



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 09:29 PM EDT

PDB ID : 1OWB
Title : Three Dimensional Structure Analysis Of The Variant R109L NADH Complex of Type II Citrate Synthase From E. Coli
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Deposited on : 2003-03-28
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

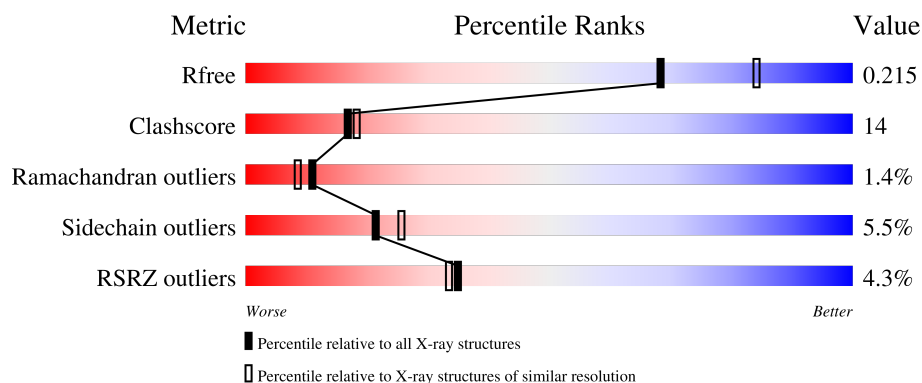
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	427	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	427	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2002	-	X	-	-
2	SO4	A	2005	-	X	-	-
2	SO4	B	2001	-	X	-	-
2	SO4	B	2003	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7335 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.

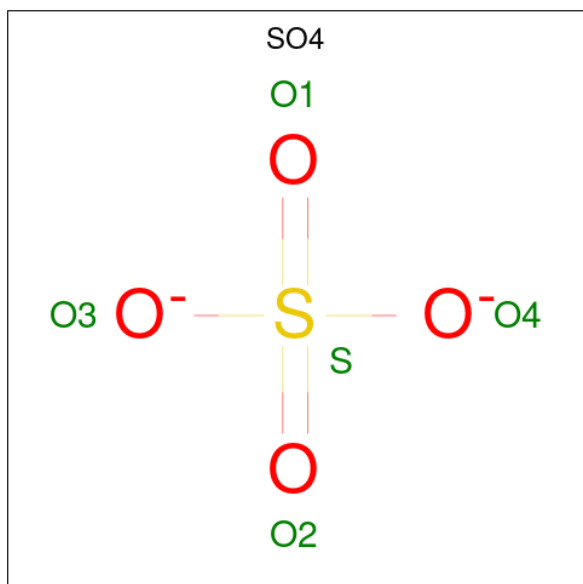
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3363	2135	576	627	25			
1	B	426	Total	C	N	O	S	0	0	0
			3363	2135	576	627	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	LEU	ARG	engineered mutation	UNP P0ABH7
B	1109	LEU	ARG	engineered mutation	UNP P0ABH7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



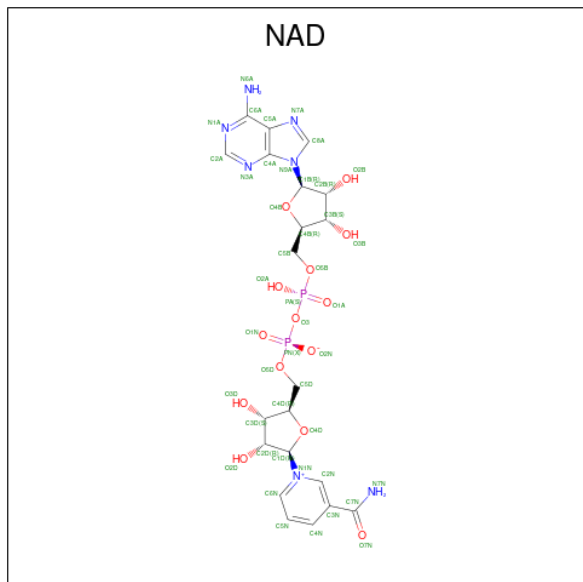
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O S	0	0
			5 4 1			

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

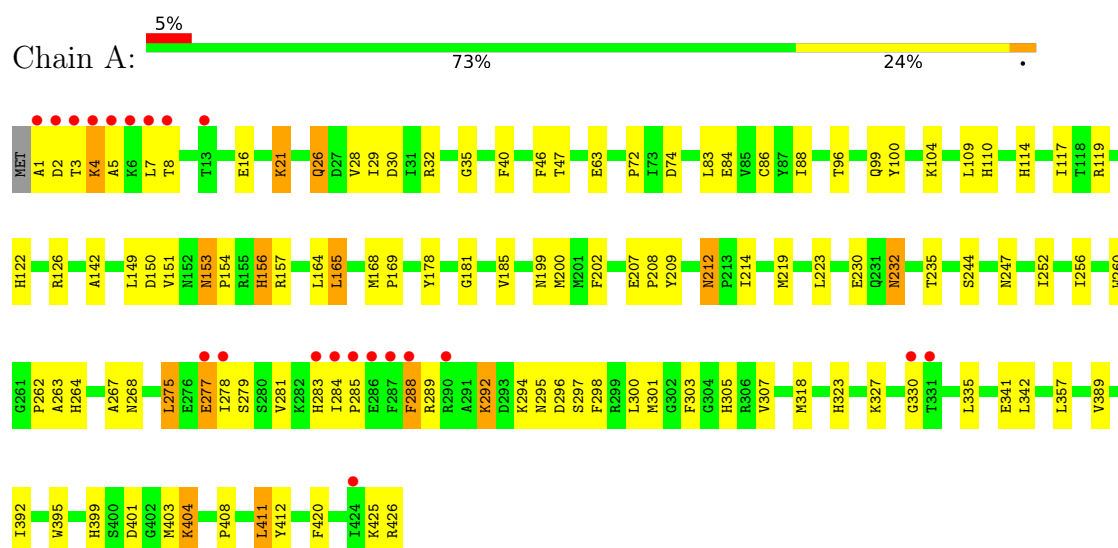
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	263	Total O 263 263	0	0
4	B	228	Total O 228 228	0	0

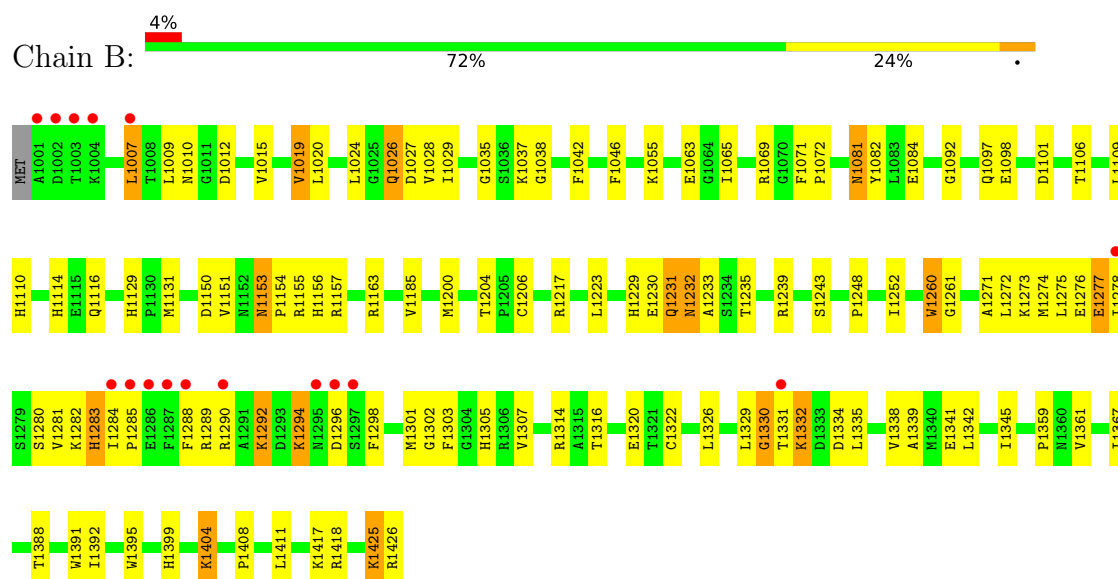
3 Residue-property plots [i](#)

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: Citrate synthase



• Molecule 1: Citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	165.00Å 165.00Å 157.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.20 14.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 90.3 (14.95-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.80 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.162 , 0.219 0.163 , 0.215	Depositor DCC
R_{free} test set	3890 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7335	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/3441	0.62	1/4651 (0.0%)
1	B	0.40	0/3441	0.63	1/4651 (0.0%)
All	All	0.39	0/6882	0.63	2/9302 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1294	LYS	N-CA-C	5.28	125.25	111.00
1	A	202	PHE	N-CA-C	5.03	124.59	111.00

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	3363	0	3311	99	0
1	B	3363	0	3308	108	0
2	A	20	0	0	1	0
2	B	10	0	0	1	0
3	A	44	0	26	1	0
3	B	44	0	26	5	0
4	A	263	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	228	0	0	6	0
All	All	7335	0	6671	191	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 14.

All (191) 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:A:425:LYS:H	1:B:1097:GLN:HE22	1.11	0.93
3:B:3001:NAD:O1A	3:B:3001:NAD:H3B	1.72	0.89
1:B:1114:HIS:HD2	1:B:1116:GLN:H	1.18	0.87
1:A:305:HIS:HD2	1:A:307:VAL:H	1.19	0.87
1:A:278:ILE:HG21	1:A:283:HIS:HB2	1.59	0.85
1:A:244:SER:HB3	1:B:1233:ALA:HB1	1.60	0.82
1:B:1204:THR:HG22	1:B:1206:CYS:H	1.45	0.81
1:A:1:ALA:HA	1:A:4:LYS:HD2	1.63	0.81
1:B:1129:HIS:HD2	1:B:1131:MET:H	1.30	0.80
1:B:1305:HIS:HD2	1:B:1307:VAL:H	1.28	0.80
1:B:1280:SER:HB3	1:B:1283:HIS:HB2	1.64	0.78
1:B:1335:LEU:H	1:B:1335:LEU:HD23	1.51	0.74
1:A:323:HIS:CE1	1:A:327:LYS:HE3	2.22	0.74
1:B:1285:PRO:HB2	1:B:1341:GLU:HG3	1.68	0.74
1:A:21:LYS:H	1:A:21:LYS:HE2	1.52	0.74
1:A:212:ASN:HD22	1:A:214:ILE:H	1.36	0.73
1:B:1425:LYS:HA	1:B:1425:LYS:HE2	1.70	0.72
1:B:1285:PRO:HB3	4:B:323:HOH:O	1.89	0.71
1:B:1154:PRO:HG3	1:B:1157:ARG:HH11	1.55	0.71
3:B:3001:NAD:H6N	3:B:3001:NAD:H52N	1.72	0.71
1:A:35:GLY:HA2	1:A:40:PHE:CE2	2.26	0.70
1:A:411:LEU:HG	1:B:1028:VAL:HG22	1.73	0.70
1:A:150:ASP:H	1:A:156:HIS:HD2	1.40	0.69
1:A:404:LYS:HD3	1:A:404:LYS:H	1.57	0.68
1:B:1114:HIS:CD2	1:B:1116:GLN:H	2.07	0.68
1:A:425:LYS:N	1:B:1097:GLN:HE22	1.90	0.68
1:B:1281:VAL:HG23	1:B:1282:LYS:HD2	1.76	0.68
1:A:212:ASN:ND2	1:A:214:ILE:H	1.92	0.68
1:B:1155:ARG:HH11	1:B:1156:HIS:HE1	1.42	0.68
1:B:1151:VAL:HG12	1:B:1395:TRP:HZ2	1.60	0.66
1:A:425:LYS:H	1:B:1097:GLN:NE2	1.91	0.66
1:B:1290:ARG:NH1	1:B:1342:LEU:HD23	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:CE1	1:B:1426:ARG:HB3	2.32	0.65
1:A:164:LEU:O	1:A:168:MET:HG2	1.97	0.65
1:B:1151:VAL:HB	1:B:1399:HIS:CE1	2.32	0.64
1:A:277:GLU:HG3	1:A:278:ILE:H	1.62	0.64
1:A:7:LEU:HB2	1:B:1010:ASN:O	1.99	0.63
1:B:1274:MET:O	1:B:1278:ILE:HB	2.00	0.62
1:B:1248:PRO:HG3	1:B:1395:TRP:CH2	2.35	0.62
1:A:30:ASP:OD1	1:A:32:ARG:HD3	2.00	0.61
1:A:21:LYS:H	1:A:21:LYS:CE	2.13	0.61
1:A:119:ARG:HA	1:A:122:HIS:HD2	1.65	0.61
1:B:1339:ALA:HB1	1:B:1367:ILE:HD13	1.84	0.60
1:A:404:LYS:H	1:A:404:LYS:CD	2.15	0.58
1:A:126:ARG:NH1	1:A:181:GLY:HA2	2.18	0.58
1:A:96:THR:H	1:A:99:GLN:HE21	1.51	0.58
1:A:165:LEU:HD13	1:A:392:ILE:HD12	1.86	0.57
1:B:1284:ILE:HB	1:B:1285:PRO:HD3	1.86	0.57
1:A:335:LEU:HD23	1:A:335:LEU:H	1.69	0.57
1:A:26:GLN:HG2	1:B:1038:GLY:O	2.05	0.56
1:A:86:CYS:HA	1:A:389:VAL:HG21	1.86	0.56
1:A:151:VAL:HB	1:A:399:HIS:NE2	2.21	0.56
1:A:297:SER:O	1:A:301:MET:HG3	2.05	0.56
1:B:1283:HIS:O	1:B:1288:PHE:HB3	2.06	0.56
1:A:263:ALA:HA	1:A:300:LEU:HD21	1.88	0.55
1:B:1243:SER:HB2	1:B:1404:LYS:O	2.06	0.55
1:B:1150:ASP:H	1:B:1156:HIS:HD2	1.55	0.55
1:B:1278:ILE:HG22	1:B:1284:ILE:HG13	1.89	0.55
1:B:1284:ILE:HB	1:B:1285:PRO:CD	2.36	0.55
1:A:252:ILE:O	1:A:256:ILE:HG13	2.08	0.54
1:A:284:ILE:HG23	1:A:289:ARG:HD3	1.89	0.54
1:B:1129:HIS:CD2	1:B:1131:MET:H	2.19	0.54
1:A:219:MET:O	1:A:223:LEU:HG	2.08	0.54
1:A:212:ASN:HD22	1:A:214:ILE:N	2.04	0.54
1:B:1278:ILE:CG2	1:B:1283:HIS:HB3	2.38	0.54
1:A:46:PHE:O	1:B:1408:PRO:HA	2.08	0.53
1:A:232:ASN:ND2	1:A:235:THR:H	2.06	0.53
1:B:1278:ILE:HG22	1:B:1283:HIS:HB3	1.90	0.53
1:A:426:ARG:HD3	1:B:1101:ASP:OD1	2.09	0.53
1:B:1151:VAL:HG11	4:B:6:HOH:O	2.08	0.53
1:B:1322:CYS:O	1:B:1326:LEU:HD13	2.08	0.53
1:B:1232:ASN:ND2	1:B:1235:THR:H	2.07	0.53
1:A:142:ALA:HB3	4:B:49:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:LEU:HD21	1:B:1029:ILE:HG23	1.90	0.53
1:A:268:ASN:HD22	1:A:300:LEU:HD22	1.73	0.53
1:A:83:LEU:CD2	1:A:104:LYS:HD2	2.38	0.52
1:A:275:LEU:HA	1:A:289:ARG:HD2	1.90	0.52
1:B:1082:TYR:CD1	1:B:1223:LEU:HB3	2.44	0.52
1:B:1335:LEU:H	1:B:1335:LEU:CD2	2.21	0.52
1:A:294:LYS:N	1:A:294:LYS:HD2	2.25	0.52
1:B:1316:THR:O	1:B:1320:GLU:HG3	2.09	0.52
1:A:284:ILE:N	1:A:285:PRO:HD2	2.25	0.51
1:B:1271:ALA:HA	1:B:1274:MET:HE3	1.91	0.51
1:B:1012:ASP:HA	4:B:461:HOH:O	2.10	0.51
1:A:185:VAL:HB	1:A:200:MET:HA	1.93	0.51
1:B:1131:MET:HG2	1:B:1260:TRP:CD2	2.46	0.51
1:A:8:THR:HG22	1:A:16:GLU:HA	1.93	0.50
1:A:150:ASP:HB3	1:A:156:HIS:CD2	2.46	0.50
1:A:283:HIS:C	1:A:288:PHE:HB3	2.32	0.50
1:A:149:LEU:HD22	1:A:247:ASN:HB2	1.94	0.50
1:A:169:PRO:HG2	4:A:3095:HOH:O	2.12	0.50
1:A:412:TYR:CD1	1:B:1024:LEU:HB2	2.47	0.50
1:B:1404:LYS:O	1:B:1404:LYS:HD3	2.12	0.50
1:A:110:HIS:CE1	3:A:3000:NAD:H51N	2.45	0.50
1:A:281:VAL:HA	1:A:285:PRO:HG3	1.94	0.50
1:A:420:PHE:HB2	1:B:1071:PHE:CD2	2.47	0.49
1:B:1007:LEU:HD11	1:B:1029:ILE:CG2	2.42	0.49
1:A:126:ARG:HD2	1:A:178:TYR:CZ	2.47	0.49
1:B:1272:LEU:HD23	1:B:1301:MET:HG2	1.94	0.49
1:B:1284:ILE:HG23	1:B:1289:ARG:HD3	1.93	0.49
3:B:3001:NAD:H52N	3:B:3001:NAD:C6N	2.42	0.49
1:B:1151:VAL:HB	1:B:1399:HIS:NE2	2.27	0.48
1:B:1388:THR:O	1:B:1392:ILE:HG13	2.14	0.48
1:B:1106:THR:O	1:B:1110:HIS:HD2	1.95	0.48
1:B:1305:HIS:HE1	2:B:2003:SO4:O1	1.97	0.48
1:A:100:TYR:HE1	1:B:1426:ARG:HB3	1.76	0.47
1:A:100:TYR:CD1	1:B:1426:ARG:HB3	2.49	0.47
1:A:232:ASN:C	1:A:232:ASN:HD22	2.18	0.47
1:B:1009:LEU:HB3	1:B:1015:VAL:HB	1.96	0.47
1:A:292:LYS:HB2	1:A:292:LYS:NZ	2.30	0.47
1:B:1285:PRO:CB	1:B:1341:GLU:HG3	2.42	0.47
1:A:283:HIS:O	1:A:288:PHE:HB3	2.14	0.47
1:A:212:ASN:HD21	1:A:214:ILE:HB	1.81	0.46
1:B:1081:ASN:ND2	1:B:1084:GLU:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HD3	1:B:1418:ARG:O	2.16	0.46
1:B:1330:GLY:C	1:B:1332:LYS:H	2.18	0.46
1:B:1425:LYS:HA	1:B:1425:LYS:CE	2.42	0.46
1:A:285:PRO:HB2	1:A:341:GLU:HG2	1.98	0.46
1:B:1329:LEU:O	1:B:1331:THR:N	2.49	0.46
1:A:212:ASN:ND2	1:A:214:ILE:HB	2.30	0.46
1:B:1302:GLY:O	1:B:1359:PRO:HA	2.16	0.45
1:A:32:ARG:HD2	1:B:1042:PHE:CD1	2.52	0.45
1:A:411:LEU:HG	1:B:1028:VAL:CG2	2.45	0.45
1:B:1278:ILE:O	1:B:1284:ILE:HD11	2.16	0.45
1:A:284:ILE:CG2	1:A:342:LEU:HD21	2.46	0.45
1:A:408:PRO:HA	1:B:1046:PHE:O	2.17	0.45
1:B:1278:ILE:HG13	1:B:1288:PHE:HE1	1.82	0.45
1:B:1285:PRO:HB2	1:B:1341:GLU:CG	2.44	0.45
1:A:83:LEU:HD22	1:A:104:LYS:HD2	1.98	0.45
1:B:1026:GLN:HE21	1:B:1027:ASP:H	1.65	0.45
1:A:29:ILE:HD12	1:A:29:ILE:N	2.33	0.44
1:A:267:ALA:HB1	1:A:295:ASN:HB3	1.99	0.44
1:B:1155:ARG:NH1	1:B:1156:HIS:HE1	2.12	0.44
1:B:1163:ARG:NE	3:B:3001:NAD:O2N	2.50	0.44
1:A:399:HIS:HD2	4:A:3184:HOH:O	2.00	0.44
1:B:1035:GLY:C	1:B:1037:LYS:H	2.19	0.44
1:A:21:LYS:H	1:A:21:LYS:CD	2.31	0.44
1:A:212:ASN:HD22	1:A:212:ASN:C	2.20	0.44
1:A:262:PRO:O	1:A:268:ASN:HB2	2.17	0.44
1:A:114:HIS:HB3	1:A:117:ILE:HG13	2.00	0.43
1:A:335:LEU:H	1:A:335:LEU:CD2	2.31	0.43
1:B:1252:ILE:HD12	1:B:1388:THR:HG23	2.01	0.43
1:B:1345:ILE:HD12	4:B:323:HOH:O	2.18	0.43
1:B:1388:THR:HA	1:B:1391:TRP:CE3	2.52	0.43
1:A:207:GLU:HB2	1:A:208:PRO:HD2	2.00	0.43
1:A:395:TRP:NE1	1:A:399:HIS:HE1	2.16	0.43
1:B:1063:GLU:HB3	1:B:1065:ILE:HG12	2.01	0.43
1:A:84:GLU:O	1:A:88:ILE:HG13	2.19	0.43
1:A:298:PHE:HB3	1:A:303:PHE:O	2.18	0.43
1:B:1273:LYS:O	1:B:1277:GLU:HG2	2.19	0.43
1:B:1007:LEU:HD11	1:B:1029:ILE:HG21	2.00	0.43
1:A:296:ASP:CG	1:A:297:SER:H	2.22	0.43
1:A:28:VAL:HG22	1:B:1411:LEU:HD13	2.01	0.42
1:A:153:ASN:HA	1:A:154:PRO:HD2	1.85	0.42
1:A:412:TYR:CE1	1:B:1024:LEU:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HE2	1:A:21:LYS:N	2.25	0.42
3:B:3001:NAD:H3B	3:B:3001:NAD:PA	2.57	0.42
1:A:284:ILE:HG12	1:A:289:ARG:HG3	2.01	0.42
1:B:1298:PHE:HB3	1:B:1303:PHE:HB2	2.01	0.42
1:B:1417:LYS:HD3	1:B:1417:LYS:C	2.39	0.42
1:B:1026:GLN:HE21	1:B:1026:GLN:CA	2.32	0.42
1:B:1231:GLN:HE22	1:B:1239:ARG:HD2	1.85	0.42
1:B:1026:GLN:HE21	1:B:1026:GLN:HA	1.85	0.42
1:B:1274:MET:HB2	1:B:1289:ARG:HG3	2.02	0.42
1:A:47:THR:HG22	1:A:47:THR:O	2.20	0.42
1:A:153:ASN:C	1:A:153:ASN:HD22	2.23	0.42
1:B:1153:ASN:HD22	1:B:1154:PRO:N	2.17	0.42
1:A:1:ALA:HB1	1:A:4:LYS:HB2	2.01	0.42
1:A:3:THR:C	1:A:5:ALA:H	2.22	0.41
1:A:157:ARG:HH11	1:A:399:HIS:HB3	1.85	0.41
1:B:1157:ARG:HG2	1:B:1395:TRP:CH2	2.55	0.41
1:B:1305:HIS:CD2	1:B:1307:VAL:H	2.20	0.41
1:B:1007:LEU:HD13	1:B:1029:ILE:HD13	2.02	0.41
1:A:264:HIS:HB2	4:A:3099:HOH:O	2.20	0.41
1:B:1154:PRO:HG3	1:B:1157:ARG:NH1	2.29	0.41
1:B:1292:LYS:HB2	1:B:1292:LYS:NZ	2.35	0.41
1:B:1290:ARG:HH11	1:B:1342:LEU:HA	1.84	0.41
1:B:1069:ARG:CD	1:B:1092:GLY:HA2	2.51	0.41
1:B:1153:ASN:HD22	1:B:1153:ASN:C	2.24	0.41
1:A:399:HIS:CD2	1:A:403:MET:SD	3.14	0.41
1:B:1314:ARG:HB2	1:B:1361:VAL:HB	2.03	0.41
1:B:1276:GLU:C	1:B:1278:ILE:H	2.24	0.41
1:A:199:ASN:HD22	1:A:209:TYR:HD1	1.69	0.40
1:A:335:LEU:HD23	1:A:335:LEU:N	2.36	0.40
1:B:1071:PHE:HA	1:B:1072:PRO:HD3	1.96	0.40
1:A:232:ASN:HD22	1:A:235:THR:H	1.69	0.40
1:A:268:ASN:HB3	1:A:300:LEU:CD2	2.50	0.40
1:B:1342:LEU:HA	4:B:323:HOH:O	2.19	0.40
2:A:2002:SO4:S	1:B:1055:LYS:HD3	2.62	0.40
1:B:1019:VAL:HA	1:B:1028:VAL:O	2.21	0.40
1:B:1185:VAL:HB	1:B:1200:MET:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/427 (99%)	392 (92%)	26 (6%)	6 (1%)	11	8
1	B	424/427 (99%)	380 (90%)	38 (9%)	6 (1%)	11	8
All	All	848/854 (99%)	772 (91%)	64 (8%)	12 (1%)	11	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	B	1330	GLY
1	A	277	GLU
1	A	330	GLY
1	A	401	ASP
1	B	1231	GLN
1	B	1261	GLY
1	B	1277	GLU
1	B	1334	ASP
1	A	279	SER
1	A	4	LYS
1	B	1338	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/362 (100%)	342 (95%)	19 (5%)	22	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	361/362 (100%)	340 (94%)	21 (6%)	20	23
All	All	722/724 (100%)	682 (94%)	40 (6%)	21	26

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	26	GLN
1	A	63	GLU
1	A	74	ASP
1	A	109	LEU
1	A	153	ASN
1	A	156	HIS
1	A	165	LEU
1	A	212	ASN
1	A	230	GLU
1	A	232	ASN
1	A	260	TRP
1	A	275	LEU
1	A	288	PHE
1	A	292	LYS
1	A	318	MET
1	A	357	LEU
1	A	404	LYS
1	A	411	LEU
1	B	1007	LEU
1	B	1019	VAL
1	B	1020	LEU
1	B	1026	GLN
1	B	1081	ASN
1	B	1098	GLU
1	B	1109	LEU
1	B	1153	ASN
1	B	1217	ARG
1	B	1229	HIS
1	B	1230	GLU
1	B	1232	ASN
1	B	1260	TRP
1	B	1275	LEU
1	B	1283	HIS
1	B	1292	LYS
1	B	1294	LYS

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Mol	Chain	Res	Type
1	B	1296	ASP
1	B	1332	LYS
1	B	1404	LYS
1	B	1425	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	99	GLN
1	A	122	HIS
1	A	153	ASN
1	A	156	HIS
1	A	182	GLN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	268	ASN
1	A	283	HIS
1	A	305	HIS
1	A	323	HIS
1	A	399	HIS
1	B	1026	GLN
1	B	1081	ASN
1	B	1097	GLN
1	B	1114	HIS
1	B	1129	HIS
1	B	1153	ASN
1	B	1156	HIS
1	B	1232	ASN
1	B	1305	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	SO4	A	2002	-	4,4,4	0.58	0	6,6,6	3.86	4 (66%)
2	SO4	B	2001	-	4,4,4	0.48	0	6,6,6	3.84	4 (66%)
2	SO4	A	2006	-	4,4,4	0.64	0	6,6,6	0.42	0
3	NAD	A	3000	-	42,48,48	2.02	10 (23%)	50,73,73	2.57	11 (22%)
2	SO4	A	2004	-	4,4,4	0.70	0	6,6,6	0.34	0
2	SO4	A	2005	-	4,4,4	0.58	0	6,6,6	3.87	4 (66%)
2	SO4	B	2003	-	4,4,4	0.51	0	6,6,6	3.86	4 (66%)
3	NAD	B	3001	-	42,48,48	2.04	9 (21%)	50,73,73	2.60	15 (30%)

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	A	3000	-	-	10/26/62/62	0/5/5/5
3	NAD	B	3001	-	-	7/26/62/62	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3001	NAD	C2N-C3N	-7.52	1.27	1.39
3	A	3000	NAD	C2N-C3N	-7.49	1.27	1.39
3	B	3001	NAD	C4N-C3N	6.10	1.49	1.39
3	A	3000	NAD	C4N-C3N	5.92	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3000	NAD	C3N-C7N	-4.11	1.44	1.50
3	B	3001	NAD	C3N-C7N	-3.97	1.44	1.50
3	B	3001	NAD	PN-O2N	-3.55	1.38	1.55
3	A	3000	NAD	PN-O2N	-3.39	1.39	1.55
3	A	3000	NAD	C2D-C1D	-3.20	1.48	1.53
3	B	3001	NAD	C6N-N1N	2.79	1.42	1.35
3	B	3001	NAD	C2D-C1D	-2.78	1.49	1.53
3	A	3000	NAD	C6N-N1N	2.63	1.41	1.35
3	B	3001	NAD	C2A-N1A	2.36	1.38	1.33
3	B	3001	NAD	C7N-N7N	2.35	1.37	1.33
3	A	3000	NAD	C2N-N1N	-2.13	1.32	1.35
3	B	3001	NAD	O4D-C1D	2.10	1.44	1.41
3	A	3000	NAD	C2A-N1A	2.07	1.37	1.33
3	A	3000	NAD	PA-O5B	-2.07	1.50	1.59
3	A	3000	NAD	C7N-N7N	2.02	1.36	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	NAD	C5N-C4N-C3N	-7.39	111.59	120.34
3	B	3001	NAD	C5N-C4N-C3N	-7.36	111.64	120.34
3	A	3000	NAD	C2N-C3N-C4N	6.63	125.77	118.26
3	B	3001	NAD	C2N-C3N-C4N	6.56	125.70	118.26
3	A	3000	NAD	C6N-N1N-C2N	6.54	127.94	121.97
3	B	3001	NAD	C6N-N1N-C2N	6.52	127.92	121.97
2	B	2003	SO4	O4-S-O1	-5.72	79.45	109.31
2	A	2005	SO4	O4-S-O1	-5.69	79.63	109.31
2	A	2002	SO4	O4-S-O1	-5.59	80.15	109.31
2	A	2002	SO4	O4-S-O3	-5.58	85.23	109.06
2	B	2001	SO4	O4-S-O1	-5.57	80.24	109.31
2	B	2003	SO4	O4-S-O3	-5.41	85.95	109.06
3	B	3001	NAD	C5N-C6N-N1N	-5.37	112.70	120.40
2	A	2005	SO4	O4-S-O3	-5.35	86.21	109.06
3	A	3000	NAD	C5N-C6N-N1N	-5.33	112.75	120.40
2	B	2001	SO4	O4-S-O3	-5.33	86.31	109.06
3	B	3001	NAD	C2N-N1N-C1D	-5.07	107.84	119.14
3	A	3000	NAD	O7N-C7N-C3N	-5.07	113.56	119.63
3	A	3000	NAD	C4N-C3N-C7N	-4.95	107.79	121.04
3	A	3000	NAD	C2N-N1N-C1D	-4.91	108.20	119.14
3	B	3001	NAD	C4N-C3N-C7N	-4.87	108.00	121.04
3	B	3001	NAD	O7N-C7N-C3N	-4.87	113.80	119.63
2	B	2001	SO4	O4-S-O2	-4.63	85.13	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2005	SO4	O4-S-O2	-4.58	85.40	109.31
2	B	2003	SO4	O4-S-O2	-4.44	86.15	109.31
2	A	2002	SO4	O4-S-O2	-4.38	86.46	109.31
3	A	3000	NAD	C6N-C5N-C4N	3.92	125.13	119.44
3	B	3001	NAD	C6N-C5N-C4N	3.90	125.11	119.44
3	A	3000	NAD	C3N-C7N-N7N	3.74	122.24	117.75
3	A	3000	NAD	C3N-C2N-N1N	-3.71	116.80	120.43
3	B	3001	NAD	C3N-C2N-N1N	-3.57	116.94	120.43
3	B	3001	NAD	C3N-C7N-N7N	3.52	121.97	117.75
3	A	3000	NAD	C2N-C3N-C7N	2.40	126.44	119.46
2	A	2005	SO4	O2-S-O1	2.37	126.93	109.43
2	B	2001	SO4	O2-S-O1	2.36	126.88	109.43
3	B	3001	NAD	C2N-C3N-C7N	2.36	126.31	119.46
2	B	2003	SO4	O2-S-O1	2.29	126.35	109.43
2	A	2002	SO4	O2-S-O1	2.26	126.15	109.43
3	B	3001	NAD	O4D-C4D-C3D	-2.17	100.82	105.11
3	B	3001	NAD	O3D-C3D-C4D	2.05	116.99	111.05
3	B	3001	NAD	O5D-C5D-C4D	2.04	116.00	108.99
3	B	3001	NAD	O4D-C4D-C5D	-2.02	102.72	109.37

There are no chirality outliers.

All (17) torsion outliers are listed below:

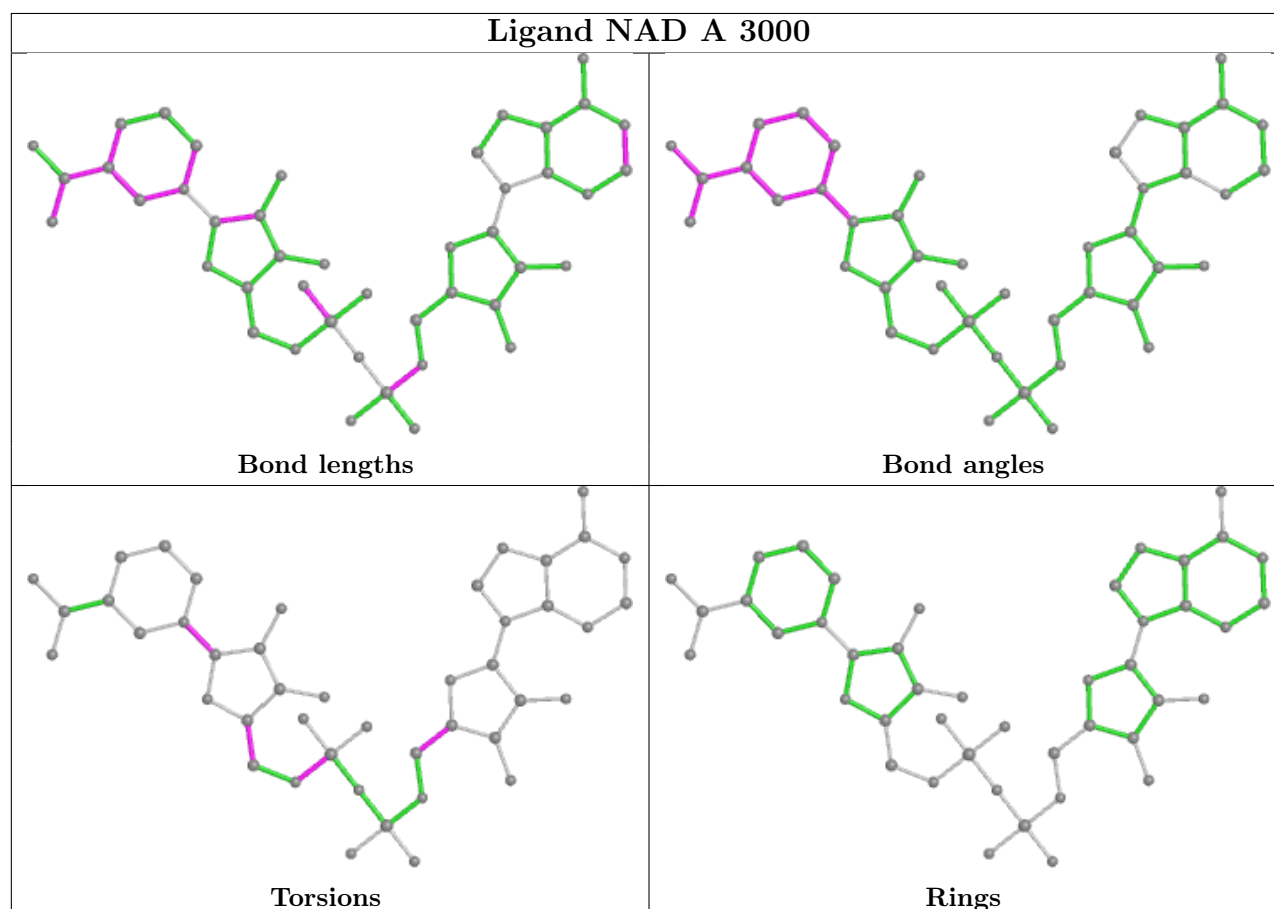
Mol	Chain	Res	Type	Atoms
3	A	3000	NAD	C5D-O5D-PN-O1N
3	A	3000	NAD	C5D-O5D-PN-O2N
3	A	3000	NAD	O4D-C1D-N1N-C2N
3	A	3000	NAD	O4D-C1D-N1N-C6N
3	A	3000	NAD	C2D-C1D-N1N-C2N
3	A	3000	NAD	C2D-C1D-N1N-C6N
3	B	3001	NAD	C5D-O5D-PN-O1N
3	B	3001	NAD	O4D-C4D-C5D-O5D
3	B	3001	NAD	C3D-C4D-C5D-O5D
3	B	3001	NAD	O4D-C1D-N1N-C6N
3	A	3000	NAD	O4D-C4D-C5D-O5D
3	B	3001	NAD	C4B-C5B-O5B-PA
3	A	3000	NAD	C3D-C4D-C5D-O5D
3	B	3001	NAD	PA-O3-PN-O5D
3	A	3000	NAD	O4B-C4B-C5B-O5B
3	B	3001	NAD	O4B-C4B-C5B-O5B
3	A	3000	NAD	C5D-O5D-PN-O3

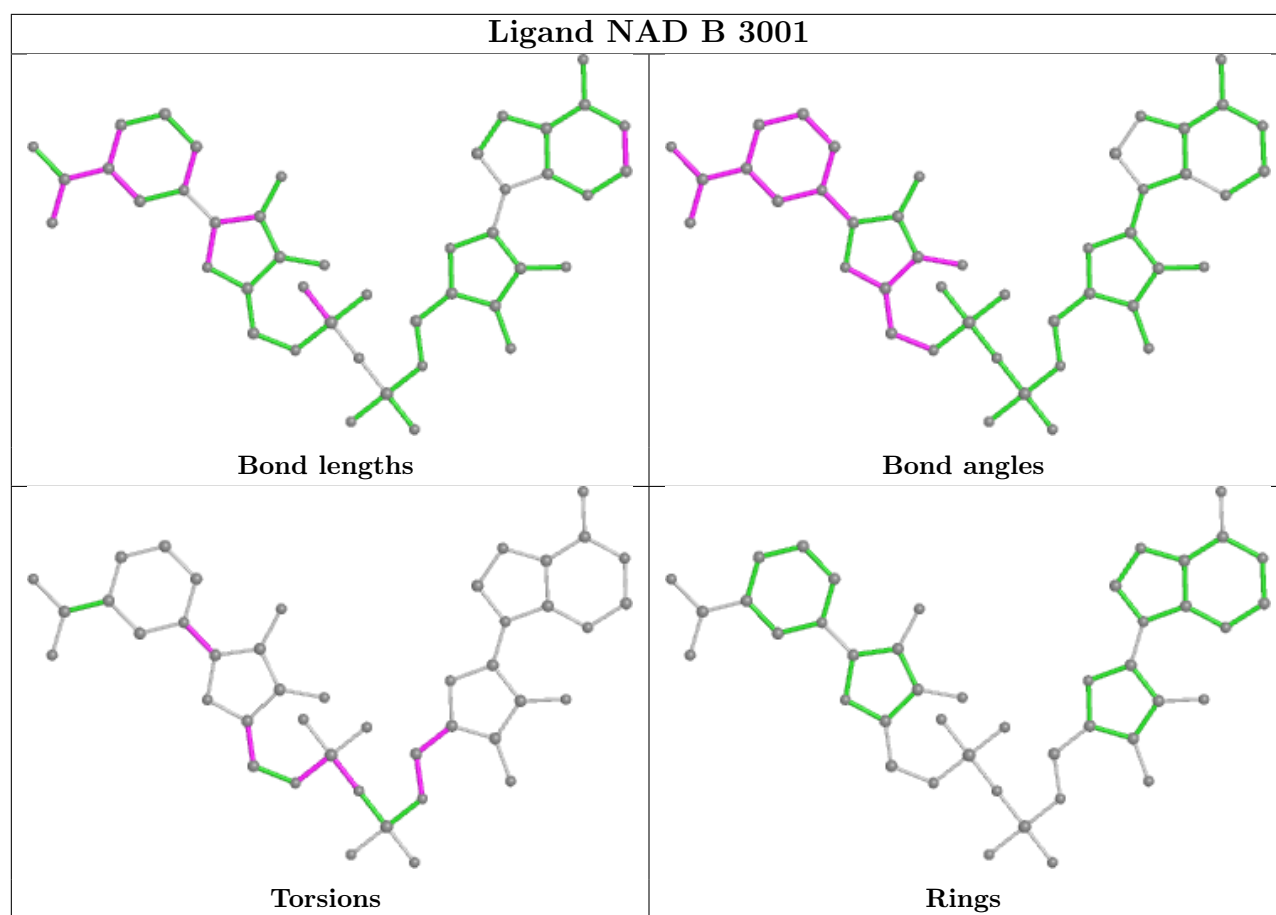
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2002	SO4	1	0
3	A	3000	NAD	1	0
2	B	2003	SO4	1	0
3	B	3001	NAD	5	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 [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	A	426/427 (99%)	-0.35	21 (4%) 29 28	8, 23, 71, 100	0
1	B	426/427 (99%)	-0.42	16 (3%) 40 38	9, 21, 66, 93	0
All	All	852/854 (99%)	-0.38	37 (4%) 35 33	8, 22, 70, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	5.9
1	A	290	ARG	5.8
1	A	285	PRO	5.6
1	B	1284	ILE	5.3
1	A	284	ILE	4.7
1	B	1290	ARG	4.7
1	A	7	LEU	4.3
1	B	1297	SER	4.3
1	B	1004	LYS	4.2
1	B	1003	THR	4.1
1	A	4	LYS	4.0
1	A	287	PHE	4.0
1	A	5	ALA	3.9
1	A	3	THR	3.9
1	B	1296	ASP	3.8
1	B	1285	PRO	3.6
1	B	1287	PHE	3.5
1	B	1278	ILE	3.4
1	B	1001	ALA	3.4
1	B	1002	ASP	3.2
1	A	331	THR	3.1
1	B	1288	PHE	3.0
1	A	2	ASP	2.9
1	A	288	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1295	ASN	2.8
1	A	13	THR	2.7
1	A	286	GLU	2.7
1	B	1007	LEU	2.6
1	A	277	GLU	2.6
1	B	1286	GLU	2.4
1	A	278	ILE	2.3
1	A	8	THR	2.3
1	A	424	ILE	2.2
1	A	330	GLY	2.2
1	A	6	LYS	2.2
1	A	283	HIS	2.1
1	B	1331	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.

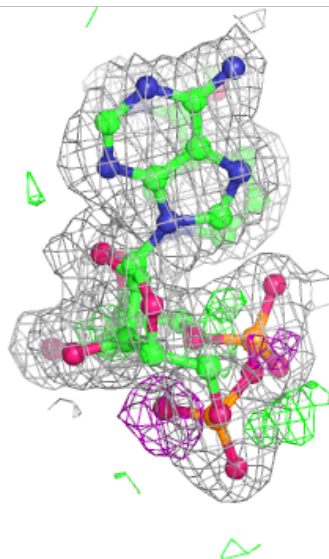
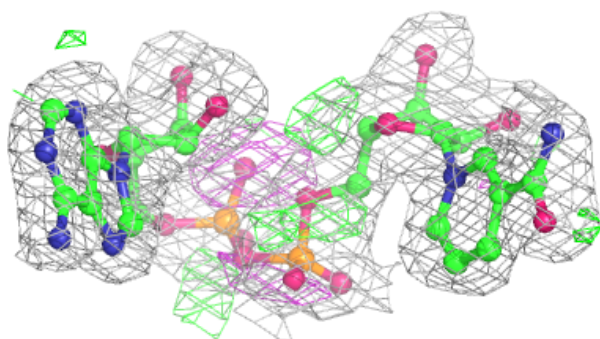
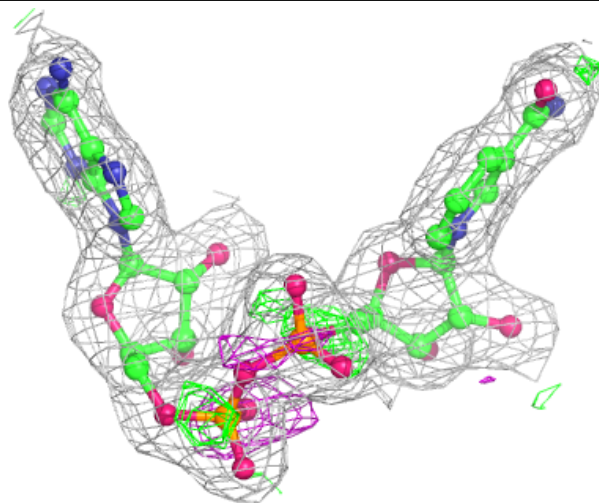
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	B	3001	44/44	0.95	0.12	26,29,35,40	0
2	SO4	A	2005	5/5	0.96	0.15	62,62,63,63	0
3	NAD	A	3000	44/44	0.98	0.11	6,12,23,24	0
2	SO4	A	2002	5/5	0.98	0.12	35,36,37,37	0
2	SO4	B	2003	5/5	0.99	0.11	32,33,33,34	0
2	SO4	A	2004	5/5	0.99	0.11	24,24,25,25	0
2	SO4	B	2001	5/5	0.99	0.12	17,17,19,21	0
2	SO4	A	2006	5/5	1.00	0.10	15,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

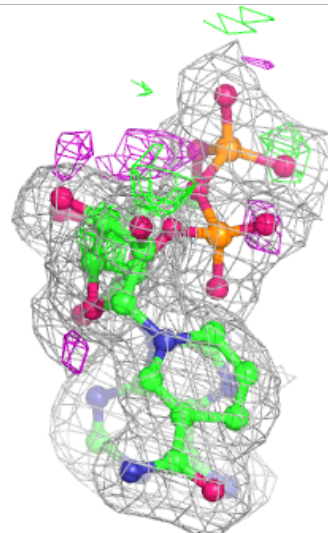
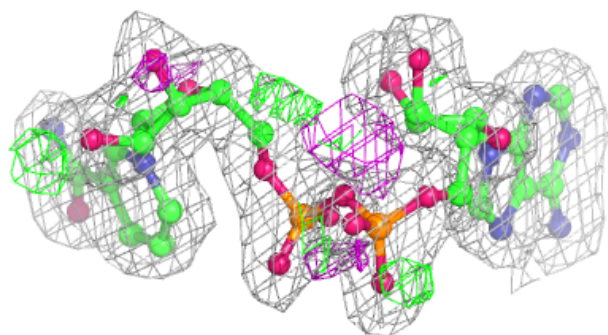
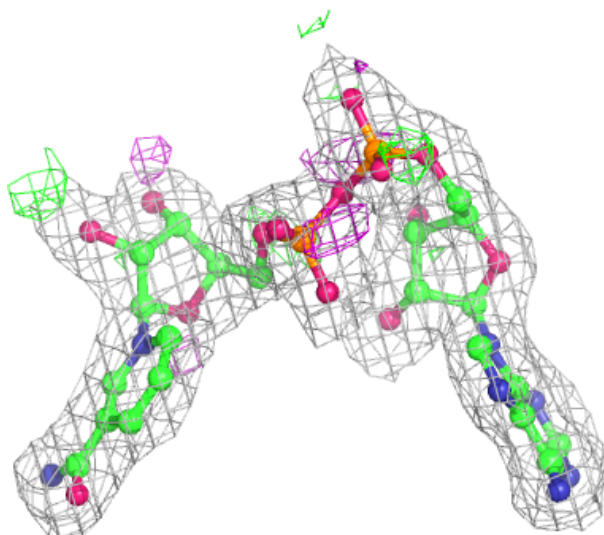
Electron density around NAD B 3001:

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



Electron density around NAD A 3000:

$2mF_o-DF_c$ (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.