



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 5DDI / pdb_00005ddi
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from pig muscle - holo enzyme - at 2.40 Angstrom resolution
Authors : Dimova, M.; Devedjiev, Y.D.
Deposited on : 2015-08-24
Resolution : 2.40 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

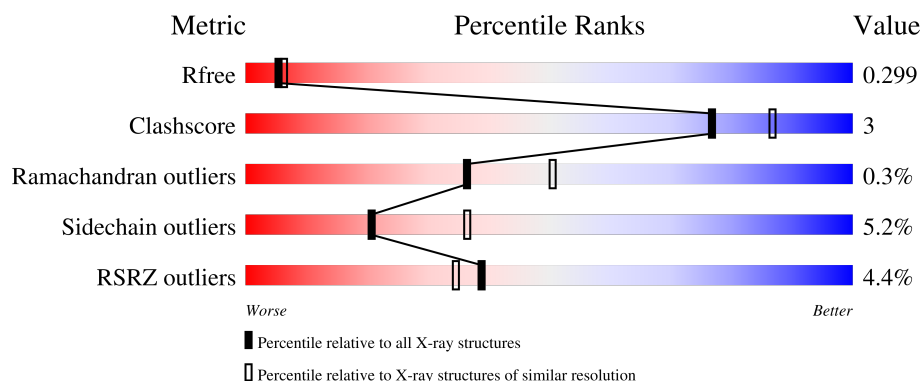
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	P	332	% 88% 10% .
1	R	332	11% 87% 12% .
1	S	332	% 88% 11% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

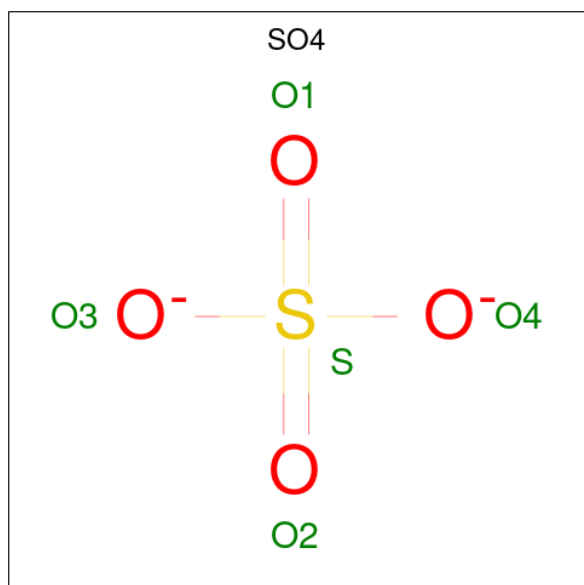
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	332	Total	C	N	O	S	0	0	0
			2511	1589	436	473	13			
1	R	332	Total	C	N	O	S	0	0	0
			2511	1589	436	473	13			
1	S	332	Total	C	N	O	S	0	0	0
			2511	1589	436	473	13			

There are 3 discrepancies between the modelled and reference sequences:

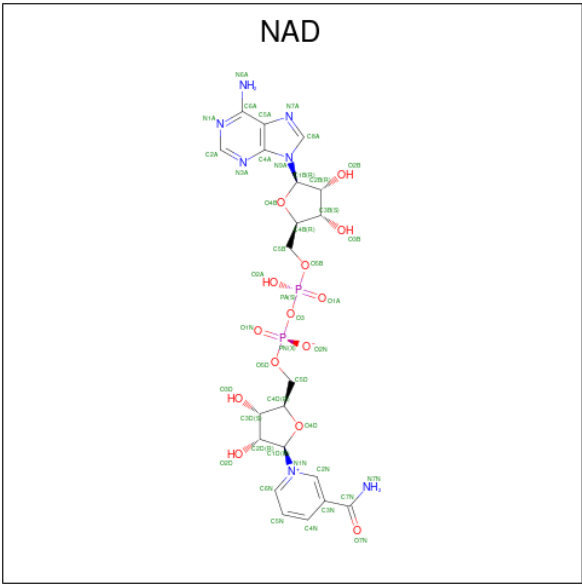
Chain	Residue	Modelled	Actual	Comment	Reference
P	257	GLN	LYS	conflict	UNP P00355
R	257	GLN	LYS	conflict	UNP P00355
S	257	GLN	LYS	conflict	UNP P00355

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	P	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	R	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	S	1	Total 44	C 21	N 7	O 14	P 2	0	0

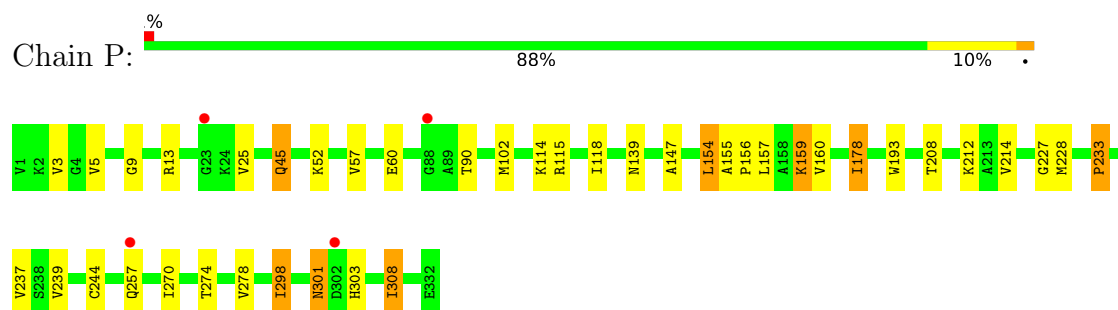
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	129	Total 129	O 129	0	0
4	R	70	Total 70	O 70	0	0
4	S	184	Total 184	O 184	0	0

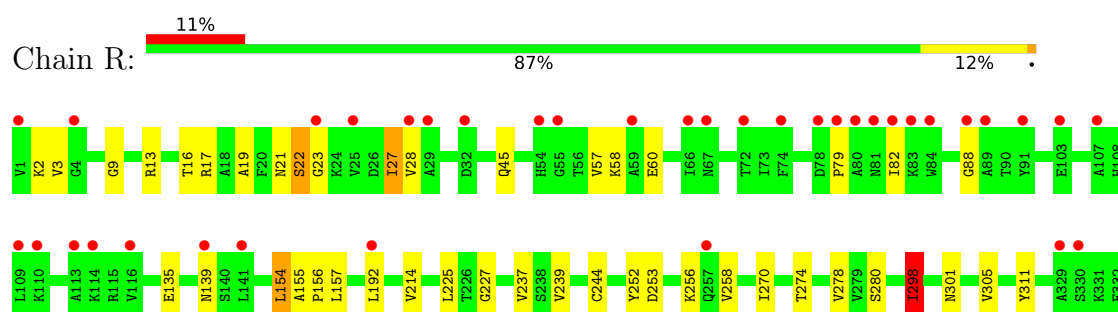
3 Residue-property plots [i](#)

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.

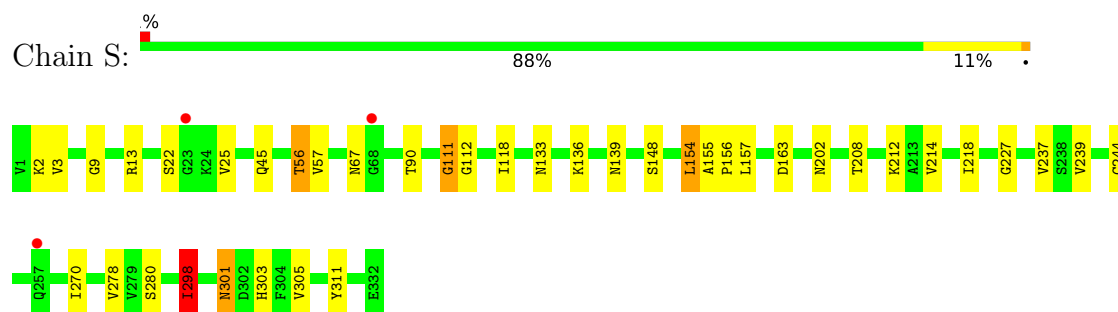
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.90Å 138.97Å 222.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.98 – 2.40 23.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (23.98-2.40) 99.1 (23.98-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.30 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.248 , 0.295 0.252 , 0.299	Depositor DCC
R_{free} test set	1699 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8078	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, SO4

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	P	1.03	1/2562 (0.0%)	1.11	12/3469 (0.3%)
1	R	0.99	0/2562	1.11	11/3469 (0.3%)
1	S	1.14	2/2562 (0.1%)	1.14	13/3469 (0.4%)
All	All	1.06	3/7686 (0.0%)	1.12	36/10407 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	280	SER	N-CA	6.22	1.53	1.46
1	P	147	ALA	CA-C	5.95	1.60	1.52
1	S	148	SER	N-CA	5.28	1.52	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	298	ILE	CB-CA-C	-6.91	102.20	111.80
1	R	298	ILE	CB-CA-C	-6.61	102.62	111.80
1	S	111	GLY	N-CA-C	6.47	122.03	113.37
1	P	298	ILE	CB-CA-C	-6.40	102.90	111.80
1	S	298	ILE	N-CA-C	6.11	116.31	107.88
1	S	278	VAL	N-CA-C	6.08	116.67	110.05
1	S	311	TYR	N-CA-C	5.95	118.08	108.32
1	S	280	SER	N-CA-C	5.91	118.20	111.11
1	S	45	GLN	N-CA-C	5.90	117.38	111.07
1	R	298	ILE	N-CA-C	5.88	116.00	107.88
1	R	274	THR	N-CA-C	5.77	117.87	108.76
1	P	274	THR	N-CA-C	5.62	117.65	108.76
1	R	244	CYS	N-CA-C	5.61	117.59	109.07
1	R	227	GLY	N-CA-C	5.59	118.75	110.42
1	P	298	ILE	N-CA-C	5.59	115.59	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	239	VAL	N-CA-C	5.45	116.51	108.45
1	R	278	VAL	N-CA-C	5.44	115.98	110.05
1	S	227	GLY	N-CA-C	5.43	118.52	110.42
1	S	202	ASN	N-CA-C	5.41	118.38	109.72
1	R	139	ASN	N-CA-C	5.35	118.91	112.38
1	P	233	PRO	N-CA-C	5.34	119.69	112.48
1	P	193	TRP	N-CA-C	5.30	117.14	111.36
1	P	308	ILE	CG1-CB-CG2	-5.26	94.92	110.70
1	P	227	GLY	N-CA-C	5.18	118.13	110.42
1	P	5	VAL	N-CA-C	5.17	115.43	107.77
1	R	311	TYR	N-CA-C	5.13	116.73	108.32
1	S	244	CYS	N-CA-C	5.13	116.87	109.07
1	S	218	ILE	CA-C-N	5.13	125.17	119.32
1	S	218	ILE	C-N-CA	5.13	125.17	119.32
1	P	239	VAL	N-CA-C	5.12	116.03	108.45
1	S	239	VAL	N-CA-C	5.06	115.94	108.45
1	R	28	VAL	N-CA-C	5.04	118.04	113.20
1	R	280	SER	N-CA-C	5.04	117.16	111.11
1	P	45	GLN	N-CA-C	5.02	116.44	111.07
1	P	278	VAL	N-CA-C	5.02	115.52	110.05
1	P	244	CYS	N-CA-C	5.01	116.69	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2511	0	2510	15	0
1	R	2511	0	2510	17	0
1	S	2511	0	2510	14	0
2	P	10	0	0	0	0
2	R	10	0	0	0	0
2	S	10	0	0	1	0
3	P	44	0	26	1	0
3	R	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	44	0	26	0	0
4	P	129	0	0	0	0
4	R	70	0	0	7	1
4	S	184	0	0	4	1
All	All	8078	0	7608	45	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (45) 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:R:17:ARG:O	1:R:21:ASN:ND2	2.02	0.93
1:R:79:PRO:O	1:R:82:ILE:HG22	1.75	0.86
1:P:178:ILE:CD1	1:P:233:PRO:HA	2.12	0.78
1:P:178:ILE:HD11	1:P:233:PRO:HA	1.65	0.78
1:S:136:LYS:HG3	4:S:675:HOH:O	1.87	0.74
1:S:163:ASP:OD2	4:S:601:HOH:O	2.05	0.73
1:R:256:LYS:HD3	4:R:601:HOH:O	1.95	0.67
1:R:19:ALA:HB3	1:R:27:ILE:HD11	1.80	0.63
1:P:3:VAL:HG21	1:P:25:VAL:HG13	1.83	0.61
1:S:3:VAL:HG21	1:S:25:VAL:HG13	1.83	0.60
1:P:114:LYS:HD2	1:P:114:LYS:N	2.17	0.59
1:R:298:ILE:HG23	4:R:625:HOH:O	2.04	0.56
1:R:16:THR:HG23	1:R:27:ILE:HD13	1.86	0.56
1:R:17:ARG:NH1	4:R:602:HOH:O	2.38	0.56
1:S:111:GLY:N	1:S:112:GLY:HA2	2.21	0.56
1:S:154:LEU:HD13	1:S:214:VAL:HG21	1.87	0.56
1:P:154:LEU:HD13	1:P:214:VAL:HG21	1.87	0.55
1:S:212:LYS:HG3	4:S:638:HOH:O	2.08	0.53
1:R:154:LEU:HD13	1:R:214:VAL:HG21	1.90	0.53
1:P:301:ASN:HD22	1:P:303:HIS:H	1.55	0.53
1:P:9:GLY:O	1:P:13:ARG:HG3	2.10	0.51
1:R:2:LYS:HD2	1:R:88:GLY:O	2.12	0.50
1:R:192:LEU:HB3	4:R:611:HOH:O	2.12	0.50
1:S:301:ASN:HD22	1:S:303:HIS:H	1.58	0.49
1:R:9:GLY:O	1:R:13:ARG:HG3	2.13	0.49
1:P:178:ILE:HD12	1:P:233:PRO:HA	1.95	0.46
1:S:9:GLY:O	1:S:13:ARG:HG3	2.15	0.46
1:R:155:ALA:HB3	1:R:156:PRO:HD3	1.99	0.45
1:S:208:THR:OG1	2:S:501:SO4:O2	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:56:THR:HG22	1:S:67:ASN:HA	1.98	0.43
1:R:252:TYR:HD2	4:R:601:HOH:O	2.02	0.43
1:P:114:LYS:N	1:P:114:LYS:CD	2.81	0.43
1:R:58:LYS:HE2	1:R:60:GLU:OE1	2.19	0.43
1:P:159:LYS:HE3	1:P:160:VAL:HA	2.01	0.42
1:R:22:SER:OG	1:R:23:GLY:N	2.52	0.42
1:P:208:THR:HG22	1:P:228:MET:HA	2.02	0.42
1:S:155:ALA:HB3	1:S:156:PRO:HD3	2.01	0.42
1:R:253:ASP:OD1	4:R:601:HOH:O	2.22	0.41
1:R:298:ILE:CG2	4:R:625:HOH:O	2.66	0.41
1:S:133:ASN:HB2	1:S:136:LYS:HE2	2.02	0.41
1:P:155:ALA:HB3	1:P:156:PRO:HD3	2.02	0.41
1:P:115:ARG:NH2	1:P:139:ASN:O	2.54	0.41
1:S:298:ILE:HG23	4:S:692:HOH:O	2.20	0.41
1:P:102:MET:HE1	1:S:139:ASN:O	2.21	0.41
1:P:9:GLY:HA3	3:P:503:NAD:O5B	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:633:HOH:O	4:R:633:HOH:O[2_555]	1.79	0.41
4:S:700:HOH:O	4:S:700:HOH:O[2_565]	2.05	0.15

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	P	330/332 (99%)	319 (97%)	10 (3%)	1 (0%)	36	50
1	R	330/332 (99%)	316 (96%)	13 (4%)	1 (0%)	36	50
1	S	330/332 (99%)	319 (97%)	10 (3%)	1 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	990/996 (99%)	954 (96%)	33 (3%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	237	VAL
1	R	237	VAL
1	S	237	VAL

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	P	268/268 (100%)	252 (94%)	16 (6%)	17	31
1	R	268/268 (100%)	254 (95%)	14 (5%)	21	36
1	S	268/268 (100%)	256 (96%)	12 (4%)	24	42
All	All	804/804 (100%)	762 (95%)	42 (5%)	21	36

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	45	GLN
1	P	52	LYS
1	P	57	VAL
1	P	60	GLU
1	P	90	THR
1	P	118	ILE
1	P	154	LEU
1	P	157	LEU
1	P	159	LYS
1	P	178	ILE
1	P	212	LYS
1	P	257	GLN
1	P	270	ILE

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Mol	Chain	Res	Type
1	P	298	ILE
1	P	301	ASN
1	P	308	ILE
1	R	3	VAL
1	R	22	SER
1	R	27	ILE
1	R	45	GLN
1	R	57	VAL
1	R	135	GLU
1	R	154	LEU
1	R	157	LEU
1	R	225	LEU
1	R	258	VAL
1	R	270	ILE
1	R	298	ILE
1	R	301	ASN
1	R	305	VAL
1	S	2	LYS
1	S	22	SER
1	S	56	THR
1	S	57	VAL
1	S	90	THR
1	S	118	ILE
1	S	154	LEU
1	S	157	LEU
1	S	270	ILE
1	S	298	ILE
1	S	301	ASN
1	S	305	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	75	GLN
1	P	134	HIS
1	P	146	ASN
1	P	201	GLN
1	P	277	GLN
1	P	301	ASN
1	R	21	ASN
1	R	134	HIS
1	R	146	ASN

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Mol	Chain	Res	Type
1	R	201	GLN
1	R	277	GLN
1	R	327	HIS
1	S	81	ASN
1	S	146	ASN
1	S	222	ASN
1	S	257	GLN
1	S	301	ASN
1	S	303	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SO4	P	501	-	4,4,4	0.47	0	6,6,6	0.42	0
2	SO4	R	502	-	4,4,4	0.55	0	6,6,6	0.28	0
3	NAD	S	503	-	46,48,48	1.50	6 (13%)	64,73,73	2.09	18 (28%)
2	SO4	R	501	-	4,4,4	0.50	0	6,6,6	0.46	0
2	SO4	S	501	-	4,4,4	0.51	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	R	503	-	46,48,48	1.43	6 (13%)	64,73,73	2.00	15 (23%)
2	SO4	S	502	-	4,4,4	0.40	0	6,6,6	0.58	0
2	SO4	P	502	-	4,4,4	0.54	0	6,6,6	0.70	0
3	NAD	P	503	-	46,48,48	1.66	8 (17%)	64,73,73	1.93	14 (21%)

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	NAD	R	503	-	-	5/30/62/62	0/5/5/5
3	NAD	S	503	-	-	7/30/62/62	0/5/5/5
3	NAD	P	503	-	-	2/30/62/62	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	503	NAD	C5A-C4A	5.12	1.48	1.39
3	P	503	NAD	C5A-C4A	4.59	1.47	1.39
3	S	503	NAD	C5A-C4A	4.50	1.47	1.39
3	P	503	NAD	PN-O3	4.07	1.63	1.59
3	P	503	NAD	O4D-C1D	4.03	1.46	1.40
3	S	503	NAD	C2N-N1N	3.86	1.39	1.35
3	R	503	NAD	C5A-C6A	3.63	1.51	1.41
3	P	503	NAD	PA-O3	3.58	1.63	1.59
3	R	503	NAD	C8A-N7A	3.56	1.38	1.31
3	S	503	NAD	C8A-N7A	3.33	1.38	1.31
3	S	503	NAD	PN-O3	3.32	1.63	1.59
3	P	503	NAD	C2N-N1N	3.27	1.38	1.35
3	S	503	NAD	C5A-C6A	3.13	1.49	1.41
3	S	503	NAD	O4D-C1D	3.12	1.45	1.40
3	P	503	NAD	C5A-C6A	2.90	1.49	1.41
3	R	503	NAD	PN-O3	2.84	1.62	1.59
3	R	503	NAD	PA-O3	2.78	1.62	1.59
3	P	503	NAD	C5A-N7A	-2.71	1.34	1.39
3	R	503	NAD	O4D-C1D	2.20	1.43	1.40
3	P	503	NAD	C8A-N7A	2.14	1.35	1.31

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	503	NAD	C5A-C4A-N3A	-7.47	116.43	126.72
3	P	503	NAD	C5A-C4A-N3A	-6.08	118.34	126.72
3	R	503	NAD	C5A-C4A-N3A	-5.76	118.78	126.72
3	P	503	NAD	C3N-C7N-N7N	5.22	124.17	117.74
3	S	503	NAD	N3A-C4A-N9A	5.22	136.04	127.17
3	R	503	NAD	C4A-C5A-N7A	-5.21	104.63	110.58
3	S	503	NAD	C2A-N3A-C4A	4.72	123.36	111.83
3	P	503	NAD	N3A-C4A-N9A	4.66	135.09	127.17
3	S	503	NAD	C4A-C5A-N7A	-4.59	105.33	110.58
3	P	503	NAD	C4A-C5A-N7A	-4.34	105.62	110.58
3	R	503	NAD	C2A-N3A-C4A	4.27	122.26	111.83
3	R	503	NAD	C3N-C7N-N7N	4.25	122.98	117.74
3	P	503	NAD	O7N-C7N-N7N	-4.04	116.78	122.62
3	R	503	NAD	C6A-C5A-N7A	3.99	139.78	132.09
3	R	503	NAD	N3A-C2A-N1A	-3.86	122.74	128.58
3	R	503	NAD	N3A-C4A-N9A	3.76	133.56	127.17
3	S	503	NAD	C5A-N7A-C8A	3.76	109.35	103.45
3	R	503	NAD	C5A-N7A-C8A	3.70	109.27	103.45
3	P	503	NAD	C2A-N3A-C4A	3.52	120.42	111.83
3	S	503	NAD	N3A-C2A-N1A	-3.47	123.33	128.58
3	P	503	NAD	C5A-N7A-C8A	3.40	108.79	103.45
3	S	503	NAD	C6N-N1N-C2N	-3.27	119.10	121.88
3	R	503	NAD	O7N-C7N-C3N	-3.17	115.72	119.60
3	S	503	NAD	C5N-C4N-C3N	-3.15	117.27	120.36
3	R	503	NAD	N9A-C8A-N7A	-3.14	109.49	113.94
3	P	503	NAD	N3A-C2A-N1A	-3.09	123.91	128.58
3	R	503	NAD	C4A-N9A-C8A	3.06	108.95	105.74
3	S	503	NAD	C6A-C5A-N7A	2.96	137.80	132.09
3	S	503	NAD	N9A-C8A-N7A	-2.94	109.76	113.94
3	S	503	NAD	C4D-O4D-C1D	2.93	112.61	109.92
3	P	503	NAD	C4A-N9A-C8A	2.89	108.78	105.74
3	R	503	NAD	C4A-N9A-C1B	-2.82	120.05	126.63
3	P	503	NAD	C6N-N1N-C2N	-2.61	119.66	121.88
3	P	503	NAD	N9A-C8A-N7A	-2.60	110.25	113.94
3	P	503	NAD	O2A-PA-O3	2.60	114.29	107.27
3	S	503	NAD	O7N-C7N-C3N	-2.55	116.48	119.60
3	S	503	NAD	O2N-PN-O3	2.54	114.14	107.27
3	S	503	NAD	C3N-C7N-N7N	2.44	120.75	117.74
3	S	503	NAD	C2N-N1N-C1D	2.39	124.40	119.13
3	P	503	NAD	O2B-C2B-C3B	2.37	119.41	111.82
3	R	503	NAD	C6N-N1N-C2N	-2.32	119.90	121.88
3	R	503	NAD	C2N-N1N-C1D	2.30	124.21	119.13
3	R	503	NAD	O2A-PA-O1A	2.23	122.83	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	503	NAD	C4A-N9A-C8A	2.18	108.03	105.74
3	S	503	NAD	O4D-C4D-C5D	2.17	116.28	109.33
3	P	503	NAD	C6A-C5A-N7A	2.13	136.20	132.09
3	S	503	NAD	O2A-PA-O3	2.06	112.85	107.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	503	NAD	O4D-C1D-N1N-C2N
3	P	503	NAD	O4D-C1D-N1N-C6N
3	R	503	NAD	O4D-C1D-N1N-C2N
3	R	503	NAD	O4D-C1D-N1N-C6N
3	R	503	NAD	C2D-C1D-N1N-C2N
3	R	503	NAD	C2D-C1D-N1N-C6N
3	S	503	NAD	O4D-C1D-N1N-C2N
3	S	503	NAD	O4D-C1D-N1N-C6N
3	S	503	NAD	C2D-C1D-N1N-C2N
3	S	503	NAD	C2D-C1D-N1N-C6N
3	S	503	NAD	O4B-C4B-C5B-O5B
3	S	503	NAD	C3B-C4B-C5B-O5B
3	S	503	NAD	C5B-O5B-PA-O2A
3	R	503	NAD	O4B-C4B-C5B-O5B

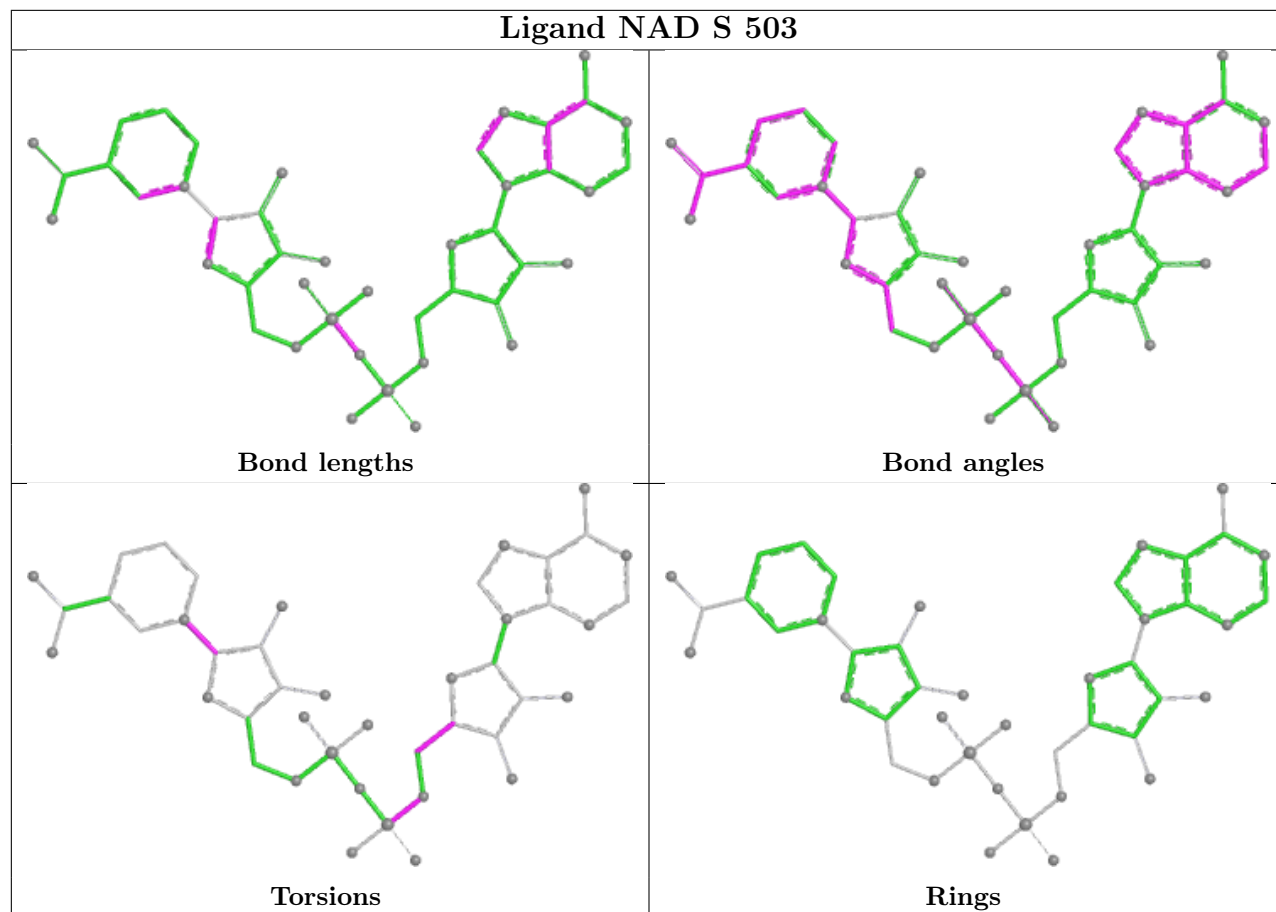
There are no ring outliers.

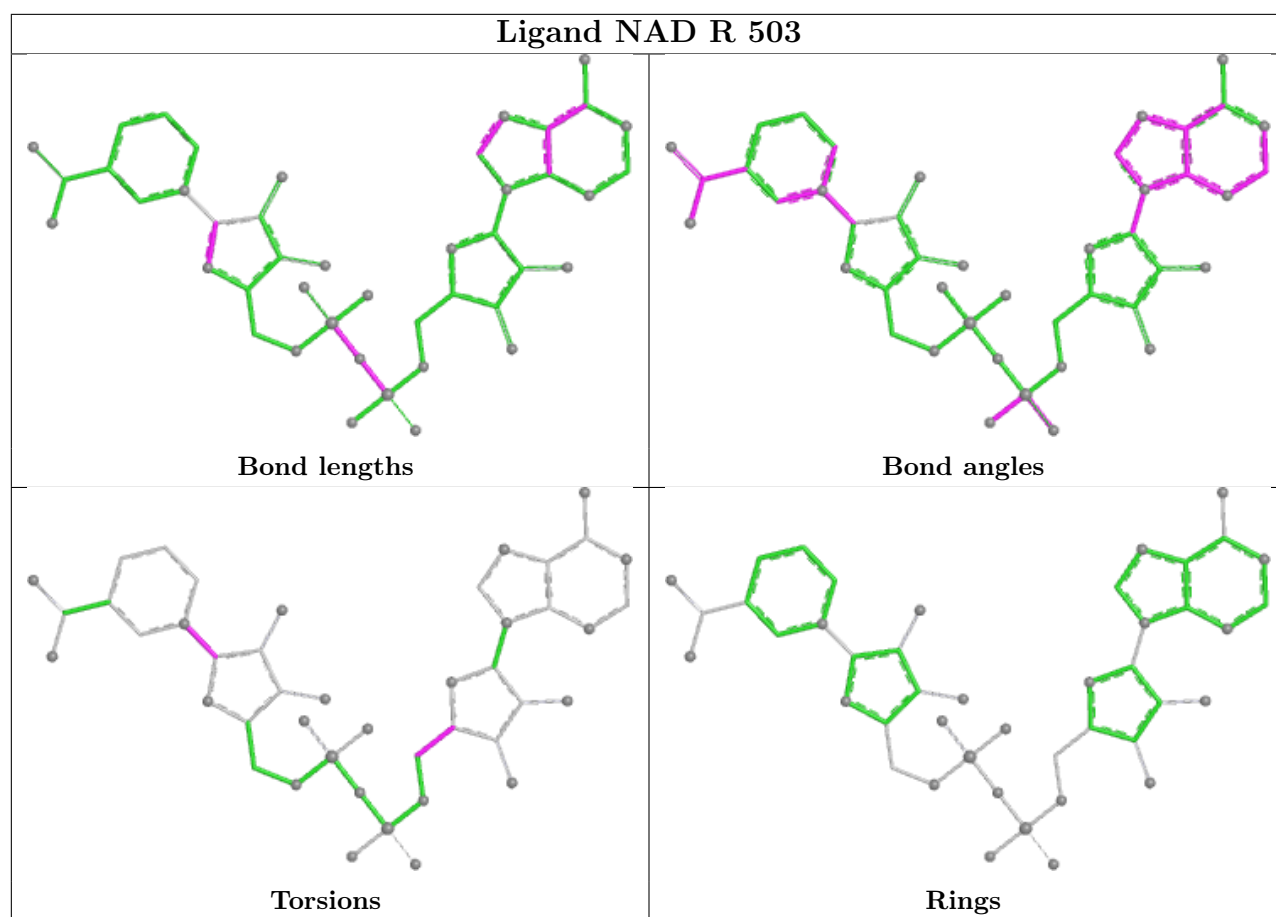
2 monomers are involved in 2 short contacts:

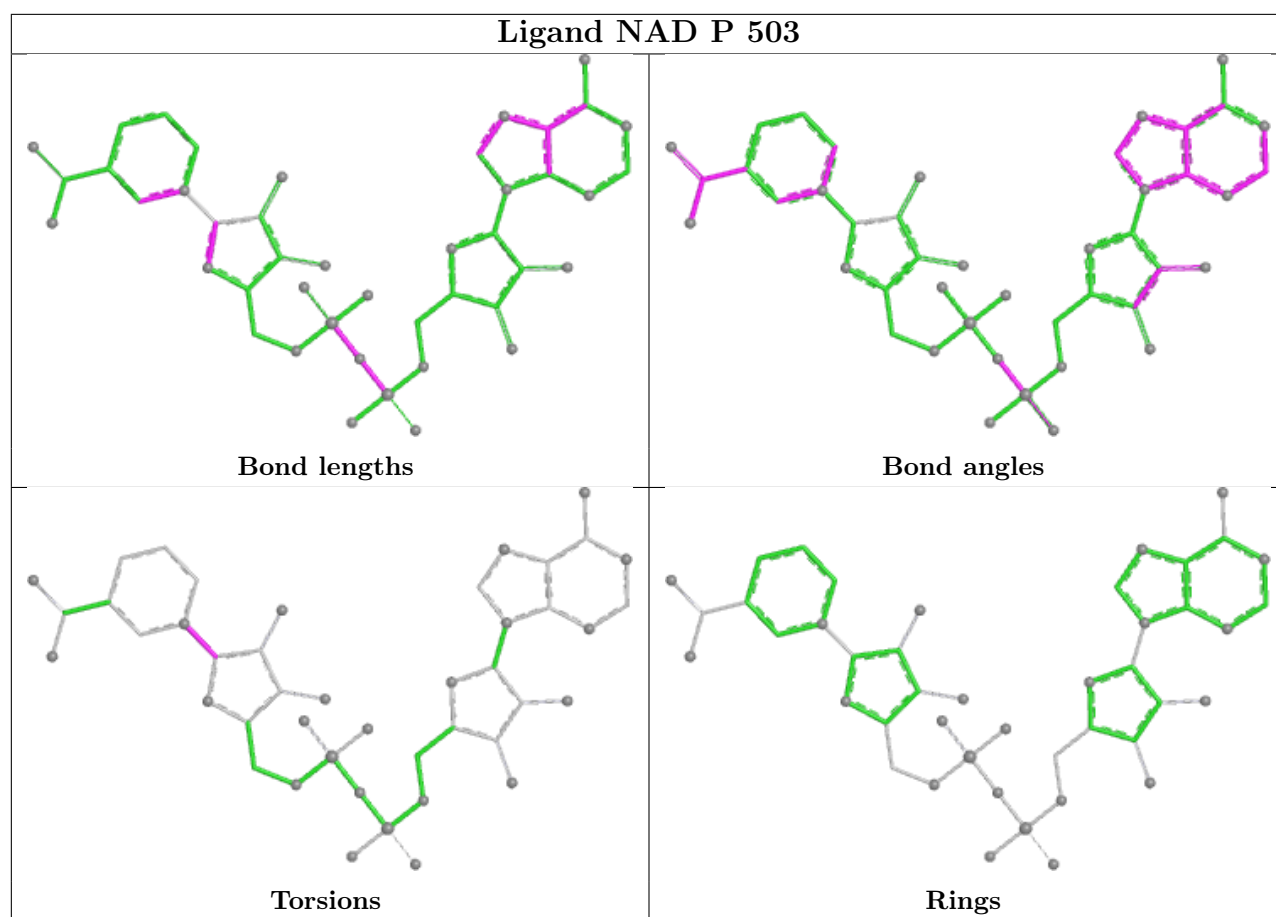
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	501	SO4	1	0
3	P	503	NAD	1	0

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

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	P	332/332 (100%)	0.15	4 (1%) 76 73	16, 34, 51, 62	0
1	R	332/332 (100%)	0.83	37 (11%) 10 7	23, 47, 83, 98	0
1	S	332/332 (100%)	-0.23	3 (0%) 81 78	5, 23, 53, 64	0
All	All	996/996 (100%)	0.25	44 (4%) 39 34	5, 35, 73, 98	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	29	ALA	4.0
1	R	80	ALA	4.0
1	R	25	VAL	3.6
1	R	23	GLY	3.1
1	R	54	HIS	2.9
1	R	79	PRO	2.9
1	R	107	ALA	2.9
1	R	28	VAL	2.8
1	R	113	ALA	2.8
1	R	89	ALA	2.7
1	R	139	ASN	2.7
1	R	82	ILE	2.7
1	R	114	LYS	2.6
1	R	329	ALA	2.5
1	P	257	GLN	2.5
1	R	330	SER	2.5
1	P	23	GLY	2.4
1	R	81	ASN	2.4
1	R	116	VAL	2.4
1	R	88	GLY	2.4
1	S	23	GLY	2.3
1	P	88	GLY	2.3
1	R	4	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	74	PHE	2.3
1	R	1	VAL	2.3
1	R	59	ALA	2.3
1	S	257	GLN	2.3
1	R	110	LYS	2.3
1	R	72	THR	2.2
1	P	302	ASP	2.2
1	R	91	TYR	2.2
1	R	66	ILE	2.2
1	R	67	ASN	2.1
1	R	109	LEU	2.1
1	R	141	LEU	2.1
1	R	32	ASP	2.1
1	R	84	TRP	2.1
1	R	257	GLN	2.1
1	R	103	GLU	2.1
1	R	83	LYS	2.1
1	R	192	LEU	2.0
1	R	55	GLY	2.0
1	S	68	GLY	2.0
1	R	78	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 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.

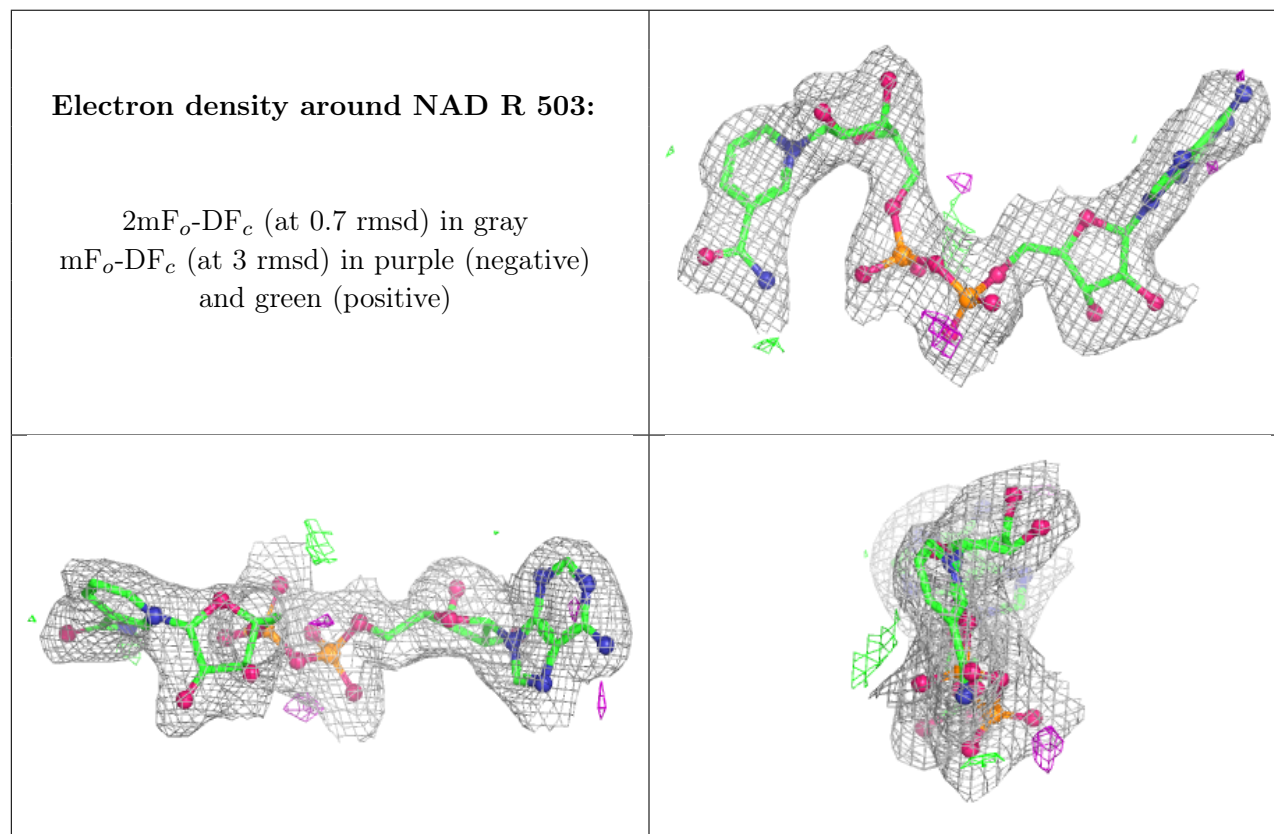
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	R	501	5/5	0.73	0.20	86,88,93,93	0
2	SO4	P	501	5/5	0.76	0.17	74,80,84,88	0

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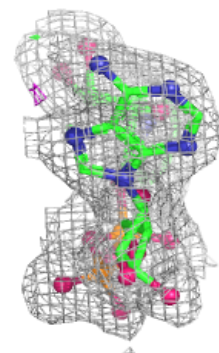
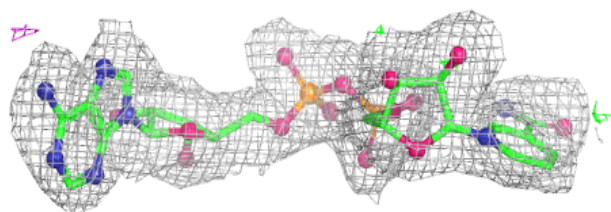
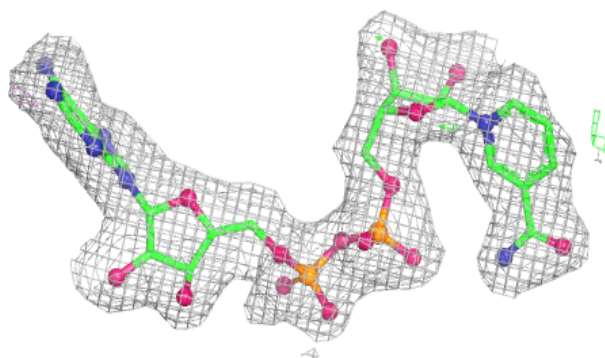
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	P	502	5/5	0.88	0.13	54,57,59,60	0
2	SO4	S	501	5/5	0.90	0.14	69,69,73,75	0
3	NAD	R	503	44/44	0.92	0.10	31,38,53,55	0
2	SO4	R	502	5/5	0.93	0.13	55,55,57,59	0
2	SO4	S	502	5/5	0.95	0.11	42,44,48,49	0
3	NAD	P	503	44/44	0.96	0.07	22,25,36,38	0
3	NAD	S	503	44/44	0.97	0.06	11,17,28,30	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.

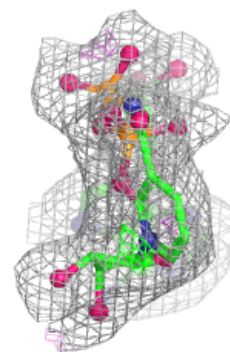
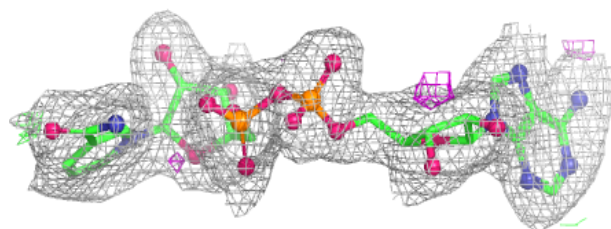
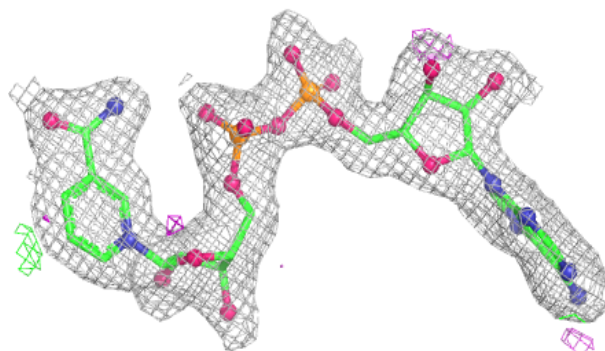


Electron density around NAD P 503:

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

**Electron density around NAD S 503:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.