Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 03:11 AM EDT

PDB ID	:	3QW2
Title	:	L-myo-inositol 1-phosphate synthase from Archaeoglobus mutant N255A
Authors	:	Neelon, K.; Roberts, M.F.; Stec, B.
Deposited on	:	2011-02-26
Resolution	:	2.59 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

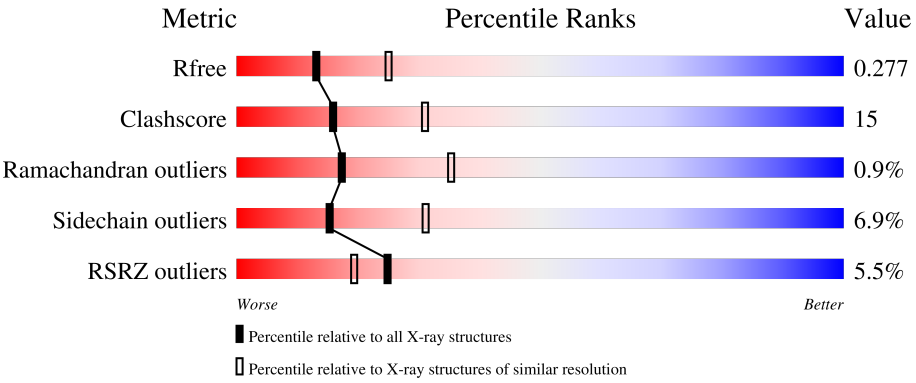
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	392	6% 67% 29% .
1	B	392	6% 68% 28% .
1	C	392	5% 72% 25% .
1	D	392	5% 72% 25% .

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
5	SO4	B	394	-	-	X	-
6	K	C	398	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13061 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.

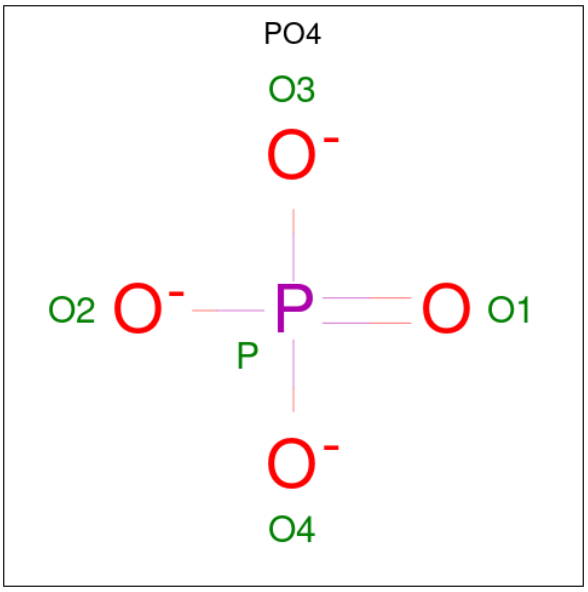
- Molecule 1 is a protein called Myo-inositol-1-phosphate synthase (Ino1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			
1	B	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			
1	C	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			
1	D	392	Total	C	N	O	S	0	0	0
			3081	1995	498	575	13			

There are 4 discrepancies between the modelled and reference sequences:

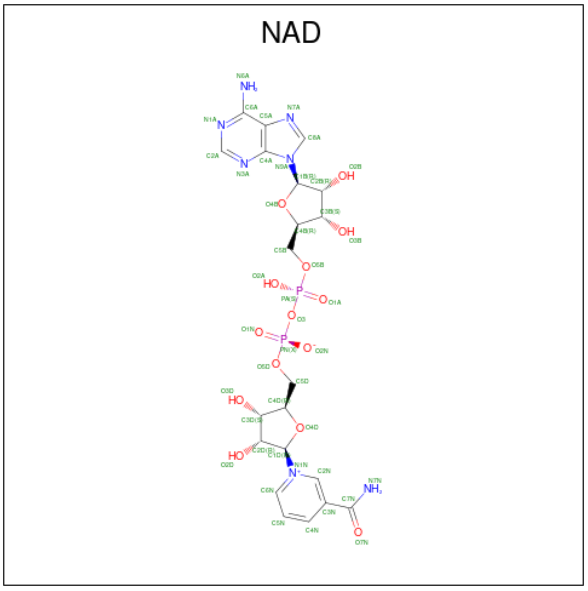
Chain	Residue	Modelled	Actual	Comment	Reference
A	255	ALA	ASN	engineered mutation	UNP O28480
B	255	ALA	ASN	engineered mutation	UNP O28480
C	255	ALA	ASN	engineered mutation	UNP O28480
D	255	ALA	ASN	engineered mutation	UNP O28480

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



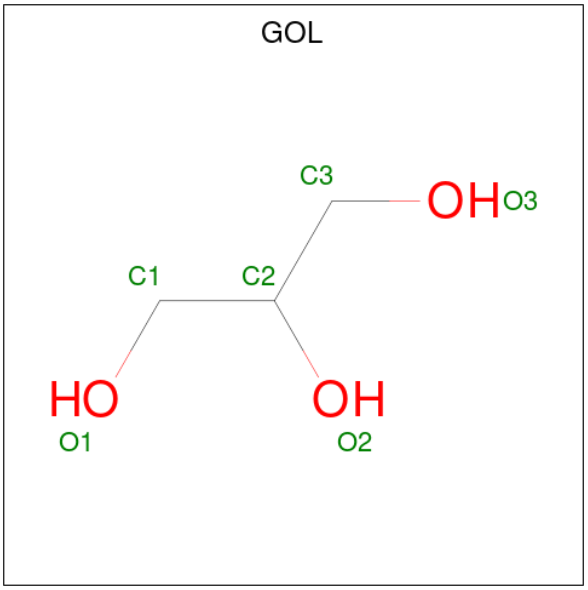
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

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



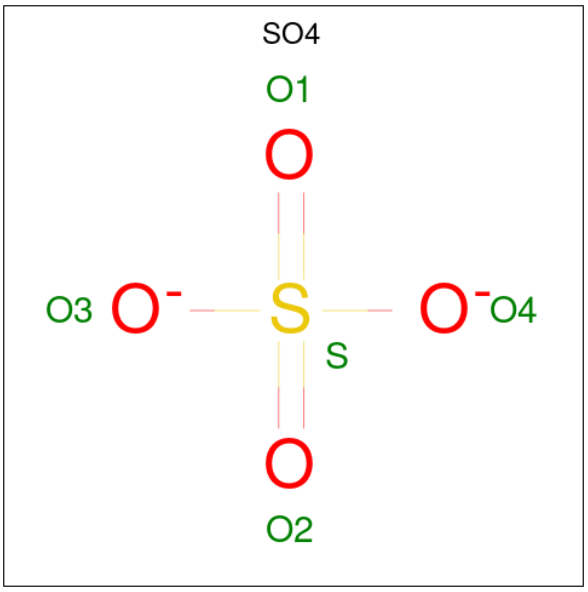
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is water.

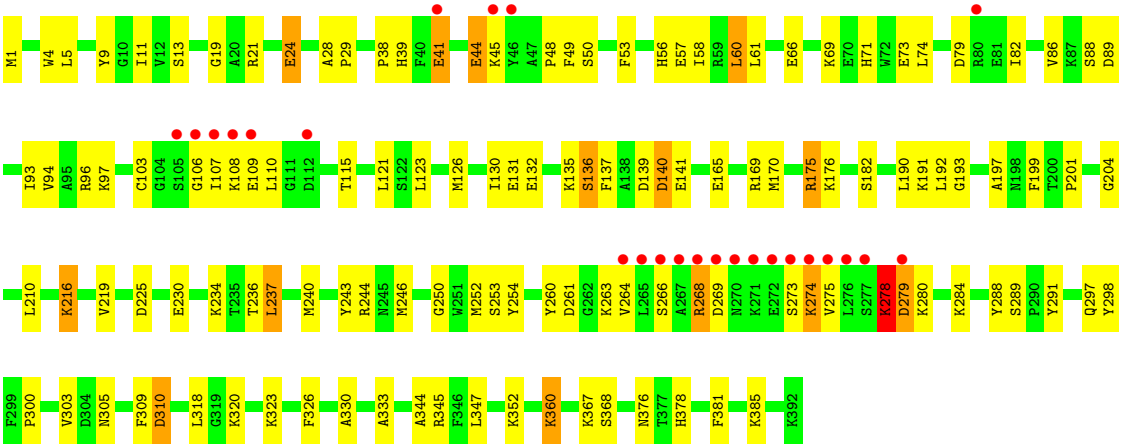
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	115	Total O 115 115	0	0
7	B	100	Total O 100 100	0	0
7	C	138	Total O 138 138	0	0
7	D	133	Total O 133 133	0	0

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.

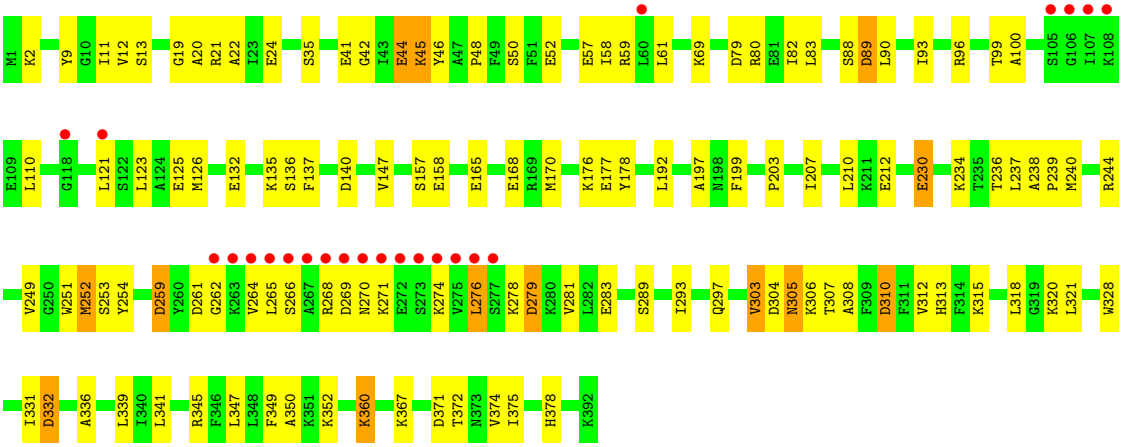
• Molecule 1: Myo-inositol-1-phosphate synthase (Ino1)

Chain A:



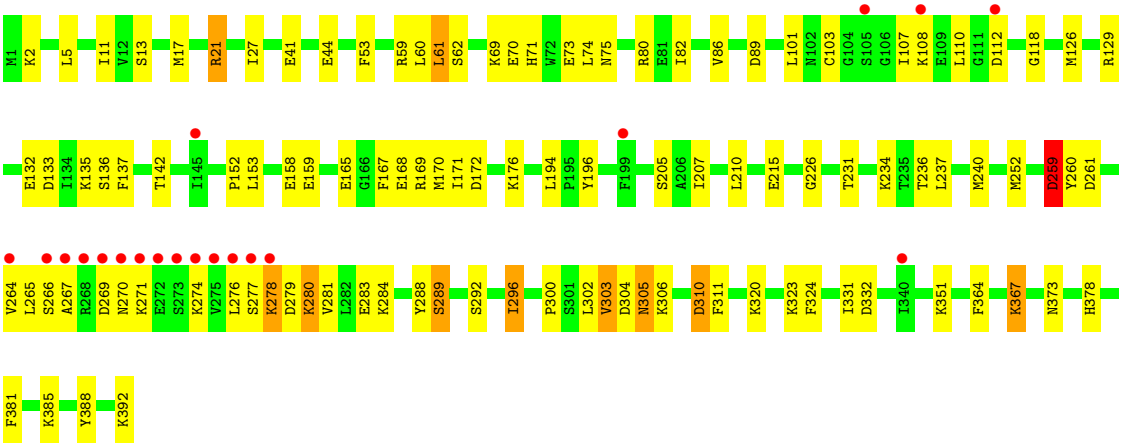
• Molecule 1: Myo-inositol-1-phosphate synthase (Ino1)

Chain B:



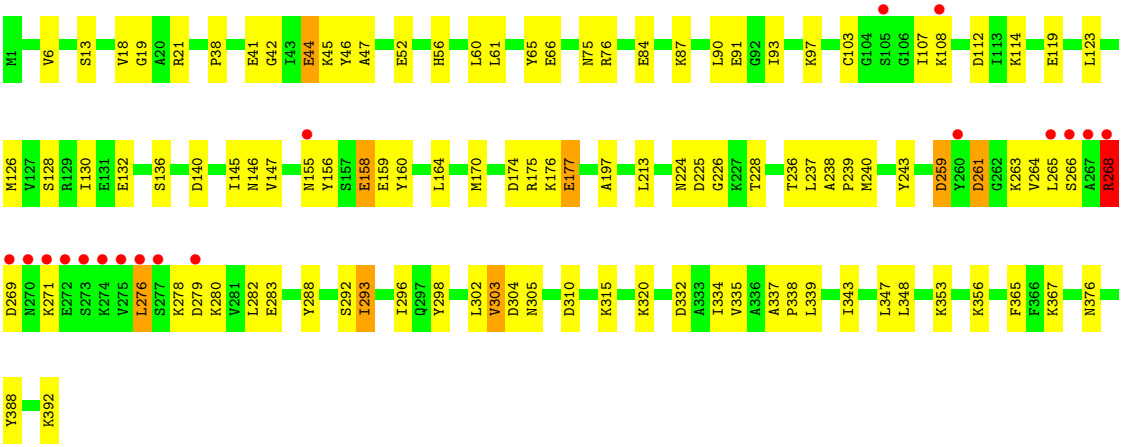
• Molecule 1: Myo-inositol-1-phosphate synthase (Ino1)

Chain C:



• Molecule 1: Myo-inositol-1-phosphate synthase (Ino1)

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	91.51Å 88.04Å 103.73Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	103.14 – 2.59 38.71 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.3 (103.14-2.59) 96.3 (38.71-2.59)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.185 , 0.267 0.193 , 0.277	Depositor DCC
R_{free} test set	2506 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13061	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 4.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, K, 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	0.72	0/3152	0.78	1/4253 (0.0%)
1	B	0.73	0/3152	0.78	2/4253 (0.0%)
1	C	0.73	0/3152	0.79	2/4253 (0.0%)
1	D	0.74	0/3152	0.78	1/4253 (0.0%)
All	All	0.73	0/12608	0.79	6/17012 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	276	LEU	CA-CB-CG	6.21	129.58	115.30
1	B	61	LEU	CA-CB-CG	6.09	129.30	115.30
1	C	61	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	60	LEU	CA-CB-CG	5.68	128.37	115.30
1	D	276	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	74	LEU	CA-CB-CG	5.30	127.48	115.30

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	3081	0	3083	103	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3081	0	3083	95	0
1	C	3081	0	3082	85	0
1	D	3081	0	3083	96	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	44	0	26	0	0
3	B	44	0	26	4	0
3	C	44	0	26	2	0
3	D	44	0	26	3	0
4	A	6	0	8	1	0
4	B	6	0	8	2	0
5	A	5	0	0	0	0
5	B	10	0	0	2	0
5	C	15	0	0	2	0
5	D	10	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	115	0	0	22	0
7	B	100	0	0	23	0
7	C	138	0	0	31	0
7	D	133	0	0	29	0
All	All	13061	0	12451	366	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 (366) 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:293:ILE:HB	7:D:512:HOH:O	1.52	1.08
1:A:253:SER:HB3	7:A:399:HOH:O	1.57	1.03
1:D:126:MET:SD	7:D:466:HOH:O	2.16	1.01
1:B:21:ARG:HD2	7:B:460:HOH:O	1.59	1.01
1:B:121:LEU:HB3	7:B:430:HOH:O	1.61	1.01
1:B:360:LYS:HG2	7:B:483:HOH:O	1.67	0.95
1:A:175:ARG:HE	1:A:175:ARG:HA	1.33	0.93
1:D:123:LEU:HD23	1:D:126:MET:HE3	1.48	0.93
1:D:259:ASP:HB3	7:D:484:HOH:O	1.67	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:HG3	7:D:458:HOH:O	1.68	0.91
1:C:215:GLU:HG3	7:C:445:HOH:O	1.69	0.91
1:A:44:GLU:HB2	1:A:48:PRO:HA	1.50	0.91
1:D:278:LYS:HE2	7:D:426:HOH:O	1.72	0.89
1:D:128:SER:O	1:D:132:GLU:HG3	1.74	0.88
1:D:123:LEU:HD23	1:D:126:MET:CE	2.03	0.87
1:D:123:LEU:HA	1:D:126:MET:CE	2.05	0.87
1:D:97:LYS:HE3	1:D:119:GLU:OE1	1.73	0.87
1:C:283:GLU:HG3	7:C:428:HOH:O	1.75	0.86
1:C:237:LEU:HB2	7:C:400:HOH:O	1.73	0.86
1:A:49:PHE:HD1	7:A:423:HOH:O	1.58	0.86
1:B:125:GLU:HB2	7:B:430:HOH:O	1.75	0.85
1:D:268:ARG:HA	1:D:271:LYS:HB3	1.60	0.83
1:C:107:ILE:HD11	7:C:520:HOH:O	1.78	0.83
1:B:230:GLU:OE2	1:B:253:SER:HB3	1.76	0.83
1:B:13:SER:HB2	1:B:147:VAL:HG21	1.59	0.82
1:B:82:ILE:HG23	7:B:491:HOH:O	1.79	0.82
1:B:254:TYR:OH	1:B:297:GLN:HG3	1.78	0.82
1:B:261:ASP:HB2	7:B:479:HOH:O	1.79	0.82
1:B:289:SER:HB2	7:B:410:HOH:O	1.80	0.81
1:A:121:LEU:O	1:A:176:LYS:NZ	2.13	0.81
1:D:259:ASP:CB	7:D:484:HOH:O	2.23	0.81
1:C:169:ARG:NH2	7:C:405:HOH:O	2.12	0.81
1:C:296:ILE:HB	7:C:502:HOH:O	1.79	0.80
1:A:123:LEU:HA	1:A:126:MET:HE3	1.64	0.79
1:B:177:GLU:HB2	7:B:447:HOH:O	1.81	0.79
1:B:237:LEU:HB2	7:B:451:HOH:O	1.84	0.78
1:D:123:LEU:HA	1:D:126:MET:HE2	1.66	0.77
1:C:260:TYR:CD1	7:C:469:HOH:O	2.38	0.77
1:D:103:CYS:HB3	1:D:107:ILE:HD11	1.67	0.75
1:A:237:LEU:HD12	7:B:451:HOH:O	1.86	0.75
1:C:159:GLU:HG3	7:C:405:HOH:O	1.85	0.75
1:D:60:LEU:HD21	1:D:114:LYS:HG3	1.66	0.75
1:A:21:ARG:HD3	1:A:89:ASP:OD1	1.87	0.75
1:D:107:ILE:HD11	7:D:498:HOH:O	1.85	0.74
1:D:280:LYS:HG3	7:D:444:HOH:O	1.86	0.74
1:D:293:ILE:HG21	7:D:514:HOH:O	1.87	0.74
1:B:197:ALA:HB2	1:B:347:LEU:HD11	1.70	0.74
1:B:41:GLU:HB2	7:B:401:HOH:O	1.87	0.73
7:C:400:HOH:O	1:D:237:LEU:HD22	1.87	0.73
1:D:276:LEU:HD23	7:D:411:HOH:O	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HB3	7:A:464:HOH:O	1.88	0.73
1:C:278:LYS:HA	1:C:281:VAL:HB	1.72	0.72
1:D:21:ARG:HD2	7:D:425:HOH:O	1.89	0.71
1:A:254:TYR:OH	1:A:297:GLN:HG3	1.89	0.71
1:B:303:VAL:HG12	1:B:304:ASP:H	1.55	0.71
1:A:243:TYR:OH	1:B:378:HIS:HD2	1.74	0.71
1:B:79:ASP:HB3	7:C:514:HOH:O	1.90	0.70
1:C:231:THR:HG21	1:C:367:LYS:HG2	1.73	0.70
1:A:243:TYR:OH	1:B:378:HIS:CD2	2.45	0.70
1:A:360:LYS:HD3	7:A:470:HOH:O	1.92	0.69
1:B:360:LYS:HE3	7:B:467:HOH:O	1.93	0.69
1:C:260:TYR:CG	7:C:469:HOH:O	2.46	0.69
1:C:165:GLU:HG3	1:C:169:ARG:HH12	1.58	0.68
1:C:351:LYS:HA	7:C:438:HOH:O	1.92	0.68
1:A:230:GLU:HG3	7:A:399:HOH:O	1.93	0.67
1:C:5:LEU:HD13	1:C:13:SER:OG	1.95	0.67
7:C:400:HOH:O	1:D:237:LEU:CD2	2.42	0.67
1:C:378:HIS:HD2	1:D:243:TYR:OH	1.79	0.66
1:A:103:CYS:HB2	1:A:107:ILE:HG13	1.77	0.66
1:B:303:VAL:HG12	1:B:304:ASP:N	2.11	0.66
1:A:140:ASP:OD2	1:A:141:GLU:HG3	1.96	0.66
1:C:152:PRO:HG3	1:C:270:ASN:HD21	1.59	0.66
1:D:123:LEU:HA	1:D:126:MET:HE3	1.78	0.66
1:C:378:HIS:CD2	1:D:243:TYR:OH	2.48	0.65
1:D:108:LYS:HB2	7:D:408:HOH:O	1.95	0.65
1:D:164:LEU:HD13	1:D:213:LEU:HB2	1.79	0.65
1:C:234:LYS:NZ	1:C:278:LYS:HG2	2.11	0.65
1:A:269:ASP:OD2	7:A:473:HOH:O	2.14	0.65
1:D:269:ASP:HB3	7:D:428:HOH:O	1.96	0.65
1:B:315:LYS:HG2	1:B:321:LEU:HD23	1.80	0.64
1:B:20:ALA:O	1:B:24:GLU:HG3	1.98	0.64
1:A:108:LYS:HA	7:A:482:HOH:O	1.98	0.64
1:A:140:ASP:HB3	7:A:466:HOH:O	1.98	0.64
1:A:320:LYS:HE2	1:B:331:ILE:HD13	1.80	0.64
1:B:274:LYS:HZ2	4:B:397:GOL:HO1	1.45	0.63
1:C:152:PRO:HG3	1:C:270:ASN:ND2	2.13	0.63
1:A:268:ARG:HB3	7:A:438:HOH:O	1.99	0.63
1:C:133:ASP:O	1:C:136:SER:HB3	1.99	0.63
1:C:265:LEU:O	1:C:271:LYS:HB2	1.98	0.63
1:B:283:GLU:HB2	1:B:289:SER:HB3	1.80	0.63
1:D:61:LEU:HD13	1:D:66:GLU:OE1	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:O	1:A:41:GLU:HG2	1.99	0.62
1:D:44:GLU:HG3	7:D:421:HOH:O	1.98	0.62
1:D:52:GLU:HG3	7:D:434:HOH:O	2.00	0.62
1:D:263:LYS:HD3	1:D:298:TYR:CE1	2.34	0.62
1:B:230:GLU:OE2	1:B:253:SER:CB	2.48	0.62
1:C:126:MET:HE1	1:C:176:LYS:HE3	1.81	0.62
1:A:175:ARG:HE	1:A:175:ARG:CA	1.99	0.61
1:C:126:MET:CE	1:C:176:LYS:HE3	2.30	0.61
1:B:374:VAL:HG23	5:B:394:SO4:O1	2.01	0.61
1:B:80:ARG:CD	7:B:463:HOH:O	2.49	0.61
1:B:123:LEU:HD23	1:B:126:MET:HE3	1.82	0.61
1:D:226:GLY:O	3:D:396:NAD:H5N	2.01	0.60
3:D:396:NAD:C4N	7:D:524:HOH:O	2.50	0.60
1:B:46:TYR:HB3	1:B:352:LYS:HD2	1.84	0.60
1:B:80:ARG:HD3	7:B:463:HOH:O	2.02	0.60
1:B:21:ARG:CD	7:B:460:HOH:O	2.33	0.60
1:A:234:LYS:HZ2	1:A:278:LYS:HG2	1.67	0.59
1:D:279:ASP:HB3	1:D:292:SER:OG	2.02	0.59
1:A:126:MET:O	1:A:130:ILE:HG13	2.01	0.59
1:B:230:GLU:HG3	1:B:308:ALA:CB	2.32	0.59
1:D:103:CYS:HB3	1:D:107:ILE:CD1	2.31	0.59
1:D:84:GLU:HG2	7:D:510:HOH:O	2.03	0.59
1:A:175:ARG:HA	1:A:175:ARG:NE	2.10	0.59
1:A:49:PHE:CD1	7:A:423:HOH:O	2.44	0.59
1:A:53:PHE:HB2	1:A:93:ILE:HD13	1.83	0.59
1:C:278:LYS:HG3	7:C:527:HOH:O	2.01	0.59
1:B:157:SER:HB2	1:B:178:TYR:CD2	2.37	0.59
1:D:46:TYR:CE2	1:D:353:LYS:HE2	2.38	0.58
1:B:265:LEU:HD23	1:B:270:ASN:O	2.03	0.58
1:D:107:ILE:HB	7:D:494:HOH:O	2.03	0.58
1:A:250:GLY:HA2	1:A:291:TYR:O	2.03	0.58
1:C:234:LYS:HZ2	1:C:278:LYS:HG2	1.69	0.58
1:D:268:ARG:HA	1:D:271:LYS:CB	2.32	0.58
1:D:38:PRO:O	1:D:41:GLU:HG2	2.04	0.58
1:C:303:VAL:HG12	1:C:304:ASP:H	1.68	0.57
1:C:252:MET:O	1:C:310:ASP:HA	2.03	0.57
1:C:2:LYS:HB3	1:C:137:PHE:CE1	2.39	0.57
7:C:400:HOH:O	1:D:237:LEU:HB3	2.05	0.57
1:D:279:ASP:HB3	1:D:292:SER:CB	2.34	0.57
1:A:345:ARG:NH1	7:A:423:HOH:O	2.38	0.57
1:C:80:ARG:NH2	7:C:514:HOH:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LYS:HE2	7:D:423:HOH:O	2.05	0.57
1:C:21:ARG:HD3	1:C:89:ASP:HB3	1.86	0.56
1:D:315:LYS:HE2	7:D:472:HOH:O	2.04	0.56
1:A:110:LEU:HD23	1:A:260:TYR:CD2	2.41	0.56
1:A:135:LYS:HG3	1:A:136:SER:N	2.21	0.56
1:C:284:LYS:HG3	7:C:428:HOH:O	2.04	0.56
1:C:107:ILE:CD1	7:C:520:HOH:O	2.46	0.55
1:C:283:GLU:HB2	1:C:289:SER:HB2	1.88	0.55
1:D:56:HIS:CE1	1:D:130:ILE:HG23	2.42	0.55
1:B:244:ARG:NH1	7:B:492:HOH:O	2.37	0.55
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.87	0.55
1:B:2:LYS:HB3	1:B:137:PHE:CE1	2.41	0.55
1:C:101:LEU:HD21	1:C:176:LYS:HG2	1.88	0.54
1:D:303:VAL:HG12	1:D:304:ASP:N	2.23	0.54
1:B:230:GLU:HG3	1:B:308:ALA:HB1	1.89	0.54
1:B:320:LYS:HB2	7:B:409:HOH:O	2.06	0.54
1:C:240:MET:HB2	1:D:236:THR:HG21	1.90	0.54
1:B:278:LYS:HA	1:B:281:VAL:HB	1.89	0.53
1:A:170:MET:HG3	1:A:175:ARG:HB2	1.91	0.53
1:D:90:LEU:HA	1:D:93:ILE:HD12	1.89	0.53
1:A:236:THR:HG21	1:B:240:MET:HB2	1.90	0.53
1:C:226:GLY:O	3:C:396:NAD:H5N	2.08	0.53
1:A:131:GLU:HB3	1:A:192:LEU:HD21	1.91	0.53
1:B:336:ALA:HB2	3:B:396:NAD:N7N	2.23	0.53
1:A:69:LYS:O	1:A:73:GLU:HG2	2.09	0.52
1:C:236:THR:HG21	1:D:240:MET:HB2	1.90	0.52
1:A:360:LYS:CD	7:A:470:HOH:O	2.54	0.52
1:A:56:HIS:HA	1:A:96:ARG:O	2.09	0.52
1:D:45:LYS:HB3	1:D:46:TYR:CD1	2.45	0.52
1:D:388:TYR:OH	1:D:392:LYS:HE3	2.10	0.52
1:A:237:LEU:HD23	1:A:240:MET:HE2	1.92	0.52
1:B:251:TRP:CD2	1:B:312:VAL:HG22	2.45	0.52
1:B:126:MET:CE	1:B:176:LYS:HE3	2.40	0.51
1:A:263:LYS:HA	7:A:492:HOH:O	2.10	0.51
1:A:240:MET:HB2	1:B:236:THR:HG21	1.92	0.51
1:C:277:SER:O	1:C:278:LYS:HD2	2.11	0.51
1:C:381:PHE:CE2	1:C:385:LYS:HE2	2.44	0.51
1:A:11:ILE:HG12	1:A:333:ALA:HB2	1.93	0.50
1:B:207:ILE:HD11	1:B:210:LEU:HG	1.93	0.50
1:D:155:ASN:HB3	7:D:491:HOH:O	2.10	0.50
1:A:45:LYS:HD3	7:A:475:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LYS:HE3	1:C:296:ILE:O	2.11	0.50
3:D:396:NAD:H4N	7:D:524:HOH:O	2.10	0.50
1:A:24:GLU:OE2	1:A:50:SER:HA	2.11	0.50
1:A:39:HIS:CG	1:A:385:LYS:HG2	2.47	0.50
1:C:132:GLU:O	1:C:136:SER:HB2	2.11	0.50
1:C:165:GLU:CG	1:C:169:ARG:HH12	2.24	0.50
1:C:303:VAL:HG12	1:C:304:ASP:N	2.26	0.50
1:A:182:SER:HA	7:A:448:HOH:O	2.12	0.50
1:B:252:MET:O	1:B:310:ASP:HA	2.11	0.50
1:B:58:ILE:HD13	1:B:100:ALA:HB2	1.94	0.49
1:B:341:LEU:O	1:B:345:ARG:HG3	2.12	0.49
1:C:27:ILE:HD12	1:C:82:ILE:HD13	1.94	0.49
1:C:373:ASN:N	5:C:397:SO4:O2	2.38	0.49
1:C:132:GLU:HB3	7:C:515:HOH:O	2.11	0.49
1:A:260:TYR:O	1:A:263:LYS:HB2	2.13	0.49
3:B:396:NAD:H2D	4:B:397:GOL:O3	2.12	0.49
1:B:69:LYS:HG3	1:B:83:LEU:HD21	1.95	0.49
1:C:331:ILE:HD12	1:D:320:LYS:HE2	1.94	0.49
1:C:311:PHE:CZ	1:C:323:LYS:HG2	2.47	0.49
1:D:114:LYS:NZ	7:D:420:HOH:O	2.46	0.48
1:D:197:ALA:HB2	1:D:347:LEU:HD11	1.94	0.48
1:D:18:VAL:HG12	1:D:19:GLY:N	2.28	0.48
1:A:5:LEU:HD13	1:A:13:SER:OG	2.13	0.48
1:A:197:ALA:HB2	1:A:347:LEU:HD11	1.96	0.48
1:B:44:GLU:HB3	1:B:48:PRO:HA	1.95	0.48
1:C:17:MET:HG2	1:C:53:PHE:CG	2.48	0.48
1:A:288:TYR:CD1	1:A:288:TYR:N	2.80	0.48
1:A:305:ASN:ND2	1:A:330:ALA:O	2.43	0.48
1:B:349:PHE:O	1:B:350:ALA:C	2.51	0.48
1:A:378:HIS:HB3	1:B:378:HIS:ND1	2.28	0.48
1:A:378:HIS:CD2	1:B:378:HIS:HB2	2.47	0.48
1:B:89:ASP:OD2	1:B:89:ASP:N	2.47	0.48
1:D:97:LYS:CE	1:D:119:GLU:OE1	2.56	0.48
1:B:305:ASN:C	1:B:305:ASN:HD22	2.17	0.48
1:D:376:ASN:OD1	1:D:376:ASN:C	2.52	0.48
1:C:44:GLU:HG3	7:C:493:HOH:O	2.13	0.47
1:C:103:CYS:HB3	7:C:520:HOH:O	2.13	0.47
1:C:283:GLU:HA	1:C:288:TYR:O	2.14	0.47
1:A:110:LEU:HD23	1:A:260:TYR:HD2	1.79	0.47
1:A:320:LYS:HE2	1:B:331:ILE:CD1	2.43	0.47
1:A:274:LYS:HB3	7:A:485:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:SER:HB2	1:B:147:VAL:CG2	2.37	0.47
1:A:323:LYS:HE3	7:B:444:HOH:O	2.15	0.47
1:C:71:HIS:O	1:C:75:ASN:HB2	2.15	0.47
1:A:28:ALA:HB1	1:A:29:PRO:HD2	1.96	0.47
1:C:2:LYS:O	1:C:142:THR:HA	2.15	0.47
1:C:110:LEU:HD23	1:C:260:TYR:CD2	2.49	0.47
1:D:45:LYS:CE	7:D:423:HOH:O	2.61	0.47
1:C:269:ASP:HB2	7:C:530:HOH:O	2.14	0.46
1:B:42:GLY:O	1:B:45:LYS:HB2	2.15	0.46
1:A:74:LEU:HG	7:A:419:HOH:O	2.16	0.46
1:D:65:TYR:CD1	1:D:87:LYS:HA	2.51	0.46
1:D:339:LEU:O	1:D:343:ILE:HG13	2.15	0.46
1:C:142:THR:HB	1:C:194:LEU:HD22	1.96	0.46
1:D:367:LYS:HE2	2:D:395:PO4:O4	2.16	0.46
1:C:302:LEU:O	1:C:305:ASN:HB3	2.16	0.46
1:A:298:TYR:CE1	1:A:300:PRO:HG3	2.50	0.46
1:D:123:LEU:CA	1:D:126:MET:HE2	2.43	0.46
1:A:132:GLU:O	1:A:136:SER:HB2	2.14	0.46
1:C:69:LYS:O	1:C:73:GLU:HG2	2.16	0.46
1:C:215:GLU:CG	7:C:445:HOH:O	2.45	0.46
1:A:9:TYR:CG	1:A:57:GLU:HG3	2.50	0.46
1:A:274:LYS:NZ	4:A:397:GOL:H11	2.31	0.46
1:B:123:LEU:HD23	1:B:126:MET:CE	2.44	0.46
1:C:280:LYS:HB3	7:C:442:HOH:O	2.15	0.46
1:D:75:ASN:O	1:D:76:ARG:C	2.54	0.46
1:B:90:LEU:HA	1:B:93:ILE:HD12	1.98	0.45
1:D:13:SER:HB2	1:D:147:VAL:HG21	1.98	0.45
1:B:279:ASP:OD2	1:B:279:ASP:N	2.50	0.45
1:D:264:VAL:HG11	7:D:467:HOH:O	2.16	0.45
1:A:252:MET:O	1:A:310:ASP:HA	2.17	0.45
1:B:59:ARG:HD3	1:B:110:LEU:HD22	1.97	0.45
1:C:169:ARG:HD2	7:C:475:HOH:O	2.16	0.45
1:D:6:VAL:HB	1:D:146:ASN:HA	1.99	0.45
1:D:174:ASP:OD2	1:D:176:LYS:NZ	2.50	0.45
1:A:97:LYS:HE2	1:A:97:LYS:HB3	1.77	0.45
1:B:135:LYS:HD3	1:B:192:LEU:CD2	2.46	0.45
1:C:11:ILE:HG13	1:C:71:HIS:HB3	1.99	0.45
1:C:167:PHE:O	1:C:170:MET:HB3	2.17	0.45
1:A:199:PHE:O	1:A:225:ASP:HA	2.16	0.44
1:D:238:ALA:N	1:D:239:PRO:CD	2.80	0.44
1:D:283:GLU:HA	1:D:288:TYR:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:OD1	1:A:376:ASN:C	2.56	0.44
1:B:262:GLY:O	1:B:266:SER:HB3	2.18	0.44
1:C:207:ILE:HD11	1:C:210:LEU:HG	1.99	0.44
1:C:269:ASP:HA	7:C:536:HOH:O	2.17	0.44
1:D:123:LEU:HB2	1:D:174:ASP:HA	1.98	0.44
1:D:261:ASP:O	1:D:265:LEU:HG	2.18	0.44
1:B:238:ALA:HB3	1:B:239:PRO:HD3	1.99	0.44
1:C:279:ASP:HB3	1:C:292:SER:HB3	1.99	0.44
1:A:106:GLY:HA2	7:A:500:HOH:O	2.18	0.44
1:A:381:PHE:CE2	1:A:385:LYS:HD2	2.53	0.44
1:C:264:VAL:HG11	7:C:468:HOH:O	2.18	0.44
1:A:182:SER:HB2	1:A:204:GLY:HA2	1.98	0.44
1:B:11:ILE:HG23	1:B:12:VAL:N	2.33	0.44
1:C:388:TYR:O	1:C:392:LYS:HB2	2.18	0.44
1:A:190:LEU:HD23	1:A:219:VAL:HG11	2.00	0.44
1:C:82:ILE:O	1:C:86:VAL:HG22	2.18	0.43
1:A:82:ILE:O	1:A:86:VAL:HG22	2.18	0.43
1:B:207:ILE:O	1:B:207:ILE:HG13	2.18	0.43
1:C:311:PHE:CE2	1:C:323:LYS:HG2	2.52	0.43
1:D:156:TYR:CD1	1:D:156:TYR:C	2.91	0.43
1:A:266:SER:HB3	1:A:298:TYR:HB2	2.00	0.43
1:B:306:LYS:HB2	1:B:332:ASP:OD1	2.18	0.43
1:B:360:LYS:H	1:B:360:LYS:HG3	1.53	0.43
1:A:71:HIS:HE1	1:A:260:TYR:CE1	2.37	0.43
1:A:109:GLU:OE2	1:A:263:LYS:HD2	2.17	0.43
1:A:61:LEU:HD12	1:A:66:GLU:HB3	1.99	0.43
1:B:9:TYR:H	1:B:57:GLU:CG	2.32	0.43
1:B:274:LYS:HB2	1:B:274:LYS:HE3	1.80	0.43
1:C:266:SER:O	1:C:271:LYS:HD3	2.18	0.43
1:A:4:TRP:HE3	1:A:137:PHE:CD1	2.37	0.43
1:A:19:GLY:HA2	1:B:318:LEU:HD21	1.99	0.43
1:B:254:TYR:HH	1:B:297:GLN:HG3	1.78	0.43
1:B:126:MET:HE2	1:B:176:LYS:HE3	1.99	0.43
1:B:307:THR:HA	1:B:328:TRP:O	2.19	0.43
1:D:228:THR:HB	1:D:335:VAL:HG23	2.01	0.43
1:A:139:ASP:C	1:A:141:GLU:H	2.21	0.43
1:B:332:ASP:OD2	3:B:396:NAD:C7N	2.67	0.43
1:C:300:PRO:HD2	7:C:449:HOH:O	2.19	0.43
1:D:279:ASP:CB	1:D:292:SER:HB3	2.49	0.43
1:D:283:GLU:O	1:D:283:GLU:HG3	2.18	0.43
1:A:243:TYR:CZ	1:B:378:HIS:HD2	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ASP:HB3	7:B:483:HOH:O	2.19	0.43
1:B:265:LEU:O	1:B:271:LYS:HE3	2.18	0.43
1:C:21:ARG:HD3	1:C:89:ASP:CB	2.49	0.42
1:A:38:PRO:O	1:A:41:GLU:CG	2.67	0.42
1:B:35:SER:OG	1:B:345:ARG:NH1	2.50	0.42
1:C:237:LEU:HD21	1:C:324:PHE:CE1	2.54	0.42
1:C:304:ASP:HA	7:C:427:HOH:O	2.18	0.42
1:D:47:ALA:CB	1:D:348:LEU:HD23	2.49	0.42
1:C:306:LYS:HB3	7:C:521:HOH:O	2.19	0.42
1:D:123:LEU:HD23	1:D:126:MET:HE1	1.98	0.42
1:A:1:MET:CE	1:A:344:ALA:HB1	2.50	0.42
1:A:230:GLU:OE1	1:A:278:LYS:NZ	2.46	0.42
1:D:42:GLY:N	7:D:421:HOH:O	2.33	0.42
1:D:279:ASP:O	1:D:282:LEU:N	2.51	0.42
1:D:302:LEU:HA	1:D:302:LEU:HD23	1.78	0.42
1:D:303:VAL:HG12	1:D:304:ASP:H	1.84	0.42
3:B:396:NAD:PN	7:B:479:HOH:O	2.77	0.42
1:B:44:GLU:H	1:B:44:GLU:CD	2.22	0.42
1:B:212:GLU:HG2	7:B:484:HOH:O	2.19	0.42
1:B:372:THR:OG1	5:B:394:SO4:O1	2.29	0.42
1:A:201:PRO:HB2	1:A:273:SER:HB3	2.01	0.42
1:A:252:MET:CE	1:A:309:PHE:O	2.68	0.42
1:C:59:ARG:HG3	3:C:396:NAD:O2B	2.20	0.42
1:B:2:LYS:HD2	1:B:52:GLU:HB2	2.02	0.42
1:A:96:ARG:NH1	7:A:431:HOH:O	2.52	0.41
1:A:141:GLU:OE2	1:A:352:LYS:NZ	2.31	0.41
1:A:275:VAL:HG13	7:A:404:HOH:O	2.20	0.41
1:D:337:ALA:N	1:D:338:PRO:HD2	2.35	0.41
1:B:234:LYS:HD2	1:B:278:LYS:HD2	2.01	0.41
1:B:264:VAL:HG23	7:B:496:HOH:O	2.19	0.41
1:B:367:LYS:NZ	2:B:395:PO4:O3	2.47	0.41
1:A:274:LYS:HD3	1:A:367:LYS:HZ2	1.86	0.41
1:B:126:MET:HE1	1:B:176:LYS:HE3	2.02	0.41
1:A:318:LEU:HD21	1:B:19:GLY:HA2	2.01	0.41
1:C:196:TYR:CE2	1:C:205:SER:HB3	2.54	0.41
1:D:283:GLU:HG2	7:D:474:HOH:O	2.20	0.41
1:A:11:ILE:HG12	1:A:333:ALA:CB	2.50	0.41
1:A:58:ILE:CG2	1:A:115:THR:HG22	2.50	0.41
1:A:244:ARG:HA	1:A:244:ARG:HD3	1.81	0.41
1:B:22:ALA:HB2	7:B:491:HOH:O	2.19	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:NZ	2:A:395:PO4:O3	2.50	0.41
1:B:199:PHE:HZ	1:B:339:LEU:HD12	1.86	0.41
1:D:145:ILE:HG12	1:D:197:ALA:HB3	2.01	0.41
1:A:264:VAL:HG23	7:A:425:HOH:O	2.20	0.41
1:D:132:GLU:HA	7:D:500:HOH:O	2.20	0.41
1:A:193:GLY:HA2	1:A:219:VAL:HG21	2.02	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.83	0.41
1:A:244:ARG:NH1	7:A:443:HOH:O	2.37	0.41
1:B:281:VAL:HG13	1:B:375:ILE:HG21	2.03	0.41
1:C:320:LYS:HG2	1:D:334:ILE:HG13	2.03	0.41
1:D:224:ASN:O	1:D:225:ASP:HB3	2.21	0.41
1:D:276:LEU:HD12	7:D:475:HOH:O	2.21	0.41
1:A:279:ASP:OD2	1:A:279:ASP:N	2.54	0.41
1:A:280:LYS:O	1:A:284:LYS:HD2	2.21	0.41
1:C:129:ARG:HA	1:C:132:GLU:HG2	2.03	0.41
1:D:123:LEU:HD23	1:D:123:LEU:HA	1.78	0.41
1:D:160:TYR:OH	1:D:175:ARG:HD3	2.21	0.41
1:D:279:ASP:CB	1:D:292:SER:CB	2.99	0.41
1:A:123:LEU:HD23	1:A:126:MET:HE3	2.03	0.40
1:D:158:GLU:HG3	1:D:159:GLU:N	2.36	0.40
1:D:60:LEU:HD12	1:D:112:ASP:HB3	2.04	0.40
1:A:274:LYS:HB2	1:A:274:LYS:HE3	1.92	0.40
1:B:249:VAL:HG23	1:B:313:HIS:HB3	2.03	0.40
1:C:80:ARG:NH2	5:C:394:SO4:O3	2.52	0.40
1:D:226:GLY:HA2	1:D:365:PHE:O	2.21	0.40
1:C:259:ASP:HB3	7:C:447:HOH:O	2.22	0.40
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.99	0.40
1:D:47:ALA:HB2	1:D:348:LEU:HD23	2.03	0.40
1:D:87:LYS:O	1:D:91:GLU:HB2	2.22	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	390/392 (100%)	362 (93%)	24 (6%)	4 (1%)	15	32
1	B	390/392 (100%)	368 (94%)	20 (5%)	2 (0%)	29	52
1	C	390/392 (100%)	363 (93%)	21 (5%)	6 (2%)	10	21
1	D	390/392 (100%)	364 (93%)	24 (6%)	2 (0%)	29	52
All	All	1560/1568 (100%)	1457 (93%)	89 (6%)	14 (1%)	17	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	267	ALA
1	C	278	LYS
1	A	216	LYS
1	A	274	LYS
1	A	278	LYS
1	C	259	ASP
1	C	364	PHE
1	A	303	VAL
1	B	259	ASP
1	B	303	VAL
1	C	303	VAL
1	D	303	VAL
1	D	268	ARG
1	C	118	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/324 (100%)	299 (92%)	25 (8%)	13	25
1	B	324/324 (100%)	298 (92%)	26 (8%)	12	24
1	C	324/324 (100%)	301 (93%)	23 (7%)	14	29
1	D	324/324 (100%)	308 (95%)	16 (5%)	25	48
All	All	1296/1296 (100%)	1206 (93%)	90 (7%)	15	31

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	41	GLU
1	A	44	GLU
1	A	60	LEU
1	A	79	ASP
1	A	88	SER
1	A	94	VAL
1	A	136	SER
1	A	140	ASP
1	A	165	GLU
1	A	169	ARG
1	A	175	ARG
1	A	191	LYS
1	A	216	LYS
1	A	237	LEU
1	A	246	MET
1	A	261	ASP
1	A	268	ARG
1	A	278	LYS
1	A	279	ASP
1	A	289	SER
1	A	310	ASP
1	A	326	PHE
1	A	360	LYS
1	A	368	SER
1	B	44	GLU
1	B	45	LYS
1	B	50	SER
1	B	88	SER
1	B	89	ASP
1	B	96	ARG
1	B	99	THR
1	B	132	GLU
1	B	136	SER
1	B	140	ASP
1	B	158	GLU
1	B	165	GLU
1	B	168	GLU
1	B	170	MET
1	B	203	PRO
1	B	230	GLU
1	B	252	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	259	ASP
1	B	268	ARG
1	B	269	ASP
1	B	276	LEU
1	B	279	ASP
1	B	305	ASN
1	B	310	ASP
1	B	332	ASP
1	B	360	LYS
1	C	21	ARG
1	C	41	GLU
1	C	60	LEU
1	C	61	LEU
1	C	62	SER
1	C	70	GLU
1	C	108	LYS
1	C	112	ASP
1	C	135	LYS
1	C	153	LEU
1	C	158	GLU
1	C	172	ASP
1	C	259	ASP
1	C	261	ASP
1	C	274	LYS
1	C	276	LEU
1	C	280	LYS
1	C	289	SER
1	C	296	ILE
1	C	305	ASN
1	C	310	ASP
1	C	332	ASP
1	C	367	LYS
1	D	44	GLU
1	D	136	SER
1	D	140	ASP
1	D	158	GLU
1	D	170	MET
1	D	177	GLU
1	D	259	ASP
1	D	261	ASP
1	D	266	SER
1	D	268	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	293	ILE
1	D	296	ILE
1	D	305	ASN
1	D	310	ASP
1	D	332	ASP
1	D	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	378	HIS
1	C	270	ASN
1	C	378	HIS
1	D	297	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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\#\|Z\|>2$
3	NAD	C	396	6	42,48,48	1.78	4 (9%)	50,73,73	1.29	5 (10%)
2	PO4	C	395	-	4,4,4	1.53	0	6,6,6	0.57	0
2	PO4	D	395	-	4,4,4	1.12	0	6,6,6	1.17	0
3	NAD	D	396	6	42,48,48	1.83	4 (9%)	50,73,73	1.45	6 (12%)
5	SO4	C	394	-	4,4,4	0.15	0	6,6,6	0.19	0
5	SO4	D	393	-	4,4,4	0.30	0	6,6,6	0.36	0
4	GOL	A	397	-	5,5,5	0.43	0	5,5,5	0.21	0
2	PO4	A	395	-	4,4,4	1.52	0	6,6,6	1.00	1 (16%)
5	SO4	B	393	-	4,4,4	0.15	0	6,6,6	0.38	0
5	SO4	D	394	-	4,4,4	0.16	0	6,6,6	0.40	0
3	NAD	A	396	-	42,48,48	1.87	5 (11%)	50,73,73	1.57	7 (14%)
4	GOL	B	397	-	5,5,5	0.46	0	5,5,5	0.17	0
5	SO4	A	393	-	4,4,4	0.16	0	6,6,6	0.55	0
2	PO4	B	395	-	4,4,4	1.12	0	6,6,6	0.81	0
5	SO4	C	393	-	4,4,4	0.16	0	6,6,6	0.53	0
3	NAD	B	396	-	42,48,48	1.86	4 (9%)	50,73,73	1.30	5 (10%)
5	SO4	C	397	-	4,4,4	0.09	0	6,6,6	0.53	0
5	SO4	B	394	-	4,4,4	0.09	0	6,6,6	0.57	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	C	396	6	-	9/26/62/62	0/5/5/5
3	NAD	D	396	6	-	9/26/62/62	0/5/5/5
4	GOL	A	397	-	-	2/4/4/4	-
3	NAD	A	396	-	-	2/26/62/62	0/5/5/5
4	GOL	B	397	-	-	2/4/4/4	-
3	NAD	B	396	-	-	8/26/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	396	NAD	O7N-C7N	9.40	1.42	1.24
3	A	396	NAD	O7N-C7N	8.86	1.41	1.24
3	D	396	NAD	O7N-C7N	8.76	1.40	1.24
3	C	396	NAD	O7N-C7N	8.40	1.40	1.24
3	D	396	NAD	C2A-N3A	5.07	1.40	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	396	NAD	C2A-N3A	3.99	1.38	1.32
3	C	396	NAD	C2A-N3A	3.82	1.38	1.32
3	A	396	NAD	C2A-N3A	3.76	1.38	1.32
3	A	396	NAD	C2N-N1N	3.73	1.39	1.35
3	C	396	NAD	C2A-N1A	3.54	1.40	1.33
3	D	396	NAD	C2A-N1A	2.78	1.39	1.33
3	A	396	NAD	C2A-N1A	2.77	1.39	1.33
3	B	396	NAD	C2A-N1A	2.70	1.38	1.33
3	C	396	NAD	C2N-N1N	2.38	1.37	1.35
3	D	396	NAD	C2N-N1N	2.28	1.37	1.35
3	B	396	NAD	C2N-N1N	2.21	1.37	1.35
3	A	396	NAD	C3N-C7N	2.08	1.53	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	396	NAD	N3A-C2A-N1A	-6.12	119.11	128.68
3	B	396	NAD	N3A-C2A-N1A	-5.65	119.85	128.68
3	D	396	NAD	N3A-C2A-N1A	-5.45	120.16	128.68
3	A	396	NAD	O7N-C7N-N7N	-4.65	115.98	122.58
3	C	396	NAD	N3A-C2A-N1A	-4.49	121.67	128.68
3	D	396	NAD	PN-O3-PA	-3.55	120.64	132.83
3	A	396	NAD	O7N-C7N-C3N	3.19	123.45	119.63
3	C	396	NAD	C3D-C2D-C1D	2.90	105.34	100.98
3	C	396	NAD	C3N-C7N-N7N	2.87	121.19	117.75
3	D	396	NAD	O7N-C7N-C3N	-2.72	116.38	119.63
3	D	396	NAD	C2N-C3N-C4N	2.62	121.22	118.26
3	C	396	NAD	O5D-PN-O1N	-2.55	99.12	109.07
3	D	396	NAD	C6N-N1N-C2N	-2.46	119.73	121.97
3	A	396	NAD	C3N-C7N-N7N	2.35	120.57	117.75
3	B	396	NAD	C3D-C2D-C1D	2.35	104.51	100.98
3	B	396	NAD	C6N-N1N-C2N	-2.25	119.93	121.97
3	A	396	NAD	O2N-PN-O1N	2.23	123.29	112.24
3	D	396	NAD	C3N-C7N-N7N	2.23	120.42	117.75
3	A	396	NAD	C3D-C2D-C1D	2.22	104.31	100.98
3	A	396	NAD	C1B-N9A-C4A	-2.20	122.77	126.64
3	B	396	NAD	O2N-PN-O1N	2.16	122.92	112.24
3	C	396	NAD	C1B-N9A-C4A	-2.08	122.99	126.64
2	A	395	PO4	O4-P-O1	-2.03	103.46	110.89
3	B	396	NAD	O3D-C3D-C4D	2.00	116.83	111.05

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	396	NAD	C5B-O5B-PA-O1A
3	B	396	NAD	C5B-O5B-PA-O2A
3	B	396	NAD	PN-O3-PA-O5B
3	B	396	NAD	O4B-C4B-C5B-O5B
3	C	396	NAD	C5B-O5B-PA-O1A
3	D	396	NAD	C5B-O5B-PA-O1A
3	D	396	NAD	PN-O3-PA-O5B
3	D	396	NAD	O4B-C4B-C5B-O5B
4	A	397	GOL	O1-C1-C2-C3
4	B	397	GOL	O1-C1-C2-C3
3	B	396	NAD	C3B-C4B-C5B-O5B
4	B	397	GOL	O1-C1-C2-O2
3	C	396	NAD	O4D-C4D-C5D-O5D
3	C	396	NAD	C3D-C4D-C5D-O5D
3	D	396	NAD	C3B-C4B-C5B-O5B
4	A	397	GOL	O1-C1-C2-O2
3	C	396	NAD	PA-O3-PN-O1N
3	C	396	NAD	PN-O3-PA-O5B
3	D	396	NAD	O4D-C4D-C5D-O5D
3	C	396	NAD	C5B-O5B-PA-O3
3	D	396	NAD	C5B-O5B-PA-O3
3	C	396	NAD	C5B-O5B-PA-O2A
3	D	396	NAD	C5B-O5B-PA-O2A
3	B	396	NAD	PA-O3-PN-O2N
3	C	396	NAD	PA-O3-PN-O2N
3	A	396	NAD	O4B-C4B-C5B-O5B
3	C	396	NAD	O4B-C4B-C5B-O5B
3	D	396	NAD	PA-O3-PN-O2N
3	B	396	NAD	C5B-O5B-PA-O3
3	D	396	NAD	C5D-O5D-PN-O3
3	A	396	NAD	PA-O3-PN-O2N
3	B	396	NAD	PA-O3-PN-O1N

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	396	NAD	2	0
2	D	395	PO4	1	0
3	D	396	NAD	3	0
5	C	394	SO4	1	0

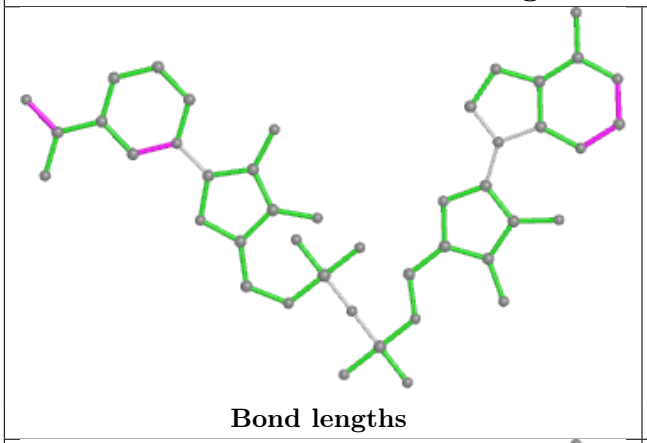
Continued on next page...

Continued from previous page...

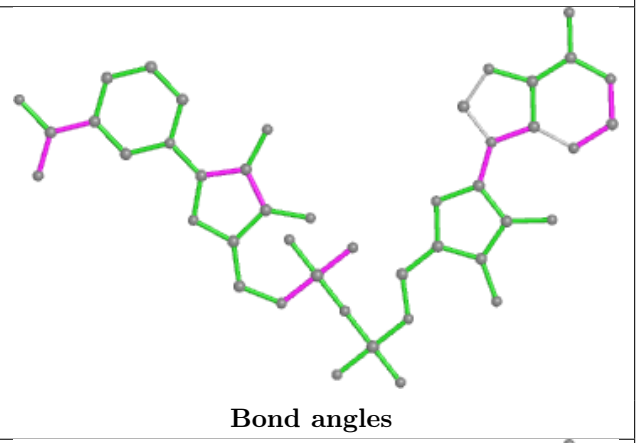
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	397	GOL	1	0
2	A	395	PO4	1	0
4	B	397	GOL	2	0
2	B	395	PO4	1	0
3	B	396	NAD	4	0
5	C	397	SO4	1	0
5	B	394	SO4	2	0

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.

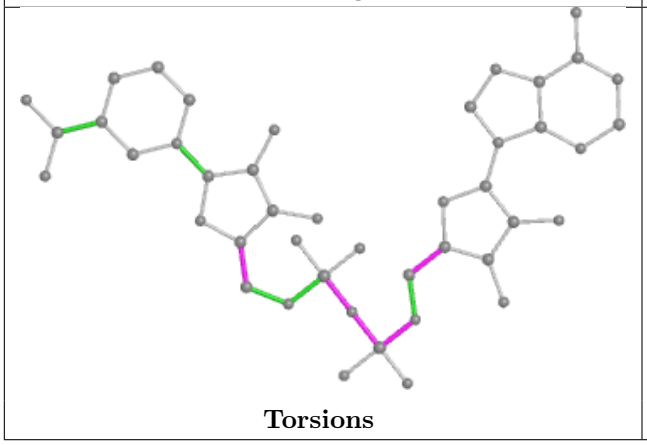
Ligand NAD C 396



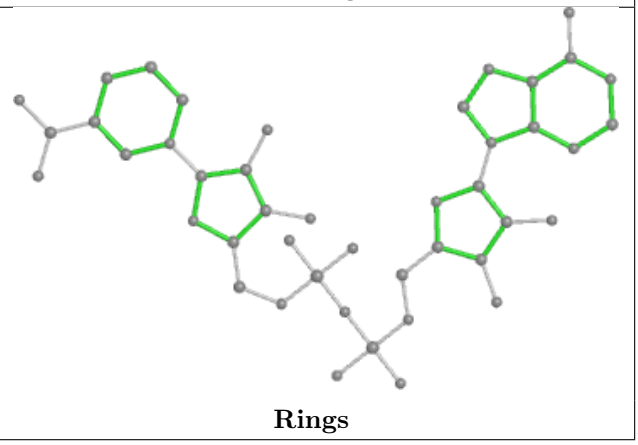
Bond lengths



Bond angles

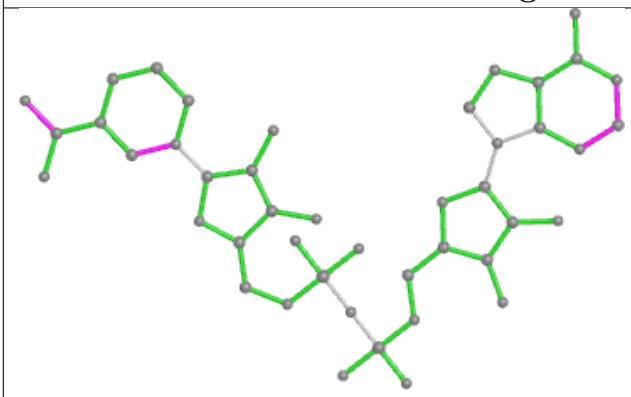


Torsions

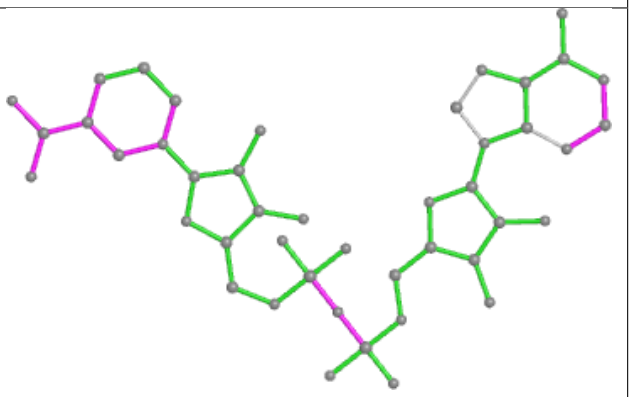


Rings

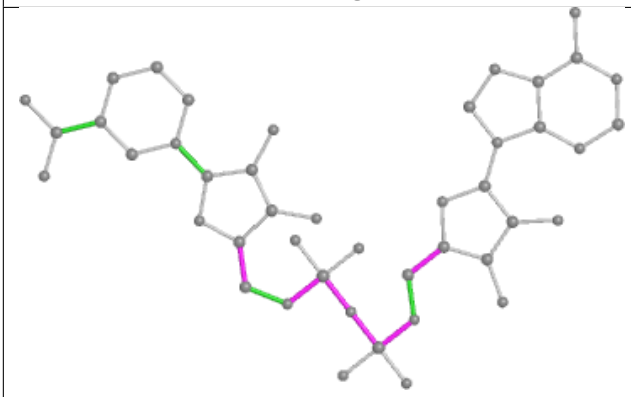
Ligand NAD D 396



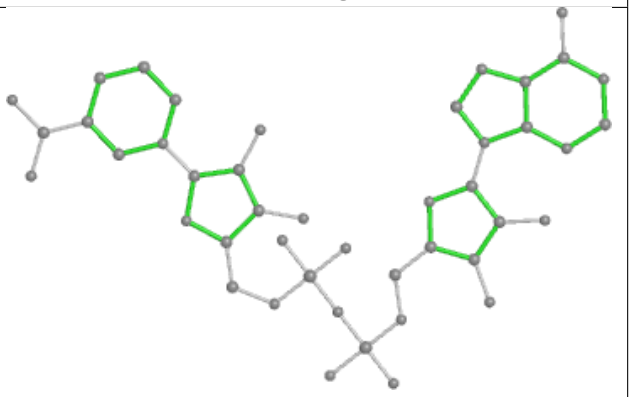
Bond lengths



Bond angles

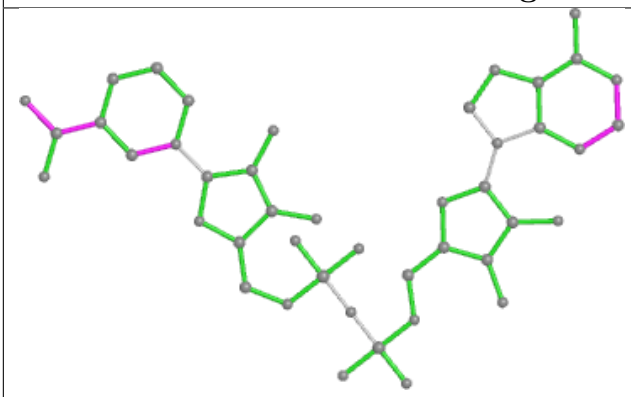


Torsions

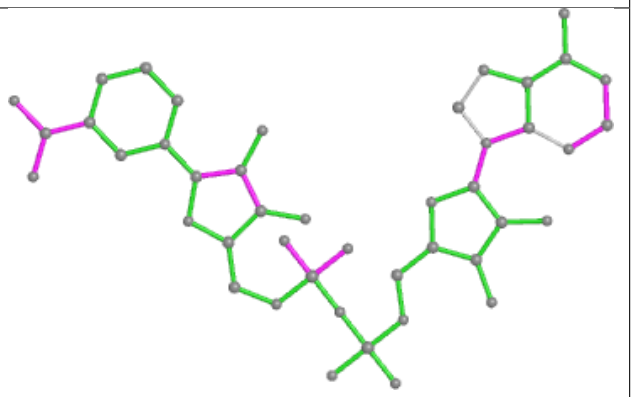


Rings

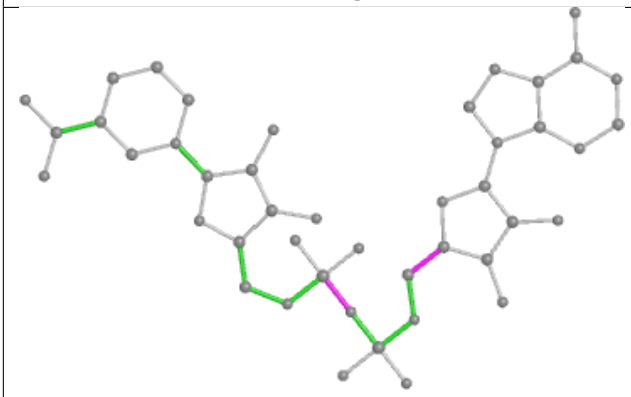
Ligand NAD A 396



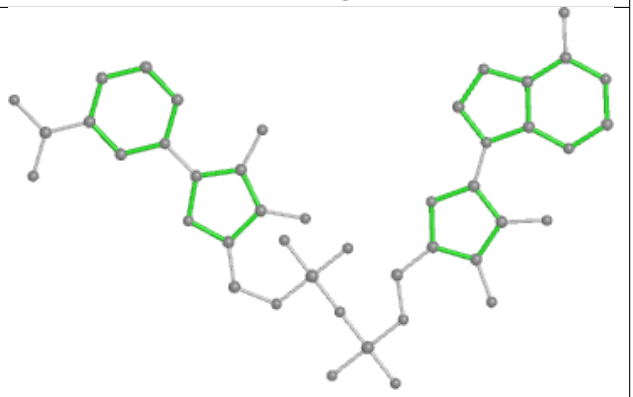
Bond lengths



Bond angles

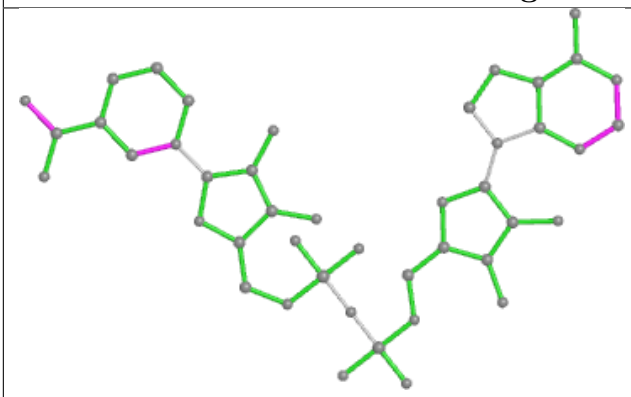


Torsions

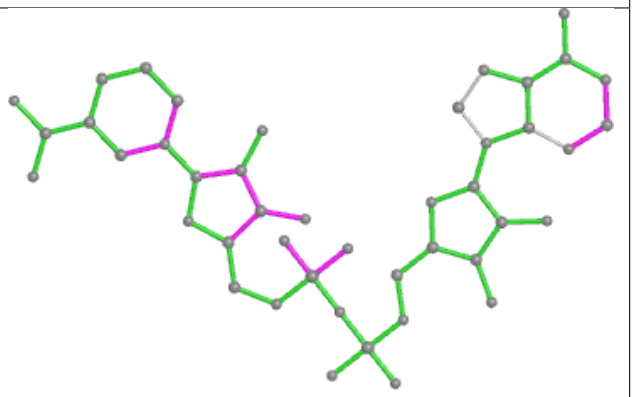


Rings

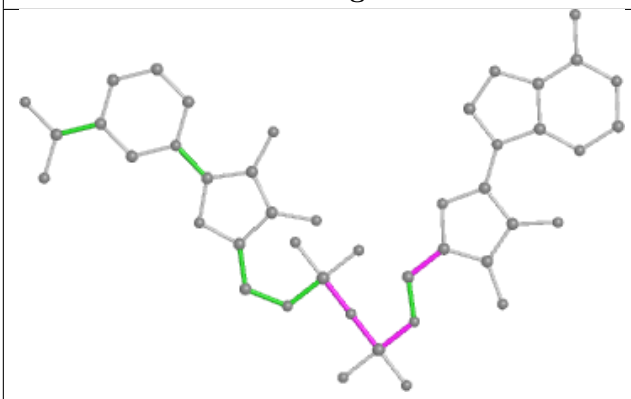
Ligand NAD B 396



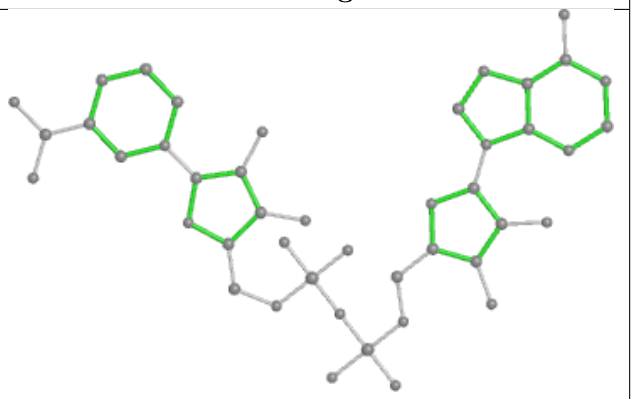
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	392/392 (100%)	0.29	25 (6%)	19	14	13, 26, 63, 100	0
1	B	392/392 (100%)	0.23	23 (5%)	22	17	11, 27, 58, 93	0
1	C	392/392 (100%)	0.24	20 (5%)	28	22	10, 22, 55, 94	0
1	D	392/392 (100%)	0.12	18 (4%)	32	26	11, 21, 55, 98	0
All	All	1568/1568 (100%)	0.22	86 (5%)	25	19	10, 24, 58, 100	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	275	VAL	15.6
1	C	273	SER	12.6
1	D	277	SER	9.9
1	D	269	ASP	8.8
1	C	276	LEU	8.5
1	A	275	VAL	8.1
1	C	267	ALA	8.1
1	D	270	ASN	7.8
1	D	273	SER	7.7
1	D	276	LEU	7.7
1	C	277	SER	7.5
1	D	275	VAL	7.4
1	B	275	VAL	7.0
1	A	269	ASP	6.9
1	D	272	GLU	6.9
1	A	277	SER	6.7
1	C	271	LYS	6.4
1	A	276	LEU	6.3
1	C	272	GLU	6.3
1	D	266	SER	6.0
1	A	274	LYS	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	270	ASN	5.8
1	B	276	LEU	5.7
1	D	279	ASP	5.4
1	B	268	ARG	5.2
1	B	271	LYS	4.9
1	B	269	ASP	4.9
1	D	267	ALA	4.9
1	C	268	ARG	4.9
1	B	267	ALA	4.8
1	A	272	GLU	4.8
1	D	260	TYR	4.6
1	A	268	ARG	4.4
1	B	266	SER	4.4
1	B	277	SER	4.4
1	D	271	LYS	4.4
1	A	273	SER	4.3
1	C	270	ASN	4.3
1	A	266	SER	4.2
1	D	274	LYS	4.1
1	D	268	ARG	4.1
1	B	264	VAL	4.1
1	A	108	LYS	4.0
1	C	264	VAL	4.0
1	B	270	ASN	4.0
1	C	266	SER	3.9
1	A	265	LEU	3.9
1	A	267	ALA	3.7
1	A	106	GLY	3.6
1	C	274	LYS	3.5
1	C	269	ASP	3.5
1	A	271	LYS	3.4
1	B	274	LYS	3.3
1	A	264	VAL	3.2
1	A	105	SER	3.2
1	B	105	SER	3.1
1	B	118	GLY	3.1
1	A	112	ASP	2.9
1	A	45	LYS	2.9
1	B	265	LEU	2.7
1	B	272	GLU	2.7
1	B	60	LEU	2.7
1	C	105	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	2.7
1	D	155	ASN	2.7
1	B	121	LEU	2.6
1	C	278	LYS	2.5
1	B	273	SER	2.5
1	A	279	ASP	2.4
1	B	107	ILE	2.3
1	B	106	GLY	2.3
1	B	108	LYS	2.3
1	A	107	ILE	2.2
1	D	105	SER	2.2
1	A	80	ARG	2.2
1	C	145	ILE	2.2
1	D	108	LYS	2.2
1	B	262	GLY	2.2
1	C	199	PHE	2.2
1	A	46	TYR	2.1
1	A	109	GLU	2.1
1	C	112	ASP	2.1
1	C	340	ILE	2.1
1	A	41	GLU	2.1
1	D	265	LEU	2.1
1	C	108	LYS	2.1

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, 95^{th} 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.

Continued on next page...

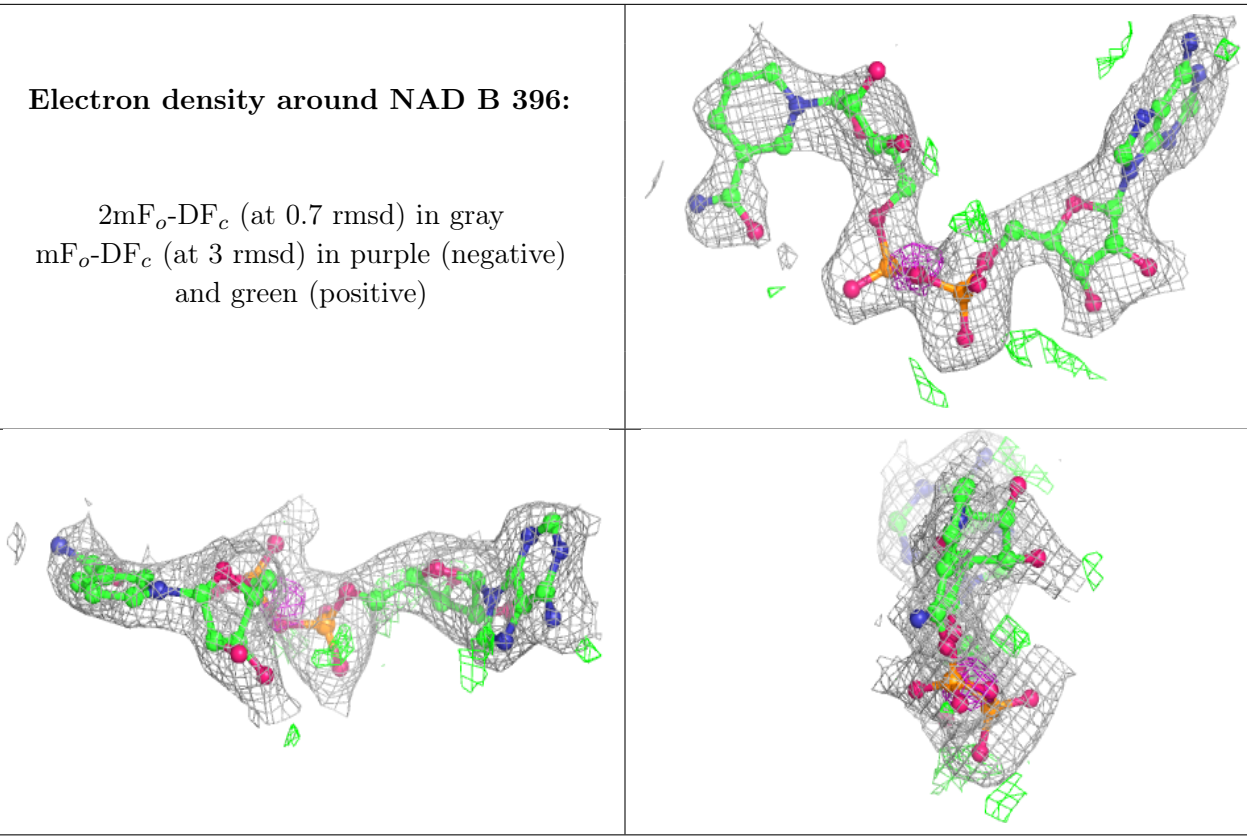
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	K	C	398	1/1	0.55	0.47	90,90,90,90	0
5	SO4	C	397	5/5	0.78	0.26	73,73,75,75	0
5	SO4	C	394	5/5	0.78	0.27	91,92,92,93	0
4	GOL	A	397	6/6	0.85	0.37	70,71,72,72	0
6	K	D	397	1/1	0.86	0.28	88,88,88,88	0
4	GOL	B	397	6/6	0.87	0.29	64,65,66,67	0
5	SO4	A	393	5/5	0.91	0.26	57,58,59,59	0
3	NAD	B	396	44/44	0.93	0.17	22,38,50,51	0
5	SO4	C	393	5/5	0.93	0.18	60,61,62,63	0
3	NAD	C	396	44/44	0.93	0.18	23,40,52,53	0
5	SO4	B	393	5/5	0.94	0.15	63,63,65,65	0
3	NAD	A	396	44/44	0.94	0.16	29,37,42,43	0
5	SO4	B	394	5/5	0.95	0.19	63,64,65,65	0
3	NAD	D	396	44/44	0.96	0.13	11,30,44,45	0
5	SO4	D	394	5/5	0.96	0.12	50,50,51,52	0
5	SO4	D	393	5/5	0.97	0.12	57,58,58,60	0
6	K	A	394	1/1	0.97	0.14	45,45,45,45	0
2	PO4	B	395	5/5	0.99	0.13	19,21,23,23	0
2	PO4	C	395	5/5	0.99	0.17	17,18,21,21	0
2	PO4	D	395	5/5	0.99	0.15	18,18,19,20	0
2	PO4	A	395	5/5	0.99	0.16	18,18,22,22	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.

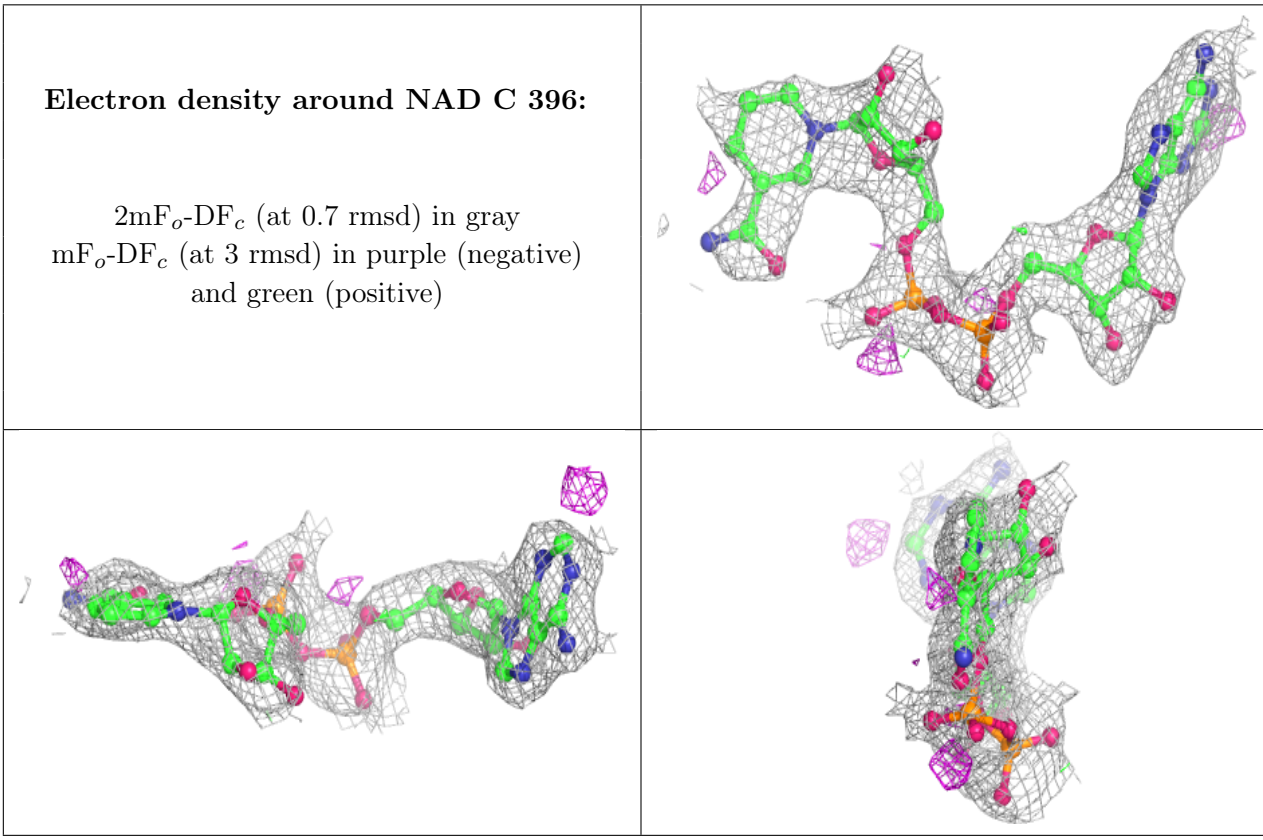
Electron density around NAD B 396:

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



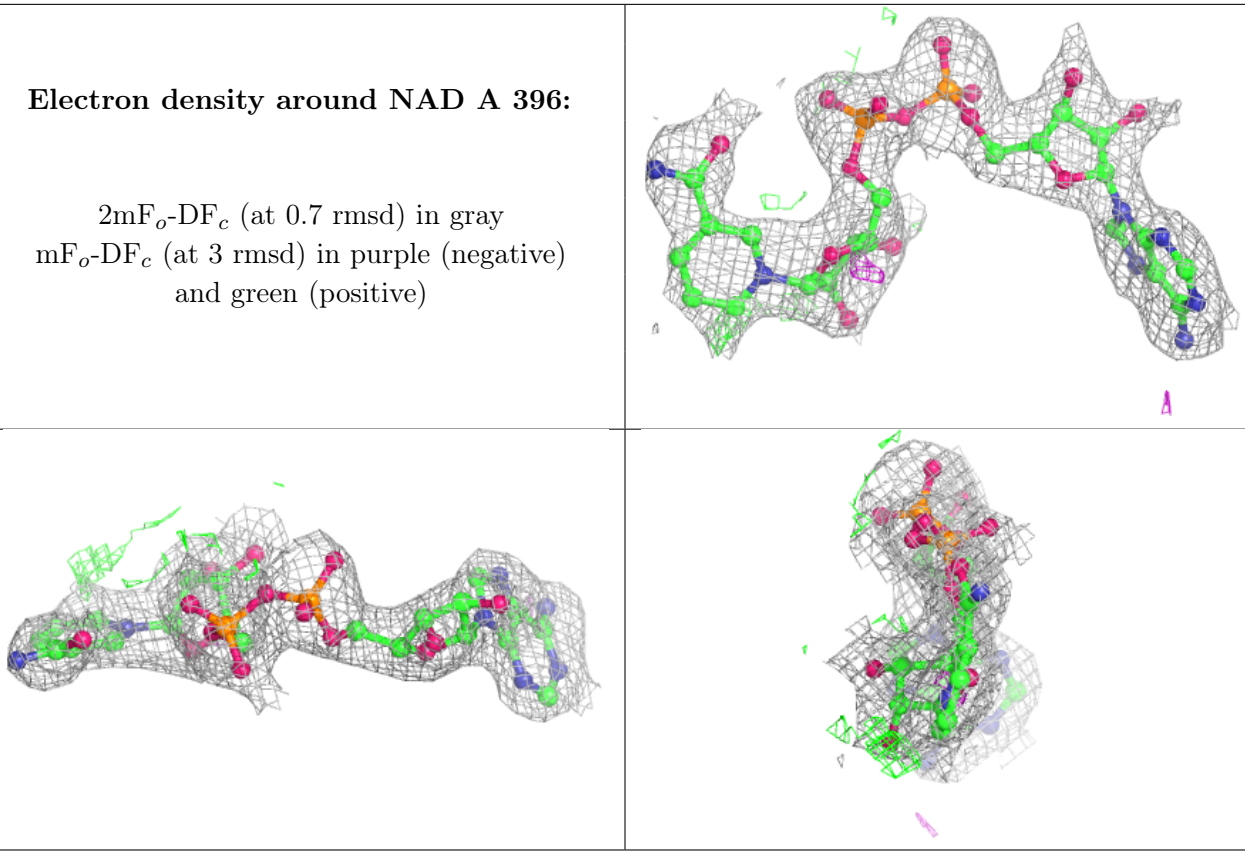
Electron density around NAD C 396:

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



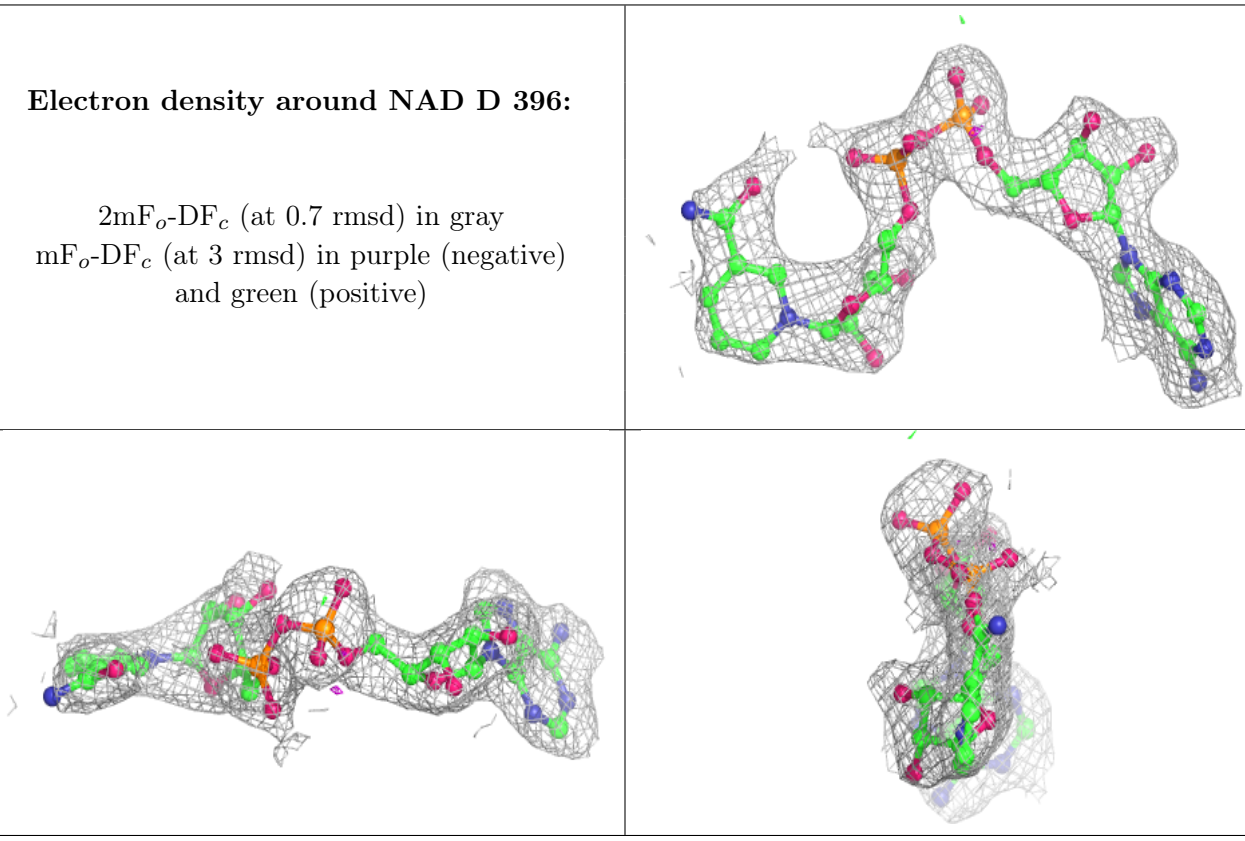
Electron density around NAD A 396:

$2mF_o$-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 396:

$2mF_o$-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.