



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2022 – 08:08 PM JST

PDB ID : 7X2Y
Title : Crystal Structure of cis-4,5-dihydrodiol phthalate dehydrogenase in complex with NAD⁺ and 3-Hydroxybenzoate
Authors : Sharma, M.; Mahto, J.K.; Kumar, P.
Deposited on : 2022-02-26
Resolution : 2.48 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	:	2.30
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)	:	2.30

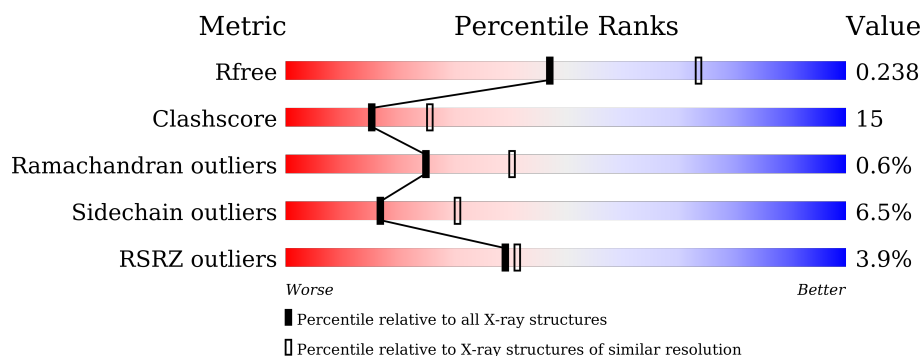
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	392	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	392	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>

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
3	GOL	A	602	-	-	X	-
3	GOL	B	601	-	-	X	-
3	GOL	B	605	-	-	X	-
4	PO4	A	604	-	-	X	-

2 Entry composition [i](#)

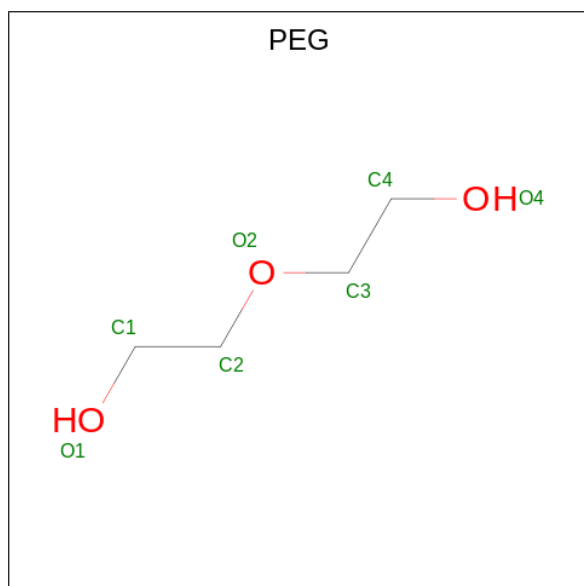
There are 7 unique types of molecules in this entry. The entry contains 5860 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4,5-dihydroxyphthalate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2668	1685	487	482	14			
1	B	342	Total	C	N	O	S	0	0	0
			2668	1685	486	483	14			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



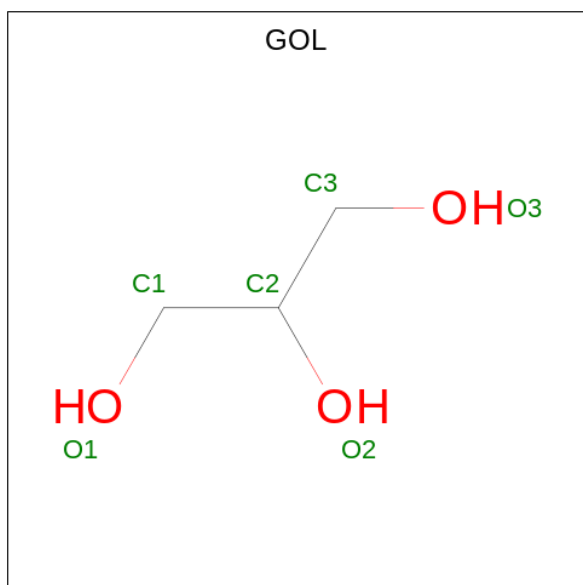
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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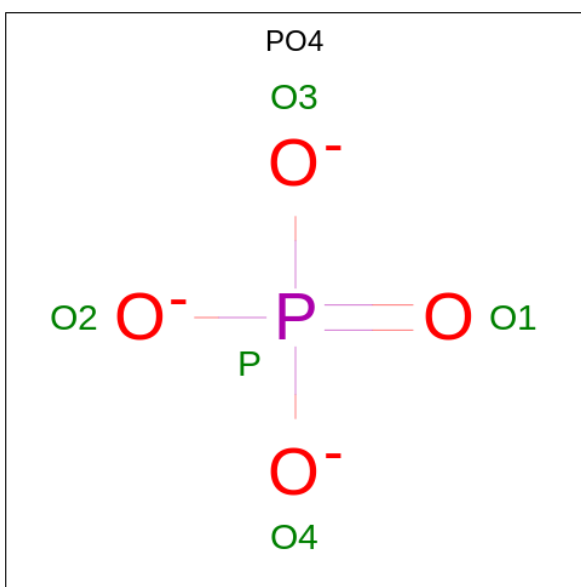
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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



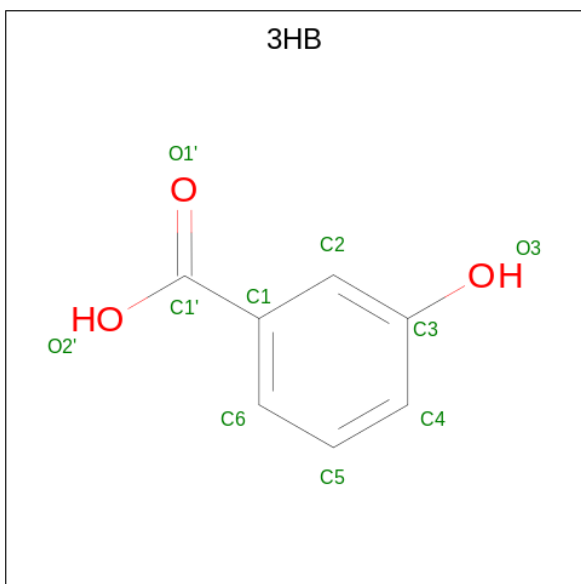
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is 3-HYDROXYBENZOIC ACID (three-letter code: 3HB) (formula: $C_7H_6O_3$) (labeled as "Ligand of Interest" by depositor).



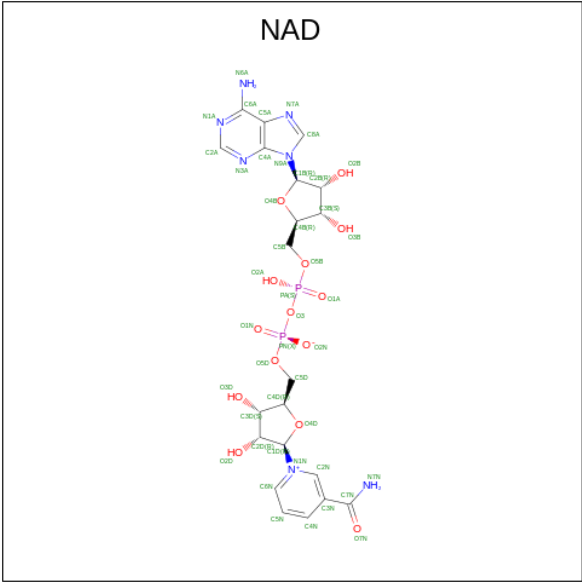
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

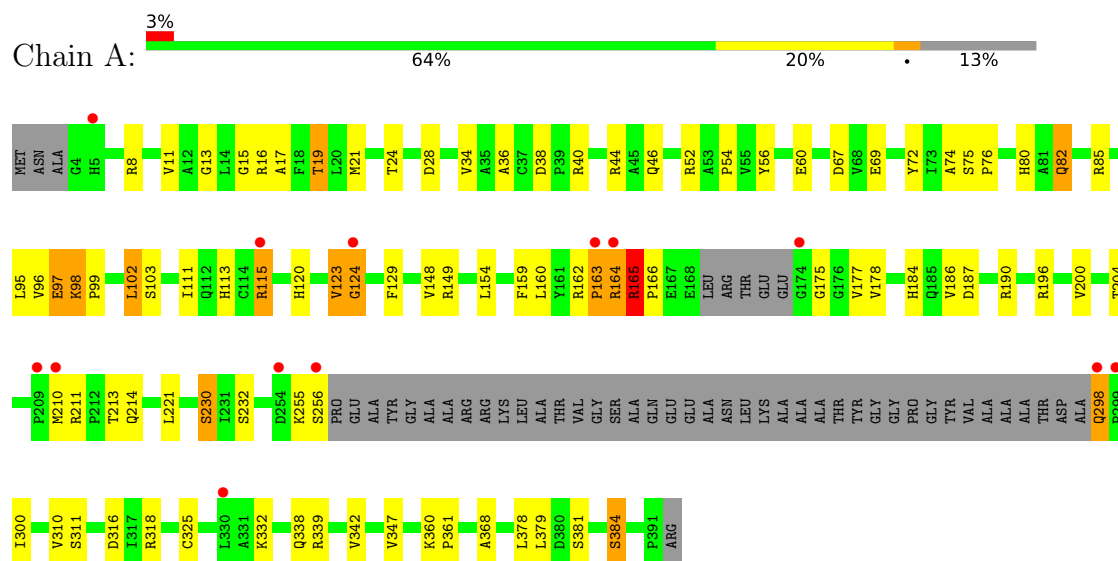
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total	O	0	0
			172	172		
7	B	162	Total	O	0	0
			162	162		

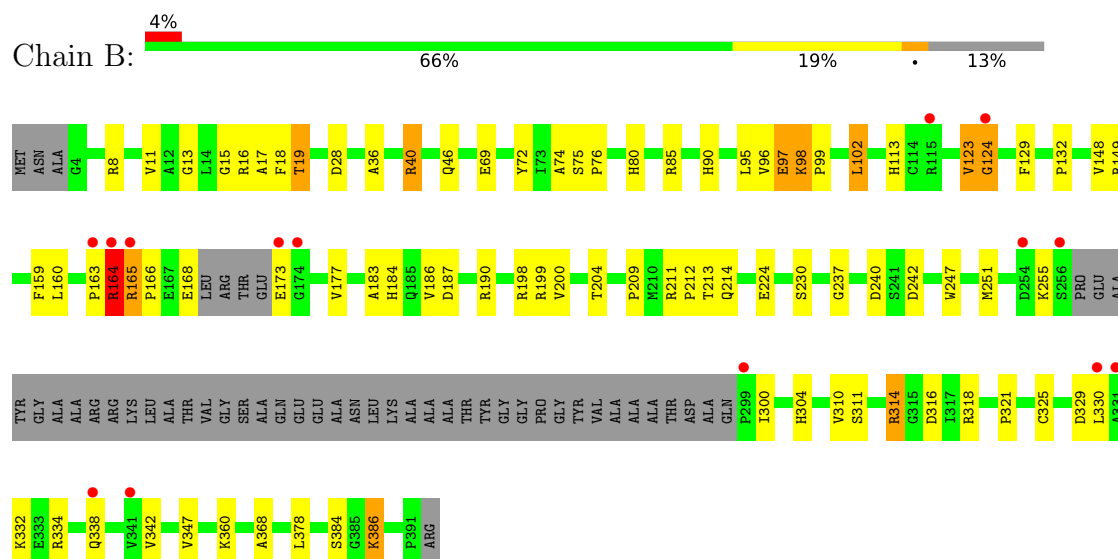
3 Residue-property plots [i](#)

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: 4,5-dihydroxyphthalate dehydrogenase



- Molecule 1: 4,5-dihydroxyphthalate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.58Å 88.31Å 162.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.18 – 2.48 27.16 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.18-2.48) 99.8 (27.16-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.235 0.193 , 0.238	Depositor DCC
R_{free} test set	1412 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5860	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8230e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, NAD, PEG, GOL, 3HB

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	0.52	1/2737 (0.0%)	0.84	3/3718 (0.1%)
1	B	0.51	2/2737 (0.1%)	0.85	3/3717 (0.1%)
All	All	0.52	3/5474 (0.1%)	0.84	6/7435 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	GLU	CD-OE2	6.83	1.33	1.25
1	B	97	GLU	CD-OE2	6.34	1.32	1.25
1	B	97	GLU	CD-OE1	5.20	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ARG	N-CA-C	-9.20	86.16	111.00
1	B	123	VAL	C-N-CA	7.86	138.81	122.30
1	B	40	ARG	CB-CA-C	7.54	125.47	110.40
1	A	123	VAL	C-N-CA	7.40	137.84	122.30
1	B	40	ARG	CG-CD-NE	-7.35	96.37	111.80
1	A	384	SER	C-N-CA	-5.53	110.70	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	ARG	Peptide

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	2668	0	2598	75	0
1	B	2668	0	2597	80	0
2	A	14	0	20	3	0
2	B	28	0	40	5	0
3	A	18	0	24	6	0
3	B	12	0	16	8	0
4	A	5	0	0	2	0
4	B	5	0	0	1	0
5	A	10	0	4	0	0
5	B	10	0	4	1	0
6	A	44	0	26	13	0
6	B	44	0	26	13	0
7	A	172	0	0	5	0
7	B	162	0	0	5	0
All	All	5860	0	5355	162	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 15.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:O	6:A:607:NAD:H6N	1.63	0.99
1:B:98:LYS:O	6:B:609:NAD:H6N	1.60	0.98
1:A:19:THR:HG21	2:A:603:PEG:H22	1.48	0.96
1:B:211:ARG:HH11	1:B:211:ARG:HA	1.32	0.92
1:A:211:ARG:HA	1:A:211:ARG:HH11	1.35	0.89
1:A:98:LYS:HE3	1:A:184:HIS:CE1	2.08	0.88
1:A:98:LYS:CE	1:A:184:HIS:CE1	2.59	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASP:HB2	3:B:605:GOL:H2	1.59	0.83
1:A:82:GLN:HG3	7:A:835:HOH:O	1.77	0.83
1:A:75:SER:O	1:A:80:HIS:HE1	1.63	0.82
1:A:163:PRO:HB2	1:A:164:ARG:O	1.79	0.81
1:B:164:ARG:HB3	6:B:609:NAD:H72N	1.44	0.80
1:B:13:GLY:HA2	6:B:609:NAD:H8A	1.62	0.79
1:A:98:LYS:HE3	1:A:184:HIS:NE2	1.99	0.78
1:B:75:SER:O	1:B:80:HIS:HE1	1.68	0.77
1:A:15:GLY:O	1:A:19:THR:HG23	1.84	0.76
1:A:159:PHE:O	1:A:163:PRO:HB3	1.87	0.75
1:A:13:GLY:HA2	6:A:607:NAD:H8A	1.67	0.74
1:B:199:ARG:HH12	2:B:607:PEG:H31	1.53	0.73
1:A:211:ARG:HA	1:A:211:ARG:NH1	2.05	0.72
1:B:211:ARG:HA	1:B:211:ARG:NH1	2.04	0.72
6:B:609:NAD:H2B	6:B:609:NAD:N3A	2.03	0.72
1:B:330:LEU:H	1:B:330:LEU:HD23	1.54	0.71
1:A:159:PHE:CE2	1:A:177:VAL:HG12	2.26	0.71
1:A:15:GLY:HA3	6:A:607:NAD:O5B	1.91	0.71
1:B:165:ARG:HD3	1:B:165:ARG:H	1.55	0.71
1:B:19:THR:HG21	2:B:602:PEG:H32	1.73	0.70
1:B:15:GLY:HA3	6:B:609:NAD:O5B	1.92	0.70
1:B:314:ARG:HH21	1:B:314:ARG:HG2	1.57	0.70
1:B:98:LYS:O	6:B:609:NAD:C6N	2.40	0.69
1:A:17:ALA:HB1	1:A:97:GLU:HG3	1.74	0.69
1:A:298:GLN:O	1:A:298:GLN:HG2	1.92	0.69
1:B:237:GLY:HA2	3:B:605:GOL:H31	1.74	0.69
1:B:46:GLN:CG	3:B:601:GOL:H2	2.23	0.69
1:B:15:GLY:O	1:B:19:THR:HG23	1.92	0.68
1:B:46:GLN:HG3	3:B:601:GOL:H2	1.76	0.68
6:A:607:NAD:H2B	6:A:607:NAD:N3A	2.08	0.68
1:B:159:PHE:CE2	1:B:177:VAL:HG12	2.29	0.68
1:B:159:PHE:O	1:B:163:PRO:HB3	1.94	0.67
1:A:200:VAL:HG22	1:A:221:LEU:CD2	2.25	0.66
1:B:98:LYS:HE3	1:B:183:ALA:HB3	1.75	0.66
1:B:13:GLY:CA	6:B:609:NAD:H8A	2.25	0.66
1:A:200:VAL:HG22	1:A:221:LEU:HD23	1.77	0.66
1:A:96:VAL:O	1:A:124:GLY:N	2.26	0.65
1:A:60:GLU:HB2	7:A:837:HOH:O	1.96	0.65
1:B:198:ARG:HD3	1:B:224:GLU:OE1	1.98	0.63
1:A:19:THR:HG21	2:A:603:PEG:C2	2.24	0.63
1:B:300:ILE:HD12	7:B:752:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:O	1:B:124:GLY:N	2.31	0.62
1:A:98:LYS:O	6:A:607:NAD:C6N	2.44	0.62
1:A:46:GLN:CG	3:A:602:GOL:H2	2.29	0.62
1:A:339:ARG:HG3	7:A:724:HOH:O	2.00	0.61
1:B:16:ARG:HE	1:B:164:ARG:HG3	1.65	0.61
6:A:607:NAD:N7N	6:A:607:NAD:O1N	2.34	0.61
1:A:46:GLN:HG3	3:A:602:GOL:H2	1.83	0.61
1:A:98:LYS:HE2	1:A:184:HIS:CE1	2.35	0.60
1:B:90:HIS:HD2	2:B:606:PEG:H32	1.66	0.60
1:A:200:VAL:HG13	1:A:378:LEU:HD23	1.84	0.59
6:B:609:NAD:H2N	6:B:609:NAD:O1N	2.02	0.59
1:B:314:ARG:HH21	1:B:314:ARG:CG	2.15	0.59
1:B:97:GLU:HA	1:B:124:GLY:HA3	1.84	0.59
1:B:90:HIS:CD2	2:B:606:PEG:H32	2.38	0.59
1:B:98:LYS:HE2	1:B:184:HIS:NE2	2.17	0.59
1:A:13:GLY:CA	6:A:607:NAD:H8A	2.32	0.58
1:B:159:PHE:CD2	1:B:177:VAL:HG12	2.39	0.58
1:B:17:ALA:HB1	1:B:97:GLU:HG3	1.85	0.58
1:A:200:VAL:CG1	1:A:378:LEU:HD23	2.34	0.57
1:B:384:SER:O	1:B:386:LYS:HE3	2.03	0.57
1:A:15:GLY:O	1:A:19:THR:CG2	2.53	0.57
1:B:75:SER:O	1:B:80:HIS:CE1	2.56	0.57
1:A:75:SER:O	1:A:80:HIS:CE1	2.52	0.56
1:A:159:PHE:CD2	1:A:177:VAL:HG12	2.41	0.56
1:A:204:THR:HB	1:A:214:GLN:HG2	1.88	0.55
1:B:242:ASP:OD2	4:B:603:PO4:O4	2.25	0.55
1:A:97:GLU:HA	1:A:124:GLY:HA3	1.88	0.55
1:B:85:ARG:HG3	1:B:113:HIS:CD2	2.41	0.55
1:B:314:ARG:HG2	1:B:314:ARG:NH2	2.21	0.55
1:B:237:GLY:CA	3:B:605:GOL:H31	2.37	0.54
3:A:602:GOL:O3	2:A:603:PEG:H32	2.07	0.54
1:B:15:GLY:O	1:B:19:THR:CG2	2.56	0.54
1:B:334:ARG:HD3	7:B:843:HOH:O	2.07	0.54
1:B:200:VAL:HG13	1:B:378:LEU:HD23	1.89	0.54
1:B:204:THR:HB	1:B:214:GLN:HG2	1.90	0.54
1:A:165:ARG:H	1:A:166:PRO:HD3	1.73	0.54
1:A:103:SER:HB3	3:A:605:GOL:H11	1.91	0.53
1:B:98:LYS:HE2	1:B:184:HIS:CE1	2.45	0.52
1:B:164:ARG:HB3	6:B:609:NAD:N7N	2.17	0.52
1:A:85:ARG:HG3	1:A:113:HIS:CD2	2.44	0.52
1:A:381:SER:O	1:A:384:SER:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:CG1	1:B:378:LEU:HD23	2.39	0.51
1:A:159:PHE:HE2	1:A:177:VAL:HG12	1.75	0.51
1:A:230:SER:HB2	7:A:795:HOH:O	2.11	0.51
1:A:164:ARG:HG3	6:A:607:NAD:O7N	2.10	0.50
1:A:211:ARG:O	1:A:213:THR:N	2.40	0.49
1:B:46:GLN:HG2	3:B:601:GOL:H2	1.93	0.49
1:A:99:PRO:HD2	6:A:607:NAD:O2D	2.12	0.49
1:B:129:PHE:CE2	1:B:347:VAL:HA	2.47	0.49
1:B:163:PRO:HD2	7:B:801:HOH:O	2.12	0.49
6:A:607:NAD:O1N	6:A:607:NAD:H2N	2.11	0.49
1:A:46:GLN:HG2	3:A:602:GOL:H2	1.94	0.48
1:B:237:GLY:C	3:B:605:GOL:H31	2.34	0.48
1:B:98:LYS:HE2	1:B:184:HIS:CD2	2.48	0.48
1:B:99:PRO:HD2	6:B:609:NAD:O2D	2.14	0.48
1:A:129:PHE:CE2	1:A:347:VAL:HA	2.49	0.48
1:A:311:SER:HA	1:A:316:ASP:OD1	2.15	0.47
1:B:90:HIS:HD2	2:B:606:PEG:C3	2.27	0.47
1:A:196:ARG:HG3	3:A:608:GOL:H32	1.97	0.47
1:B:311:SER:HA	1:B:316:ASP:OD1	2.16	0.46
1:A:186:VAL:O	1:A:190:ARG:HG3	2.16	0.46
1:B:310:VAL:O	1:B:316:ASP:HA	2.15	0.46
1:A:38:ASP:OD1	1:A:40:ARG:HB2	2.15	0.45
1:A:123:VAL:HG21	1:A:368:ALA:CB	2.46	0.45
1:B:8:ARG:N	1:B:69:GLU:OE1	2.40	0.45
6:B:609:NAD:O1N	6:B:609:NAD:N7N	2.47	0.45
1:A:13:GLY:O	1:A:74:ALA:HB3	2.16	0.45
1:A:255:LYS:O	1:A:256:SER:C	2.54	0.45
1:B:132:PRO:HG2	7:B:781:HOH:O	2.17	0.45
1:A:28:ASP:HB2	1:A:342:VAL:HG11	1.98	0.45
1:A:361:PRO:HD2	4:A:604:PO4:O3	2.17	0.45
1:B:165:ARG:NH1	1:B:166:PRO:HD3	2.31	0.45
1:A:318:ARG:HB3	1:A:325:CYS:HB2	1.99	0.45
1:B:186:VAL:O	1:B:190:ARG:HG3	2.17	0.44
1:B:148:VAL:O	1:B:149:ARG:HD2	2.17	0.44
1:A:300:ILE:HD13	7:A:774:HOH:O	2.17	0.44
1:B:72:TYR:HA	1:B:95:LEU:O	2.18	0.44
1:A:72:TYR:HA	1:A:95:LEU:O	2.18	0.44
1:B:123:VAL:HG21	1:B:368:ALA:CB	2.48	0.44
1:B:211:ARG:O	1:B:213:THR:N	2.40	0.44
1:A:11:VAL:O	1:A:36:ALA:HA	2.18	0.44
1:A:120:HIS:ND1	4:A:604:PO4:O1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ARG:N	1:A:69:GLU:OE1	2.39	0.43
1:A:164:ARG:CB	6:A:607:NAD:H72N	2.31	0.43
1:B:247:TRP:HB3	1:B:255:LYS:O	2.17	0.43
1:B:28:ASP:HB2	1:B:342:VAL:HG11	2.01	0.43
1:A:76:PRO:HA	6:A:607:NAD:H4D	2.01	0.43
1:B:204:THR:CB	1:B:214:GLN:HG2	2.48	0.43
1:A:44:ARG:HD3	1:A:56:TYR:O	2.19	0.42
1:B:11:VAL:O	1:B:36:ALA:HA	2.19	0.42
1:B:304:HIS:CD2	1:B:321:PRO:HG3	2.54	0.42
1:B:98:LYS:O	6:B:609:NAD:H1D	2.18	0.42
1:A:148:VAL:O	1:A:149:ARG:HD2	2.19	0.42
1:A:204:THR:CB	1:A:214:GLN:HG2	2.48	0.42
1:A:310:VAL:O	1:A:316:ASP:HA	2.18	0.42
1:B:164:ARG:HH11	1:B:251:MET:HE2	1.85	0.42
1:B:164:ARG:N	1:B:164:ARG:HD3	2.34	0.42
1:B:164:ARG:HH11	1:B:251:MET:CE	2.31	0.42
1:B:184:HIS:HE2	5:B:608:3HB:C2	2.32	0.42
1:A:34:VAL:O	1:A:54:PRO:HD2	2.21	0.41
1:A:111:ILE:O	1:A:115:ARG:HB2	2.20	0.41
1:B:74:ALA:HB1	7:B:703:HOH:O	2.20	0.41
1:A:21:MET:O	1:A:24:THR:HB	2.20	0.41
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.85	0.41
1:B:76:PRO:HA	6:B:609:NAD:H4D	2.02	0.41
1:B:164:ARG:NH1	1:B:251:MET:HE2	2.36	0.41
1:B:102:LEU:HD12	1:B:102:LEU:HA	1.83	0.41
1:A:164:ARG:HB2	6:A:607:NAD:N7N	2.36	0.41
1:B:18:PHE:HE2	3:B:601:GOL:H32	1.84	0.41
1:B:318:ARG:HB3	1:B:325:CYS:HB2	2.03	0.41
1:A:98:LYS:HE3	1:A:184:HIS:CD2	2.55	0.41
1:A:178:VAL:HG11	1:A:379:LEU:HG	2.03	0.41
1:A:154:LEU:HA	1:A:232:SER:O	2.21	0.40
1:B:209:PRO:O	1:B:212:PRO:HD3	2.21	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	336/392 (86%)	324 (96%)	9 (3%)	3 (1%)	17	29
1	B	336/392 (86%)	327 (97%)	8 (2%)	1 (0%)	41	59
All	All	672/784 (86%)	651 (97%)	17 (2%)	4 (1%)	25	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	GLY
1	B	124	GLY
1	A	175	GLY
1	A	165	ARG

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	279/310 (90%)	260 (93%)	19 (7%)	16	28
1	B	279/310 (90%)	262 (94%)	17 (6%)	18	34
All	All	558/620 (90%)	522 (94%)	36 (6%)	17	31

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	THR
1	A	52	ARG
1	A	67	ASP
1	A	82	GLN
1	A	98	LYS
1	A	102	LEU
1	A	115	ARG

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	162	ARG
1	A	163	PRO
1	A	165	ARG
1	A	187	ASP
1	A	210	MET
1	A	230	SER
1	A	298	GLN
1	A	332	LYS
1	A	338	GLN
1	A	360	LYS
1	B	19	THR
1	B	40	ARG
1	B	98	LYS
1	B	102	LEU
1	B	160	LEU
1	B	164	ARG
1	B	165	ARG
1	B	168	GLU
1	B	173	GLU
1	B	187	ASP
1	B	230	SER
1	B	314	ARG
1	B	329	ASP
1	B	332	LYS
1	B	338	GLN
1	B	360	LYS
1	B	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	GLN
1	A	90	HIS
1	A	353	HIS
1	A	357	ASN
1	B	80	HIS
1	B	83	GLN
1	B	90	HIS
1	B	113	HIS
1	B	338	GLN

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Mol	Chain	Res	Type
1	B	353	HIS
1	B	357	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	GOL	A	605	-	5,5,5	0.19	0	5,5,5	0.75	0
6	NAD	A	607	-	42,48,48	0.61	0	50,73,73	0.98	4 (8%)
2	PEG	B	602	-	6,6,6	0.27	0	5,5,5	0.17	0
5	3HB	A	606	-	10,10,10	2.74	3 (30%)	13,13,13	0.87	0
6	NAD	B	609	-	42,48,48	0.71	1 (2%)	50,73,73	1.10	3 (6%)
2	PEG	A	601	-	6,6,6	0.48	0	5,5,5	0.42	0
3	GOL	A	608	-	5,5,5	0.15	0	5,5,5	0.37	0
3	GOL	B	601	-	5,5,5	0.13	0	5,5,5	0.45	0
5	3HB	B	608	-	10,10,10	2.31	3 (30%)	13,13,13	1.08	1 (7%)
4	PO4	A	604	-	4,4,4	0.83	0	6,6,6	0.56	0
2	PEG	A	603	-	6,6,6	0.25	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	602	-	5,5,5	0.20	0	5,5,5	0.50	0
2	PEG	B	606	-	6,6,6	0.39	0	5,5,5	0.33	0
2	PEG	B	604	-	6,6,6	0.22	0	5,5,5	0.22	0
2	PEG	B	607	-	6,6,6	0.29	0	5,5,5	0.16	0
4	PO4	B	603	-	4,4,4	0.81	0	6,6,6	0.55	0
3	GOL	B	605	-	5,5,5	0.05	0	5,5,5	0.36	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
3	GOL	A	605	-	-	4/4/4/4	-
6	NAD	A	607	-	-	18/26/62/62	0/5/5/5
2	PEG	B	602	-	-	2/4/4/4	-
5	3HB	A	606	-	-	4/4/4/4	0/1/1/1
6	NAD	B	609	-	-	16/26/62/62	0/5/5/5
2	PEG	A	601	-	-	2/4/4/4	-
3	GOL	A	608	-	-	4/4/4/4	-
3	GOL	B	601	-	-	1/4/4/4	-
5	3HB	B	608	-	-	4/4/4/4	0/1/1/1
2	PEG	A	603	-	-	3/4/4/4	-
3	GOL	A	602	-	-	2/4/4/4	-
2	PEG	B	606	-	-	3/4/4/4	-
2	PEG	B	604	-	-	2/4/4/4	-
2	PEG	B	607	-	-	2/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	3HB	O3-C3	-6.06	1.22	1.37
5	B	608	3HB	O3-C3	-5.29	1.24	1.37
5	A	606	3HB	C2-C3	4.82	1.46	1.39
5	A	606	3HB	O2'-C1'	-3.31	1.20	1.30
5	B	608	3HB	O2'-C1'	-3.24	1.20	1.30
5	B	608	3HB	C2-C3	3.11	1.43	1.39
6	B	609	NAD	O4D-C1D	2.34	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	609	NAD	C6N-N1N-C2N	-3.56	118.72	121.97
6	B	609	NAD	C5A-C6A-N6A	3.27	125.33	120.35
6	A	607	NAD	C6N-N1N-C2N	-3.24	119.02	121.97
6	A	607	NAD	C5A-C6A-N6A	2.53	124.20	120.35
5	B	608	3HB	C4-C3-C2	-2.44	117.51	120.17
6	A	607	NAD	PN-O3-PA	2.39	141.02	132.83
6	B	609	NAD	C3B-C2B-C1B	2.33	104.49	100.98
6	A	607	NAD	C3B-C2B-C1B	2.23	104.34	100.98

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	GOL	O1-C1-C2-C3
3	A	605	GOL	C1-C2-C3-O3
3	A	608	GOL	C1-C2-C3-O3
3	A	608	GOL	O2-C2-C3-O3
6	A	607	NAD	C5B-O5B-PA-O1A
6	A	607	NAD	PN-O3-PA-O5B
6	A	607	NAD	C5D-O5D-PN-O1N
6	A	607	NAD	C5D-O5D-PN-O2N
6	A	607	NAD	O4D-C1D-N1N-C2N
6	A	607	NAD	O4D-C1D-N1N-C6N
6	B	609	NAD	C5B-O5B-PA-O1A
6	B	609	NAD	PN-O3-PA-O5B
6	B	609	NAD	C5D-O5D-PN-O3
6	B	609	NAD	O4D-C1D-N1N-C2N
6	B	609	NAD	O4D-C1D-N1N-C6N
5	B	608	3HB	C2-C1-C1'-O1'
5	B	608	3HB	C6-C1-C1'-O1'
5	B	608	3HB	C2-C1-C1'-O2'
5	B	608	3HB	C6-C1-C1'-O2'
2	B	606	PEG	C1-C2-O2-C3
5	A	606	3HB	C6-C1-C1'-O1'
5	A	606	3HB	C2-C1-C1'-O1'
5	A	606	3HB	C6-C1-C1'-O2'
5	A	606	3HB	C2-C1-C1'-O2'
2	A	603	PEG	O2-C3-C4-O4
6	A	607	NAD	O4B-C4B-C5B-O5B
6	A	607	NAD	C3B-C4B-C5B-O5B
6	B	609	NAD	O4B-C4B-C5B-O5B

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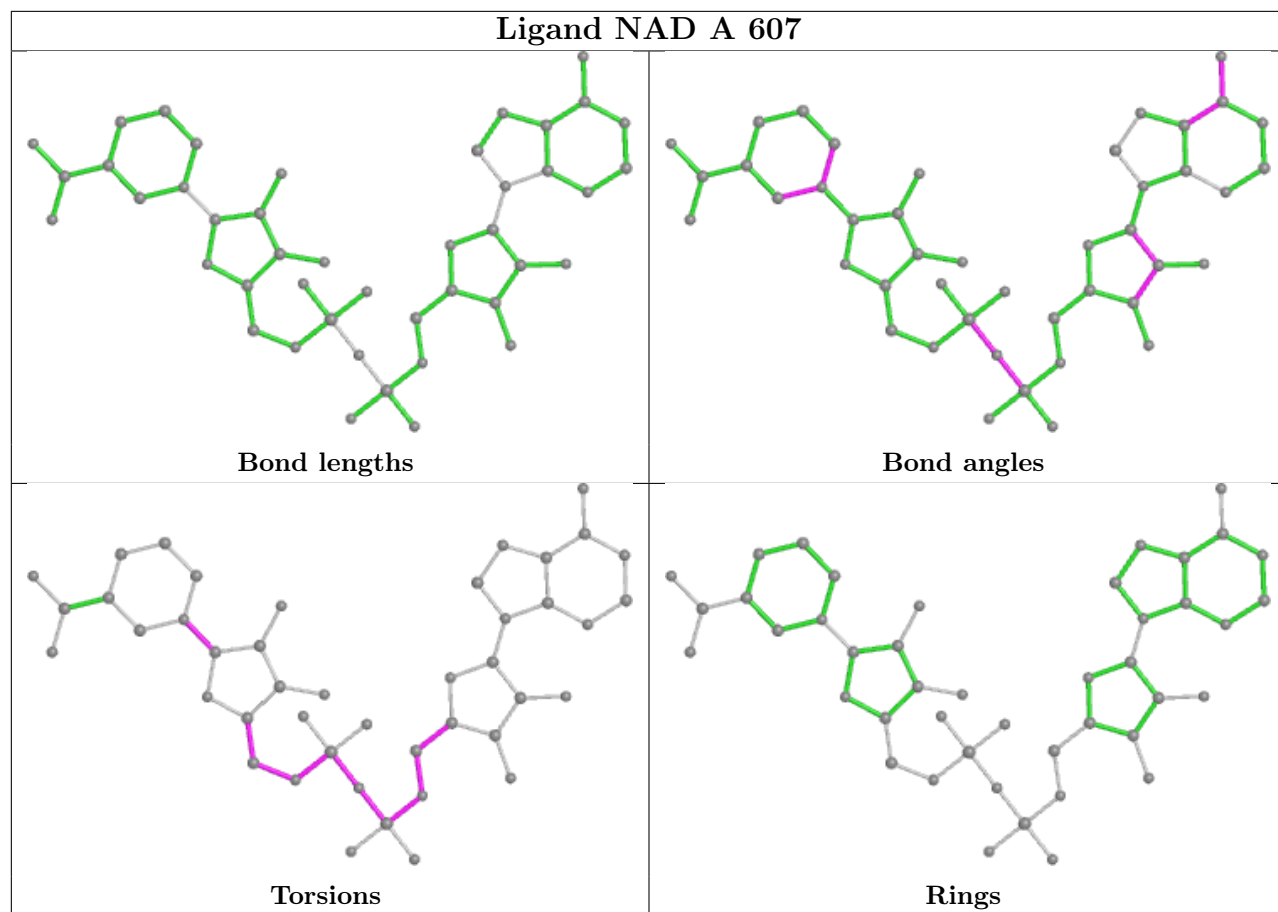
Mol	Chain	Res	Type	Atoms
6	B	609	NAD	C3B-C4B-C5B-O5B
3	A	605	GOL	O2-C2-C3-O3
6	A	607	NAD	O4D-C4D-C5D-O5D
6	A	607	NAD	C3D-C4D-C5D-O5D
6	B	609	NAD	O4D-C4D-C5D-O5D
6	B	609	NAD	C3D-C4D-C5D-O5D
2	A	601	PEG	O2-C3-C4-O4
3	A	608	GOL	O1-C1-C2-C3
3	B	605	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-O2
3	A	608	GOL	O1-C1-C2-O2
2	B	607	PEG	O1-C1-C2-O2
3	A	602	GOL	O2-C2-C3-O3
2	B	606	PEG	O1-C1-C2-O2
6	A	607	NAD	PA-O3-PN-O5D
6	B	609	NAD	PA-O3-PN-O5D
2	B	602	PEG	O1-C1-C2-O2
2	B	607	PEG	C4-C3-O2-C2
6	A	607	NAD	C4D-C5D-O5D-PN
2	B	606	PEG	C4-C3-O2-C2
2	B	604	PEG	C4-C3-O2-C2
6	A	607	NAD	C5B-O5B-PA-O3
6	A	607	NAD	C5D-O5D-PN-O3
3	A	602	GOL	C1-C2-C3-O3
6	B	609	NAD	C4D-C5D-O5D-PN
6	A	607	NAD	C5B-O5B-PA-O2A
6	B	609	NAD	C5B-O5B-PA-O2A
6	B	609	NAD	C5D-O5D-PN-O1N
2	B	602	PEG	C1-C2-O2-C3
3	B	601	GOL	O2-C2-C3-O3
2	A	601	PEG	O1-C1-C2-O2
2	A	603	PEG	O1-C1-C2-O2
2	B	604	PEG	O2-C3-C4-O4
3	B	605	GOL	O1-C1-C2-O2
6	A	607	NAD	PA-O3-PN-O1N
6	B	609	NAD	C4B-C5B-O5B-PA
6	B	609	NAD	PA-O3-PN-O1N
2	A	603	PEG	C4-C3-O2-C2
6	A	607	NAD	C4B-C5B-O5B-PA
6	A	607	NAD	C2D-C1D-N1N-C6N
6	B	609	NAD	C5B-O5B-PA-O3

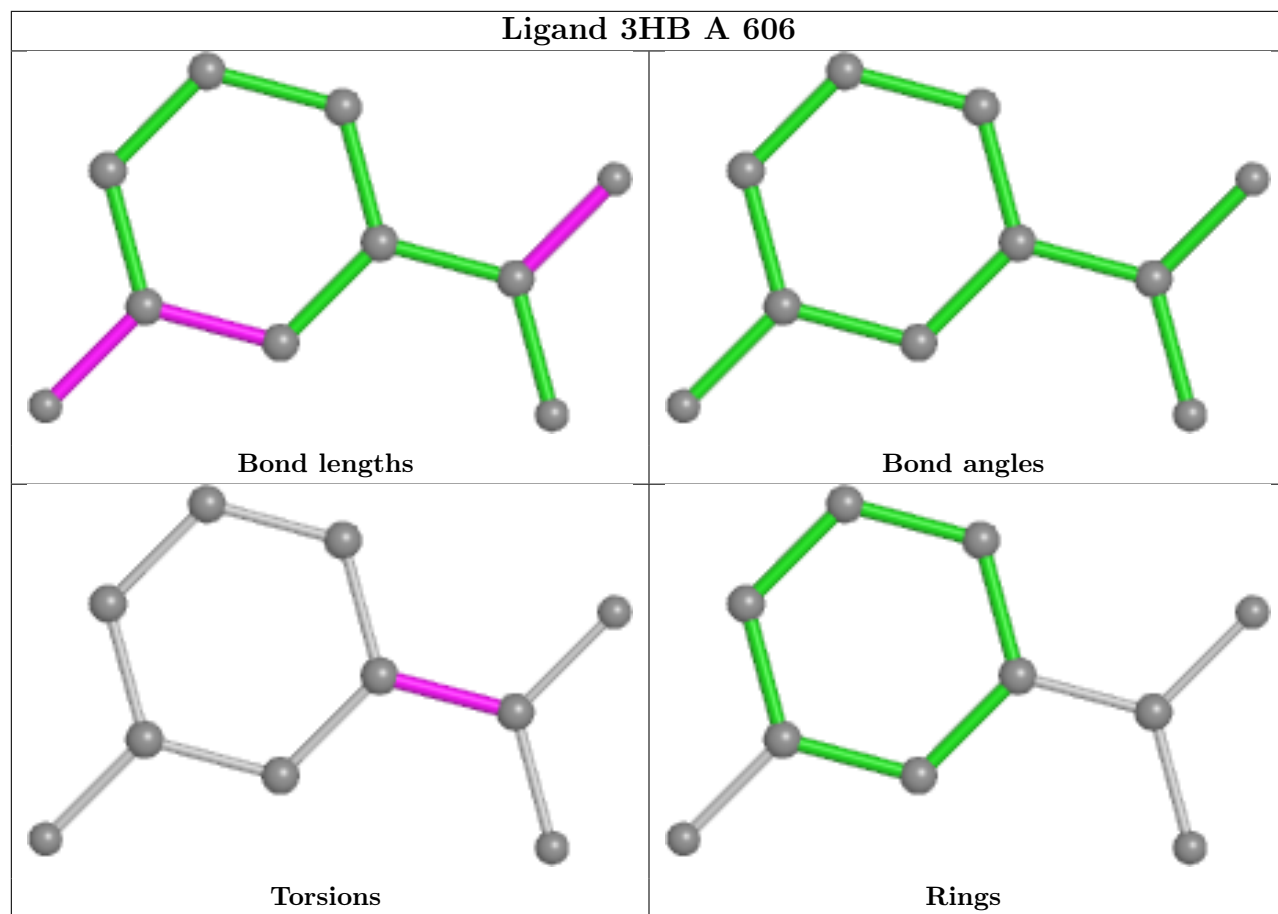
There are no ring outliers.

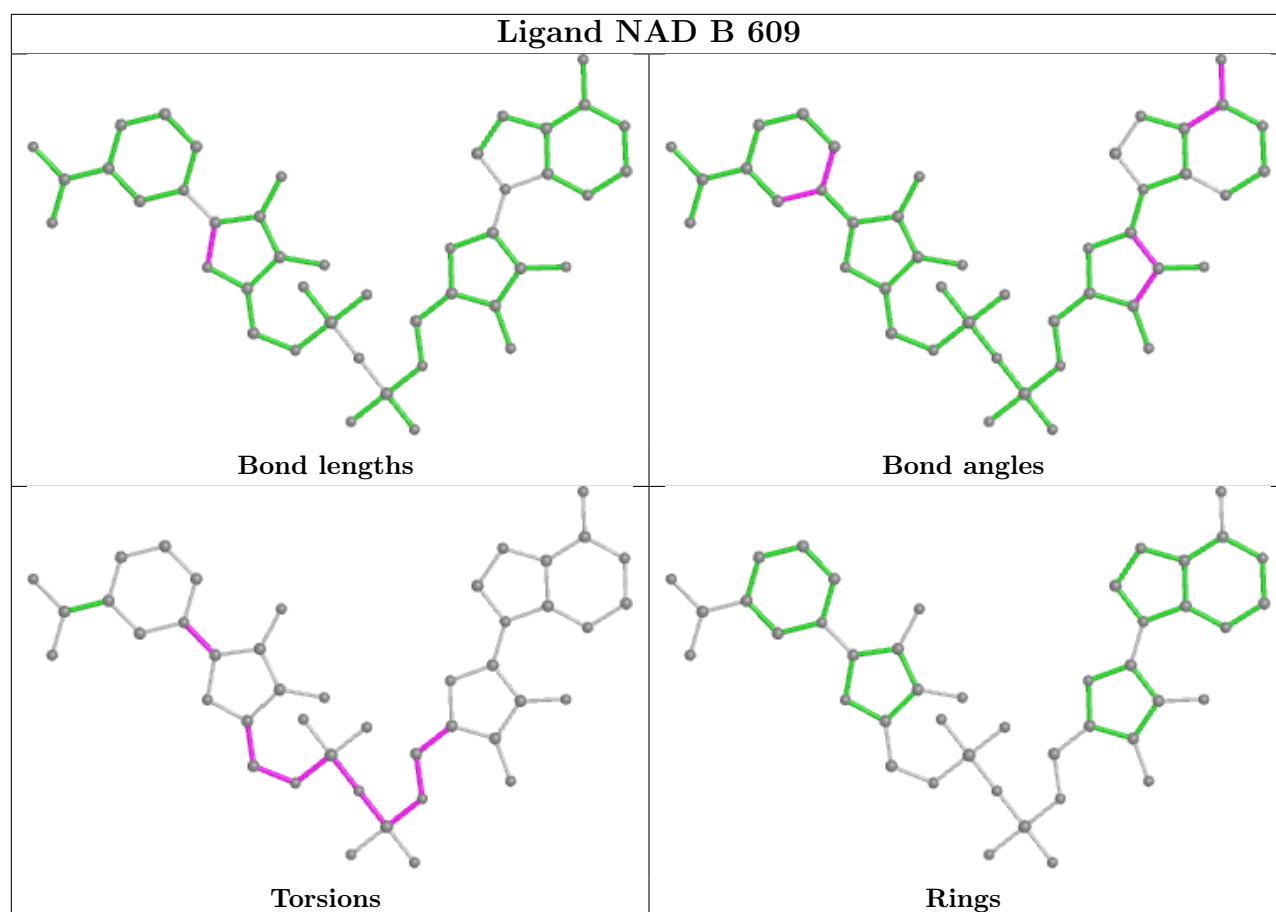
14 monomers are involved in 51 short contacts:

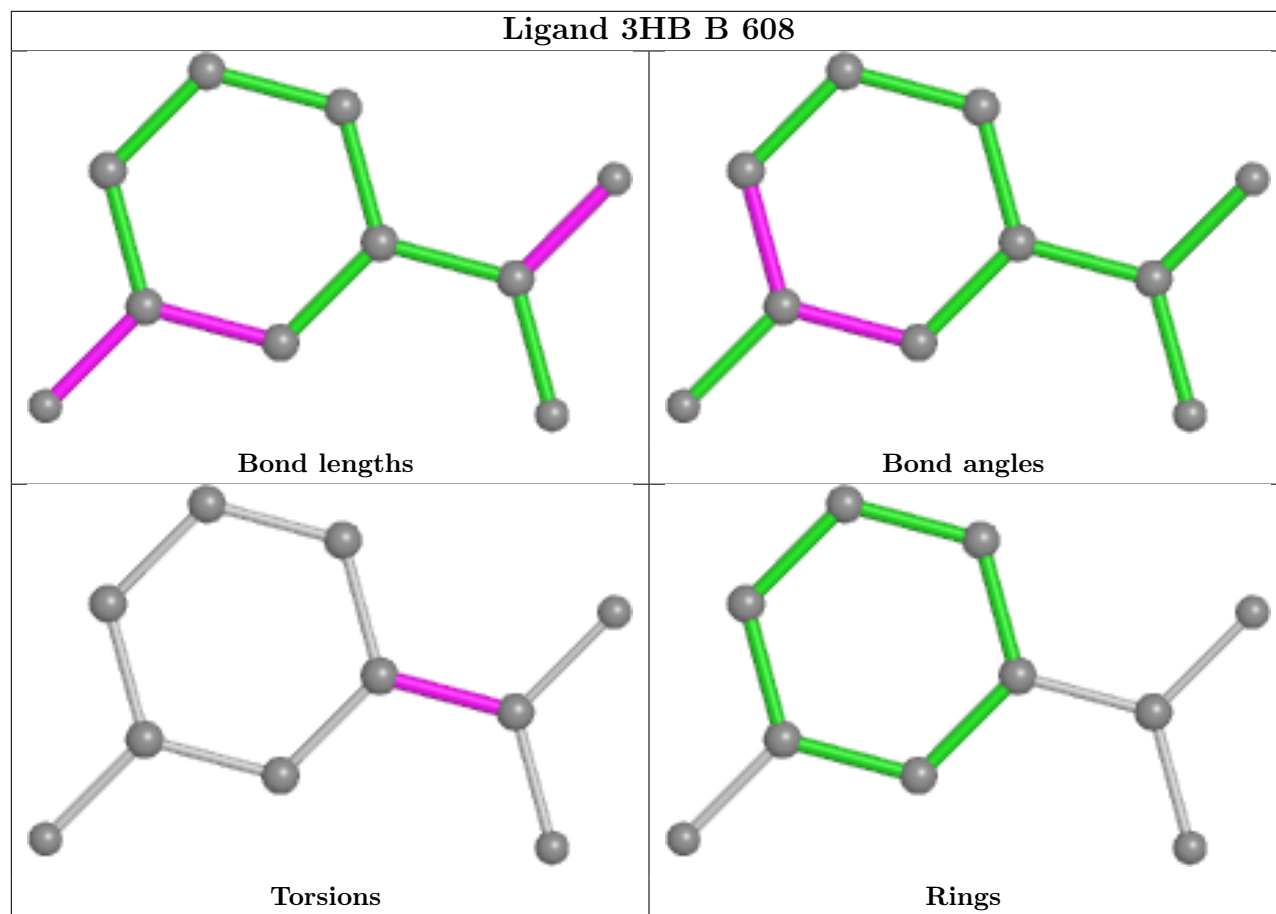
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	GOL	1	0
6	A	607	NAD	13	0
2	B	602	PEG	1	0
6	B	609	NAD	13	0
3	A	608	GOL	1	0
3	B	601	GOL	4	0
5	B	608	3HB	1	0
4	A	604	PO4	2	0
2	A	603	PEG	3	0
3	A	602	GOL	4	0
2	B	606	PEG	3	0
2	B	607	PEG	1	0
4	B	603	PO4	1	0
3	B	605	GOL	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/392 (87%)	-0.17	13 (3%) 40 42	6, 16, 47, 82	0
1	B	342/392 (87%)	-0.14	14 (4%) 37 39	6, 16, 44, 95	0
All	All	684/784 (87%)	-0.16	27 (3%) 39 41	6, 16, 48, 95	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	GLN	4.7
1	B	330	LEU	4.4
1	A	299	PRO	4.0
1	A	330	LEU	4.0
1	B	256	SER	3.9
1	A	209	PRO	3.5
1	A	164	ARG	3.5
1	B	173	GLU	3.3
1	B	165	ARG	3.3
1	B	331	ALA	3.1
1	A	256	SER	3.0
1	B	163	PRO	2.9
1	A	124	GLY	2.8
1	B	299	PRO	2.8
1	A	163	PRO	2.8
1	A	210	MET	2.7
1	B	254	ASP	2.6
1	B	164	ARG	2.4
1	A	115	ARG	2.4
1	B	174	GLY	2.4
1	B	341	VAL	2.4
1	B	338	GLN	2.2
1	A	5	HIS	2.1
1	B	124	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	115	ARG	2.0
1	A	174	GLY	2.0
1	A	254	ASP	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.

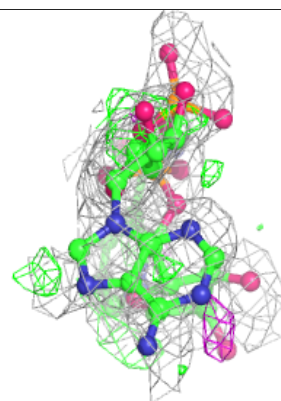
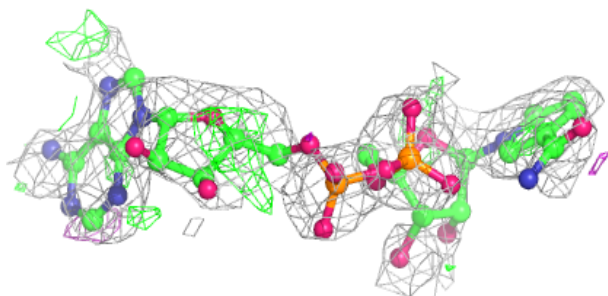
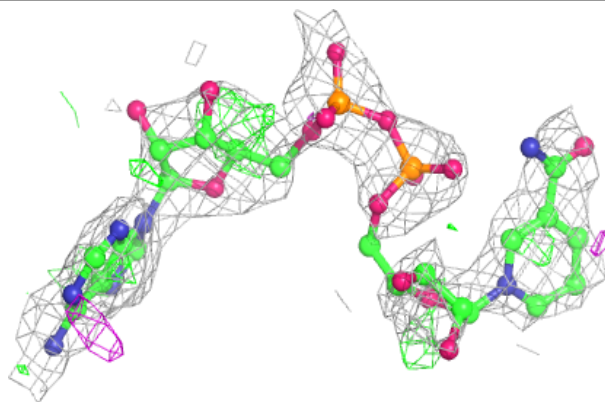
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	605	6/6	0.81	0.29	38,45,49,50	0
2	PEG	B	607	7/7	0.83	0.18	39,47,54,55	0
2	PEG	A	603	7/7	0.83	0.16	49,49,54,54	0
6	NAD	B	609	44/44	0.83	0.29	22,32,44,51	44
2	PEG	B	602	7/7	0.84	0.20	37,44,53,54	0
6	NAD	A	607	44/44	0.86	0.24	30,46,69,73	44
5	3HB	A	606	10/10	0.86	0.30	25,30,34,46	0
2	PEG	A	601	7/7	0.87	0.12	26,28,29,31	0
3	GOL	A	602	6/6	0.88	0.15	29,32,34,35	0
5	3HB	B	608	10/10	0.88	0.28	26,31,34,49	0
2	PEG	B	604	7/7	0.89	0.15	33,38,45,45	0
4	PO4	B	603	5/5	0.90	0.28	49,55,59,61	0
2	PEG	B	606	7/7	0.91	0.25	23,33,45,46	0
4	PO4	A	604	5/5	0.93	0.23	56,58,62,78	0
3	GOL	B	601	6/6	0.93	0.13	28,30,31,32	0
3	GOL	B	605	6/6	0.94	0.20	38,52,55,55	0
3	GOL	A	608	6/6	0.96	0.18	31,40,43,49	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.

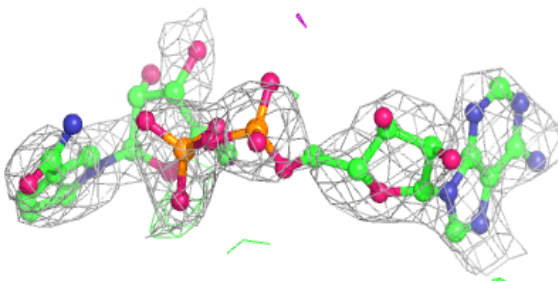
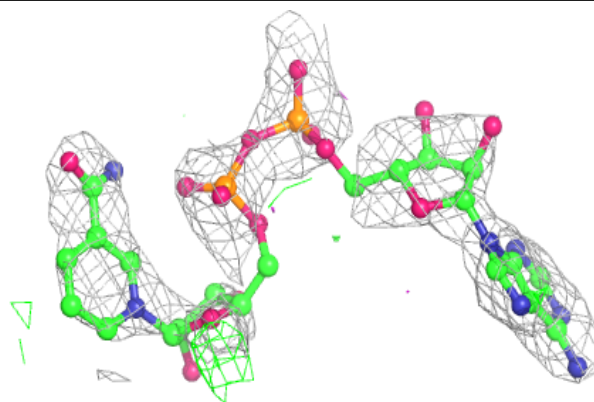
Electron density around NAD B 609:

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



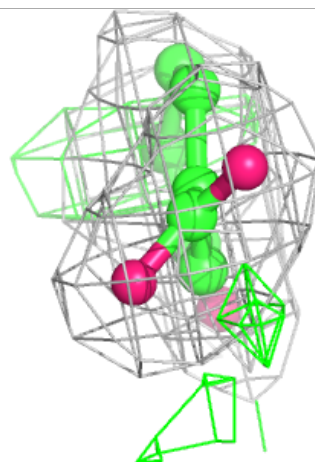
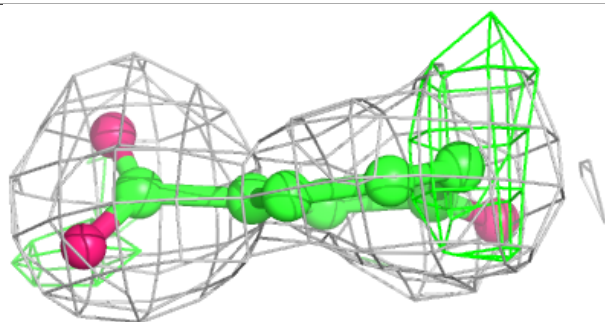
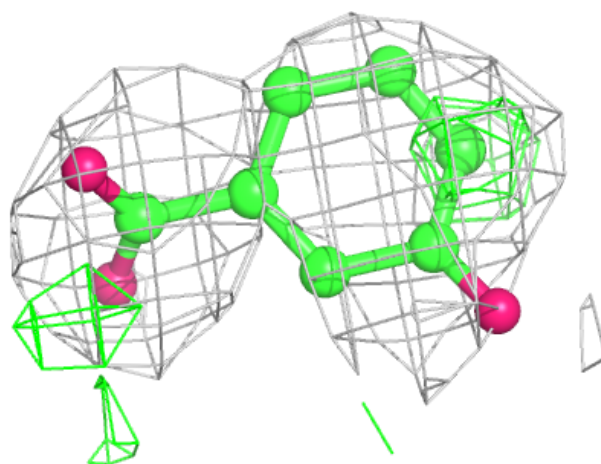
Electron density around NAD A 607:

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



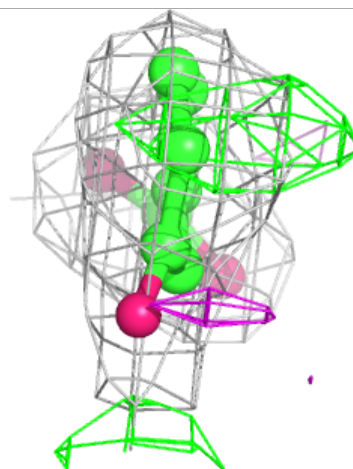
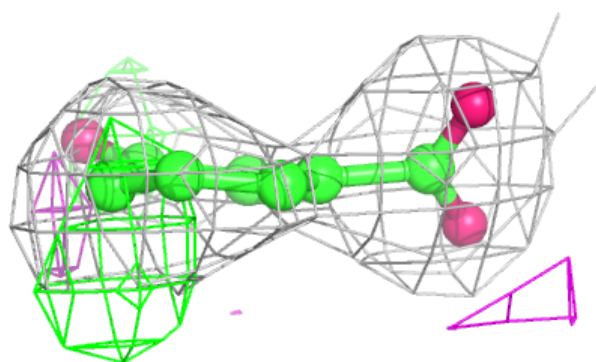
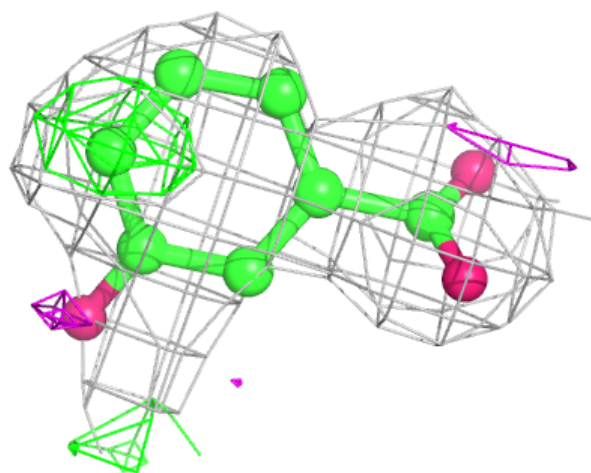
Electron density around 3HB A 606:

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



Electron density around 3HB B 608:

$2mF_o-DF_c$ (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.