Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 03:16 AM EDT

PDB ID	:	1TAE
Title	:	Structural rearrangement accompanying NAD+ synthesis within a bacterial DNA ligase crystal
Authors	:	Gajiwala, K.S.; Pinko, C.
Deposited on	:	2004-05-19
Resolution	:	2.70 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:

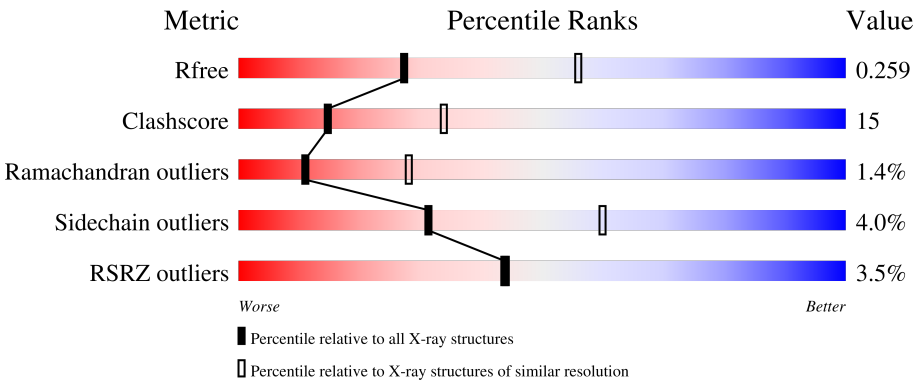
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	332	3% 67% 27% • •
1	B	332	2% 67% 29% • •
1	C	332	5% 68% 27% • •
1	D	332	3% 58% 35% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10774 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.

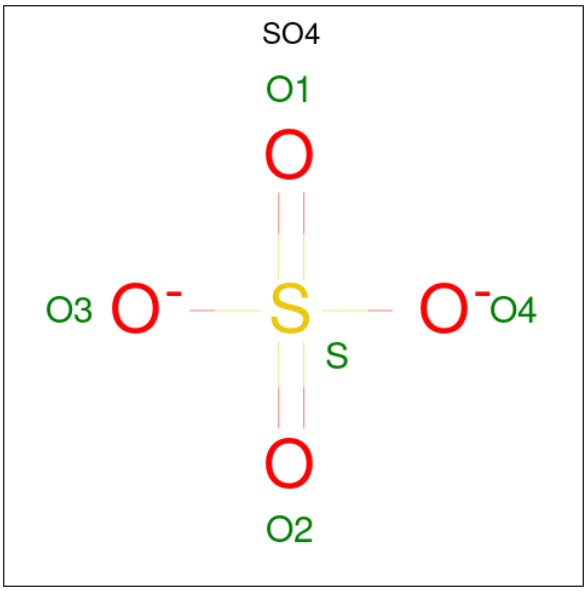
- Molecule 1 is a protein called DNA ligase, NAD-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2575	1631	436	500	8	0	0	0
1	B	321	2575	1631	436	500	8	0	0	0
1	C	321	2575	1631	436	500	8	0	0	0
1	D	321	2575	1631	436	500	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	HIS	-	expression tag	UNP Q837V6
B	275	HIS	-	expression tag	GB 29375318
C	275	HIS	-	expression tag	GB 29375318
D	275	HIS	-	expression tag	GB 29375318

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



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

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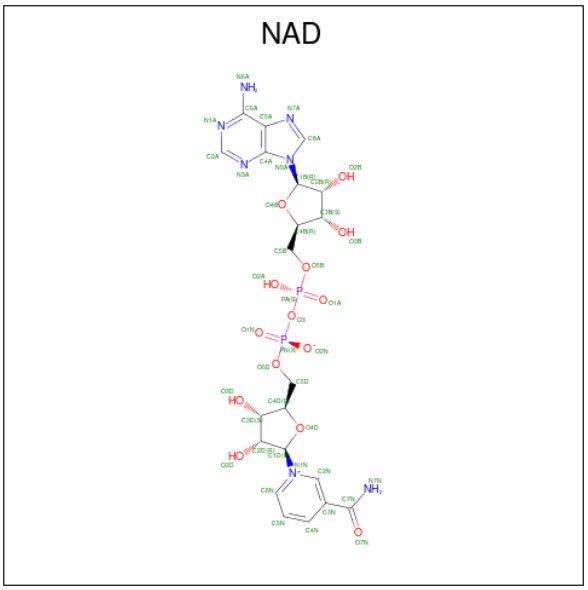
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	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	A	1	44	21	7	14	2	0	0

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	B	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is water.

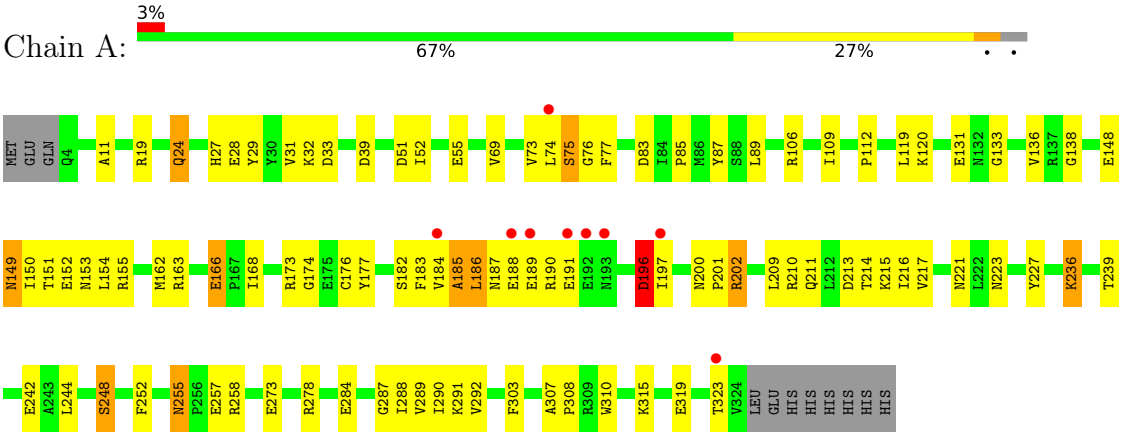
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	51	51	51	0	0
5	B	51	51	51	0	0
5	C	35	35	35	0	0
5	D	39	39	39	0	0

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.

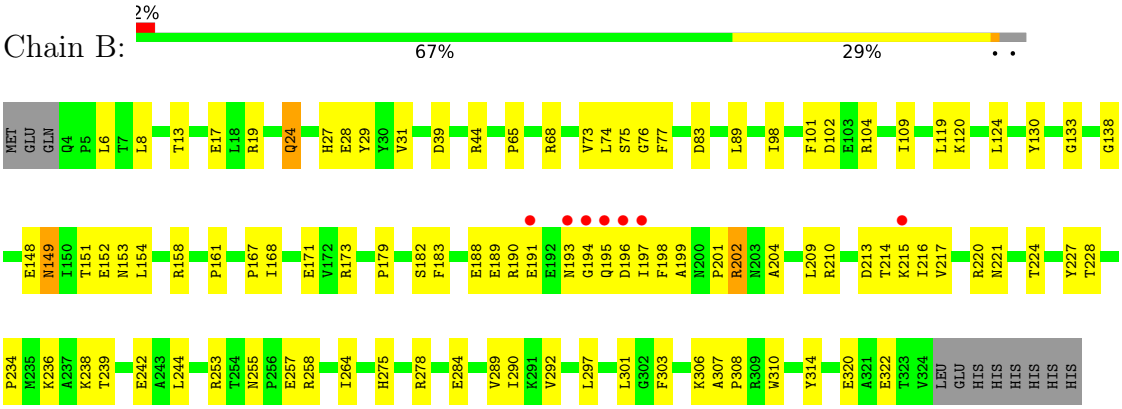
• Molecule 1: DNA ligase, NAD-dependent

Chain A:



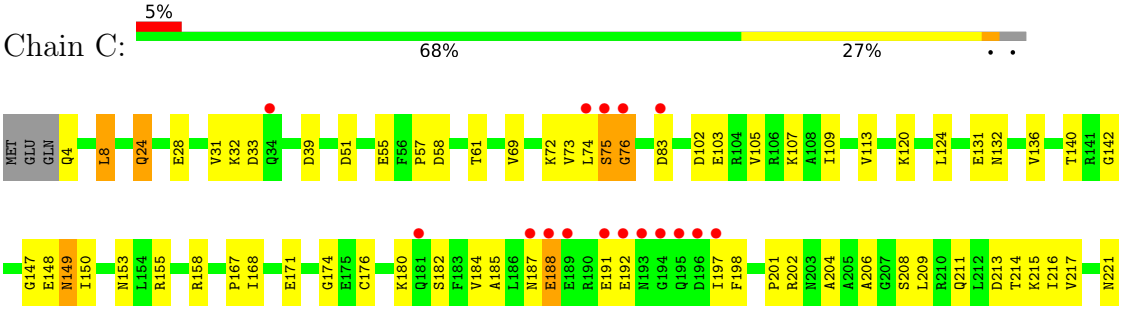
• Molecule 1: DNA ligase, NAD-dependent

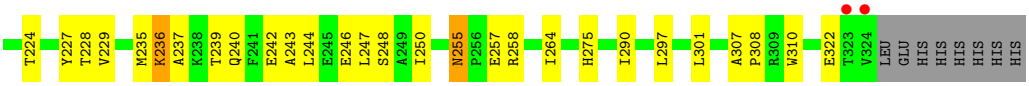
Chain B:



• Molecule 1: DNA ligase, NAD-dependent

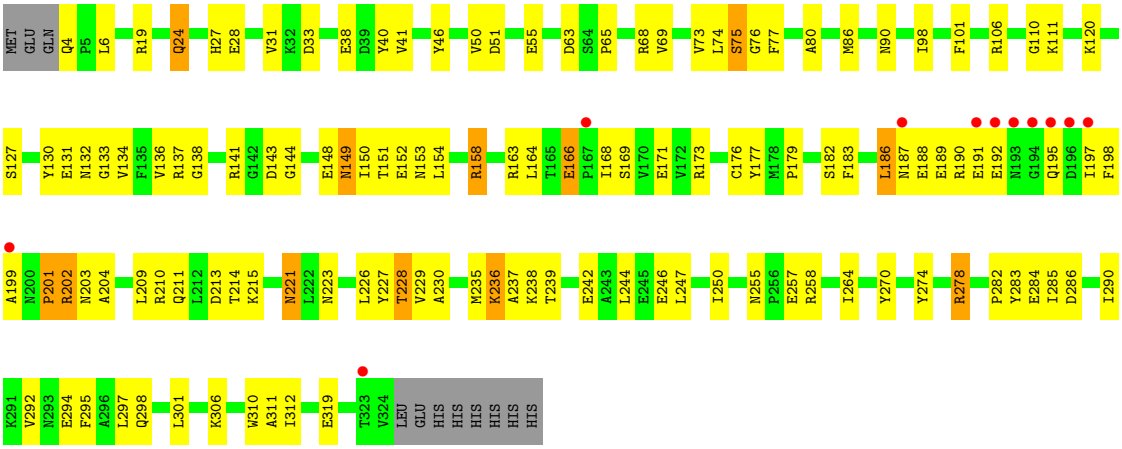
Chain C:





• Molecule 1: DNA ligase, NAD-dependent

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.30Å 135.18Å 115.80Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	24.77 – 2.70 24.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.77-2.70) 95.7 (24.76-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 2.72Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.202 , 0.263 0.200 , 0.259	Depositor DCC
R_{free} test set	5065 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10774	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: NA, NAD, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.38	0/2629	0.63	0/3563
1	B	0.37	0/2629	0.62	0/3563
1	C	0.37	0/2629	0.62	0/3563
1	D	0.35	0/2629	0.61	0/3563
All	All	0.37	0/10516	0.62	0/14252

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2575	0	2526	78	0
1	B	2575	0	2526	65	0
1	C	2575	0	2526	78	0
1	D	2575	0	2526	104	0
2	A	30	0	0	0	0
2	B	35	0	0	1	0
2	C	25	0	0	1	0
2	D	30	0	0	0	0
3	A	44	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	3	0
3	C	44	0	26	2	0
3	D	44	0	26	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	51	0	0	2	0
5	B	51	0	0	1	0
5	C	35	0	0	3	0
5	D	39	0	0	0	0
All	All	10774	0	10208	319	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 15.

All (319) 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:C:236:LYS:H	1:C:236:LYS:HD3	1.13	1.09
1:B:98:ILE:HG22	1:B:264:ILE:HD11	1.40	1.00
1:D:190:ARG:HB3	1:D:195:GLN:HB2	1.53	0.89
1:D:98:ILE:HG22	1:D:264:ILE:HD11	1.53	0.88
1:B:73:VAL:HG12	1:B:75:SER:H	1.42	0.84
1:D:236:LYS:H	1:D:236:LYS:HD3	1.44	0.81
1:A:133:GLY:O	1:A:163:ARG:HA	1.82	0.79
1:C:236:LYS:HD3	1:C:236:LYS:N	1.93	0.79
1:A:185:ALA:O	1:A:188:GLU:HG3	1.83	0.79
1:A:166:GLU:HB3	1:A:168:ILE:HG23	1.66	0.78
1:B:201:PRO:HG2	1:B:284:GLU:HG3	1.68	0.76
1:C:191:GLU:HG2	1:C:197:ILE:HG21	1.68	0.76
1:A:153:ASN:ND2	1:A:217:VAL:HG21	2.03	0.74
1:A:74:LEU:HB2	1:A:210:ARG:HH11	1.52	0.73
1:A:236:LYS:H	1:A:236:LYS:HD3	1.53	0.73
1:A:85:PRO:HD3	1:C:8:LEU:HD23	1.71	0.72
1:D:213:ASP:OD2	1:D:215:LYS:HB2	1.88	0.72
1:D:173:ARG:HB2	1:D:228:THR:HG23	1.72	0.71
1:D:166:GLU:HB3	1:D:168:ILE:HG23	1.71	0.71
1:C:73:VAL:HG13	1:C:148:GLU:HG2	1.73	0.71
1:A:73:VAL:HG13	1:A:148:GLU:HG2	1.73	0.71
1:D:73:VAL:HG13	1:D:148:GLU:HG2	1.73	0.70
1:D:229:VAL:HG22	1:D:247:LEU:HD21	1.73	0.70
1:A:319:GLU:O	1:A:323:THR:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:THR:OG1	1:D:242:GLU:HG3	1.93	0.69
1:D:236:LYS:HD3	1:D:236:LYS:N	2.08	0.68
1:D:301:LEU:HD12	1:D:310:TRP:HB3	1.74	0.68
1:A:106:ARG:NH2	1:A:112:PRO:HG3	2.10	0.67
1:A:213:ASP:OD2	1:A:215:LYS:HB2	1.95	0.66
1:D:149:ASN:HD22	1:D:149:ASN:C	1.99	0.65
1:D:201:PRO:HG2	1:D:284:GLU:HG3	1.78	0.65
1:A:73:VAL:HG13	1:A:148:GLU:CG	2.26	0.65
1:B:171:GLU:HG3	5:B:556:HOH:O	1.96	0.65
1:D:149:ASN:ND2	1:D:151:THR:H	1.94	0.65
1:C:131:GLU:HG3	1:C:136:VAL:HG21	1.79	0.64
1:B:102:ASP:HB2	1:B:264:ILE:HD13	1.79	0.64
1:C:227:TYR:HD2	1:C:228:THR:HG23	1.63	0.63
1:C:236:LYS:H	1:C:236:LYS:CD	2.02	0.63
1:C:24:GLN:O	1:C:28:GLU:HG3	1.98	0.63
1:D:73:VAL:HG13	1:D:148:GLU:CG	2.29	0.63
1:B:29:TYR:OH	1:B:202:ARG:HD2	1.98	0.63
1:C:211:GLN:CD	1:C:216:ILE:HD12	2.19	0.63
1:D:138:GLY:HA3	1:D:154:LEU:HD12	1.81	0.63
1:B:239:THR:OG1	1:B:242:GLU:HG3	1.99	0.63
1:A:187:ASN:OD1	1:A:197:ILE:HB	1.98	0.63
1:C:239:THR:OG1	1:C:242:GLU:HG3	1.99	0.63
1:D:46:TYR:O	1:D:50:VAL:HG23	1.99	0.63
1:D:198:PHE:CD2	1:D:204:ALA:HA	2.34	0.62
1:A:290:ILE:HD12	1:A:290:ILE:N	2.15	0.62
1:B:149:ASN:C	1:B:149:ASN:HD22	2.02	0.62
1:D:176:CYS:SG	1:D:209:LEU:HD11	2.39	0.62
1:C:191:GLU:HG2	1:C:197:ILE:CG2	2.29	0.62
1:C:132:ASN:HA	1:C:167:PRO:O	2.00	0.61
1:C:120:LYS:HE2	3:C:403:NAD:H52A	1.81	0.61
1:D:227:TYR:CD2	1:D:228:THR:HG22	2.35	0.61
1:C:237:ALA:HB2	1:C:246:GLU:OE2	2.01	0.61
1:D:74:LEU:HB2	1:D:210:ARG:NH1	2.14	0.61
1:D:164:LEU:HD22	1:D:250:ILE:HG22	1.82	0.60
1:D:51:ASP:O	1:D:55:GLU:HG3	2.01	0.60
1:D:131:GLU:HG3	1:D:136:VAL:HG21	1.82	0.60
1:B:182:SER:OG	1:B:221:ASN:ND2	2.34	0.60
1:A:255:ASN:HD21	1:A:257:GLU:HG2	1.67	0.59
1:C:74:LEU:HB3	1:C:148:GLU:OE2	2.02	0.59
1:B:153:ASN:OD1	1:B:217:VAL:HG21	2.02	0.59
1:C:73:VAL:HG13	1:C:148:GLU:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:CYS:SG	1:C:209:LEU:HD11	2.42	0.59
1:B:301:LEU:HD12	1:B:310:TRP:HB3	1.84	0.59
1:A:119:LEU:HD11	1:A:257:GLU:HG3	1.85	0.58
1:A:106:ARG:CZ	1:A:112:PRO:HG3	2.33	0.58
1:D:19:ARG:HG2	1:D:65:PRO:HD2	1.83	0.58
1:D:74:LEU:HB3	1:D:148:GLU:OE2	2.03	0.58
1:C:72:LYS:HG3	5:C:454:HOH:O	2.03	0.58
1:B:98:ILE:HD11	1:B:314:TYR:HD2	1.69	0.58
1:B:120:LYS:HE2	3:B:402:NAD:H52A	1.85	0.58
1:A:255:ASN:ND2	1:A:257:GLU:H	2.02	0.58
1:B:183:PHE:CD2	1:B:201:PRO:HA	2.38	0.58
1:D:4:GLN:NE2	1:D:55:GLU:HB3	2.18	0.58
1:A:236:LYS:HD3	1:A:236:LYS:N	2.17	0.58
1:A:31:VAL:HG12	1:A:31:VAL:O	2.03	0.58
1:C:213:ASP:OD2	1:C:215:LYS:HB2	2.04	0.57
1:A:307:ALA:HB1	1:A:308:PRO:HD2	1.85	0.57
1:B:191:GLU:HG3	1:B:197:ILE:CG2	2.34	0.57
1:C:301:LEU:HD12	1:C:310:TRP:HB3	1.84	0.57
1:D:202:ARG:HG3	1:D:203:ASN:N	2.19	0.57
1:C:51:ASP:O	1:C:55:GLU:HG3	2.04	0.57
1:D:149:ASN:HD22	1:D:151:THR:H	1.52	0.57
1:D:75:SER:O	1:D:77:PHE:N	2.37	0.56
1:C:255:ASN:ND2	1:C:257:GLU:H	2.03	0.56
1:B:148:GLU:OE2	1:B:210:ARG:NH2	2.37	0.56
1:C:187:ASN:OD1	1:C:197:ILE:HB	2.05	0.56
1:B:74:LEU:HD22	1:B:210:ARG:NH1	2.20	0.56
1:B:224:THR:O	1:B:253:ARG:HD3	2.06	0.56
1:A:138:GLY:HA3	1:A:154:LEU:HD12	1.87	0.56
1:C:31:VAL:HG12	1:C:31:VAL:O	2.06	0.56
1:D:27:HIS:O	1:D:31:VAL:HB	2.06	0.56
1:A:149:ASN:C	1:A:149:ASN:HD22	2.10	0.55
1:D:74:LEU:HB2	1:D:210:ARG:HH12	1.71	0.55
1:D:153:ASN:OD1	1:D:214:THR:HG22	2.06	0.55
1:A:155:ARG:HG2	1:A:162:MET:SD	2.47	0.55
1:B:124:LEU:HD23	1:B:209:LEU:HD12	1.89	0.55
1:A:24:GLN:O	1:A:28:GLU:HG3	2.07	0.55
1:A:176:CYS:SG	1:A:209:LEU:HD11	2.47	0.55
1:D:148:GLU:OE1	1:D:210:ARG:NH2	2.40	0.55
1:A:213:ASP:OD2	1:A:216:ILE:HG13	2.06	0.54
1:D:133:GLY:O	1:D:163:ARG:HA	2.07	0.54
1:B:179:PRO:HG3	2:B:417:SO4:O4	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ALA:O	1:C:247:LEU:HG	2.07	0.54
1:B:198:PHE:CD2	1:B:204:ALA:HA	2.42	0.54
1:D:255:ASN:HD21	1:D:257:GLU:HB2	1.72	0.54
1:B:153:ASN:OD1	1:B:214:THR:HG22	2.07	0.54
1:D:294:GLU:HB2	1:D:297:LEU:HD12	1.89	0.54
1:B:190:ARG:HD3	1:B:196:ASP:O	2.08	0.54
1:B:104:ARG:HH21	1:B:104:ARG:HG3	1.73	0.54
1:C:103:GLU:HG2	1:C:107:LYS:HE3	1.89	0.54
1:D:187:ASN:O	1:D:197:ILE:HG22	2.08	0.54
1:D:182:SER:CB	1:D:221:ASN:HD22	2.21	0.53
1:A:255:ASN:HD22	1:A:257:GLU:H	1.54	0.53
1:C:211:GLN:HG2	1:C:216:ILE:HB	1.90	0.53
1:B:290:ILE:N	1:B:290:ILE:HD12	2.23	0.53
1:A:75:SER:O	1:A:77:PHE:N	2.42	0.53
1:D:77:PHE:CE2	1:D:150:ILE:HG22	2.44	0.53
1:D:182:SER:HB3	1:D:221:ASN:HD22	1.74	0.52
1:B:13:THR:O	1:B:17:GLU:HG3	2.08	0.52
1:D:188:GLU:HG3	1:D:189:GLU:N	2.24	0.52
1:A:74:LEU:HB3	1:A:148:GLU:OE2	2.09	0.52
1:A:185:ALA:O	1:A:186:LEU:C	2.48	0.52
1:A:120:LYS:HE3	1:A:315:LYS:HE2	1.91	0.52
1:C:208:SER:O	1:C:211:GLN:HB3	2.10	0.52
1:D:171:GLU:O	1:D:230:ALA:HB3	2.09	0.52
1:B:188:GLU:HG3	1:B:189:GLU:N	2.24	0.52
1:B:244:LEU:HD13	1:B:258:ARG:HD3	1.91	0.52
1:D:110:GLY:O	1:D:111:LYS:HB3	2.10	0.52
1:A:149:ASN:HD22	1:A:150:ILE:N	2.07	0.52
1:A:153:ASN:HD21	1:A:217:VAL:HG21	1.73	0.52
1:C:213:ASP:OD1	1:C:215:LYS:HG2	2.09	0.51
1:D:63:ASP:HB2	1:D:68:ARG:HH21	1.76	0.51
1:D:149:ASN:HD22	1:D:150:ILE:N	2.08	0.51
1:B:227:TYR:HD2	1:B:228:THR:HG1	1.57	0.51
1:D:98:ILE:O	1:D:101:PHE:HB3	2.11	0.51
1:C:140:THR:CG2	1:C:150:ILE:HD13	2.40	0.51
1:D:134:VAL:HG22	1:D:163:ARG:NH2	2.25	0.51
1:B:307:ALA:HB1	1:B:308:PRO:HD2	1.91	0.51
1:A:120:LYS:HE2	3:A:401:NAD:H52A	1.91	0.51
1:B:89:LEU:HD12	3:B:402:NAD:H52A	1.92	0.51
1:B:109:ILE:HG22	1:B:109:ILE:O	2.11	0.51
1:C:153:ASN:OD1	1:C:217:VAL:HG21	2.11	0.50
1:A:186:LEU:O	1:A:189:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:THR:HG22	5:C:459:HOH:O	2.10	0.50
1:C:102:ASP:HB2	1:C:264:ILE:HD13	1.94	0.50
1:C:39:ASP:OD2	3:C:403:NAD:H2N	2.11	0.50
1:D:244:LEU:HB3	1:D:258:ARG:HH21	1.77	0.50
1:D:237:ALA:HB2	1:D:246:GLU:OE2	2.12	0.50
1:B:191:GLU:O	1:B:194:GLY:N	2.39	0.49
1:C:240:GLN:HE21	1:C:240:GLN:HA	1.77	0.49
1:D:98:ILE:HG22	1:D:264:ILE:CD1	2.33	0.49
1:B:189:GLU:HG2	1:B:193:ASN:HD21	1.77	0.49
1:C:198:PHE:CD2	1:C:204:ALA:HA	2.47	0.49
1:C:244:LEU:HA	1:C:247:LEU:HD12	1.93	0.49
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.12	0.49
1:A:162:MET:H	1:D:158:ARG:NH2	2.10	0.49
1:A:221:ASN:HA	5:A:459:HOH:O	2.11	0.49
1:A:303:PHE:HB2	1:C:57:PRO:CG	2.42	0.49
1:D:143:ASP:C	1:D:143:ASP:OD2	2.51	0.49
1:B:39:ASP:OD2	3:B:402:NAD:H2N	2.13	0.49
1:C:168:ILE:HD11	1:C:250:ILE:HD13	1.95	0.49
1:A:174:GLY:HA2	1:A:227:TYR:CZ	2.48	0.48
1:B:27:HIS:O	1:B:31:VAL:HB	2.13	0.48
1:D:278:ARG:NE	1:D:319:GLU:HB3	2.28	0.48
1:D:130:TYR:O	1:D:169:SER:HA	2.13	0.48
1:D:134:VAL:O	1:D:136:VAL:HG13	2.12	0.48
1:D:149:ASN:ND2	1:D:151:THR:OG1	2.45	0.48
1:D:182:SER:HB3	1:D:221:ASN:ND2	2.29	0.48
1:C:235:MET:HE3	1:C:246:GLU:HG2	1.96	0.48
1:C:244:LEU:HB3	1:C:258:ARG:HH21	1.79	0.48
1:C:307:ALA:HB1	1:C:308:PRO:HD2	1.95	0.48
1:D:69:VAL:HG21	1:D:144:GLY:HA3	1.96	0.48
1:D:186:LEU:O	1:D:189:GLU:HB3	2.14	0.48
1:B:255:ASN:HD21	1:B:257:GLU:HG2	1.79	0.48
1:C:229:VAL:HG22	1:C:247:LEU:HD21	1.96	0.48
1:D:226:LEU:N	1:D:226:LEU:HD22	2.29	0.47
1:A:131:GLU:HG3	1:A:136:VAL:HG21	1.96	0.47
1:A:149:ASN:ND2	1:A:151:THR:H	2.12	0.47
1:B:149:ASN:ND2	1:B:151:THR:H	2.12	0.47
1:A:27:HIS:CE1	1:A:31:VAL:HG11	2.49	0.47
1:A:183:PHE:CD2	1:A:201:PRO:HA	2.49	0.47
1:B:152:GLU:HB3	1:B:214:THR:HG21	1.95	0.47
1:C:109:ILE:HD12	1:C:297:LEU:HD22	1.97	0.47
1:A:287:GLY:O	1:A:288:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ILE:N	1:D:290:ILE:HD12	2.29	0.47
1:C:105:VAL:HG11	1:C:113:VAL:HG21	1.97	0.47
1:C:211:GLN:OE1	1:C:216:ILE:HD12	2.14	0.47
1:C:240:GLN:HA	1:C:240:GLN:NE2	2.30	0.47
1:B:173:ARG:HB2	1:B:228:THR:HB	1.97	0.47
1:D:227:TYR:HD2	1:D:228:THR:HG22	1.79	0.47
1:A:51:ASP:O	1:A:55:GLU:HG3	2.15	0.47
1:C:149:ASN:C	1:C:149:ASN:HD22	2.17	0.47
1:C:185:ALA:HA	1:C:188:GLU:HG3	1.95	0.47
1:C:142:GLY:HA3	1:C:147:GLY:HA2	1.96	0.47
1:D:244:LEU:HB3	1:D:258:ARG:NH2	2.30	0.47
1:C:171:GLU:HG2	2:C:423:SO4:O4	2.14	0.47
1:C:255:ASN:HD22	1:C:257:GLU:H	1.62	0.46
1:A:109:ILE:O	1:C:107:LYS:HD3	2.15	0.46
1:C:4:GLN:HA	1:C:4:GLN:OE1	2.15	0.46
1:D:282:PRO:HG2	1:D:283:TYR:HD1	1.79	0.46
1:A:196:ASP:N	1:A:196:ASP:OD2	2.48	0.46
1:B:109:ILE:HG23	1:B:297:LEU:HD22	1.97	0.46
1:C:290:ILE:HD12	1:C:290:ILE:N	2.30	0.46
1:D:69:VAL:HG12	1:D:306:LYS:HB2	1.98	0.46
1:A:290:ILE:N	1:A:290:ILE:CD1	2.78	0.46
1:D:177:TYR:CE2	1:D:179:PRO:HG3	2.51	0.46
1:B:24:GLN:O	1:B:28:GLU:HG3	2.16	0.46
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.81	0.46
1:D:235:MET:CE	1:D:246:GLU:HG2	2.46	0.46
1:A:74:LEU:O	1:A:75:SER:C	2.54	0.46
1:A:201:PRO:HG2	1:A:284:GLU:HG3	1.98	0.46
1:B:8:LEU:HD13	1:B:8:LEU:O	2.16	0.45
1:B:120:LYS:HB2	1:B:289:VAL:HG23	1.98	0.45
1:B:213:ASP:OD2	1:B:216:ILE:HG13	2.16	0.45
1:A:153:ASN:OD1	1:A:214:THR:HG22	2.16	0.45
1:A:166:GLU:HB3	1:A:168:ILE:CG2	2.43	0.45
1:C:140:THR:O	1:C:147:GLY:HA3	2.16	0.45
1:A:303:PHE:HB2	1:C:57:PRO:HG3	1.99	0.45
1:A:24:GLN:HA	1:A:24:GLN:OE1	2.15	0.45
1:A:31:VAL:O	1:A:31:VAL:CG1	2.63	0.45
1:B:130:TYR:OH	1:B:161:PRO:HG2	2.17	0.45
1:C:31:VAL:C	1:C:32:LYS:HG3	2.36	0.45
1:C:255:ASN:HD21	1:C:257:GLU:HG2	1.82	0.45
1:D:131:GLU:O	1:D:132:ASN:HB2	2.17	0.45
1:D:270:TYR:CE1	1:D:274:TYR:CE2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLY:HA3	1:B:154:LEU:HD12	1.99	0.45
1:C:174:GLY:HA2	1:C:227:TYR:CZ	2.52	0.45
1:D:292:VAL:HB	1:D:310:TRP:HB2	1.97	0.45
1:A:289:VAL:HG11	1:A:291:LYS:HE3	1.98	0.45
1:D:235:MET:HE3	1:D:246:GLU:HG2	1.99	0.45
1:B:149:ASN:C	1:B:149:ASN:ND2	2.68	0.44
1:D:4:GLN:OE1	1:D:4:GLN:HA	2.17	0.44
1:D:189:GLU:HA	1:D:192:GLU:OE2	2.17	0.44
1:B:275:HIS:CE1	1:B:322:GLU:OE1	2.71	0.44
1:B:133:GLY:HA3	1:B:167:PRO:HA	1.99	0.44
1:B:213:ASP:OD2	1:B:215:LYS:HB2	2.18	0.44
1:C:182:SER:OG	1:C:221:ASN:ND2	2.51	0.44
1:D:80:ALA:HB1	1:D:137:ARG:CZ	2.48	0.44
1:B:190:ARG:HG3	1:B:195:GLN:HB2	1.99	0.44
1:B:119:LEU:HD11	1:B:257:GLU:HG3	1.98	0.44
1:B:303:PHE:CE2	1:B:308:PRO:HB3	2.52	0.44
1:A:173:ARG:HD2	1:A:173:ARG:N	2.33	0.44
1:A:75:SER:O	1:A:77:PHE:O	2.36	0.44
1:B:168:ILE:HG22	1:B:234:PRO:HG3	2.00	0.43
1:C:250:ILE:O	1:C:250:ILE:HG22	2.17	0.43
1:A:190:ARG:HG2	1:A:190:ARG:HH21	1.83	0.43
1:A:323:THR:O	1:A:323:THR:HG23	2.18	0.43
1:C:153:ASN:OD1	1:C:214:THR:HG22	2.18	0.43
1:C:188:GLU:O	1:C:192:GLU:HG3	2.18	0.43
1:D:86:MET:HE3	1:D:173:ARG:CG	2.48	0.43
1:D:183:PHE:CD2	1:D:201:PRO:HA	2.53	0.43
1:B:44:ARG:HG3	1:B:44:ARG:HH11	1.82	0.43
1:D:86:MET:HE3	1:D:127:SER:HB2	2.00	0.43
1:A:11:ALA:HB1	1:A:52:ILE:HG23	1.99	0.43
1:A:248:SER:HA	1:A:252:PHE:O	2.19	0.43
1:C:155:ARG:NH2	5:C:451:HOH:O	2.40	0.43
1:A:32:LYS:O	1:A:33:ASP:C	2.57	0.43
1:A:89:LEU:HD12	3:A:401:NAD:H52A	2.01	0.43
1:B:74:LEU:HB2	1:B:148:GLU:OE2	2.19	0.43
1:A:239:THR:OG1	1:A:242:GLU:HG3	2.19	0.43
1:D:33:ASP:OD2	1:D:210:ARG:HD3	2.19	0.43
1:A:87:TYR:CE2	1:C:58:ASP:HB3	2.54	0.43
1:A:182:SER:OG	1:A:221:ASN:ND2	2.51	0.42
1:A:74:LEU:CB	1:A:148:GLU:OE2	2.67	0.42
1:C:180:LYS:O	1:C:184:VAL:HG23	2.20	0.42
1:D:120:LYS:HG2	1:D:286:ASP:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLU:O	1:D:250:ILE:HG12	2.18	0.42
1:A:211:GLN:OE1	1:A:216:ILE:HD12	2.18	0.42
1:A:244:LEU:HD13	1:A:258:ARG:HD2	2.01	0.42
1:A:73:VAL:HG13	1:A:148:GLU:HG3	2.00	0.42
1:C:275:HIS:CE1	1:C:322:GLU:OE1	2.73	0.42
1:D:106:ARG:CB	1:D:106:ARG:NH2	2.82	0.42
1:D:298:GLN:HE21	1:D:298:GLN:HB3	1.52	0.42
1:B:75:SER:O	1:B:77:PHE:N	2.53	0.42
1:C:140:THR:HG22	1:C:150:ILE:HD13	2.01	0.42
1:D:191:GLU:HG2	1:D:197:ILE:CG2	2.49	0.42
1:B:19:ARG:HG2	1:B:65:PRO:HD2	2.01	0.42
1:C:176:CYS:HA	1:C:224:THR:HG22	2.01	0.42
1:D:141:ARG:NH1	3:D:404:NAD:O1N	2.42	0.42
1:A:29:TYR:OH	1:A:202:ARG:HD2	2.19	0.42
1:D:250:ILE:HG22	1:D:250:ILE:O	2.20	0.42
1:D:290:ILE:O	1:D:311:ALA:HA	2.20	0.42
1:B:98:ILE:O	1:B:101:PHE:HB3	2.19	0.42
1:C:185:ALA:O	1:C:188:GLU:HG3	2.19	0.42
1:D:38:GLU:HG2	1:D:40:TYR:CE2	2.55	0.42
1:D:211:GLN:HA	1:D:211:GLN:NE2	2.35	0.42
1:C:209:LEU:C	1:C:211:GLN:H	2.23	0.41
1:D:177:TYR:HE2	1:D:179:PRO:HG3	1.84	0.41
1:D:120:LYS:HE2	3:D:404:NAD:H52A	2.03	0.41
1:D:238:LYS:C	1:D:295:PHE:HD2	2.23	0.41
1:B:74:LEU:O	1:B:76:GLY:N	2.48	0.41
1:D:86:MET:HE3	1:D:173:ARG:HG3	2.02	0.41
1:D:106:ARG:HB3	1:D:106:ARG:HH21	1.86	0.41
1:D:285:ILE:O	1:D:285:ILE:HG13	2.19	0.41
1:D:131:GLU:HG3	1:D:136:VAL:CG2	2.49	0.41
1:D:213:ASP:CG	1:D:215:LYS:HB2	2.39	0.41
1:B:292:VAL:HG21	1:B:301:LEU:CD1	2.50	0.41
1:C:75:SER:O	1:C:76:GLY:C	2.59	0.41
1:A:177:TYR:CZ	1:A:223:ASN:HB3	2.55	0.41
1:A:39:ASP:OD2	3:A:401:NAD:H2N	2.21	0.41
1:B:255:ASN:ND2	1:B:257:GLU:HG2	2.35	0.41
1:C:124:LEU:HD22	1:C:206:ALA:HA	2.03	0.41
1:C:124:LEU:HD23	1:C:209:LEU:HD12	2.03	0.41
1:D:90:ASN:O	1:D:312:ILE:HG13	2.21	0.41
1:D:238:LYS:C	1:D:295:PHE:CD2	2.95	0.41
1:D:38:GLU:HB3	1:D:41:VAL:HG23	2.02	0.41
1:A:183:PHE:CE2	1:A:200:ASN:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:O	1:B:306:LYS:HG3	2.21	0.40
1:C:191:GLU:OE2	1:C:197:ILE:HG23	2.21	0.40
1:A:19:ARG:NH1	5:A:437:HOH:O	2.48	0.40
1:D:27:HIS:ND1	1:D:31:VAL:HG21	2.36	0.40
1:D:177:TYR:CZ	1:D:223:ASN:HB3	2.55	0.40
1:D:24:GLN:O	1:D:28:GLU:HG3	2.21	0.40
1:A:292:VAL:HB	1:A:310:TRP:HB2	2.04	0.40
1:C:32:LYS:O	1:C:33:ASP:C	2.59	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	319/332 (96%)	293 (92%)	18 (6%)	8 (2%)	5 14
1	B	319/332 (96%)	299 (94%)	18 (6%)	2 (1%)	25 50
1	C	319/332 (96%)	294 (92%)	23 (7%)	2 (1%)	25 50
1	D	319/332 (96%)	295 (92%)	18 (6%)	6 (2%)	8 20
All	All	1276/1328 (96%)	1181 (93%)	77 (6%)	18 (1%)	11 28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	A	76	GLY
1	A	196	ASP
1	C	75	SER
1	D	75	SER
1	D	76	GLY
1	A	185	ALA

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Mol	Chain	Res	Type
1	B	199	ALA
1	C	76	GLY
1	D	186	LEU
1	D	278	ARG
1	A	278	ARG
1	B	278	ARG
1	A	186	LEU
1	A	273	GLU
1	D	221	ASN
1	D	199	ALA
1	A	184	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	278/289 (96%)	266 (96%)	12 (4%)	29	57
1	B	278/289 (96%)	269 (97%)	9 (3%)	39	68
1	C	278/289 (96%)	265 (95%)	13 (5%)	26	54
1	D	278/289 (96%)	268 (96%)	10 (4%)	35	64
All	All	1112/1156 (96%)	1068 (96%)	44 (4%)	31	60

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	69	VAL
1	A	83	ASP
1	A	149	ASN
1	A	152	GLU
1	A	166	GLU
1	A	191	GLU
1	A	196	ASP
1	A	202	ARG
1	A	236	LYS

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Mol	Chain	Res	Type
1	A	248	SER
1	A	255	ASN
1	B	6	LEU
1	B	24	GLN
1	B	83	ASP
1	B	149	ASN
1	B	158	ARG
1	B	202	ARG
1	B	236	LYS
1	B	238	LYS
1	B	320	GLU
1	C	8	LEU
1	C	24	GLN
1	C	61	THR
1	C	69	VAL
1	C	83	ASP
1	C	149	ASN
1	C	158	ARG
1	C	188	GLU
1	C	201	PRO
1	C	202	ARG
1	C	236	LYS
1	C	248	SER
1	C	255	ASN
1	D	6	LEU
1	D	24	GLN
1	D	149	ASN
1	D	152	GLU
1	D	158	ARG
1	D	166	GLU
1	D	201	PRO
1	D	202	ARG
1	D	228	THR
1	D	236	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	149	ASN
1	A	221	ASN
1	A	240	GLN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	298	GLN
1	B	16	GLN
1	B	132	ASN
1	B	149	ASN
1	B	193	ASN
1	B	211	GLN
1	B	221	ASN
1	B	240	GLN
1	B	255	ASN
1	B	275	HIS
1	B	298	GLN
1	C	21	GLN
1	C	132	ASN
1	C	149	ASN
1	C	221	ASN
1	C	240	GLN
1	C	255	ASN
1	C	298	GLN
1	D	132	ASN
1	D	149	ASN
1	D	193	ASN
1	D	221	ASN
1	D	240	GLN
1	D	255	ASN
1	D	298	GLN

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)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	411	-	4,4,4	1.86	2 (50%)	6,6,6	0.93	0
3	NAD	C	403	-	42,48,48	2.35	14 (33%)	50,73,73	1.90	14 (28%)
3	NAD	B	402	-	42,48,48	2.24	12 (28%)	50,73,73	1.92	18 (36%)
2	SO4	A	405	-	4,4,4	1.86	2 (50%)	6,6,6	0.89	0
2	SO4	D	426	-	4,4,4	1.90	2 (50%)	6,6,6	0.88	0
2	SO4	D	430	-	4,4,4	1.91	2 (50%)	6,6,6	0.89	0
2	SO4	B	415	-	4,4,4	1.88	2 (50%)	6,6,6	0.89	0
2	SO4	D	429	-	4,4,4	1.91	2 (50%)	6,6,6	0.88	0
2	SO4	B	412	-	4,4,4	1.84	2 (50%)	6,6,6	0.93	0
2	SO4	C	410	-	4,4,4	1.91	2 (50%)	6,6,6	0.88	0
2	SO4	C	423	-	4,4,4	1.87	2 (50%)	6,6,6	0.91	0
2	SO4	A	409	-	4,4,4	1.79	2 (50%)	6,6,6	0.92	0
3	NAD	D	404	-	42,48,48	2.26	11 (26%)	50,73,73	1.85	14 (28%)
3	NAD	A	401	-	42,48,48	2.34	12 (28%)	50,73,73	1.88	14 (28%)
2	SO4	B	418	-	4,4,4	1.87	2 (50%)	6,6,6	0.93	0
2	SO4	A	408	-	4,4,4	1.83	1 (25%)	6,6,6	0.94	0
2	SO4	A	406	-	4,4,4	1.89	2 (50%)	6,6,6	0.90	0
2	SO4	C	422	-	4,4,4	1.86	2 (50%)	6,6,6	0.91	0
2	SO4	D	428	-	4,4,4	1.81	2 (50%)	6,6,6	0.93	0
2	SO4	B	413	-	4,4,4	1.87	2 (50%)	6,6,6	0.95	0
2	SO4	A	407	-	4,4,4	1.86	2 (50%)	6,6,6	0.92	0
2	SO4	B	419	-	4,4,4	1.90	2 (50%)	6,6,6	0.90	0
2	SO4	C	424	-	4,4,4	1.84	2 (50%)	6,6,6	0.90	0
2	SO4	B	420	-	4,4,4	1.87	2 (50%)	6,6,6	0.88	0
2	SO4	B	417	-	4,4,4	1.92	2 (50%)	6,6,6	0.88	0
2	SO4	D	425	-	4,4,4	1.84	2 (50%)	6,6,6	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	427	-	4,4,4	1.88	2 (50%)	6,6,6	0.89	0
2	SO4	C	421	-	4,4,4	1.86	2 (50%)	6,6,6	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	401	-	-	12/26/62/62	0/5/5/5
3	NAD	C	403	-	-	9/26/62/62	0/5/5/5
3	NAD	B	402	-	-	11/26/62/62	0/5/5/5
3	NAD	D	404	-	-	11/26/62/62	0/5/5/5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C2N-N1N	7.32	1.43	1.35
3	B	402	NAD	C2N-N1N	6.72	1.43	1.35
3	C	403	NAD	C2N-N1N	6.57	1.43	1.35
3	D	404	NAD	C2N-N1N	6.44	1.42	1.35
3	D	404	NAD	C4N-C3N	5.67	1.49	1.39
3	B	402	NAD	C4N-C3N	5.57	1.48	1.39
3	C	403	NAD	C4N-C3N	5.56	1.48	1.39
3	A	401	NAD	C4N-C3N	5.42	1.48	1.39
3	C	403	NAD	O4D-C1D	5.17	1.48	1.41
3	D	404	NAD	C6N-N1N	4.63	1.46	1.35
3	A	401	NAD	C6N-N1N	4.61	1.46	1.35
3	B	402	NAD	O4D-C1D	4.61	1.47	1.41
3	B	402	NAD	PA-O5B	-4.55	1.40	1.59
3	D	404	NAD	O4D-C1D	4.44	1.47	1.41
3	B	402	NAD	C6N-N1N	4.36	1.46	1.35
3	A	401	NAD	O4D-C1D	4.31	1.47	1.41
3	A	401	NAD	PA-O5B	-4.26	1.42	1.59
3	D	404	NAD	PA-O5B	-4.25	1.42	1.59
3	C	403	NAD	PA-O5B	-4.18	1.42	1.59
3	C	403	NAD	C6N-N1N	4.15	1.45	1.35
3	C	403	NAD	C2A-N1A	3.88	1.41	1.33
3	A	401	NAD	C2D-C1D	-3.85	1.47	1.53
3	D	404	NAD	C2A-N1A	3.76	1.40	1.33
3	C	403	NAD	C2D-C1D	-3.74	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C2A-N1A	3.72	1.40	1.33
3	B	402	NAD	C2A-N1A	3.63	1.40	1.33
2	B	419	SO4	O1-S	3.19	1.63	1.46
2	C	410	SO4	O1-S	3.18	1.63	1.46
2	D	429	SO4	O1-S	3.18	1.63	1.46
2	D	430	SO4	O1-S	3.17	1.63	1.46
2	B	417	SO4	O1-S	3.16	1.63	1.46
2	D	426	SO4	O1-S	3.14	1.63	1.46
2	D	427	SO4	O1-S	3.13	1.63	1.46
2	A	406	SO4	O1-S	3.11	1.62	1.46
2	B	418	SO4	O1-S	3.11	1.62	1.46
2	B	415	SO4	O1-S	3.10	1.62	1.46
2	A	411	SO4	O1-S	3.10	1.62	1.46
2	B	413	SO4	O1-S	3.10	1.62	1.46
2	B	420	SO4	O1-S	3.09	1.62	1.46
2	C	422	SO4	O1-S	3.09	1.62	1.46
2	C	423	SO4	O1-S	3.09	1.62	1.46
3	D	404	NAD	C2D-C1D	-3.08	1.49	1.53
2	A	407	SO4	O1-S	3.07	1.62	1.46
3	C	403	NAD	PA-O1A	3.06	1.61	1.50
2	A	405	SO4	O1-S	3.05	1.62	1.46
2	C	421	SO4	O1-S	3.05	1.62	1.46
2	D	425	SO4	O1-S	3.03	1.62	1.46
2	A	408	SO4	O1-S	3.02	1.62	1.46
2	C	424	SO4	O1-S	3.01	1.62	1.46
2	B	412	SO4	O1-S	2.98	1.62	1.46
2	D	428	SO4	O1-S	2.98	1.62	1.46
3	D	404	NAD	PA-O1A	2.96	1.61	1.50
3	A	401	NAD	PA-O1A	2.93	1.61	1.50
2	A	409	SO4	O1-S	2.90	1.61	1.46
3	B	402	NAD	PA-O1A	2.83	1.61	1.50
3	B	402	NAD	PN-O1N	2.62	1.60	1.50
3	D	404	NAD	PN-O1N	2.61	1.60	1.50
3	C	403	NAD	PN-O1N	2.59	1.60	1.50
3	D	404	NAD	C5N-C4N	2.59	1.44	1.38
3	A	401	NAD	PN-O1N	2.55	1.59	1.50
3	B	402	NAD	C2D-C1D	-2.53	1.49	1.53
3	A	401	NAD	C5N-C4N	2.51	1.44	1.38
3	C	403	NAD	C3N-C7N	2.50	1.54	1.50
3	A	401	NAD	C6N-C5N	2.50	1.44	1.38
3	D	404	NAD	C6N-C5N	2.43	1.44	1.38
3	B	402	NAD	C5N-C4N	2.42	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	NAD	C2A-N3A	2.37	1.35	1.32
3	B	402	NAD	C2A-N3A	2.24	1.35	1.32
3	C	403	NAD	C5N-C4N	2.18	1.43	1.38
3	C	403	NAD	C6N-C5N	2.18	1.43	1.38
2	B	417	SO4	O3-S	-2.13	1.30	1.47
3	A	401	NAD	C2A-N3A	2.12	1.35	1.32
2	A	406	SO4	O3-S	-2.10	1.30	1.47
3	C	403	NAD	O7N-C7N	-2.10	1.20	1.24
2	B	415	SO4	O3-S	-2.09	1.30	1.47
2	C	423	SO4	O3-S	-2.08	1.30	1.47
2	D	426	SO4	O3-S	-2.08	1.30	1.47
2	B	412	SO4	O3-S	-2.08	1.30	1.47
2	A	405	SO4	O3-S	-2.08	1.30	1.47
2	C	410	SO4	O3-S	-2.07	1.30	1.47
2	D	429	SO4	O3-S	-2.07	1.30	1.47
2	C	424	SO4	O3-S	-2.07	1.30	1.47
2	D	430	SO4	O3-S	-2.06	1.30	1.47
2	B	413	SO4	O3-S	-2.05	1.31	1.47
2	A	409	SO4	O3-S	-2.05	1.31	1.47
2	C	421	SO4	O3-S	-2.05	1.31	1.47
2	B	420	SO4	O3-S	-2.05	1.31	1.47
2	C	422	SO4	O3-S	-2.04	1.31	1.47
2	A	407	SO4	O3-S	-2.04	1.31	1.47
2	D	427	SO4	O3-S	-2.04	1.31	1.47
3	B	402	NAD	C6N-C5N	2.03	1.43	1.38
2	D	428	SO4	O3-S	-2.03	1.31	1.47
2	B	419	SO4	O3-S	-2.02	1.31	1.47
2	B	418	SO4	O3-S	-2.02	1.31	1.47
2	D	425	SO4	O3-S	-2.02	1.31	1.47
2	A	411	SO4	O3-S	-2.00	1.31	1.47

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	NAD	PA-O5B-C5B	5.17	152.00	121.68
3	D	404	NAD	PA-O5B-C5B	5.06	151.36	121.68
3	A	401	NAD	PA-O5B-C5B	4.98	150.86	121.68
3	C	403	NAD	PA-O5B-C5B	4.89	150.33	121.68
3	A	401	NAD	C3B-C2B-C1B	4.20	107.30	100.98
3	C	403	NAD	C3B-C2B-C1B	4.13	107.20	100.98
3	B	402	NAD	N3A-C2A-N1A	-4.05	122.35	128.68
3	D	404	NAD	N3A-C2A-N1A	-4.05	122.36	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	404	NAD	C3B-C2B-C1B	3.98	106.97	100.98
3	B	402	NAD	C3B-C2B-C1B	3.94	106.91	100.98
3	A	401	NAD	N3A-C2A-N1A	-3.88	122.61	128.68
3	C	403	NAD	N3A-C2A-N1A	-3.80	122.75	128.68
3	C	403	NAD	C3N-C7N-N7N	3.57	122.03	117.75
3	B	402	NAD	C3N-C7N-N7N	3.43	121.86	117.75
3	D	404	NAD	C5A-C6A-N6A	3.38	125.49	120.35
3	B	402	NAD	C5A-C6A-N6A	3.34	125.43	120.35
3	C	403	NAD	C5A-C6A-N6A	3.34	125.43	120.35
3	A	401	NAD	C5A-C6A-N6A	3.29	125.35	120.35
3	B	402	NAD	PN-O5D-C5D	-3.29	102.39	121.68
3	D	404	NAD	PN-O5D-C5D	-3.23	102.75	121.68
3	C	403	NAD	PN-O5D-C5D	-3.20	102.92	121.68
3	B	402	NAD	O7N-C7N-C3N	-3.18	115.83	119.63
3	A	401	NAD	PN-O5D-C5D	-3.10	103.49	121.68
3	A	401	NAD	C3N-C7N-N7N	3.09	121.46	117.75
3	A	401	NAD	O7N-C7N-C3N	-3.04	115.99	119.63
3	D	404	NAD	C3N-C7N-N7N	2.79	121.10	117.75
3	C	403	NAD	O7N-C7N-C3N	-2.78	116.30	119.63
3	A	401	NAD	C1B-N9A-C4A	2.75	131.48	126.64
3	D	404	NAD	C2A-N1A-C6A	2.74	123.44	118.75
3	B	402	NAD	C2A-N1A-C6A	2.71	123.39	118.75
3	C	403	NAD	C2A-N1A-C6A	2.71	123.38	118.75
3	A	401	NAD	C2N-C3N-C4N	2.69	121.30	118.26
3	C	403	NAD	C1B-N9A-C4A	2.66	131.32	126.64
3	A	401	NAD	C2A-N1A-C6A	2.63	123.25	118.75
3	C	403	NAD	C5A-C6A-N1A	-2.60	114.46	120.35
3	D	404	NAD	O7N-C7N-C3N	-2.59	116.53	119.63
3	D	404	NAD	C2N-C3N-C4N	2.58	121.18	118.26
3	A	401	NAD	C5A-C6A-N1A	-2.57	114.52	120.35
3	D	404	NAD	C5A-C6A-N1A	-2.55	114.58	120.35
3	B	402	NAD	C5A-C6A-N1A	-2.54	114.58	120.35
3	B	402	NAD	C2N-C3N-C4N	2.54	121.13	118.26
3	B	402	NAD	PN-O3-PA	-2.45	124.43	132.83
3	D	404	NAD	O5D-PN-O1N	-2.41	99.64	109.07
3	B	402	NAD	C3D-C2D-C1D	2.36	104.54	100.98
3	C	403	NAD	C2N-C3N-C4N	2.35	120.93	118.26
3	A	401	NAD	O5D-PN-O1N	-2.34	99.92	109.07
3	D	404	NAD	C1B-N9A-C4A	2.33	130.74	126.64
3	C	403	NAD	O4D-C1D-C2D	-2.27	103.61	106.93
3	B	402	NAD	O4B-C1B-C2B	-2.27	103.61	106.93
3	B	402	NAD	O5D-PN-O1N	-2.22	100.39	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	403	NAD	O5D-PN-O1N	-2.21	100.43	109.07
3	B	402	NAD	C3N-C2N-N1N	-2.12	118.36	120.43
3	C	403	NAD	PN-O3-PA	-2.12	125.56	132.83
3	B	402	NAD	C1B-N9A-C4A	2.11	130.35	126.64
3	A	401	NAD	PN-O3-PA	-2.10	125.60	132.83
3	B	402	NAD	O2A-PA-O5B	2.09	117.45	107.75
3	D	404	NAD	C5N-C6N-N1N	-2.06	117.45	120.40
3	B	402	NAD	C5N-C6N-N1N	-2.02	117.50	120.40
3	A	401	NAD	C3N-C2N-N1N	-2.02	118.45	120.43
3	D	404	NAD	PN-O3-PA	-2.02	125.90	132.83

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAD	C5B-O5B-PA-O1A
3	A	401	NAD	C5B-O5B-PA-O2A
3	A	401	NAD	C3B-C4B-C5B-O5B
3	A	401	NAD	C5D-O5D-PN-O3
3	A	401	NAD	C5D-O5D-PN-O2N
3	B	402	NAD	C5B-O5B-PA-O1A
3	B	402	NAD	C5B-O5B-PA-O2A
3	B	402	NAD	PN-O3-PA-O5B
3	B	402	NAD	C3B-C4B-C5B-O5B
3	B	402	NAD	C5D-O5D-PN-O3
3	B	402	NAD	C5D-O5D-PN-O2N
3	C	403	NAD	C5B-O5B-PA-O1A
3	C	403	NAD	C5B-O5B-PA-O2A
3	C	403	NAD	PN-O3-PA-O5B
3	C	403	NAD	C3B-C4B-C5B-O5B
3	D	404	NAD	C5B-O5B-PA-O1A
3	D	404	NAD	C5B-O5B-PA-O2A
3	D	404	NAD	C3B-C4B-C5B-O5B
3	D	404	NAD	C5D-O5D-PN-O3
3	D	404	NAD	C5D-O5D-PN-O1N
3	D	404	NAD	C5D-O5D-PN-O2N
3	A	401	NAD	O4B-C4B-C5B-O5B
3	C	403	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	O4B-C4B-C5B-O5B
3	D	404	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	C4D-C5D-O5D-PN
3	C	403	NAD	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
3	A	401	NAD	PN-O3-PA-O5B
3	D	404	NAD	PN-O3-PA-O5B
3	A	401	NAD	C4D-C5D-O5D-PN
3	A	401	NAD	PA-O3-PN-O2N
3	B	402	NAD	PA-O3-PN-O2N
3	C	403	NAD	PA-O3-PN-O2N
3	D	404	NAD	PA-O3-PN-O2N
3	D	404	NAD	C4D-C5D-O5D-PN
3	A	401	NAD	C5D-O5D-PN-O1N
3	B	402	NAD	C5D-O5D-PN-O1N
3	C	403	NAD	C5D-O5D-PN-O2N
3	A	401	NAD	C5B-O5B-PA-O3
3	B	402	NAD	C5B-O5B-PA-O3
3	C	403	NAD	C5B-O5B-PA-O3
3	D	404	NAD	C5B-O5B-PA-O3
3	A	401	NAD	PA-O3-PN-O1N

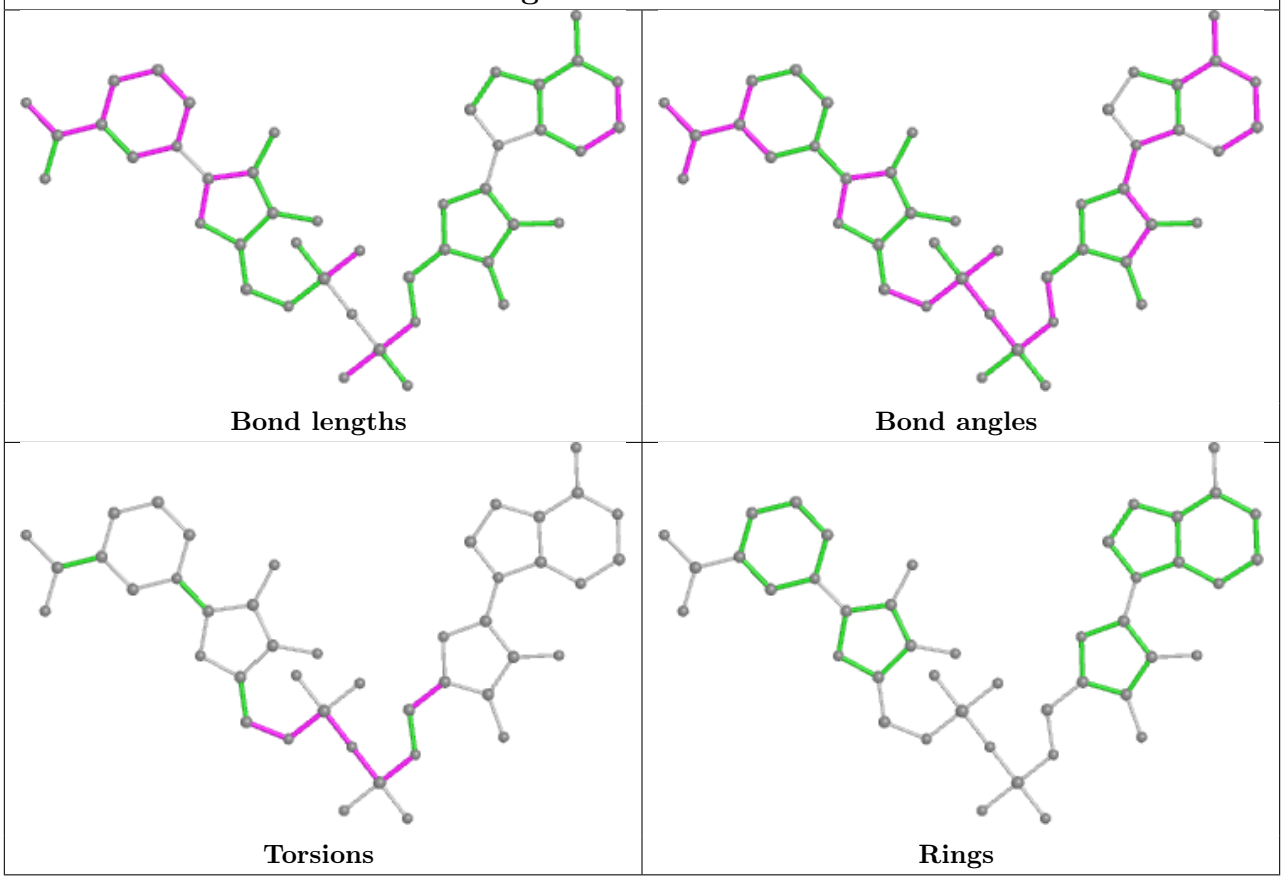
There are no ring outliers.

6 monomers are involved in 12 short contacts:

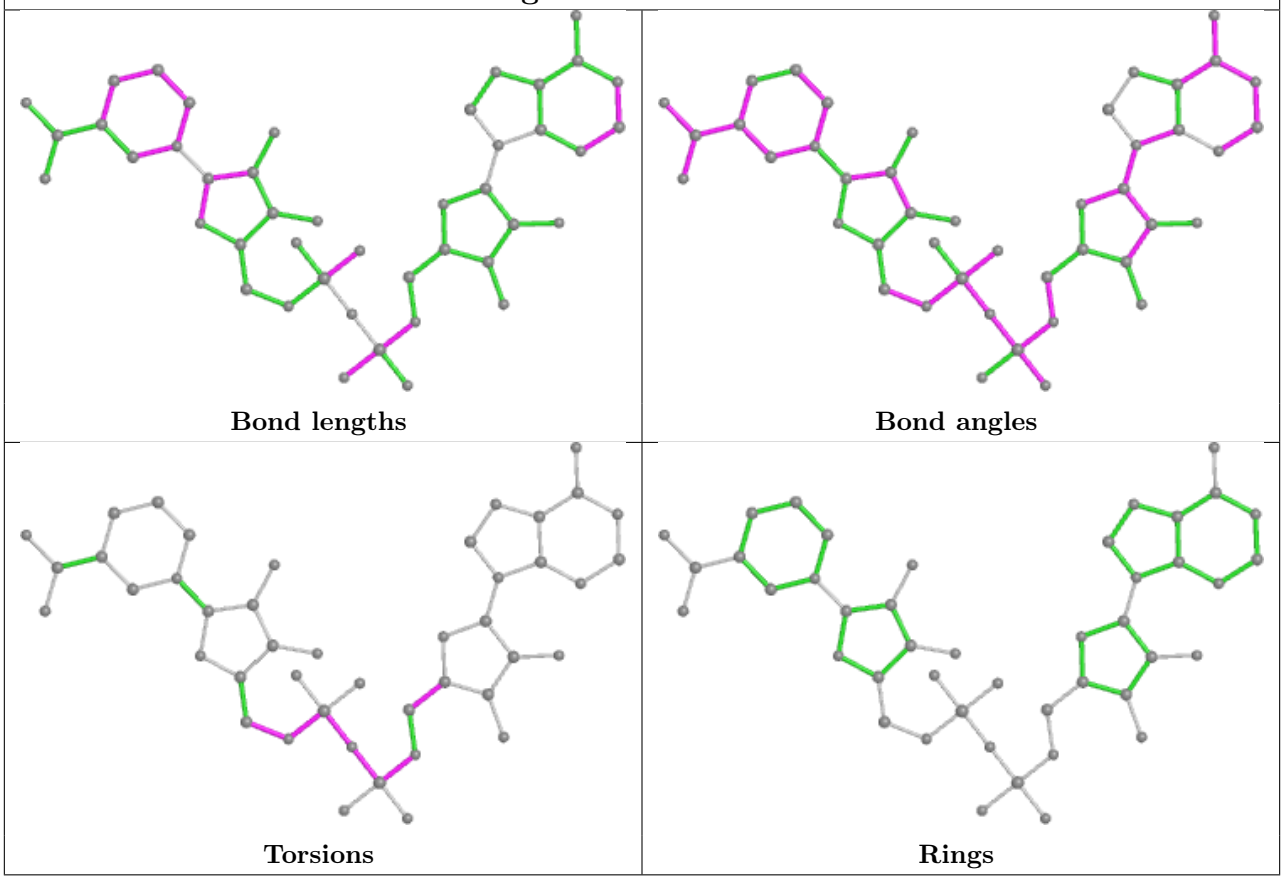
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	NAD	2	0
3	B	402	NAD	3	0
2	C	423	SO4	1	0
3	D	404	NAD	2	0
3	A	401	NAD	3	0
2	B	417	SO4	1	0

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 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.

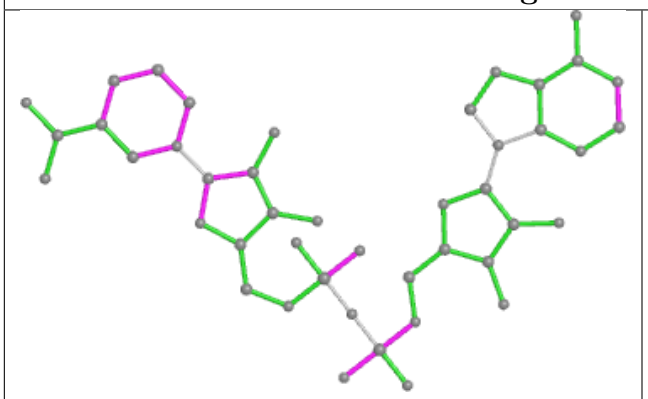
Ligand NAD C 403



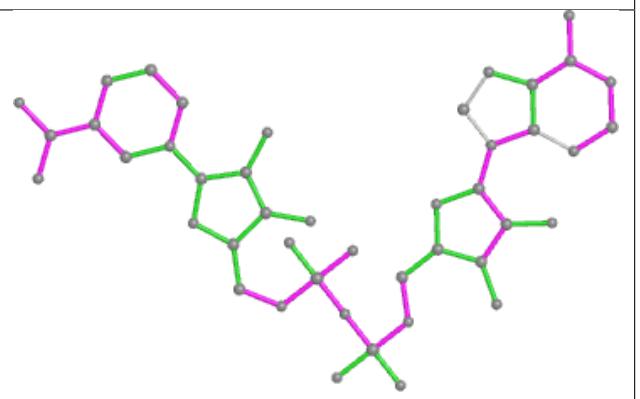
Ligand NAD B 402



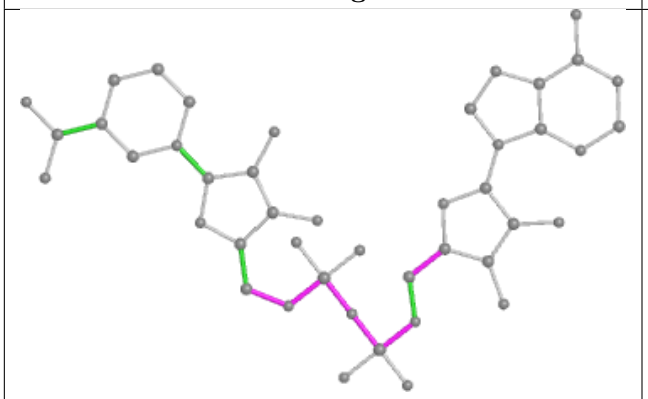
Ligand NAD D 404



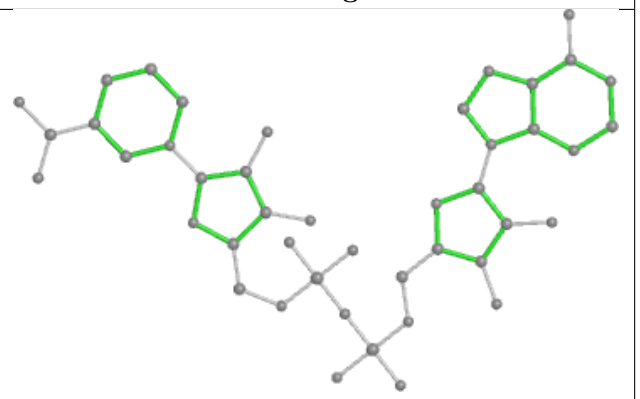
Bond lengths



Bond angles

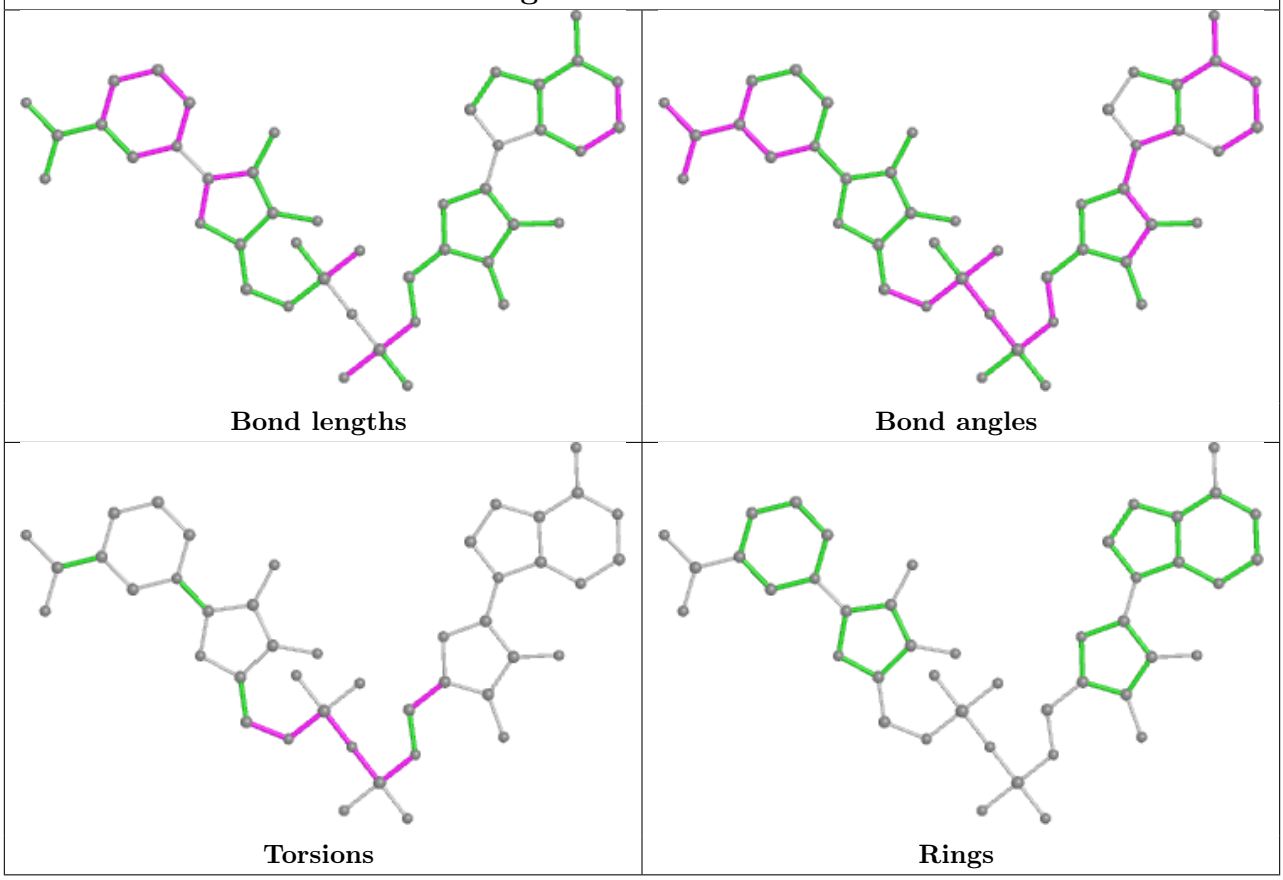


Torsions



Rings

Ligand NAD A 401



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	321/332 (96%)	-0.26	9 (2%)	53	54	8, 32, 76, 142	0
1	B	321/332 (96%)	-0.19	7 (2%)	62	63	14, 34, 85, 127	0
1	C	321/332 (96%)	-0.11	18 (5%)	24	23	11, 35, 89, 151	0
1	D	321/332 (96%)	-0.05	11 (3%)	45	45	15, 42, 88, 141	0
All	All	1284/1328 (96%)	-0.16	45 (3%)	44	44	8, 36, 86, 151	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ASN	5.6
1	C	188	GLU	4.8
1	A	191	GLU	4.7
1	D	191	GLU	4.7
1	C	191	GLU	4.3
1	B	193	ASN	3.8
1	C	196	ASP	3.7
1	D	193	ASN	3.7
1	A	197	ILE	3.7
1	D	194	GLY	3.7
1	B	194	GLY	3.6
1	B	191	GLU	3.5
1	C	192	GLU	3.4
1	D	195	GLN	3.2
1	C	75	SER	3.1
1	C	189	GLU	3.1
1	C	194	GLY	3.0
1	D	196	ASP	3.0
1	C	195	GLN	3.0
1	C	193	ASN	3.0
1	D	187	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	323	THR	3.0
1	B	195	GLN	2.9
1	A	188	GLU	2.9
1	A	74	LEU	2.9
1	D	199	ALA	2.8
1	B	197	ILE	2.8
1	A	189	GLU	2.7
1	C	197	ILE	2.7
1	D	192	GLU	2.5
1	C	324	VAL	2.5
1	D	197	ILE	2.4
1	C	76	GLY	2.4
1	B	196	ASP	2.4
1	C	83	ASP	2.4
1	C	187	ASN	2.3
1	A	323	THR	2.3
1	A	192	GLU	2.3
1	C	181	GLN	2.2
1	C	74	LEU	2.2
1	C	34	GLN	2.2
1	B	215	LYS	2.1
1	D	167	PRO	2.1
1	A	184	VAL	2.0
1	D	323	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)

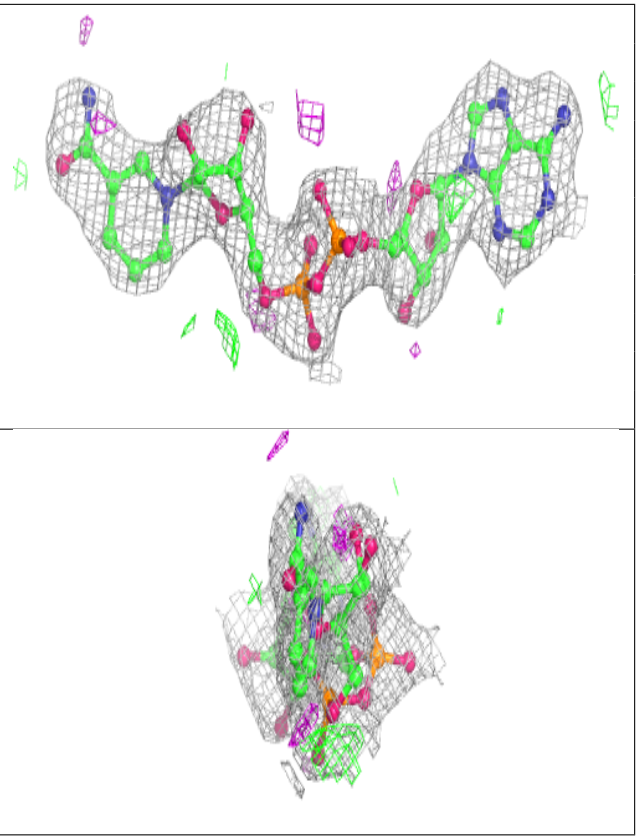
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	429	5/5	0.69	0.37	113,113,113,113	0
2	SO4	B	419	5/5	0.74	0.37	111,111,111,111	0
2	SO4	A	406	5/5	0.80	0.27	103,103,103,103	0
2	SO4	D	430	5/5	0.82	0.34	100,100,100,100	0
2	SO4	C	410	5/5	0.83	0.24	113,113,113,113	0
2	SO4	D	426	5/5	0.85	0.23	109,109,109,109	0
2	SO4	D	427	5/5	0.85	0.16	112,112,112,112	0
2	SO4	B	418	5/5	0.87	0.28	96,96,96,96	0
2	SO4	C	422	5/5	0.87	0.27	102,102,102,102	0
2	SO4	A	411	5/5	0.88	0.25	97,97,97,97	0
2	SO4	D	428	5/5	0.89	0.18	115,115,115,115	0
2	SO4	A	409	5/5	0.89	0.25	87,87,87,87	0
2	SO4	B	415	5/5	0.89	0.17	110,110,110,110	0
2	SO4	C	424	5/5	0.90	0.32	98,98,98,98	0
2	SO4	C	423	5/5	0.90	0.24	112,112,112,112	0
2	SO4	B	413	5/5	0.91	0.21	77,77,77,77	0
4	NA	B	531	1/1	0.93	0.23	29,29,29,29	0
3	NAD	C	403	44/44	0.94	0.17	36,36,36,36	0
3	NAD	A	401	44/44	0.95	0.16	32,32,32,32	0
2	SO4	A	408	5/5	0.95	0.15	73,73,73,73	0
2	SO4	A	407	5/5	0.95	0.14	89,89,89,89	0
3	NAD	D	404	44/44	0.96	0.14	37,37,37,37	0
3	NAD	B	402	44/44	0.96	0.15	35,35,35,35	0
4	NA	D	532	1/1	0.96	0.14	34,34,34,34	0
2	SO4	D	425	5/5	0.97	0.16	62,62,62,62	0
2	SO4	A	405	5/5	0.98	0.15	51,51,51,51	0
2	SO4	B	412	5/5	0.98	0.12	49,49,49,49	0
2	SO4	B	420	5/5	0.98	0.10	64,64,64,64	0
2	SO4	B	417	5/5	0.98	0.11	46,46,46,46	0
2	SO4	C	421	5/5	0.98	0.11	47,47,47,47	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.

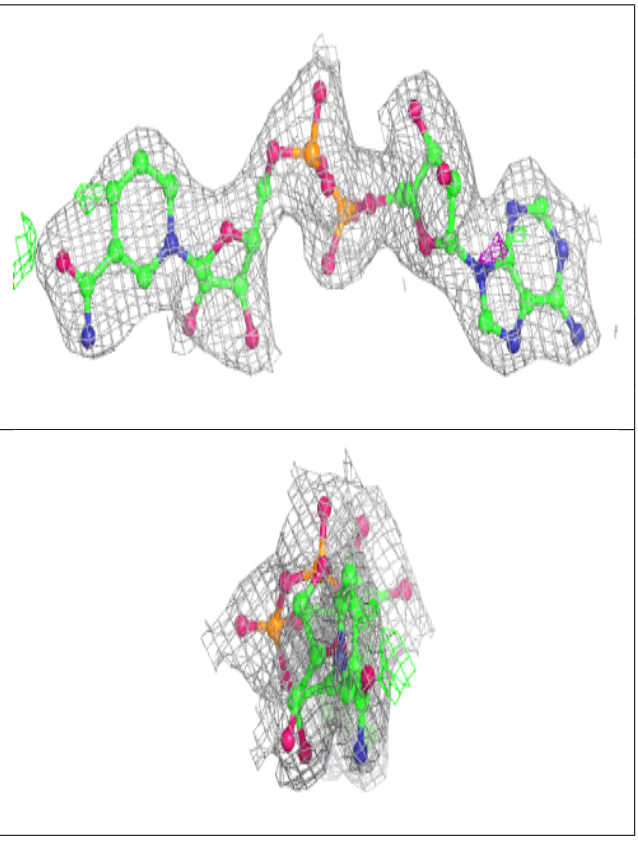
Electron density around NAD C 403:

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



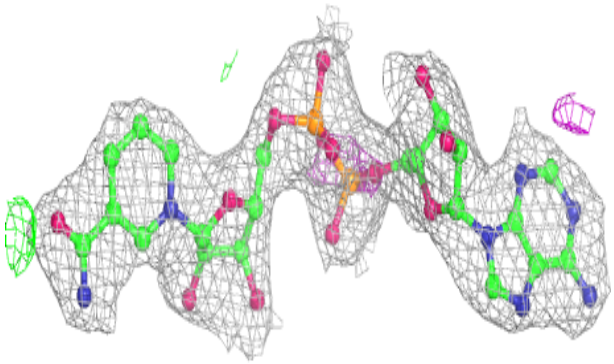
Electron density around NAD A 401:

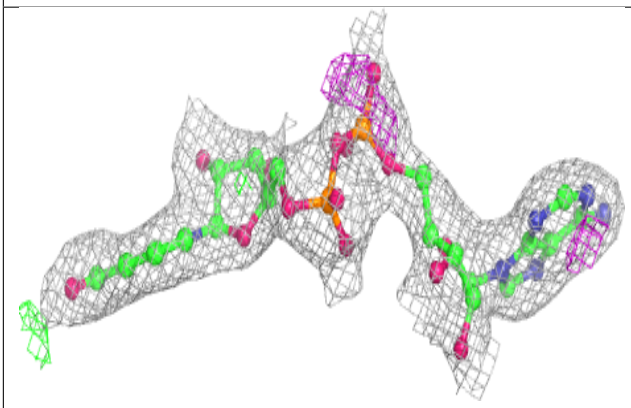
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

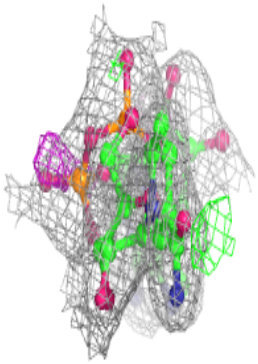


Electron density around NAD D 404:

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

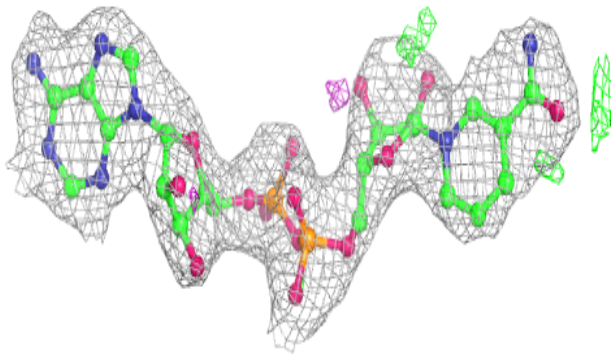


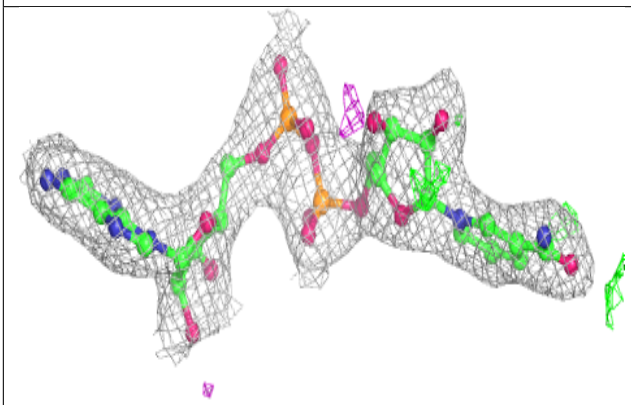


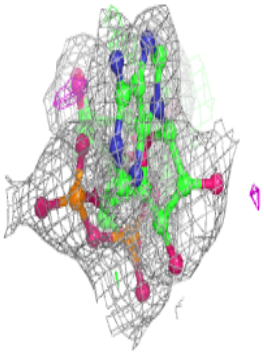


Electron density around NAD B 402:

$2mF_o$-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.