



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:57 PM UTC

PDB ID : 7QK8 / pdb_00007qk8
Title : Crystal structure of the ALDH1A3-NAD⁺ complex
Authors : Castellvi, A.; Farres, J.
Deposited on : 2021-12-17
Resolution : 1.89 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

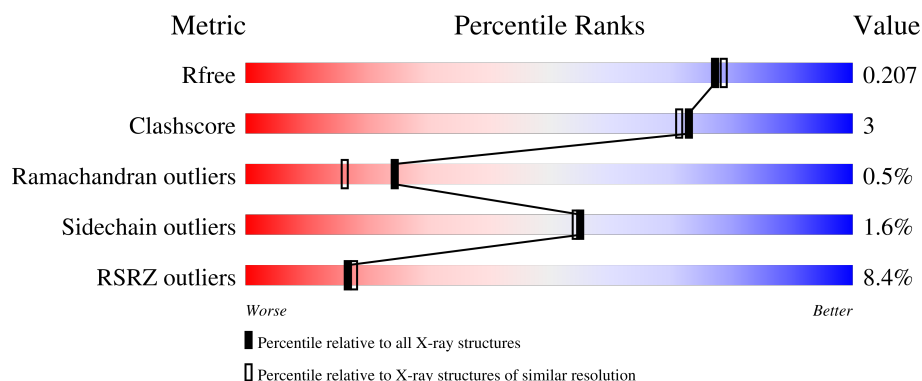
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	529	
1	B	529	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	603[A]	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8193 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 Aldehyde dehydrogenase family 1 member A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	3	0
			3702	2366	630	685	21			
1	B	489	Total	C	N	O	S	0	4	0
			3698	2360	630	686	22			

There are 34 discrepancies between the modelled and reference sequences:

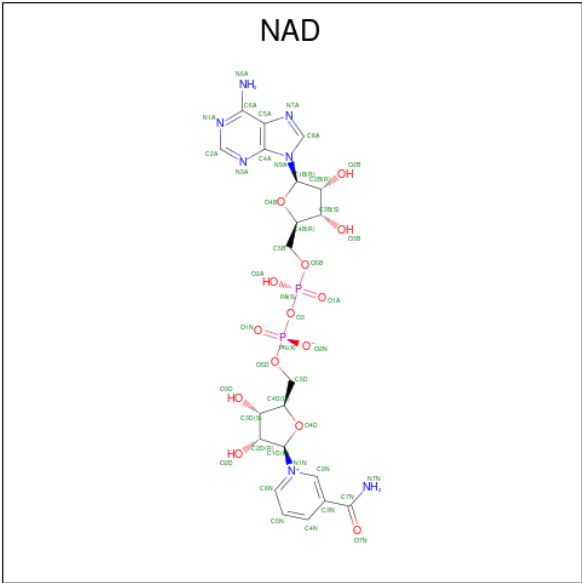
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP P47895
A	-15	HIS	-	expression tag	UNP P47895
A	-14	HIS	-	expression tag	UNP P47895
A	-13	HIS	-	expression tag	UNP P47895
A	-12	HIS	-	expression tag	UNP P47895
A	-11	HIS	-	expression tag	UNP P47895
A	-10	LEU	-	expression tag	UNP P47895
A	-9	GLU	-	expression tag	UNP P47895
A	-8	SER	-	expression tag	UNP P47895
A	-7	THR	-	expression tag	UNP P47895
A	-6	SER	-	expression tag	UNP P47895
A	-5	LEU	-	expression tag	UNP P47895
A	-4	TYR	-	expression tag	UNP P47895
A	-3	LYS	-	expression tag	UNP P47895
A	-2	LYS	-	expression tag	UNP P47895
A	-1	ALA	-	expression tag	UNP P47895
A	0	GLY	-	expression tag	UNP P47895
B	-16	HIS	-	expression tag	UNP P47895
B	-15	HIS	-	expression tag	UNP P47895
B	-14	HIS	-	expression tag	UNP P47895
B	-13	HIS	-	expression tag	UNP P47895
B	-12	HIS	-	expression tag	UNP P47895
B	-11	HIS	-	expression tag	UNP P47895
B	-10	LEU	-	expression tag	UNP P47895
B	-9	GLU	-	expression tag	UNP P47895

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP P47895
B	-7	THR	-	expression tag	UNP P47895
B	-6	SER	-	expression tag	UNP P47895
B	-5	LEU	-	expression tag	UNP P47895
B	-4	TYR	-	expression tag	UNP P47895
B	-3	LYS	-	expression tag	UNP P47895
B	-2	LYS	-	expression tag	UNP P47895
B	-1	ALA	-	expression tag	UNP P47895
B	0	GLY	-	expression tag	UNP P47895

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).





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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



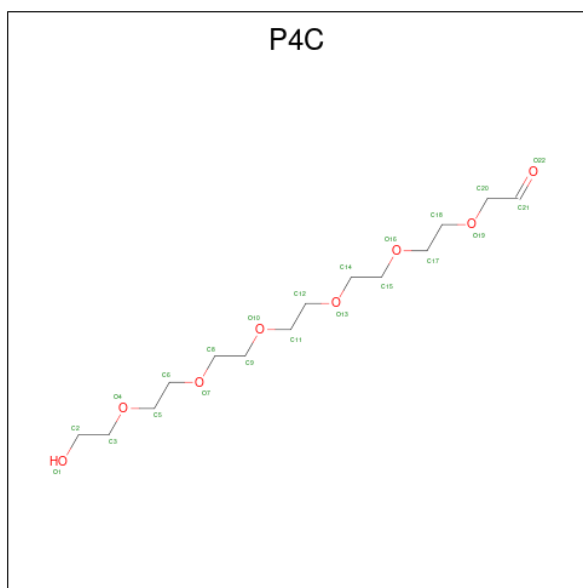
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		

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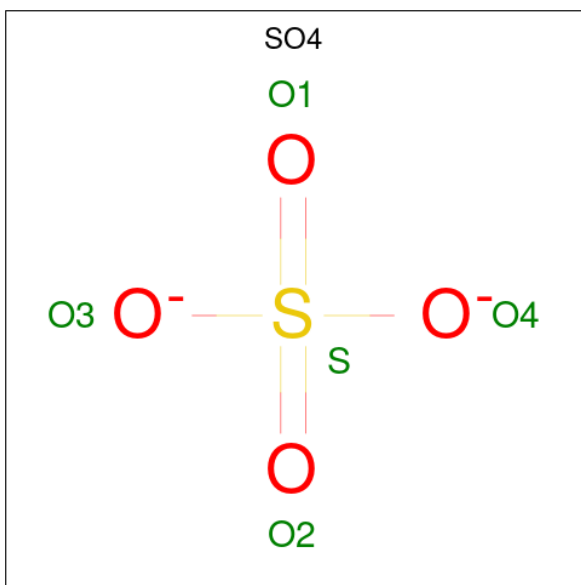
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is O-ACETALDEHYDYL-HEXAETHYLENE GLYCOL (CCD ID: P4C) (formula: $C_{14}H_{28}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

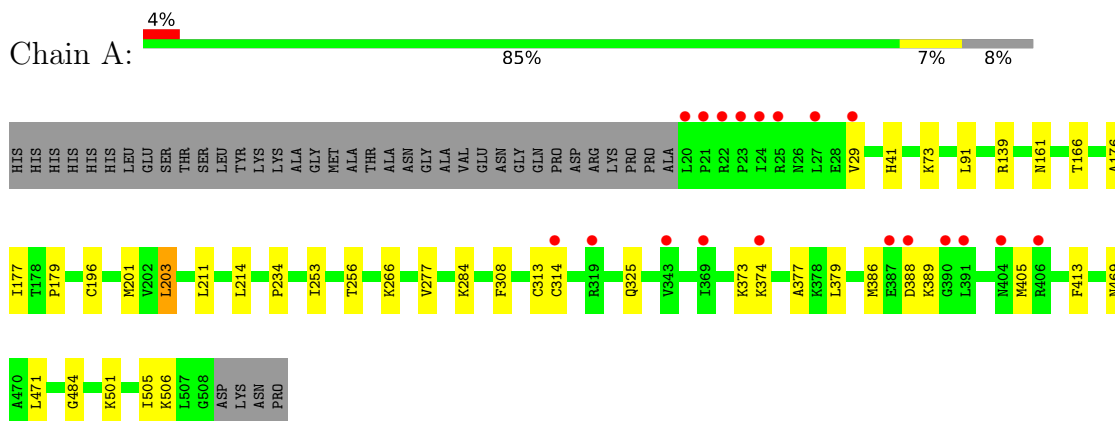
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	301	Total	O	0	5
			306	306		
7	B	292	Total	O	0	2
			294	294		

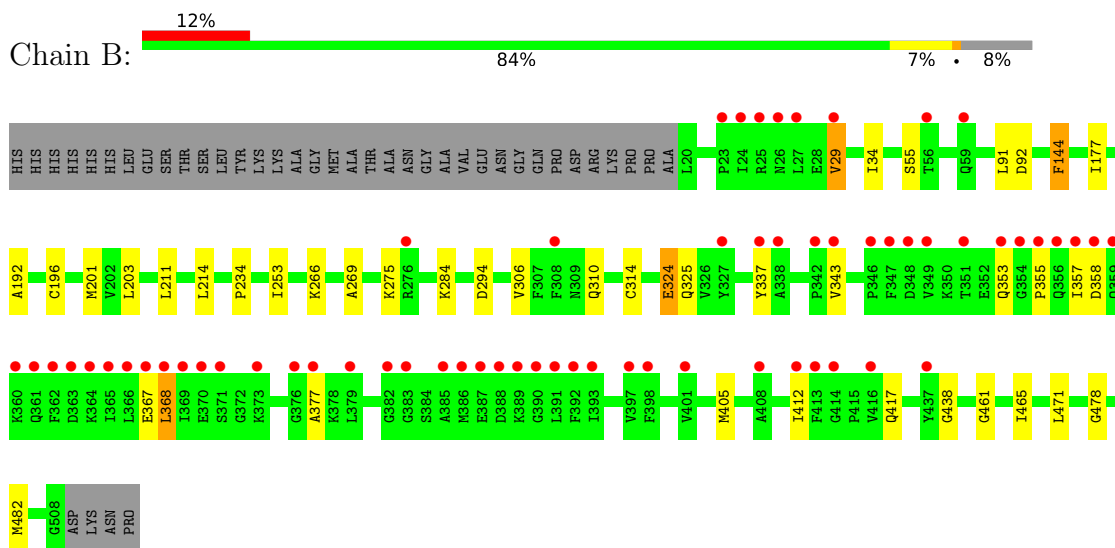
3 Residue-property plots [i](#)

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: Aldehyde dehydrogenase family 1 member A3



- Molecule 1: Aldehyde dehydrogenase family 1 member A3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.58Å 89.52Å 158.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.53 – 1.89 45.53 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.53-1.89) 98.8 (45.53-1.89)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.89Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
R, R_{free}	0.180 , 0.204 0.181 , 0.207	Depositor DCC
R_{free} test set	4477 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtrriage
Anisotropy	0.590	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8193	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: NAD, GOL, P4C, SO4, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/3780	0.98	4/5135 (0.1%)
1	B	0.72	1/3775 (0.0%)	0.99	9/5128 (0.2%)
All	All	0.71	1/7555 (0.0%)	0.98	13/10263 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	MET	SD-CE	-5.58	1.65	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LEU	N-CA-C	7.58	119.19	111.07
1	A	211	LEU	N-CA-C	6.85	118.40	111.07
1	B	294	ASP	N-CA-C	-5.78	98.29	108.23
1	B	284	LYS	N-CA-C	-5.68	99.12	108.49
1	A	284	LYS	N-CA-C	-5.61	99.23	108.49
1	A	201	MET	N-CA-C	5.57	117.86	109.23
1	B	29	VAL	N-CA-CB	5.56	116.59	110.53
1	B	144	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	201	MET	N-CA-C	5.33	117.49	109.23
1	B	367	GLU	CA-C-N	5.30	131.66	121.54
1	B	367	GLU	C-N-CA	5.30	131.66	121.54
1	A	484	GLY	N-CA-C	5.16	117.10	110.96
1	B	92	ASP	CA-CB-CG	5.09	117.69	112.60

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	3702	0	3634	27	0
1	B	3698	0	3627	21	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
3	A	7	0	10	1	0
3	B	7	0	10	0	0
4	A	30	0	40	7	0
4	B	30	0	40	0	0
5	A	16	0	19	5	0
5	B	10	0	11	2	0
6	B	5	0	0	0	0
7	A	306	0	0	1	0
7	B	294	0	0	0	0
All	All	8193	0	7443	48	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 (48) 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:377:ALA:HB2	1:B:405:MET:HE1	1.56	0.85
1:A:377:ALA:HB2	1:A:405:MET:HE1	1.58	0.85
1:A:266:LYS:NZ	4:A:603[A]:GOL:H11	2.02	0.75
1:A:266:LYS:HZ3	4:A:603[A]:GOL:H11	1.58	0.67
4:A:603[A]:GOL:C2	1:B:266:LYS:HZ1	2.08	0.66
4:A:603[A]:GOL:H2	1:B:266:LYS:HZ1	1.60	0.66
1:A:161:ASN:ND2	1:A:506:LYS:HZ3	1.94	0.66
5:A:605:P4C:H21	7:A:847:HOH:O	1.96	0.65
1:A:471:LEU:HD12	5:A:605:P4C:H151	1.79	0.64
1:A:161:ASN:ND2	1:A:506:LYS:NZ	2.47	0.62
1:B:310:GLN:HG3	1:B:353:GLN:HG3	1.82	0.60
1:B:368:LEU:HD13	1:B:412:ILE:HG12	1.85	0.57
1:A:373:LYS:HE2	1:A:379:LEU:HD22	1.88	0.56
1:B:177:ILE:HD12	1:B:253:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:CE1	1:A:73:LYS:HZ3	2.26	0.54
1:A:325:GLN:NE2	1:A:325:GLN:H	2.06	0.54
1:A:41:HIS:CE1	1:A:73:LYS:NZ	2.78	0.52
1:B:269:ALA:HB1	1:B:275:LYS:HG3	1.91	0.51
1:A:41:HIS:ND1	1:A:73:LYS:NZ	2.58	0.50
1:A:314:CYS:SG	5:A:605:P4C:H21	2.51	0.50
1:A:266:LYS:HZ1	4:A:603[A]:GOL:H11	1.76	0.50
1:B:325:GLN:NE2	1:B:325:GLN:H	2.11	0.49
1:A:179:PRO:HD3	1:A:256:THR:HB	1.94	0.49
1:A:377:ALA:CB	1:A:405:MET:HE1	2.37	0.48
1:B:377:ALA:HB2	1:B:405:MET:CE	2.37	0.47
1:B:214:LEU:HD21	1:B:234:PRO:HG3	1.96	0.47
1:B:471:LEU:HD12	5:B:1306:P4C:H181	1.96	0.46
1:B:55:SER:HA	1:B:355:PRO:HG3	1.98	0.46
1:A:505:ILE:HG12	1:B:465:ILE:HD12	1.98	0.46
1:A:314:CYS:SG	5:A:605:P4C:C21	3.04	0.45
1:A:139:ARG:HD2	3:A:602:PEG:H41	1.99	0.45
1:A:469:ASN:HD22	5:A:605:P4C:H82	1.81	0.44
1:B:461:GLY:HA3	1:B:478:GLY:O	2.18	0.44
1:B:306:VAL:HG11	1:B:417:GLN:HB2	2.00	0.44
1:A:176:ALA:HB3	1:A:203:LEU:HD12	2.00	0.43
1:A:277:VAL:O	4:A:603[B]:GOL:O3	2.37	0.43
1:B:343:VAL:HG22	1:B:353:GLN:HB3	2.01	0.42
1:B:357:ILE:HG23	1:B:358:ASP:N	2.34	0.42
1:A:177:ILE:HD12	1:A:253:ILE:HD11	2.02	0.41
1:B:314:CYS:SG	5:B:1306:P4C:O22	2.79	0.41
1:A:214:LEU:HD21	1:A:234:PRO:HG3	2.02	0.41
1:B:34:ILE:HG12	1:B:234:PRO:HD2	2.02	0.41
1:A:166:THR:HA	1:A:501:LYS:O	2.21	0.41
1:A:308:PHE:CD2	1:A:313[B]:CYS:SG	3.14	0.41
1:B:324:GLU:HG3	1:B:325:GLN:HE22	1.86	0.41
1:A:405:MET:HE2	1:A:405:MET:HB3	1.92	0.40
1:A:266:LYS:HZ3	4:A:603[B]:GOL:H12	1.86	0.40
1:B:144:PHE:HB2	1:B:192:ALA:HB1	2.02	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	490/529 (93%)	472 (96%)	15 (3%)	3 (1%)	21	13
1	B	491/529 (93%)	474 (96%)	15 (3%)	2 (0%)	30	22
All	All	981/1058 (93%)	946 (96%)	30 (3%)	5 (0%)	24	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	B	368	LEU
1	A	389	LYS
1	A	386	MET
1	B	438	GLY

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	379/437 (87%)	373 (98%)	6 (2%)	55	54
1	B	379/437 (87%)	373 (98%)	6 (2%)	55	54
All	All	758/874 (87%)	746 (98%)	12 (2%)	55	54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL

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Mol	Chain	Res	Type
1	A	91	LEU
1	A	196	CYS
1	A	203	LEU
1	A	374	LYS
1	A	413	PHE
1	B	29	VAL
1	B	91	LEU
1	B	196	CYS
1	B	203	LEU
1	B	324	GLU
1	B	337	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	38	ASN
1	A	102	GLN
1	A	128	HIS
1	A	161	ASN
1	A	325	GLN
1	A	356	GLN
1	B	325	GLN
1	B	356	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

17 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	$\# Z > 2$
6	SO4	B	1307	-	4,4,4	0.26	0	6,6,6	0.14	0
4	GOL	B	1305	-	5,5,5	0.03	0	5,5,5	0.19	0
5	P4C	B	1306	-	9,9,21	0.58	0	8,8,20	0.80	0
4	GOL	B	1308	-	5,5,5	0.15	0	5,5,5	0.35	0
5	P4C	A	605	-	15,15,21	0.57	0	14,14,20	0.53	0
3	PEG	A	602	-	6,6,6	0.15	0	5,5,5	0.15	0
4	GOL	A	603[B]	-	5,5,5	0.10	0	5,5,5	0.20	0
4	GOL	A	604	-	5,5,5	0.05	0	5,5,5	0.13	0
4	GOL	A	607	-	5,5,5	0.08	0	5,5,5	0.20	0
4	GOL	B	1301	-	5,5,5	0.07	0	5,5,5	0.45	0
4	GOL	B	1309	-	5,5,5	0.05	0	5,5,5	0.32	0
4	GOL	A	603[A]	-	5,5,5	0.14	0	5,5,5	0.48	0
3	PEG	B	1303	-	6,6,6	0.16	0	5,5,5	0.19	0
4	GOL	B	1304	-	5,5,5	0.08	0	5,5,5	0.17	0
2	NAD	A	601	-	46,48,48	0.35	0	64,73,73	0.81	2 (3%)
2	NAD	B	1302	-	46,48,48	0.36	0	64,73,73	0.70	2 (3%)
4	GOL	A	606	-	5,5,5	0.09	0	5,5,5	0.19	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	GOL	B	1305	-	-	2/4/4/4	-
5	P4C	B	1306	-	-	2/6/7/19	-
4	GOL	B	1308	-	-	2/4/4/4	-
5	P4C	A	605	-	-	6/12/13/19	-
3	PEG	A	602	-	-	0/4/4/4	-
4	GOL	A	603[B]	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	604	-	-	0/4/4/4	-
4	GOL	A	607	-	-	2/4/4/4	-
4	GOL	B	1301	-	-	2/4/4/4	-
4	GOL	B	1309	-	-	2/4/4/4	-
4	GOL	A	603[A]	-	-	0/4/4/4	-
3	PEG	B	1303	-	-	2/4/4/4	-
4	GOL	B	1304	-	-	0/4/4/4	-
2	NAD	A	601	-	-	5/30/62/62	0/5/5/5
2	NAD	B	1302	-	-	4/30/62/62	0/5/5/5
4	GOL	A	606	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1302	NAD	C4D-O4D-C1D	-3.60	106.63	109.92
2	A	601	NAD	C4D-O4D-C1D	-3.49	106.73	109.92
2	A	601	NAD	O2A-PA-O3	3.03	115.47	107.27
2	B	1302	NAD	O2A-PA-O3	2.06	112.84	107.27

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	PN-O3-PA-O5B
2	B	1302	NAD	PN-O3-PA-O5B
4	A	606	GOL	O1-C1-C2-C3
4	A	607	GOL	C1-C2-C3-O3
4	B	1305	GOL	C1-C2-C3-O3
5	A	605	P4C	O10-C11-C12-O13
2	B	1302	NAD	O4D-C4D-C5D-O5D
4	A	603[B]	GOL	C1-C2-C3-O3
4	B	1301	GOL	C1-C2-C3-O3
4	B	1308	GOL	O1-C1-C2-C3
4	B	1309	GOL	O1-C1-C2-C3
4	B	1309	GOL	C1-C2-C3-O3
4	A	606	GOL	O1-C1-C2-O2
4	A	607	GOL	O2-C2-C3-O3
4	B	1308	GOL	O1-C1-C2-O2

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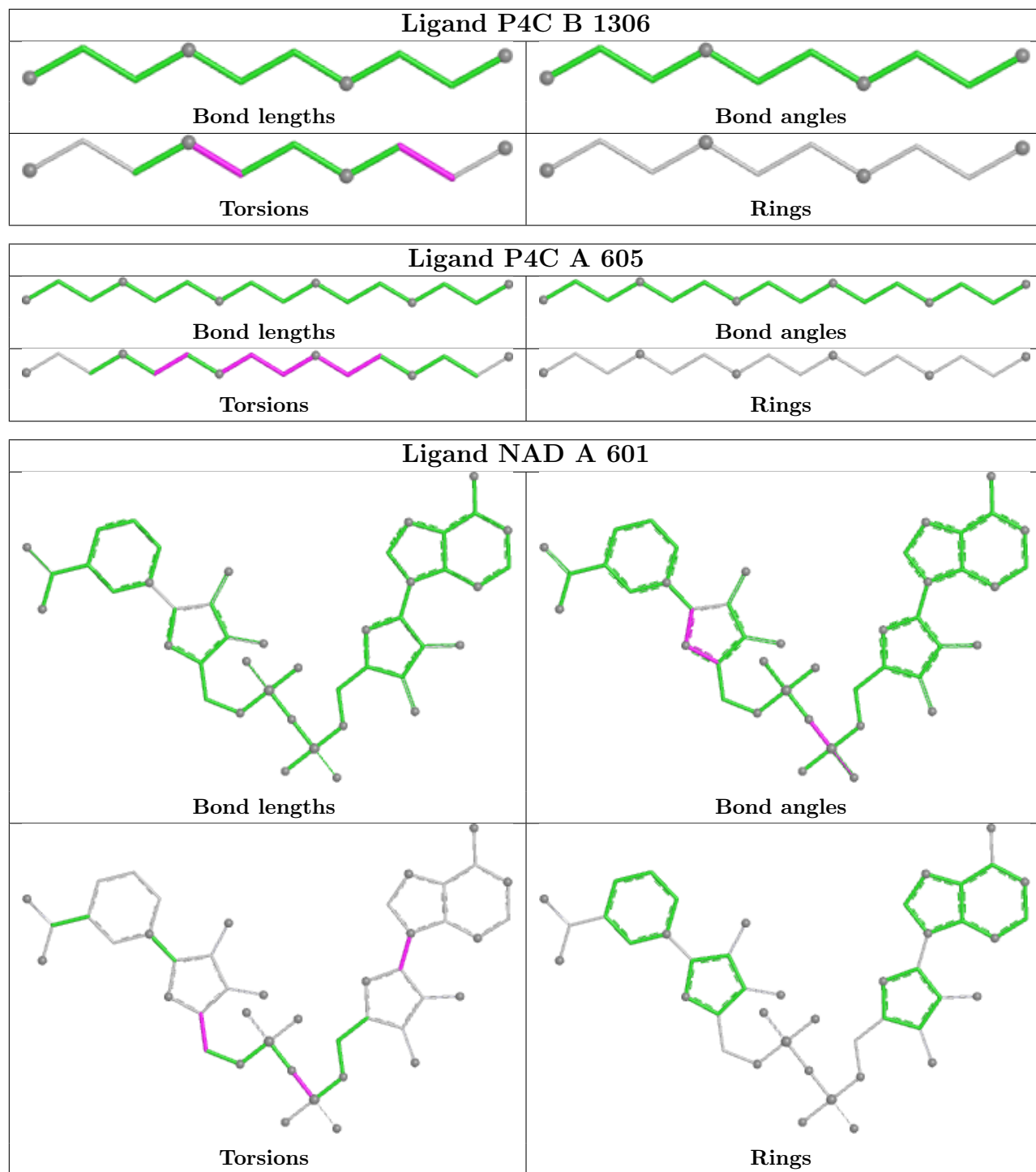
Mol	Chain	Res	Type	Atoms
5	A	605	P4C	O16-C17-C18-O19
2	B	1302	NAD	C3D-C4D-C5D-O5D
5	A	605	P4C	O13-C14-C15-O16
5	B	1306	P4C	O13-C14-C15-O16
5	A	605	P4C	C15-C14-O13-C12
3	B	1303	PEG	C1-C2-O2-C3
2	A	601	NAD	C2B-C1B-N9A-C8A
5	A	605	P4C	C14-C15-O16-C17
3	B	1303	PEG	O1-C1-C2-O2
4	B	1301	GOL	O2-C2-C3-O3
5	B	1306	P4C	C17-C18-O19-C20
4	B	1305	GOL	O2-C2-C3-O3
2	B	1302	NAD	C2B-C1B-N9A-C8A
2	A	601	NAD	O4D-C4D-C5D-O5D
5	A	605	P4C	C11-C12-O13-C14
2	A	601	NAD	O4B-C1B-N9A-C8A
2	A	601	NAD	C3D-C4D-C5D-O5D

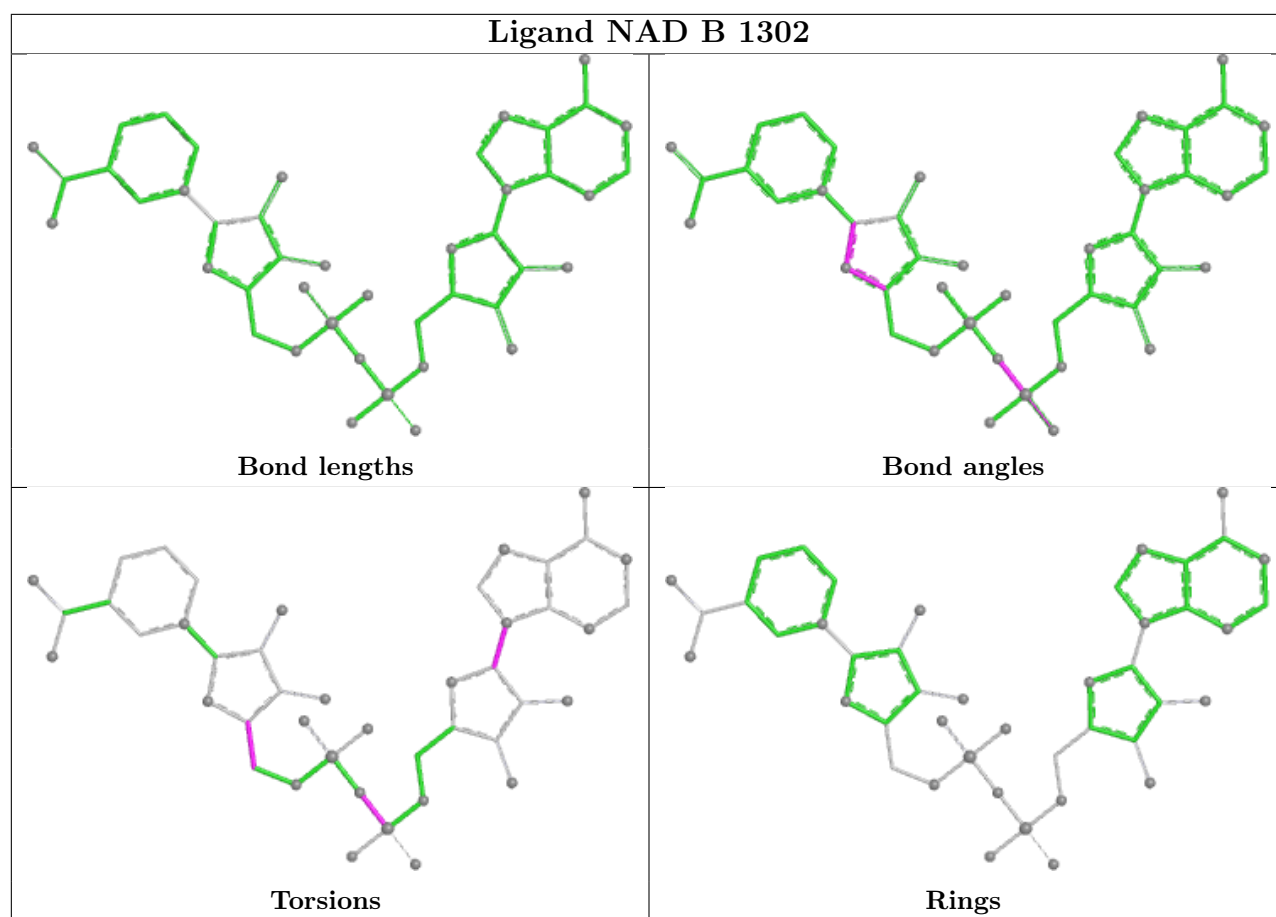
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1306	P4C	2	0
5	A	605	P4C	5	0
3	A	602	PEG	1	0
4	A	603[B]	GOL	2	0
4	A	603[A]	GOL	5	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	489/529 (92%)	0.19	19 (3%) 43 46	14, 35, 60, 75	4 (0%)
1	B	489/529 (92%)	0.51	63 (12%) 7 7	14, 36, 79, 91	5 (1%)
All	All	978/1058 (92%)	0.35	82 (8%) 17 18	14, 36, 75, 91	9 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	PHE	7.0
1	B	365	ILE	6.7
1	B	369	ILE	5.1
1	B	368	LEU	4.8
1	B	364	LYS	4.8
1	B	338	ALA	4.8
1	B	357	ILE	4.7
1	B	24	ILE	4.6
1	B	366	LEU	4.5
1	B	391	LEU	4.2
1	B	343	VAL	3.8
1	B	361	GLN	3.8
1	B	393	ILE	3.7
1	B	347	PHE	3.6
1	B	360	LYS	3.5
1	A	24	ILE	3.4
1	B	392	PHE	3.4
1	B	388	ASP	3.3
1	B	25	ARG	3.3
1	B	363	ASP	3.3
1	B	390	GLY	3.2
1	B	358	ASP	3.2
1	B	337	TYR	3.2
1	B	346	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	388	ASP	3.1
1	A	343	VAL	3.0
1	A	23	PRO	3.0
1	A	22	ARG	3.0
1	B	356	GLN	3.0
1	B	414	GLY	3.0
1	B	416	VAL	2.9
1	B	354	GLY	2.9
1	B	349	VAL	2.8
1	B	27	LEU	2.8
1	B	373	LYS	2.8
1	B	413	PHE	2.8
1	B	359	GLN	2.8
1	A	21	PRO	2.8
1	B	408	ALA	2.7
1	A	314	CYS	2.7
1	B	412	ILE	2.7
1	B	377	ALA	2.7
1	B	398	PHE	2.6
1	B	389	LYS	2.6
1	A	25	ARG	2.6
1	A	390	GLY	2.6
1	B	56	THR	2.6
1	B	383	GLY	2.5
1	A	387	GLU	2.5
1	B	23	PRO	2.4
1	B	308	PHE	2.4
1	B	401	VAL	2.4
1	B	386	MET	2.4
1	A	29	VAL	2.4
1	A	374	LYS	2.4
1	A	391	LEU	2.3
1	B	371	SER	2.3
1	B	348	ASP	2.3
1	B	376	GLY	2.3
1	A	406	ARG	2.3
1	B	370	GLU	2.3
1	B	342	PRO	2.2
1	B	382	GLY	2.2
1	B	385	ALA	2.2
1	B	276[A]	ARG	2.2
1	B	327	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	437	TYR	2.2
1	A	404	ASN	2.2
1	A	319[A]	ARG	2.2
1	B	367	GLU	2.2
1	A	27	LEU	2.2
1	B	59	GLN	2.2
1	B	353	GLN	2.2
1	A	20	LEU	2.1
1	B	26	ASN	2.1
1	B	29	VAL	2.1
1	A	369	ILE	2.1
1	B	351	THR	2.1
1	B	387	GLU	2.0
1	B	355	PRO	2.0
1	B	379	LEU	2.0
1	B	397	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	604	6/6	0.71	0.17	83,83,83,83	0
4	GOL	A	603[B]	6/6	0.75	0.23	20,21,22,22	6
4	GOL	A	603[A]	6/6	0.75	0.23	51,51,52,52	6
4	GOL	B	1309	6/6	0.77	0.14	75,75,76,76	0
4	GOL	A	606	6/6	0.78	0.18	56,57,57,57	0
4	GOL	B	1304	6/6	0.81	0.16	74,74,74,74	0
4	GOL	B	1305	6/6	0.83	0.13	71,71,71,71	0

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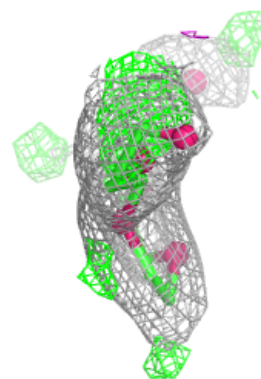
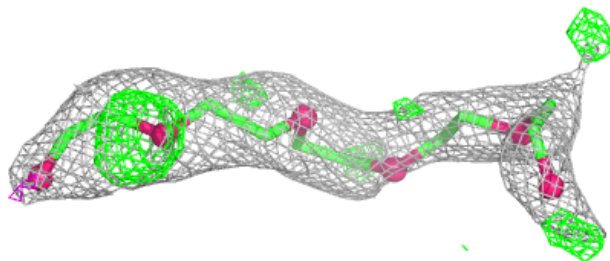
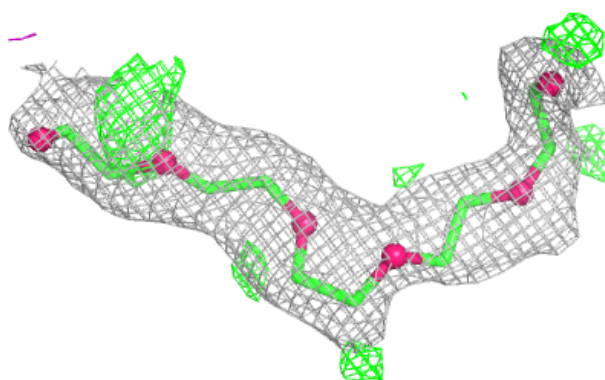
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	P4C	A	605	16/22	0.83	0.22	73,76,78,78	0
5	P4C	B	1306	10/22	0.84	0.17	67,68,68,68	0
6	SO4	B	1307	5/5	0.86	0.09	84,85,85,85	0
4	GOL	B	1301	6/6	0.87	0.13	61,62,62,62	0
4	GOL	B	1308	6/6	0.88	0.15	57,57,58,58	0
4	GOL	A	607	6/6	0.91	0.13	49,51,51,51	0
3	PEG	B	1303	7/7	0.92	0.13	41,43,46,46	0
2	NAD	A	601	44/44	0.92	0.11	31,40,50,50	17
3	PEG	A	602	7/7	0.93	0.10	41,43,45,46	0
2	NAD	B	1302	44/44	0.94	0.11	29,38,52,52	17

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.

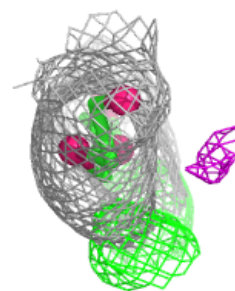
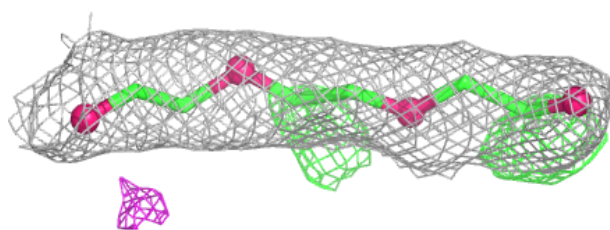
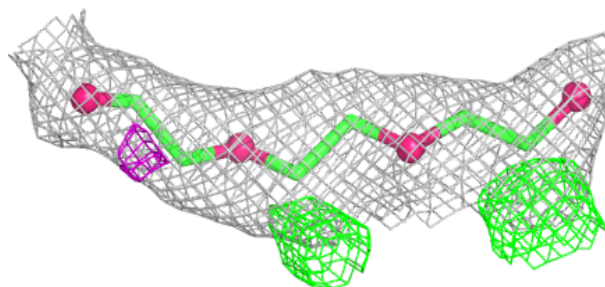
Electron density around P4C A 605:

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

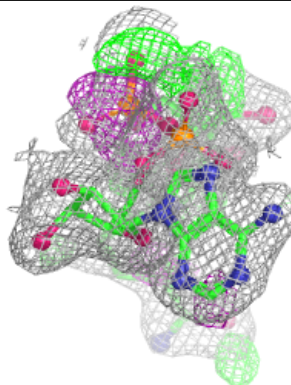
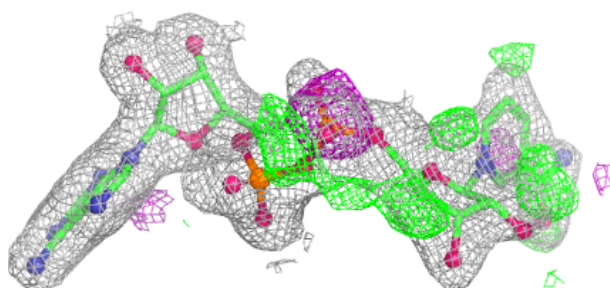
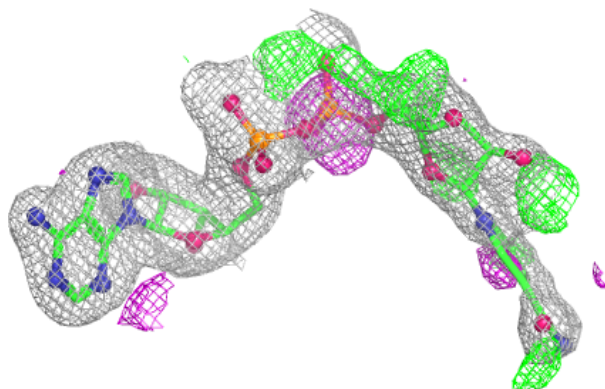


Electron density around P4C B 1306:

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

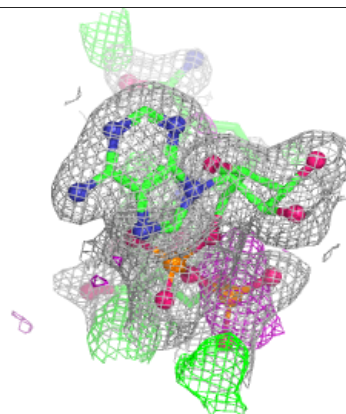
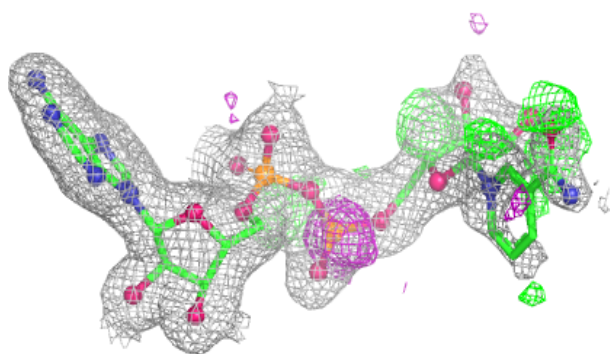
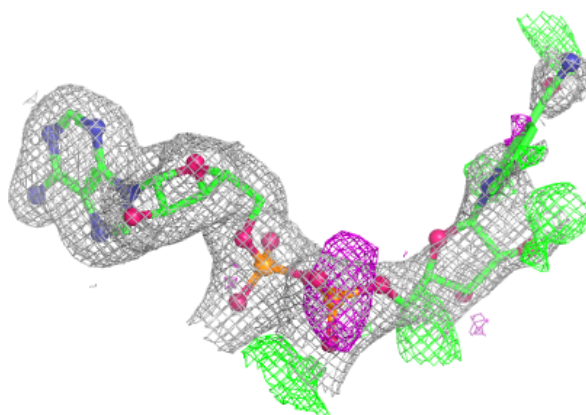
**Electron density around NAD A 601:**

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



Electron density around NAD B 1302:

$2mF_o-DF_c$ (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.