



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:27 AM UTC

PDB ID : 1YBA / pdb_00001yba
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 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

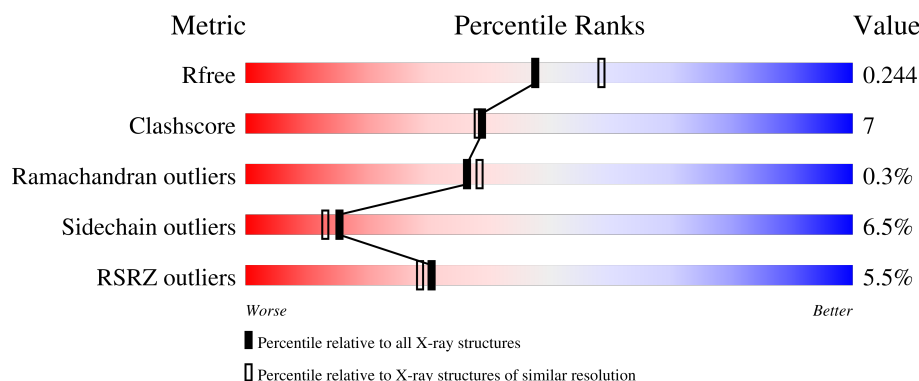
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (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 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	410	 6% 84% 13% ..
1	B	410	 3% 83% 14% ..
1	C	410	 3% 85% 12% ..
1	D	410	 8% 83% 13% ..

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	A	413	-	X	-	-
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:

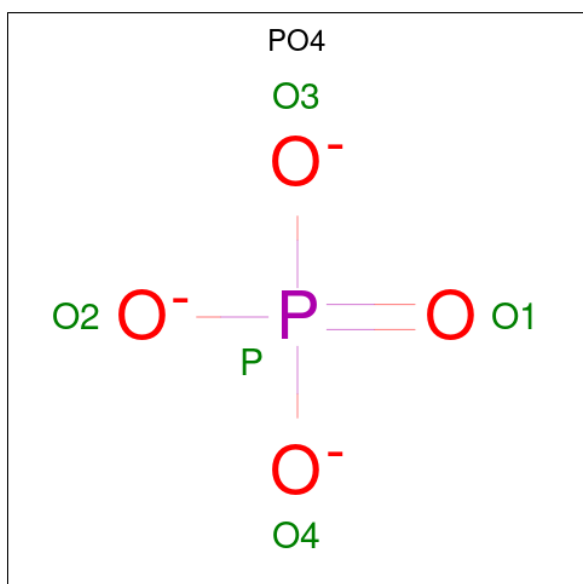
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MSE	MET	modified residue	UNP P08328
A	203	MSE	MET	modified residue	UNP P08328
A	220	MSE	MET	modified residue	UNP P08328
A	221	MSE	MET	modified residue	UNP P08328
A	229	MSE	MET	modified residue	UNP P08328
A	341	MSE	MET	modified residue	UNP P08328
A	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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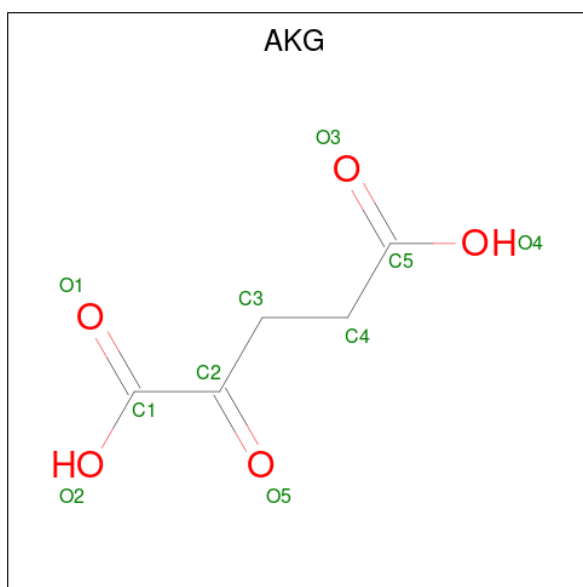
Chain	Residue	Modelled	Actual	Comment	Reference
C	341	MSE	MET	modified residue	UNP P08328
C	376	MSE	MET	modified residue	UNP P08328
C	397	MSE	MET	modified residue	UNP P08328
D	175	MSE	MET	modified residue	UNP P08328
D	203	MSE	MET	modified residue	UNP P08328
D	220	MSE	MET	modified residue	UNP P08328
D	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 (CCD ID: PO4) (formula: O_4P).



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

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).

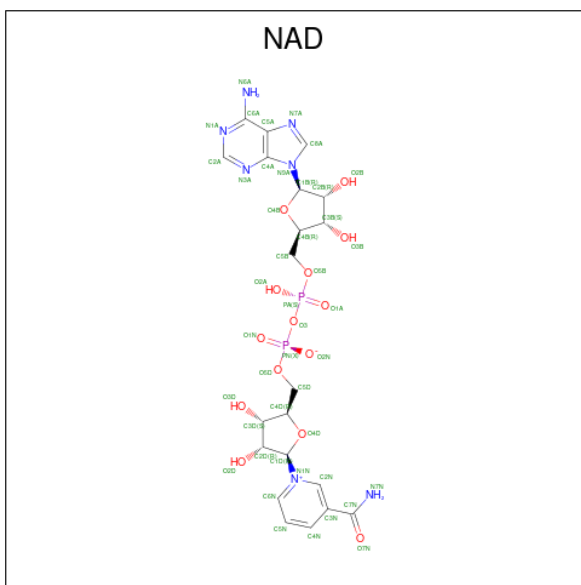


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

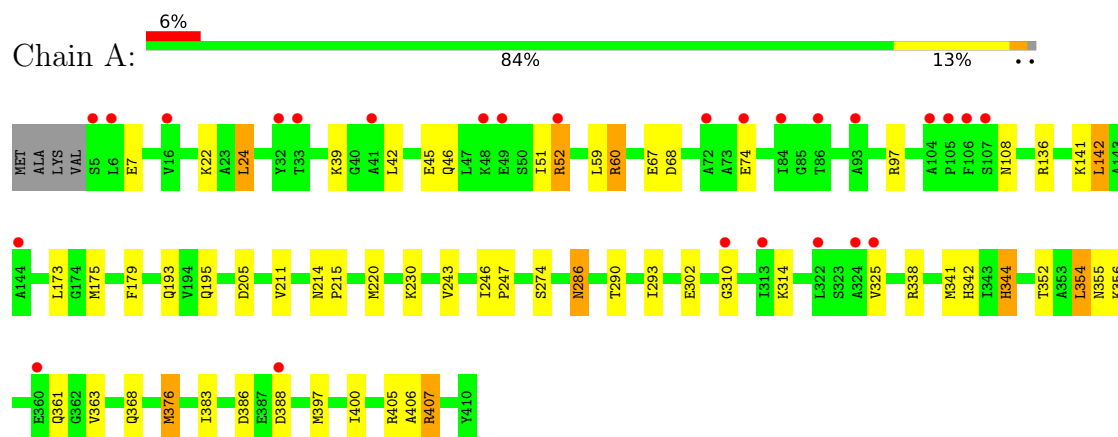
- Molecule 6 is water.

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

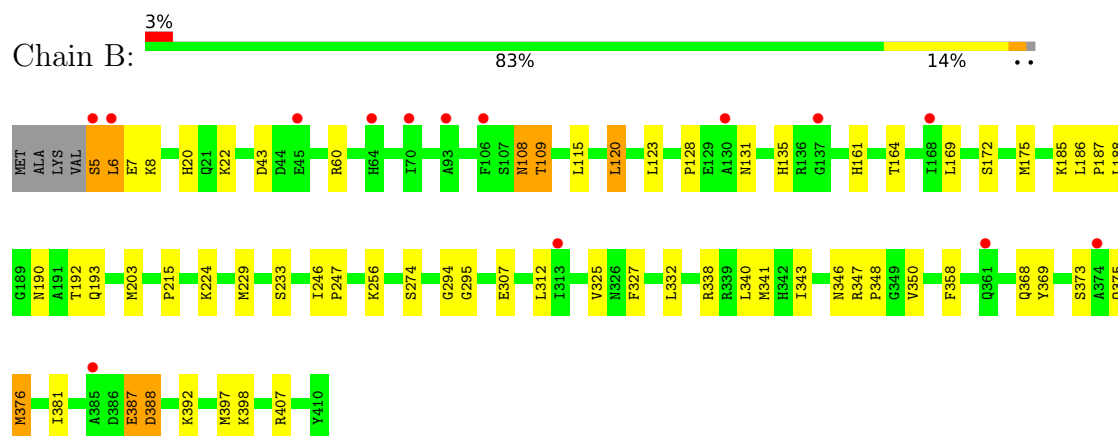
3 Residue-property plots [i](#)

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

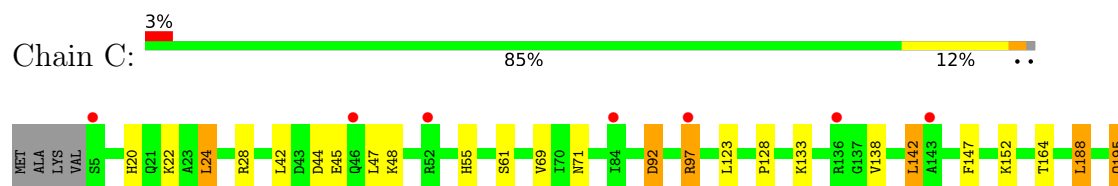
- Molecule 1: D-3-phosphoglycerate dehydrogenase

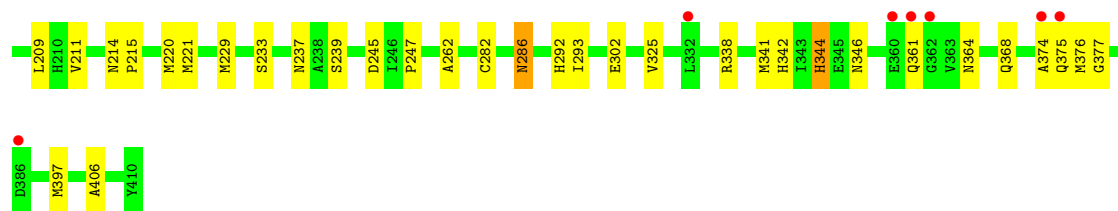


- Molecule 1: D-3-phosphoglycerate dehydrogenase

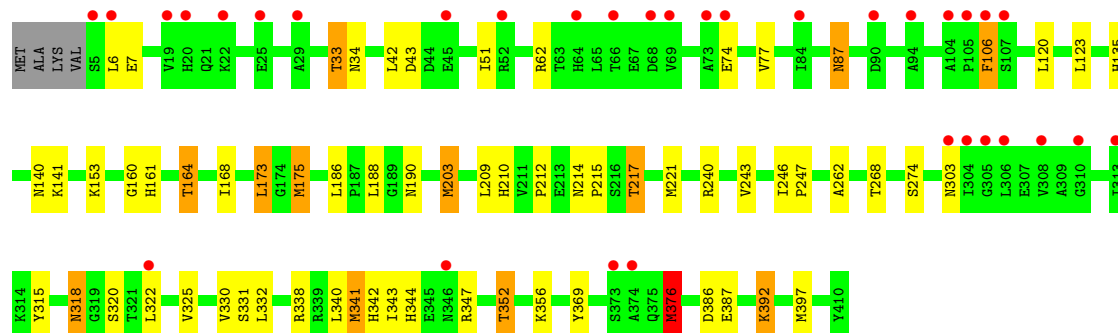
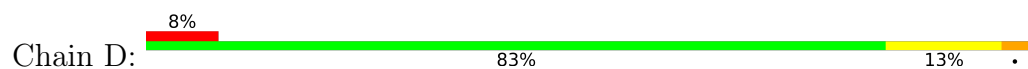


- Molecule 1: D-3-phosphoglycerate dehydrogenase





● 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	76.16Å 76.16Å 354.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 50.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.24) 94.2 (50.00-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	32.92 (at 2.24Å)	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 (4.72%)	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)	0.36 , 45.6	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	0.91	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, PO4, NAD, AKG

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	0.95	2/3128 (0.1%)	1.00	3/4224 (0.1%)
1	B	0.97	2/3131 (0.1%)	1.02	4/4228 (0.1%)
1	C	0.95	1/3141 (0.0%)	0.98	1/4239 (0.0%)
1	D	0.99	3/3139 (0.1%)	1.00	3/4239 (0.1%)
All	All	0.97	8/12539 (0.1%)	1.00	11/16930 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	MSE	SE-CE	12.90	2.34	1.95
1	D	376	MSE	SE-CE	8.59	2.21	1.95
1	A	376	MSE	SE-CE	7.52	2.18	1.95
1	D	175	MSE	SE-CE	7.02	2.16	1.95
1	A	175	MSE	SE-CE	6.17	2.13	1.95
1	B	175	MSE	SE-CE	5.88	2.13	1.95
1	B	203	MSE	SE-CE	5.75	2.12	1.95
1	C	376	MSE	SE-CE	5.43	2.11	1.95

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	LEU	N-CA-C	-7.93	104.05	112.93
1	A	363	VAL	N-CA-C	7.22	118.42	108.89
1	B	109	THR	N-CA-C	7.06	118.62	111.07
1	A	344	HIS	N-CA-C	6.02	118.28	108.76
1	B	350	VAL	N-CA-C	-5.81	104.67	111.00
1	D	106	PHE	CB-CA-C	-5.79	103.16	112.07
1	B	108	ASN	CA-CB-CG	5.70	118.30	112.60
1	D	186	LEU	CA-C-N	-5.41	114.38	119.85
1	D	186	LEU	C-N-CA	-5.41	114.38	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	HIS	N-CA-C	5.26	117.07	109.07
1	A	211	VAL	N-CA-C	5.01	113.40	107.84

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	36	0
1	B	3086	0	3121	37	0
1	C	3097	0	3135	57	0
1	D	3094	0	3124	44	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	1	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	7	0
6	C	350	0	0	7	0
6	D	366	0	0	7	0
All	All	14017	0	12620	173	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 (173) 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:CE	1:D:175:MSE:SE	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
1:D:203:MSE:SE	1:D:203:MSE:CE	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:HE21	1:C:375[B]:GLN:N	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:141:LYS:HZ1	3:B:412:AKG:H31	1.57	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:C2	4:D:414:UNL:O4	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:D:341:MSE:HE2	1:D:341:MSE:C	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:ASN:ND2	1:D:190:ASN:HD21	1.95	0.62
1:B:340:LEU:HD22	1:B:397:MSE:HE1	1.81	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:D:318:ASN:C	1:D:318:ASN:HD22	2.08	0.60
1:A:24:LEU:HD23	1:A:24:LEU:N	2.15	0.60
1:C:20:HIS:HD2	1:C:22:LYS:H	1.50	0.60
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:C:142:LEU:C	1:C:142:LEU:CD2	2.76	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: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:O3	4:B:413:UNL:C2	2.52	0.56
1:D:341:MSE:HE2	1:D:342:HIS:N	2.20	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:209:LEU:HD22	1:C:220:MSE:HE3	1.89	0.54
4:C:414:UNL:O4	4:C:414:UNL:C2	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:D:210:HIS:HD2	6:D:482:HOH:O	1.91	0.53
1:A:142:LEU:O	1:A:142:LEU:HD23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:ASN:N	1:D:87:ASN:OD1	2.43	0.51
1:A:59:LEU:N	1:A:59:LEU:HD23	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
4:D:414:UNL:O2	4:D:414:UNL:C5	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:B:120:LEU:C	1:B:120:LEU:HD12	2.36	0.49
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:141:LYS:NZ	3:B:412:AKG:H31	2.26	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:D:318:ASN:C	1:D:318:ASN:ND2	2.70	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:C:142:LEU:HD22	1:C:142:LEU:C	2.40	0.46
1:D:120:LEU:HD12	1:D:120:LEU:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:51:ILE:O	1:A:52:ARG:C	2.60	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:43:ASP:OD1	1:D:43:ASP:C	2.61	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
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:C:293:ILE:C	1:C:293:ILE:HD12	2.44	0.43
1:A:397:MSE:HE2	1:A:406:ALA:HB1	2.01	0.43
1:A:97:ARG:HD3	6:A:557:HOH:O	2.20	0.42
1:A:246:ILE:HB	1:A:247:PRO:HD3	2.02	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:D:34:ASN:C	1:D:34:ASN:HD22	2.27	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:A:361:GLN:O	1:A:361:GLN:CD	2.64	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:NE2	1:A:46:GLN:HA	2.36	0.41
1:A:179:PHE:CZ	1:A:193:GLN:HB2	2.56	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:77:VAL:HG12	1:D:315:TYR:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:LEU:HD13	1:D:369:TYR:HB2	2.02	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:B:398:LYS:NZ	6:B:628:HOH:O	2.54	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
1:D:123:LEU:HD11	1:D:262:ALA:HB2	2.03	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	405/410 (99%)	386 (95%)	18 (4%)	1 (0%)	43	48
1	B	405/410 (99%)	389 (96%)	14 (4%)	2 (0%)	24	23
1	C	406/410 (99%)	393 (97%)	13 (3%)	0	100	100
1	D	406/410 (99%)	383 (94%)	21 (5%)	2 (0%)	24	23
All	All	1622/1640 (99%)	1551 (96%)	66 (4%)	5 (0%)	36	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	GLU
1	B	43	ASP
1	D	6	LEU

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Mol	Chain	Res	Type
1	A	386	ASP
1	B	215	PRO

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	329/323 (102%)	305 (93%)	24 (7%)	13	10
1	B	329/323 (102%)	306 (93%)	23 (7%)	14	11
1	C	330/323 (102%)	317 (96%)	13 (4%)	28	33
1	D	330/323 (102%)	305 (92%)	25 (8%)	12	9
All	All	1318/1292 (102%)	1233 (94%)	85 (6%)	15	14

All (85) 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	60	ARG
1	A	67	GLU
1	A	68	ASP
1	A	74	GLU
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	325	VAL
1	A	341	MSE

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Mol	Chain	Res	Type
1	A	352	THR
1	A	354	LEU
1	A	356	LYS
1	A	388	ASP
1	A	407	ARG
1	B	5	SER
1	B	6	LEU
1	B	109	THR
1	B	120	LEU
1	B	192	THR
1	B	224	LYS
1	B	256	LYS
1	B	274	SER
1	B	307	GLU
1	B	312	LEU
1	B	325	VAL
1	B	327	PHE
1	B	338	ARG
1	B	341	MSE
1	B	346	ASN
1	B	347	ARG
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	42	LEU
1	C	45	GLU
1	C	92	ASP
1	C	97	ARG
1	C	142	LEU
1	C	188	LEU
1	C	195	GLN
1	C	286	ASN
1	C	325	VAL
1	C	338	ARG
1	C	341	MSE
1	C	361	GLN
1	D	7	GLU

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Mol	Chain	Res	Type
1	D	33	THR
1	D	42	LEU
1	D	51	ILE
1	D	62	ARG
1	D	87	ASN
1	D	106	PHE
1	D	140	ASN
1	D	164	THR
1	D	173	LEU
1	D	217	THR
1	D	268	THR
1	D	274	SER
1	D	318	ASN
1	D	322	LEU
1	D	325	VAL
1	D	331	SER
1	D	338	ARG
1	D	341	MSE
1	D	347	ARG
1	D	352	THR
1	D	376	MSE
1	D	386	ASP
1	D	387	GLU
1	D	392	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	46	GLN
1	A	55	HIS
1	A	87	ASN
1	A	108	ASN
1	A	140	ASN
1	A	165	GLN
1	A	195	GLN
1	A	273	ASN
1	A	286	ASN
1	A	303	ASN
1	A	342	HIS
1	A	344	HIS
1	A	346	ASN

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Mol	Chain	Res	Type
1	A	368	GLN
1	A	375	GLN
1	B	20	HIS
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	202	ASN
1	B	257	HIS
1	B	273	ASN
1	B	303	ASN
1	B	335	HIS
1	B	346	ASN
1	B	355	ASN
1	C	34	ASN
1	C	55	HIS
1	C	71	ASN
1	C	108	ASN
1	C	140	ASN
1	C	165	GLN
1	C	184	ASN
1	C	190	ASN
1	C	237	ASN
1	C	273	ASN
1	C	286	ASN
1	C	318	ASN
1	C	335	HIS
1	C	342	HIS
1	C	344	HIS
1	C	346	ASN
1	C	361	GLN
1	C	364	ASN
1	C	368	GLN
1	D	34	ASN
1	D	135	HIS
1	D	140	ASN
1	D	161	HIS
1	D	190	ASN
1	D	210	HIS
1	D	257	HIS

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Mol	Chain	Res	Type
1	D	273	ASN
1	D	303	ASN
1	D	318	ASN
1	D	335	HIS
1	D	342	HIS
1	D	344	HIS
1	D	346	ASN
1	D	355	ASN
1	D	364	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 oligosaccharides 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	A	413	-	9,9,9	1.40	1 (11%)	11,11,11	1.86	4 (36%)
2	PO4	D	411	-	4,4,4	1.26	1 (25%)	6,6,6	2.05	2 (33%)
3	AKG	D	412	-	9,9,9	1.46	1 (11%)	11,11,11	1.77	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAD	B	414	-	46,48,48	1.91	8 (17%)	64,73,73	1.77	17 (26%)
5	NAD	C	415	-	46,48,48	1.91	7 (15%)	64,73,73	1.73	14 (21%)
3	AKG	C	412	-	9,9,9	1.89	2 (22%)	11,11,11	2.03	4 (36%)
2	PO4	A	412	-	4,4,4	0.75	0	6,6,6	0.48	0
2	PO4	A	411	-	4,4,4	1.69	1 (25%)	6,6,6	1.11	0
3	AKG	B	412	-	9,9,9	1.44	1 (11%)	11,11,11	1.78	3 (27%)
5	NAD	A	416	-	46,48,48	2.10	8 (17%)	64,73,73	1.76	10 (15%)
5	NAD	D	415	-	46,48,48	1.83	6 (13%)	64,73,73	1.78	14 (21%)
2	PO4	B	411	-	4,4,4	0.98	0	6,6,6	2.44	3 (50%)
2	PO4	C	411	-	4,4,4	1.06	0	6,6,6	1.10	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	A	413	-	-	7/9/9/9	-
3	AKG	D	412	-	-	2/9/9/9	-
5	NAD	B	414	-	-	8/30/62/62	0/5/5/5
5	NAD	C	415	-	-	6/30/62/62	0/5/5/5
3	AKG	C	412	-	-	4/9/9/9	-
3	AKG	B	412	-	-	5/9/9/9	-
5	NAD	A	416	-	-	7/30/62/62	0/5/5/5
5	NAD	D	415	-	-	6/30/62/62	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	416	NAD	O7N-C7N	9.91	1.42	1.24
5	D	415	NAD	O7N-C7N	9.54	1.41	1.24
5	C	415	NAD	O7N-C7N	9.34	1.41	1.24
5	B	414	NAD	O7N-C7N	8.36	1.39	1.24
5	A	416	NAD	PN-O3	4.55	1.64	1.59
5	B	414	NAD	PA-O3	4.54	1.64	1.59
5	A	416	NAD	C2A-N3A	3.84	1.40	1.33
3	C	412	AKG	C2-C1	-3.84	1.47	1.53
5	D	415	NAD	PA-O3	3.72	1.63	1.59
3	A	413	AKG	C2-C1	-3.68	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	412	AKG	C2-C1	-3.63	1.48	1.53
5	A	416	NAD	C2N-N1N	3.58	1.38	1.35
5	C	415	NAD	C2N-N1N	3.49	1.38	1.35
5	B	414	NAD	PN-O3	3.49	1.63	1.59
3	C	412	AKG	C3-C2	3.20	1.54	1.51
5	B	414	NAD	C2A-N3A	3.16	1.39	1.33
5	A	416	NAD	PA-O3	3.15	1.62	1.59
5	B	414	NAD	C2A-N1A	3.14	1.39	1.33
5	D	415	NAD	PN-O3	3.10	1.62	1.59
3	D	412	AKG	C3-C2	3.02	1.54	1.51
5	C	415	NAD	C2A-N3A	3.00	1.39	1.33
5	B	414	NAD	O4D-C1D	2.95	1.44	1.40
5	D	415	NAD	C8A-N7A	2.95	1.37	1.31
5	C	415	NAD	C5A-N7A	-2.89	1.33	1.39
5	C	415	NAD	PA-O3	2.75	1.62	1.59
5	A	416	NAD	C2A-N1A	2.73	1.38	1.33
5	C	415	NAD	C8A-N7A	2.68	1.36	1.31
5	A	416	NAD	C8A-N7A	2.66	1.36	1.31
2	A	411	PO4	P-O4	-2.62	1.47	1.54
5	B	414	NAD	C5A-N7A	-2.48	1.34	1.39
5	B	414	NAD	C2N-N1N	2.24	1.37	1.35
2	D	411	PO4	P-O4	-2.13	1.48	1.54
5	A	416	NAD	C5A-N7A	-2.11	1.35	1.39
5	C	415	NAD	O4D-C1D	2.09	1.43	1.40
5	D	415	NAD	O4B-C4B	-2.09	1.40	1.45
5	D	415	NAD	C2N-N1N	2.07	1.37	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	415	NAD	N3A-C2A-N1A	-5.50	120.26	128.58
5	A	416	NAD	C4A-C5A-N7A	-5.38	104.43	110.58
5	A	416	NAD	C5A-C4A-N3A	-5.23	119.52	126.72
5	A	416	NAD	C5A-N7A-C8A	4.96	111.24	103.45
5	C	415	NAD	N3A-C2A-N1A	-4.73	121.43	128.58
5	C	415	NAD	C5A-C4A-N3A	-4.69	120.26	126.72
5	B	414	NAD	N9A-C8A-N7A	-4.66	107.32	113.94
5	B	414	NAD	N3A-C2A-N1A	-4.63	121.57	128.58
5	A	416	NAD	N9A-C8A-N7A	-4.63	107.37	113.94
5	C	415	NAD	O7N-C7N-C3N	-4.51	114.09	119.60
5	D	415	NAD	N9A-C8A-N7A	-4.48	107.57	113.94
5	D	415	NAD	C5A-C4A-N3A	-4.38	120.69	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	PO4	O4-P-O1	-4.33	95.63	110.95
5	C	415	NAD	N9A-C8A-N7A	-4.10	108.12	113.94
5	C	415	NAD	C3N-C7N-N7N	4.09	122.78	117.74
5	A	416	NAD	C6A-C5A-C4A	4.02	122.67	117.18
5	B	414	NAD	O3-PA-O1A	-3.79	99.29	110.70
3	B	412	AKG	O1-C1-C2	3.79	126.53	121.81
5	D	415	NAD	C5A-N7A-C8A	3.79	109.40	103.45
5	D	415	NAD	C4A-C5A-N7A	-3.75	106.29	110.58
5	B	414	NAD	C4A-N9A-C8A	3.61	109.53	105.74
3	A	413	AKG	O2-C1-C2	3.51	123.32	113.59
5	D	415	NAD	C2A-N3A-C4A	3.50	120.37	111.83
2	B	411	PO4	O2-P-O1	3.49	123.30	110.95
5	B	414	NAD	C5A-N7A-C8A	3.47	108.91	103.45
3	C	412	AKG	O1-C1-C2	-3.45	117.52	121.81
5	A	416	NAD	N3A-C2A-N1A	-3.43	123.38	128.58
5	B	414	NAD	C5A-C4A-N3A	-3.43	122.00	126.72
5	C	415	NAD	C5A-N7A-C8A	3.42	108.82	103.45
2	D	411	PO4	O3-P-O1	-3.34	99.14	110.95
5	A	416	NAD	C5A-C4A-N9A	3.20	109.30	105.81
5	D	415	NAD	O3-PA-O1A	-3.19	101.09	110.70
5	C	415	NAD	C2A-N3A-C4A	3.01	119.18	111.83
3	C	412	AKG	O2-C1-C2	2.98	121.85	113.59
2	D	411	PO4	O3-P-O2	2.96	117.11	107.91
3	B	412	AKG	O5-C2-C1	2.94	123.87	119.67
5	B	414	NAD	O7N-C7N-N7N	-2.91	118.41	122.62
3	D	412	AKG	C3-C2-C1	2.90	120.79	115.86
3	A	413	AKG	O1-C1-C2	-2.85	118.27	121.81
5	D	415	NAD	C4A-N9A-C8A	2.82	108.70	105.74
5	B	414	NAD	O4B-C1B-N9A	-2.79	102.72	108.09
5	A	416	NAD	C2A-N3A-C4A	2.67	118.34	111.83
5	C	415	NAD	C4A-C5A-N7A	-2.65	107.55	110.58
5	C	415	NAD	C5A-C4A-N9A	2.62	108.66	105.81
5	B	414	NAD	C3N-C7N-N7N	2.55	120.88	117.74
3	C	412	AKG	O4-C5-C4	2.55	122.05	114.00
5	B	414	NAD	N3A-C4A-N9A	2.54	131.49	127.17
5	D	415	NAD	O4B-C4B-C5B	-2.50	101.32	109.33
3	D	412	AKG	O4-C5-C4	2.50	121.89	114.00
5	B	414	NAD	C4A-C5A-N7A	-2.48	107.74	110.58
5	B	414	NAD	O2A-PA-O3	2.47	113.96	107.27
5	C	415	NAD	C6A-C5A-C4A	2.45	120.52	117.18
5	D	415	NAD	N3A-C4A-N9A	2.42	131.29	127.17
5	B	414	NAD	C2A-N3A-C4A	2.42	117.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	415	NAD	O2A-PA-O5B	2.36	118.28	107.57
5	B	414	NAD	C6A-C5A-C4A	2.35	120.39	117.18
5	A	416	NAD	N3A-C4A-N9A	2.35	131.16	127.17
3	A	413	AKG	O2-C1-O1	-2.32	118.37	123.90
3	A	413	AKG	C3-C4-C5	-2.31	107.53	113.67
5	C	415	NAD	N3A-C4A-N9A	2.29	131.06	127.17
3	C	412	AKG	C3-C4-C5	-2.27	107.64	113.67
5	D	415	NAD	C2N-C3N-C4N	2.21	120.82	118.26
5	C	415	NAD	C2N-C3N-C4N	2.20	120.82	118.26
3	D	412	AKG	O4-C5-O3	-2.20	117.67	123.33
3	B	412	AKG	O4-C5-O3	-2.20	117.68	123.33
5	B	414	NAD	C6N-N1N-C2N	-2.15	120.05	121.88
5	B	414	NAD	C5A-C6A-N6A	-2.14	117.98	123.29
5	D	415	NAD	O2N-PN-O1N	2.12	122.31	112.44
5	C	415	NAD	C4D-O4D-C1D	2.11	111.86	109.92
5	D	415	NAD	O2A-PA-O1A	2.09	122.19	112.44
2	B	411	PO4	O4-P-O3	2.04	114.27	107.91
5	D	415	NAD	C5A-C4A-N9A	2.03	108.02	105.81
5	A	416	NAD	O5B-C5B-C4B	-2.01	102.15	108.99
5	B	414	NAD	O2N-PN-O3	-2.01	101.85	107.27

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	413	AKG	O1-C1-C2-C3
3	A	413	AKG	O2-C1-C2-C3
3	A	413	AKG	C2-C3-C4-C5
3	B	412	AKG	C1-C2-C3-C4
3	B	412	AKG	C2-C3-C4-C5
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
5	C	415	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
5	D	415	NAD	O4D-C1D-N1N-C6N
3	A	413	AKG	O5-C2-C3-C4
5	D	415	NAD	C4N-C3N-C7N-N7N
3	A	413	AKG	O1-C1-C2-O5
3	C	412	AKG	O1-C1-C2-O5
5	D	415	NAD	C4N-C3N-C7N-O7N
3	D	412	AKG	C2-C3-C4-C5
3	C	412	AKG	O2-C1-C2-O5
5	A	416	NAD	PN-O3-PA-O1A
5	B	414	NAD	PN-O3-PA-O1A
5	B	414	NAD	PN-O3-PA-O2A
3	C	412	AKG	O2-C1-C2-C3
5	D	415	NAD	C2D-C1D-N1N-C2N
5	D	415	NAD	C2D-C1D-N1N-C6N
5	C	415	NAD	O4B-C4B-C5B-O5B
5	D	415	NAD	O4D-C1D-N1N-C2N
3	B	412	AKG	C3-C4-C5-O3
3	B	412	AKG	C3-C4-C5-O4
5	C	415	NAD	C2B-C1B-N9A-C8A
3	B	412	AKG	O1-C1-C2-O5
3	C	412	AKG	O1-C1-C2-C3
3	A	413	AKG	C3-C4-C5-O3
5	B	414	NAD	O4B-C4B-C5B-O5B
5	A	416	NAD	C2B-C1B-N9A-C8A
5	A	416	NAD	O4B-C4B-C5B-O5B
5	B	414	NAD	C2B-C1B-N9A-C8A
3	A	413	AKG	C3-C4-C5-O4
3	D	412	AKG	C3-C4-C5-O4

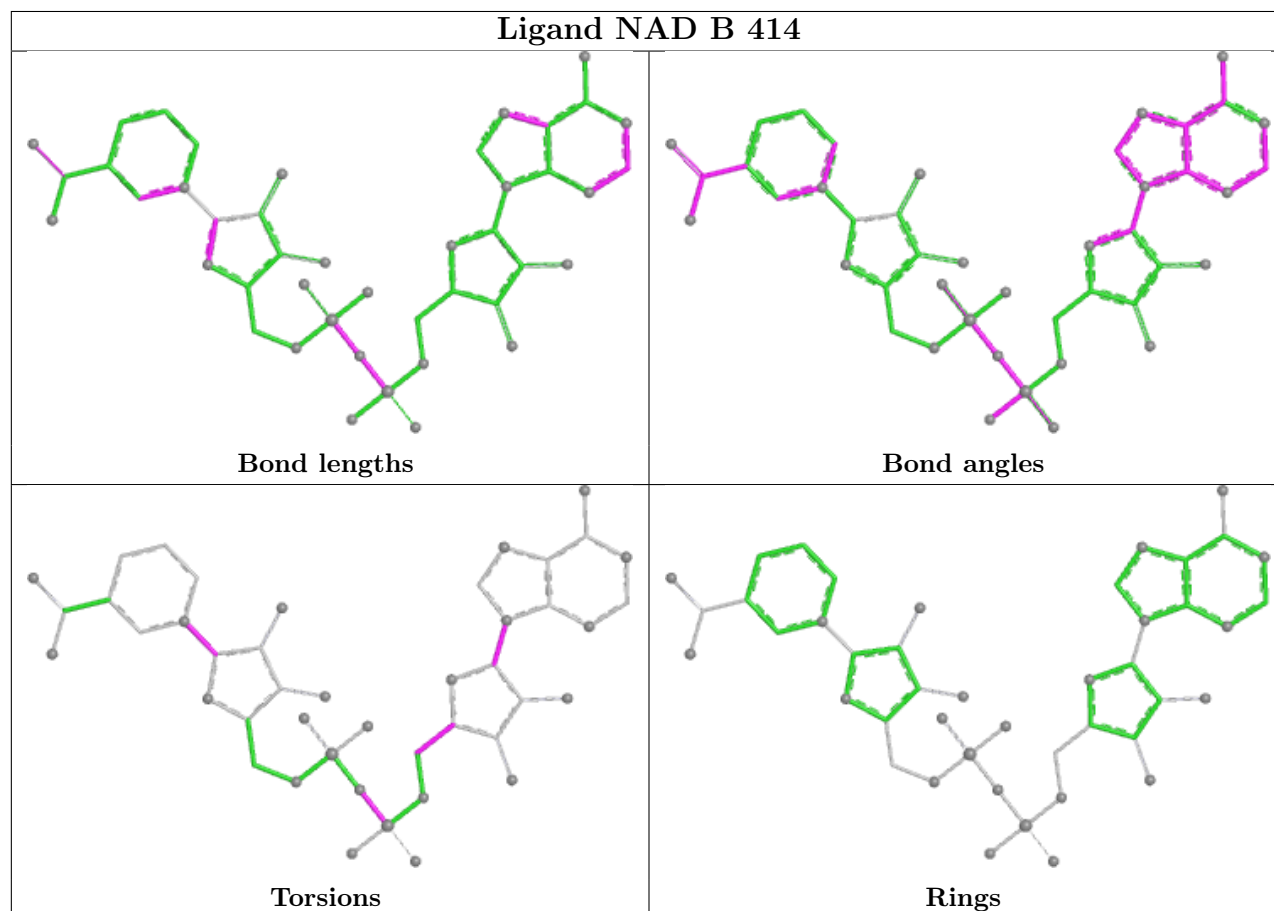
There are no ring outliers.

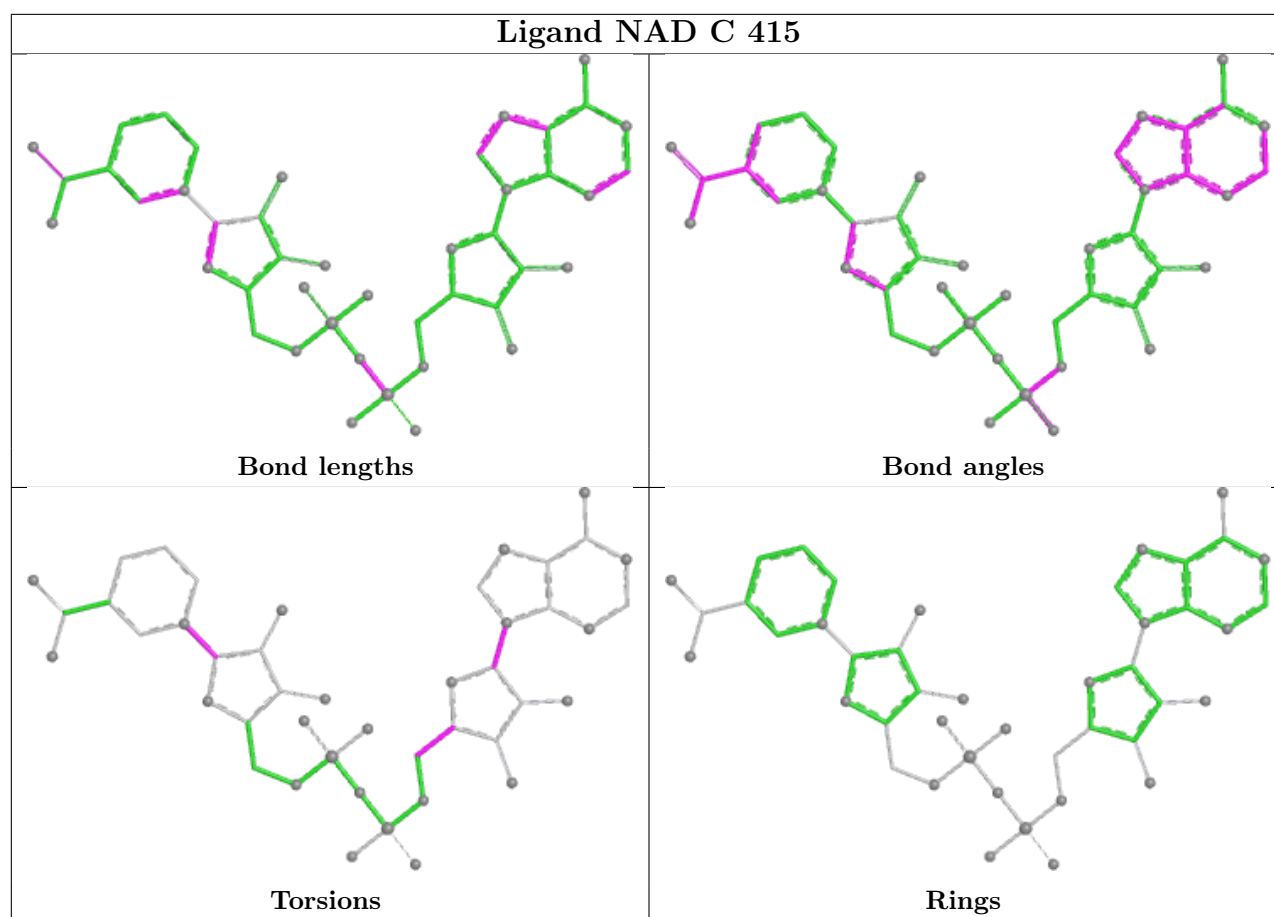
3 monomers are involved in 6 short contacts:

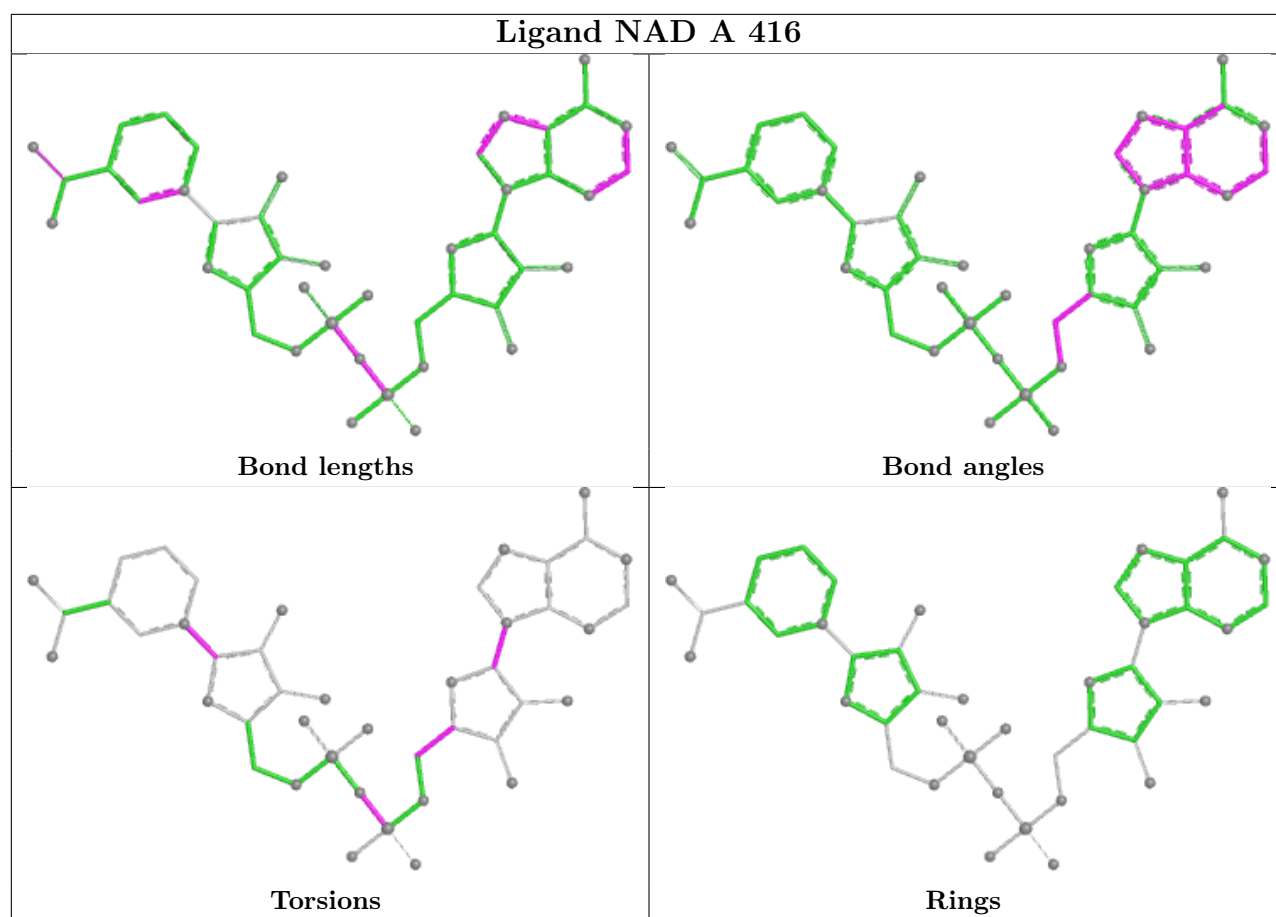
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	414	NAD	1	0
3	C	412	AKG	1	0
3	B	412	AKG	4	0

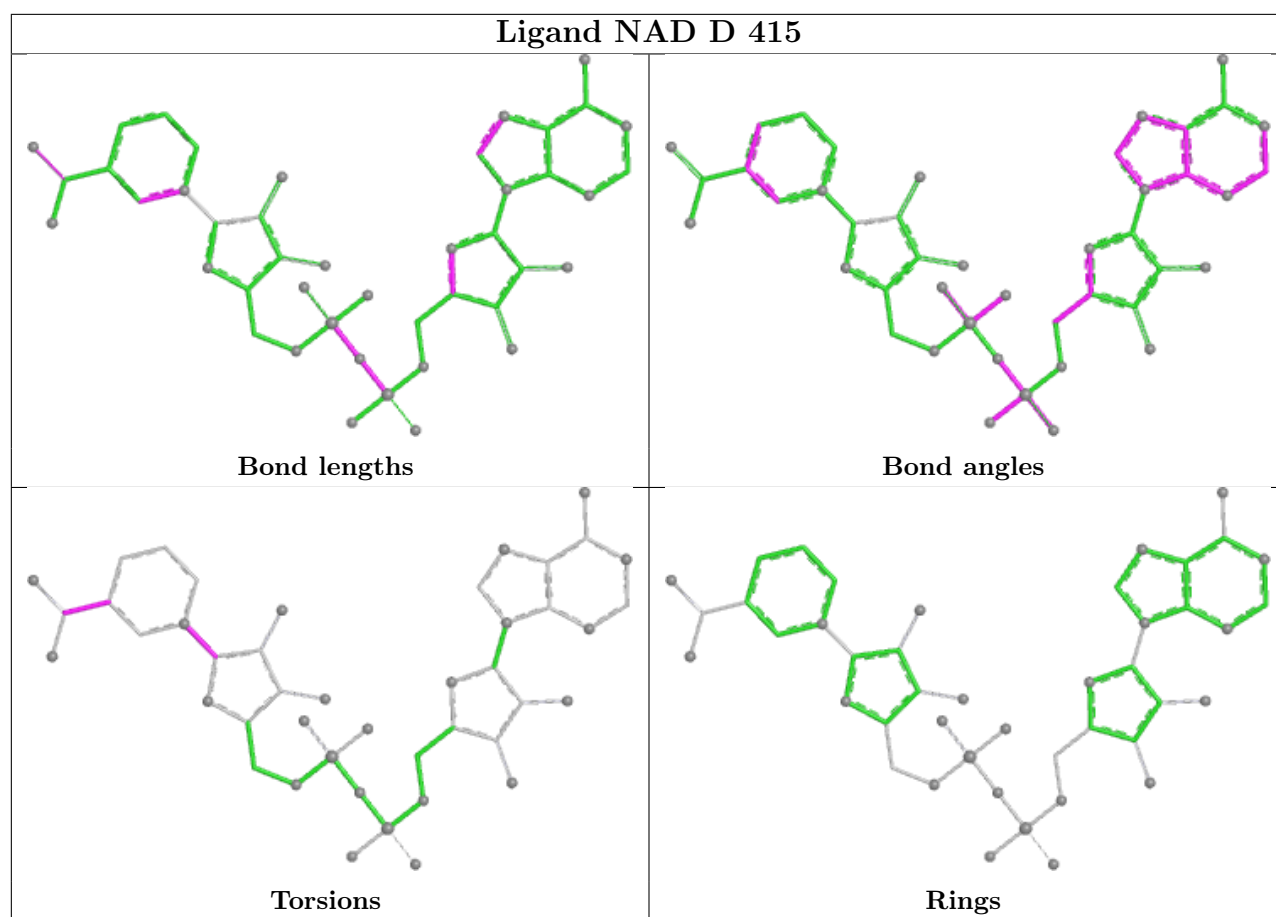
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

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	398/410 (97%)	0.79	26 (6%)	25 23	24, 43, 50, 55	1 (0%)
1	B	398/410 (97%)	0.79	14 (3%)	47 46	20, 43, 51, 69	1 (0%)
1	C	398/410 (97%)	0.56	14 (3%)	47 46	18, 43, 51, 56	2 (0%)
1	D	398/410 (97%)	0.77	33 (8%)	17 15	20, 43, 50, 65	2 (0%)
All	All	1592/1640 (97%)	0.73	87 (5%)	30 29	18, 43, 51, 69	6 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	SER	4.4
1	D	6	LEU	4.3
1	B	6	LEU	4.3
1	D	303	ASN	4.0
1	A	105	PRO	3.6
1	D	5	SER	3.4
1	A	106	PHE	3.3
1	D	45	GLU	3.3
1	C	375[A]	GLN	3.3
1	B	5	SER	3.3
1	D	107	SER	3.3
1	D	306	LEU	3.2
1	A	6	LEU	3.0
1	D	304	ILE	2.9
1	D	73	ALA	2.9
1	B	64	HIS	2.8
1	C	374	ALA	2.8
1	A	93	ALA	2.8
1	D	66	THR	2.8
1	A	322	LEU	2.8
1	D	19	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	45[A]	GLU	2.7
1	D	105	PRO	2.6
1	D	29	ALA	2.6
1	D	373	SER	2.6
1	D	22	LYS	2.5
1	A	74	GLU	2.4
1	D	64	HIS	2.4
1	D	106	PHE	2.4
1	A	41	ALA	2.4
1	A	72	ALA	2.4
1	A	310	GLY	2.4
1	C	362	GLY	2.4
1	C	360	GLU	2.4
1	D	310	GLY	2.3
1	A	313	ILE	2.3
1	B	313	ILE	2.3
1	C	84	ILE	2.3
1	D	313	ILE	2.3
1	A	325	VAL	2.3
1	D	374	ALA	2.3
1	A	33	THR	2.3
1	B	137	GLY	2.3
1	A	104	ALA	2.3
1	A	144	ALA	2.3
1	B	93	ALA	2.3
1	D	104	ALA	2.3
1	D	68	ASP	2.2
1	C	97	ARG	2.2
1	A	360	GLU	2.2
1	D	20	HIS	2.2
1	D	94	ALA	2.2
1	A	107[A]	SER	2.2
1	C	46	GLN	2.2
1	B	106	PHE	2.2
1	A	324	ALA	2.2
1	B	361	GLN	2.2
1	B	385	ALA	2.2
1	C	386	ASP	2.2
1	D	69	VAL	2.2
1	B	130	ALA	2.2
1	C	52	ARG	2.1
1	D	52	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	84	ILE	2.1
1	A	16	VAL	2.1
1	D	90	ASP	2.1
1	C	143	ALA	2.1
1	A	52	ARG	2.1
1	A	48	LYS	2.1
1	A	84	ILE	2.1
1	A	388	ASP	2.1
1	D	25	GLU	2.1
1	C	136[A]	ARG	2.1
1	C	332	LEU	2.1
1	D	74	GLU	2.1
1	B	70	ILE	2.1
1	B	374	ALA	2.1
1	A	49	GLU	2.1
1	C	361	GLN	2.1
1	A	32	TYR	2.1
1	D	308	VAL	2.1
1	D	305	GLY	2.1
1	C	5	SER	2.0
1	B	168	ILE	2.0
1	A	86	THR	2.0
1	D	322	LEU	2.0
1	D	346	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

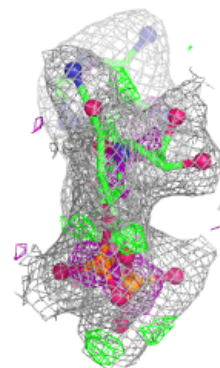
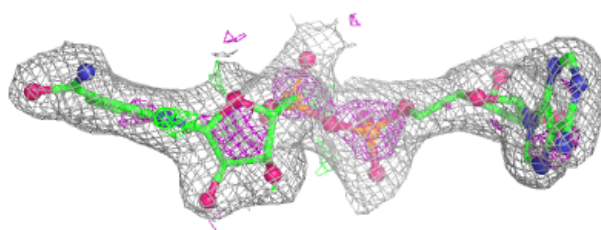
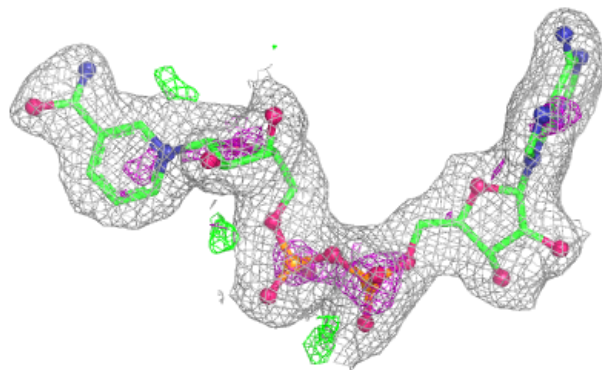
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	412	5/5	0.65	0.14	100,101,101,102	0
3	AKG	A	413	10/10	0.74	0.18	63,64,69,71	0
4	UNL	A	415	10/-	0.75	0.15	68,71,74,76	0
3	AKG	B	412	10/10	0.79	0.15	55,58,61,63	0
4	UNL	B	413	10/-	0.79	0.15	80,83,86,86	0
4	UNL	D	414	10/-	0.79	0.15	67,79,80,82	0
4	UNL	C	413	10/-	0.80	0.16	52,63,76,77	0
4	UNL	C	414	10/-	0.81	0.14	62,69,77,79	0
3	AKG	C	412	10/10	0.81	0.17	54,67,73,74	0
3	AKG	D	412	10/10	0.82	0.17	45,60,66,69	0
4	UNL	A	414	10/-	0.83	0.15	57,61,71,74	0
4	UNL	D	413	10/-	0.91	0.12	25,51,62,65	0
5	NAD	B	414	44/44	0.93	0.10	34,42,47,48	0
5	NAD	A	416	44/44	0.95	0.08	28,31,36,38	0
5	NAD	C	415	44/44	0.95	0.08	27,35,38,40	0
5	NAD	D	415	44/44	0.95	0.09	33,39,41,42	0
2	PO4	B	411	5/5	0.97	0.14	33,36,42,42	0
2	PO4	A	411	5/5	0.98	0.12	27,28,29,31	0
2	PO4	C	411	5/5	0.98	0.11	32,33,34,34	0
2	PO4	D	411	5/5	0.98	0.11	27,31,35,39	0

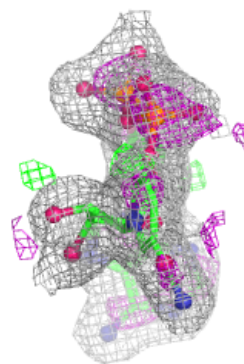
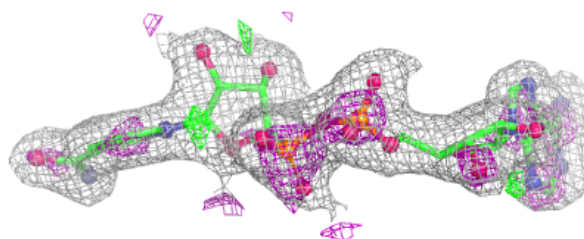
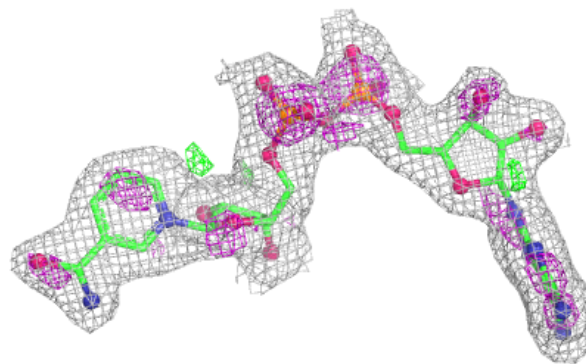
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 414:

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

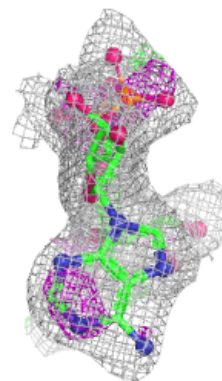
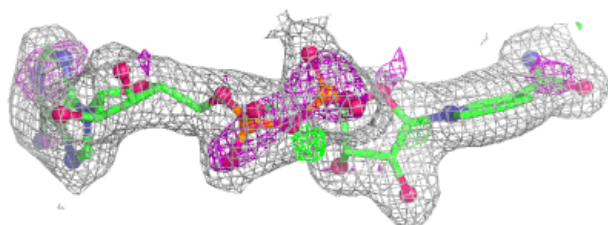
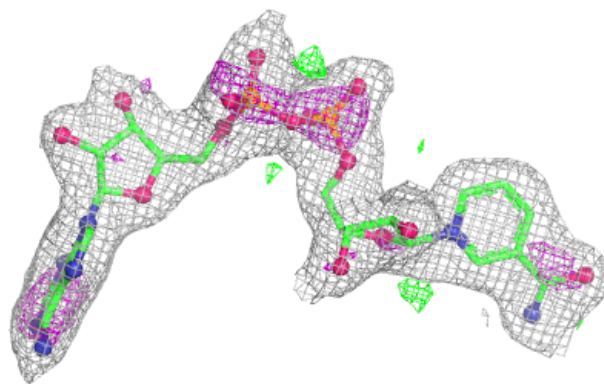
**Electron density around NAD A 416:**

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

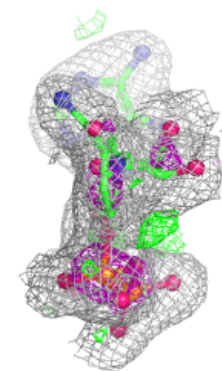
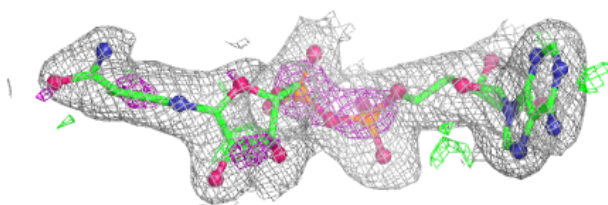
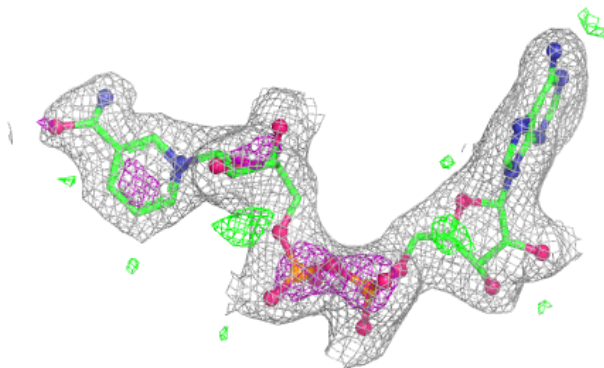


Electron density around NAD C 415:

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

**Electron density around NAD D 415:**

$2mF_o-DF_c$ (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.