



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2023 – 10:24 PM JST

PDB ID : 8HRT
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from *Corynebacterium glutamicum* ATCC13032 (L36S/T37K/F100V/P192S) in complex with NADP
Authors : Son, H.F.; Kim, K.J.
Deposited on : 2022-12-15
Resolution : 1.99 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

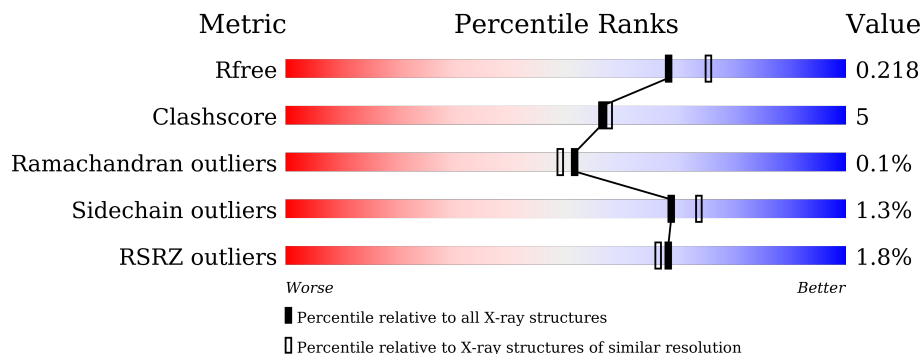
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	342	 % 89% 8% ..
1	B	342	 % 86% 11% ..
1	C	342	 2% 87% 11% ..
1	D	342	 3% 89% 8% .

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11172 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2541	1588	441	506	6	0	0	0
1	B	336	2551	1594	444	507	6	0	0	0
1	C	335	2541	1588	441	506	6	0	0	0
1	D	334	2532	1583	440	503	6	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

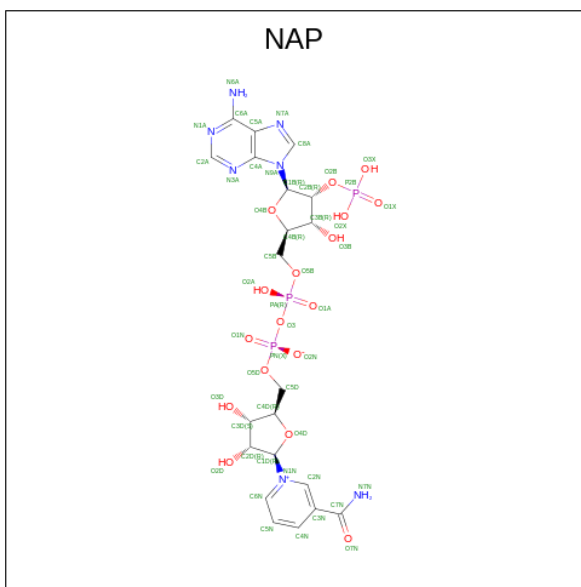
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	SER	LEU	engineered mutation	UNP A0A8G0CHY2
A	37	LYS	THR	engineered mutation	UNP A0A8G0CHY2
A	100	VAL	PHE	engineered mutation	UNP A0A8G0CHY2
A	192	SER	PRO	engineered mutation	UNP A0A8G0CHY2
A	335	LEU	-	expression tag	UNP A0A8G0CHY2
A	336	GLU	-	expression tag	UNP A0A8G0CHY2
A	337	HIS	-	expression tag	UNP A0A8G0CHY2
A	338	HIS	-	expression tag	UNP A0A8G0CHY2
A	339	HIS	-	expression tag	UNP A0A8G0CHY2
A	340	HIS	-	expression tag	UNP A0A8G0CHY2
A	341	HIS	-	expression tag	UNP A0A8G0CHY2
A	342	HIS	-	expression tag	UNP A0A8G0CHY2
B	36	SER	LEU	engineered mutation	UNP A0A8G0CHY2
B	37	LYS	THR	engineered mutation	UNP A0A8G0CHY2
B	100	VAL	PHE	engineered mutation	UNP A0A8G0CHY2
B	192	SER	PRO	engineered mutation	UNP A0A8G0CHY2
B	335	LEU	-	expression tag	UNP A0A8G0CHY2
B	336	GLU	-	expression tag	UNP A0A8G0CHY2
B	337	HIS	-	expression tag	UNP A0A8G0CHY2
B	338	HIS	-	expression tag	UNP A0A8G0CHY2
B	339	HIS	-	expression tag	UNP A0A8G0CHY2

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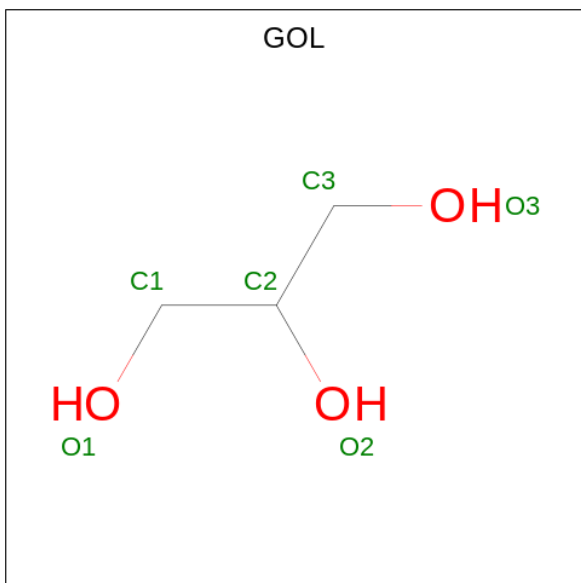
Chain	Residue	Modelled	Actual	Comment	Reference
B	340	HIS	-	expression tag	UNP A0A8G0CHY2
B	341	HIS	-	expression tag	UNP A0A8G0CHY2
B	342	HIS	-	expression tag	UNP A0A8G0CHY2
C	36	SER	LEU	engineered mutation	UNP A0A8G0CHY2
C	37	LYS	THR	engineered mutation	UNP A0A8G0CHY2
C	100	VAL	PHE	engineered mutation	UNP A0A8G0CHY2
C	192	SER	PRO	engineered mutation	UNP A0A8G0CHY2
C	335	LEU	-	expression tag	UNP A0A8G0CHY2
C	336	GLU	-	expression tag	UNP A0A8G0CHY2
C	337	HIS	-	expression tag	UNP A0A8G0CHY2
C	338	HIS	-	expression tag	UNP A0A8G0CHY2
C	339	HIS	-	expression tag	UNP A0A8G0CHY2
C	340	HIS	-	expression tag	UNP A0A8G0CHY2
C	341	HIS	-	expression tag	UNP A0A8G0CHY2
C	342	HIS	-	expression tag	UNP A0A8G0CHY2
D	36	SER	LEU	engineered mutation	UNP A0A8G0CHY2
D	37	LYS	THR	engineered mutation	UNP A0A8G0CHY2
D	100	VAL	PHE	engineered mutation	UNP A0A8G0CHY2
D	192	SER	PRO	engineered mutation	UNP A0A8G0CHY2
D	335	LEU	-	expression tag	UNP A0A8G0CHY2
D	336	GLU	-	expression tag	UNP A0A8G0CHY2
D	337	HIS	-	expression tag	UNP A0A8G0CHY2
D	338	HIS	-	expression tag	UNP A0A8G0CHY2
D	339	HIS	-	expression tag	UNP A0A8G0CHY2
D	340	HIS	-	expression tag	UNP A0A8G0CHY2
D	341	HIS	-	expression tag	UNP A0A8G0CHY2
D	342	HIS	-	expression tag	UNP A0A8G0CHY2

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



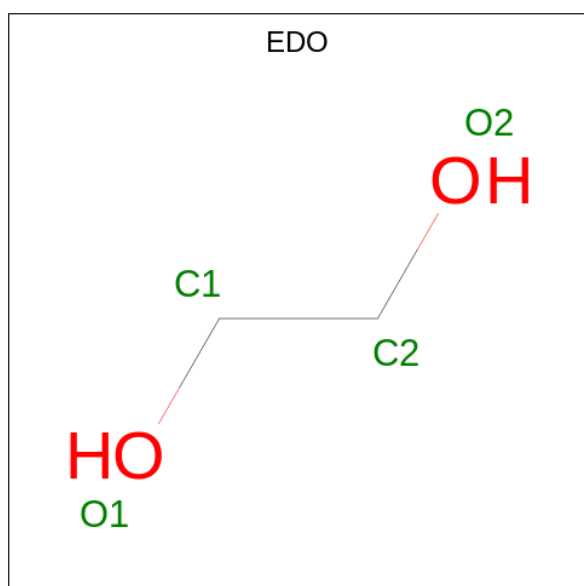
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

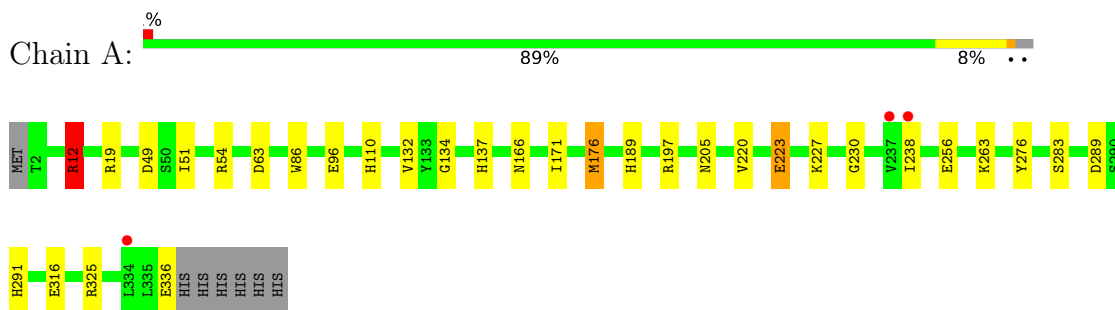
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	229	Total	O	0	0
			229	229		
5	B	235	Total	O	0	0
			235	235		
5	C	191	Total	O	0	0
			191	191		
5	D	132	Total	O	0	0
			132	132		

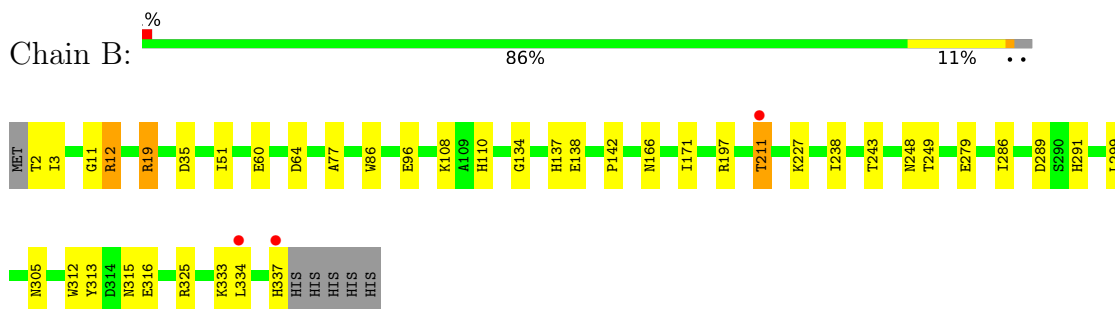
3 Residue-property plots [i](#)

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.

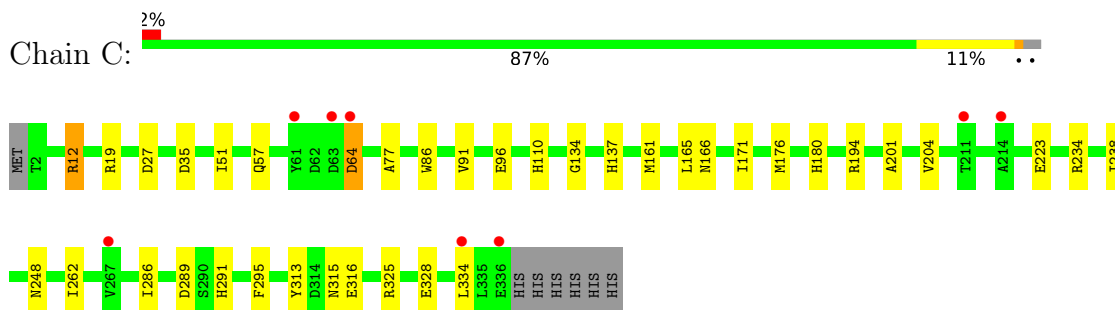
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



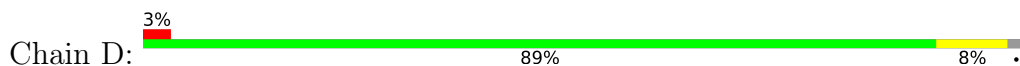
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

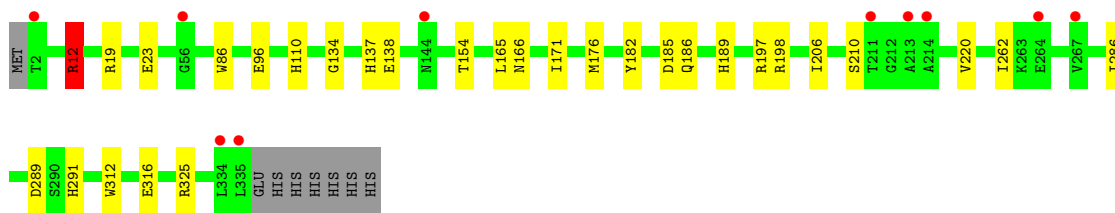


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.97Å 119.99Å 144.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.72 – 1.99 36.69 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.9 (36.72-1.99) 96.9 (36.69-1.99)	Depositor EDS
R_{merge}	0.98	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.168 , 0.215 0.177 , 0.218	Depositor DCC
R_{free} test set	4642 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11172	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, GOL, NAP

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	0.44	1/2582 (0.0%)	0.73	2/3508 (0.1%)
1	B	0.43	0/2593	0.77	5/3523 (0.1%)
1	C	0.38	0/2582	0.76	4/3508 (0.1%)
1	D	0.38	0/2573	0.74	3/3496 (0.1%)
All	All	0.41	1/10330 (0.0%)	0.75	14/14035 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLU	CD-OE2	-5.33	1.19	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	NE-CZ-NH1	-9.96	115.32	120.30
1	C	12	ARG	NE-CZ-NH2	9.01	124.81	120.30
1	B	12	ARG	NE-CZ-NH1	-8.71	115.94	120.30
1	B	19	ARG	NE-CZ-NH2	-7.89	116.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	C	19	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	19	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	19	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	C	12	ARG	NE-CZ-NH1	-7.53	116.54	120.30
1	A	12	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	D	12	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	B	12	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	B	211	THR	CA-CB-CG2	5.33	119.86	112.40
1	D	19	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	205	ASN	Peptide
1	A	325	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	325	ARG	Sidechain
1	C	325	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	325	ARG	Sidechain

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	2541	0	2509	25	0
1	B	2551	0	2516	32	0
1	C	2541	0	2509	27	0
1	D	2532	0	2503	22	0
2	A	48	0	25	0	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	1	0
3	B	6	0	8	2	0
3	C	6	0	8	2	0
4	B	4	0	6	0	0
5	A	229	0	0	5	0
5	B	235	0	0	7	0
5	C	191	0	0	2	0
5	D	132	0	0	3	0
All	All	11172	0	10175	102	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 (102) 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:B:12:ARG:HD3	1:B:316:GLU:OE2	1.64	0.97
1:A:12:ARG:HD3	1:A:316:GLU:OE2	1.75	0.86
1:A:166:ASN:HD22	1:A:171:ILE:H	1.22	0.84
1:C:57:GLN:OE1	3:C:402:GOL:H11	1.78	0.83
1:D:12:ARG:HD3	1:D:316:GLU:OE2	1.79	0.82
1:C:12:ARG:HD3	1:C:316:GLU:OE2	1.80	0.79
1:D:166:ASN:HD22	1:D:171:ILE:H	1.32	0.77
1:D:86:TRP:HE1	1:D:110:HIS:HD2	1.33	0.76
1:B:19:ARG:HD2	5:B:694:HOH:O	1.86	0.75
1:A:12:ARG:CD	1:A:316:GLU:OE2	2.40	0.70
1:B:279:GLU:OE1	3:B:403:GOL:O1	2.10	0.70
1:C:194:ARG:NH1	5:C:501:HOH:O	2.26	0.69
1:C:64:ASP:HA	5:C:555:HOH:O	1.93	0.69
1:C:204:VAL:HG12	1:C:204:VAL:O	1.93	0.68
1:B:289:ASP:OD1	1:B:291:HIS:HD2	1.78	0.67
1:C:86:TRP:HE1	1:C:110:HIS:HD2	1.41	0.67
1:C:166:ASN:HD22	1:C:171:ILE:H	1.43	0.67
1:B:86:TRP:HE1	1:B:110:HIS:HD2	1.41	0.66
1:D:86:TRP:HE1	1:D:110:HIS:CD2	2.13	0.66
1:C:315:ASN:HD22	2:C:401:NAP:H72N	1.41	0.66
1:A:86:TRP:HE1	1:A:110:HIS:HD2	1.44	0.65
1:B:227:LYS:HE2	5:B:570:HOH:O	1.97	0.65
1:A:134:GLY:H	1:A:137:HIS:CD2	2.16	0.64
1:B:315:ASN:HD22	2:B:401:NAP:H72N	1.45	0.64
1:B:86:TRP:HE1	1:B:110:HIS:CD2	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASN:HD22	1:B:171:ILE:H	1.46	0.62
1:B:3:ILE:HD12	1:B:3:ILE:N	2.15	0.61
1:C:134:GLY:H	1:C:137:HIS:HD2	1.48	0.61
1:C:289:ASP:OD1	1:C:291:HIS:HD2	1.84	0.61
1:D:165:LEU:HD21	1:D:262:ILE:CD1	2.30	0.61
1:D:185:ASP:OD2	1:D:198:ARG:NH2	2.34	0.60
1:A:256:GLU:HG3	5:A:633:HOH:O	2.01	0.60
1:A:336:GLU:C	5:A:507:HOH:O	2.39	0.60
1:C:134:GLY:H	1:C:137:HIS:CD2	2.19	0.60
1:A:289:ASP:OD1	1:A:291:HIS:HD2	1.85	0.59
1:B:96:GLU:OE2	1:B:110:HIS:HE1	1.85	0.59
1:A:96:GLU:OE2	1:A:110:HIS:HE1	1.87	0.58
1:C:57:GLN:OE1	3:C:402:GOL:C1	2.52	0.58
1:D:12:ARG:CD	1:D:316:GLU:OE2	2.50	0.57
1:C:51:ILE:HD11	1:C:238:ILE:HG12	1.86	0.57
1:A:86:TRP:HE1	1:A:110:HIS:CD2	2.23	0.56
1:A:227:LYS:NZ	5:A:505:HOH:O	2.40	0.55
1:B:134:GLY:H	1:B:137:HIS:CD2	2.25	0.55
1:C:262:ILE:HD13	1:C:295:PHE:CZ	2.41	0.55
1:A:51:ILE:HD11	1:A:238:ILE:HG12	1.87	0.55
1:D:23:GLU:OE2	5:D:501:HOH:O	2.18	0.54
1:B:134:GLY:H	1:B:137:HIS:HD2	1.56	0.53
1:B:334:LEU:HD12	5:B:635:HOH:O	2.07	0.53
1:B:291:HIS:HE1	5:B:698:HOH:O	1.90	0.52
1:C:96:GLU:OE2	1:C:110:HIS:HE1	1.91	0.52
1:C:289:ASP:OD1	1:C:291:HIS:CD2	2.61	0.52
1:A:63:ASP:OD1	3:A:403:GOL:O3	2.26	0.51
1:A:166:ASN:ND2	1:A:171:ILE:H	1.99	0.50
1:B:35:ASP:O	1:B:77:ALA:HA	2.11	0.50
1:B:64:ASP:HA	5:B:569:HOH:O	2.12	0.50
1:B:248:ASN:HD21	1:C:248:ASN:HB3	1.77	0.49
1:D:138:GLU:HG2	5:D:597:HOH:O	2.10	0.49
1:A:176:MET:HG3	1:A:230:GLY:HA3	1.92	0.49
1:D:134:GLY:H	1:D:137:HIS:HD2	1.61	0.49
1:C:165:LEU:HD21	1:C:262:ILE:HD11	1.94	0.49
1:C:204:VAL:O	1:C:204:VAL:CG1	2.61	0.49
1:A:12:ARG:NH1	1:A:49:ASP:OD2	2.35	0.48
1:A:134:GLY:H	1:A:137:HIS:HD2	1.59	0.48
1:D:154:THR:HG21	1:D:176:MET:HE1	1.94	0.48
1:A:54:ARG:HH22	3:B:403:GOL:H11	1.79	0.48
1:C:86:TRP:HE1	1:C:110:HIS:CD2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:HG2	5:B:677:HOH:O	2.13	0.47
1:B:289:ASP:OD1	1:B:291:HIS:CD2	2.64	0.47
1:A:263:LYS:HD3	1:A:276:TYR:CE2	2.50	0.47
1:D:166:ASN:ND2	1:D:171:ILE:H	2.07	0.47
1:B:12:ARG:HD2	1:D:189:HIS:ND1	2.30	0.46
1:A:289:ASP:OD1	1:A:291:HIS:CD2	2.67	0.46
1:D:182:TYR:HA	1:D:186:GLN:OE1	2.16	0.45
1:C:180:HIS:O	1:C:234:ARG:HA	2.17	0.45
1:D:289:ASP:OD1	1:D:291:HIS:HD2	1.99	0.45
1:B:166:ASN:ND2	1:B:171:ILE:H	2.11	0.45
1:D:165:LEU:HD21	1:D:262:ILE:HD11	1.97	0.45
1:B:51:ILE:HD11	1:B:238:ILE:HG12	1.98	0.45
1:B:249:THR:O	1:B:305:ASN:HB3	2.17	0.44
1:B:337:HIS:CD2	1:B:337:HIS:C	2.90	0.44
1:B:142:PRO:HG3	1:B:333:LYS:HE2	1.98	0.44
1:A:132:VAL:HG23	1:A:220:VAL:HG21	2.00	0.44
1:A:189:HIS:HD2	5:A:632:HOH:O	2.00	0.44
1:D:165:LEU:HD21	1:D:262:ILE:HD12	1.97	0.44
1:C:27:ASP:OD1	1:C:328:GLU:OE2	2.36	0.44
1:B:11:GLY:HA3	2:B:401:NAP:O5B	2.18	0.43
1:C:286:ILE:C	1:C:286:ILE:HD12	2.38	0.43
1:A:189:HIS:CD2	1:C:12:ARG:HD2	2.53	0.43
1:D:134:GLY:H	1:D:137:HIS:CD2	2.36	0.43
1:B:3:ILE:N	1:B:3:ILE:CD1	2.81	0.43
1:B:243:THR:HG23	1:B:313:TYR:CE1	2.54	0.43
1:C:35:ASP:O	1:C:77:ALA:HA	2.18	0.42
1:B:60:GLU:CG	5:B:724:HOH:O	2.68	0.42
1:D:96:GLU:OE2	1:D:110:HIS:HE1	2.02	0.42
1:D:210:SER:HA	5:D:605:HOH:O	2.20	0.42
1:A:283:SER:HB3	1:D:206:ILE:HB	2.02	0.41
1:C:86:TRP:HB3	1:C:91:VAL:HB	2.02	0.41
1:A:291:HIS:HE1	5:A:692:HOH:O	2.03	0.41
1:B:286:ILE:HG12	1:B:312:TRP:HB3	2.02	0.41
1:C:165:LEU:HD21	1:C:262:ILE:CD1	2.51	0.40
1:D:286:ILE:HG12	1:D:312:TRP:HB3	2.03	0.40
1:B:2:THR:C	1:B:3:ILE:HD12	2.42	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	333/342 (97%)	320 (96%)	13 (4%)	0	100	100
1	B	334/342 (98%)	321 (96%)	13 (4%)	0	100	100
1	C	333/342 (97%)	317 (95%)	15 (4%)	1 (0%)	41	37
1	D	332/342 (97%)	322 (97%)	10 (3%)	0	100	100
All	All	1332/1368 (97%)	1280 (96%)	51 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	ALA

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	273/280 (98%)	270 (99%)	3 (1%)	73	78
1	B	274/280 (98%)	271 (99%)	3 (1%)	73	78
1	C	273/280 (98%)	267 (98%)	6 (2%)	52	55
1	D	272/280 (97%)	270 (99%)	2 (1%)	84	88
All	All	1092/1120 (98%)	1078 (99%)	14 (1%)	69	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	176	MET
1	A	223	GLU
1	B	108	LYS
1	B	211	THR
1	B	299	LEU
1	C	64	ASP
1	C	161	MET
1	C	176	MET
1	C	223	GLU
1	C	313	TYR
1	C	334	LEU
1	D	12	ARG
1	D	220	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	137	HIS
1	A	166	ASN
1	A	189	HIS
1	A	205	ASN
1	A	291	HIS
1	B	57	GLN
1	B	110	HIS
1	B	137	HIS
1	B	166	ASN
1	B	189	HIS
1	B	205	ASN
1	B	248	ASN
1	B	291	HIS
1	B	315	ASN
1	B	337	HIS
1	C	110	HIS
1	C	137	HIS
1	C	166	ASN
1	C	205	ASN
1	C	291	HIS
1	D	57	GLN
1	D	110	HIS
1	D	137	HIS
1	D	166	ASN

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Mol	Chain	Res	Type
1	D	205	ASN
1	D	291	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	GOL	C	402	-	5,5,5	0.12	0	5,5,5	0.41	0
4	EDO	B	402	-	3,3,3	0.10	0	2,2,2	0.23	0
2	NAP	A	401	-	45,52,52	0.93	2 (4%)	56,80,80	0.90	1 (1%)
2	NAP	C	401	-	45,52,52	0.86	1 (2%)	56,80,80	0.90	2 (3%)
3	GOL	B	403	-	5,5,5	0.11	0	5,5,5	0.34	0
3	GOL	A	402	-	5,5,5	0.08	0	5,5,5	0.29	0
3	GOL	A	403	-	5,5,5	0.45	0	5,5,5	0.79	0
2	NAP	D	401	-	45,52,52	0.77	1 (2%)	56,80,80	0.88	3 (5%)
2	NAP	B	401	-	45,52,52	0.85	1 (2%)	56,80,80	0.94	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
3	GOL	C	402	-	-	4/4/4/4	-
4	EDO	B	402	-	-	1/1/1/1	-
2	NAP	A	401	-	-	8/31/67/67	0/5/5/5
2	NAP	C	401	-	-	8/31/67/67	0/5/5/5
3	GOL	B	403	-	-	3/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
2	NAP	D	401	-	-	9/31/67/67	0/5/5/5
2	NAP	B	401	-	-	8/31/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAP	C2N-N1N	3.20	1.38	1.35
2	A	401	NAP	C2N-N1N	3.19	1.38	1.35
2	C	401	NAP	C2N-N1N	2.99	1.38	1.35
2	B	401	NAP	C2N-N1N	2.74	1.38	1.35
2	A	401	NAP	P2B-O2B	2.28	1.63	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C6N-N1N-C2N	-2.74	119.47	121.97
2	C	401	NAP	C5A-C6A-N6A	2.71	124.47	120.35
2	B	401	NAP	C6N-N1N-C2N	-2.68	119.53	121.97
2	D	401	NAP	C6N-N1N-C2N	-2.39	119.80	121.97
2	B	401	NAP	O2N-PN-O1N	2.25	123.35	112.24
2	B	401	NAP	C5A-C6A-N6A	2.07	123.50	120.35
2	C	401	NAP	C6N-N1N-C2N	-2.06	120.10	121.97
2	B	401	NAP	O7N-C7N-C3N	2.05	122.08	119.63
2	D	401	NAP	C5A-C6A-N6A	2.01	123.40	120.35
2	D	401	NAP	O2X-P2B-O2B	-2.00	97.03	105.99

There are no chirality outliers.

All (43) torsion outliers are listed below:

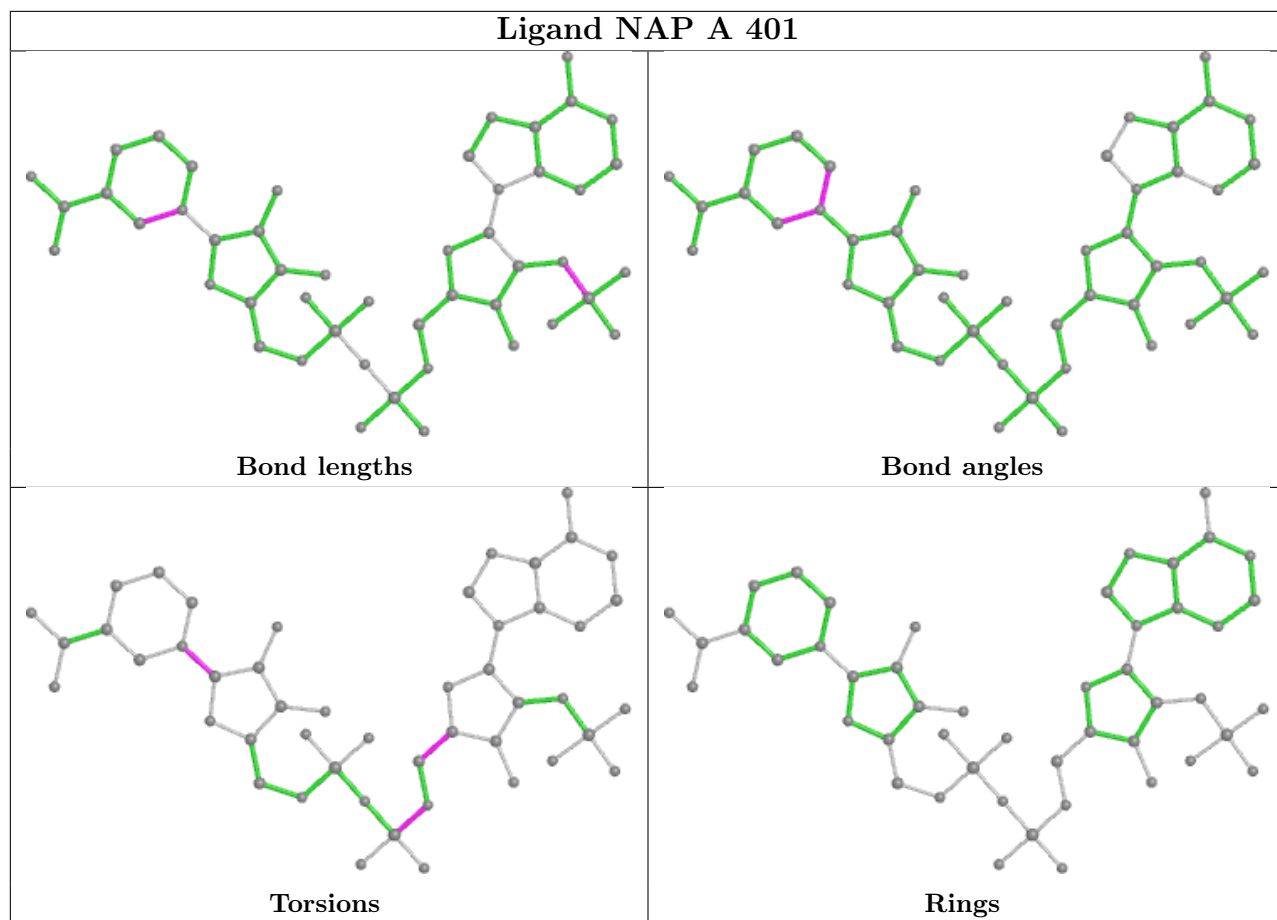
Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2D-C1D-N1N-C2N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	B	401	NAP	C5B-O5B-PA-O2A
2	B	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	C2D-C1D-N1N-C2N
2	B	401	NAP	C2D-C1D-N1N-C6N
2	C	401	NAP	C5B-O5B-PA-O2A
2	C	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	C2D-C1D-N1N-C2N
2	C	401	NAP	C2D-C1D-N1N-C6N
2	D	401	NAP	C5B-O5B-PA-O1A
2	D	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	C2D-C1D-N1N-C2N
2	D	401	NAP	C2D-C1D-N1N-C6N
3	A	402	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	C	402	GOL	C1-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
4	B	402	EDO	O1-C1-C2-O2
2	B	401	NAP	C5B-O5B-PA-O3
2	C	401	NAP	C5B-O5B-PA-O3
2	D	401	NAP	C5B-O5B-PA-O3
2	A	401	NAP	C5B-O5B-PA-O2A
2	B	401	NAP	C5B-O5B-PA-O1A
2	D	401	NAP	C5B-O5B-PA-O2A
2	B	401	NAP	O4B-C4B-C5B-O5B
2	C	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	O4B-C4B-C5B-O5B
3	B	403	GOL	O1-C1-C2-C3
3	C	402	GOL	O2-C2-C3-O3
2	A	401	NAP	C5B-O5B-PA-O3
2	D	401	NAP	PA-O3-PN-O1N
2	A	401	NAP	C5B-O5B-PA-O1A
2	C	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	O4B-C4B-C5B-O5B

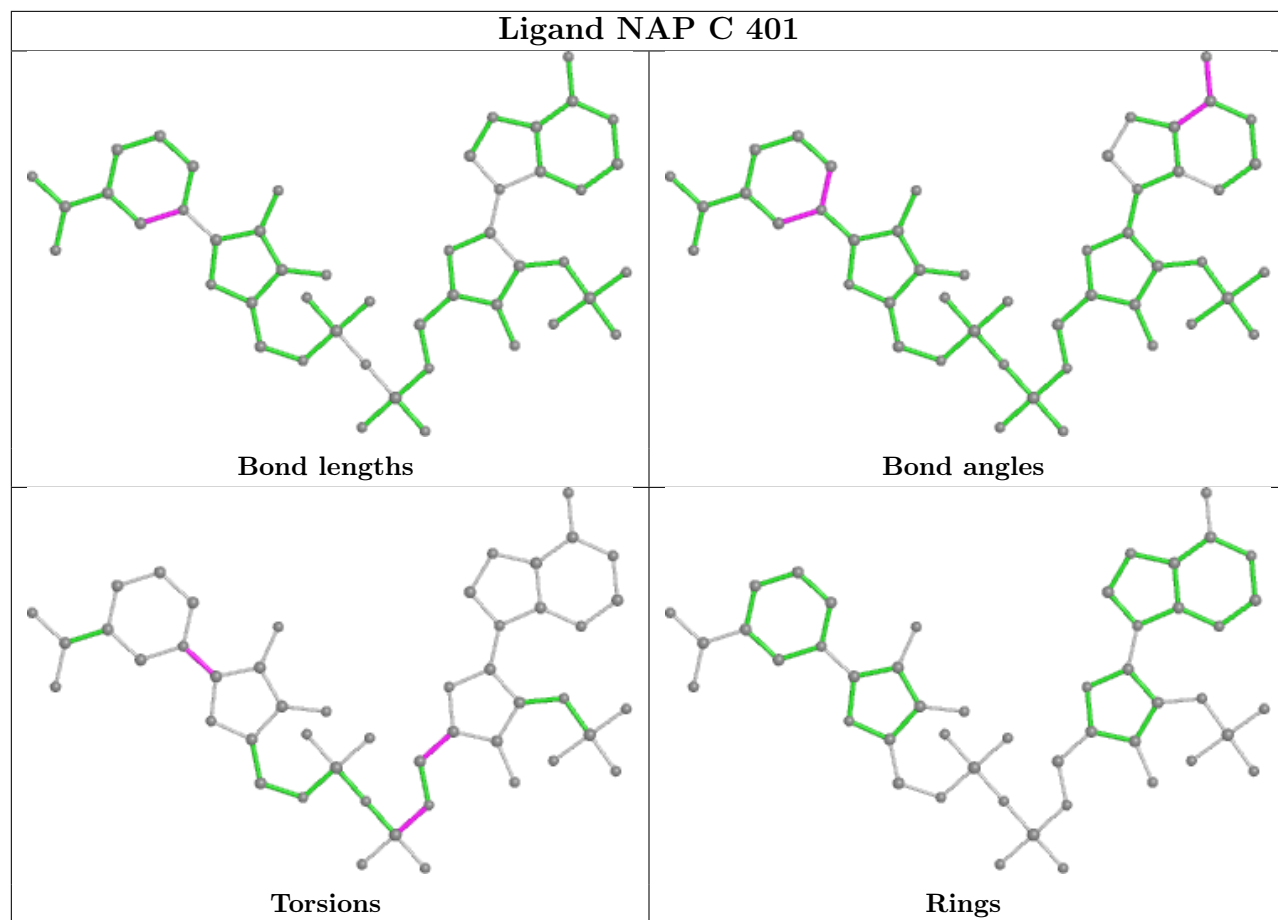
There are no ring outliers.

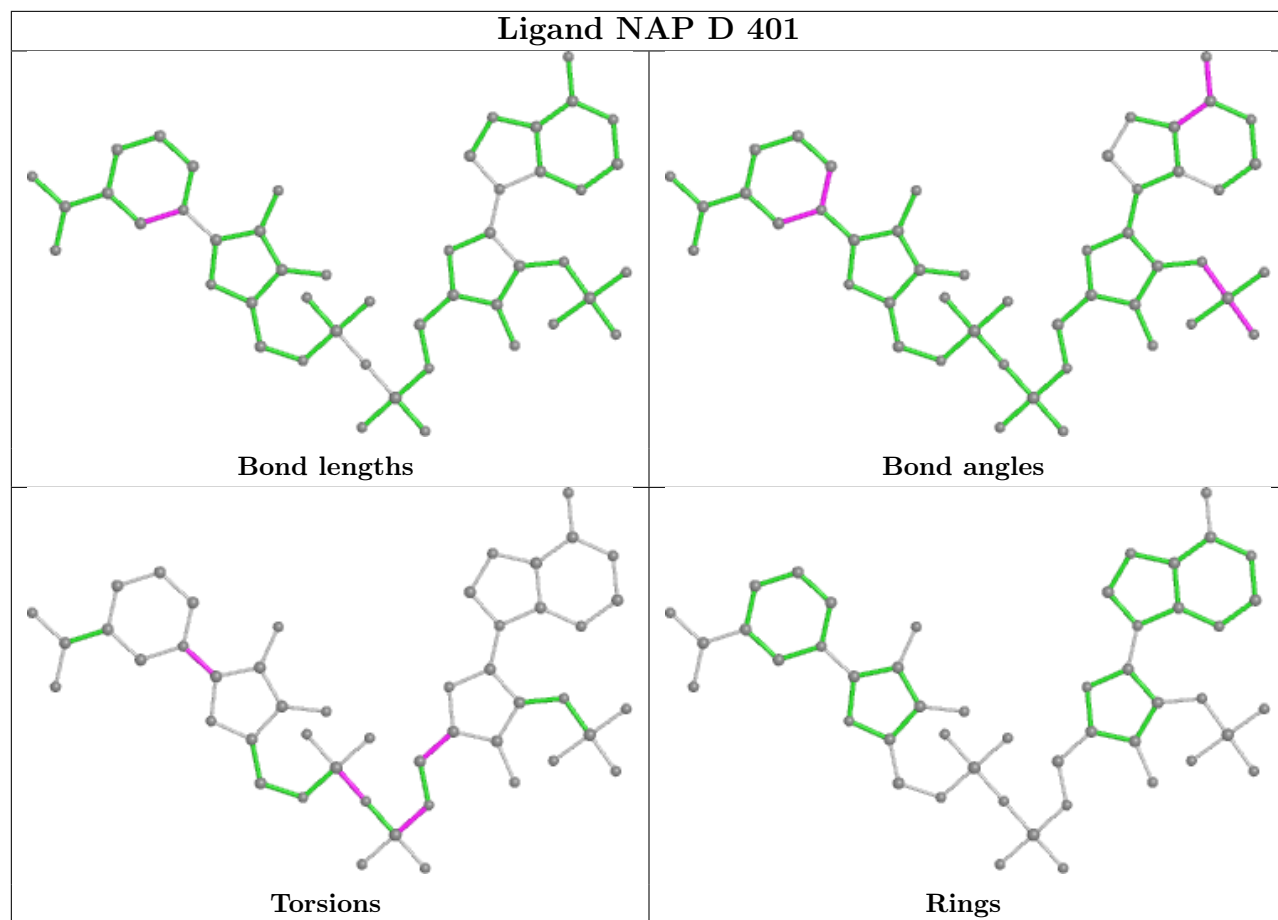
5 monomers are involved in 8 short contacts:

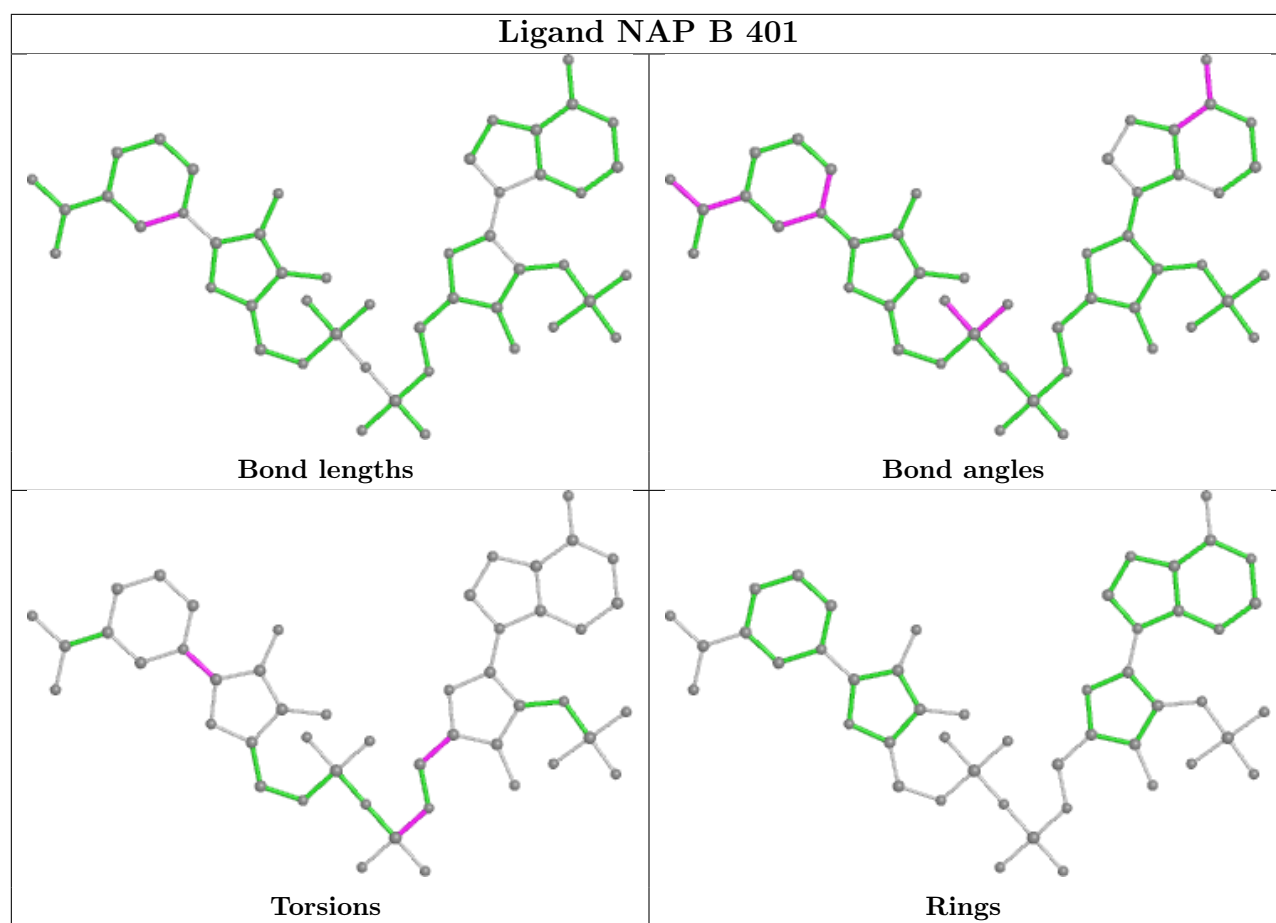
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	GOL	2	0
2	C	401	NAP	1	0
3	B	403	GOL	2	0
3	A	403	GOL	1	0
2	B	401	NAP	2	0

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









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	335/342 (97%)	-0.10	3 (0%) 84 83	15, 22, 36, 56	0
1	B	336/342 (98%)	-0.16	3 (0%) 84 83	16, 21, 35, 79	0
1	C	335/342 (97%)	0.08	8 (2%) 59 57	15, 24, 41, 61	0
1	D	334/342 (97%)	0.16	10 (2%) 50 49	16, 29, 49, 72	0
All	All	1340/1368 (97%)	-0.00	24 (1%) 68 66	15, 23, 43, 79	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	334	LEU	6.7
1	B	337	HIS	5.7
1	B	334	LEU	4.9
1	C	334	LEU	4.7
1	A	334	LEU	4.2
1	B	211	THR	4.1
1	C	211	THR	3.8
1	C	267	VAL	3.5
1	D	213	ALA	3.2
1	D	211	THR	3.1
1	D	214	ALA	3.0
1	D	56	GLY	2.9
1	C	336	GLU	2.8
1	C	61	TYR	2.6
1	A	238	ILE	2.6
1	D	2	THR	2.3
1	D	264	GLU	2.3
1	C	63	ASP	2.3
1	C	214	ALA	2.2
1	C	64	ASP	2.2
1	D	267	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	335	LEU	2.1
1	A	237	VAL	2.1
1	D	144	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 monosaccharides in this entry.

6.4 Ligands [i](#)

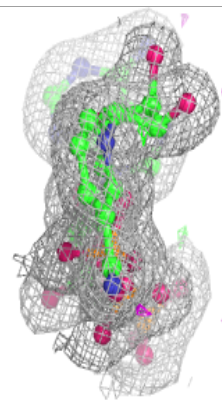
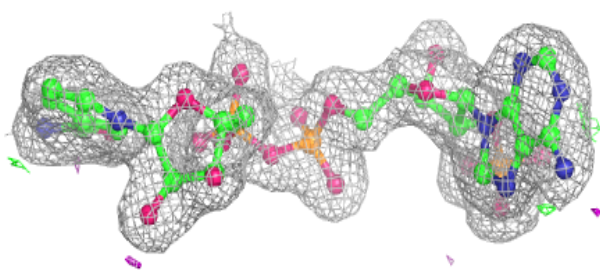
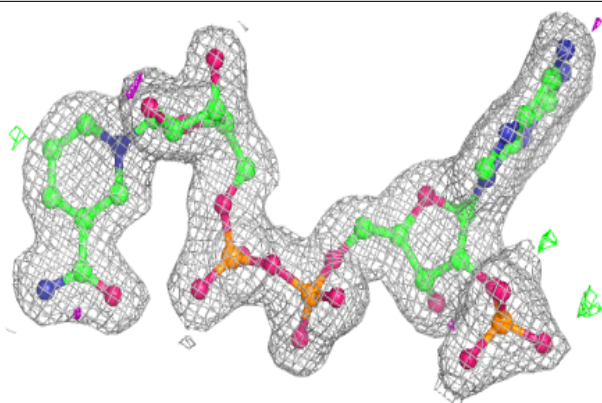
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	402	6/6	0.56	0.27	53,55,55,57	0
3	GOL	A	402	6/6	0.64	0.22	52,56,60,65	0
3	GOL	B	403	6/6	0.78	0.26	53,56,57,60	0
3	GOL	A	403	6/6	0.88	0.27	28,34,37,38	0
4	EDO	B	402	4/4	0.94	0.13	43,47,48,51	0
2	NAP	C	401	48/48	0.97	0.10	16,20,27,34	0
2	NAP	D	401	48/48	0.98	0.08	19,23,31,32	0
2	NAP	B	401	48/48	0.98	0.08	16,19,25,28	0
2	NAP	A	401	48/48	0.98	0.08	16,20,23,26	0

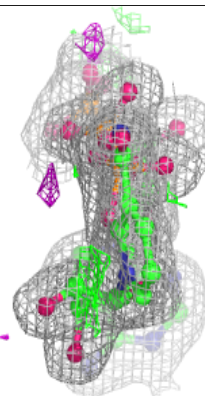
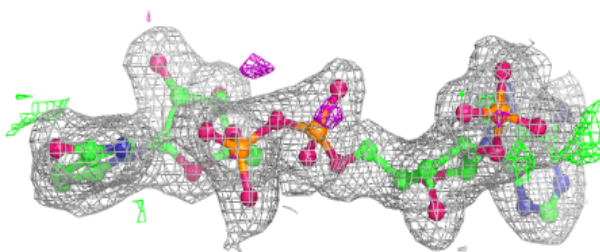
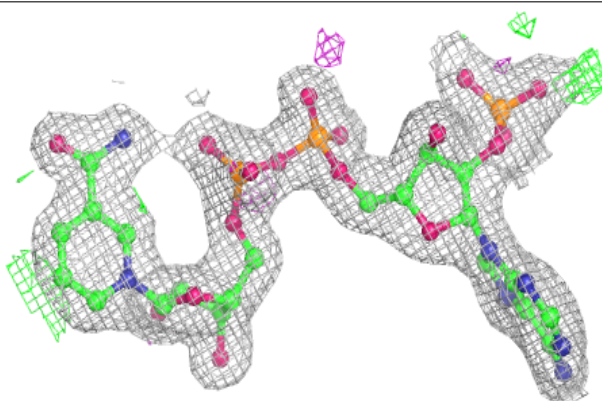
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

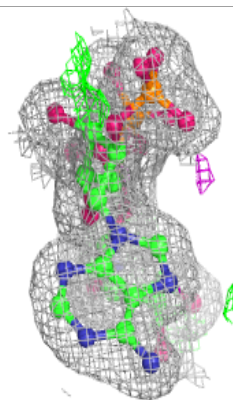
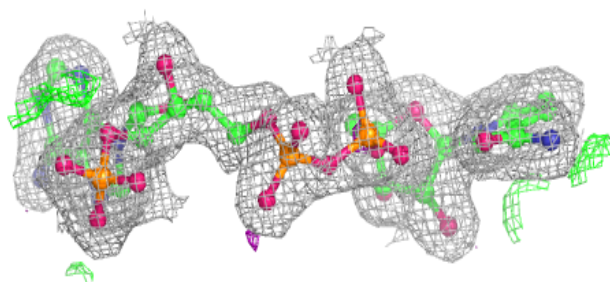
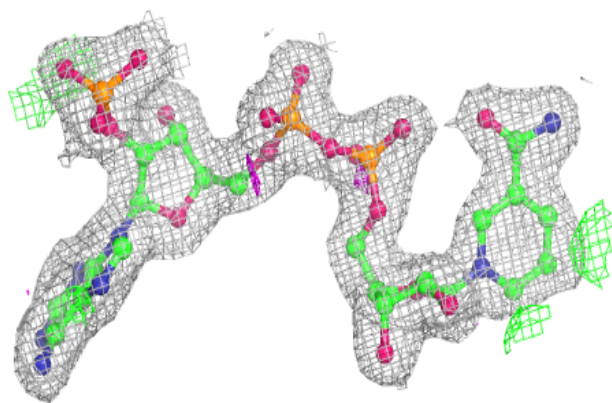
**Electron density around NAP D 401:**

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

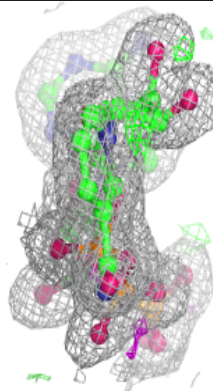
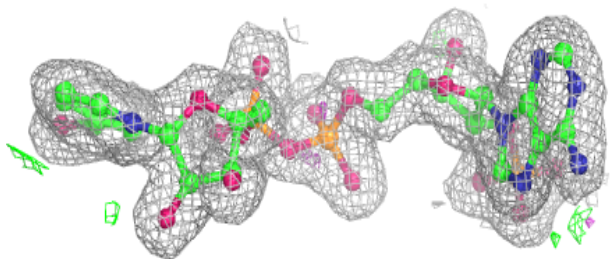
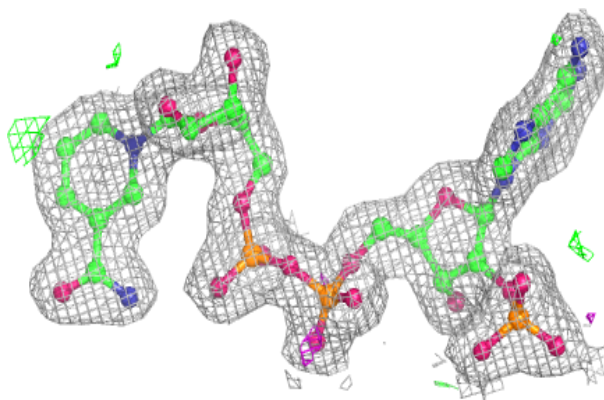


Electron density around NAP B 401:

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

**Electron density around NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.