



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:36 am BST

PDB ID : 1YBA
Title : The active form of phosphoglycerate dehydrogenase
Authors : Thompson, J.R.; Banaszak, L.J.
Deposited on : 2004-12-20
Resolution : 2.24 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 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 : 2.11
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) : 2.11

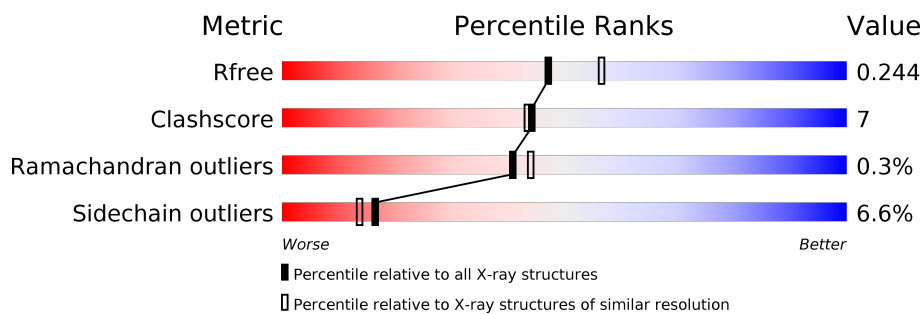
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	410	
1	B	410	
1	C	410	
1	D	410	

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	AKG	B	412	-	-	X	-
4	UNL	C	414	-	-	X	-
4	UNL	D	414	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14017 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	Se	0	1	0
			3083	1950	535	586	4	8			
1	B	406	Total	C	N	O	S	Se	0	1	0
			3086	1952	535	587	4	8			
1	C	406	Total	C	N	O	S	Se	0	2	0
			3097	1958	540	587	4	8			
1	D	406	Total	C	N	O	S	Se	0	2	0
			3094	1956	536	590	4	8			

There are 32 discrepancies between the modelled and reference sequences:

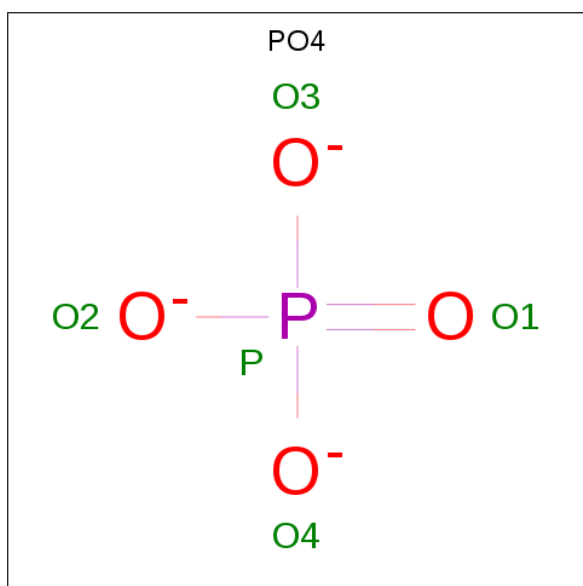
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
A	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
B	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	229	MSE	MET	MODIFIED RESIDUE	UNP P08328

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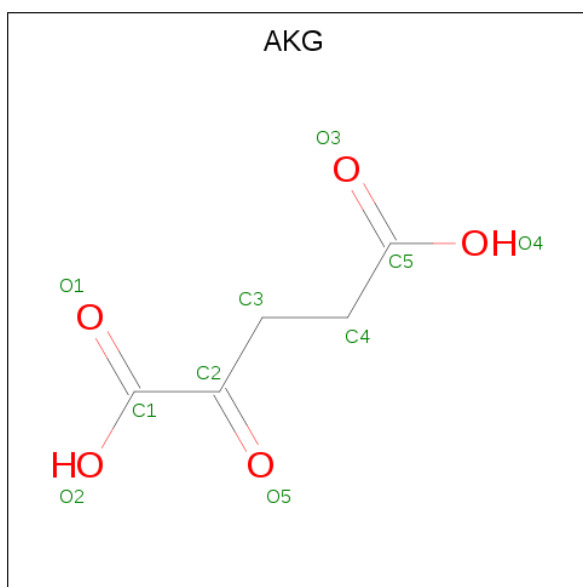
Chain	Residue	Modelled	Actual	Comment	Reference
C	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
C	397	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	175	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	203	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	220	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	221	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	229	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	341	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	376	MSE	MET	MODIFIED RESIDUE	UNP P08328
D	397	MSE	MET	MODIFIED RESIDUE	UNP P08328

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).

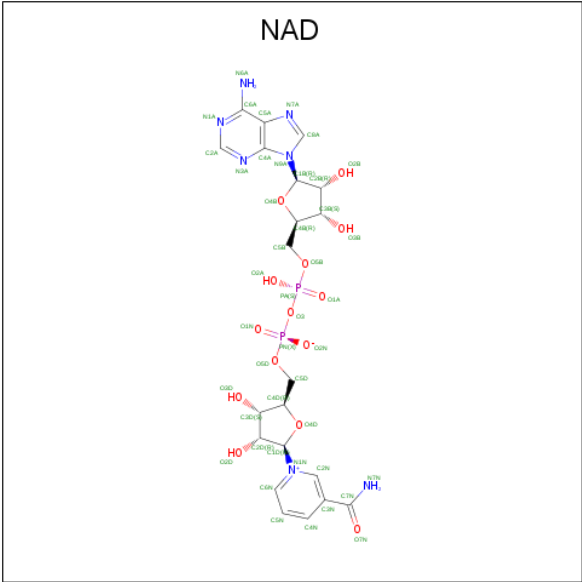


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	5	5		
4	A	2	Total	C	O	0	0
			20	10	10		
4	D	2	Total	C	O	0	0
			20	10	10		
4	C	2	Total	C	O	0	0
			20	10	10		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

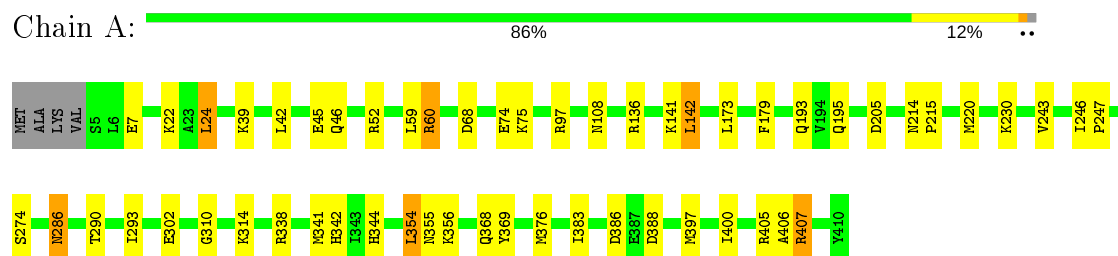
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		
6	B	330	Total	O	0	0
			330	330		
6	C	350	Total	O	0	0
			350	350		
6	D	366	Total	O	0	0
			366	366		

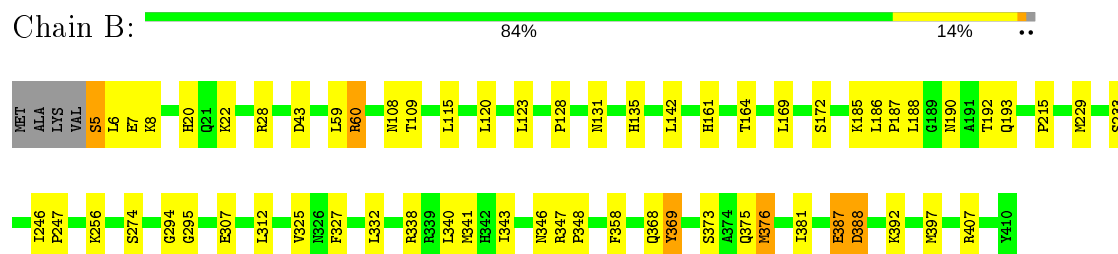
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

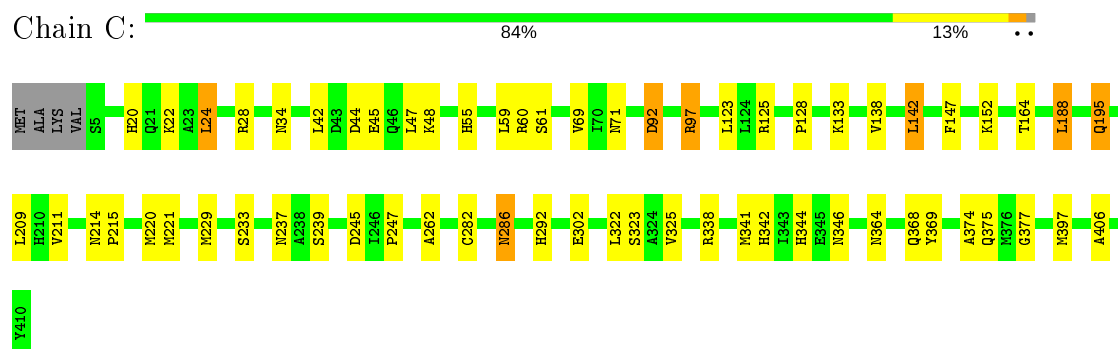
• Molecule 1: D-3-phosphoglycerate dehydrogenase



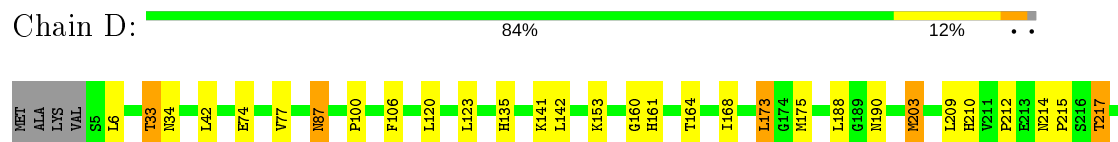
• Molecule 1: D-3-phosphoglycerate dehydrogenase



• Molecule 1: D-3-phosphoglycerate dehydrogenase



• Molecule 1: D-3-phosphoglycerate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	76.16 Å 76.16 Å 354.14 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 49.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.24) 94.2 (49.00-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	32.92 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.235 0.204 , 0.244	Depositor DCC
R_{free} test set	4538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14017	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: AKG, PO4, UNL, NAD

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	0.74	0/3128	0.81	2/4224 (0.0%)
1	B	0.78	0/3131	0.81	4/4228 (0.1%)
1	C	0.75	0/3141	0.79	2/4239 (0.0%)
1	D	0.77	1/3139 (0.0%)	0.79	0/4239
All	All	0.76	1/12539 (0.0%)	0.80	8/16930 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	MSE	SE-CE	6.56	2.34	1.95

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	60	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	60	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	28	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	322	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	60	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	28	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	60	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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	3083	0	3120	34	0
1	B	3086	0	3121	36	0
1	C	3097	0	3135	57	0
1	D	3094	0	3124	42	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	4	0
3	C	10	0	4	2	0
3	D	10	0	4	0	0
4	A	20	0	0	0	0
4	B	10	0	0	1	0
4	C	20	0	0	2	0
4	D	20	0	0	2	0
5	A	44	0	26	0	0
5	B	44	0	26	1	0
5	C	44	0	26	0	0
5	D	44	0	26	0	0
6	A	300	0	0	5	0
6	B	330	0	0	6	0
6	C	350	0	0	7	0
6	D	366	0	0	7	0
All	All	14017	0	12620	168	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 7.

All (168) 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:D:175:MSE:SE	1:D:175:MSE:CE	2.16	1.42
1:A:376:MSE:SE	1:A:376:MSE:CE	2.18	1.41
1:D:376:MSE:SE	1:D:376:MSE:CE	2.21	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:MSE:CE	1:D:203:MSE:SE	2.34	1.25
1:D:212:PRO:O	1:D:217:THR:HG21	1.66	0.96
1:C:97:ARG:HD3	6:C:671:HOH:O	1.66	0.95
1:A:355:ASN:HD21	1:A:368:GLN:HE22	1.12	0.92
1:C:375[B]:GLN:NE2	1:C:375[B]:GLN:H	1.66	0.92
1:C:375[B]:GLN:H	1:C:375[B]:GLN:HE21	0.94	0.91
1:B:348:PRO:HB3	1:C:364:ASN:ND2	1.88	0.88
1:B:343:ILE:HG23	1:B:376:MSE:HE3	1.59	0.84
1:B:190:ASN:HD21	1:D:190:ASN:HD21	1.27	0.82
1:B:348:PRO:HB3	1:C:364:ASN:HD21	1.41	0.81
1:C:375[B]:GLN:N	1:C:375[B]:GLN:HE21	1.77	0.80
1:C:342:HIS:HD2	1:C:344:HIS:HD2	1.26	0.80
1:B:387:GLU:HB2	6:B:674:HOH:O	1.81	0.78
1:B:340:LEU:HD13	1:B:397:MSE:HE1	1.72	0.70
1:C:214:ASN:HB2	1:C:215:PRO:HD2	1.73	0.70
1:A:342:HIS:HD2	1:A:344:HIS:HD2	1.39	0.70
1:C:342:HIS:HD2	1:C:344:HIS:CD2	2.10	0.69
1:D:341:MSE:HE3	1:D:343:ILE:HG13	1.73	0.69
1:A:24:LEU:H	1:A:24:LEU:HD23	1.57	0.69
3:B:412:AKG:O4	3:B:412:AKG:C2	2.41	0.68
1:B:164:THR:HG23	1:B:188:LEU:CD1	2.25	0.67
1:C:142:LEU:O	1:C:142:LEU:HD22	1.95	0.66
1:A:286:ASN:HD22	1:A:286:ASN:H	1.43	0.66
1:D:303:ASN:HB3	6:D:718:HOH:O	1.95	0.65
1:A:22:LYS:HE2	1:A:302:GLU:OE2	1.97	0.65
1:A:355:ASN:ND2	1:A:368:GLN:HE22	1.92	0.65
1:C:375[B]:GLN:HG2	6:C:500:HOH:O	1.96	0.64
4:D:414:UNL:O4	4:D:414:UNL:C2	2.44	0.64
1:C:71:ASN:HD21	1:C:97:ARG:NH2	1.96	0.63
1:C:397:MSE:HE2	1:C:406:ALA:HB1	1.80	0.63
1:C:342:HIS:CD2	1:C:344:HIS:HD2	2.13	0.63
1:C:22:LYS:HG3	1:C:302:GLU:HG3	1.80	0.62
1:A:342:HIS:HD2	1:A:344:HIS:CD2	2.17	0.62
1:B:186:LEU:HD12	1:B:187:PRO:HD2	1.81	0.62
4:C:414:UNL:O2	4:C:414:UNL:O4	2.18	0.62
1:B:340:LEU:HD22	1:B:397:MSE:HE1	1.81	0.62
1:B:190:ASN:ND2	1:D:190:ASN:HD21	1.95	0.62
1:D:153:LYS:HE2	1:D:203:MSE:HE2	1.81	0.61
1:B:340:LEU:HD22	1:B:397:MSE:CE	2.30	0.61
1:A:24:LEU:N	1:A:24:LEU:HD23	2.15	0.60
1:C:20:HIS:HD2	1:C:22:LYS:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HD22	1:B:295:GLY:HA3	1.66	0.60
1:C:47:LEU:HB3	1:C:48:LYS:HE3	1.84	0.60
1:B:20:HIS:HD2	1:B:22:LYS:H	1.50	0.60
1:D:33:THR:HG22	6:D:762:HOH:O	2.01	0.59
1:C:71:ASN:HD21	1:C:97:ARG:HH21	1.51	0.59
1:A:214:ASN:HB2	1:A:215:PRO:HD2	1.83	0.59
1:B:332:LEU:HD13	1:B:369:TYR:HB2	1.85	0.59
1:C:375[B]:GLN:CG	6:C:500:HOH:O	2.51	0.58
1:B:161:HIS:HD2	5:B:414:NAD:O2A	1.86	0.58
1:D:217:THR:HG22	6:D:531:HOH:O	2.03	0.58
1:B:164:THR:HG23	1:B:188:LEU:HD12	1.86	0.58
1:D:341:MSE:C	1:D:341:MSE:HE2	2.24	0.58
1:A:405:ARG:HD3	6:A:707:HOH:O	2.04	0.57
1:C:286:ASN:H	1:C:286:ASN:HD22	1.50	0.57
1:A:60:ARG:HD3	6:A:507:HOH:O	2.03	0.57
1:D:217:THR:HG23	1:D:243:VAL:HG22	1.86	0.57
4:B:413:UNL:C2	4:B:413:UNL:O3	2.52	0.56
1:D:341:MSE:HE2	1:D:342:HIS:N	2.20	0.56
1:D:318:ASN:C	1:D:318:ASN:HD22	2.08	0.56
1:C:44:ASP:O	1:C:48:LYS:HG2	2.06	0.55
1:B:185:LYS:H	1:B:193:GLN:HE22	1.54	0.55
1:C:92:ASP:OD2	1:C:92:ASP:N	2.40	0.55
1:B:387:GLU:OE2	1:B:387:GLU:HA	2.06	0.55
1:C:61:SER:HG	3:C:412:AKG:C5	2.19	0.54
1:C:209:LEU:HD22	1:C:220:MSE:HE3	1.89	0.54
4:C:414:UNL:C2	4:C:414:UNL:O4	2.55	0.54
1:C:209:LEU:CD2	1:C:220:MSE:HE3	2.38	0.54
1:C:211:VAL:HG21	1:C:220:MSE:HE2	1.90	0.54
1:C:142:LEU:C	1:C:142:LEU:CD2	2.76	0.54
1:D:210:HIS:HD2	6:D:482:HOH:O	1.91	0.53
1:A:142:LEU:HD23	1:A:142:LEU:O	2.09	0.53
1:A:290:THR:HB	1:A:293:ILE:HD11	1.91	0.53
3:B:412:AKG:H42	6:B:559:HOH:O	2.09	0.53
1:A:141:LYS:HZ1	3:B:412:AKG:H31	1.74	0.52
1:D:164:THR:HG23	1:D:188:LEU:HD22	1.91	0.52
1:B:388:ASP:OD2	1:B:388:ASP:N	2.40	0.51
1:D:87:ASN:N	1:D:87:ASN:OD1	2.43	0.51
1:A:59:LEU:HD23	1:A:59:LEU:N	2.25	0.51
1:C:20:HIS:HE1	6:C:681:HOH:O	1.92	0.51
1:C:142:LEU:O	1:C:142:LEU:CD2	2.59	0.51
1:B:115:LEU:HD22	1:B:294:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:414:UNL:C5	4:D:414:UNL:O2	2.58	0.51
1:B:20:HIS:CD2	1:B:22:LYS:H	2.29	0.51
1:B:368:GLN:NE2	1:C:368:GLN:HE21	2.09	0.50
1:B:108:ASN:ND2	1:B:295:GLY:HA3	2.26	0.50
1:A:205:ASP:OD1	1:A:230:LYS:HE2	2.12	0.50
1:C:237:ASN:ND2	1:C:239:SER:H	2.08	0.50
1:B:169:LEU:O	1:B:172:SER:HB2	2.11	0.50
1:A:24:LEU:N	1:A:24:LEU:CD2	2.74	0.50
1:A:141:LYS:NZ	3:B:412:AKG:H31	2.26	0.50
1:C:209:LEU:HD11	1:C:221:MSE:HG3	1.94	0.49
1:D:341:MSE:HE2	1:D:342:HIS:CA	2.42	0.49
1:A:310:GLY:O	1:A:314:LYS:HG3	2.13	0.49
1:C:342:HIS:CD2	1:C:344:HIS:CD2	2.97	0.49
1:D:342:HIS:HD2	1:D:344:HIS:CD2	2.30	0.49
1:B:131:ASN:O	1:B:135:HIS:HD2	1.96	0.49
1:B:5:SER:HA	1:B:8:LYS:HB2	1.94	0.48
1:C:147:PHE:HB3	1:C:152:LYS:HE2	1.95	0.48
1:C:71:ASN:ND2	1:C:97:ARG:HH21	2.12	0.47
1:B:246:ILE:HB	1:B:247:PRO:HD3	1.97	0.46
1:A:22:LYS:CE	1:A:302:GLU:OE2	2.62	0.46
1:B:123:LEU:HD23	1:B:128:PRO:HG2	1.98	0.46
1:B:120:LEU:C	1:B:120:LEU:HD12	2.36	0.46
1:D:352:THR:O	1:D:356:LYS:HB2	2.16	0.46
1:C:292:HIS:HB3	1:D:141:LYS:HE2	1.98	0.46
1:B:229:MSE:HE2	1:B:233:SER:OG	2.16	0.46
1:D:209:LEU:HD11	1:D:221:MSE:HG3	1.98	0.45
1:A:342:HIS:HB2	1:A:397:MSE:HE3	1.98	0.45
1:C:245:ASP:OD1	1:C:247:PRO:HD2	2.16	0.45
1:D:330:VAL:HG13	1:D:369:TYR:CG	2.52	0.45
1:B:368:GLN:HE21	1:C:368:GLN:HE21	1.64	0.45
1:D:246:ILE:HB	1:D:247:PRO:HD3	1.97	0.45
1:B:407:ARG:HG3	6:B:702:HOH:O	2.17	0.45
1:C:342:HIS:ND1	1:C:397:MSE:HE3	2.32	0.45
1:A:354:LEU:HD13	1:A:400:ILE:CD1	2.47	0.45
1:C:164:THR:HG23	1:C:188:LEU:HG	1.99	0.45
1:A:407:ARG:CD	6:A:707:HOH:O	2.65	0.44
1:D:342:HIS:HE1	1:D:397:MSE:O	2.00	0.44
1:A:338:ARG:HB2	1:A:383:ILE:HG13	2.00	0.44
1:D:318:ASN:ND2	1:D:318:ASN:C	2.70	0.44
1:C:24:LEU:O	1:C:28:ARG:HG3	2.18	0.43
1:C:282:CYS:O	1:D:135:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LYS:HB3	1:C:138:VAL:HB	2.00	0.43
1:B:185:LYS:NZ	6:B:696:HOH:O	2.51	0.43
1:B:358:PHE:CZ	1:B:397:MSE:HE2	2.53	0.43
1:C:55:HIS:HD2	6:C:606:HOH:O	2.00	0.43
1:D:214:ASN:HB2	1:D:215:PRO:CD	2.48	0.43
1:D:340:LEU:HD22	1:D:397:MSE:SE	2.68	0.43
1:C:346:ASN:HD21	1:C:377:GLY:HA3	1.83	0.43
1:C:374:ALA:CB	1:C:375[B]:GLN:NE2	2.82	0.43
1:C:123:LEU:HD23	1:C:128:PRO:HG2	2.01	0.43
1:C:48:LYS:HE2	1:C:69:VAL:HG22	2.01	0.43
1:A:397:MSE:HE2	1:A:406:ALA:HB1	2.01	0.43
1:A:246:ILE:HB	1:A:247:PRO:HD3	2.02	0.42
1:A:97:ARG:HD3	6:A:557:HOH:O	2.20	0.42
1:C:61:SER:OG	3:C:412:AKG:C5	2.67	0.42
1:D:160:GLY:O	1:D:164:THR:HB	2.19	0.42
1:A:342:HIS:CD2	1:A:344:HIS:HD2	2.28	0.42
1:D:161:HIS:CG	6:D:656:HOH:O	2.73	0.42
1:A:344:HIS:HE1	6:A:435:HOH:O	2.02	0.42
1:D:240:ARG:HD3	6:D:768:HOH:O	2.19	0.42
1:C:195:GLN:NE2	6:C:595:HOH:O	2.52	0.41
1:C:211:VAL:HG11	1:C:220:MSE:HE1	2.02	0.41
1:D:318:ASN:HD21	1:D:320:SER:HB2	1.85	0.41
1:C:142:LEU:C	1:C:142:LEU:HD22	2.40	0.41
1:D:120:LEU:HD12	1:D:120:LEU:C	2.41	0.41
1:C:344:HIS:HE1	6:C:537:HOH:O	2.04	0.41
1:D:168:ILE:HD11	1:D:188:LEU:HD23	2.02	0.41
1:A:46:GLN:HA	1:A:46:GLN:NE2	2.36	0.41
1:C:209:LEU:HD22	1:C:220:MSE:CE	2.50	0.41
1:C:229:MSE:HE2	1:C:233:SER:OG	2.21	0.41
1:D:332:LEU:HD13	1:D:369:TYR:HB2	2.02	0.41
1:D:77:VAL:HG12	1:D:315:TYR:HE2	1.86	0.41
1:A:179:PHE:CZ	1:A:193:GLN:HB2	2.56	0.41
1:D:392:LYS:HE2	6:D:661:HOH:O	2.21	0.41
1:A:354:LEU:HD13	1:A:400:ILE:HD13	2.03	0.41
1:A:220:MSE:HG2	1:A:243:VAL:HG13	2.04	0.40
1:B:60:ARG:HD3	6:B:423:HOH:O	2.20	0.40
1:C:123:LEU:HD11	1:C:262:ALA:HB2	2.03	0.40
1:D:173:LEU:HD12	1:D:173:LEU:HA	1.91	0.40
1:D:318:ASN:ND2	1:D:320:SER:H	2.20	0.40
1:B:7:GLU:HB2	6:B:661:HOH:O	2.22	0.40
1:C:374:ALA:HB3	1:C:375[B]:GLN:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD11	1:D:262:ALA:HB2	2.03	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	405/410 (99%)	386 (95%)	18 (4%)	1 (0%)	47	53
1	B	405/410 (99%)	389 (96%)	14 (4%)	2 (0%)	29	28
1	C	406/410 (99%)	393 (97%)	13 (3%)	0	100	100
1	D	406/410 (99%)	383 (94%)	21 (5%)	2 (0%)	29	28
All	All	1622/1640 (99%)	1551 (96%)	66 (4%)	5 (0%)	41	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	GLU
1	B	43	ASP
1	D	6	LEU
1	A	386	ASP
1	B	215	PRO

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	329/323 (102%)	307 (93%)	22 (7%)	16	13
1	B	329/323 (102%)	305 (93%)	24 (7%)	14	10
1	C	330/323 (102%)	313 (95%)	17 (5%)	23	22
1	D	330/323 (102%)	307 (93%)	23 (7%)	15	12
All	All	1318/1292 (102%)	1232 (94%)	86 (6%)	16	14

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	24	LEU
1	A	39	LYS
1	A	42	LEU
1	A	45	GLU
1	A	52	ARG
1	A	68	ASP
1	A	74	GLU
1	A	75	LYS
1	A	108	ASN
1	A	136	ARG
1	A	142	LEU
1	A	173	LEU
1	A	195	GLN
1	A	274	SER
1	A	286	ASN
1	A	341	MSE
1	A	354	LEU
1	A	356	LYS
1	A	369	TYR
1	A	388	ASP
1	A	407	ARG
1	B	5	SER
1	B	6	LEU
1	B	59	LEU
1	B	109	THR
1	B	142	LEU
1	B	192	THR
1	B	256	LYS
1	B	274	SER
1	B	307	GLU
1	B	312	LEU
1	B	325	VAL

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Mol	Chain	Res	Type
1	B	327	PHE
1	B	338	ARG
1	B	341	MSE
1	B	346	ASN
1	B	347	ARG
1	B	369	TYR
1	B	373	SER
1	B	375	GLN
1	B	376	MSE
1	B	381	ILE
1	B	387	GLU
1	B	388	ASP
1	B	392	LYS
1	C	24	LEU
1	C	34	ASN
1	C	42	LEU
1	C	45	GLU
1	C	59	LEU
1	C	92	ASP
1	C	97	ARG
1	C	125	ARG
1	C	142	LEU
1	C	188	LEU
1	C	195	GLN
1	C	286	ASN
1	C	323	SER
1	C	325	VAL
1	C	338	ARG
1	C	341	MSE
1	C	369	TYR
1	D	33	THR
1	D	34	ASN
1	D	42	LEU
1	D	87	ASN
1	D	100	PRO
1	D	106	PHE
1	D	142	LEU
1	D	173	LEU
1	D	217	THR
1	D	268	THR
1	D	274	SER
1	D	318	ASN

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Mol	Chain	Res	Type
1	D	327	PHE
1	D	331	SER
1	D	338	ARG
1	D	341	MSE
1	D	347	ARG
1	D	352	THR
1	D	369	TYR
1	D	376	MSE
1	D	386	ASP
1	D	387	GLU
1	D	392	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	87	ASN
1	A	108	ASN
1	A	273	ASN
1	A	286	ASN
1	A	303	ASN
1	A	342	HIS
1	A	344	HIS
1	A	346	ASN
1	A	368	GLN
1	B	20	HIS
1	B	46	GLN
1	B	55	HIS
1	B	71	ASN
1	B	161	HIS
1	B	184	ASN
1	B	190	ASN
1	B	193	GLN
1	B	257	HIS
1	B	273	ASN
1	B	303	ASN
1	B	346	ASN
1	B	355	ASN
1	B	368	GLN
1	B	395	GLN
1	C	20	HIS
1	C	34	ASN

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Mol	Chain	Res	Type
1	C	46	GLN
1	C	71	ASN
1	C	108	ASN
1	C	140	ASN
1	C	190	ASN
1	C	195	GLN
1	C	237	ASN
1	C	273	ASN
1	C	286	ASN
1	C	303	ASN
1	C	342	HIS
1	C	344	HIS
1	C	346	ASN
1	C	364	ASN
1	D	34	ASN
1	D	140	ASN
1	D	161	HIS
1	D	210	HIS
1	D	257	HIS
1	D	273	ASN
1	D	303	ASN
1	D	318	ASN
1	D	342	HIS
1	D	346	ASN
1	D	355	ASN
1	D	368	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 7 are unknown - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AKG	C	412	-	3,9,9	1.73	1 (33%)	4,11,11	2.27	2 (50%)
3	AKG	B	412	-	3,9,9	1.53	1 (33%)	4,11,11	1.38	1 (25%)
5	NAD	D	415	-	42,48,48	1.72	3 (7%)	50,73,73	1.67	10 (20%)
2	PO4	A	411	-	4,4,4	1.62	1 (25%)	6,6,6	1.08	0
2	PO4	C	411	-	4,4,4	1.02	0	6,6,6	1.06	0
2	PO4	B	411	-	4,4,4	0.95	0	6,6,6	2.36	2 (33%)
5	NAD	C	415	-	42,48,48	1.92	4 (9%)	50,73,73	1.54	7 (14%)
3	AKG	A	413	-	3,9,9	0.26	0	4,11,11	1.89	1 (25%)
5	NAD	A	416	-	42,48,48	2.02	5 (11%)	50,73,73	1.36	6 (12%)
5	NAD	B	414	-	42,48,48	1.75	5 (11%)	50,73,73	1.39	7 (14%)
3	AKG	D	412	-	3,9,9	1.84	2 (66%)	4,11,11	1.39	1 (25%)
2	PO4	D	411	-	4,4,4	1.22	1 (25%)	6,6,6	1.97	2 (33%)
2	PO4	A	412	-	4,4,4	0.71	0	6,6,6	0.45	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	AKG	C	412	-	-	0/3/9/9	-
5	NAD	B	414	-	-	7/26/62/62	0/5/5/5
5	NAD	D	415	-	-	6/26/62/62	0/5/5/5
5	NAD	C	415	-	-	5/26/62/62	0/5/5/5
3	AKG	A	413	-	-	3/3/9/9	-
5	NAD	A	416	-	-	6/26/62/62	0/5/5/5
3	AKG	B	412	-	-	3/3/9/9	-
3	AKG	D	412	-	-	1/3/9/9	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	416	NAD	O7N-C7N	9.63	1.42	1.24
5	D	415	NAD	O7N-C7N	9.27	1.41	1.24
5	C	415	NAD	O7N-C7N	9.08	1.41	1.24
5	B	414	NAD	O7N-C7N	8.12	1.39	1.24
5	A	416	NAD	C2A-N3A	5.37	1.40	1.32
5	B	414	NAD	C2A-N3A	4.62	1.39	1.32
5	C	415	NAD	C2A-N3A	4.44	1.39	1.32
5	A	416	NAD	C2N-N1N	3.25	1.38	1.35
5	C	415	NAD	C2N-N1N	3.17	1.38	1.35
5	B	414	NAD	C2A-N1A	3.01	1.39	1.33
5	B	414	NAD	O4D-C1D	2.64	1.44	1.41
5	A	416	NAD	C2A-N1A	2.63	1.38	1.33
5	A	416	NAD	C2B-C1B	-2.59	1.49	1.53
5	D	415	NAD	C2A-N3A	2.53	1.36	1.32
2	A	411	PO4	P-O4	-2.52	1.47	1.54
3	C	412	AKG	C3-C2	2.48	1.54	1.51
3	D	412	AKG	C3-C2	2.34	1.54	1.51
3	B	412	AKG	O5-C2	2.33	1.26	1.22
3	D	412	AKG	O5-C2	2.15	1.25	1.22
5	C	415	NAD	C2B-C1B	-2.09	1.50	1.53
5	D	415	NAD	O4B-C4B	-2.08	1.40	1.45
2	D	411	PO4	P-O4	-2.05	1.48	1.54
5	B	414	NAD	C2N-N1N	2.04	1.37	1.35

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	415	NAD	O4D-C1D-C2D	-5.69	98.62	106.93
5	D	415	NAD	N3A-C2A-N1A	-5.38	120.26	128.68
5	A	416	NAD	C4A-C5A-N7A	-4.77	104.43	109.40
5	C	415	NAD	N3A-C2A-N1A	-4.64	121.43	128.68
5	C	415	NAD	O7N-C7N-C3N	-4.63	114.09	119.63
5	B	414	NAD	N3A-C2A-N1A	-4.55	121.57	128.68
5	C	415	NAD	C3N-C7N-N7N	4.19	122.78	117.75
2	B	411	PO4	O4-P-O1	-4.17	95.63	110.89
5	A	416	NAD	O4D-C1D-C2D	-3.70	101.52	106.93
2	B	411	PO4	O2-P-O1	3.39	123.30	110.89
5	A	416	NAD	N3A-C2A-N1A	-3.39	123.38	128.68
2	D	411	PO4	O3-P-O1	-3.21	99.14	110.89
3	A	413	AKG	C3-C4-C5	-3.07	107.53	112.67
5	B	414	NAD	O4D-C1D-C2D	-3.02	102.52	106.93
3	C	412	AKG	C3-C4-C5	-3.00	107.64	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	415	NAD	C4A-C5A-N7A	-2.98	106.29	109.40
5	B	414	NAD	O7N-C7N-N7N	-2.94	118.41	122.58
2	D	411	PO4	O3-P-O2	2.85	117.11	107.97
5	C	415	NAD	O4D-C1D-C2D	-2.82	102.81	106.93
5	D	415	NAD	PN-O3-PA	-2.69	123.61	132.83
3	C	412	AKG	O5-C2-C3	2.65	124.90	120.38
5	B	414	NAD	C3N-C7N-N7N	2.61	120.88	117.75
3	B	412	AKG	C3-C2-C1	-2.58	114.90	121.32
5	B	414	NAD	C1B-N9A-C4A	-2.54	122.18	126.64
5	D	415	NAD	C1B-N9A-C4A	-2.53	122.20	126.64
5	D	415	NAD	O4B-C4B-C5B	-2.45	101.32	109.37
3	D	412	AKG	C3-C4-C5	-2.39	108.67	112.67
5	C	415	NAD	O4B-C1B-C2B	-2.36	103.48	106.93
5	C	415	NAD	O2A-PA-O5B	2.27	118.28	107.75
5	D	415	NAD	C2N-C3N-C4N	2.26	120.82	118.26
5	C	415	NAD	C2N-C3N-C4N	2.26	120.82	118.26
5	A	416	NAD	C5A-C6A-N6A	2.17	123.65	120.35
5	B	414	NAD	C6N-N1N-C2N	-2.11	120.05	121.97
5	A	416	NAD	PN-O3-PA	-2.09	125.65	132.83
5	D	415	NAD	C5A-C6A-N6A	2.07	123.49	120.35
5	B	414	NAD	C3D-C2D-C1D	-2.05	97.90	100.98
5	D	415	NAD	O2N-PN-O1N	2.04	122.31	112.24
5	A	416	NAD	O4B-C1B-C2B	-2.02	103.97	106.93
5	D	415	NAD	O2A-PA-O1A	2.01	122.19	112.24

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	412	AKG	C2-C3-C4-C5
5	D	415	NAD	O4D-C1D-N1N-C6N
5	A	416	NAD	O4D-C1D-N1N-C2N
5	A	416	NAD	O4D-C1D-N1N-C6N
5	A	416	NAD	C2D-C1D-N1N-C2N
5	A	416	NAD	C2D-C1D-N1N-C6N
5	B	414	NAD	O4D-C1D-N1N-C2N
5	B	414	NAD	O4D-C1D-N1N-C6N
5	B	414	NAD	C2D-C1D-N1N-C2N
5	B	414	NAD	C2D-C1D-N1N-C6N
5	C	415	NAD	O4D-C1D-N1N-C2N
5	C	415	NAD	O4D-C1D-N1N-C6N
5	C	415	NAD	C2D-C1D-N1N-C2N

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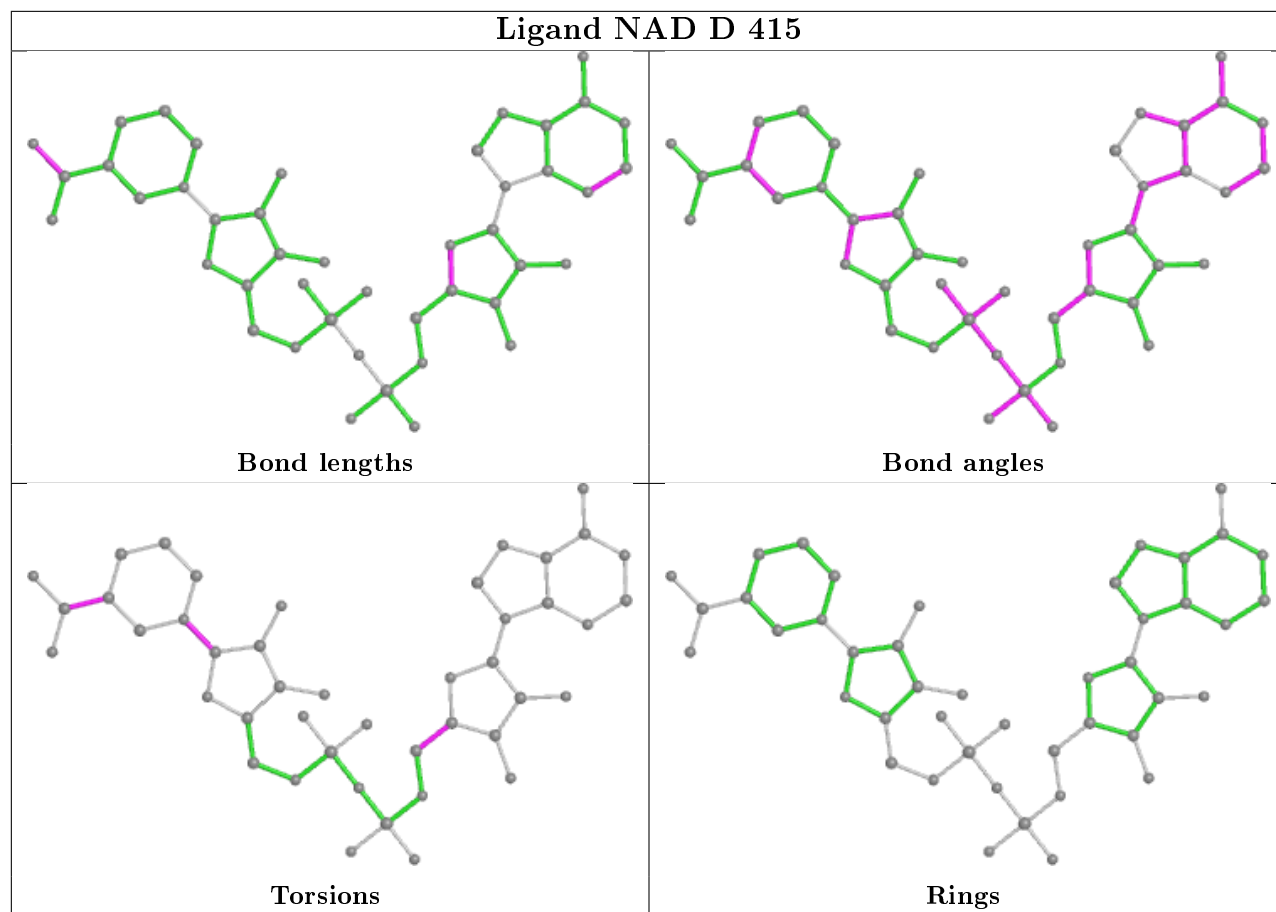
Mol	Chain	Res	Type	Atoms
5	C	415	NAD	C2D-C1D-N1N-C6N
3	A	413	AKG	C2-C3-C4-C5
3	A	413	AKG	O5-C2-C3-C4
3	A	413	AKG	C1-C2-C3-C4
3	B	412	AKG	C1-C2-C3-C4
5	D	415	NAD	C4N-C3N-C7N-N7N
5	D	415	NAD	C4N-C3N-C7N-O7N
3	B	412	AKG	O5-C2-C3-C4
5	C	415	NAD	O4B-C4B-C5B-O5B
3	D	412	AKG	C2-C3-C4-C5
5	A	416	NAD	PN-O3-PA-O1A
5	B	414	NAD	PN-O3-PA-O1A
5	B	414	NAD	PN-O3-PA-O2A
5	B	414	NAD	O4B-C4B-C5B-O5B
5	A	416	NAD	O4B-C4B-C5B-O5B
5	D	415	NAD	C2D-C1D-N1N-C2N
5	D	415	NAD	C2D-C1D-N1N-C6N
5	D	415	NAD	O4B-C4B-C5B-O5B

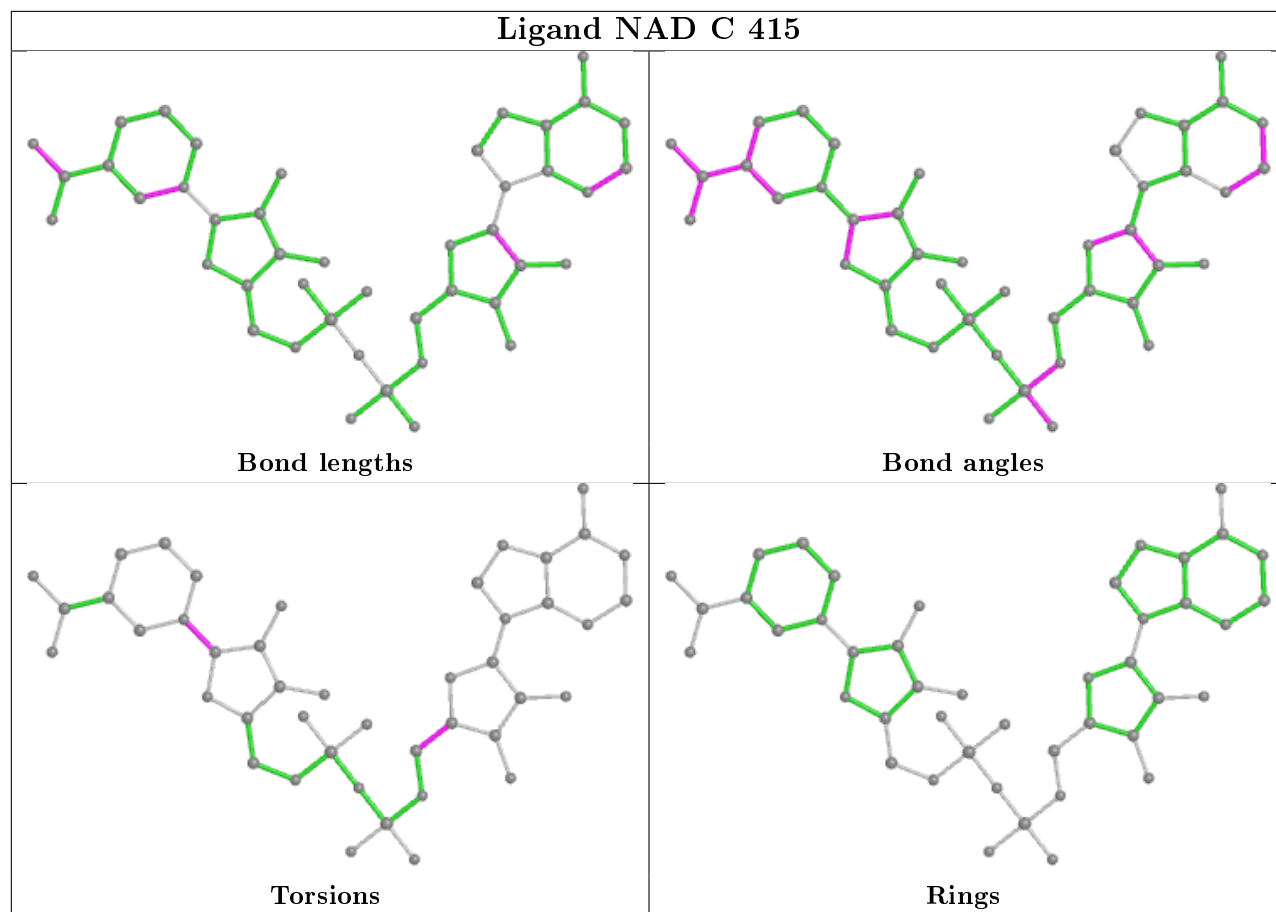
There are no ring outliers.

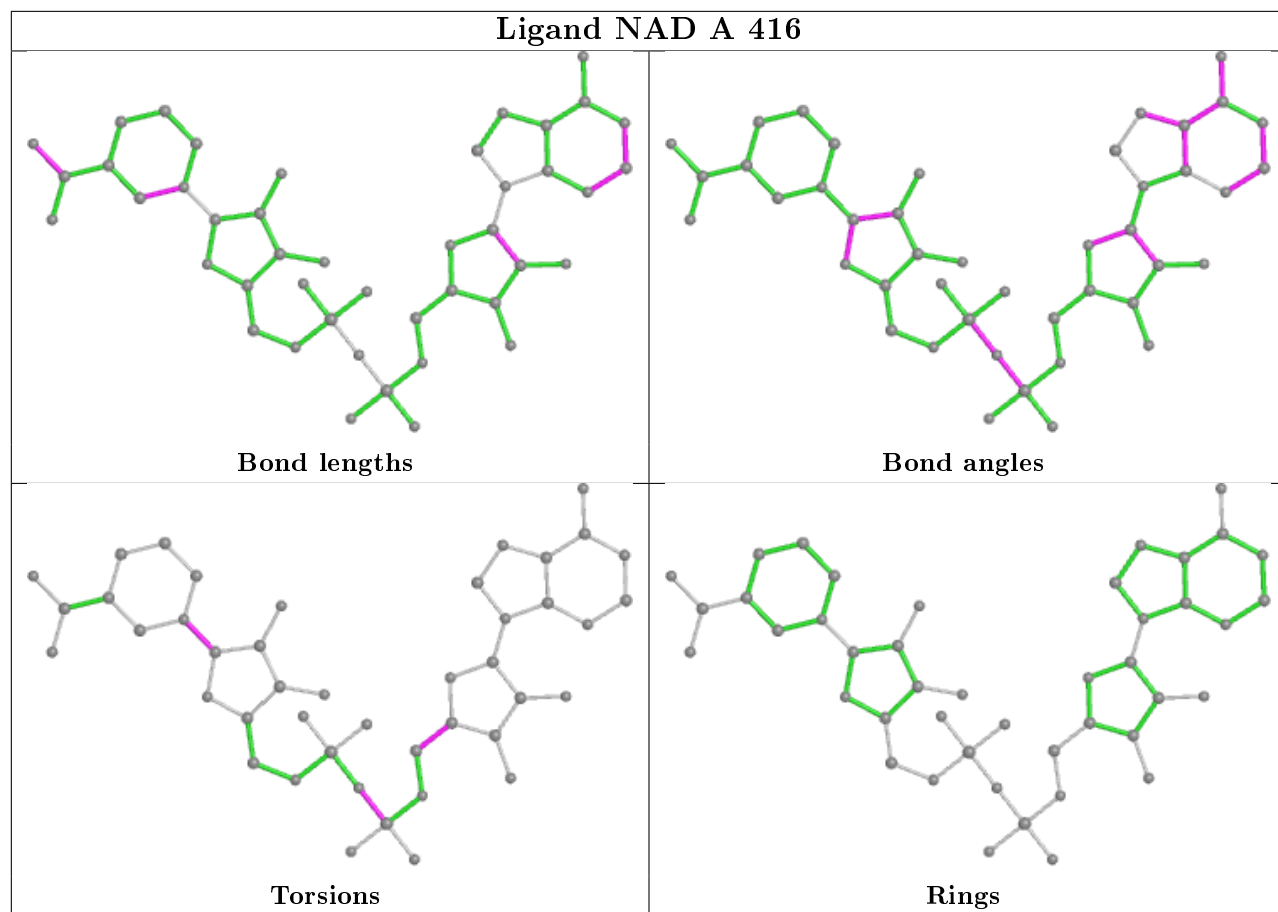
3 monomers are involved in 7 short contacts:

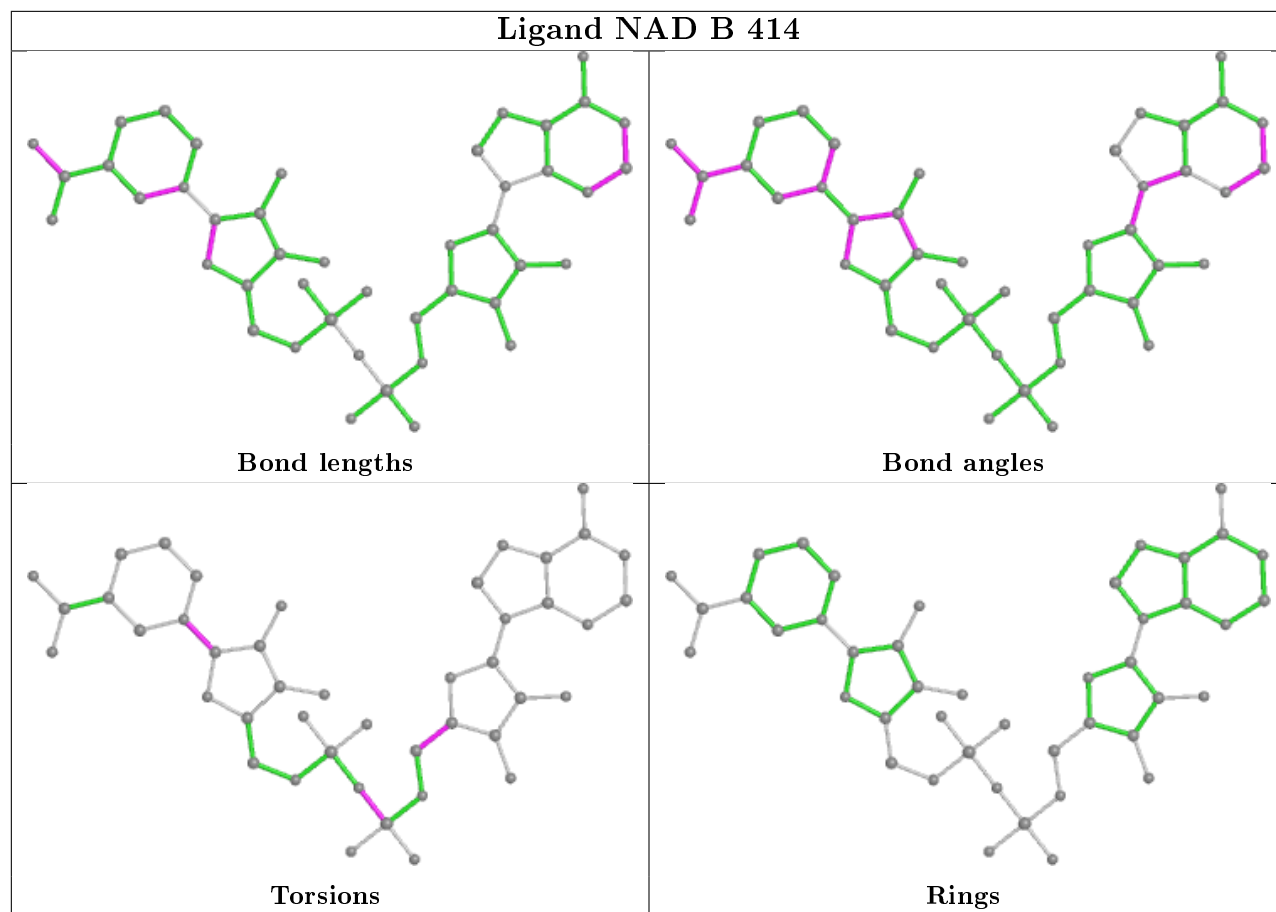
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	412	AKG	2	0
3	B	412	AKG	4	0
5	B	414	NAD	1	0

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









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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

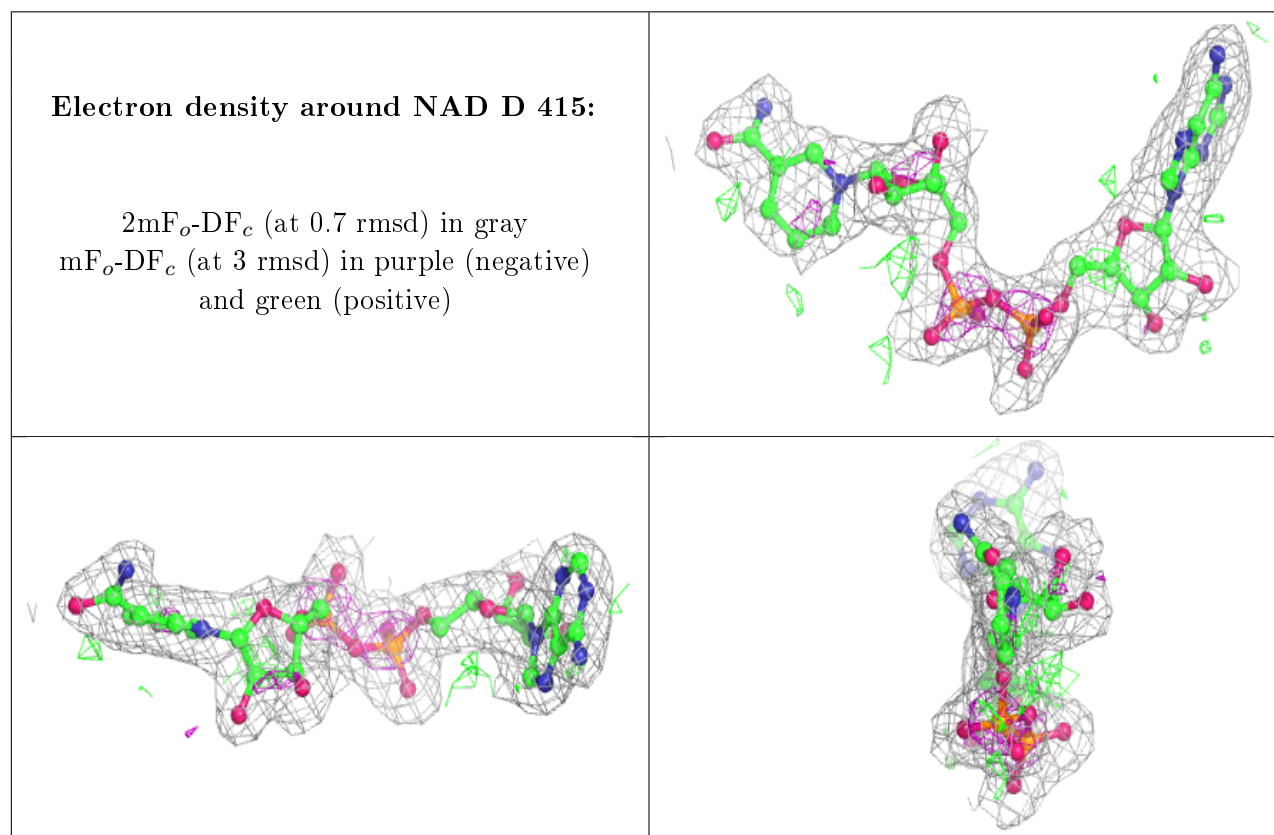
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

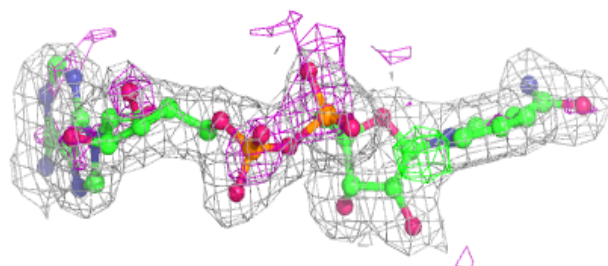
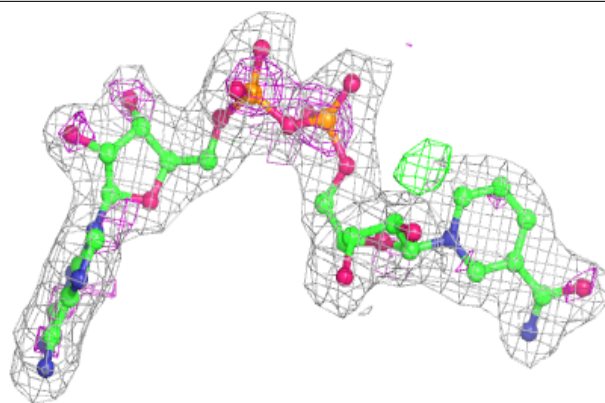
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

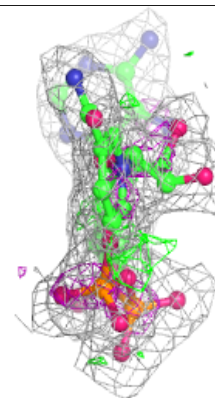
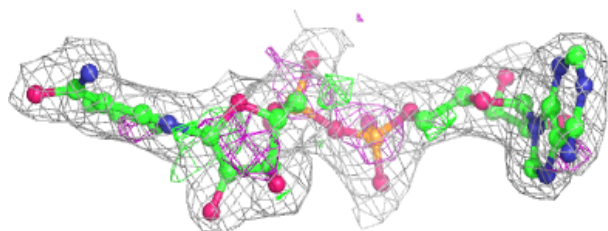
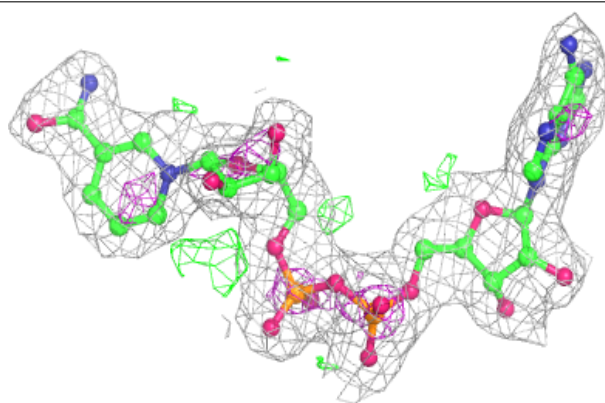


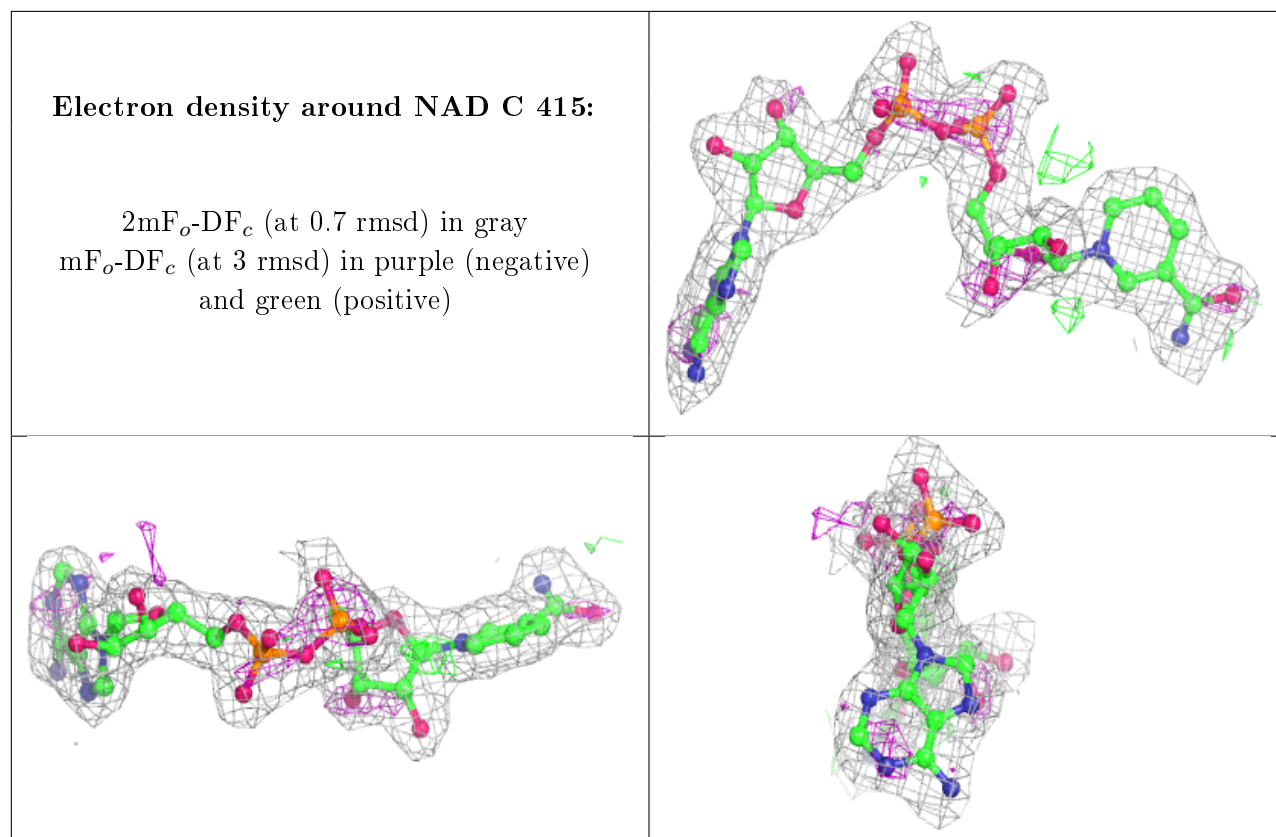
Electron density around NAD A 416:

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

**Electron density around NAD B 414:**

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





6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.