Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 03:07 PM EDT

PDB ID	:	5TSO
Title	:	CRYSTAL STRUCTURE OF GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE FROM PIG MUSCLE COMPLEXED WITH ORTHOPHENANTHROLINE AT 1.90 ANGSTROM RESOLUTION
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Deposited on	:	2016-10-30
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

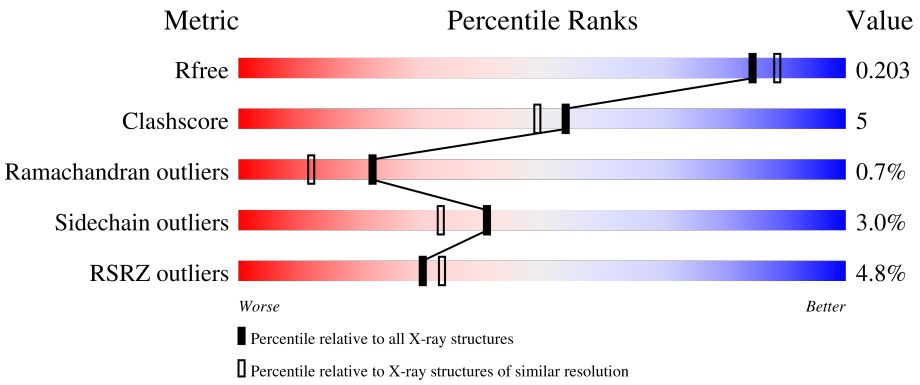
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	333	6% 89% 9%
1	R	333	8% 88% 10%
1	S	333	% 89% 9%

2 Entry composition (i)

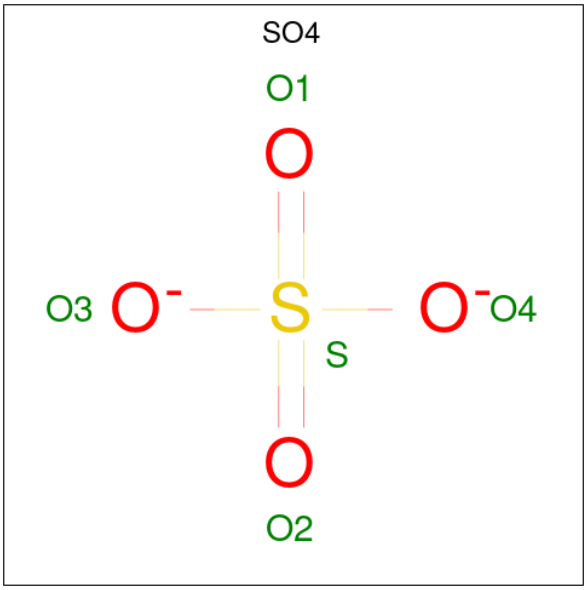
There are 6 unique types of molecules in this entry. The entry contains 8698 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	P	332	2510	1590	435	472	13	0	0	0
1	R	332	2510	1590	435	472	13	0	0	0
1	S	332	2510	1590	435	472	13	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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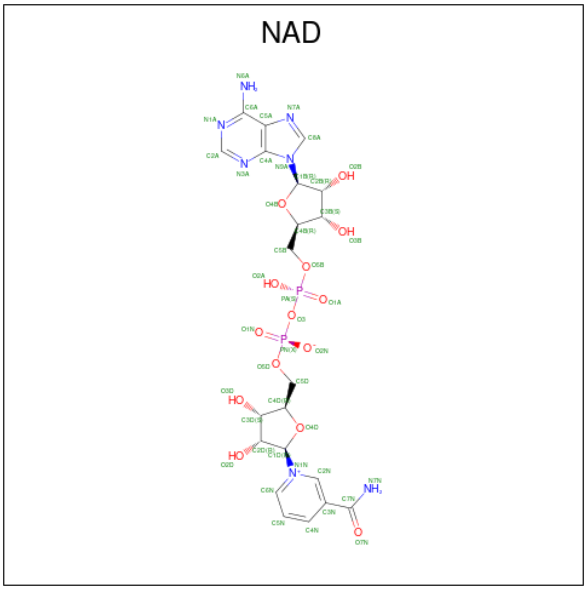
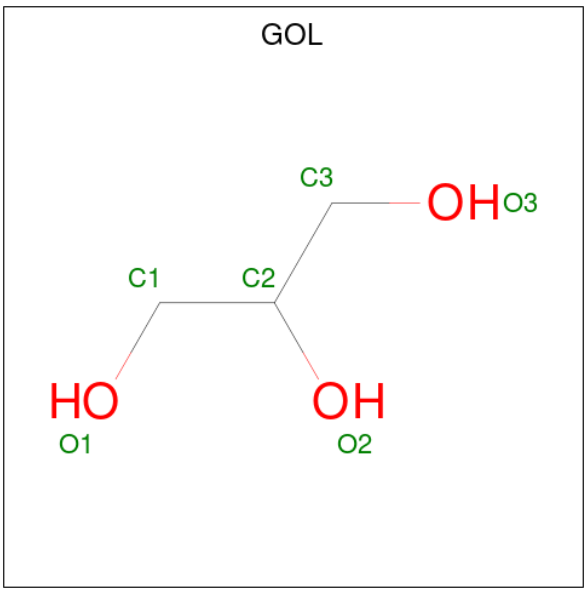
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	P	1	5	4	1		0	0
			Total	O	S			
2	P	1	5	4	1		0	0
			Total	O	S			
2	R	1	5	4	1		0	0
			Total	O	S			
2	R	1	5	4	1		0	0
			Total	O	S			
2	R	1	5	4	1		0	0
			Total	O	S			
2	R	1	5	4	1		0	0
			Total	O	S			
2	S	1	5	4	1		0	0
			Total	O	S			
2	S	1	5	4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

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



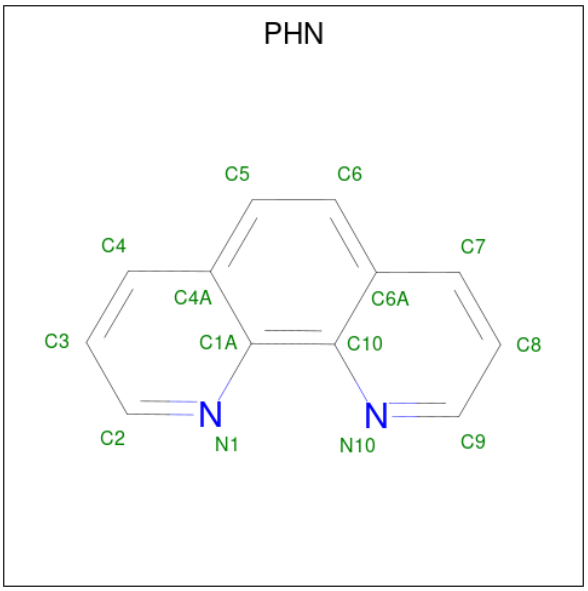
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	P	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	R	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	S	1	44	21	7	14	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	P	1	6	3	3	0	0
4	R	1	6	3	3	0	0
4	R	1	6	3	3	0	0
4	S	1	6	3	3	0	0
4	S	1	6	3	3	0	0
4	S	1	6	3	3	0	0
4	S	1	6	3	3	0	0

- Molecule 5 is 1,10-PHENANTHROLINE (three-letter code: PHN) (formula: $C_{12}H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	1	Total C N 14 12 2	0	0
5	R	1	Total C N 14 12 2	0	0
5	S	1	Total C N 14 12 2	0	0
5	S	1	Total C N 14 12 2	0	0

- Molecule 6 is water.

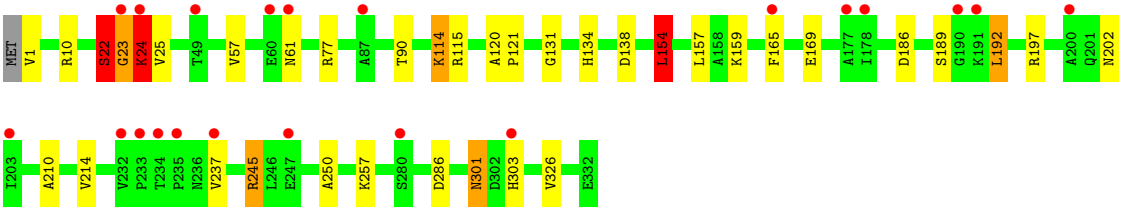
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	288	Total O 288 288	0	0
6	R	225	Total O 225 225	0	0
6	S	370	Total O 370 370	0	0

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.

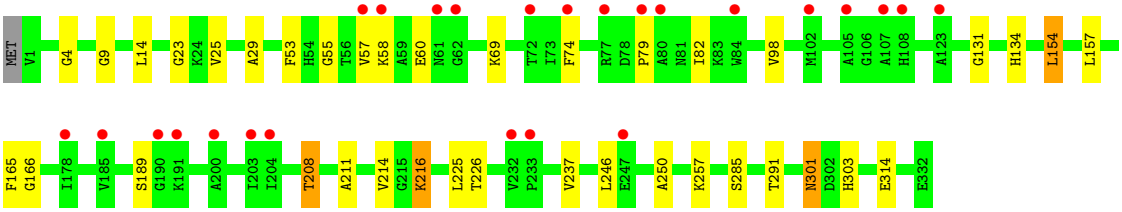
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain P:



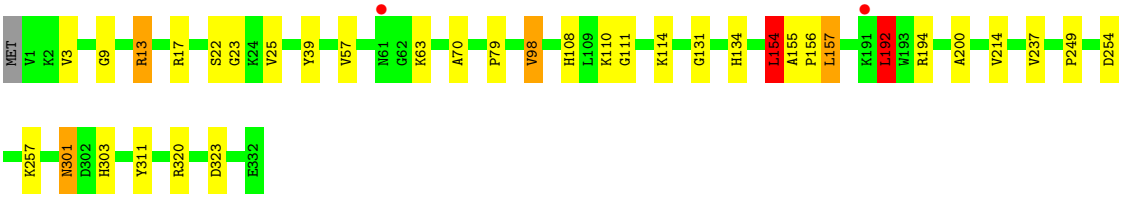
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain R:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	86.48Å 133.52Å 210.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.54 – 1.90 43.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (43.54-1.90) 93.6 (43.54-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.132 , 0.200 0.136 , 0.203	Depositor DCC
R_{free} test set	1319 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAD, SO4, PHN, GOL

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	0.90	1/2561 (0.0%)	1.02	11/3467 (0.3%)
1	R	0.87	1/2561 (0.0%)	0.87	0/3467
1	S	1.02	1/2561 (0.0%)	1.04	11/3467 (0.3%)
All	All	0.93	3/7683 (0.0%)	0.98	22/10401 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	3
1	R	0	1
1	S	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	257	LYS	CD-CE	-7.26	1.33	1.51
1	S	257	LYS	CD-CE	-6.51	1.34	1.51
1	R	257	LYS	CD-CE	-6.46	1.35	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	22	SER	O-C-N	-14.97	97.76	123.20
1	P	22	SER	CA-C-N	11.71	139.62	116.20
1	S	157	LEU	CB-CG-CD2	6.88	122.69	111.00
1	S	57	VAL	CB-CA-C	-6.83	98.42	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	13	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	S	320	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	S	320	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	S	98	VAL	CG1-CB-CG2	6.36	121.08	110.90
1	P	186	ASP	CB-CG-OD1	6.18	123.86	118.30
1	P	10	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	P	197	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	S	194	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	P	10	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	P	154	LEU	CB-CG-CD2	5.74	120.76	111.00
1	P	286	ASP	CB-CG-OD1	5.68	123.41	118.30
1	S	154	LEU	CB-CG-CD2	5.55	120.44	111.00
1	P	57	VAL	CB-CA-C	-5.54	100.88	111.40
1	P	115	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	S	17	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	P	115	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	S	192	LEU	CB-CG-CD2	5.26	119.94	111.00
1	S	323	ASP	CB-CG-OD1	-5.02	113.78	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	202	ASN	Peptide
1	P	22	SER	Mainchain
1	P	24	LYS	Peptide
1	R	23	GLY	Peptide
1	S	23	GLY	Peptide

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	2510	0	2510	37	0
1	R	2510	0	2510	19	0
1	S	2510	0	2510	20	0
2	P	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	20	0	0	1	0
2	S	10	0	0	1	0
3	P	44	0	26	0	0
3	R	44	0	26	1	0
3	S	44	0	26	0	0
4	P	6	0	8	0	0
4	R	12	0	16	3	0
4	S	24	0	32	3	0
5	R	28	0	16	0	0
5	S	28	0	16	2	0
6	P	288	0	0	5	0
6	R	225	0	0	4	0
6	S	370	0	0	7	0
All	All	8698	0	7696	82	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 5.

All (82) 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:P:24:LYS:HG3	1:P:326:VAL:HG21	1.36	1.00
1:S:192:LEU:H	1:S:192:LEU:HD23	1.31	0.96
1:P:154:LEU:HD13	1:P:214:VAL:HG21	1.58	0.83
1:P:24:LYS:CE	1:P:326:VAL:HG11	2.08	0.83
1:P:24:LYS:CG	1:P:326:VAL:HG21	2.09	0.83
1:P:24:LYS:NZ	1:P:326:VAL:HG11	1.93	0.82
1:P:22:SER:O	1:P:24:LYS:N	2.13	0.81
1:P:24:LYS:HE3	1:P:326:VAL:HG21	1.62	0.80
1:S:200:ALA:HB3	6:S:824:HOH:O	1.81	0.80
1:P:23:GLY:HA2	6:P:607:HOH:O	1.81	0.79
1:P:24:LYS:HE3	1:P:326:VAL:CB	2.13	0.78
1:P:24:LYS:HG3	1:P:326:VAL:CG2	2.14	0.78
1:P:24:LYS:HE3	1:P:326:VAL:HG11	1.64	0.77
1:S:22:SER:HB2	6:S:785:HOH:O	1.85	0.77
1:S:192:LEU:H	1:S:192:LEU:CD2	1.99	0.75
1:S:154:LEU:HD13	1:S:214:VAL:HG21	1.70	0.73
1:P:24:LYS:HE3	1:P:326:VAL:CG2	2.20	0.71
1:R:285:SER:OG	6:R:501:HOH:O	2.08	0.71
1:P:24:LYS:HE3	1:P:326:VAL:CG1	2.21	0.71
1:P:22:SER:OG	1:P:24:LYS:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:57:VAL:O	1:R:58:LYS:HG2	1.93	0.68
1:P:192:LEU:H	1:P:192:LEU:CD1	2.07	0.68
1:P:169:GLU:OE2	1:P:245:ARG:NH1	2.29	0.66
1:P:24:LYS:CE	1:P:326:VAL:HG21	2.27	0.65
1:S:301:ASN:HB2	4:S:406:GOL:H2	1.79	0.64
1:P:165:PHE:CD1	1:P:250:ALA:HB2	2.33	0.63
1:S:301:ASN:HD22	1:S:303:HIS:H	1.46	0.63
4:R:409:GOL:H11	6:R:512:HOH:O	1.99	0.62
1:P:24:LYS:CD	1:P:326:VAL:HG21	2.30	0.61
1:S:192:LEU:CD2	1:S:192:LEU:N	2.64	0.59
1:R:154:LEU:HD13	1:R:214:VAL:HG21	1.84	0.58
1:S:131:GLY:H	1:S:134:HIS:CD2	2.20	0.58
5:S:402:PHN:C7	4:S:409:GOL:H32	2.33	0.58
1:P:192:LEU:CD1	1:P:192:LEU:N	2.67	0.58
1:P:22:SER:C	1:P:24:LYS:H	2.06	0.57
1:R:301:ASN:HD22	1:R:303:HIS:H	1.51	0.57
6:P:649:HOH:O	1:S:114:LYS:HD2	2.05	0.56
1:P:131:GLY:H	1:P:134:HIS:CD2	2.24	0.56
1:P:24:LYS:HZ2	1:P:326:VAL:HG11	1.68	0.56
1:P:22:SER:OG	1:P:24:LYS:CB	2.54	0.55
1:P:192:LEU:N	1:P:192:LEU:HD12	2.21	0.55
1:P:189:SER:O	1:P:192:LEU:HD13	2.07	0.55
1:P:90:THR:HG23	1:P:114:LYS:HG3	1.89	0.54
1:S:192:LEU:HD23	1:S:192:LEU:N	2.11	0.53
1:P:120:ALA:HB1	1:P:121:PRO:HD2	1.91	0.52
1:S:111:GLY:HA3	6:S:521:HOH:O	2.10	0.52
1:R:291:THR:HG21	4:R:409:GOL:H12	1.91	0.52
1:P:301:ASN:HD22	1:P:303:HIS:H	1.57	0.52
1:S:79:PRO:HB3	1:S:108:HIS:CE1	2.46	0.51
1:P:77:ARG:NH1	2:P:504:SO4:O3	2.43	0.51
1:R:25:VAL:O	6:R:502:HOH:O	2.19	0.51
1:S:63:LYS:HD2	1:S:70:ALA:HB1	1.93	0.51
1:R:211:ALA:HB3	1:R:226:THR:HA	1.91	0.51
1:R:79:PRO:HA	1:R:82:ILE:CD1	2.42	0.50
1:R:53:PHE:CE2	1:R:55:GLY:HA3	2.47	0.49
5:S:401:PHN:H4	6:S:798:HOH:O	2.12	0.49
1:P:192:LEU:H	1:P:192:LEU:HD12	1.77	0.48
6:P:823:HOH:O	1:S:110:LYS:HD3	2.14	0.48
1:R:9:GLY:HA3	3:R:405:NAD:O5B	2.15	0.47
1:R:165:PHE:CD1	1:R:250:ALA:HB2	2.50	0.47
1:R:189:SER:O	1:R:189:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:409:GOL:C1	6:R:512:HOH:O	2.61	0.46
1:S:155:ALA:HB3	1:S:156:PRO:HD3	1.97	0.46
1:S:254:ASP:OD2	6:S:501:HOH:O	2.20	0.46
1:P:22:SER:O	1:P:23:GLY:C	2.48	0.45
1:R:216:LYS:HD2	1:R:216:LYS:N	2.31	0.45
1:S:249:PRO:HB3	1:S:303:HIS:NE2	2.32	0.45
1:P:1:VAL:N	6:P:610:HOH:O	2.49	0.45
4:S:406:GOL:H11	6:S:609:HOH:O	2.15	0.45
1:R:14:LEU:CD1	1:R:314:GLU:HB3	2.48	0.44
1:R:246:LEU:O	1:R:303:HIS:HD2	2.01	0.43
1:P:159:LYS:HE3	6:P:753:HOH:O	2.18	0.43
1:S:3:VAL:HG21	1:S:25:VAL:HG13	2.00	0.43
1:R:208:THR:OG1	2:R:403:SO4:O1	2.25	0.42
1:P:24:LYS:HE3	1:P:326:VAL:HB	1.97	0.42
1:P:192:LEU:H	1:P:192:LEU:HD13	1.82	0.41
1:R:131:GLY:H	1:R:134:HIS:CD2	2.38	0.41
1:P:210:ALA:O	1:P:214:VAL:HG23	2.20	0.41
1:S:9:GLY:O	1:S:13:ARG:HG3	2.21	0.41
2:S:403:SO4:O4	6:S:502:HOH:O	2.22	0.40
1:R:74:PHE:CD2	1:R:82:ILE:HG23	2.56	0.40
1:R:4:GLY:HA2	1:R:29:ALA:O	2.21	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	P	330/333 (99%)	315 (96%)	11 (3%)	4 (1%)	13 4
1	R	330/333 (99%)	318 (96%)	10 (3%)	2 (1%)	25 15
1	S	330/333 (99%)	319 (97%)	10 (3%)	1 (0%)	41 31
All	All	990/999 (99%)	952 (96%)	31 (3%)	7 (1%)	22 12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	23	GLY
1	P	25	VAL
1	P	24	LYS
1	P	237	VAL
1	S	237	VAL
1	R	237	VAL
1	R	166	GLY

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	P	267/269 (99%)	259 (97%)	8 (3%)	41	33
1	R	267/269 (99%)	258 (97%)	9 (3%)	37	28
1	S	267/269 (99%)	260 (97%)	7 (3%)	46	39
All	All	801/807 (99%)	777 (97%)	24 (3%)	41	33

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	61	ASN
1	P	114	LYS
1	P	138	ASP
1	P	154	LEU
1	P	157	LEU
1	P	192	LEU
1	P	245	ARG
1	P	301	ASN
1	R	60	GLU
1	R	69	LYS
1	R	98	VAL
1	R	154	LEU
1	R	157	LEU
1	R	208	THR

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Mol	Chain	Res	Type
1	R	216	LYS
1	R	225	LEU
1	R	301	ASN
1	S	39	TYR
1	S	98	VAL
1	S	154	LEU
1	S	157	LEU
1	S	192	LEU
1	S	301	ASN
1	S	311	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	75	GLN
1	P	134	HIS
1	P	139	ASN
1	P	261	GLN
1	P	301	ASN
1	R	134	HIS
1	R	301	ASN
1	R	327	HIS
1	S	134	HIS
1	S	146	ASN
1	S	222	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

25 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	504	-	4,4,4	0.77	0	6,6,6	0.64	0
2	SO4	P	501	-	4,4,4	0.69	0	6,6,6	0.50	0
2	SO4	P	506	-	4,4,4	0.55	0	6,6,6	0.54	0
2	SO4	R	407	-	4,4,4	0.47	0	6,6,6	0.47	0
2	SO4	S	404	-	4,4,4	0.19	0	6,6,6	1.24	0
2	SO4	R	404	-	4,4,4	0.10	0	6,6,6	0.78	0
3	NAD	R	405	-	42,48,48	1.22	4 (9%)	50,73,73	1.51	10 (20%)
3	NAD	P	503	-	42,48,48	1.20	7 (16%)	50,73,73	1.59	8 (16%)
2	SO4	P	505	-	4,4,4	0.45	0	6,6,6	0.93	0
4	GOL	S	408	-	5,5,5	0.59	0	5,5,5	0.72	0
2	SO4	R	403	-	4,4,4	0.53	0	6,6,6	0.71	0
5	PHN	R	401	-	16,16,16	1.97	4 (25%)	22,22,22	1.41	3 (13%)
4	GOL	S	406	-	5,5,5	0.39	0	5,5,5	1.92	1 (20%)
4	GOL	S	407	-	5,5,5	0.86	0	5,5,5	1.93	2 (40%)
5	PHN	S	402	-	16,16,16	1.80	3 (18%)	22,22,22	1.88	4 (18%)
4	GOL	P	507	-	5,5,5	0.69	0	5,5,5	1.60	1 (20%)
2	SO4	R	406	-	4,4,4	0.31	0	6,6,6	0.88	0
2	SO4	P	502	-	4,4,4	0.59	0	6,6,6	0.61	0
5	PHN	R	402	-	16,16,16	1.79	2 (12%)	22,22,22	1.56	3 (13%)
2	SO4	S	403	-	4,4,4	0.83	0	6,6,6	0.94	0
3	NAD	S	405	-	42,48,48	1.30	3 (7%)	50,73,73	1.65	11 (22%)
4	GOL	R	408	-	5,5,5	0.89	0	5,5,5	1.32	1 (20%)
5	PHN	S	401	-	16,16,16	2.11	5 (31%)	22,22,22	1.92	4 (18%)
4	GOL	S	409	-	5,5,5	0.80	0	5,5,5	1.50	1 (20%)
4	GOL	R	409	-	5,5,5	1.13	0	5,5,5	1.36	1 (20%)

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	405	-	-	5/26/62/62	0/5/5/5
4	GOL	S	408	-	-	2/4/4/4	-
4	GOL	P	507	-	-	0/4/4/4	-
5	PHN	R	401	-	-	-	0/3/3/3
4	GOL	S	406	-	-	0/4/4/4	-
4	GOL	R	408	-	-	4/4/4/4	-
5	PHN	R	402	-	-	-	0/3/3/3
4	GOL	S	407	-	-	2/4/4/4	-
5	PHN	S	401	-	-	-	0/3/3/3
4	GOL	S	409	-	-	2/4/4/4	-
5	PHN	S	402	-	-	-	0/3/3/3
3	NAD	S	405	-	-	5/26/62/62	0/5/5/5
3	NAD	P	503	-	-	5/26/62/62	0/5/5/5
4	GOL	R	409	-	-	0/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	401	PHN	C6A-C10	4.69	1.50	1.41
3	S	405	NAD	C2N-N1N	4.52	1.40	1.35
5	R	402	PHN	C6A-C10	4.51	1.50	1.41
5	R	401	PHN	C6A-C10	4.47	1.50	1.41
5	S	401	PHN	C4A-C1A	4.41	1.50	1.41
5	S	402	PHN	C6A-C10	4.29	1.50	1.41
5	R	401	PHN	C4A-C1A	3.92	1.49	1.41
5	R	402	PHN	C4A-C1A	3.37	1.48	1.41
3	P	503	NAD	C2N-N1N	3.20	1.38	1.35
3	S	405	NAD	C2B-C1B	3.10	1.58	1.53
3	S	405	NAD	C2A-N3A	3.00	1.36	1.32
3	R	405	NAD	C2A-N3A	2.84	1.36	1.32
5	S	402	PHN	C4A-C1A	2.83	1.47	1.41
3	R	405	NAD	C5A-C4A	2.60	1.47	1.40
3	R	405	NAD	C2N-N1N	2.49	1.38	1.35
5	S	401	PHN	C2-N1	2.45	1.37	1.32
3	R	405	NAD	O4D-C1D	2.31	1.44	1.41
5	S	401	PHN	C1A-C10	2.30	1.50	1.43
5	R	401	PHN	C9-N10	2.28	1.37	1.32
5	S	401	PHN	C9-N10	2.19	1.36	1.32
3	P	503	NAD	C5A-C4A	2.16	1.46	1.40
3	P	503	NAD	PA-O2A	-2.12	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	503	NAD	C2A-N3A	2.11	1.35	1.32
3	P	503	NAD	C3N-C7N	2.10	1.53	1.50
3	P	503	NAD	C2B-C1B	2.09	1.56	1.53
3	P	503	NAD	O4B-C1B	-2.05	1.38	1.41
5	R	401	PHN	C2-N1	2.03	1.36	1.32
5	S	402	PHN	C5-C4A	-2.01	1.37	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	401	PHN	C1A-C10-N10	5.12	124.50	118.23
5	S	402	PHN	C10-C1A-N1	4.98	124.32	118.23
5	S	401	PHN	C10-C1A-N1	4.71	124.00	118.23
3	R	405	NAD	O7N-C7N-N7N	-4.49	116.19	122.58
5	R	402	PHN	C10-C1A-N1	4.32	123.52	118.23
3	S	405	NAD	N3A-C2A-N1A	-4.25	122.03	128.68
3	P	503	NAD	C6N-N1N-C2N	-4.24	118.11	121.97
5	S	402	PHN	C1A-C10-N10	3.71	122.77	118.23
3	R	405	NAD	C3N-C7N-N7N	3.64	122.11	117.75
5	R	401	PHN	C10-C1A-N1	3.62	122.66	118.23
3	S	405	NAD	C1B-N9A-C4A	-3.59	120.34	126.64
4	S	406	GOL	O1-C1-C2	-3.53	93.27	110.20
3	P	503	NAD	C3N-C7N-N7N	3.49	121.94	117.75
3	P	503	NAD	N3A-C2A-N1A	-3.49	123.23	128.68
5	S	402	PHN	C2-N1-C1A	3.44	123.27	117.12
3	P	503	NAD	C1B-N9A-C4A	-3.43	120.61	126.64
3	P	503	NAD	O7N-C7N-C3N	-3.37	115.60	119.63
3	S	405	NAD	C2A-N1A-C6A	3.30	124.41	118.75
3	S	405	NAD	O2N-PN-O1N	3.28	128.47	112.24
3	S	405	NAD	C6N-N1N-C2N	-3.21	119.05	121.97
4	S	407	GOL	C3-C2-C1	-3.08	99.73	111.70
5	S	401	PHN	C4A-C1A-N1	-2.97	117.25	122.51
5	R	401	PHN	C1A-C10-N10	2.96	121.85	118.23
5	S	402	PHN	C4A-C1A-N1	-2.89	117.40	122.51
3	P	503	NAD	O5D-PN-O1N	-2.82	98.03	109.07
3	S	405	NAD	C2N-C3N-C4N	2.68	121.30	118.26
3	P	503	NAD	C2A-N1A-C6A	2.67	123.33	118.75
3	R	405	NAD	C2N-C3N-C4N	-2.67	115.23	118.26
4	S	409	GOL	O2-C2-C3	2.60	120.56	109.12
4	S	407	GOL	O3-C3-C2	-2.52	98.11	110.20
5	R	401	PHN	C2-N1-C1A	2.51	121.61	117.12
3	R	405	NAD	C3N-C2N-N1N	2.51	122.88	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	507	GOL	O1-C1-C2	-2.50	98.24	110.20
3	R	405	NAD	O4B-C1B-C2B	-2.42	103.40	106.93
3	R	405	NAD	N6A-C6A-N1A	2.33	123.40	118.57
3	R	405	NAD	C1B-N9A-C4A	-2.31	122.58	126.64
5	S	401	PHN	C6A-C10-N10	-2.24	118.56	122.51
3	S	405	NAD	N6A-C6A-N1A	2.21	123.17	118.57
3	S	405	NAD	O2A-PA-O1A	2.21	123.17	112.24
3	R	405	NAD	O2N-PN-O5D	2.21	117.99	107.75
4	R	409	GOL	O1-C1-C2	2.18	120.66	110.20
3	R	405	NAD	PN-O3-PA	-2.16	125.42	132.83
5	R	402	PHN	C4A-C1A-C10	-2.14	115.98	119.18
3	S	405	NAD	C5N-C6N-N1N	2.14	123.47	120.40
3	P	503	NAD	O2N-PN-O5D	2.13	117.63	107.75
3	R	405	NAD	N3A-C2A-N1A	-2.08	125.43	128.68
3	S	405	NAD	C2B-C3B-C4B	2.06	106.65	102.64
4	R	408	GOL	O3-C3-C2	2.03	119.95	110.20
5	R	402	PHN	C7-C8-C9	2.01	121.53	118.93
3	S	405	NAD	O7N-C7N-C3N	-2.01	117.23	119.63

There are no chirality outliers.

All (25) 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	P	503	NAD	C2D-C1D-N1N-C2N
3	P	503	NAD	C2D-C1D-N1N-C6N
3	R	405	NAD	O4D-C1D-N1N-C2N
3	R	405	NAD	O4D-C1D-N1N-C6N
3	R	405	NAD	C2D-C1D-N1N-C2N
3	R	405	NAD	C2D-C1D-N1N-C6N
3	S	405	NAD	O4D-C1D-N1N-C2N
3	S	405	NAD	O4D-C1D-N1N-C6N
3	S	405	NAD	C2D-C1D-N1N-C6N
4	S	407	GOL	C1-C2-C3-O3
4	S	408	GOL	O1-C1-C2-C3
4	S	408	GOL	O1-C1-C2-O2
4	R	408	GOL	C1-C2-C3-O3
4	R	408	GOL	O2-C2-C3-O3
4	S	407	GOL	O2-C2-C3-O3
4	S	409	GOL	O2-C2-C3-O3
4	S	409	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	R	408	GOL	O1-C1-C2-O2
4	R	408	GOL	O1-C1-C2-C3
3	S	405	NAD	O4B-C4B-C5B-O5B
3	S	405	NAD	C2D-C1D-N1N-C2N
3	R	405	NAD	O4B-C4B-C5B-O5B
3	P	503	NAD	O4B-C4B-C5B-O5B

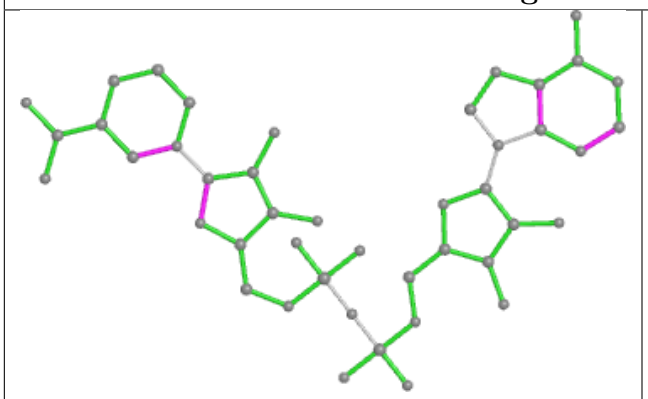
There are no ring outliers.

9 monomers are involved in 11 short contacts:

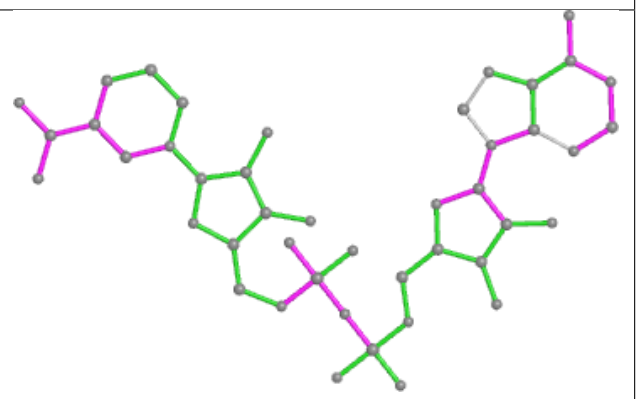
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	504	SO4	1	0
3	R	405	NAD	1	0
2	R	403	SO4	1	0
4	S	406	GOL	2	0
5	S	402	PHN	1	0
2	S	403	SO4	1	0
5	S	401	PHN	1	0
4	S	409	GOL	1	0
4	R	409	GOL	3	0

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 then 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.

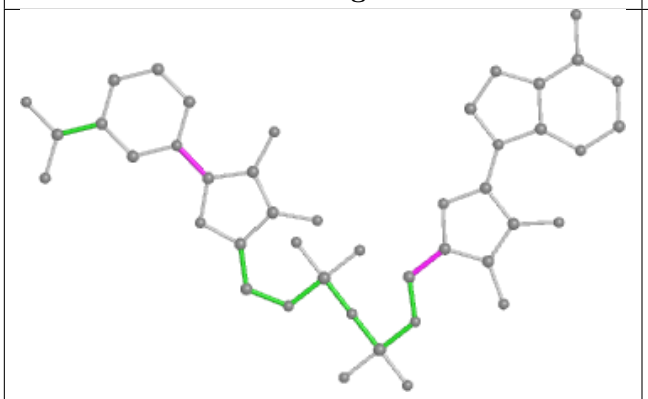
Ligand NAD R 405



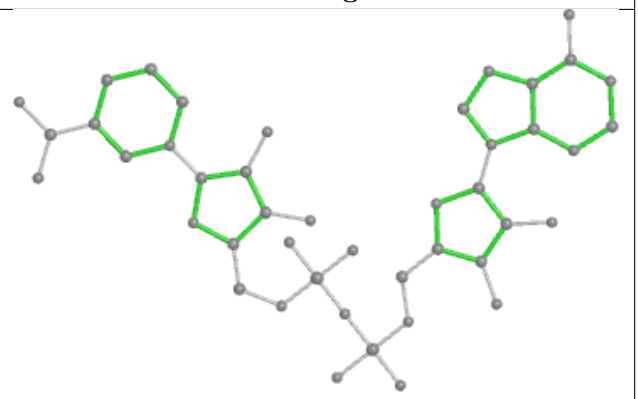
Bond lengths



Bond angles

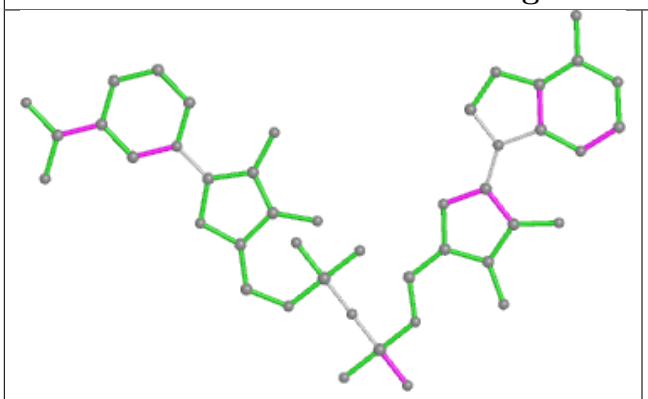


Torsions

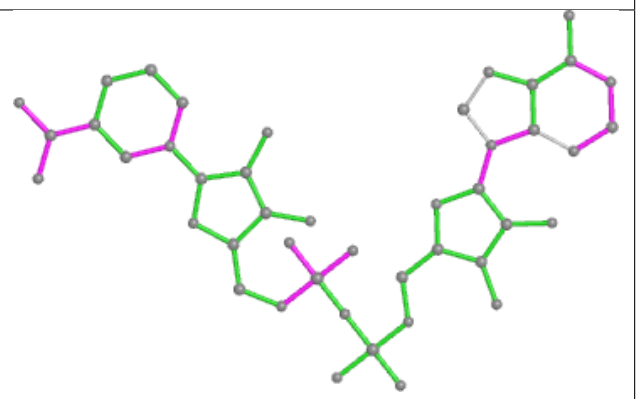


Rings

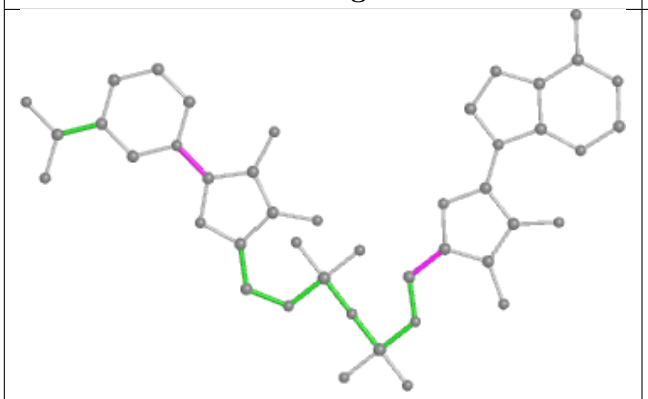
Ligand NAD P 503



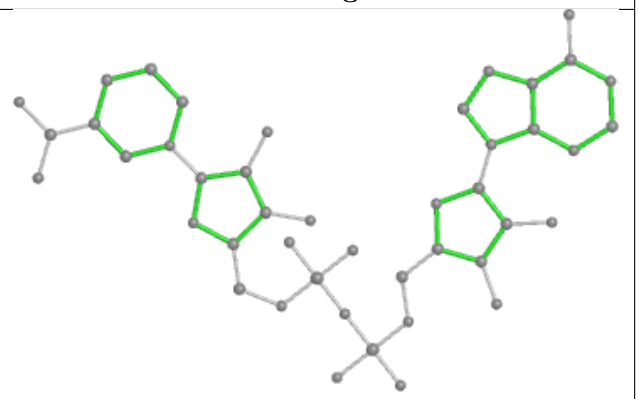
Bond lengths



Bond angles

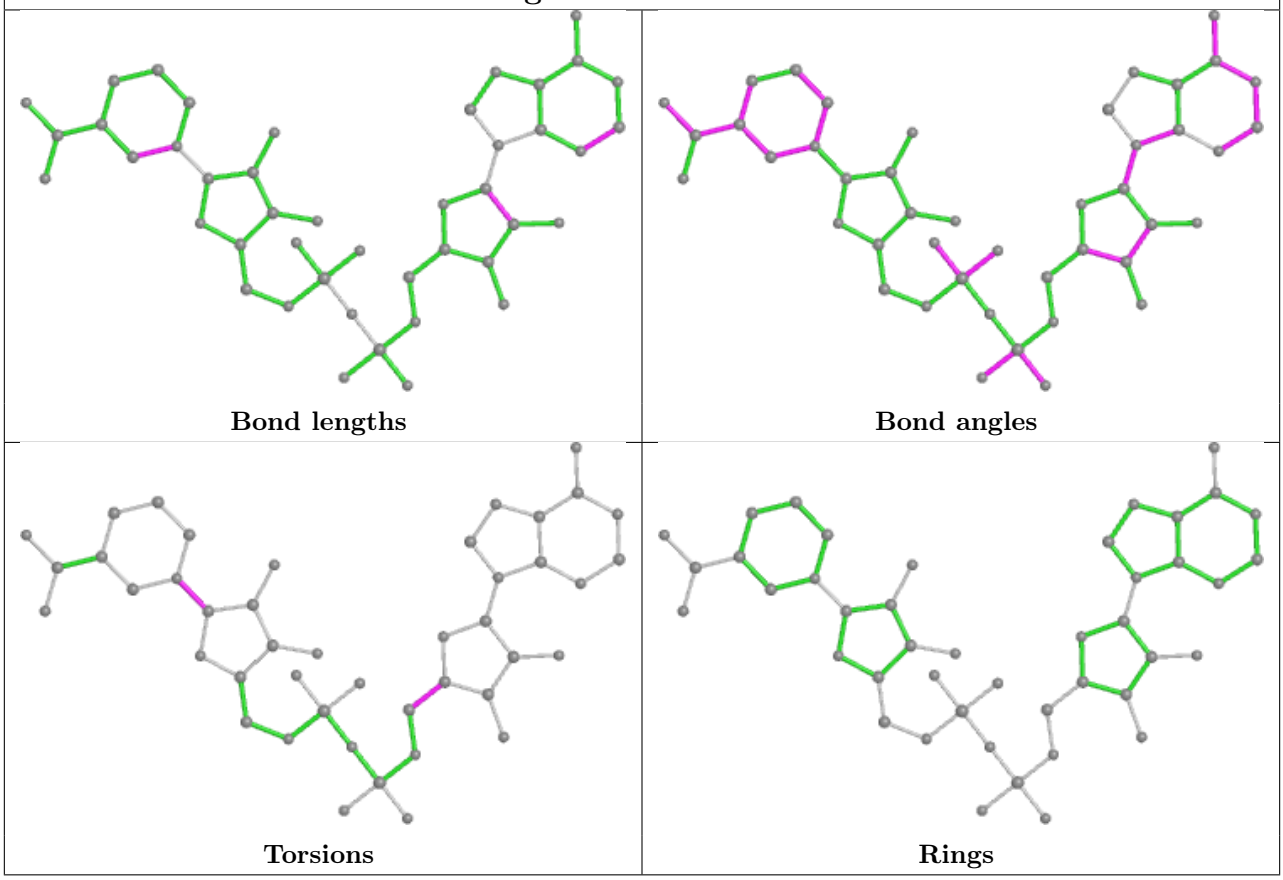


Torsions



Rings

Ligand NAD S 405



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	P	332/333 (99%)	0.15	21 (6%)	20	22	24, 33, 56, 96	0
1	R	332/333 (99%)	0.32	25 (7%)	14	15	26, 40, 58, 83	0
1	S	332/333 (99%)	-0.17	2 (0%)	89	90	15, 23, 43, 69	0
All	All	996/999 (99%)	0.10	48 (4%)	30	33	15, 33, 55, 96	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	24	LYS	6.8
1	P	23	GLY	4.4
1	P	190	GLY	4.1
1	R	80	ALA	4.0
1	R	74	PHE	3.8
1	P	178	ILE	3.7
1	P	234	THR	3.4
1	R	107	ALA	3.4
1	P	233	PRO	3.2
1	R	61	ASN	3.2
1	P	235	PRO	3.1
1	P	232	VAL	3.0
1	P	61	ASN	2.9
1	R	233	PRO	2.9
1	R	77	ARG	2.9
1	P	87	ALA	2.8
1	R	232	VAL	2.8
1	R	62	GLY	2.8
1	R	203	ILE	2.7
1	R	105	ALA	2.6
1	S	191	LYS	2.6
1	P	60	GLU	2.5
1	R	57	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	200	ALA	2.4
1	S	61	ASN	2.4
1	R	204	ILE	2.4
1	P	237	VAL	2.4
1	R	185	VAL	2.4
1	R	108	HIS	2.4
1	P	203	ILE	2.4
1	P	200	ALA	2.3
1	R	178	ILE	2.3
1	P	165	PHE	2.3
1	P	191	LYS	2.3
1	P	177	ALA	2.3
1	R	190	GLY	2.3
1	R	191	LYS	2.3
1	P	247	GLU	2.2
1	R	102	MET	2.2
1	R	72	THR	2.1
1	R	247	GLU	2.1
1	R	123	ALA	2.1
1	R	79	PRO	2.1
1	P	303	HIS	2.1
1	R	84	TRP	2.1
1	R	58	LYS	2.1
1	P	280	SER	2.0
1	P	49	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

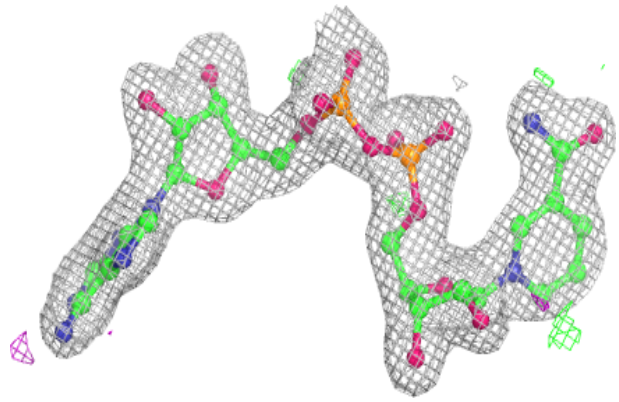
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

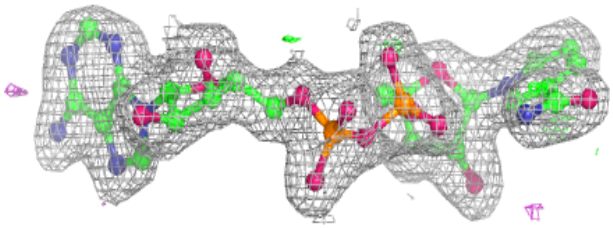
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	R	409	6/6	0.82	0.19	49,58,60,62	0
4	GOL	R	408	6/6	0.84	0.15	55,63,66,67	0
2	SO4	R	406	5/5	0.85	0.25	38,47,52,55	5
5	PHN	S	401	14/14	0.89	0.18	47,63,75,77	0
5	PHN	R	401	14/14	0.90	0.15	46,58,70,71	0
4	GOL	S	409	6/6	0.91	0.15	51,55,57,69	0
4	GOL	S	407	6/6	0.91	0.14	44,48,51,61	0
4	GOL	S	408	6/6	0.91	0.15	38,57,65,68	0
2	SO4	P	504	5/5	0.92	0.23	51,59,80,87	0
4	GOL	S	406	6/6	0.93	0.14	44,49,57,64	0
2	SO4	P	505	5/5	0.94	0.32	67,74,83,83	0
2	SO4	R	407	5/5	0.94	0.26	60,68,85,85	0
2	SO4	P	506	5/5	0.95	0.25	68,71,82,85	0
4	GOL	P	507	6/6	0.97	0.13	50,54,57,62	0
2	SO4	P	501	5/5	0.97	0.07	47,50,55,57	0
5	PHN	R	402	14/14	0.97	0.13	37,43,55,61	0
3	NAD	R	405	44/44	0.97	0.09	27,36,40,45	0
5	PHN	S	402	14/14	0.97	0.13	30,35,41,46	0
2	SO4	R	403	5/5	0.98	0.09	53,54,58,77	0
2	SO4	S	403	5/5	0.98	0.08	39,44,49,51	0
3	NAD	P	503	44/44	0.98	0.09	21,27,31,34	0
3	NAD	S	405	44/44	0.99	0.09	15,19,25,26	0
2	SO4	S	404	5/5	0.99	0.10	33,34,38,41	0
2	SO4	R	404	5/5	0.99	0.07	45,47,57,62	0
2	SO4	P	502	5/5	0.99	0.09	42,45,52,53	0

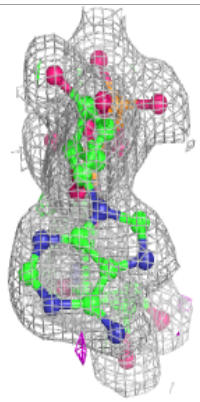
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD R 405:

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

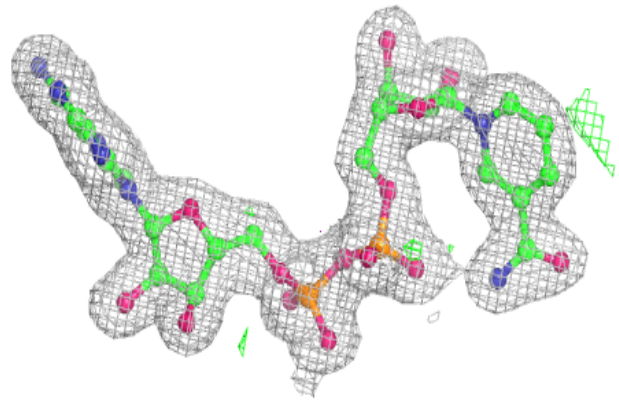


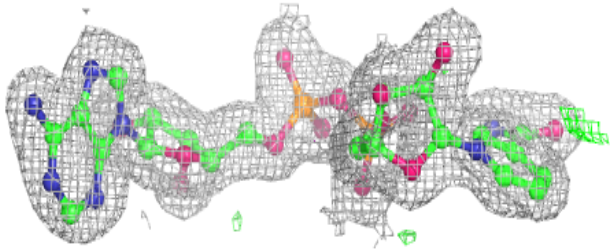


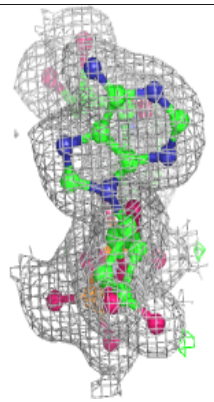


Electron density around NAD P 503:

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

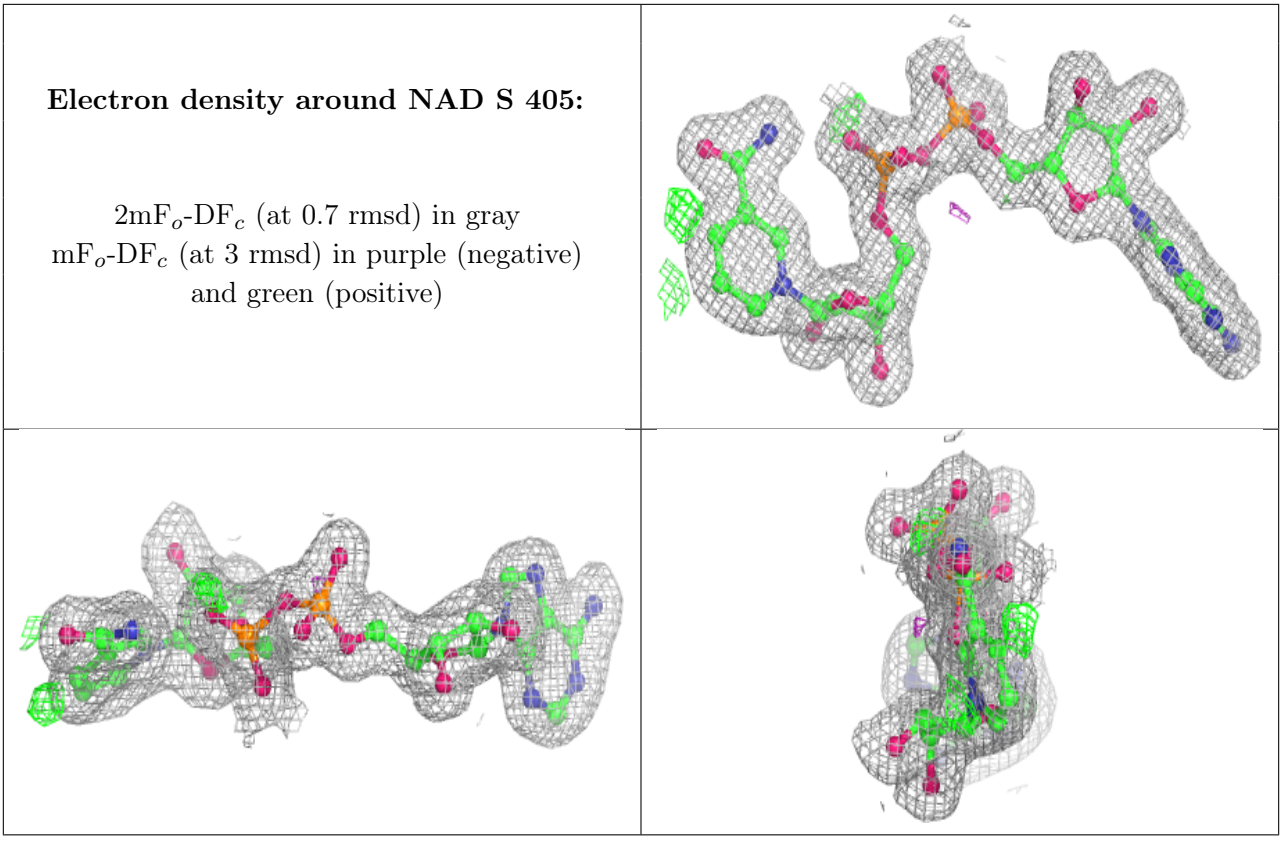






Electron density around NAD S 405:

$2mF_o$-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.