



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:05 PM UTC

PDB ID : 4E5K / pdb_00004e5k
Title : Thermostable phosphite dehydrogenase in complex with NAD and sulfite
Authors : Zou, Y.; Zhang, H.; Nair, S.K.
Deposited on : 2012-03-14
Resolution : 1.95 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

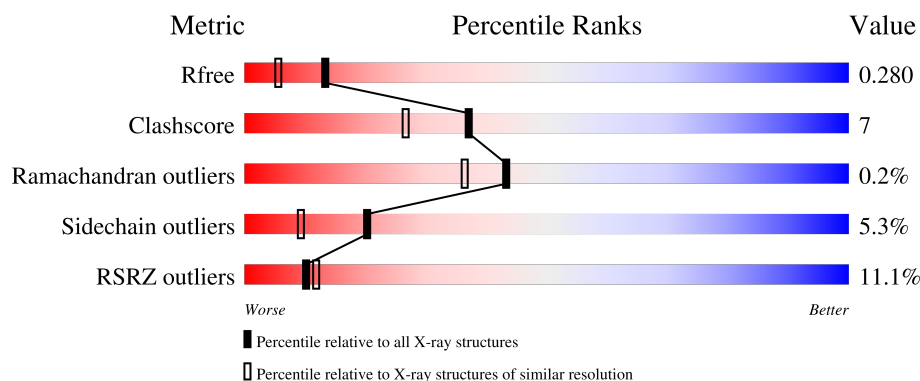
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	329	3% 84% 15% .
1	B	329	4% 83% 15% .
1	C	329	18% 77% 21% .
1	D	329	19% 81% 17% .

2 Entry composition ⓘ

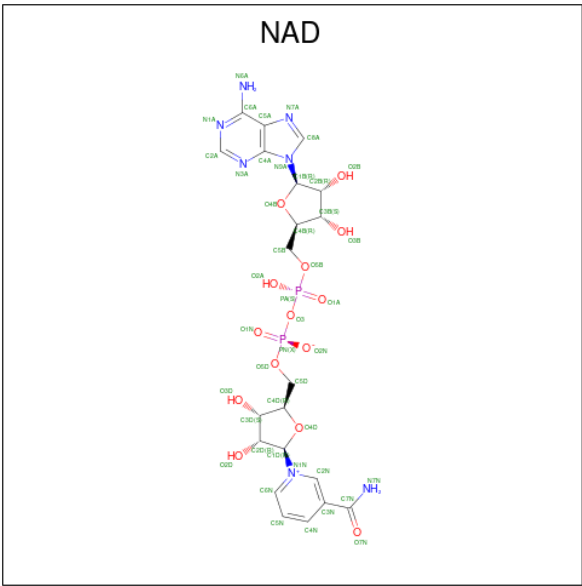
There are 4 unique types of molecules in this entry. The entry contains 10830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphite dehydrogenase (thermostable variant).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			
1	B	329	Total	C	N	O	S	0	0	0
			2515	1589	456	455	15			
1	C	328	Total	C	N	O	S	0	0	0
			2515	1589	455	456	15			
1	D	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



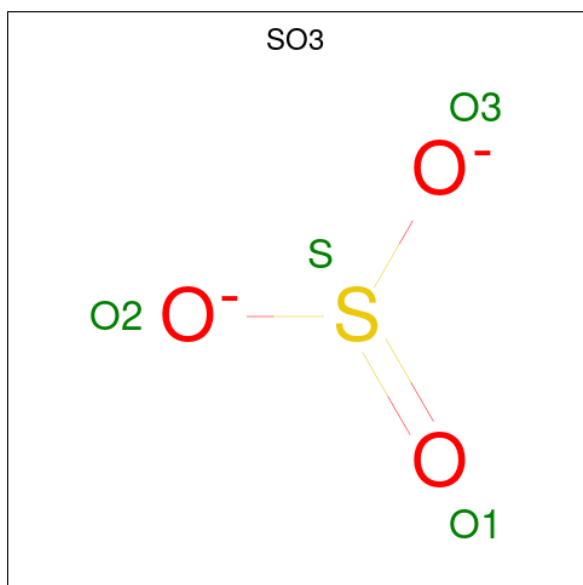
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			4 3 1			
3	B	1	Total	O S	0	0
			4 3 1			
3	C	1	Total	O S	0	0
			4 3 1			
3	D	1	Total	O S	0	0
			4 3 1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172 172			
4	B	233	Total	O	0	0
			233 233			
4	C	97	Total	O	0	0
			97 97			

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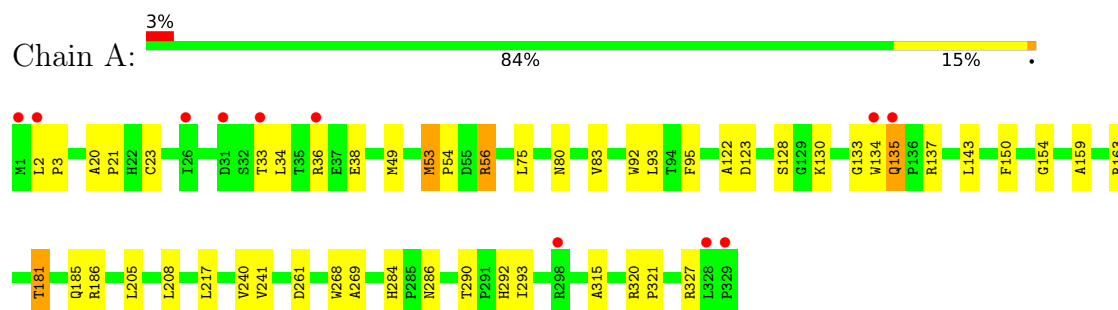
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	68	Total	O	0	0
			68	68		

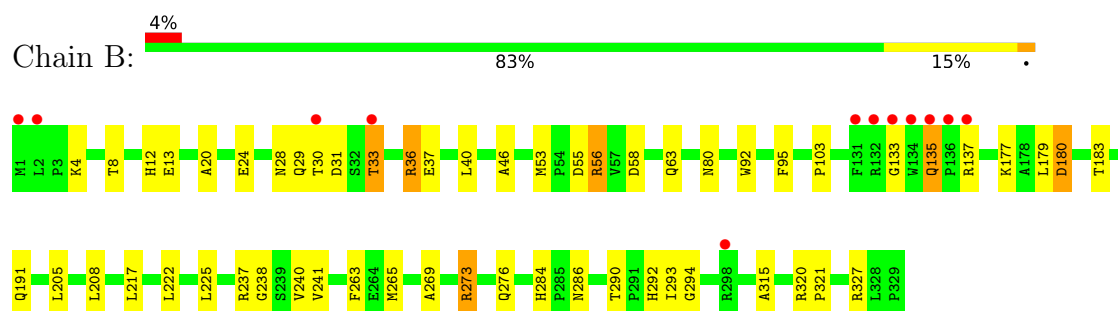
3 Residue-property plots [i](#)

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.

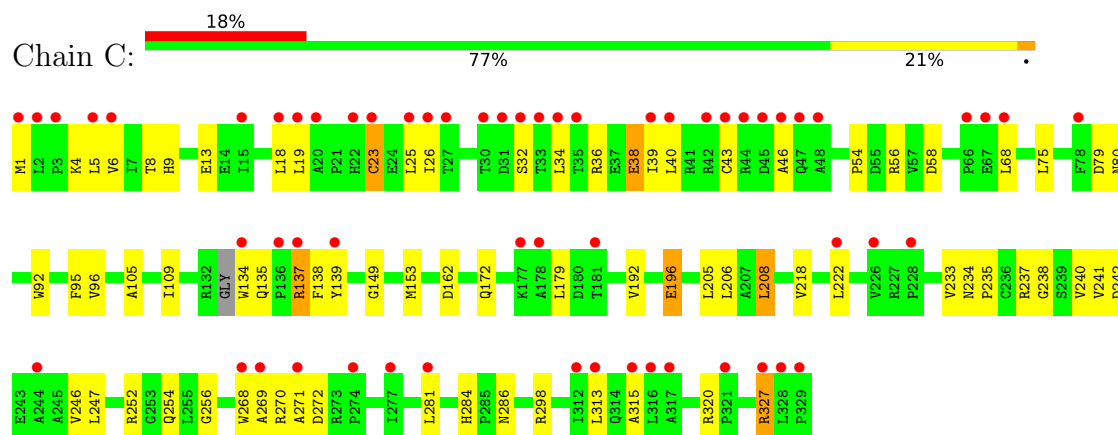
- Molecule 1: Phosphite dehydrogenase (thermostable variant)



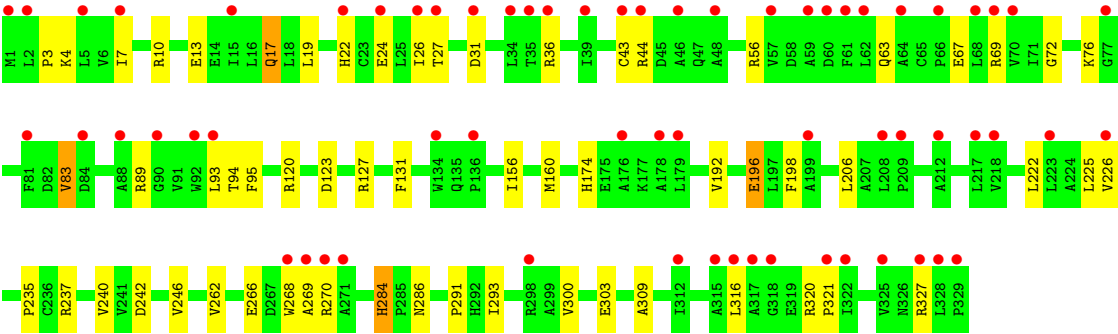
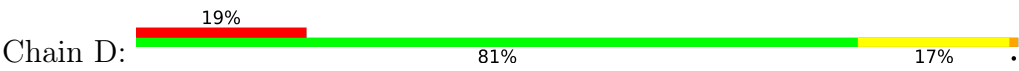
- Molecule 1: Phosphite dehydrogenase (thermostable variant)



- Molecule 1: Phosphite dehydrogenase (thermostable variant)



- Molecule 1: Phosphite dehydrogenase (thermostable variant)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.06Å 114.18Å 88.31Å 90.00° 112.33° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 25.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-1.95) 97.9 (25.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.267 (Not available) , 0.280	Depositor DCC
R_{free} test set	4766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10830	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.03% 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: NAD, SO3

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	0.82	1/2566 (0.0%)	0.97	1/3490 (0.0%)
1	B	0.86	0/2562	0.98	3/3485 (0.1%)
1	C	0.74	0/2561	0.93	3/3482 (0.1%)
1	D	0.63	0/2566	0.90	2/3490 (0.1%)
All	All	0.76	1/10255 (0.0%)	0.94	9/13947 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	VAL	CA-CB	6.29	1.63	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLY	N-CA-C	-7.00	102.75	112.13
1	B	133	GLY	N-CA-C	-6.64	104.81	111.85
1	D	284	HIS	CA-C-N	6.00	125.70	119.05
1	D	284	HIS	C-N-CA	6.00	125.70	119.05
1	B	20	ALA	CA-C-N	-5.92	113.88	120.45
1	B	20	ALA	C-N-CA	-5.92	113.88	120.45
1	C	23	CYS	N-CA-C	5.20	117.16	108.99
1	C	96	VAL	CA-C-N	5.12	124.73	119.05
1	C	96	VAL	C-N-CA	5.12	124.73	119.05

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	2519	0	2540	42	0
1	B	2515	0	2536	41	0
1	C	2515	0	2536	41	1
1	D	2519	0	2540	33	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	2	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
4	A	172	0	0	2	0
4	B	233	0	0	5	2
4	C	97	0	0	6	1
4	D	68	0	0	1	0
All	All	10830	0	10256	145	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 7.

All (145) 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:B:265:MET:HE3	1:B:276:GLN:HA	1.23	1.14
1:A:181:THR:CG2	1:B:273:ARG:NH2	2.15	1.10
1:A:181:THR:HG21	1:B:273:ARG:HH21	1.20	1.06
1:C:25:LEU:HD23	4:C:518:HOH:O	1.64	0.98
1:C:5:LEU:HB3	4:C:518:HOH:O	1.65	0.96
1:A:181:THR:HG21	1:B:273:ARG:NH2	1.80	0.95
1:A:3:PRO:O	1:A:23:CYS:HB2	1.71	0.91
1:B:265:MET:CE	1:B:276:GLN:HA	2.01	0.90
1:B:56:ARG:NH1	1:B:58:ASP:HB3	1.92	0.84
1:A:181:THR:CG2	1:B:273:ARG:HH22	1.90	0.83
1:D:192:VAL:HB	1:D:196:GLU:HG2	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:THR:HG23	1:B:273:ARG:NH2	2.01	0.73
1:B:265:MET:HE3	1:B:276:GLN:CA	2.12	0.70
1:A:185:GLN:OE1	1:B:273:ARG:NH1	2.25	0.70
1:B:53:MET:HE1	4:B:676:HOH:O	1.94	0.68
1:D:222:LEU:HD12	1:D:225:LEU:HD12	1.75	0.68
1:A:83:VAL:HG22	1:A:93:LEU:HD23	1.76	0.65
1:B:56:ARG:HH11	1:B:58:ASP:HB3	1.58	0.65
1:D:123:ASP:OD2	1:D:127:ARG:NE	2.25	0.63
1:B:284:HIS:HD2	1:B:286:ASN:H	1.47	0.62
1:C:36:ARG:HA	1:C:39:ILE:HD12	1.80	0.62
1:C:237:ARG:NH1	3:C:402:SO3:O1	2.29	0.62
1:D:63:GLN:HA	1:D:89:ARG:NH2	2.14	0.62
1:B:208:LEU:H	1:B:208:LEU:HD23	1.65	0.60
1:A:2:LEU:HB3	1:A:23:CYS:HA	1.82	0.60
1:A:34:LEU:HD22	1:A:38:GLU:HG2	1.82	0.60
1:A:135:GLN:HG3	1:A:137:ARG:HD3	1.83	0.60
1:A:83:VAL:HG22	1:A:93:LEU:CD2	2.31	0.60
1:C:153:MET:HG2	1:C:179:LEU:HD11	1.84	0.59
1:C:138:PHE:HD2	4:C:521:HOH:O	1.86	0.59
1:C:8:THR:HG23	4:C:519:HOH:O	2.02	0.58
1:A:123:ASP:OD2	1:D:120:ARG:HD3	2.02	0.58
1:A:53:MET:HE1	4:A:581:HOH:O	2.03	0.58
1:A:36:ARG:HH22	1:A:56:ARG:CG	2.17	0.57
1:A:128:SER:OG	1:A:130:LYS:HG3	2.04	0.57
1:D:156:ILE:HG22	1:D:160:MET:HE2	1.86	0.57
1:C:6:VAL:HG12	4:C:519:HOH:O	2.05	0.57
1:C:205:LEU:HD23	1:C:233:VAL:HB	1.87	0.57
1:A:3:PRO:O	1:A:23:CYS:CB	2.49	0.57
1:D:17:GLN:HE21	1:D:17:GLN:HA	1.69	0.57
4:A:553:HOH:O	1:D:127:ARG:HD3	2.03	0.56
1:C:34:LEU:HD22	1:C:38:GLU:HG2	1.88	0.56
1:C:149:GLY:HA2	1:C:172:GLN:O	2.06	0.56
1:B:53:MET:HE2	3:B:402:SO3:O3	2.05	0.56
1:C:247:LEU:HD13	1:C:281:LEU:HA	1.87	0.56
1:B:92:TRP:CH2	1:B:320:ARG:HG3	2.43	0.54
1:B:180:ASP:OD1	1:B:183:THR:HB	2.07	0.54
1:D:291:PRO:HD2	1:D:293:ILE:HG12	1.90	0.53
1:A:53:MET:HE3	1:A:53:MET:H	1.74	0.53
1:D:206:LEU:O	1:D:235:PRO:HD2	2.09	0.53
1:C:208:LEU:HD23	1:C:208:LEU:H	1.75	0.52
1:B:315:ALA:HB2	1:B:321:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:HD2	1:D:286:ASN:H	1.57	0.52
1:C:13:GLU:HB3	4:C:572:HOH:O	2.10	0.52
1:B:180:ASP:OD1	1:B:183:THR:CB	2.59	0.51
1:C:252:ARG:NH1	1:C:254:GLN:OE1	2.44	0.51
1:A:53:MET:HE2	1:A:75:LEU:HB3	1.92	0.51
1:A:320:ARG:HH21	1:A:327:ARG:HB3	1.75	0.51
1:B:265:MET:O	1:B:273:ARG:NH1	2.36	0.51
1:A:150:PHE:CE1	1:A:205:LEU:HD12	2.45	0.51
1:D:19:LEU:HD21	1:D:309:ALA:HB1	1.92	0.51
1:C:75:LEU:C	1:C:75:LEU:HD12	2.36	0.50
1:C:153:MET:CG	1:C:179:LEU:HD11	2.41	0.50
1:B:222:LEU:HD12	1:B:225:LEU:HD12	1.94	0.50
1:B:284:HIS:CD2	1:B:286:ASN:H	2.29	0.49
1:A:181:THR:HG23	1:B:273:ARG:HH22	1.69	0.49
1:B:292:HIS:CE1	4:B:557:HOH:O	2.65	0.49
1:A:36:ARG:HH22	1:A:56:ARG:HG2	1.76	0.49
1:A:284:HIS:HD2	1:A:286:ASN:H	1.60	0.49
1:B:208:LEU:HD23	1:B:208:LEU:N	2.28	0.48
1:B:28:ASN:C	1:B:30:THR:H	2.22	0.48
1:B:4:LYS:HB3	1:B:46:ALA:HA	1.95	0.48
1:D:83:VAL:HG13	1:D:93:LEU:HD23	1.95	0.48
1:A:20:ALA:N	1:A:21:PRO:HD2	2.29	0.48
1:C:19:LEU:HD23	1:C:313:LEU:HD21	1.95	0.47
1:C:256:GLY:O	1:C:286:ASN:HB3	2.14	0.47
1:C:43:CYS:HB3	1:C:68:LEU:HD21	1.95	0.47
1:C:218:VAL:HB	1:C:241:VAL:HA	1.95	0.47
1:C:92:TRP:CD1	1:C:315:ALA:HB1	2.50	0.47
1:C:9:HIS:HE2	1:C:54:PRO:HG2	1.79	0.46
1:B:36:ARG:O	1:B:40:LEU:HD12	2.15	0.46
1:D:131:PHE:HB3	4:D:509:HOH:O	2.15	0.46
1:A:159:ALA:O	1:A:163:ARG:HD2	2.15	0.46
1:B:24:GLU:HA	4:B:662:HOH:O	2.14	0.46
1:B:135:GLN:HG3	1:B:137:ARG:HG2	1.97	0.46
1:A:36:ARG:HH12	1:A:56:ARG:HG3	1.81	0.45
1:A:92:TRP:CH2	1:A:320:ARG:HG3	2.52	0.45
1:C:192:VAL:HB	1:C:196:GLU:HG3	1.98	0.45
1:C:247:LEU:HB2	1:C:281:LEU:HD13	1.97	0.45
1:A:284:HIS:CD2	1:A:286:ASN:H	2.35	0.45
1:D:262:VAL:HA	1:D:266:GLU:OE1	2.17	0.45
1:A:186:ARG:HD3	1:B:33:THR:HG21	1.98	0.45
1:C:80:ASN:ND2	1:C:269:ALA:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:PRO:HD2	1:D:22:HIS:O	2.17	0.45
1:D:4:LYS:HE3	1:D:26:ILE:HG13	1.99	0.45
1:A:54:PRO:HA	1:A:268:TRP:HE1	1.81	0.44
1:C:268:TRP:CD1	1:C:268:TRP:H	2.36	0.44
1:D:237:ARG:O	1:D:240:VAL:HG22	2.16	0.44
1:A:122:ALA:HB1	1:D:291:PRO:HD3	2.00	0.44
1:B:12:HIS:HB3	4:B:698:HOH:O	2.18	0.44
1:C:56:ARG:CZ	1:C:58:ASP:HB3	2.48	0.44
1:D:242:ASP:OD1	1:D:242:ASP:C	2.61	0.44
1:A:56:ARG:HG3	1:A:56:ARG:O	2.17	0.44
1:D:7:ILE:HD12	1:D:27:THR:HG22	2.00	0.44
1:A:135:GLN:HG3	1:A:137:ARG:CD	2.49	0.43
1:B:290:THR:HB	1:B:293:ILE:HG12	2.00	0.43
1:B:63:GLN:OE1	1:C:298:ARG:HD3	2.18	0.43
1:A:80:ASN:ND2	1:A:269:ALA:H	2.16	0.43
1:D:56:ARG:HH11	1:D:56:ARG:HG3	1.83	0.43
1:D:72:GLY:HA2	1:D:94:THR:OG1	2.19	0.43
1:A:123:ASP:OD2	1:D:120:ARG:CD	2.66	0.42
1:D:56:ARG:HE	1:D:269:ALA:HA	1.84	0.42
1:A:290:THR:HB	1:A:293:ILE:HG12	2.02	0.42
1:A:315:ALA:HB2	1:A:321:PRO:HG3	2.00	0.42
1:C:205:LEU:CD2	1:C:233:VAL:HB	2.49	0.42
1:B:191:GLN:HG3	4:B:529:HOH:O	2.20	0.41
1:B:238:GLY:HA3	1:B:263:PHE:C	2.44	0.41
1:C:6:VAL:HA	1:C:26:ILE:O	2.20	0.41
1:B:103:PRO:HB2	1:B:294:GLY:O	2.20	0.41
1:C:4:LYS:HB3	1:C:46:ALA:HA	2.01	0.41
1:C:284:HIS:HD2	1:C:286:ASN:H	1.69	0.41
1:C:137:ARG:HB3	1:C:139:TYR:CD2	2.56	0.41
1:A:261:ASP:O	1:A:292:HIS:HA	2.20	0.41
1:C:80:ASN:HD22	1:C:269:ALA:H	1.69	0.41
1:C:234:ASN:HD21	1:C:238:GLY:HA2	1.86	0.41
1:C:242:ASP:O	1:C:246:VAL:HG23	2.21	0.41
1:D:300:VAL:O	1:D:303:GLU:N	2.53	0.41
1:A:133:GLY:O	1:A:134:TRP:C	2.64	0.41
1:D:76:LYS:NZ	2:D:402:NAD:O1N	2.45	0.41
1:D:174:HIS:O	2:D:402:NAD:H2A	2.21	0.41
1:B:4:LYS:HA	1:B:24:GLU:HG3	2.03	0.41
1:B:80:ASN:ND2	1:B:269:ALA:H	2.18	0.41
1:C:206:LEU:O	1:C:235:PRO:HD2	2.21	0.41
1:C:320:ARG:HH21	1:C:327:ARG:NE	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:HH12	1:D:316:LEU:HA	1.86	0.41
1:A:143:LEU:HD12	1:A:143:LEU:N	2.36	0.41
1:C:105:ALA:O	1:C:109:ILE:HG12	2.21	0.41
1:C:238:GLY:O	1:C:241:VAL:HG22	2.21	0.41
1:B:8:THR:OG1	1:B:55:ASP:OD2	2.37	0.40
1:D:43:CYS:O	1:D:44:ARG:C	2.64	0.40
1:D:242:ASP:O	1:D:246:VAL:HG23	2.22	0.40
1:A:33:THR:O	1:A:33:THR:HG23	2.21	0.40
1:B:237:ARG:O	1:B:240:VAL:HG22	2.21	0.40
1:D:198:PHE:O	1:D:226:VAL:HA	2.21	0.40
1:D:320:ARG:HA	1:D:321:PRO:HD3	1.95	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)
1:C:134:TRP:NE1	4:B:548:HOH:O[2_545]	1.68	0.52
4:B:719:HOH:O	4:C:588:HOH:O[2_555]	2.17	0.03

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	327/329 (99%)	317 (97%)	10 (3%)	0	100	100
1	B	327/329 (99%)	315 (96%)	11 (3%)	1 (0%)	36	28
1	C	324/329 (98%)	309 (95%)	13 (4%)	2 (1%)	21	12
1	D	327/329 (99%)	307 (94%)	20 (6%)	0	100	100
All	All	1305/1316 (99%)	1248 (96%)	54 (4%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	ALA
1	C	272	ASP
1	B	29	GLN

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	259/259 (100%)	250 (96%)	9 (4%)	32	22
1	B	258/259 (100%)	242 (94%)	16 (6%)	16	6
1	C	259/259 (100%)	242 (93%)	17 (7%)	15	5
1	D	259/259 (100%)	246 (95%)	13 (5%)	22	11
All	All	1035/1036 (100%)	980 (95%)	55 (5%)	20	9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MET
1	A	53	MET
1	A	56	ARG
1	A	95	PHE
1	A	135	GLN
1	A	181	THR
1	A	208	LEU
1	A	217	LEU
1	A	241	VAL
1	B	13	GLU
1	B	31	ASP
1	B	33	THR
1	B	36	ARG
1	B	37	GLU
1	B	56	ARG
1	B	95	PHE
1	B	135	GLN
1	B	177	LYS
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	180	ASP
1	B	205	LEU
1	B	217	LEU
1	B	241	VAL
1	B	273	ARG
1	B	327	ARG
1	C	1	MET
1	C	18	LEU
1	C	23	CYS
1	C	32	SER
1	C	38	GLU
1	C	40	LEU
1	C	79	ASP
1	C	95	PHE
1	C	135	GLN
1	C	137	ARG
1	C	162	ASP
1	C	196	GLU
1	C	208	LEU
1	C	222	LEU
1	C	240	VAL
1	C	270	ARG
1	C	327	ARG
1	D	10	ARG
1	D	13	GLU
1	D	17	GLN
1	D	24	GLU
1	D	31	ASP
1	D	36	ARG
1	D	67	GLU
1	D	83	VAL
1	D	95	PHE
1	D	196	GLU
1	D	268	TRP
1	D	270	ARG
1	D	327	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	165	GLN
1	A	182	GLN
1	A	284	HIS
1	B	28	ASN
1	B	80	ASN
1	B	135	GLN
1	B	145	ASN
1	B	165	GLN
1	B	185	GLN
1	B	276	GLN
1	B	284	HIS
1	C	22	HIS
1	C	80	ASN
1	C	165	GLN
1	C	234	ASN
1	C	284	HIS
1	D	17	GLN
1	D	22	HIS
1	D	28	ASN
1	D	80	ASN
1	D	118	HIS
1	D	145	ASN
1	D	165	GLN
1	D	172	GLN
1	D	284	HIS

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO3	A	402	-	1,3,3	1.02	0	0,3,3	-	-
2	NAD	B	401	-	46,48,48	1.03	4 (8%)	64,73,73	1.62	11 (17%)
3	SO3	C	402	-	1,3,3	0.85	0	0,3,3	-	-
2	NAD	D	402	-	46,48,48	1.04	4 (8%)	64,73,73	1.65	9 (14%)
3	SO3	B	402	-	1,3,3	1.07	0	0,3,3	-	-
3	SO3	D	401	-	1,3,3	0.77	0	0,3,3	-	-
2	NAD	A	401	-	46,48,48	1.01	3 (6%)	64,73,73	1.78	14 (21%)
2	NAD	C	401	-	46,48,48	1.12	3 (6%)	64,73,73	1.59	9 (14%)

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
2	NAD	D	402	-	-	4/30/62/62	0/5/5/5
2	NAD	A	401	-	-	3/30/62/62	0/5/5/5
2	NAD	C	401	-	-	2/30/62/62	0/5/5/5
2	NAD	B	401	-	-	2/30/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAD	PN-O3	3.66	1.63	1.59
2	B	401	NAD	PA-O3	3.15	1.62	1.59
2	D	402	NAD	PN-O3	3.08	1.62	1.59
2	C	401	NAD	PA-O3	2.81	1.62	1.59
2	A	401	NAD	C4A-N9A	-2.80	1.31	1.37
2	C	401	NAD	C8A-N7A	2.65	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	NAD	C8A-N7A	2.53	1.36	1.31
2	B	401	NAD	C5A-N7A	-2.38	1.34	1.39
2	D	402	NAD	C4A-N9A	-2.37	1.32	1.37
2	B	401	NAD	C8A-N7A	2.36	1.36	1.31
2	A	401	NAD	C8A-N7A	2.34	1.36	1.31
2	D	402	NAD	PA-O3	2.26	1.61	1.59
2	B	401	NAD	C4A-N9A	-2.18	1.33	1.37
2	A	401	NAD	PA-O3	2.10	1.61	1.59

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	N3A-C2A-N1A	-6.26	119.10	128.58
2	D	402	NAD	N3A-C2A-N1A	-5.59	120.12	128.58
2	C	401	NAD	C5A-C4A-N3A	-5.20	119.55	126.72
2	B	401	NAD	N3A-C2A-N1A	-4.74	121.41	128.58
2	B	401	NAD	C5A-C4A-N3A	-4.73	120.21	126.72
2	A	401	NAD	C4A-N9A-C8A	4.65	110.62	105.74
2	C	401	NAD	N3A-C2A-N1A	-4.60	121.61	128.58
2	A	401	NAD	N9A-C8A-N7A	-4.47	107.59	113.94
2	D	402	NAD	N9A-C8A-N7A	-4.43	107.65	113.94
2	D	402	NAD	C5A-C4A-N3A	-4.30	120.79	126.72
2	C	401	NAD	N9A-C8A-N7A	-4.01	108.25	113.94
2	D	402	NAD	C4A-N9A-C8A	3.70	109.62	105.74
2	C	401	NAD	N3A-C4A-N9A	3.65	133.38	127.17
2	A	401	NAD	C5A-C4A-N3A	-3.51	121.89	126.72
2	B	401	NAD	N9A-C8A-N7A	-3.49	108.98	113.94
2	D	402	NAD	C2A-N3A-C4A	3.47	120.31	111.83
2	C	401	NAD	C4A-N9A-C8A	3.32	109.22	105.74
2	B	401	NAD	N3A-C4A-N9A	3.23	132.66	127.17
2	A	401	NAD	C2A-N3A-C4A	3.22	119.69	111.83
2	C	401	NAD	C2A-N3A-C4A	3.20	119.66	111.83
2	A	401	NAD	C2A-N1A-C6A	3.03	123.70	118.73
2	B	401	NAD	C3N-C7N-N7N	3.00	121.44	117.74
2	B	401	NAD	O4B-C1B-N9A	2.91	113.67	108.09
2	A	401	NAD	C4A-N9A-C1B	-2.90	119.84	126.63
2	B	401	NAD	C2A-N3A-C4A	2.88	118.88	111.83
2	C	401	NAD	C5A-N7A-C8A	2.77	107.80	103.45
2	B	401	NAD	C4A-N9A-C8A	2.76	108.63	105.74
2	D	402	NAD	N3A-C4A-N9A	2.74	131.83	127.17
2	D	402	NAD	C5A-N7A-C8A	2.71	107.72	103.45
2	C	401	NAD	O2D-C2D-C3D	-2.68	103.24	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	N3A-C4A-N9A	2.61	131.61	127.17
2	D	402	NAD	C4A-C5A-N7A	-2.59	107.62	110.58
2	C	401	NAD	C4A-C5A-N7A	-2.55	107.66	110.58
2	A	401	NAD	C6N-N1N-C2N	-2.53	119.72	121.88
2	A	401	NAD	C5A-N7A-C8A	2.48	107.34	103.45
2	B	401	NAD	C5A-N7A-C8A	2.30	107.06	103.45
2	A	401	NAD	C4A-C5A-N7A	-2.29	107.96	110.58
2	B	401	NAD	O2A-PA-O1A	2.24	122.85	112.44
2	D	402	NAD	C4A-N9A-C1B	-2.21	121.46	126.63
2	A	401	NAD	C4B-O4B-C1B	-2.16	104.69	109.47
2	A	401	NAD	C5N-C4N-C3N	-2.16	118.24	120.36
2	B	401	NAD	C4A-C5A-N7A	-2.11	108.17	110.58
2	A	401	NAD	C2N-C3N-C4N	2.06	120.65	118.26

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	D	402	NAD	O4D-C1D-N1N-C2N
2	D	402	NAD	O4D-C1D-N1N-C6N
2	D	402	NAD	C2D-C1D-N1N-C2N
2	D	402	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	C2B-C1B-N9A-C8A

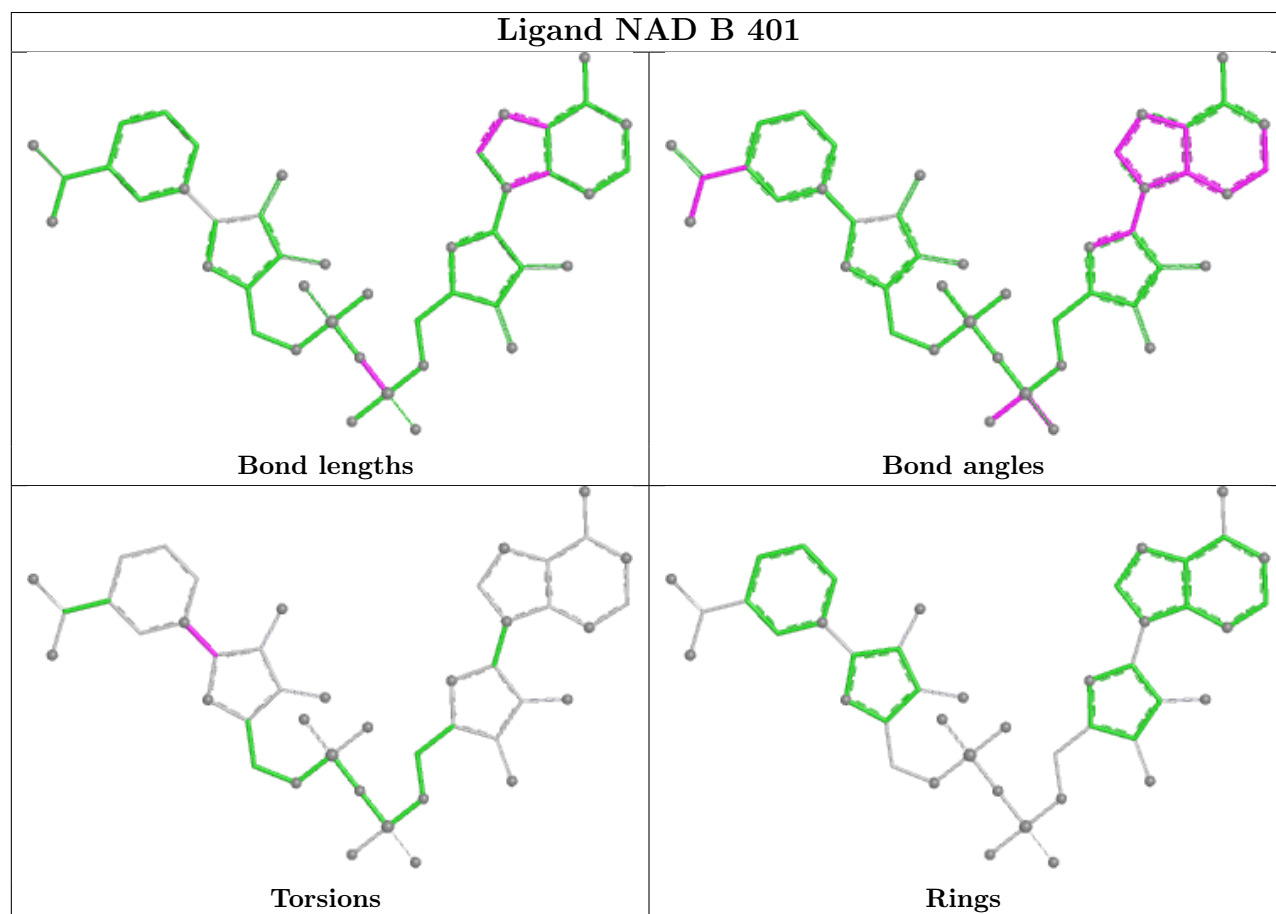
There are no ring outliers.

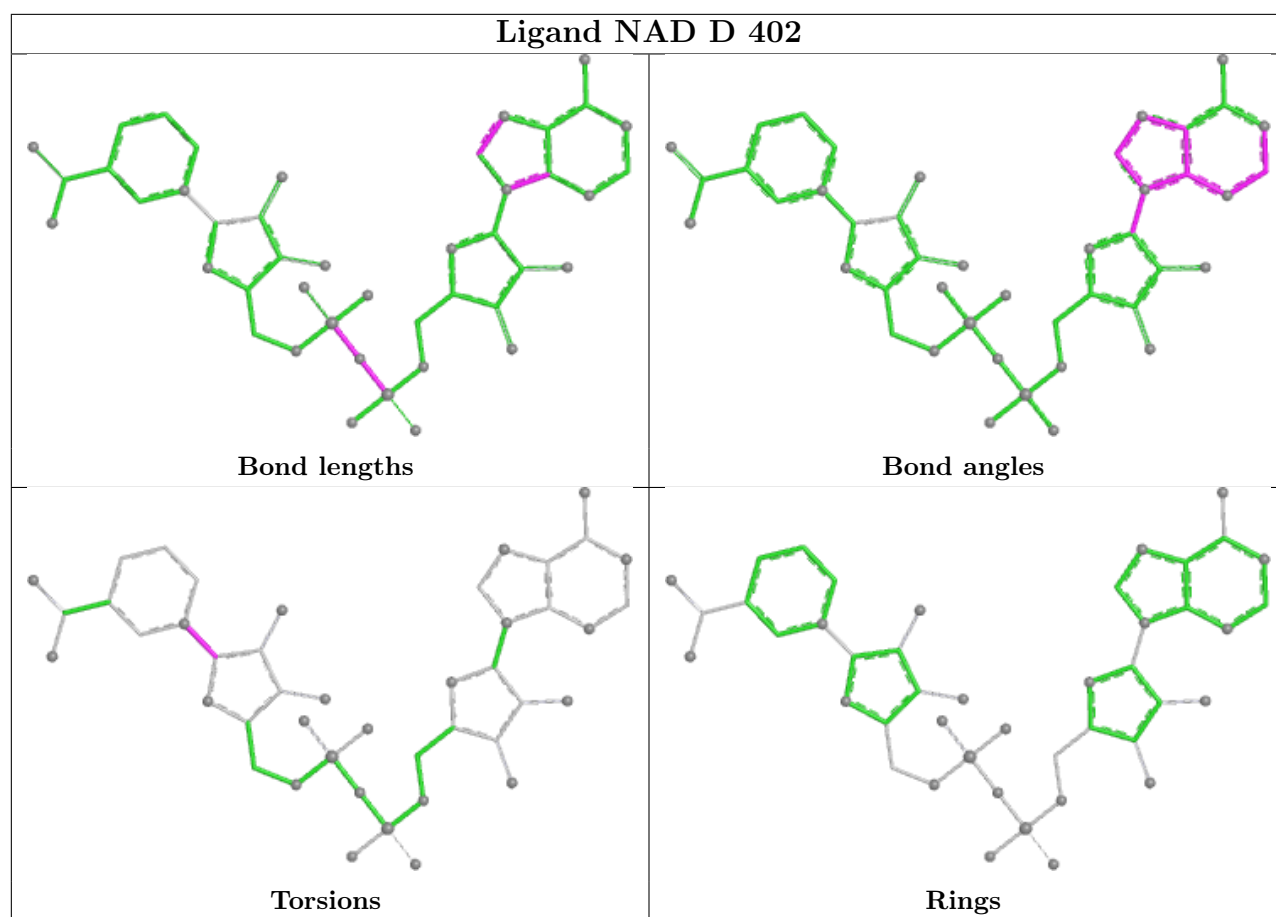
3 monomers are involved in 4 short contacts:

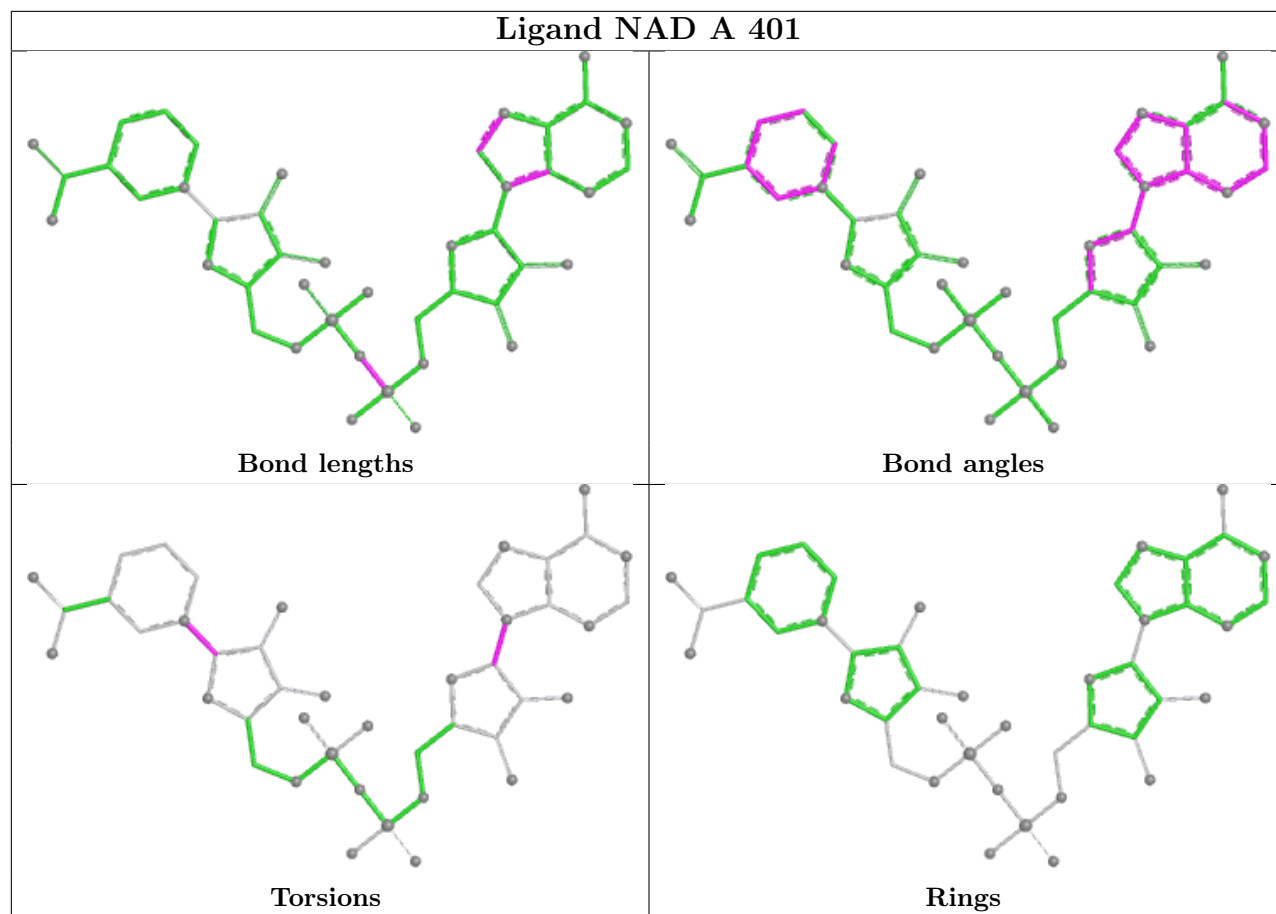
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	SO3	1	0
2	D	402	NAD	2	0
3	B	402	SO3	1	0

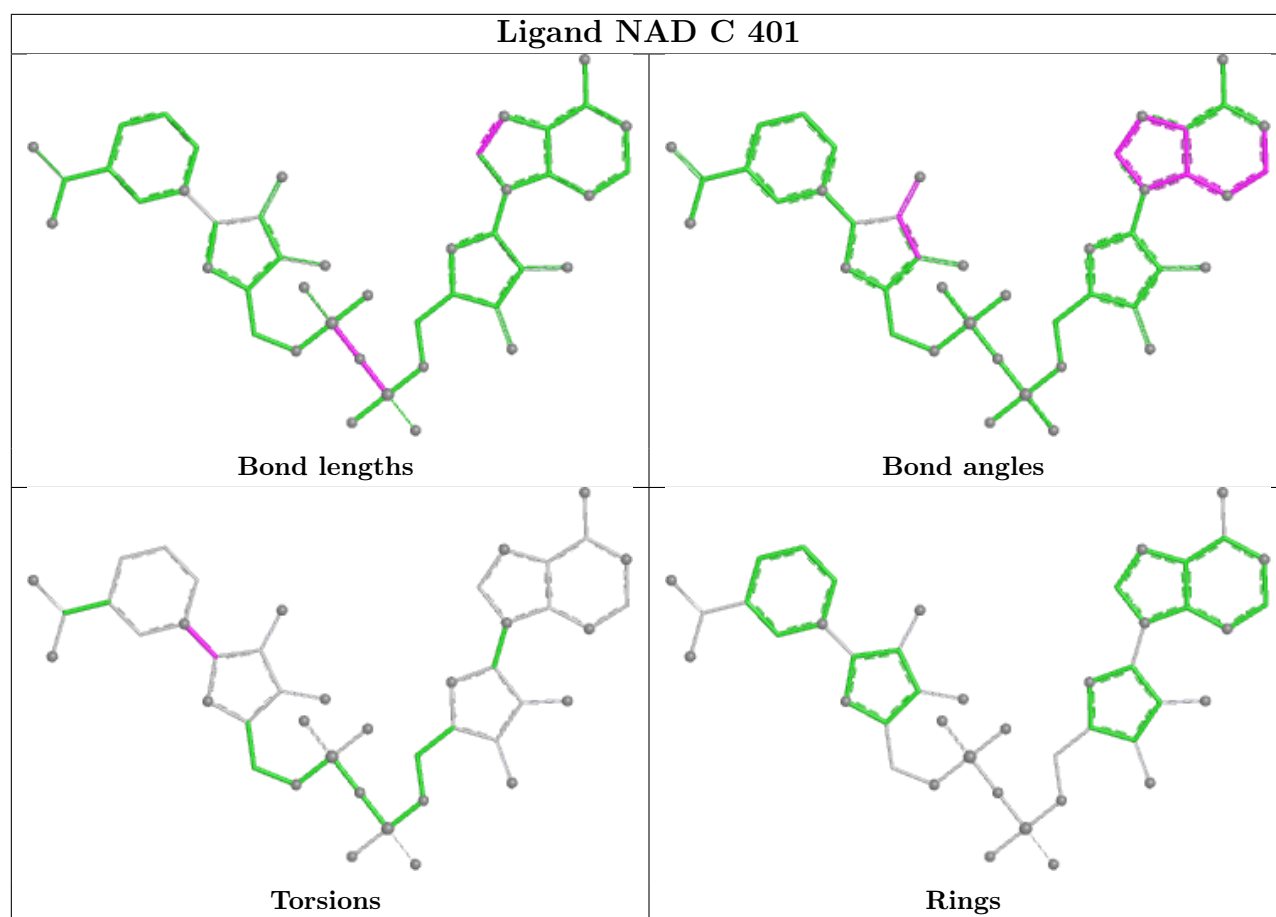
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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	A	329/329 (100%)	0.41	11 (3%)	49	55	16, 27, 50, 67	0
1	B	329/329 (100%)	0.35	12 (3%)	46	53	15, 27, 53, 81	0
1	C	328/329 (99%)	1.18	59 (17%)	3	3	19, 46, 75, 89	0
1	D	329/329 (100%)	1.34	64 (19%)	3	3	28, 51, 74, 87	0
All	All	1315/1316 (99%)	0.82	146 (11%)	10	12	15, 37, 70, 89	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	TRP	5.3
1	D	329	PRO	4.8
1	D	271	ALA	4.6
1	D	268	TRP	4.4
1	C	33	THR	4.4
1	C	43	CYS	4.3
1	C	2	LEU	4.3
1	C	329	PRO	4.3
1	C	139	TYR	4.2
1	B	134	TRP	4.1
1	C	1	MET	3.9
1	B	132	ARG	3.8
1	C	20	ALA	3.8
1	C	23	CYS	3.8
1	D	269	ALA	3.8
1	C	39	ILE	3.8
1	B	1	MET	3.7
1	C	271	ALA	3.7
1	C	315	ALA	3.6
1	A	1	MET	3.6
1	D	316	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	312	ILE	3.5
1	A	329	PRO	3.4
1	C	27	THR	3.4
1	C	328	LEU	3.4
1	C	316	LEU	3.3
1	D	328	LEU	3.3
1	D	92	TRP	3.3
1	C	5	LEU	3.2
1	C	134	TRP	3.2
1	C	26	ILE	3.2
1	C	68	LEU	3.2
1	B	135	GLN	3.2
1	D	48	ALA	3.1
1	C	34	LEU	3.1
1	A	31	ASP	3.0
1	D	322	ILE	3.0
1	C	25	LEU	3.0
1	A	33	THR	3.0
1	C	268	TRP	3.0
1	C	32	SER	2.9
1	D	1	MET	2.9
1	B	33	THR	2.8
1	B	137	ARG	2.8
1	B	298	ARG	2.8
1	C	18	LEU	2.8
1	D	2	LEU	2.8
1	D	44	ARG	2.8
1	C	30	THR	2.8
1	C	181	THR	2.8
1	B	136	PRO	2.8
1	C	137	ARG	2.8
1	C	46	ALA	2.7
1	C	228	PRO	2.7
1	C	269	ALA	2.7
1	C	40	LEU	2.7
1	C	277	ILE	2.7
1	D	39	ILE	2.7
1	D	218	VAL	2.7
1	B	131	PHE	2.6
1	C	3	PRO	2.6
1	D	208	LEU	2.6
1	C	22	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	313	LEU	2.6
1	D	270	ARG	2.6
1	D	134	TRP	2.6
1	D	176	ALA	2.6
1	A	36	ARG	2.5
1	C	45	ASP	2.5
1	C	222	LEU	2.5
1	D	5	LEU	2.5
1	D	15	ILE	2.5
1	C	226	VAL	2.5
1	B	30	THR	2.5
1	D	69	ARG	2.5
1	C	317	ALA	2.5
1	D	88	ALA	2.5
1	D	317	ALA	2.5
1	C	35	THR	2.5
1	A	298	ARG	2.5
1	D	315	ALA	2.5
1	C	15	ILE	2.4
1	C	178	ALA	2.4
1	D	66	PRO	2.4
1	A	135	GLN	2.4
1	D	61	PHE	2.4
1	D	31	ASP	2.4
1	D	212	ALA	2.4
1	D	34	LEU	2.4
1	A	26	ILE	2.4
1	D	226	VAL	2.4
1	C	44	ARG	2.3
1	C	281	LEU	2.3
1	D	64	ALA	2.3
1	D	321	PRO	2.3
1	D	318	GLY	2.3
1	C	177	LYS	2.3
1	D	179	LEU	2.3
1	C	66	PRO	2.2
1	D	312	ILE	2.2
1	C	47	GLN	2.2
1	D	90	GLY	2.2
1	D	60	ASP	2.2
1	B	2	LEU	2.2
1	D	62	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	ASP	2.2
1	D	77	GLY	2.2
1	C	78	PHE	2.2
1	D	26	ILE	2.2
1	C	327	ARG	2.2
1	D	36	ARG	2.2
1	D	325	VAL	2.2
1	D	84	ASP	2.2
1	C	136	PRO	2.2
1	C	321	PRO	2.2
1	C	48	ALA	2.2
1	D	27	THR	2.1
1	D	43	CYS	2.1
1	C	42	ARG	2.1
1	D	217	LEU	2.1
1	C	6	VAL	2.1
1	C	67	GLU	2.1
1	D	93	LEU	2.1
1	D	223	LEU	2.1
1	D	59	ALA	2.1
1	D	7	ILE	2.1
1	B	133	GLY	2.1
1	D	57	VAL	2.1
1	D	136	PRO	2.1
1	A	2	LEU	2.1
1	A	328	LEU	2.1
1	D	298	ARG	2.1
1	D	327	ARG	2.1
1	D	35	THR	2.0
1	C	274	PRO	2.0
1	D	70	VAL	2.0
1	D	209	PRO	2.0
1	C	19	LEU	2.0
1	D	68	LEU	2.0
1	C	244	ALA	2.0
1	D	46	ALA	2.0
1	D	178	ALA	2.0
1	D	199	ALA	2.0
1	D	24	GLU	2.0
1	D	22	HIS	2.0
1	D	81	PHE	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](#)

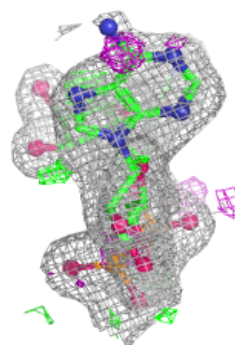
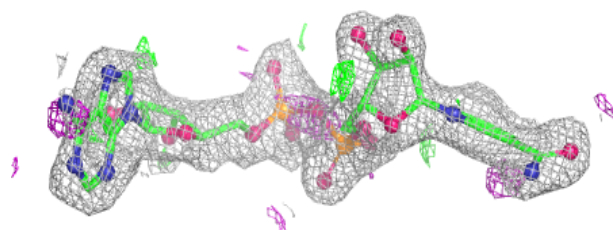
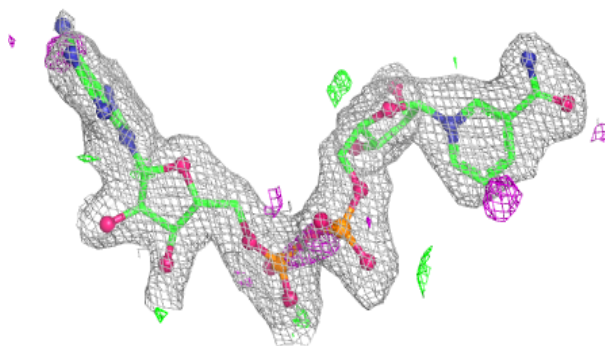
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAD	D	402	44/44	0.89	0.09	28,32,33,35	0
3	SO3	B	402	4/4	0.91	0.17	25,29,32,38	0
3	SO3	C	402	4/4	0.94	0.15	30,32,33,34	0
3	SO3	D	401	4/4	0.94	0.13	33,33,34,35	0
2	NAD	C	401	44/44	0.95	0.08	23,27,32,33	0
3	SO3	A	402	4/4	0.96	0.11	26,26,29,33	0
2	NAD	A	401	44/44	0.96	0.07	19,22,25,26	0
2	NAD	B	401	44/44	0.97	0.06	18,21,23,23	0

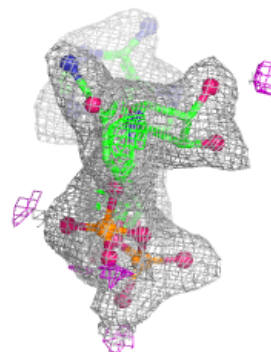
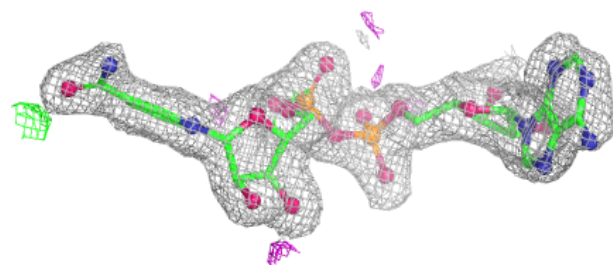
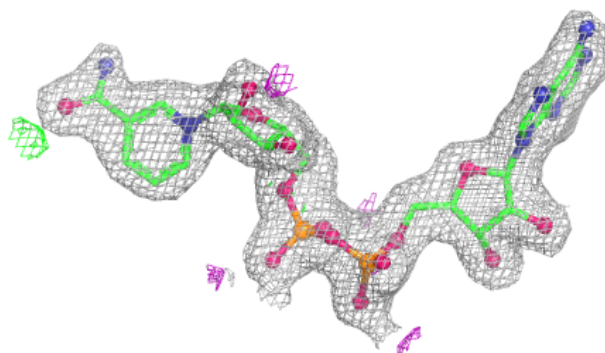
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 402:

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

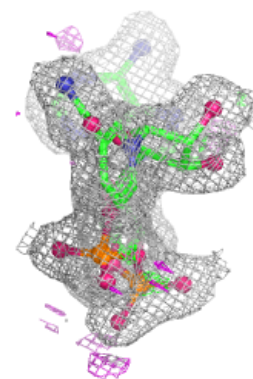
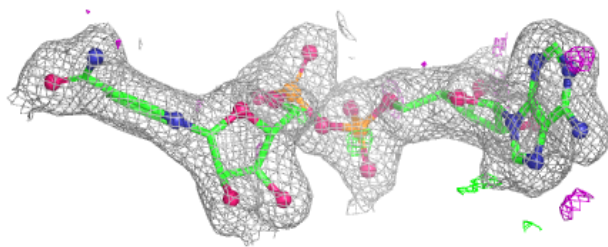
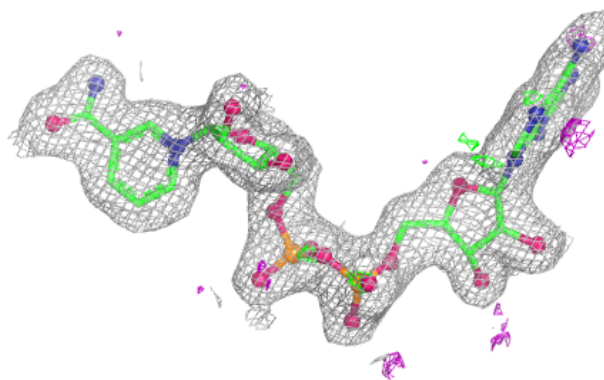
**Electron density around NAD C 401:**

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

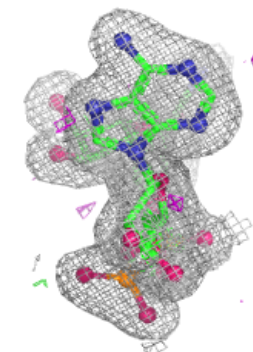
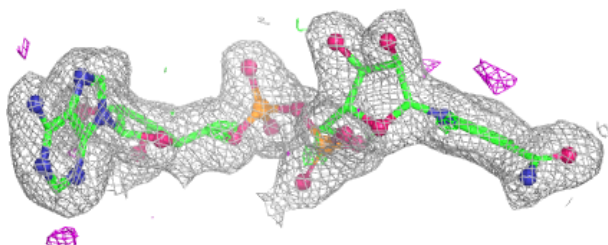
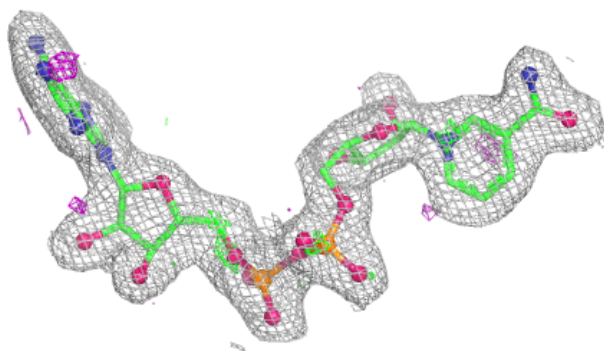


Electron density around NAD A 401:

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

**Electron density around NAD B 401:**

$2mF_o-DF_c$ (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.