Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 PM UTC

PDB ID	:	4OE2 / pdb_00004oe2
Title	:	2.00 Angstroms X-ray crystal structure of E268A 2-aminomuconate 6-semialdehyde dehydrogenase from Pseudomonas fluorescens
Authors	:	Huo, L.; Davis, I.; Liu, F.; Esaki, S.; Iwaki, H.; Hasegawa, Y.; Liu, A.
Deposited on	:	2014-01-11
Resolution	:	2.00 Å(reported)

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

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

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

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

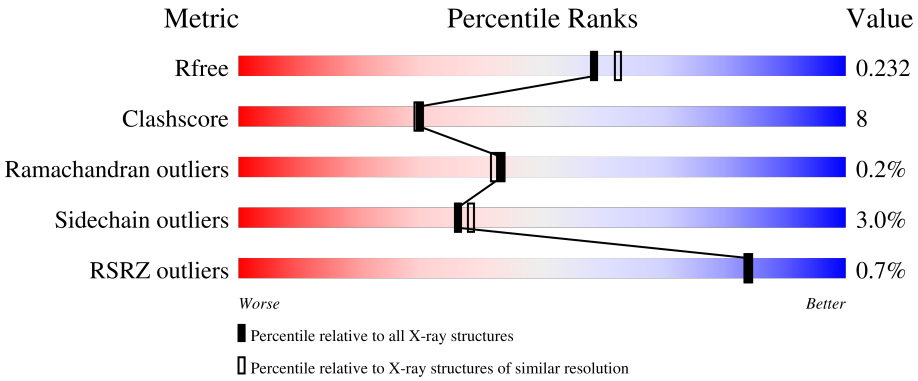
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	483	89% 10%
1	B	483	85% 13%
1	C	483	81% 17%
1	D	483	89% 10%

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
4	GOL	A	603	-	-	X	-
4	GOL	B	603	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16164 atoms, of which 104 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.

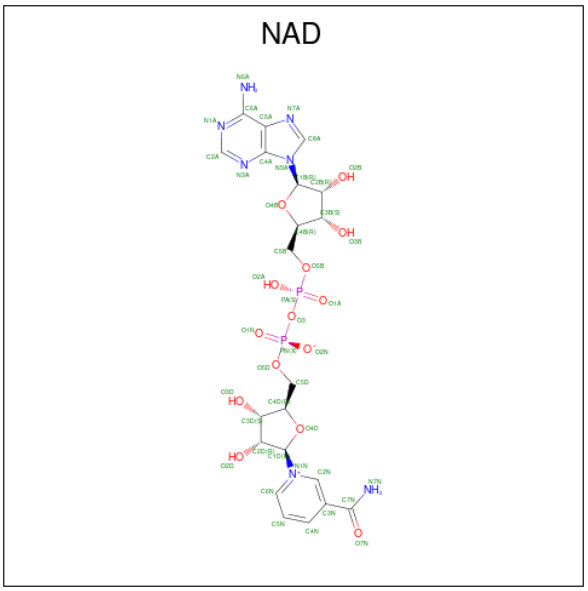
- Molecule 1 is a protein called 2-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total 3667	C 2319	N 637	O 699	S 12	0	0	0
1	B	483	Total 3667	C 2319	N 637	O 699	S 12	0	0	0
1	C	483	Total 3667	C 2319	N 637	O 699	S 12	0	0	0
1	D	483	Total 3667	C 2319	N 637	O 699	S 12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	GLU	engineered mutation	UNP Q83V33
B	268	ALA	GLU	engineered mutation	UNP Q83V33
C	268	ALA	GLU	engineered mutation	UNP Q83V33
D	268	ALA	GLU	engineered mutation	UNP Q83V33

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

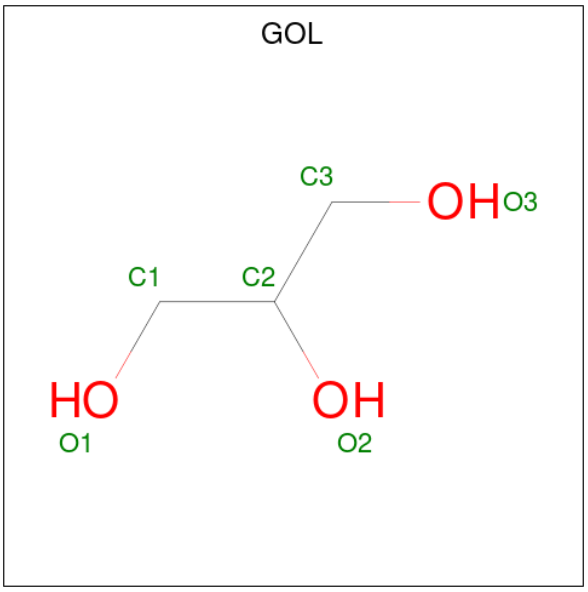


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

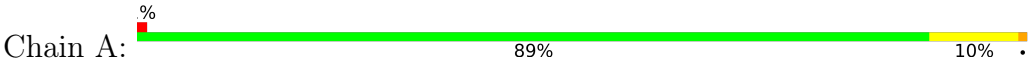
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	338	Total O 338 338	0	0
5	B	311	Total O 311 311	0	0
5	C	228	Total O 228 228	0	0
5	D	311	Total O 311 311	0	0

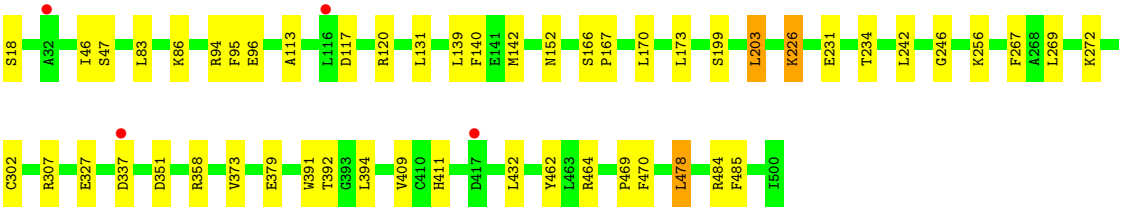
3 Residue-property plots (i)

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: 2-aminomuconate 6-semialdehyde dehydrogenase

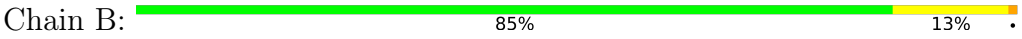
Chain A:

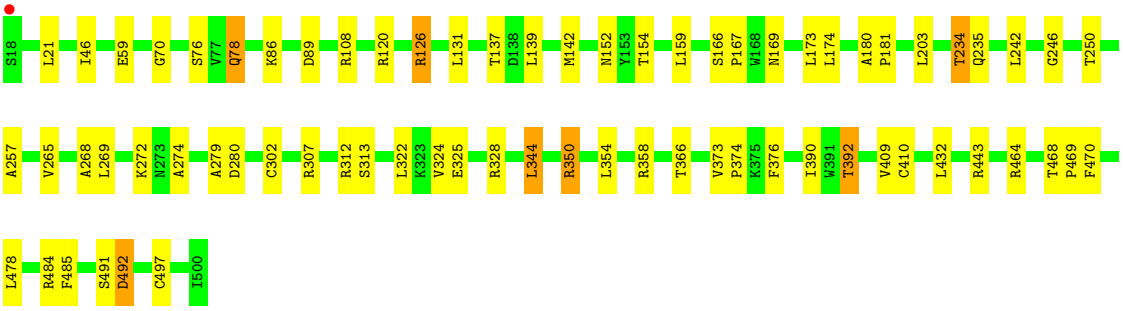




• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

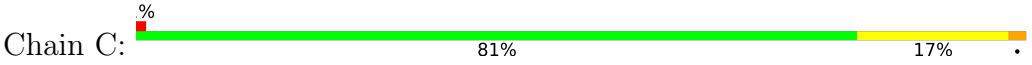
Chain B:

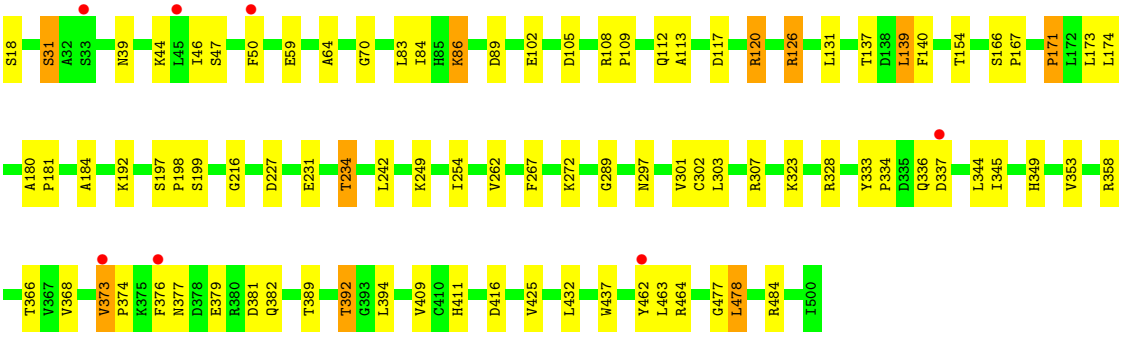




• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

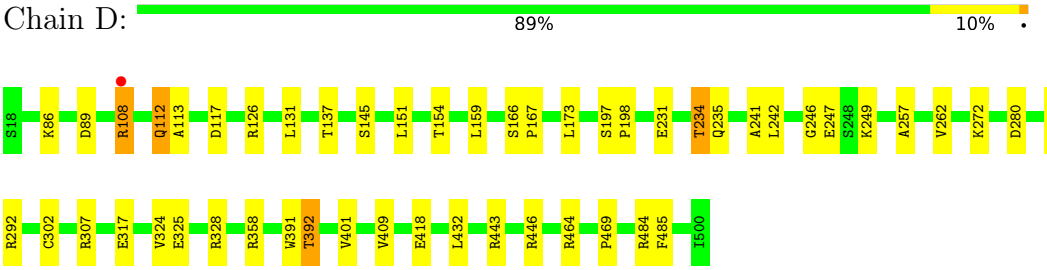
Chain C:





• Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.53Å 141.98Å 173.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.74 – 2.00 41.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (41.74-2.00) 86.4 (41.74-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.195 , 0.237 0.192 , 0.232	Depositor DCC
R_{free} test set	7372 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.4	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	0.96	EDS
Total number of atoms	16164	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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: NA, NAD, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/3746	0.76	2/5093 (0.0%)
1	B	0.48	0/3746	0.80	4/5093 (0.1%)
1	C	0.43	0/3746	0.78	3/5093 (0.1%)
1	D	0.48	0/3746	0.77	0/5093
All	All	0.47	0/14984	0.78	9/20372 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	46	ILE	CB-CA-C	-7.14	102.94	111.94
1	C	70	GLY	CA-C-N	6.21	126.40	119.32
1	C	70	GLY	C-N-CA	6.21	126.40	119.32
1	A	46	ILE	CB-CA-C	-5.72	104.73	111.94
1	B	169	ASN	N-CA-C	5.61	117.20	111.14
1	A	199	SER	N-CA-C	5.24	116.79	111.14
1	B	70	GLY	CA-C-N	5.09	124.88	119.28
1	B	70	GLY	C-N-CA	5.09	124.88	119.28
1	C	477	GLY	N-CA-C	5.03	116.98	110.45

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	3667	0	3604	51	0
1	B	3667	0	3604	72	0
1	C	3667	0	3604	73	0
1	D	3667	0	3604	52	0
2	A	44	26	26	7	0
2	B	44	26	24	13	0
2	C	44	26	26	8	0
2	D	44	26	25	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	5	0
4	B	6	0	8	6	0
4	C	6	0	8	3	0
4	D	6	0	8	2	0
5	A	338	0	0	10	0
5	B	311	0	0	10	0
5	C	228	0	0	7	0
5	D	311	0	0	6	0
All	All	16060	104	14549	249	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 8.

All (249) 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:142:MET:CE	1:B:152:ASN:HD21	1.42	1.31
1:B:142:MET:CE	1:B:152:ASN:ND2	2.09	1.15
1:C:18:SER:HB3	1:C:47:SER:HB3	1.20	1.14
1:B:142:MET:HE2	1:B:152:ASN:ND2	1.62	1.12
1:A:142:MET:HE2	1:A:152:ASN:HD21	1.15	1.08
1:A:18:SER:HB3	1:A:47:SER:HB3	1.42	1.00
1:C:366:THR:HB	1:C:392:THR:HG22	1.42	1.00
1:D:280:ASP:OD2	1:D:443:ARG:NH1	1.97	0.98
1:A:142:MET:HE2	1:A:152:ASN:ND2	1.76	0.98
1:C:302:CYS:SG	2:C:601:NAD:C4N	2.54	0.96
1:B:142:MET:HE1	1:B:152:ASN:HD21	1.32	0.95
1:B:366:THR:HB	1:B:392:THR:HG22	1.53	0.88
1:A:302:CYS:SG	2:A:601:NAD:C4N	2.63	0.87
1:B:302:CYS:SG	2:B:601:NAD:C4N	2.62	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:OD2	1:B:443:ARG:NH1	2.08	0.86
1:C:328:ARG:NE	5:C:902:HOH:O	2.09	0.86
1:D:288:GLU:OE2	1:D:292:ARG:NE	2.12	0.82
1:A:231:GLU:O	1:A:234:THR:HG22	1.78	0.82
1:D:325:GLU:OE2	1:D:328:ARG:NH2	2.13	0.81
1:A:226:LYS:HE2	5:A:928:HOH:O	1.80	0.81
1:A:379:GLU:OE1	5:A:1003:HOH:O	1.99	0.81
1:C:108:ARG:HD2	1:C:297:ASN:OD1	1.81	0.80
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.62	0.80
1:D:464:ARG:HH11	4:D:603:GOL:H2	1.48	0.78
1:A:234:THR:HG21	5:A:943:HOH:O	1.82	0.78
1:D:234:THR:HG21	5:D:854:HOH:O	1.83	0.77
1:A:142:MET:CE	1:A:152:ASN:HD21	1.96	0.77
4:A:603:GOL:H11	5:A:945:HOH:O	1.84	0.77
1:B:325:GLU:OE1	1:B:328:ARG:NH1	2.18	0.76
1:B:142:MET:HE2	5:B:980:HOH:O	1.86	0.76
1:C:102:GLU:OE2	1:C:171:PRO:HB2	1.85	0.76
1:C:231:GLU:O	1:C:234:THR:HG22	1.85	0.76
1:C:109:PRO:HB2	1:C:112:GLN:HG3	1.69	0.76
1:D:108:ARG:CD	1:D:112:GLN:HG2	2.15	0.75
1:C:302:CYS:SG	2:C:601:NAD:H4N	2.25	0.75
1:D:108:ARG:HD3	1:D:112:GLN:CD	2.13	0.74
1:A:351:ASP:OD2	5:A:874:HOH:O	2.04	0.74
1:B:78:GLN:H	1:B:78:GLN:CD	1.94	0.73
1:C:18:SER:CB	1:C:47:SER:HB3	2.10	0.73
1:D:108:ARG:HD3	1:D:112:GLN:NE2	2.02	0.73
1:A:464:ARG:HE	4:A:603:GOL:H12	1.54	0.73
2:A:601:NAD:O1N	5:A:722:HOH:O	2.06	0.72
1:D:108:ARG:CG	1:D:112:GLN:HG2	2.19	0.72
1:D:358:ARG:NH2	5:D:877:HOH:O	2.23	0.71
1:B:246:GLY:HA2	2:B:601:NAD:O4D	1.90	0.71
1:C:358:ARG:HG3	1:C:358:ARG:HH11	1.55	0.71
1:C:416:ASP:OD1	5:C:797:HOH:O	2.07	0.71
1:B:142:MET:HE2	1:B:152:ASN:HD22	1.51	0.70
1:B:120:ARG:NH2	4:B:603:GOL:O2	2.24	0.70
1:B:250:THR:OG1	5:B:989:HOH:O	2.09	0.69
1:C:113:ALA:HA	1:C:117:ASP:HB2	1.72	0.69
1:B:234:THR:HG21	5:B:766:HOH:O	1.93	0.69
1:D:108:ARG:CD	1:D:112:GLN:CG	2.71	0.69
1:C:109:PRO:HB2	1:C:112:GLN:CG	2.24	0.68
1:D:262:VAL:O	5:D:705:HOH:O	2.12	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:CYS:SG	2:D:601:NAD:C4N	2.82	0.67
1:B:358:ARG:NH2	5:B:876:HOH:O	2.25	0.66
1:C:44:LYS:NZ	5:C:834:HOH:O	2.29	0.66
1:C:120:ARG:NH2	4:C:603:GOL:O3	2.28	0.66
1:C:373:VAL:HG23	1:C:374:PRO:HD2	1.77	0.66
1:D:108:ARG:HD2	1:D:117:ASP:OD1	1.95	0.66
1:B:120:ARG:NH1	4:B:603:GOL:O1	2.28	0.65
1:C:366:THR:HB	1:C:392:THR:CG2	2.23	0.65
1:D:418:GLU:OE2	1:D:446:ARG:HD2	1.96	0.65
1:C:18:SER:HB3	1:C:47:SER:CB	2.13	0.65
1:B:59:GLU:OE1	5:B:868:HOH:O	2.15	0.64
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.77	0.64
1:B:491:SER:O	5:B:703:HOH:O	2.14	0.64
2:B:601:NAD:O2N	5:B:708:HOH:O	2.15	0.63
1:B:464:ARG:HE	4:B:603:GOL:H2	1.64	0.63
1:D:108:ARG:CD	1:D:112:GLN:CD	2.71	0.63
1:B:89:ASP:OD1	1:B:126:ARG:NH2	2.22	0.63
1:A:462:TYR:HE1	1:A:464:ARG:HG3	1.64	0.62
1:A:18:SER:CB	1:A:47:SER:HB3	2.25	0.62
1:B:234:THR:HG23	1:B:257:ALA:CB	2.30	0.62
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.80	0.62
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.34	0.62
1:C:358:ARG:HG3	1:C:358:ARG:NH1	2.10	0.61
1:B:302:CYS:SG	2:B:601:NAD:H4N	2.40	0.61
1:C:302:CYS:HB3	2:C:601:NAD:C4N	2.30	0.61
1:C:333:TYR:HB2	1:C:336:GLN:HB2	1.82	0.61
1:A:327:GLU:OE1	5:A:1010:HOH:O	2.17	0.61
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.83	0.60
1:C:105:ASP:OD2	1:C:199:SER:HB2	2.01	0.60
1:C:462:TYR:HE1	1:C:464:ARG:HG3	1.67	0.59
1:C:120:ARG:NH2	4:C:603:GOL:O2	2.28	0.59
1:B:344:LEU:HD23	1:B:350:ARG:HA	1.84	0.59
1:B:374:PRO:HG2	1:B:376:PHE:CE2	2.37	0.58
1:B:234:THR:HG23	1:B:257:ALA:HB1	1.86	0.58
1:B:265:VAL:HG23	1:B:478:LEU:HD21	1.85	0.58
1:A:464:ARG:HE	4:A:603:GOL:C1	2.16	0.58
1:C:302:CYS:CB	2:C:601:NAD:C4N	2.82	0.58
1:D:325:GLU:CD	1:D:328:ARG:HH21	2.12	0.58
1:B:350:ARG:HD3	1:B:354:LEU:HD11	1.85	0.57
1:C:59:GLU:OE1	5:C:798:HOH:O	2.17	0.57
1:A:462:TYR:CE1	1:A:464:ARG:HG3	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:VAL:HG12	1:C:303:LEU:H	1.69	0.57
1:D:108:ARG:HD2	1:D:112:GLN:CG	2.35	0.57
1:D:108:ARG:HG3	1:D:112:GLN:HG2	1.86	0.57
1:A:267:PHE:CD2	1:A:478:LEU:CD2	2.88	0.56
1:A:267:PHE:CD2	1:A:478:LEU:HD21	2.41	0.56
1:D:247:GLU:OE1	1:D:249:LYS:HE3	2.05	0.56
1:D:113:ALA:HA	1:D:117:ASP:HB2	1.87	0.56
1:D:108:ARG:HB2	1:D:108:ARG:CZ	2.35	0.56
1:B:302:CYS:HB3	2:B:601:NAD:C5N	2.35	0.56
1:C:302:CYS:HB3	2:C:601:NAD:C5N	2.34	0.56
1:B:324:VAL:O	1:B:328:ARG:HG3	2.06	0.55
1:A:302:CYS:SG	2:A:601:NAD:H4N	2.47	0.55
1:D:231:GLU:O	1:D:234:THR:HG22	2.07	0.55
1:A:246:GLY:HA2	2:A:601:NAD:O4D	2.06	0.54
1:A:120:ARG:NH2	4:A:603:GOL:O2	2.31	0.53
1:A:83:LEU:O	1:A:86:LYS:HB3	2.08	0.53
1:C:89:ASP:OD1	1:C:126:ARG:NH2	2.33	0.53
1:D:302:CYS:SG	2:D:601:NAD:C3N	2.96	0.53
1:D:166:SER:HB2	1:D:167:PRO:HD2	1.91	0.53
1:D:246:GLY:HA2	2:D:601:NAD:O4D	2.09	0.53
1:C:358:ARG:HH11	1:C:358:ARG:CG	2.21	0.52
1:A:391:TRP:CH2	1:A:409:VAL:HG21	2.44	0.52
1:D:89:ASP:OD1	1:D:126:ARG:NH2	2.40	0.52
1:A:256:LYS:NZ	5:A:925:HOH:O	2.42	0.52
1:A:166:SER:HB2	1:A:167:PRO:HD2	1.92	0.52
1:C:462:TYR:CE1	1:C:464:ARG:HG3	2.45	0.52
1:D:272:LYS:HG3	1:D:307:ARG:CD	2.39	0.51
1:D:464:ARG:NH1	4:D:603:GOL:H2	2.22	0.50
1:A:272:LYS:HG3	1:A:307:ARG:CD	2.42	0.50
1:C:323:LYS:HD2	1:C:368:VAL:CG1	2.42	0.50
1:C:31:SER:OG	1:C:50:PHE:HB3	2.11	0.50
1:C:227:ASP:N	1:C:231:GLU:OE1	2.25	0.50
1:A:484:ARG:HE	1:B:484:ARG:NH1	2.10	0.49
1:B:166:SER:HB2	1:B:167:PRO:HD2	1.94	0.49
1:B:302:CYS:HB3	2:B:601:NAD:C4N	2.42	0.49
1:C:302:CYS:SG	2:C:601:NAD:C3N	3.00	0.49
1:B:464:ARG:HE	4:B:603:GOL:C2	2.25	0.49
1:B:78:GLN:CD	1:B:78:GLN:N	2.69	0.49
1:A:96:GLU:OE1	5:A:902:HOH:O	2.20	0.49
1:B:152:ASN:OD1	1:B:497:CYS:HB2	2.13	0.48
1:B:269:LEU:O	2:B:601:NAD:H2N	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:CYS:HB3	2:C:601:NAD:C3N	2.43	0.48
1:C:197:SER:N	1:C:198:PRO:HD3	2.27	0.48
1:C:302:CYS:CB	2:C:601:NAD:C3N	2.91	0.48
1:C:345:ILE:O	5:C:906:HOH:O	2.19	0.48
1:B:470:PHE:HE1	2:B:601:NAD:H72N	1.60	0.48
1:B:350:ARG:HD3	1:B:354:LEU:CD1	2.43	0.48
1:C:484:ARG:NH1	1:D:484:ARG:NH1	2.61	0.48
1:B:142:MET:HE3	1:B:152:ASN:ND2	2.21	0.48
1:B:302:CYS:CB	2:B:601:NAD:C4N	2.92	0.48
1:B:312:ARG:HG3	1:B:313:SER:N	2.29	0.47
1:C:262:VAL:O	1:C:262:VAL:HG12	2.12	0.47
1:C:139:LEU:HD13	1:C:140:PHE:N	2.29	0.47
1:C:349:HIS:O	1:C:353:VAL:HG23	2.13	0.47
1:C:166:SER:HB2	1:C:167:PRO:HD2	1.95	0.47
1:B:469:PRO:HB3	1:B:485:PHE:CE2	2.50	0.47
1:A:18:SER:HB3	1:A:47:SER:CB	2.29	0.47
1:B:246:GLY:CA	2:B:601:NAD:O4D	2.60	0.47
1:C:389:THR:HB	1:C:409:VAL:HG23	1.97	0.47
1:A:272:LYS:CG	1:A:307:ARG:HD2	2.45	0.47
1:C:139:LEU:HD13	1:C:139:LEU:C	2.40	0.47
1:B:234:THR:CG2	1:B:257:ALA:CB	2.94	0.46
1:C:64:ALA:HA	1:C:216:GLY:O	2.15	0.46
1:A:113:ALA:HA	1:A:117:ASP:HB2	1.97	0.46
1:A:166:SER:HB2	1:A:167:PRO:CD	2.46	0.46
1:B:265:VAL:HG23	1:B:478:LEU:CD2	2.44	0.46
1:A:302:CYS:SG	2:A:601:NAD:C3N	3.03	0.46
1:D:469:PRO:HB3	1:D:485:PHE:CE2	2.50	0.46
1:B:159:LEU:HD12	1:B:492:ASP:OD1	2.15	0.46
1:A:267:PHE:HB2	1:A:478:LEU:CD2	2.46	0.46
1:A:358:ARG:NH2	5:A:823:HOH:O	2.43	0.46
1:B:234:THR:CG2	1:B:257:ALA:HB1	2.45	0.46
1:A:469:PRO:HB3	1:A:485:PHE:CE2	2.51	0.46
1:B:322:LEU:HG	1:B:390:ILE:HD11	1.97	0.46
1:D:234:THR:HG23	1:D:257:ALA:HB1	1.98	0.45
1:B:268:ALA:HB1	2:B:601:NAD:C7N	2.47	0.45
1:A:246:GLY:O	1:A:269:LEU:HA	2.16	0.45
1:C:328:ARG:CZ	5:C:902:HOH:O	2.57	0.45
1:C:379:GLU:O	1:C:382:GLN:HB2	2.15	0.45
1:D:86:LYS:HD3	5:D:981:HOH:O	2.16	0.45
1:B:302:CYS:HB3	2:B:601:NAD:C6N	2.46	0.45
1:D:108:ARG:HD3	1:D:112:GLN:CG	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD13	1:A:140:PHE:N	2.32	0.45
1:C:376:PHE:O	5:C:885:HOH:O	2.21	0.45
1:C:109:PRO:HB2	1:C:112:GLN:HG2	1.99	0.45
1:C:174:LEU:HD23	4:C:603:GOL:H11	1.99	0.44
1:C:377:ASN:N	1:C:381:ASP:OD2	2.45	0.44
1:A:470:PHE:HE1	2:A:601:NAD:H72N	1.64	0.44
1:B:120:ARG:HG3	1:B:173:LEU:HG	1.98	0.44
1:B:464:ARG:HH21	4:B:603:GOL:H2	1.82	0.44
1:C:272:LYS:HG3	1:C:307:ARG:CD	2.47	0.44
1:A:139:LEU:HD13	1:A:139:LEU:C	2.43	0.44
1:C:323:LYS:HD2	1:C:368:VAL:HG12	1.99	0.44
1:C:478:LEU:HD23	1:C:478:LEU:O	2.18	0.44
1:D:108:ARG:HD2	1:D:112:GLN:CD	2.43	0.44
1:B:443:ARG:NE	5:B:871:HOH:O	2.14	0.43
1:D:302:CYS:HB3	2:D:601:NAD:C2N	2.48	0.43
1:C:83:LEU:O	1:C:86:LYS:HB2	2.18	0.43
1:B:21:LEU:N	1:B:21:LEU:HD12	2.33	0.43
1:B:234:THR:HG22	1:B:235:GLN:HG3	2.01	0.43
1:D:392:THR:HG21	5:D:970:HOH:O	2.18	0.43
1:B:137:THR:HB	1:B:154:THR:OG1	2.19	0.43
1:B:139:LEU:HD13	1:B:139:LEU:C	2.44	0.43
1:B:272:LYS:O	1:B:307:ARG:HD3	2.17	0.43
1:A:269:LEU:O	2:A:601:NAD:H2N	2.19	0.43
1:A:478:LEU:HD23	1:A:478:LEU:O	2.19	0.43
1:C:180:ALA:HB3	1:C:181:PRO:CD	2.49	0.43
1:D:108:ARG:HD3	1:D:112:GLN:HG2	1.96	0.43
1:B:76:SER:OG	1:B:78:GLN:HG2	2.19	0.43
1:B:268:ALA:HB1	2:B:601:NAD:N7N	2.34	0.43
1:C:463:LEU:HD23	1:C:463:LEU:HA	1.93	0.42
1:A:267:PHE:CD2	1:A:478:LEU:HD22	2.54	0.42
1:C:39:ASN:HB2	1:C:46:ILE:HD11	2.00	0.42
1:D:151:LEU:HD21	5:D:869:HOH:O	2.19	0.42
1:D:234:THR:HG22	1:D:235:GLN:HG3	2.01	0.42
4:B:603:GOL:H11	5:B:931:HOH:O	2.19	0.42
1:C:289:GLY:HA3	1:C:437:TRP:CZ2	2.55	0.42
1:C:234:THR:OG1	1:C:254:ILE:HG23	2.20	0.42
1:C:307:ARG:NH2	1:C:425:VAL:HA	2.35	0.42
1:C:267:PHE:CD2	1:C:478:LEU:HD22	2.54	0.42
1:D:166:SER:HB2	1:D:167:PRO:CD	2.50	0.42
1:A:173:LEU:C	1:A:173:LEU:HD23	2.44	0.42
1:D:324:VAL:O	1:D:328:ARG:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.88	0.42
1:D:391:TRP:CZ3	1:D:409:VAL:HG21	2.54	0.42
1:C:394:LEU:HB2	1:C:411:HIS:NE2	2.35	0.41
1:D:159:LEU:CD2	1:D:241:ALA:HB2	2.50	0.41
1:D:173:LEU:HD23	1:D:173:LEU:C	2.45	0.41
1:D:283:LEU:HD21	1:D:317:GLU:HG2	2.01	0.41
1:B:166:SER:HB2	1:B:167:PRO:CD	2.50	0.41
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.90	0.41
1:C:173:LEU:C	1:C:173:LEU:HD23	2.45	0.41
1:B:409:VAL:HG22	1:B:410:CYS:N	2.35	0.41
1:D:197:SER:N	1:D:198:PRO:HD3	2.36	0.41
1:D:231:GLU:O	1:D:235:GLN:HG3	2.21	0.41
1:A:94:ARG:O	1:A:95:PHE:C	2.62	0.41
1:C:84:ILE:CD1	1:C:184:ALA:HA	2.51	0.41
1:B:272:LYS:HG3	1:B:307:ARG:CD	2.50	0.41
1:C:137:THR:HB	1:C:154:THR:OG1	2.21	0.41
1:D:137:THR:HB	1:D:154:THR:OG1	2.21	0.41
1:A:120:ARG:HH12	4:A:603:GOL:HO1	1.64	0.41
1:A:391:TRP:CZ3	1:A:409:VAL:HG21	2.56	0.41
1:B:180:ALA:N	1:B:181:PRO:HD2	2.36	0.41
1:C:197:SER:N	1:C:198:PRO:CD	2.84	0.41
1:B:274:ALA:HA	1:B:307:ARG:O	2.21	0.41
1:A:140:PHE:CD1	1:B:468:THR:HG22	2.56	0.40
1:B:173:LEU:C	1:B:173:LEU:HD23	2.46	0.40
1:C:109:PRO:HA	1:C:334:PRO:HA	2.02	0.40
1:A:394:LEU:HB2	1:A:411:HIS:NE2	2.36	0.40
1:B:279:ALA:HB3	5:B:943:HOH:O	2.21	0.40
1:B:470:PHE:CD1	1:B:470:PHE:C	2.99	0.40
1:C:307:ARG:HH22	1:C:425:VAL:HA	1.87	0.40
1:D:302:CYS:CB	2:D:601:NAD:C3N	2.99	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	481/483 (100%)	462 (96%)	18 (4%)	1 (0%)	43	42
1	B	481/483 (100%)	462 (96%)	19 (4%)	0	100	100
1	C	481/483 (100%)	461 (96%)	18 (4%)	2 (0%)	30	27
1	D	481/483 (100%)	466 (97%)	15 (3%)	0	100	100
All	All	1924/1932 (100%)	1851 (96%)	70 (4%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	337	ASP
1	A	337	ASP
1	C	171	PRO

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	391/391 (100%)	382 (98%)	9 (2%)	44	49
1	B	391/391 (100%)	377 (96%)	14 (4%)	31	31
1	C	391/391 (100%)	376 (96%)	15 (4%)	29	29
1	D	391/391 (100%)	382 (98%)	9 (2%)	44	49
All	All	1564/1564 (100%)	1517 (97%)	47 (3%)	36	38

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	170	LEU
1	A	203	LEU
1	A	226	LYS
1	A	242	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	373	VAL
1	A	392	THR
1	A	432	LEU
1	A	478	LEU
1	B	78	GLN
1	B	86	LYS
1	B	108	ARG
1	B	126	ARG
1	B	131	LEU
1	B	203	LEU
1	B	234	THR
1	B	242	LEU
1	B	344	LEU
1	B	350	ARG
1	B	373	VAL
1	B	392	THR
1	B	432	LEU
1	B	492	ASP
1	C	31	SER
1	C	86	LYS
1	C	120	ARG
1	C	126	ARG
1	C	131	LEU
1	C	139	LEU
1	C	192	LYS
1	C	234	THR
1	C	242	LEU
1	C	249	LYS
1	C	344	LEU
1	C	373	VAL
1	C	392	THR
1	C	432	LEU
1	C	478	LEU
1	D	108	ARG
1	D	112	GLN
1	D	131	LEU
1	D	145	SER
1	D	234	THR
1	D	242	LEU
1	D	392	THR
1	D	401	VAL
1	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	B	92	GLN
1	B	152	ASN
1	C	377	ASN
1	C	495	ASN
1	D	112	GLN
1	D	377	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.23	0
2	NAD	A	601	-	46,48,48	1.61	7 (15%)	64,73,73	2.29	13 (20%)
4	GOL	B	603	-	5,5,5	0.43	0	5,5,5	0.49	0
2	NAD	B	601	-	46,48,48	1.65	7 (15%)	64,73,73	2.22	16 (25%)
4	GOL	C	603	-	5,5,5	0.31	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	D	603	-	5,5,5	0.41	0	5,5,5	0.32	0
2	NAD	D	601	-	46,48,48	1.61	4 (8%)	64,73,73	2.03	16 (25%)
2	NAD	C	601	-	46,48,48	1.62	6 (13%)	64,73,73	2.40	14 (21%)

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
4	GOL	A	603	-	-	0/4/4/4	-
2	NAD	A	601	-	-	5/30/62/62	0/5/5/5
4	GOL	B	603	-	-	2/4/4/4	-
2	NAD	B	601	-	-	4/30/62/62	0/5/5/5
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	D	603	-	-	3/4/4/4	-
2	NAD	D	601	-	-	3/30/62/62	0/5/5/5
2	NAD	C	601	-	-	4/30/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	C7N-N7N	6.12	1.44	1.33
2	A	601	NAD	C7N-N7N	5.95	1.43	1.33
2	B	601	NAD	C7N-N7N	5.77	1.43	1.33
2	C	601	NAD	C7N-N7N	5.62	1.43	1.33
2	C	601	NAD	C6A-N6A	3.80	1.43	1.34
2	A	601	NAD	C6A-N6A	3.75	1.43	1.34
2	B	601	NAD	C6A-N6A	3.69	1.43	1.34
2	D	601	NAD	C6A-N6A	3.56	1.43	1.34
2	D	601	NAD	C5A-N7A	-3.51	1.32	1.39
2	A	601	NAD	C5A-N7A	-2.94	1.33	1.39
2	C	601	NAD	C5A-N7A	-2.94	1.33	1.39
2	B	601	NAD	C5A-N7A	-2.77	1.34	1.39
2	B	601	NAD	O4B-C4B	-2.54	1.39	1.45
2	C	601	NAD	O4D-C4D	-2.54	1.39	1.45
2	B	601	NAD	C2D-C3D	-2.49	1.46	1.53
2	A	601	NAD	C2D-C3D	-2.27	1.47	1.53
2	C	601	NAD	C2D-C3D	-2.27	1.47	1.53
2	B	601	NAD	PA-O3	-2.26	1.57	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	O4B-C4B	-2.25	1.40	1.45
2	D	601	NAD	PA-O3	-2.13	1.57	1.59
2	A	601	NAD	C2N-N1N	2.06	1.37	1.35
2	A	601	NAD	O4D-C4D	-2.05	1.40	1.45
2	B	601	NAD	C2N-N1N	2.02	1.37	1.35
2	A	601	NAD	PA-O1A	2.00	1.57	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	NAD	O3-PA-O1A	-8.18	86.09	110.70
2	B	601	NAD	C4D-O4D-C1D	-8.01	102.59	109.92
2	A	601	NAD	O3-PA-O1A	-7.78	87.31	110.70
2	D	601	NAD	C5A-C4A-N3A	-6.86	117.27	126.72
2	A	601	NAD	O2A-PA-O1A	-6.48	82.29	112.44
2	C	601	NAD	O2A-PA-O1A	-6.26	83.30	112.44
2	C	601	NAD	C4D-O4D-C1D	-6.24	104.22	109.92
2	C	601	NAD	O5B-PA-O1A	-5.88	85.64	108.94
2	B	601	NAD	O4D-C4D-C5D	5.81	127.96	109.33
2	D	601	NAD	N3A-C4A-N9A	5.59	136.68	127.17
2	A	601	NAD	O2A-PA-O3	5.55	122.27	107.27
2	A	601	NAD	O5B-PA-O1A	-5.54	86.99	108.94
2	C	601	NAD	C5A-C4A-N3A	-5.50	119.15	126.72
2	A	601	NAD	C5A-C4A-N3A	-5.43	119.25	126.72
2	B	601	NAD	C5A-C4A-N3A	-5.38	119.30	126.72
2	D	601	NAD	C2B-C1B-N9A	5.29	126.45	113.30
2	A	601	NAD	N3A-C2A-N1A	-5.12	120.83	128.58
2	B	601	NAD	N3A-C2A-N1A	-5.06	120.93	128.58
2	C	601	NAD	N3A-C2A-N1A	-5.04	120.95	128.58
2	D	601	NAD	O4B-C1B-N9A	5.00	117.70	108.09
2	C	601	NAD	O2A-PA-O3	4.96	120.69	107.27
2	D	601	NAD	N3A-C2A-N1A	-4.78	121.35	128.58
2	C	601	NAD	C5A-N7A-C8A	4.11	109.90	103.45
2	A	601	NAD	C5A-N7A-C8A	3.94	109.64	103.45
2	C	601	NAD	N3A-C4A-N9A	3.90	133.79	127.17
2	B	601	NAD	C5A-N7A-C8A	3.79	109.41	103.45
2	D	601	NAD	C2A-N3A-C4A	3.78	121.06	111.83
2	C	601	NAD	C4A-C5A-N7A	-3.77	106.27	110.58
2	B	601	NAD	O4B-C4B-C5B	3.72	121.24	109.33
2	A	601	NAD	C4A-C5A-N7A	-3.69	106.36	110.58
2	A	601	NAD	C4D-O4D-C1D	-3.68	106.56	109.92
2	B	601	NAD	N3A-C4A-N9A	3.67	133.40	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	NAD	N3A-C4A-N9A	3.53	133.16	127.17
2	C	601	NAD	C2A-N3A-C4A	3.51	120.41	111.83
2	A	601	NAD	C2A-N3A-C4A	3.50	120.39	111.83
2	D	601	NAD	C5A-N7A-C8A	3.50	108.95	103.45
2	B	601	NAD	C2D-C3D-C4D	-3.48	95.89	102.61
2	B	601	NAD	C2A-N3A-C4A	3.46	120.27	111.83
2	B	601	NAD	C4A-C5A-N7A	-3.44	106.65	110.58
2	B	601	NAD	O4D-C4D-C3D	3.39	111.88	105.15
2	B	601	NAD	C2B-C3B-C4B	-3.30	96.22	102.61
2	B	601	NAD	O4B-C4B-C3B	3.05	111.20	105.15
2	B	601	NAD	N9A-C8A-N7A	-2.91	109.81	113.94
2	D	601	NAD	C4D-O4D-C1D	-2.89	107.27	109.92
2	C	601	NAD	N9A-C8A-N7A	-2.79	109.98	113.94
2	D	601	NAD	O4B-C1B-C2B	2.78	112.57	106.62
2	A	601	NAD	N9A-C8A-N7A	-2.70	110.11	113.94
2	A	601	NAD	O2A-PA-O5B	2.68	119.70	107.57
2	B	601	NAD	C4B-O4B-C1B	-2.52	103.90	109.47
2	D	601	NAD	C1B-N9A-C8A	-2.52	121.51	127.09
2	D	601	NAD	C4A-C5A-N7A	-2.42	107.81	110.58
2	C	601	NAD	O2A-PA-O5B	2.39	118.41	107.57
2	D	601	NAD	C4A-N9A-C1B	2.38	132.20	126.63
2	D	601	NAD	C6A-C5A-C4A	2.35	120.39	117.18
2	D	601	NAD	C3N-C7N-N7N	2.26	120.53	117.74
2	B	601	NAD	C5B-C4B-C3B	2.15	122.96	115.21
2	C	601	NAD	C3N-C7N-N7N	2.14	120.38	117.74
2	D	601	NAD	N9A-C8A-N7A	-2.06	111.02	113.94
2	D	601	NAD	C5A-C6A-N6A	-2.00	118.33	123.29

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C5B-O5B-PA-O3
2	B	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	O4D-C1D-N1N-C6N
2	C	601	NAD	C5B-O5B-PA-O1A
2	C	601	NAD	C5B-O5B-PA-O3
2	D	601	NAD	C5B-O5B-PA-O3
4	B	603	GOL	O1-C1-C2-C3
4	C	603	GOL	C1-C2-C3-O3
4	D	603	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	603	GOL	O1-C1-C2-O2
4	C	603	GOL	O1-C1-C2-O2
4	C	603	GOL	O2-C2-C3-O3
4	B	603	GOL	O1-C1-C2-O2
4	D	603	GOL	O2-C2-C3-O3
2	B	601	NAD	PN-O3-PA-O5B
2	C	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C5B-O5B-PA-O1A
2	A	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	O4B-C4B-C5B-O5B
2	D	601	NAD	O4B-C1B-N9A-C8A
2	B	601	NAD	C4D-C5D-O5D-PN
2	C	601	NAD	C2B-C1B-N9A-C8A
2	A	601	NAD	C2B-C1B-N9A-C8A

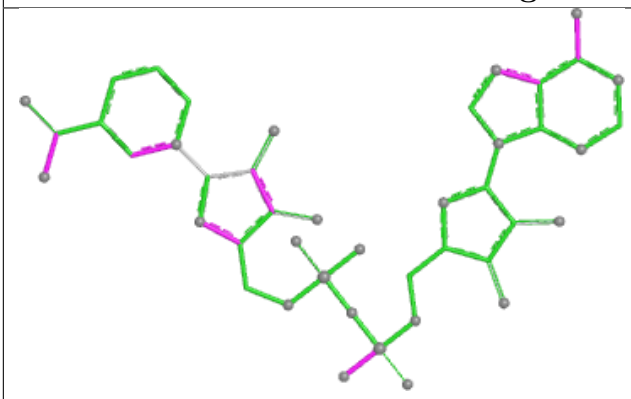
There are no ring outliers.

8 monomers are involved in 49 short contacts:

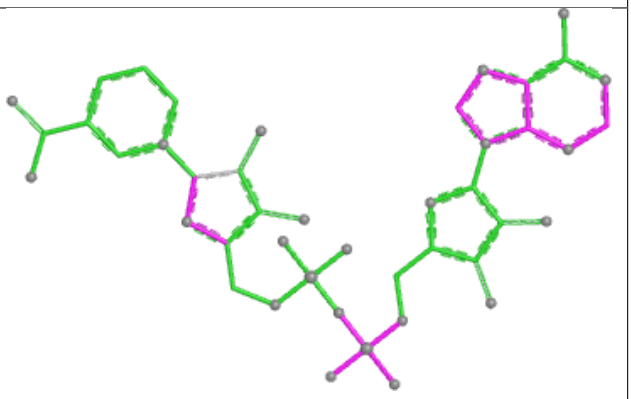
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	5	0
2	A	601	NAD	7	0
4	B	603	GOL	6	0
2	B	601	NAD	13	0
4	C	603	GOL	3	0
4	D	603	GOL	2	0
2	D	601	NAD	5	0
2	C	601	NAD	8	0

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.

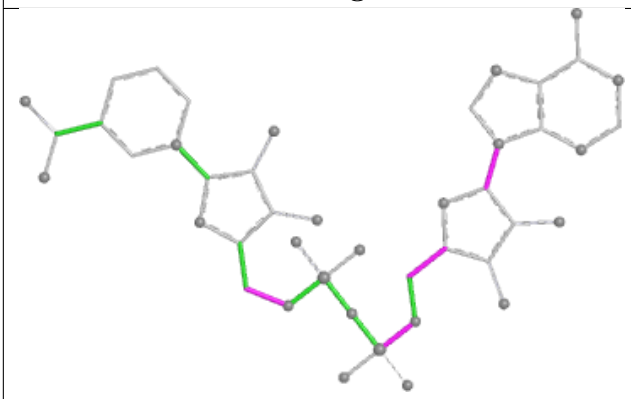
Ligand NAD A 601



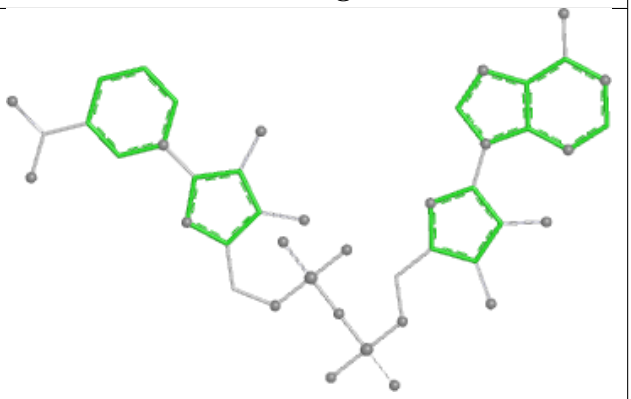
Bond lengths



Bond angles

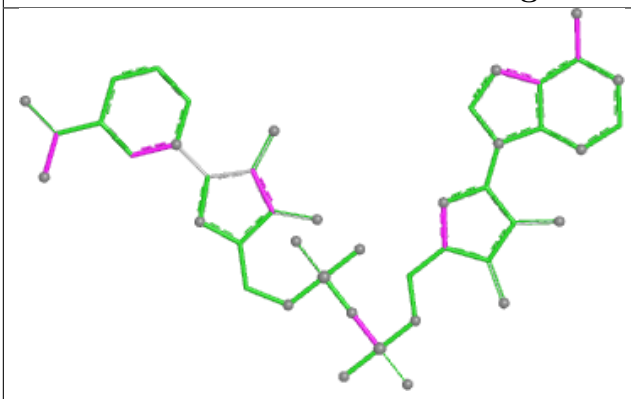


Torsions

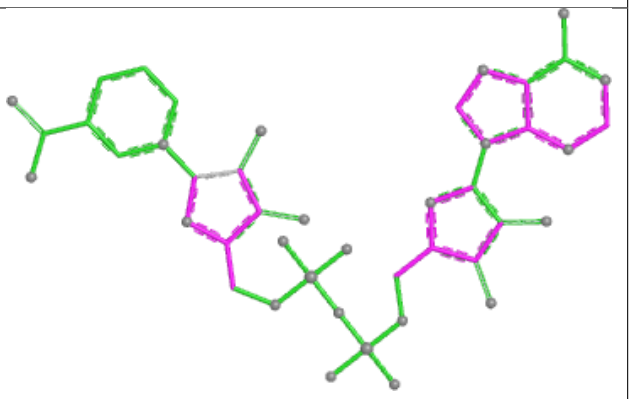


Rings

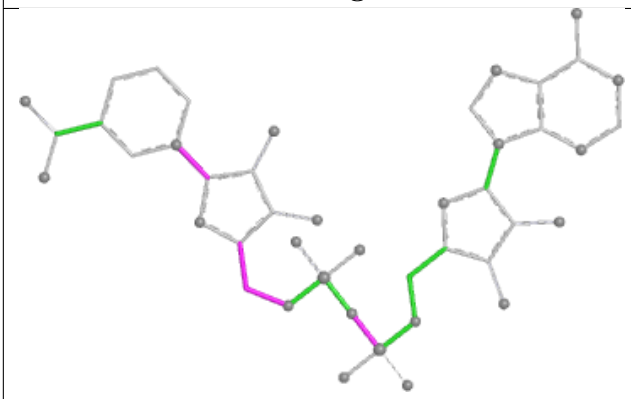
Ligand NAD B 601



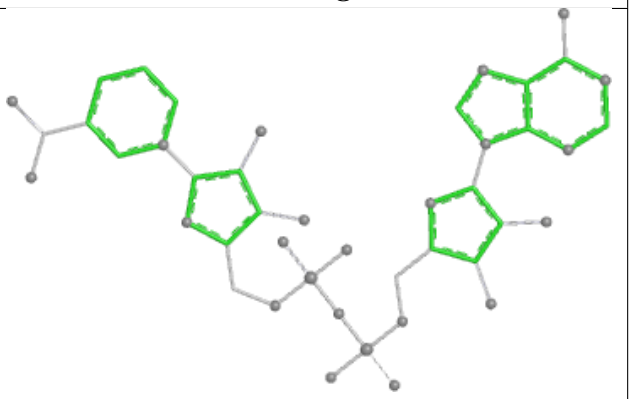
Bond lengths



Bond angles

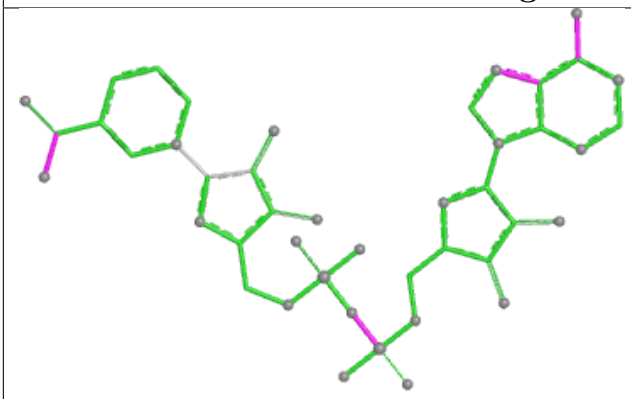


Torsions

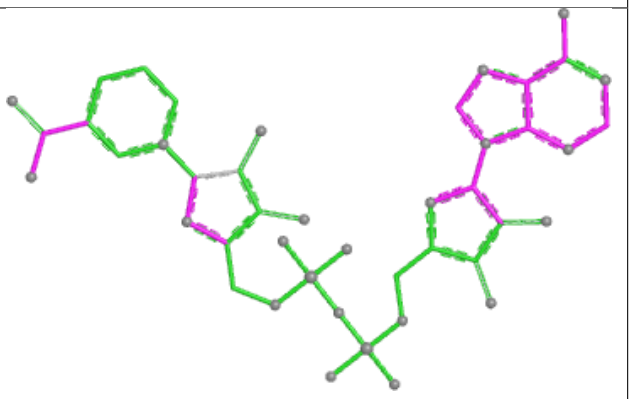


Rings

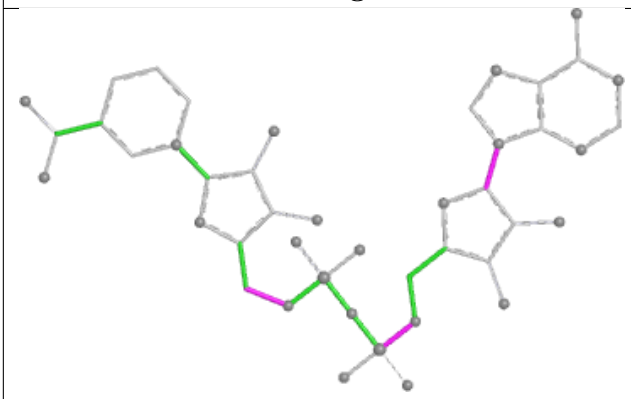
Ligand NAD D 601



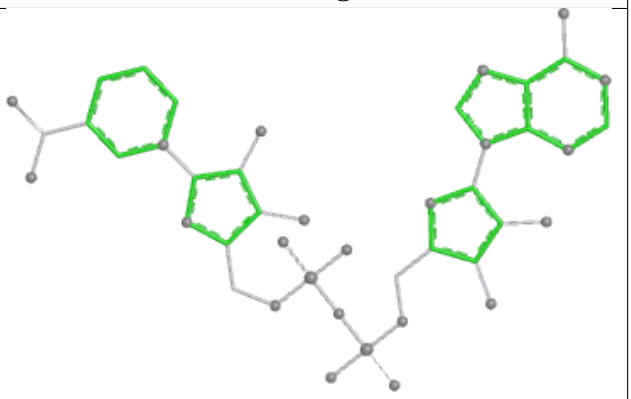
Bond lengths



Bond angles

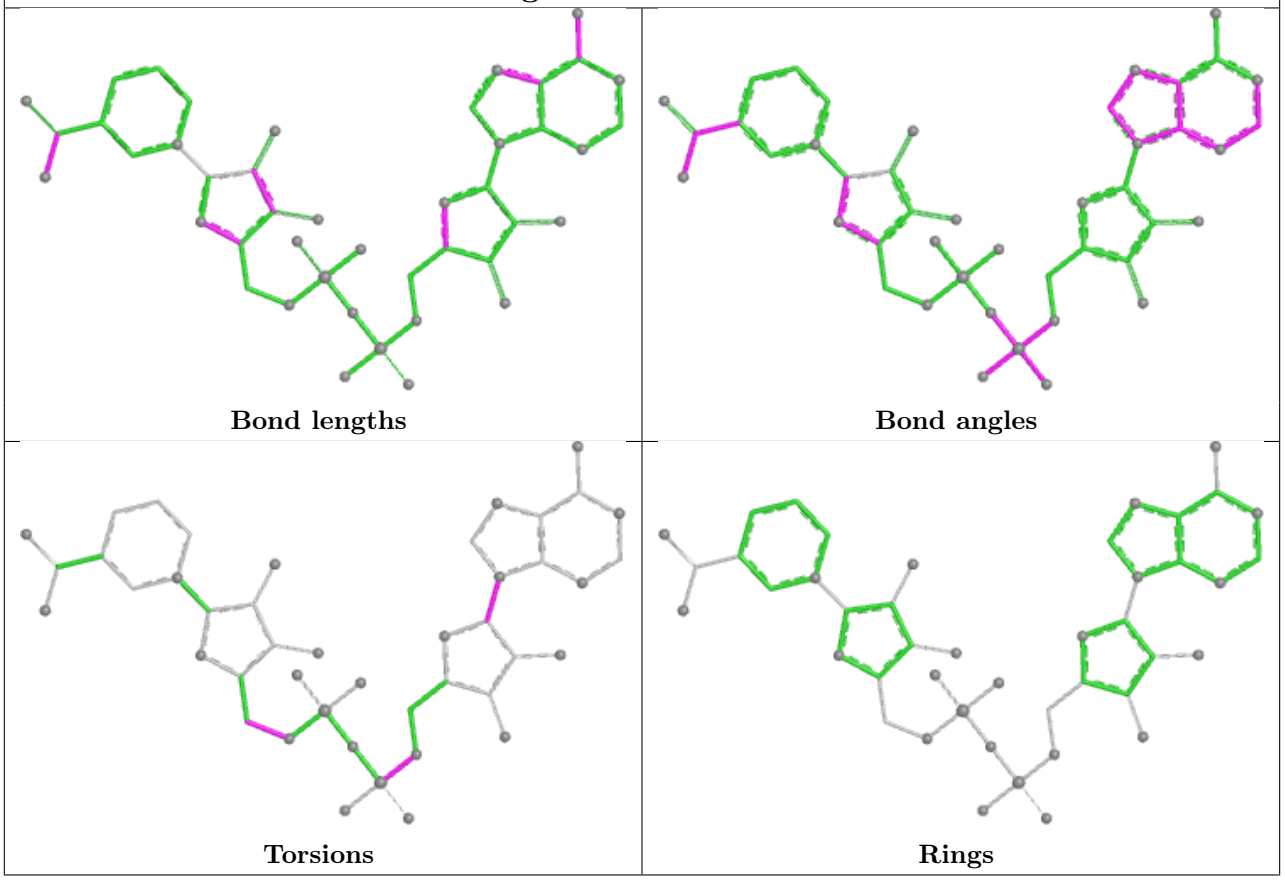


Torsions



Rings

Ligand NAD C 601



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	483/483 (100%)	-0.19	4 (0%)	82	82	19, 29, 40, 52	0
1	B	483/483 (100%)	-0.21	1 (0%)	91	90	18, 29, 39, 56	0
1	C	483/483 (100%)	0.26	7 (1%)	73	73	20, 36, 50, 69	0
1	D	483/483 (100%)	-0.16	1 (0%)	91	90	20, 30, 40, 49	0
All	All	1932/1932 (100%)	-0.08	13 (0%)	84	84	18, 30, 45, 69	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	SER	4.8
1	A	32	ALA	3.2
1	A	116	LEU	3.2
1	A	337	ASP	2.9
1	C	337	ASP	2.3
1	C	45	LEU	2.3
1	C	462	TYR	2.3
1	C	376	PHE	2.2
1	D	108	ARG	2.2
1	C	50	PHE	2.2
1	C	373	VAL	2.1
1	C	33	SER	2.0
1	A	417	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

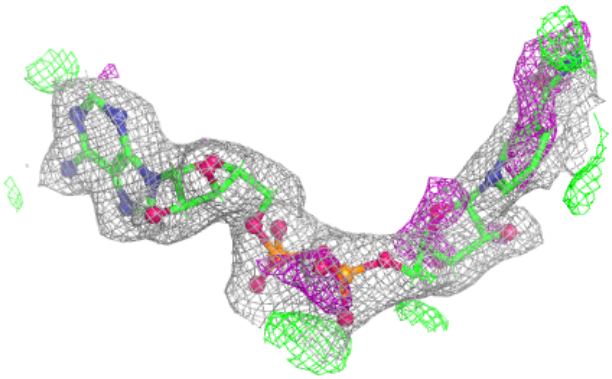
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

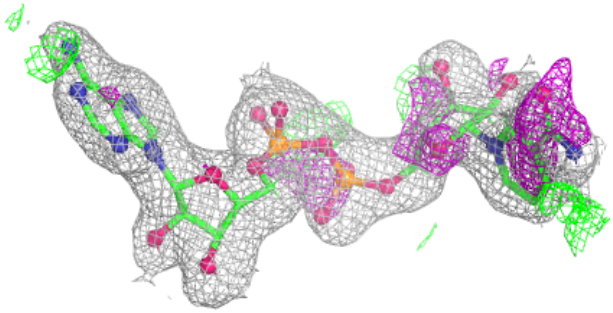
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	603	6/6	0.80	0.17	33,38,41,43	0
3	NA	C	602	1/1	0.83	0.13	42,42,42,42	0
4	GOL	C	603	6/6	0.85	0.11	42,43,47,50	0
2	NAD	C	601	44/44	0.87	0.11	32,43,52,57	0
4	GOL	D	603	6/6	0.88	0.14	36,38,43,48	0
3	NA	D	602	1/1	0.89	0.09	30,30,30,30	0
2	NAD	D	601	44/44	0.89	0.11	28,38,48,54	0
4	GOL	A	603	6/6	0.90	0.14	38,40,46,50	0
2	NAD	B	601	44/44	0.91	0.10	22,33,45,49	0
2	NAD	A	601	44/44	0.94	0.08	23,34,44,46	0
3	NA	A	602	1/1	0.95	0.06	30,30,30,30	0
3	NA	B	602	1/1	0.96	0.06	31,31,31,31	0

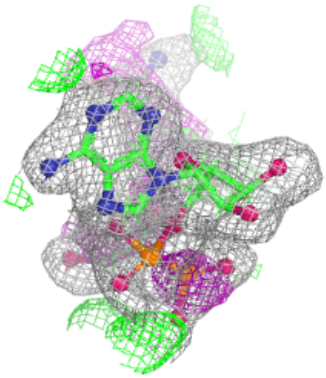
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 601:

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

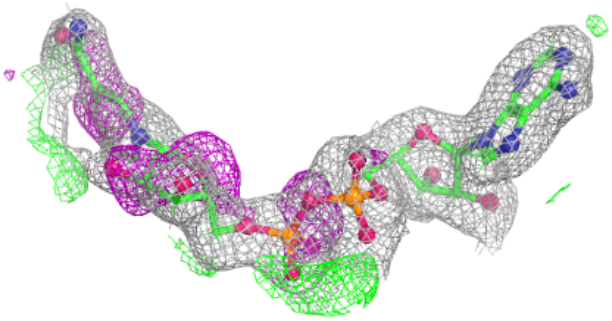


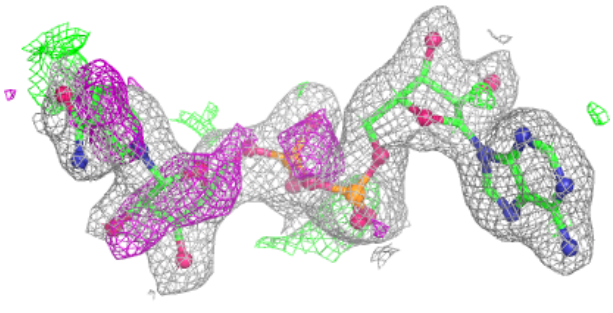


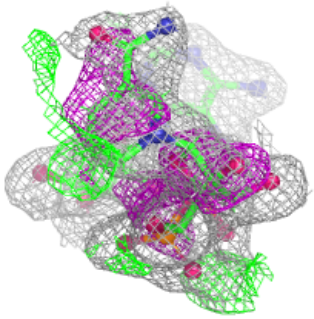


Electron density around NAD D 601:

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

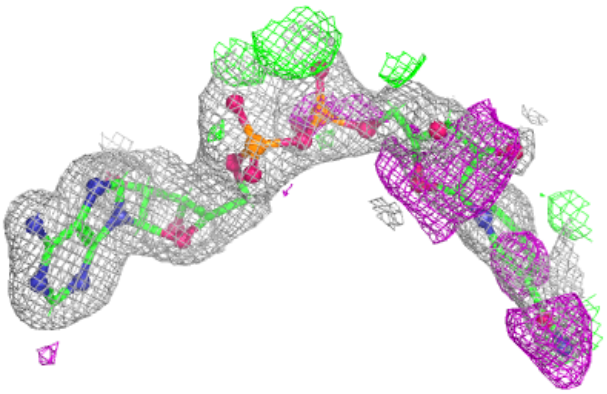


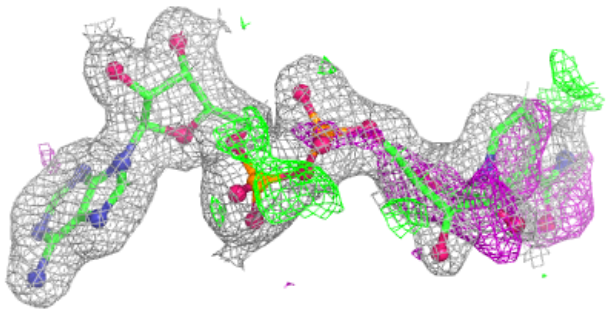


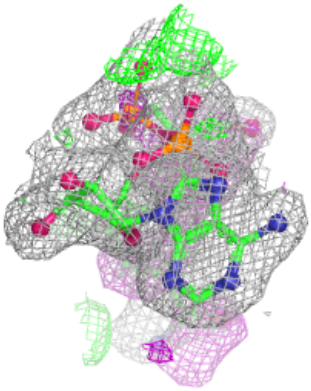


Electron density around NAD B 601:

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

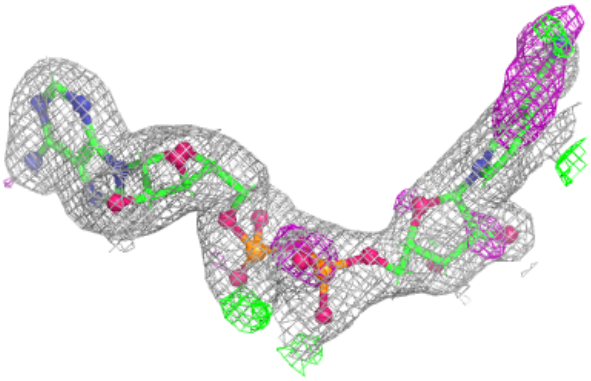


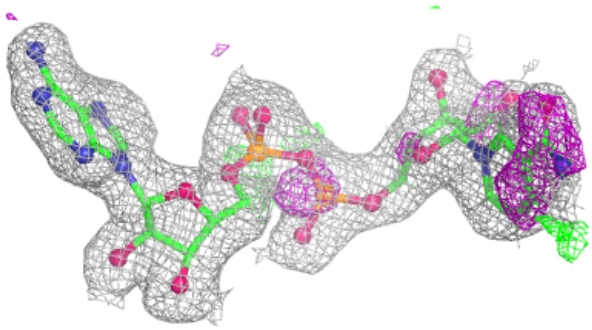


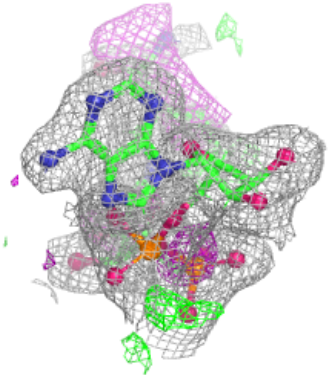


Electron density around NAD A 601:

$2mF_o$-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.