Q0P8I7
D	315	GLU	-	expression tag	UNP Q0P8I7
D	316	HIS	-	expression tag	UNP Q0P8I7
D	317	HIS	-	expression tag	UNP Q0P8I7
D	318	HIS	-	expression tag	UNP Q0P8I7
D	319	HIS	-	expression tag	UNP Q0P8I7
D	320	HIS	-	expression tag	UNP Q0P8I7
D	321	HIS	-	expression tag	UNP Q0P8I7

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



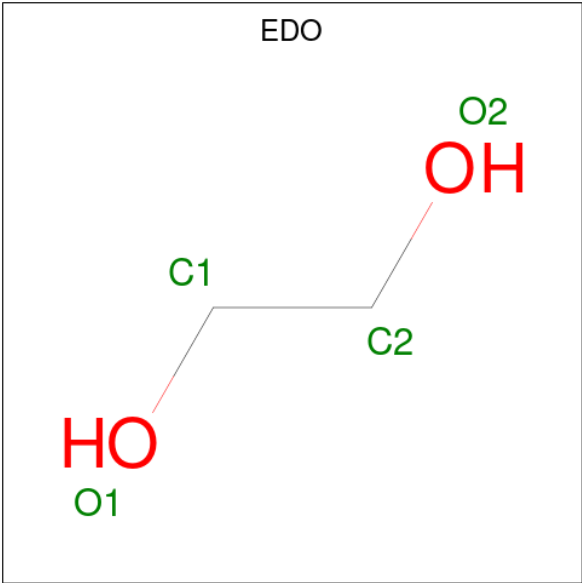
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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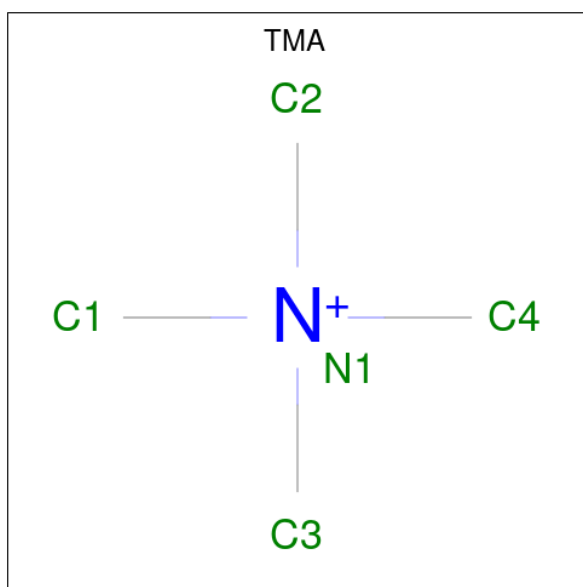
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is TETRAMETHYLAMMONIUM ION (CCD ID: TMA) (formula: C₄H₁₂N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	4	1		
6	B	1	Total	C	N	0	0
			5	4	1		
6	B	1	Total	C	N	0	0
			5	4	1		
6	C	1	Total	C	N	0	0
			5	4	1		
6	D	1	Total	C	N	0	0
			5	4	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	298	Total	O	0	0
			298	298		
8	B	337	Total	O	0	0
			337	337		
8	C	299	Total	O	0	0
			299	299		

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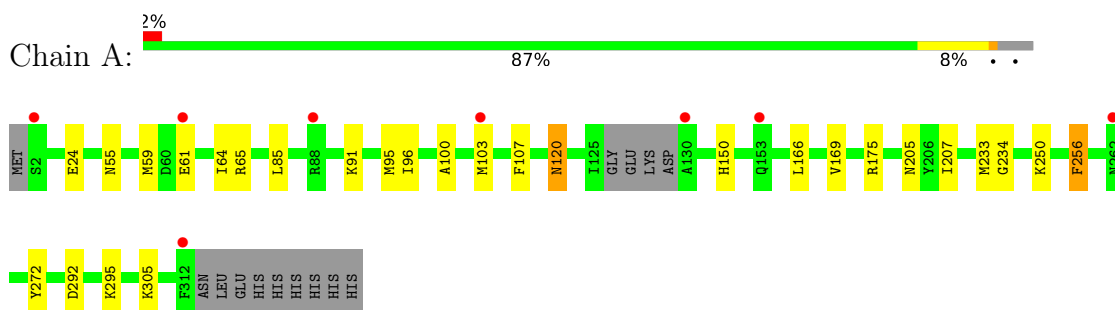
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	363	Total 363	O 363	0	0

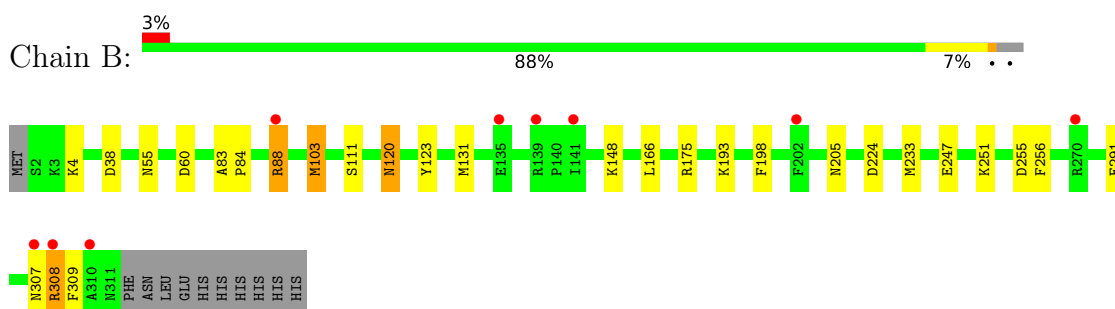
3 Residue-property plots [i](#)

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

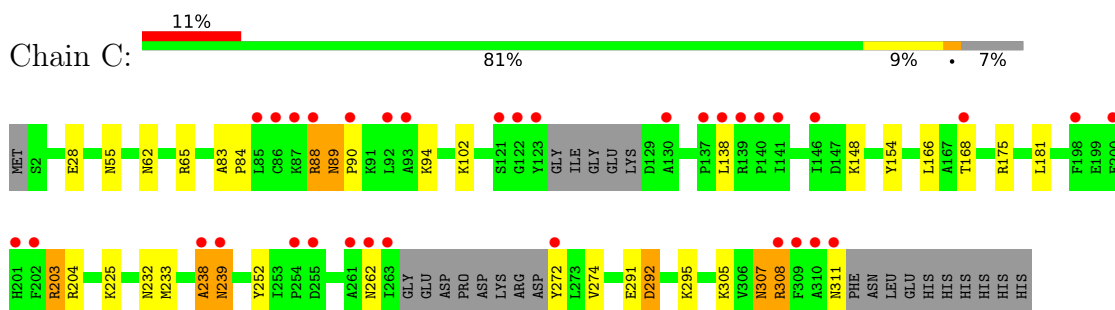
- Molecule 1: Putative sugar-nucleotide epimerase/dehydratase



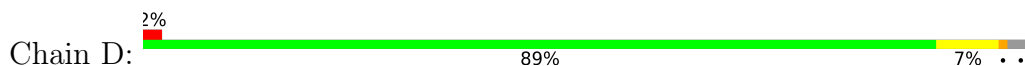
- Molecule 1: Putative sugar-nucleotide epimerase/dehydratase

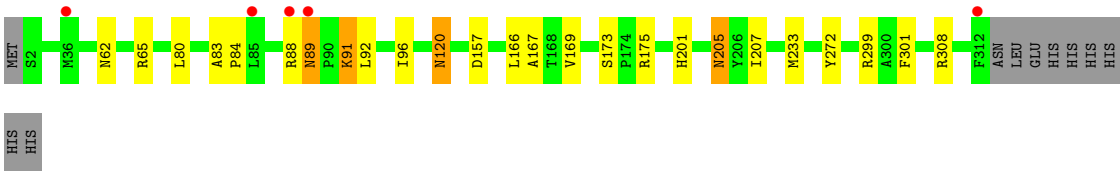


- Molecule 1: Putative sugar-nucleotide epimerase/dehydratase



- Molecule 1: Putative sugar-nucleotide epimerase/dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.61Å 84.34Å 135.45Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	35.14 – 1.50 35.14 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.14-1.50) 97.5 (35.14-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.163 , 0.189 0.164 , 0.190	Depositor DCC
R_{free} test set	11613 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11506	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GDP, NAI, NA, TMA, CL

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	1.05	1/2533 (0.0%)	1.22	2/3415 (0.1%)
1	B	1.07	2/2613 (0.1%)	1.27	7/3522 (0.2%)
1	C	1.10	5/2455 (0.2%)	1.32	9/3308 (0.3%)
1	D	1.09	2/2554 (0.1%)	1.21	2/3443 (0.1%)
All	All	1.08	10/10155 (0.1%)	1.25	20/13688 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308[A]	ARG	C-O	8.35	1.34	1.24
1	B	308[B]	ARG	C-O	8.35	1.34	1.24
1	C	308[A]	ARG	C-O	6.74	1.32	1.24
1	C	308[B]	ARG	C-O	6.74	1.32	1.24
1	D	173	SER	CA-CB	-6.09	1.45	1.54
1	C	232	ASN	C-O	5.68	1.30	1.23
1	C	292	ASP	CG-OD2	5.55	1.35	1.25
1	D	301	PHE	C-O	-5.24	1.17	1.24
1	A	234	GLY	C-O	5.16	1.29	1.23
1	C	274	VAL	C-O	-5.02	1.18	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308[A]	ARG	N-CA-C	14.27	130.14	113.01
1	B	308[B]	ARG	N-CA-C	14.27	130.14	113.01
1	C	308[A]	ARG	N-CA-C	12.15	124.61	111.36
1	C	308[B]	ARG	N-CA-C	12.15	124.61	111.36
1	C	308[A]	ARG	CA-C-O	11.31	132.41	120.42
1	C	308[B]	ARG	CA-C-O	11.31	132.41	120.42
1	C	292	ASP	CA-CB-CG	9.63	122.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308[A]	ARG	CA-C-O	8.40	129.97	119.05
1	B	308[B]	ARG	CA-C-O	8.40	129.97	119.05
1	B	307	ASN	CB-CA-C	6.49	120.47	109.75
1	C	89	ASN	CA-CB-CG	6.06	118.66	112.60
1	C	90	PRO	N-CA-C	6.02	121.46	113.40
1	C	308[A]	ARG	O-C-N	-5.83	115.50	122.15
1	C	308[B]	ARG	O-C-N	-5.83	115.50	122.15
1	B	256	PHE	CA-CB-CG	5.61	119.41	113.80
1	D	299	ARG	CG-CD-NE	5.39	123.86	112.00
1	A	292	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	60	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	256	PHE	CA-CB-CG	5.15	118.95	113.80
1	D	157	ASP	CA-CB-CG	5.11	117.71	112.60

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	2472	0	2496	19	0
1	B	2532	0	2572	23	0
1	C	2397	0	2431	34	0
1	D	2497	0	2520	20	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
3	A	28	0	12	0	0
3	D	28	0	12	2	0
4	A	16	0	24	0	0
4	B	16	0	23	3	0
4	C	12	0	18	0	0
4	D	8	0	12	0	0
5	A	1	0	0	0	0
6	A	5	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	24	3	0
6	C	5	0	12	0	0
6	D	5	0	12	0	0
7	D	1	0	0	0	0
8	A	298	0	0	3	0
8	B	337	0	0	11	0
8	C	299	0	0	10	0
8	D	363	0	0	3	0
All	All	11506	0	10288	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (96) 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)
3:D:402:GDP:H5'	8:D:501:HOH:O	1.48	1.11
1:C:88[A]:ARG:HE	1:C:89:ASN:ND2	1.50	1.08
1:B:255[A]:ASP:OD2	8:B:502:HOH:O	1.78	1.01
1:C:166:LEU:CD2	1:C:233:MET:HE3	1.94	0.96
1:C:204:ARG:O	1:C:239:ASN:HA	1.66	0.95
1:C:88[A]:ARG:HE	1:C:89:ASN:HD21	0.97	0.93
1:D:166:LEU:CD2	1:D:233:MET:HE3	1.99	0.93
1:C:292:ASP:OD1	8:C:501:HOH:O	1.89	0.90
1:C:88[A]:ARG:NE	1:C:89:ASN:HD21	1.73	0.85
1:B:198:PHE:CD2	6:B:407:TMA:H21	2.13	0.83
1:C:168:THR:HG22	8:C:534:HOH:O	1.77	0.82
1:C:28:GLU:OE1	8:C:502:HOH:O	1.97	0.82
1:C:238:ALA:HA	8:C:647:HOH:O	1.80	0.82
1:B:247[A]:GLU:OE2	8:B:503:HOH:O	1.97	0.81
1:D:166:LEU:HD22	1:D:233:MET:HE3	1.63	0.80
1:B:111:SER:HA	4:B:404:EDO:H21	1.64	0.78
1:C:166:LEU:HD21	1:C:233:MET:HE3	1.69	0.75
1:B:224:ASP:OD1	8:B:504:HOH:O	2.06	0.73
1:A:59[A]:MET:SD	1:A:96:ILE:HD13	2.29	0.73
1:A:59[A]:MET:SD	1:A:96:ILE:CD1	2.79	0.71
1:B:120:ASN:C	1:B:120:ASN:HD22	1.99	0.69
1:D:62:ASN:HD22	1:D:65:ARG:NH1	1.90	0.69
3:D:402:GDP:O2B	8:D:501:HOH:O	2.12	0.67
1:D:166:LEU:CD2	1:D:233:MET:CE	2.73	0.65
1:A:120:ASN:HD22	1:A:120:ASN:C	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LYS:NZ	1:B:291:GLU:OE2	2.21	0.62
1:C:166:LEU:HD22	1:C:233:MET:HE3	1.79	0.62
1:D:62:ASN:ND2	1:D:65:ARG:HH12	1.98	0.61
4:B:402:EDO:H21	8:B:610:HOH:O	2.00	0.61
1:C:88[B]:ARG:NH2	8:C:503:HOH:O	2.33	0.61
1:C:62:ASN:HD22	1:C:65:ARG:HH12	1.48	0.61
1:C:203:ARG:HH11	1:C:203:ARG:HG3	1.65	0.60
4:B:403:EDO:H22	8:B:540:HOH:O	2.03	0.59
1:D:62:ASN:HD22	1:D:65:ARG:HH12	1.49	0.59
1:D:120:ASN:C	1:D:120:ASN:HD22	2.10	0.59
1:B:123:TYR:O	8:B:505:HOH:O	2.17	0.59
1:B:166:LEU:CD2	1:B:233:MET:HE3	2.33	0.58
1:D:166:LEU:HD21	1:D:233:MET:HE3	1.81	0.58
1:D:62:ASN:ND2	1:D:65:ARG:NH1	2.54	0.55
1:D:201:HIS:HE1	8:D:756:HOH:O	1.89	0.55
1:C:168:THR:HG21	1:C:181:LEU:HB3	1.89	0.54
1:D:166:LEU:HD21	1:D:233:MET:CE	2.36	0.54
1:B:55:ASN:OD1	1:C:88[A]:ARG:NH2	2.36	0.54
1:B:166:LEU:HD22	1:B:233:MET:HE3	1.90	0.54
1:B:4[C]:LYS:HD3	8:B:508:HOH:O	2.07	0.53
1:C:295:LYS:NZ	8:C:505:HOH:O	2.35	0.53
1:C:88[A]:ARG:NE	1:C:89:ASN:ND2	2.35	0.53
1:A:64:ILE:HG13	1:A:103:MET:HE1	1.90	0.52
1:B:308[B]:ARG:HG2	1:D:308:ARG:HE	1.75	0.52
1:A:250:LYS:NZ	1:A:256:PHE:O	2.41	0.51
1:A:61:GLU:HG3	8:A:692:HOH:O	2.11	0.51
1:C:238:ALA:HB3	8:C:573:HOH:O	2.11	0.50
1:A:59[A]:MET:SD	1:A:96:ILE:HD11	2.50	0.50
1:B:198:PHE:CZ	6:B:407:TMA:H31	2.46	0.50
1:C:307:ASN:ND2	1:C:307:ASN:C	2.70	0.49
1:D:80:LEU:HD13	1:D:96:ILE:HG21	1.95	0.48
1:D:92:LEU:O	1:D:96:ILE:HG22	2.13	0.48
1:C:94:LYS:HD2	8:C:664:HOH:O	2.13	0.48
1:A:85:LEU:HD22	1:C:311:ASN:HB3	1.96	0.47
1:C:62:ASN:ND2	1:C:65:ARG:HH12	2.12	0.47
1:A:166:LEU:CD2	1:A:233:MET:HE3	2.44	0.47
1:A:295:LYS:NZ	8:A:506:HOH:O	2.47	0.46
1:B:198:PHE:CG	6:B:407:TMA:H21	2.51	0.46
1:C:55:ASN:HD22	1:C:55:ASN:C	2.24	0.46
1:B:166:LEU:CD2	1:B:233:MET:CE	2.93	0.45
1:A:120:ASN:C	1:A:120:ASN:ND2	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LYS:O	1:C:308[A]:ARG:HD2	2.16	0.45
1:C:272:TYR:N	8:C:514:HOH:O	2.50	0.45
1:A:166:LEU:CD2	1:A:233:MET:CE	2.95	0.45
1:C:307:ASN:ND2	1:C:307:ASN:O	2.50	0.45
1:B:4[B]:LYS:NZ	8:B:515:HOH:O	2.50	0.44
1:A:55:ASN:C	1:A:55:ASN:HD22	2.25	0.43
1:B:193:LYS:HE3	8:B:683:HOH:O	2.18	0.43
1:C:166:LEU:HD21	1:C:233:MET:CE	2.43	0.43
1:C:102:LYS:HG3	1:C:154:TYR:CZ	2.54	0.43
1:A:150:HIS:HD2	8:A:637:HOH:O	2.02	0.43
1:A:65:ARG:HG3	1:A:107:PHE:CD1	2.53	0.43
1:D:83:ALA:N	1:D:84:PRO:CD	2.82	0.42
1:B:309:PHE:N	8:B:501:HOH:O	1.77	0.42
1:A:59[A]:MET:SD	1:A:95:MET:HE2	2.60	0.42
1:D:89:ASN:OD1	1:D:89:ASN:N	2.53	0.42
1:B:103:MET:HB3	1:B:103:MET:HE2	1.86	0.41
1:C:252:TYR:OH	1:C:291:GLU:OE1	2.27	0.41
1:C:308[B]:ARG:HH11	1:C:308[B]:ARG:HD3	1.72	0.41
1:B:88:ARG:NH1	8:B:509:HOH:O	2.46	0.41
1:D:167:ALA:HB1	1:D:205:ASN:C	2.45	0.41
1:D:88:ARG:C	1:D:89:ASN:OD1	2.64	0.41
1:D:169:VAL:HA	1:D:207:ILE:O	2.21	0.41
1:B:83:ALA:N	1:B:84:PRO:CD	2.84	0.41
1:C:83:ALA:HB3	1:C:84:PRO:HD3	2.03	0.40
1:C:292:ASP:HA	8:C:501:HOH:O	2.20	0.40
1:D:91:LYS:N	1:D:91:LYS:HD3	2.35	0.40
1:A:59[B]:MET:SD	1:A:100:ALA:HB2	2.61	0.40
1:C:83:ALA:N	1:C:84:PRO:CD	2.85	0.40
1:A:169:VAL:HA	1:A:207:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	307/321 (96%)	300 (98%)	7 (2%)	0	100	100
1	B	318/321 (99%)	309 (97%)	9 (3%)	0	100	100
1	C	295/321 (92%)	284 (96%)	9 (3%)	2 (1%)	18	5
1	D	311/321 (97%)	303 (97%)	8 (3%)	0	100	100
All	All	1231/1284 (96%)	1196 (97%)	33 (3%)	2 (0%)	43	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	238	ALA
1	C	262	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	263 (97%)	7 (3%)	40	13
1	B	279/280 (100%)	271 (97%)	8 (3%)	37	10
1	C	262/280 (94%)	252 (96%)	10 (4%)	29	6
1	D	272/280 (97%)	266 (98%)	6 (2%)	45	17
All	All	1083/1120 (97%)	1052 (97%)	31 (3%)	39	10

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24[A]	GLU
1	A	24[B]	GLU
1	A	91	LYS
1	A	120	ASN
1	A	175	ARG
1	A	205	ASN
1	A	272	TYR
1	B	38	ASP
1	B	88	ARG

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Mol	Chain	Res	Type
1	B	103	MET
1	B	120	ASN
1	B	131	MET
1	B	148	LYS
1	B	175	ARG
1	B	205	ASN
1	C	88[A]	ARG
1	C	88[B]	ARG
1	C	138	LEU
1	C	148	LYS
1	C	175	ARG
1	C	203	ARG
1	C	225	LYS
1	C	239	ASN
1	C	305	LYS
1	C	307	ASN
1	D	89	ASN
1	D	91	LYS
1	D	120	ASN
1	D	175	ARG
1	D	205	ASN
1	D	272	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	120	ASN
1	A	150	HIS
1	A	205	ASN
1	B	120	ASN
1	B	205	ASN
1	B	262	ASN
1	B	276	ASN
1	B	307	ASN
1	C	55	ASN
1	C	62	ASN
1	C	89	ASN
1	C	307	ASN
1	D	55	ASN
1	D	62	ASN
1	D	120	ASN

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Mol	Chain	Res	Type
1	D	153	GLN
1	D	201	HIS
1	D	205	ASN
1	D	276	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	$\# Z > 2$
6	TMA	B	407	-	4,4,4	0.21	0	6,6,6	0.20	0
6	TMA	B	406	-	4,4,4	0.37	0	6,6,6	0.05	0
3	GDP	D	402	-	29,30,30	1.16	2 (6%)	45,47,47	1.45	9 (20%)
4	EDO	C	402	-	3,3,3	0.42	0	2,2,2	0.32	0
4	EDO	B	402	-	3,3,3	0.09	0	2,2,2	0.27	0
6	TMA	A	408	-	4,4,4	0.34	0	6,6,6	0.09	0
4	EDO	C	403	-	3,3,3	0.41	0	2,2,2	0.60	0
4	EDO	D	405	-	3,3,3	0.29	0	2,2,2	0.09	0
4	EDO	A	404	-	3,3,3	0.15	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAI	D	401	-	47,48,48	0.96	2 (4%)	64,73,73	0.83	2 (3%)
2	NAI	B	401	-	47,48,48	0.98	3 (6%)	64,73,73	0.78	0
6	TMA	D	406	-	4,4,4	0.23	0	6,6,6	0.12	0
4	EDO	D	404	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	A	406	-	3,3,3	0.10	0	2,2,2	0.07	0
3	GDP	A	402	-	29,30,30	1.18	5 (17%)	45,47,47	1.24	4 (8%)
4	EDO	A	405	-	3,3,3	0.28	0	2,2,2	0.06	0
4	EDO	B	403	-	3,3,3	0.27	0	2,2,2	0.56	0
4	EDO	C	404	-	3,3,3	0.51	0	2,2,2	0.35	0
6	TMA	C	405	-	4,4,4	0.33	0	6,6,6	0.09	0
4	EDO	B	405	-	3,3,3	0.61	0	2,2,2	1.22	0
2	NAI	A	401	-	47,48,48	0.92	2 (4%)	64,73,73	0.68	0
4	EDO	A	403	-	3,3,3	0.18	0	2,2,2	0.14	0
4	EDO	B	404	-	3,3,3	0.80	0	2,2,2	0.78	0
2	NAI	C	401	-	47,48,48	1.25	5 (10%)	64,73,73	0.90	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	D	402	-	-	2/16/32/32	0/3/3/3
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
2	NAI	D	401	-	-	5/29/72/72	0/5/5/5
2	NAI	B	401	-	-	4/29/72/72	0/5/5/5
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
3	GDP	A	402	-	-	1/16/32/32	0/3/3/3
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	C	404	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
2	NAI	A	401	-	-	4/29/72/72	0/5/5/5
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	C	401	-	-	2/29/72/72	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAI	C4N-C5N	-4.34	1.37	1.49
2	C	401	NAI	PN-O3	3.98	1.63	1.59
2	A	401	NAI	C4N-C3N	-3.93	1.42	1.50
2	D	401	NAI	C4N-C3N	-3.84	1.42	1.50
2	B	401	NAI	C4N-C5N	-3.39	1.40	1.49
2	C	401	NAI	PA-O3	3.12	1.62	1.59
2	A	401	NAI	C4N-C5N	-2.95	1.41	1.49
2	B	401	NAI	PN-O3	2.90	1.62	1.59
3	D	402	GDP	C5-C4	2.68	1.46	1.38
3	A	402	GDP	C6-N1	-2.57	1.34	1.38
2	C	401	NAI	C4N-C3N	-2.54	1.45	1.50
2	D	401	NAI	C4N-C5N	-2.52	1.42	1.49
3	A	402	GDP	C5-C4	2.51	1.45	1.38
3	D	402	GDP	O4'-C1'	2.43	1.47	1.42
3	A	402	GDP	C5-N7	-2.43	1.34	1.39
2	B	401	NAI	C4N-C3N	-2.29	1.45	1.50
3	A	402	GDP	O3'-C3'	2.11	1.48	1.43
2	C	401	NAI	PN-O1N	-2.02	1.46	1.55
3	A	402	GDP	PB-O2B	-2.01	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	GDP	C6-C5-N7	3.13	135.98	130.29
3	A	402	GDP	C5-C4-N3	-2.91	123.75	128.39
3	D	402	GDP	C2-N3-C4	2.86	117.23	112.30
3	D	402	GDP	O2A-PA-O1A	2.76	125.30	112.44
3	D	402	GDP	O3A-PA-O1A	-2.65	102.73	110.70
3	D	402	GDP	N9-C4-N3	2.60	131.16	125.95
3	A	402	GDP	N9-C4-N3	2.56	131.08	125.95
3	D	402	GDP	C5-C4-N3	-2.55	124.33	128.39
2	D	401	NAI	O7N-C7N-C3N	-2.51	116.18	120.90
2	D	401	NAI	C3N-C2N-N1N	-2.47	119.58	123.20
3	D	402	GDP	O6-C6-C5	-2.44	120.10	126.53
3	D	402	GDP	O2B-PB-O1B	2.41	120.21	110.83
3	D	402	GDP	C6-C5-C4	-2.32	115.33	118.83
3	A	402	GDP	C2-N3-C4	2.23	116.14	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	GDP	C6-C5-N7	2.15	134.21	130.29
2	C	401	NAI	O3-PA-O1A	-2.02	104.64	110.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

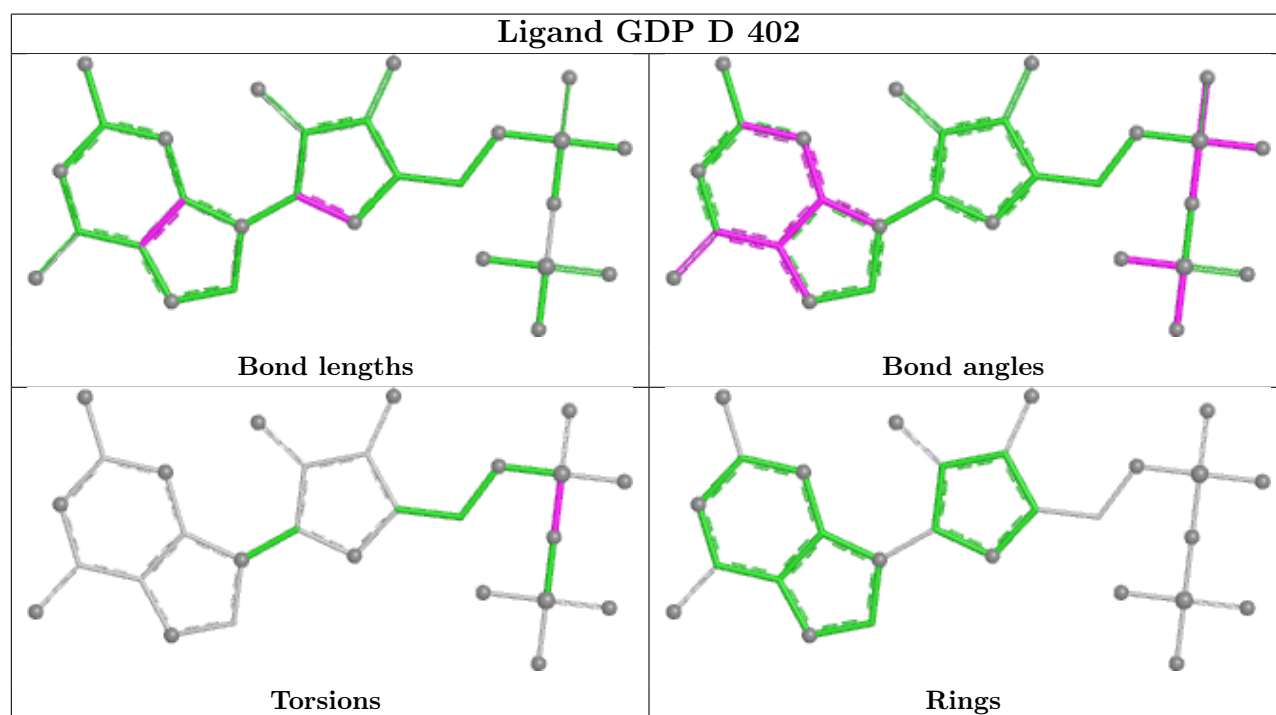
Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	C5D-O5D-PN-O2N
2	C	401	NAI	C5D-O5D-PN-O2N
2	D	401	NAI	C5B-O5B-PA-O1A
2	D	401	NAI	C5D-O5D-PN-O2N
2	A	401	NAI	O4D-C1D-N1N-C6N
4	B	403	EDO	O1-C1-C2-O2
2	D	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	C5D-O5D-PN-O3
2	D	401	NAI	C5B-O5B-PA-O2A
2	D	401	NAI	C5B-O5B-PA-O3
4	C	403	EDO	O1-C1-C2-O2
2	A	401	NAI	C2N-C3N-C7N-N7N
3	D	402	GDP	PB-O3A-PA-O2A
4	B	405	EDO	O1-C1-C2-O2
2	A	401	NAI	O4B-C4B-C5B-O5B
4	A	405	EDO	O1-C1-C2-O2
4	C	404	EDO	O1-C1-C2-O2
3	D	402	GDP	PB-O3A-PA-O1A
3	A	402	GDP	PB-O3A-PA-O2A

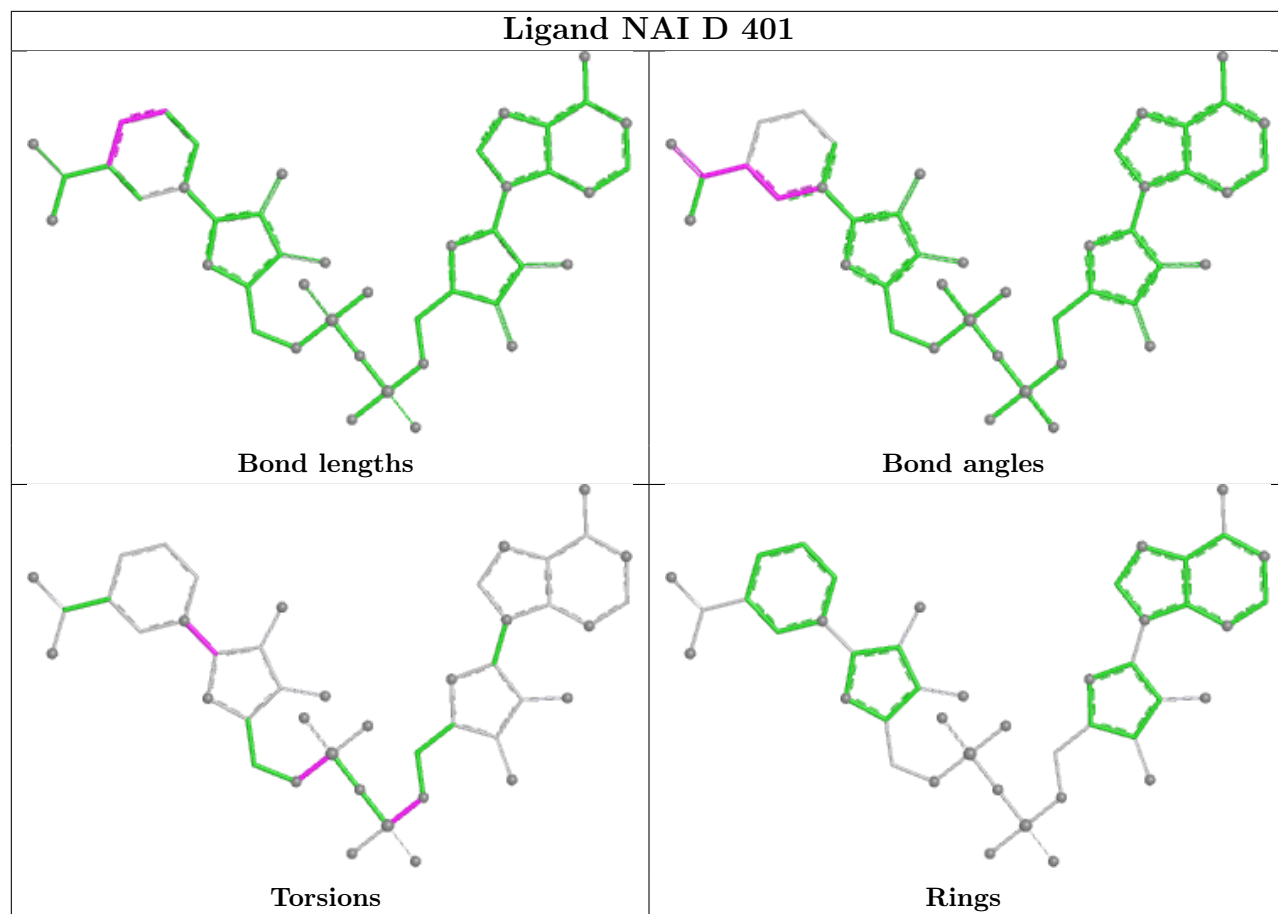
There are no ring outliers.

5 monomers are involved in 8 short contacts:

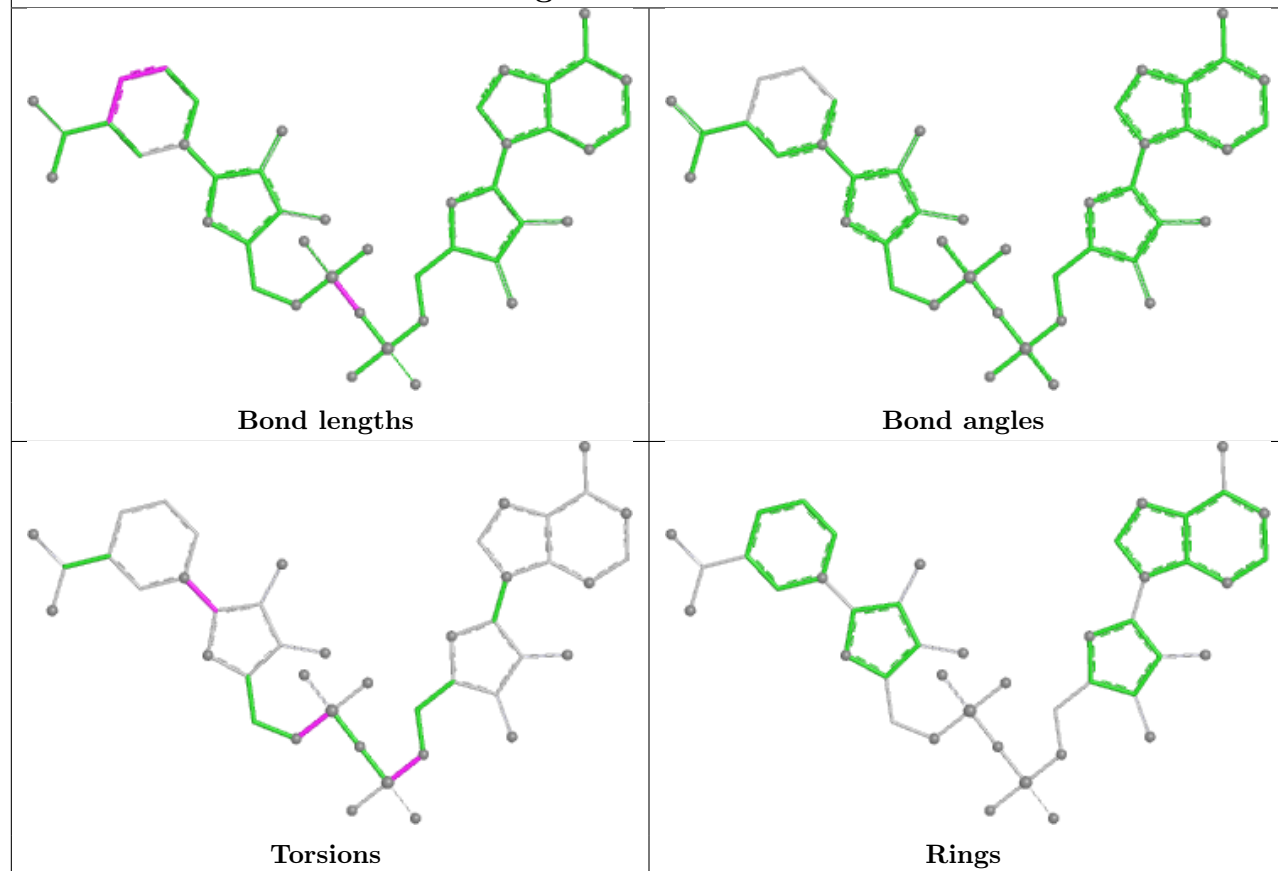
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	407	TMA	3	0
3	D	402	GDP	2	0
4	B	402	EDO	1	0
4	B	403	EDO	1	0
4	B	404	EDO	1	0

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.

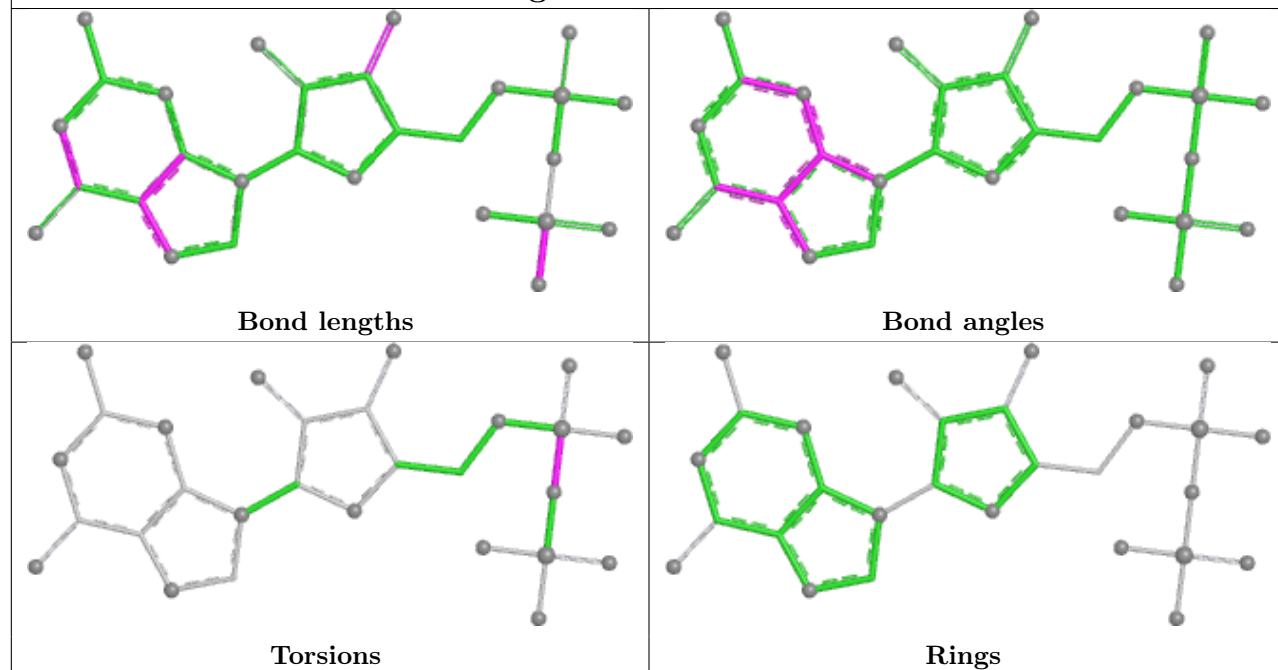


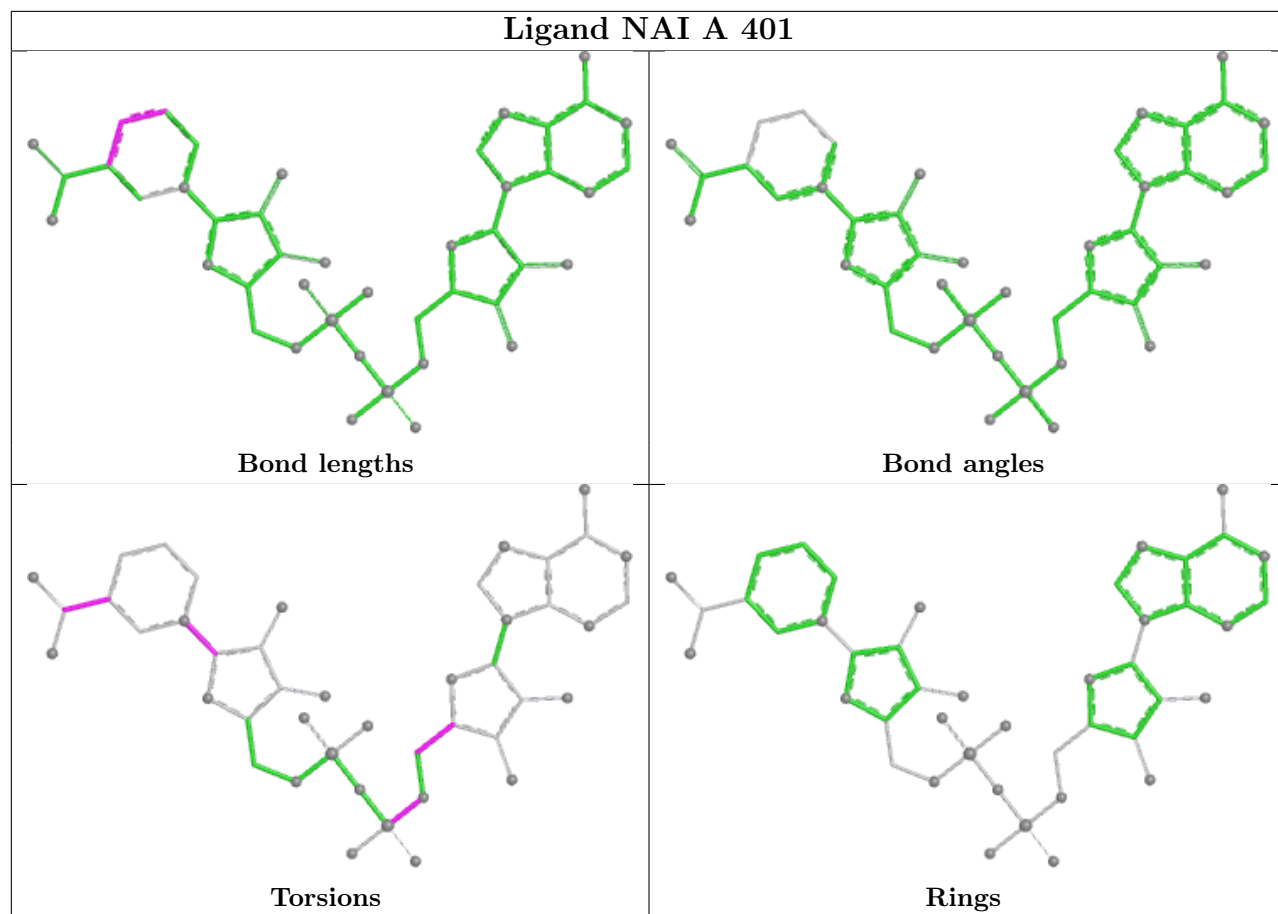


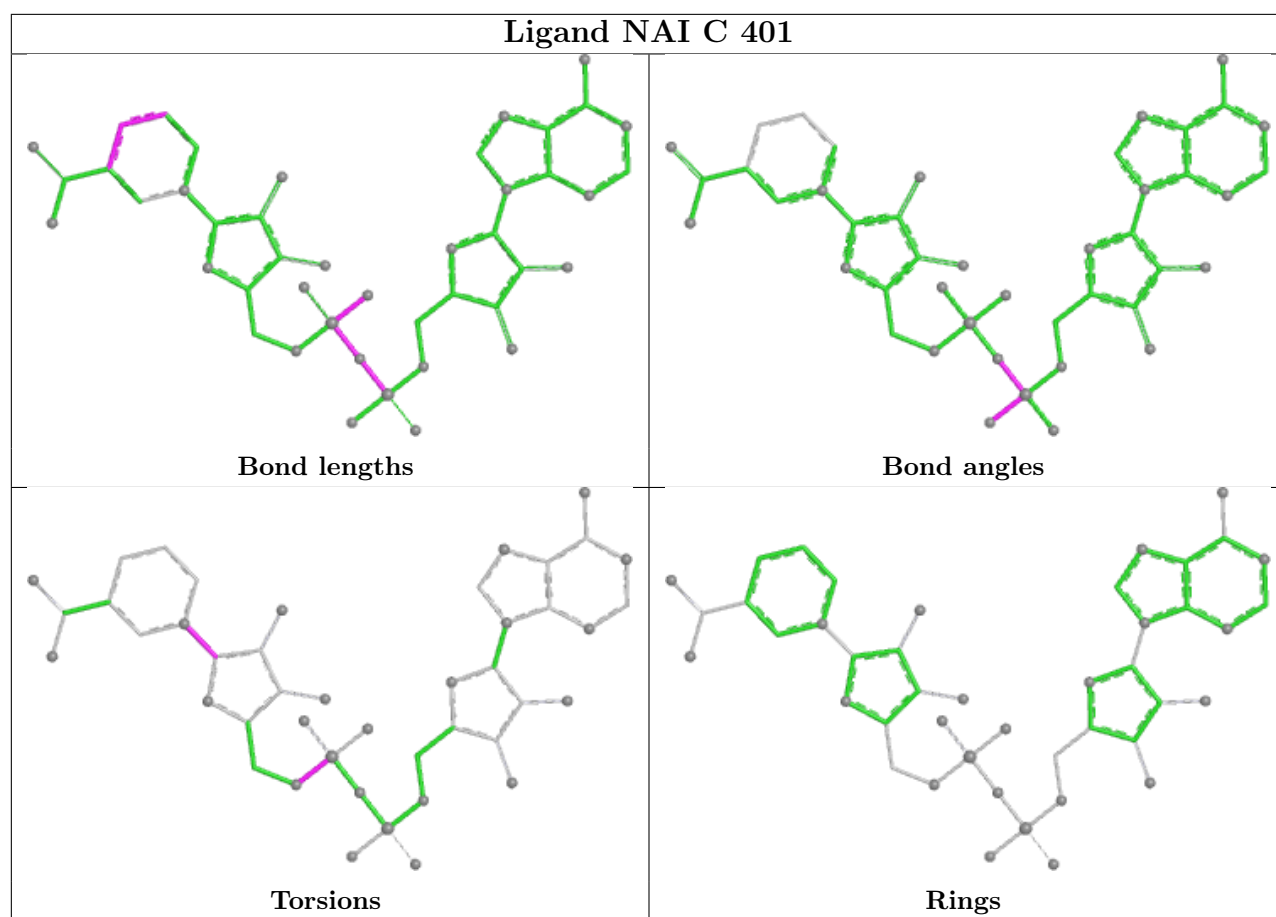
Ligand NAI B 401



Ligand GDP A 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	307/321 (95%)	0.26	8 (2%) 57 61	11, 19, 32, 60	4 (1%)
1	B	310/321 (96%)	0.02	9 (2%) 53 58	9, 16, 29, 46	10 (3%)
1	C	297/321 (92%)	0.45	34 (11%) 10 10	10, 18, 41, 65	4 (1%)
1	D	311/321 (96%)	0.04	5 (1%) 70 74	10, 17, 32, 52	2 (0%)
All	All	1225/1284 (95%)	0.19	56 (4%) 37 41	9, 17, 34, 65	20 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	310	ALA	7.9
1	C	238	ALA	7.8
1	C	138	LEU	6.8
1	C	202	PHE	5.7
1	C	272	TYR	5.5
1	C	201	HIS	5.0
1	D	312	PHE	4.9
1	C	263	ILE	4.5
1	C	141	ILE	3.9
1	A	130	ALA	3.7
1	B	310	ALA	3.7
1	B	308[A]	ARG	3.6
1	C	239	ASN	3.6
1	C	90	PRO	3.5
1	A	312	PHE	3.4
1	B	141	ILE	3.3
1	C	122	GLY	3.2
1	C	262	ASN	3.2
1	C	121	SER	3.1
1	D	89	ASN	3.1
1	A	153	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	311	ASN	3.0
1	C	123	TYR	2.9
1	C	140	PRO	2.8
1	B	139	ARG	2.7
1	C	137	PRO	2.7
1	C	88[A]	ARG	2.6
1	D	88	ARG	2.6
1	C	308[A]	ARG	2.5
1	D	85	LEU	2.5
1	C	93	ALA	2.4
1	C	130	ALA	2.4
1	C	92	LEU	2.4
1	A	61	GLU	2.4
1	C	168	THR	2.4
1	C	139	ARG	2.4
1	C	254	PRO	2.4
1	C	198	PHE	2.4
1	B	88	ARG	2.3
1	C	87	LYS	2.3
1	C	309	PHE	2.2
1	A	103	MET	2.2
1	C	146	ILE	2.1
1	A	262	ASN	2.1
1	A	2	SER	2.1
1	C	261	ALA	2.1
1	B	307	ASN	2.1
1	C	255	ASP	2.1
1	D	36	MET	2.1
1	B	202	PHE	2.1
1	C	200	GLU	2.1
1	C	85	LEU	2.1
1	B	135	GLU	2.1
1	A	88	ARG	2.0
1	B	270	ARG	2.0
1	C	86	CYS	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

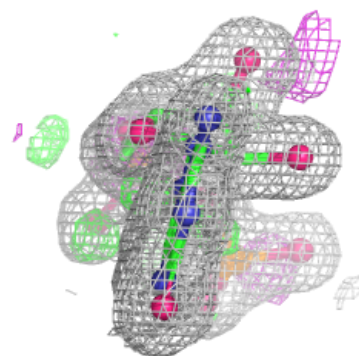
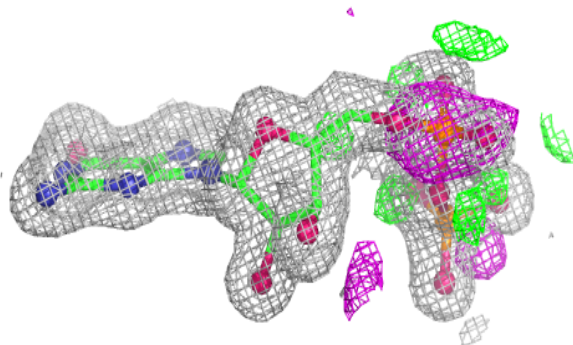
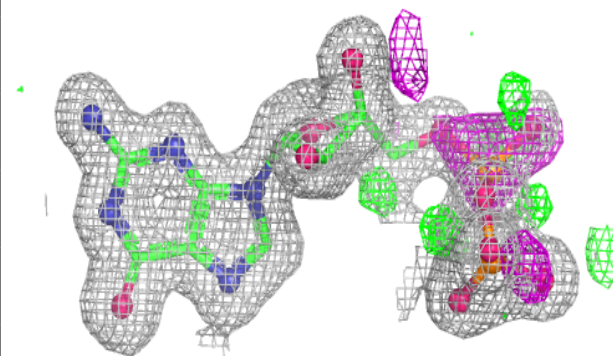
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	406	4/4	0.78	0.14	44,52,52,54	0
4	EDO	B	405	4/4	0.78	0.17	35,36,37,37	0
4	EDO	D	405	4/4	0.81	0.15	28,31,34,37	0
6	TMA	B	407	5/5	0.81	0.26	38,43,49,49	0
6	TMA	A	408	5/5	0.84	0.19	51,54,56,56	0
6	TMA	B	406	5/5	0.85	0.21	63,67,68,69	0
6	TMA	C	405	5/5	0.88	0.14	43,47,48,49	0
4	EDO	C	403	4/4	0.89	0.15	25,29,33,34	0
4	EDO	B	404	4/4	0.89	0.29	28,28,28,30	0
4	EDO	A	405	4/4	0.89	0.11	32,33,34,37	0
6	TMA	D	406	5/5	0.89	0.13	30,35,35,36	0
4	EDO	C	404	4/4	0.90	0.11	28,28,30,33	0
4	EDO	A	404	4/4	0.91	0.09	33,38,42,44	0
4	EDO	B	402	4/4	0.91	0.10	35,37,37,40	0
4	EDO	C	402	4/4	0.93	0.08	24,25,27,29	0
4	EDO	B	403	4/4	0.95	0.12	22,26,30,34	0
3	GDP	D	402	28/28	0.95	0.07	13,16,20,21	0
4	EDO	A	403	4/4	0.97	0.07	20,21,21,21	0
4	EDO	D	404	4/4	0.97	0.06	16,16,16,17	0
3	GDP	A	402	28/28	0.98	0.05	14,16,19,20	0
7	NA	D	403	1/1	0.98	0.04	17,17,17,17	0
2	NAI	A	401	44/44	0.99	0.04	12,13,16,18	0
2	NAI	B	401	44/44	0.99	0.04	10,12,13,14	0
2	NAI	C	401	44/44	0.99	0.04	11,12,13,14	0
5	CL	A	407	1/1	0.99	0.04	21,21,21,21	0
2	NAI	D	401	44/44	0.99	0.04	10,12,15,18	0

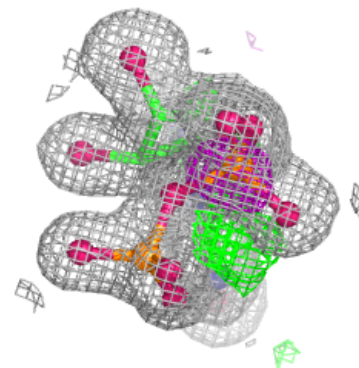
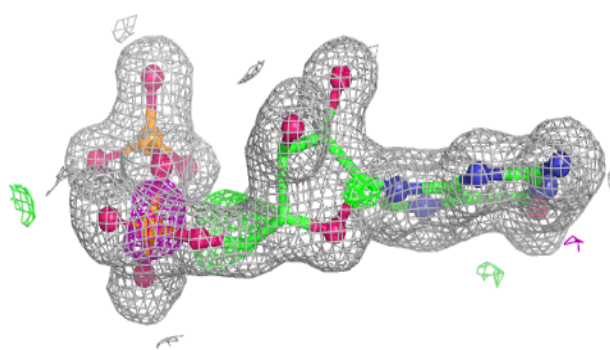
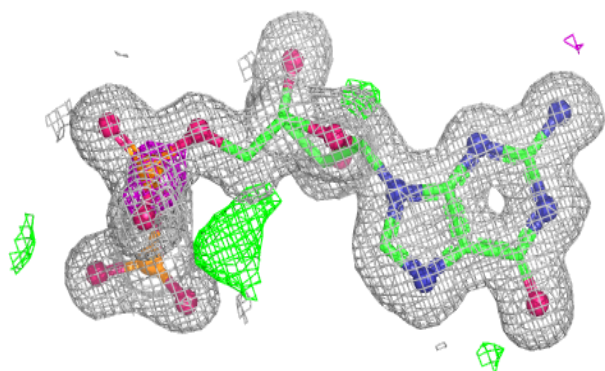
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP 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)

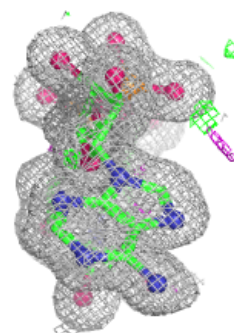
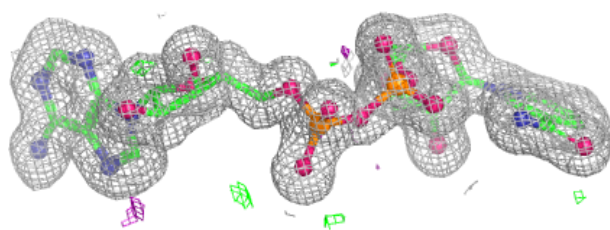
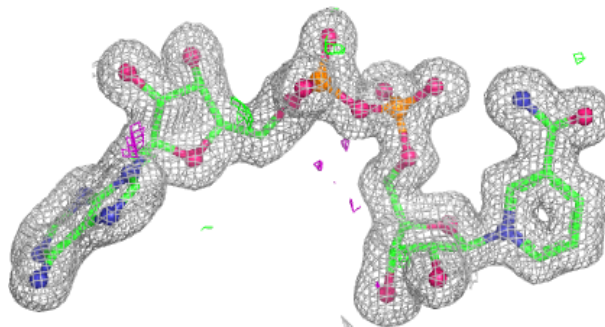
**Electron density around GDP A 402:**

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

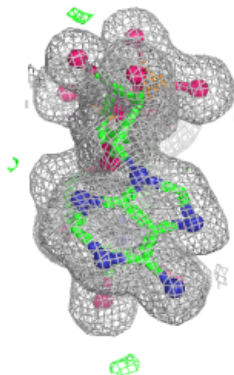
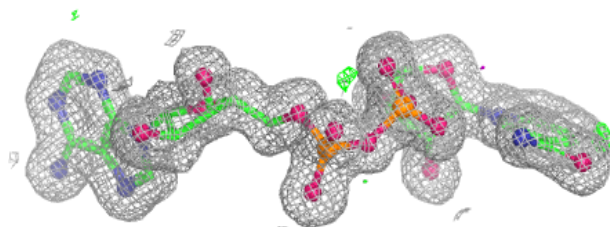
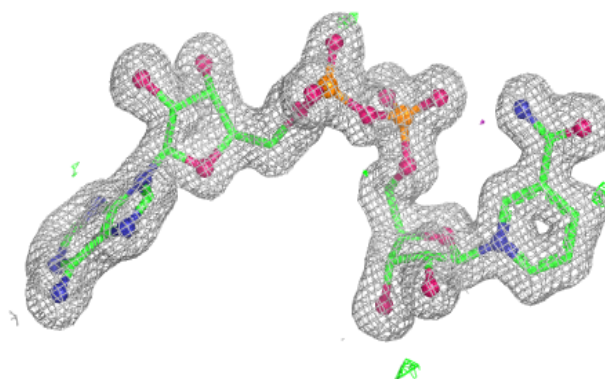


Electron density around NAI A 401:

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

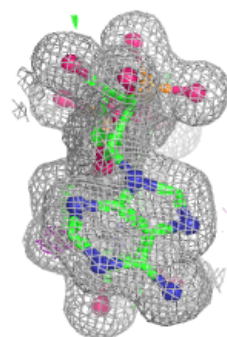
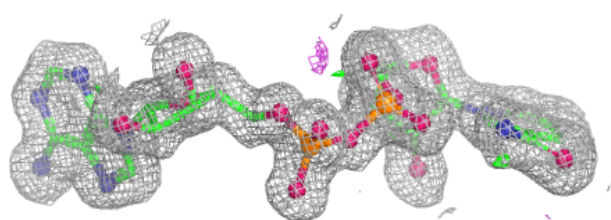
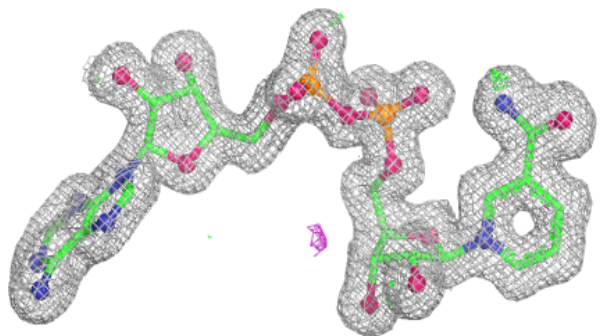
**Electron density around NAI B 401:**

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

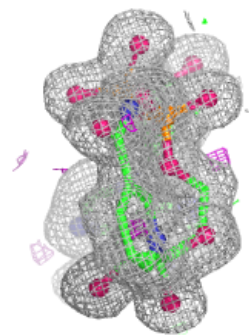
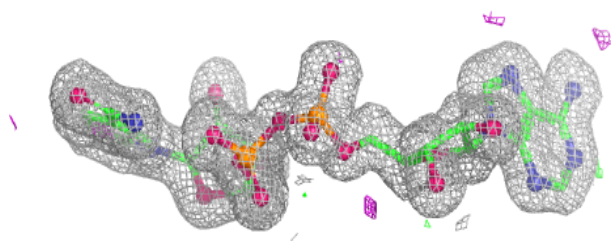
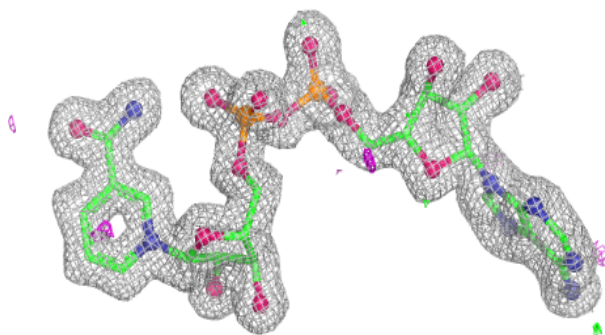


Electron density around NAI C 401:

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

**Electron density around NAI D 401:**

$2mF_o-DF_c$ (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.