



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:12 PM UTC

PDB ID : 2P5U / pdb_00002p5u
Title : Crystal structure of Thermus thermophilus HB8 UDP-glucose 4-epimerase complex with NAD
Authors : Fu, Z.-Q.; Chen, L.; Ebihara, A.; Shinkai, A.; Kuramitsu, S.; Yokoyama, S.; Zhao, M.; Dillard, B.; Chrzas, J.; Rose, J.P.; Wang, B.-C.; South-east Collaboratory for Structural Genomics (SECSG); RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-16
Resolution : 2.37 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)

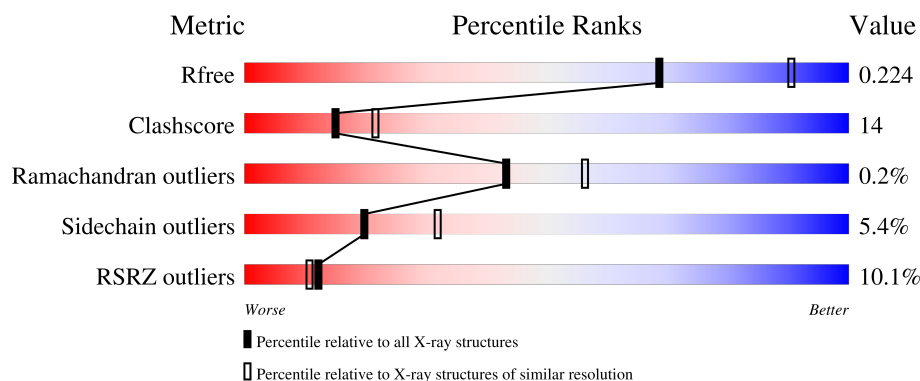
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	311	8% 74% 23% .
1	B	311	14% 73% 24% .
1	C	311	13% 69% 28% .

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	311	6% 69% 29%

2 Entry composition [i](#)

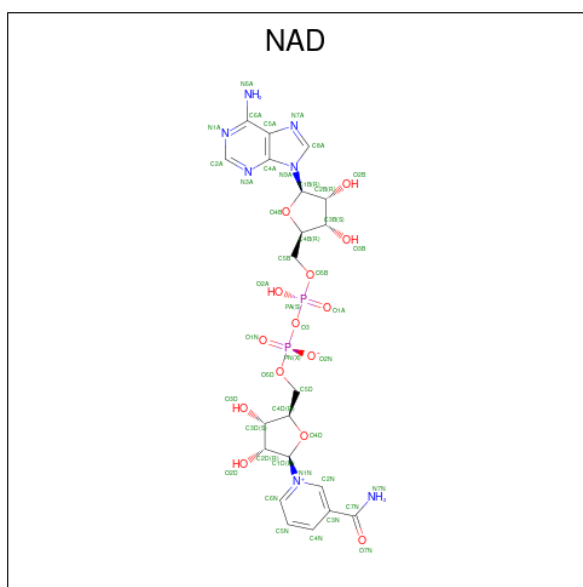
There are 3 unique types of molecules in this entry. The entry contains 10139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glucose 4-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	B	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	C	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	D	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			

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



Continued from previous page...

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

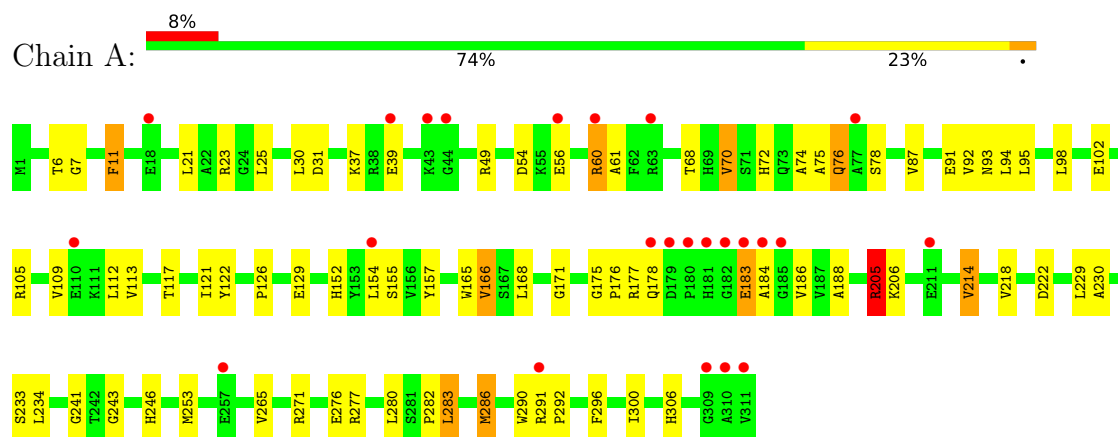
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	99	Total	O	0	0
			99	99		
3	C	78	Total	O	0	0
			78	78		
3	D	122	Total	O	0	0
			122	122		

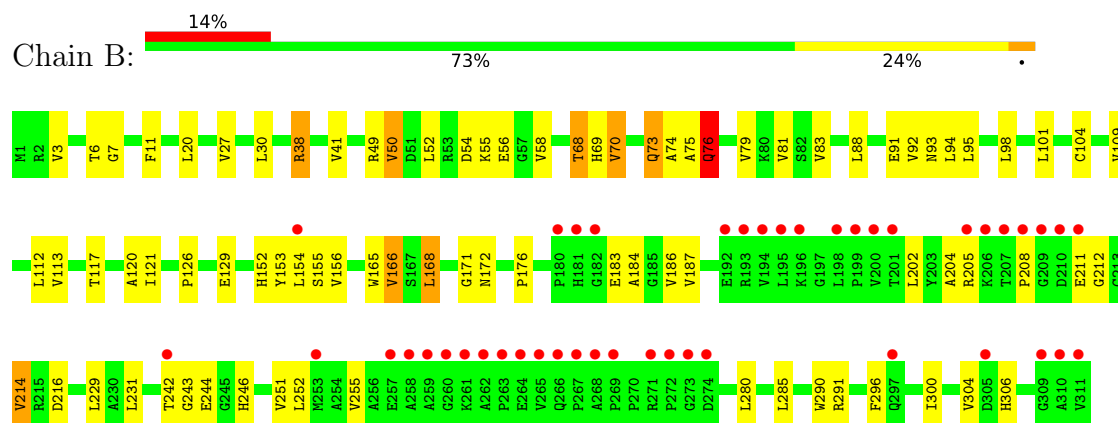
3 Residue-property plots [i](#)

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.

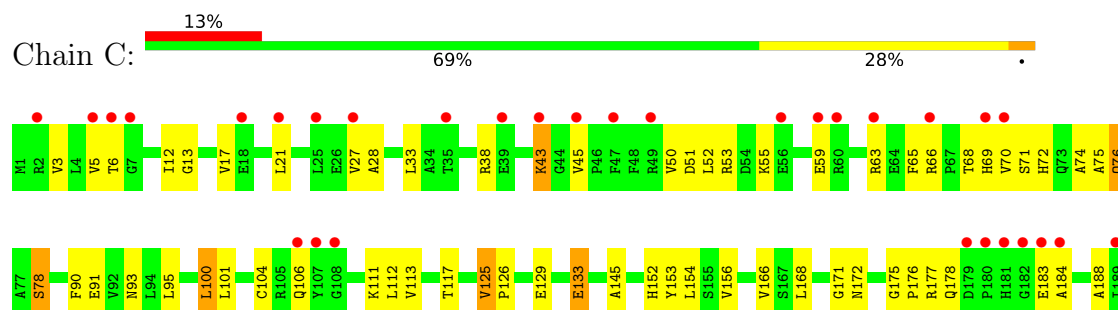
• Molecule 1: UDP-glucose 4-epimerase

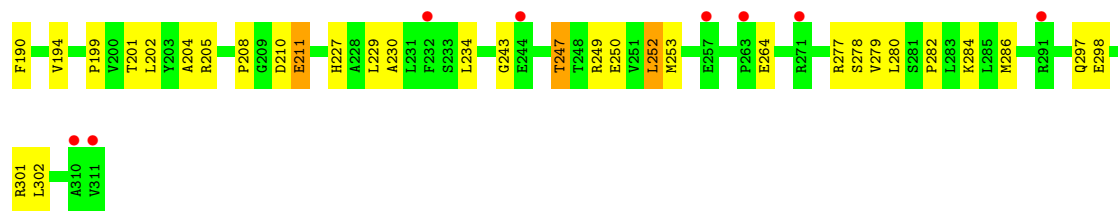


• Molecule 1: UDP-glucose 4-epimerase

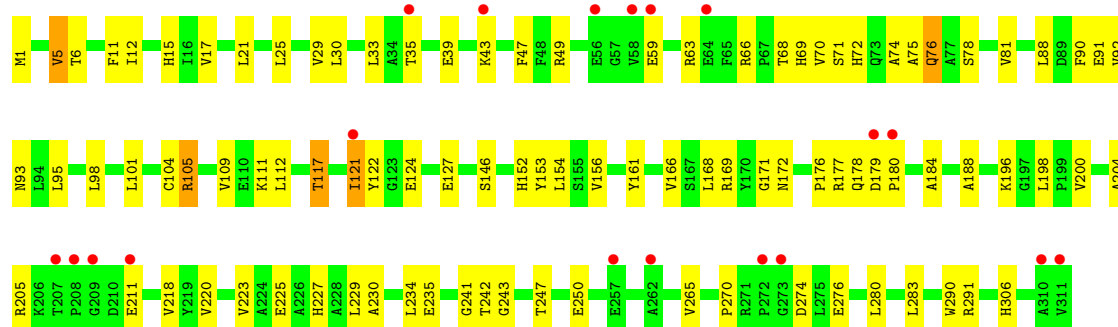


• Molecule 1: UDP-glucose 4-epimerase





● Molecule 1: UDP-glucose 4-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	250.92Å 250.92Å 121.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.37 49.85 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.85-2.37) 99.7 (49.85-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.57 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.261 0.226 , 0.224	Depositor DCC
R_{free} test set	4519 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10139	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.46	1/2446 (0.0%)	0.90	5/3320 (0.2%)
1	B	0.42	0/2446	0.86	4/3320 (0.1%)
1	C	0.41	0/2446	0.86	5/3320 (0.2%)
1	D	0.46	0/2446	0.90	3/3320 (0.1%)
All	All	0.44	1/9784 (0.0%)	0.88	17/13280 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	MET	SD-CE	-5.53	1.65	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	GLY	N-CA-C	-6.28	101.84	112.77
1	D	265	VAL	N-CA-C	6.22	117.54	108.58
1	A	205	ARG	N-CA-C	-5.93	105.13	112.90
1	D	171	GLY	N-CA-C	-5.88	102.53	112.77
1	D	76	GLN	N-CA-C	-5.80	97.78	107.99
1	A	265	VAL	N-CA-C	5.77	116.61	108.36
1	A	171	GLY	N-CA-C	-5.76	102.75	112.77
1	A	68	THR	N-CA-C	-5.57	106.61	113.41
1	B	68	THR	N-CA-C	-5.49	106.72	113.41
1	B	171	GLY	N-CA-C	-5.48	103.23	112.77
1	C	76	GLN	N-CA-C	-5.47	99.61	108.41
1	C	45	VAL	N-CA-C	5.45	113.31	108.63
1	C	205	ARG	N-CA-C	-5.42	105.28	111.14
1	A	76	GLN	N-CA-C	-5.26	98.73	107.99
1	C	78	SER	N-CA-C	5.19	117.42	109.07
1	B	27	VAL	N-CA-C	5.12	116.73	108.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	GLN	N-CA-C	-5.05	100.28	108.41

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	2388	0	2370	69	0
1	B	2388	0	2370	64	0
1	C	2388	0	2370	72	0
1	D	2388	0	2370	68	0
2	A	44	0	26	3	0
2	B	44	0	25	3	0
2	C	44	0	25	1	0
2	D	44	0	25	3	0
3	A	112	0	0	3	0
3	B	99	0	0	5	0
3	C	78	0	0	3	0
3	D	122	0	0	7	0
All	All	10139	0	9581	265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (265) 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:D:218:VAL:HG11	1:D:241:GLY:HA2	1.52	0.91
1:C:247:THR:HG22	1:C:250:GLU:H	1.42	0.84
1:B:216:ASP:OD1	1:B:242:THR:HG22	1.76	0.84
1:A:76:GLN:HB2	1:A:92:VAL:HG21	1.59	0.84
1:B:76:GLN:HE22	1:B:81:VAL:HB	1.43	0.84
1:A:183:GLU:HA	1:A:271:ARG:HH12	1.42	0.84
1:A:76:GLN:HE22	1:A:78:SER:HB3	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:HG3	1:B:291:ARG:HH21	1.46	0.81
1:D:76:GLN:HB2	1:D:92:VAL:HG11	1.64	0.80
1:D:218:VAL:HG12	1:D:242:THR:HG23	1.65	0.79
1:C:230:ALA:HA	1:C:234:LEU:HB2	1.64	0.78
1:A:54:ASP:OD2	1:A:56:GLU:HG2	1.83	0.77
1:B:76:GLN:HB3	1:B:92:VAL:HG11	1.67	0.76
1:A:152:HIS:HE1	1:D:152:HIS:HE1	1.32	0.76
1:B:76:GLN:O	1:B:76:GLN:HG3	1.86	0.75
1:B:242:THR:HG23	1:B:244:GLU:H	1.53	0.73
1:A:152:HIS:CE1	1:D:152:HIS:HE1	2.07	0.71
1:C:297:GLN:HG2	1:C:301:ARG:HH22	1.54	0.71
1:D:63:ARG:HA	1:D:66:ARG:NH2	2.05	0.71
1:A:117:THR:HG23	1:A:121:ILE:HG23	1.73	0.70
1:A:178:GLN:HG3	1:A:188:ALA:HB2	1.72	0.70
1:D:172:ASN:HB3	1:D:184:ALA:HB2	1.75	0.69
1:C:12:ILE:HD11	2:C:1118:NAD:H71N	1.58	0.69
1:D:290:TRP:O	1:D:291:ARG:HG3	1.95	0.67
1:C:297:GLN:HG2	1:C:301:ARG:NH2	2.10	0.66
1:B:290:TRP:O	1:B:291:ARG:HG3	1.95	0.65
1:B:172:ASN:HB3	1:B:184:ALA:HB2	1.78	0.65
1:A:11:PHE:HB3	2:A:1118:NAD:O2N	1.97	0.65
1:A:113:VAL:HA	1:A:166:VAL:HG13	1.77	0.65
1:D:291:ARG:HG3	1:D:291:ARG:HH11	1.63	0.63
1:B:291:ARG:HG3	1:B:291:ARG:NH2	2.12	0.63
1:C:43:LYS:HA	1:C:43:LYS:NZ	2.14	0.63
1:B:154:LEU:HD13	1:B:165:TRP:CE3	2.33	0.63
1:C:75:ALA:HB1	1:C:93:ASN:OD1	2.00	0.62
1:C:126:PRO:HG2	1:C:129:GLU:CD	2.25	0.62
1:B:211:GLU:H	1:B:211:GLU:CD	2.08	0.62
1:C:76:GLN:NE2	1:C:78:SER:H	1.98	0.61
1:A:154:LEU:HD13	1:A:165:TRP:CD2	2.34	0.61
1:C:76:GLN:HE22	1:C:78:SER:HB3	1.65	0.60
1:A:218:VAL:HG21	1:A:241:GLY:HA2	1.83	0.60
1:A:154:LEU:HD13	1:A:165:TRP:CE3	2.36	0.60
1:A:282:PRO:HG2	1:A:286:MET:HE2	1.83	0.59
1:D:127:GLU:HG3	3:D:1129:HOH:O	2.02	0.59
1:A:102:GLU:OE1	1:A:105:ARG:HD3	2.03	0.59
1:A:183:GLU:HA	1:A:271:ARG:NH1	2.16	0.59
1:C:125:VAL:CG1	1:C:278:SER:HA	2.33	0.59
1:C:91:GLU:O	1:C:95:LEU:HB3	2.02	0.58
1:D:39:GLU:HG3	3:D:1214:HOH:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:HG23	1:B:244:GLU:N	2.17	0.58
1:D:218:VAL:CG1	1:D:241:GLY:HA2	2.31	0.58
1:D:88:LEU:O	1:D:92:VAL:HG12	2.04	0.58
1:C:125:VAL:HG12	1:C:277:ARG:O	2.03	0.58
1:D:29:VAL:HG23	1:D:47:PHE:HD1	1.68	0.57
1:B:41:VAL:HB	3:B:1158:HOH:O	2.04	0.57
1:C:43:LYS:HA	1:C:43:LYS:HZ3	1.68	0.57
1:A:152:HIS:HE1	1:D:152:HIS:CE1	2.19	0.57
1:A:218:VAL:CG2	1:A:241:GLY:HA2	2.35	0.57
1:C:211:GLU:O	1:C:247:THR:HG23	2.04	0.57
1:B:154:LEU:HD13	1:B:165:TRP:CD2	2.39	0.57
1:B:176:PRO:HB3	1:B:306:HIS:HB2	1.87	0.56
1:C:6:THR:O	1:C:74:ALA:HB2	2.04	0.56
1:B:300:ILE:O	1:B:304:VAL:HG23	2.05	0.56
1:B:75:ALA:HB1	1:B:93:ASN:OD1	2.05	0.56
1:B:113:VAL:HA	1:B:166:VAL:HG13	1.87	0.56
1:C:74:ALA:O	1:C:75:ALA:HB2	2.05	0.56
1:B:76:GLN:HE22	1:B:81:VAL:CB	2.16	0.56
1:B:126:PRO:HG2	1:B:129:GLU:CD	2.31	0.56
1:C:3:VAL:HB	1:C:27:VAL:HG12	1.88	0.56
1:A:6:THR:HG1	1:A:72:HIS:HD2	1.54	0.55
1:B:154:LEU:HD12	1:B:155:SER:N	2.21	0.55
1:A:76:GLN:HB2	1:A:92:VAL:CG2	2.35	0.55
1:C:172:ASN:HB3	1:C:184:ALA:HB2	1.87	0.55
1:C:243:GLY:HA2	1:C:280:LEU:O	2.06	0.55
1:D:105:ARG:HD3	1:D:161:TYR:CG	2.42	0.55
1:D:112:LEU:C	1:D:112:LEU:HD23	2.32	0.55
1:C:113:VAL:HA	1:C:166:VAL:HG13	1.89	0.54
1:A:112:LEU:C	1:A:112:LEU:HD23	2.33	0.54
1:D:15:HIS:HE1	1:D:176:PRO:O	1.91	0.54
1:C:112:LEU:C	1:C:112:LEU:HD23	2.33	0.54
1:B:251:VAL:O	1:B:255:VAL:HG23	2.07	0.54
1:D:121:ILE:HD13	1:D:169:ARG:CZ	2.38	0.53
1:A:178:GLN:CG	1:A:188:ALA:HB2	2.39	0.53
1:D:291:ARG:HG3	1:D:291:ARG:NH1	2.21	0.53
1:C:153:TYR:HA	1:C:156:VAL:HG22	1.91	0.53
1:D:93:ASN:HB2	1:D:146:SER:OG	2.08	0.53
1:C:175:GLY:O	1:C:178:GLN:HG2	2.09	0.53
1:D:243:GLY:HA2	1:D:280:LEU:O	2.09	0.53
1:A:6:THR:OG1	1:A:72:HIS:HD2	1.92	0.53
1:C:70:VAL:HG23	1:C:112:LEU:HG	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:H	1:A:178:GLN:NE2	2.07	0.53
1:A:176:PRO:O	1:A:177:ARG:HB2	2.08	0.53
1:B:74:ALA:O	1:B:75:ALA:HB2	2.09	0.53
1:C:125:VAL:HG11	1:C:278:SER:HA	1.91	0.53
1:A:246:HIS:HD2	3:A:1128:HOH:O	1.91	0.52
1:C:176:PRO:O	1:C:177:ARG:HB2	2.08	0.52
1:D:5:VAL:HG11	1:D:17:VAL:HG22	1.89	0.52
1:B:152:HIS:HE1	1:C:152:HIS:NE2	2.07	0.52
1:D:176:PRO:O	1:D:177:ARG:HB2	2.10	0.52
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.74	0.52
1:A:184:ALA:C	1:A:186:VAL:H	2.18	0.52
1:A:205:ARG:HD3	1:A:276:GLU:HB3	1.91	0.52
1:D:70:VAL:HG12	1:D:109:VAL:HG11	1.92	0.52
1:D:71:SER:OG	1:D:227:HIS:HE1	1.93	0.52
1:D:71:SER:OG	1:D:227:HIS:CE1	2.63	0.51
1:D:127:GLU:OE1	3:D:1151:HOH:O	2.19	0.51
1:B:55:LYS:HE2	3:B:1151:HOH:O	2.09	0.51
1:B:38:ARG:CZ	3:B:1158:HOH:O	2.57	0.51
1:A:91:GLU:O	1:A:95:LEU:HB3	2.10	0.51
1:A:243:GLY:HA2	1:A:280:LEU:O	2.10	0.51
1:B:113:VAL:HG22	1:B:166:VAL:CG1	2.40	0.51
1:D:91:GLU:O	1:D:95:LEU:HB3	2.10	0.51
1:A:30:LEU:C	1:A:30:LEU:HD23	2.35	0.50
1:A:253:MET:HE3	3:A:1160:HOH:O	2.11	0.50
1:D:12:ILE:HD11	2:D:1118:NAD:H71N	1.76	0.50
1:D:204:ALA:HB3	1:D:270:PRO:HD3	1.93	0.50
1:C:247:THR:HG23	1:C:249:ARG:H	1.75	0.50
1:C:199:PRO:HB3	1:C:264:GLU:HG3	1.94	0.50
1:C:5:VAL:HG11	1:C:17:VAL:HG22	1.93	0.50
1:D:124:GLU:HG3	3:D:1189:HOH:O	2.12	0.50
1:B:38:ARG:HD3	1:B:49:ARG:NH2	2.27	0.50
1:A:291:ARG:HG3	1:A:291:ARG:NH1	2.27	0.50
1:A:205:ARG:HD2	1:A:206:LYS:HD2	1.94	0.49
1:C:183:GLU:HB2	3:C:1145:HOH:O	2.13	0.49
1:A:7:GLY:HA2	1:A:31:ASP:OD2	2.12	0.49
1:D:30:LEU:C	1:D:30:LEU:HD23	2.37	0.49
1:B:6:THR:HG1	1:B:73:GLN:H	1.61	0.49
1:A:290:TRP:O	1:A:291:ARG:HG3	2.13	0.49
1:D:70:VAL:HG11	1:D:104:CYS:SG	2.53	0.49
1:D:218:VAL:HG11	1:D:241:GLY:CA	2.35	0.48
1:D:153:TYR:HA	1:D:156:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HG2	1:A:271:ARG:NH1	2.29	0.48
1:D:121:ILE:HD11	1:D:122:TYR:CZ	2.48	0.48
1:D:63:ARG:HA	1:D:66:ARG:HH21	1.77	0.48
1:B:246:HIS:HD2	3:B:1131:HOH:O	1.96	0.48
1:C:68:THR:OG1	1:C:69:HIS:HD2	1.97	0.48
1:A:11:PHE:HB3	2:A:1118:NAD:PN	2.53	0.48
1:B:153:TYR:HA	1:B:156:VAL:HG22	1.96	0.48
1:A:113:VAL:HG22	1:A:166:VAL:CG1	2.44	0.48
1:B:70:VAL:HG11	1:B:104:CYS:SG	2.54	0.47
1:C:190:PHE:O	1:C:194:VAL:HG23	2.14	0.47
1:C:63:ARG:HG3	1:C:66:ARG:NH2	2.29	0.47
1:C:6:THR:OG1	1:C:72:HIS:HA	2.15	0.47
1:C:125:VAL:HG11	1:C:279:VAL:H	1.80	0.47
1:D:117:THR:O	1:D:121:ILE:HG12	2.14	0.47
1:A:70:VAL:HG12	1:A:109:VAL:HG11	1.96	0.47
1:C:247:THR:CG2	1:C:249:ARG:H	2.28	0.47
1:C:55:LYS:O	1:C:59:GLU:HG2	2.15	0.47
1:C:71:SER:OG	1:C:227:HIS:CE1	2.68	0.47
1:D:59:GLU:O	1:D:63:ARG:HG3	2.14	0.47
1:A:154:LEU:HD12	1:A:155:SER:N	2.31	0.46
1:B:38:ARG:HH11	1:B:38:ARG:CG	2.29	0.46
1:B:112:LEU:HD23	1:B:112:LEU:C	2.40	0.46
1:C:282:PRO:HG2	1:C:286:MET:HE2	1.97	0.46
1:B:30:LEU:HG	1:B:50:VAL:HG22	1.97	0.46
1:B:79:VAL:O	1:B:83:VAL:HG23	2.15	0.46
1:D:68:THR:OG1	1:D:69:HIS:HD2	1.97	0.46
1:D:74:ALA:O	1:D:75:ALA:HB2	2.15	0.46
1:D:166:VAL:HG22	1:D:235:GLU:HA	1.97	0.46
1:D:205:ARG:HD2	3:D:1145:HOH:O	2.15	0.46
1:B:3:VAL:HA	1:B:69:HIS:O	2.15	0.46
1:D:247:THR:OG1	1:D:250:GLU:HG2	2.16	0.46
1:B:68:THR:OG1	1:B:69:HIS:HD2	1.98	0.46
1:C:6:THR:HG21	1:C:100:LEU:HD11	1.96	0.46
1:A:70:VAL:HG13	1:A:112:LEU:HG	1.98	0.46
1:B:166:VAL:HG22	1:B:168:LEU:HD13	1.97	0.45
1:C:13:GLY:O	1:C:17:VAL:HG23	2.16	0.45
1:D:230:ALA:HA	1:D:234:LEU:HB2	1.98	0.45
1:C:21:LEU:HD13	1:C:27:VAL:HG22	1.98	0.45
1:D:196:LYS:HB3	1:D:198:LEU:HD13	1.98	0.45
1:A:74:ALA:O	1:A:75:ALA:HB2	2.16	0.45
1:A:92:VAL:HG23	1:A:93:ASN:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HG11	1:B:20:LEU:HD13	1.99	0.45
1:A:205:ARG:HG3	1:A:206:LYS:HG3	1.99	0.45
1:B:183:GLU:HB2	2:B:1118:NAD:H71N	1.81	0.45
1:B:252:LEU:C	1:B:252:LEU:HD13	2.41	0.45
1:A:75:ALA:HB1	1:A:93:ASN:OD1	2.16	0.45
1:C:168:LEU:N	1:C:168:LEU:HD22	2.32	0.45
1:A:205:ARG:HG3	1:A:206:LYS:N	2.32	0.45
1:D:112:LEU:HD22	1:D:154:LEU:HD21	1.98	0.45
1:A:98:LEU:HD22	1:D:90:PHE:CG	2.52	0.44
1:C:76:GLN:HE22	1:C:78:SER:H	1.61	0.44
1:D:43:LYS:N	1:D:43:LYS:HD2	2.32	0.44
1:B:243:GLY:HA2	1:B:280:LEU:O	2.17	0.44
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.77	0.44
1:D:78:SER:HB3	1:D:81:VAL:HB	1.99	0.44
1:D:179:ASP:HB2	1:D:180:PRO:HD2	1.99	0.44
1:A:11:PHE:CE2	1:A:178:GLN:HB3	2.53	0.44
1:D:220:VAL:O	1:D:223:VAL:HG22	2.18	0.44
1:B:70:VAL:HG12	1:B:109:VAL:HG11	2.00	0.44
1:B:296:PHE:O	1:B:300:ILE:HD13	2.17	0.44
1:A:113:VAL:HG22	1:A:166:VAL:HG11	2.00	0.44
1:B:117:THR:HG23	1:B:121:ILE:HG23	2.00	0.44
1:B:202:LEU:HA	3:B:1198:HOH:O	2.17	0.44
1:A:283:LEU:HD13	1:A:286:MET:CE	2.48	0.43
1:A:60:ARG:HG3	1:A:61:ALA:N	2.32	0.43
1:D:176:PRO:HB3	1:D:306:HIS:HB2	2.00	0.43
1:D:166:VAL:HG11	1:D:230:ALA:HB1	2.01	0.43
1:D:205:ARG:NH2	1:D:276:GLU:OE2	2.51	0.43
1:B:98:LEU:HD22	1:C:90:PHE:CG	2.52	0.43
1:B:204:ALA:HB2	1:B:208:PRO:HA	2.01	0.43
1:B:205:ARG:HB2	1:B:212:GLY:C	2.43	0.43
1:A:23:ARG:HB2	1:A:25:LEU:HD23	2.01	0.43
1:A:39:GLU:H	1:A:39:GLU:CD	2.27	0.43
1:C:38:ARG:HA	1:C:38:ARG:HD2	1.91	0.43
1:D:35:THR:HG22	2:D:1118:NAD:H2B	2.00	0.43
1:A:87:VAL:HG22	1:D:98:LEU:HD11	2.01	0.43
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.84	0.43
1:B:88:LEU:O	1:B:92:VAL:HG12	2.18	0.43
1:A:222:ASP:CG	1:A:292:PRO:HA	2.44	0.42
1:B:7:GLY:N	1:B:74:ALA:HB2	2.35	0.42
1:B:75:ALA:HB3	2:B:1118:NAD:O3D	2.19	0.42
1:B:117:THR:CG2	1:B:120:ALA:HB3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:VAL:HG12	1:C:51:ASP:N	2.34	0.42
1:C:133:GLU:HG3	1:C:284:LYS:HD2	2.01	0.42
1:A:214:VAL:HA	1:A:246:HIS:O	2.19	0.42
1:A:296:PHE:O	1:A:300:ILE:HD13	2.20	0.42
1:C:211:GLU:OE2	1:C:249:ARG:HD2	2.20	0.42
1:C:252:LEU:HD13	1:C:253:MET:CE	2.49	0.42
1:A:176:PRO:HB3	1:A:306:HIS:HB2	2.02	0.42
1:C:227:HIS:HD2	3:C:1126:HOH:O	2.02	0.42
1:D:1:MET:HG3	1:D:69:HIS:CD2	2.55	0.42
1:D:6:THR:OG1	1:D:72:HIS:HD2	2.03	0.42
1:D:111:LYS:HG2	1:D:112:LEU:N	2.34	0.42
1:B:54:ASP:O	1:B:58:VAL:HG23	2.19	0.42
1:C:33:LEU:HD12	1:C:33:LEU:N	2.34	0.42
1:C:101:LEU:HD21	1:C:154:LEU:CD1	2.50	0.42
1:C:113:VAL:HG22	1:C:166:VAL:CG1	2.50	0.42
1:A:121:ILE:HD11	1:A:122:TYR:CE2	2.55	0.42
1:B:231:LEU:C	1:B:231:LEU:HD13	2.44	0.42
1:A:105:ARG:HD2	1:A:157:TYR:CE1	2.54	0.42
1:A:214:VAL:HG13	1:A:277:ARG:HA	2.02	0.42
1:C:298:GLU:O	1:C:302:LEU:HD13	2.20	0.42
1:C:210:ASP:HB2	3:C:1175:HOH:O	2.18	0.41
1:C:71:SER:OG	1:C:227:HIS:HE1	2.02	0.41
1:D:75:ALA:HB3	2:D:1118:NAD:O3D	2.20	0.41
1:D:105:ARG:NH2	3:D:1187:HOH:O	2.53	0.41
1:D:227:HIS:HD2	3:D:1121:HOH:O	2.03	0.41
1:B:91:GLU:O	1:B:95:LEU:HB3	2.20	0.41
1:C:204:ALA:HB2	1:C:208:PRO:HA	2.01	0.41
1:A:75:ALA:HB3	2:A:1118:NAD:H3D	2.02	0.41
1:A:282:PRO:HG2	1:A:286:MET:CE	2.49	0.41
1:A:126:PRO:HG2	1:A:129:GLU:CD	2.45	0.41
1:C:111:LYS:HG2	1:C:112:LEU:N	2.35	0.41
1:C:252:LEU:HD13	1:C:253:MET:HE2	2.03	0.41
1:D:92:VAL:HG13	1:D:93:ASN:N	2.35	0.41
1:D:178:GLN:HG3	1:D:188:ALA:HB2	2.03	0.41
1:B:11:PHE:HB3	2:B:1118:NAD:PN	2.61	0.41
1:B:166:VAL:CG2	1:B:168:LEU:HD13	2.51	0.41
1:C:178:GLN:HG3	1:C:188:ALA:HB2	2.02	0.41
1:B:76:GLN:HB3	1:B:92:VAL:CG1	2.43	0.40
1:B:156:VAL:HG11	1:C:145:ALA:HB2	2.03	0.40
1:C:21:LEU:HD12	1:C:21:LEU:HA	1.91	0.40
1:C:70:VAL:HG21	1:C:104:CYS:SG	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:CD	1:C:133:GLU:H	2.28	0.40
1:C:172:ASN:CB	1:C:184:ALA:HB2	2.50	0.40
1:A:230:ALA:HA	1:A:234:LEU:HB2	2.03	0.40
1:B:186:VAL:HG13	1:B:187:VAL:N	2.36	0.40
1:B:214:VAL:HG23	1:B:246:HIS:H	1.86	0.40
1:C:5:VAL:O	1:C:5:VAL:HG13	2.21	0.40
1:C:100:LEU:O	1:C:100:LEU:HD23	2.21	0.40
1:D:49:ARG:HH11	1:D:49:ARG:HG2	1.86	0.40
1:D:29:VAL:CG2	1:D:47:PHE:HD1	2.34	0.40
1:C:117:THR:HG23	1:C:117:THR:O	2.21	0.40
1:A:233:SER:HB2	3:A:1222:HOH:O	2.22	0.40
1:C:28:ALA:HB2	1:C:65:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/311 (99%)	297 (96%)	11 (4%)	1 (0%)	36	48
1	B	309/311 (99%)	300 (97%)	9 (3%)	0	100	100
1	C	309/311 (99%)	298 (96%)	11 (4%)	0	100	100
1	D	309/311 (99%)	299 (97%)	9 (3%)	1 (0%)	36	48
All	All	1236/1244 (99%)	1194 (97%)	40 (3%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	11	PHE
1	A	11	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/244 (100%)	232 (95%)	12 (5%)	22	36
1	B	244/244 (100%)	231 (95%)	13 (5%)	20	33
1	C	244/244 (100%)	231 (95%)	13 (5%)	20	33
1	D	244/244 (100%)	229 (94%)	15 (6%)	17	27
All	All	976/976 (100%)	923 (95%)	53 (5%)	20	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	37	LYS
1	A	60	ARG
1	A	70	VAL
1	A	94	LEU
1	A	166	VAL
1	A	168	LEU
1	A	183	GLU
1	A	205	ARG
1	A	214	VAL
1	A	229	LEU
1	A	283	LEU
1	B	38	ARG
1	B	50	VAL
1	B	52	LEU
1	B	56	GLU
1	B	70	VAL
1	B	73	GLN
1	B	76	GLN
1	B	101	LEU
1	B	166	VAL
1	B	168	LEU
1	B	214	VAL
1	B	229	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	285	LEU
1	C	43	LYS
1	C	52	LEU
1	C	53	ARG
1	C	100	LEU
1	C	106	GLN
1	C	125	VAL
1	C	133	GLU
1	C	201	THR
1	C	202	LEU
1	C	211	GLU
1	C	229	LEU
1	C	247	THR
1	C	252	LEU
1	D	5	VAL
1	D	21	LEU
1	D	25	LEU
1	D	33	LEU
1	D	101	LEU
1	D	105	ARG
1	D	117	THR
1	D	121	ILE
1	D	168	LEU
1	D	200	VAL
1	D	211	GLU
1	D	225	GLU
1	D	229	LEU
1	D	274	ASP
1	D	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	72	HIS
1	A	76	GLN
1	A	106	GLN
1	A	152	HIS
1	A	159	GLN
1	A	178	GLN
1	A	181	HIS
1	A	239	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	246	HIS
1	A	288	HIS
1	B	15	HIS
1	B	69	HIS
1	B	72	HIS
1	B	76	GLN
1	B	152	HIS
1	B	159	GLN
1	B	172	ASN
1	B	181	HIS
1	B	239	ASN
1	B	246	HIS
1	B	266	GLN
1	C	69	HIS
1	C	76	GLN
1	C	159	GLN
1	C	172	ASN
1	C	227	HIS
1	C	239	ASN
1	C	297	GLN
1	D	15	HIS
1	D	69	HIS
1	D	72	HIS
1	D	106	GLN
1	D	152	HIS
1	D	159	GLN
1	D	172	ASN
1	D	227	HIS
1	D	239	ASN
1	D	288	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	B	1118	-	46,48,48	1.98	8 (17%)	64,73,73	2.44	18 (28%)
2	NAD	D	1118	-	46,48,48	2.00	8 (17%)	64,73,73	2.35	19 (29%)
2	NAD	A	1118	-	46,48,48	1.94	8 (17%)	64,73,73	2.41	20 (31%)
2	NAD	C	1118	-	46,48,48	1.87	8 (17%)	64,73,73	2.31	22 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	1118	-	-	10/30/62/62	0/5/5/5
2	NAD	D	1118	-	-	12/30/62/62	0/5/5/5
2	NAD	A	1118	-	-	9/30/62/62	0/5/5/5
2	NAD	C	1118	-	-	9/30/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1118	NAD	C2N-N1N	8.22	1.44	1.35
2	B	1118	NAD	C2N-N1N	8.12	1.43	1.35
2	D	1118	NAD	C2N-N1N	7.96	1.43	1.35
2	A	1118	NAD	C2N-N1N	7.89	1.43	1.35
2	D	1118	NAD	PA-O3	6.62	1.66	1.59
2	A	1118	NAD	PA-O3	6.41	1.66	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1118	NAD	PN-O3	4.68	1.64	1.59
2	B	1118	NAD	PA-O3	4.60	1.64	1.59
2	D	1118	NAD	PN-O3	4.23	1.64	1.59
2	C	1118	NAD	PN-O3	3.82	1.63	1.59
2	B	1118	NAD	C5A-N7A	-3.39	1.32	1.39
2	A	1118	NAD	C5A-N7A	-3.37	1.32	1.39
2	C	1118	NAD	PA-O3	3.36	1.63	1.59
2	C	1118	NAD	C5A-N7A	-3.33	1.33	1.39
2	D	1118	NAD	C5A-N7A	-3.28	1.33	1.39
2	B	1118	NAD	C6N-N1N	3.16	1.42	1.35
2	B	1118	NAD	O4D-C1D	3.06	1.44	1.40
2	C	1118	NAD	C6N-N1N	3.04	1.42	1.35
2	A	1118	NAD	C6N-N1N	2.86	1.41	1.35
2	D	1118	NAD	C6N-N1N	2.84	1.41	1.35
2	A	1118	NAD	O4D-C1D	2.72	1.44	1.40
2	C	1118	NAD	C3N-C7N	2.60	1.54	1.50
2	C	1118	NAD	O4D-C1D	2.55	1.44	1.40
2	B	1118	NAD	C4A-N9A	-2.34	1.32	1.37
2	B	1118	NAD	C5D-C4D	2.32	1.58	1.51
2	A	1118	NAD	C3N-C7N	2.27	1.54	1.50
2	C	1118	NAD	C4A-N9A	-2.18	1.33	1.37
2	A	1118	NAD	C4A-N9A	-2.16	1.33	1.37
2	D	1118	NAD	C4A-N9A	-2.13	1.33	1.37
2	A	1118	NAD	C5D-C4D	2.13	1.58	1.51
2	D	1118	NAD	C3N-C7N	2.09	1.53	1.50
2	D	1118	NAD	C5D-C4D	2.05	1.57	1.51

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1118	NAD	C4D-O4D-C1D	8.29	117.51	109.92
2	B	1118	NAD	C4D-O4D-C1D	7.11	116.44	109.92
2	C	1118	NAD	C4D-O4D-C1D	6.86	116.21	109.92
2	A	1118	NAD	C4D-O4D-C1D	6.59	115.96	109.92
2	B	1118	NAD	O4D-C4D-C5D	6.48	130.08	109.33
2	A	1118	NAD	C5A-C4A-N3A	-6.29	118.06	126.72
2	D	1118	NAD	C5A-C4A-N3A	-6.19	118.20	126.72
2	C	1118	NAD	C5A-C4A-N3A	-6.04	118.41	126.72
2	B	1118	NAD	C5A-C4A-N3A	-5.93	118.56	126.72
2	D	1118	NAD	N3A-C2A-N1A	-5.50	120.25	128.58
2	A	1118	NAD	N3A-C2A-N1A	-5.44	120.34	128.58
2	A	1118	NAD	O4B-C1B-N9A	5.44	118.53	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1118	NAD	N3A-C4A-N9A	5.41	136.37	127.17
2	B	1118	NAD	N3A-C2A-N1A	-5.39	120.42	128.58
2	D	1118	NAD	N3A-C4A-N9A	5.35	136.26	127.17
2	B	1118	NAD	N3A-C4A-N9A	5.34	136.24	127.17
2	C	1118	NAD	N3A-C2A-N1A	-5.32	120.52	128.58
2	C	1118	NAD	N3A-C4A-N9A	5.31	136.19	127.17
2	D	1118	NAD	O4B-C1B-N9A	4.98	117.66	108.09
2	A	1118	NAD	O5D-C5D-C4D	4.98	125.95	108.99
2	C	1118	NAD	O4D-C4D-C5D	4.62	124.13	109.33
2	D	1118	NAD	O4D-C4D-C5D	4.31	123.15	109.33
2	A	1118	NAD	O4D-C4D-C5D	4.25	122.93	109.33
2	B	1118	NAD	O4B-C1B-N9A	4.21	116.17	108.09
2	C	1118	NAD	O4B-C1B-N9A	4.18	116.12	108.09
2	A	1118	NAD	O4D-C4D-C3D	-4.13	96.96	105.15
2	D	1118	NAD	C2A-N3A-C4A	4.01	121.61	111.83
2	A	1118	NAD	C2A-N3A-C4A	3.93	121.42	111.83
2	B	1118	NAD	O4D-C4D-C3D	-3.86	97.48	105.15
2	B	1118	NAD	C6N-N1N-C2N	-3.79	118.65	121.88
2	C	1118	NAD	C2A-N3A-C4A	3.74	120.96	111.83
2	B	1118	NAD	C2A-N3A-C4A	3.74	120.95	111.83
2	B	1118	NAD	O5D-C5D-C4D	3.62	121.31	108.99
2	A	1118	NAD	C6N-N1N-C2N	-3.34	119.03	121.88
2	C	1118	NAD	C6A-C5A-N7A	-3.34	125.65	132.09
2	A	1118	NAD	C6A-C5A-N7A	-3.33	125.68	132.09
2	B	1118	NAD	C6A-C5A-N7A	-3.32	125.70	132.09
2	A	1118	NAD	C6A-C5A-C4A	3.26	121.63	117.18
2	B	1118	NAD	C6A-C5A-C4A	3.11	121.43	117.18
2	C	1118	NAD	C6N-N1N-C2N	-3.11	119.23	121.88
2	C	1118	NAD	O5D-C5D-C4D	3.10	119.56	108.99
2	C	1118	NAD	C6A-C5A-C4A	3.09	121.40	117.18
2	D	1118	NAD	C3N-C7N-N7N	-3.04	113.99	117.74
2	B	1118	NAD	C2N-N1N-C1D	3.03	125.81	119.13
2	D	1118	NAD	C6A-C5A-C4A	2.92	121.17	117.18
2	C	1118	NAD	O4B-C4B-C5B	2.87	118.54	109.33
2	D	1118	NAD	C6A-C5A-N7A	-2.80	126.69	132.09
2	C	1118	NAD	C2N-N1N-C1D	2.78	125.27	119.13
2	B	1118	NAD	O4B-C4B-C5B	2.72	118.06	109.33
2	D	1118	NAD	C6N-N1N-C1D	-2.68	114.46	119.73
2	D	1118	NAD	C2N-N1N-C1D	2.67	125.04	119.13
2	A	1118	NAD	C4B-O4B-C1B	2.66	115.34	109.47
2	C	1118	NAD	O4D-C4D-C3D	-2.59	100.00	105.15
2	A	1118	NAD	C2N-N1N-C1D	2.58	124.83	119.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1118	NAD	C6N-N1N-C1D	-2.57	114.68	119.73
2	A	1118	NAD	C6N-N1N-C1D	-2.55	114.72	119.73
2	D	1118	NAD	PN-O5D-C5D	2.47	135.51	121.35
2	C	1118	NAD	O7N-C7N-C3N	2.46	122.61	119.60
2	A	1118	NAD	O3-PN-O1N	-2.45	103.33	110.70
2	C	1118	NAD	C3N-C7N-N7N	-2.44	114.73	117.74
2	C	1118	NAD	C2B-C1B-N9A	2.38	119.22	113.30
2	D	1118	NAD	C6N-N1N-C2N	-2.37	119.86	121.88
2	B	1118	NAD	PN-O5D-C5D	2.35	134.81	121.35
2	A	1118	NAD	O4B-C1B-C2B	-2.27	101.76	106.62
2	C	1118	NAD	C4B-O4B-C1B	2.26	114.45	109.47
2	B	1118	NAD	O2N-PN-O3	2.25	113.35	107.27
2	A	1118	NAD	C2A-N1A-C6A	2.20	122.34	118.73
2	B	1118	NAD	C2A-N1A-C6A	2.19	122.33	118.73
2	D	1118	NAD	C2A-N1A-C6A	2.19	122.33	118.73
2	C	1118	NAD	C6N-N1N-C1D	-2.17	115.46	119.73
2	D	1118	NAD	C4B-O4B-C1B	2.17	114.26	109.47
2	C	1118	NAD	C5N-C4N-C3N	2.17	122.50	120.36
2	A	1118	NAD	O4B-C4B-C3B	-2.15	100.88	105.15
2	D	1118	NAD	C5N-C4N-C3N	2.14	122.47	120.36
2	C	1118	NAD	C2A-N1A-C6A	2.10	122.18	118.73
2	A	1118	NAD	O2N-PN-O1N	2.06	122.02	112.44
2	D	1118	NAD	O7N-C7N-C3N	2.06	122.11	119.60
2	C	1118	NAD	O4B-C1B-C2B	-2.03	102.27	106.62
2	D	1118	NAD	O3-PN-O1N	-2.02	104.64	110.70

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1118	NAD	PN-O3-PA-O5B
2	A	1118	NAD	O4D-C1D-N1N-C2N
2	A	1118	NAD	O4D-C1D-N1N-C6N
2	A	1118	NAD	C2D-C1D-N1N-C6N
2	B	1118	NAD	O4D-C1D-N1N-C2N
2	B	1118	NAD	O4D-C1D-N1N-C6N
2	B	1118	NAD	C2D-C1D-N1N-C6N
2	B	1118	NAD	C2N-C3N-C7N-O7N
2	C	1118	NAD	O4D-C1D-N1N-C2N
2	C	1118	NAD	O4D-C1D-N1N-C6N
2	D	1118	NAD	C5D-O5D-PN-O3
2	D	1118	NAD	O4D-C1D-N1N-C2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1118	NAD	O4D-C1D-N1N-C6N
2	D	1118	NAD	C2D-C1D-N1N-C6N
2	B	1118	NAD	C4N-C3N-C7N-O7N
2	B	1118	NAD	C4N-C3N-C7N-N7N
2	B	1118	NAD	C2N-C3N-C7N-N7N
2	C	1118	NAD	C3D-C4D-C5D-O5D
2	D	1118	NAD	C4N-C3N-C7N-O7N
2	D	1118	NAD	C4N-C3N-C7N-N7N
2	C	1118	NAD	C4N-C3N-C7N-O7N
2	C	1118	NAD	C4N-C3N-C7N-N7N
2	D	1118	NAD	PA-O3-PN-O1N
2	B	1118	NAD	PN-O3-PA-O5B
2	D	1118	NAD	PN-O3-PA-O5B
2	A	1118	NAD	PA-O3-PN-O2N
2	C	1118	NAD	O4D-C4D-C5D-O5D
2	A	1118	NAD	C5D-O5D-PN-O3
2	A	1118	NAD	C5D-O5D-PN-O1N
2	A	1118	NAD	C5D-O5D-PN-O2N
2	D	1118	NAD	C5D-O5D-PN-O1N
2	B	1118	NAD	PA-O3-PN-O2N
2	D	1118	NAD	PA-O3-PN-O2N
2	D	1118	NAD	C2D-C1D-N1N-C2N
2	B	1118	NAD	C3D-C4D-C5D-O5D
2	C	1118	NAD	C2N-C3N-C7N-O7N
2	C	1118	NAD	C2N-C3N-C7N-N7N
2	A	1118	NAD	PA-O3-PN-O1N
2	D	1118	NAD	O4B-C4B-C5B-O5B
2	C	1118	NAD	O4B-C4B-C5B-O5B

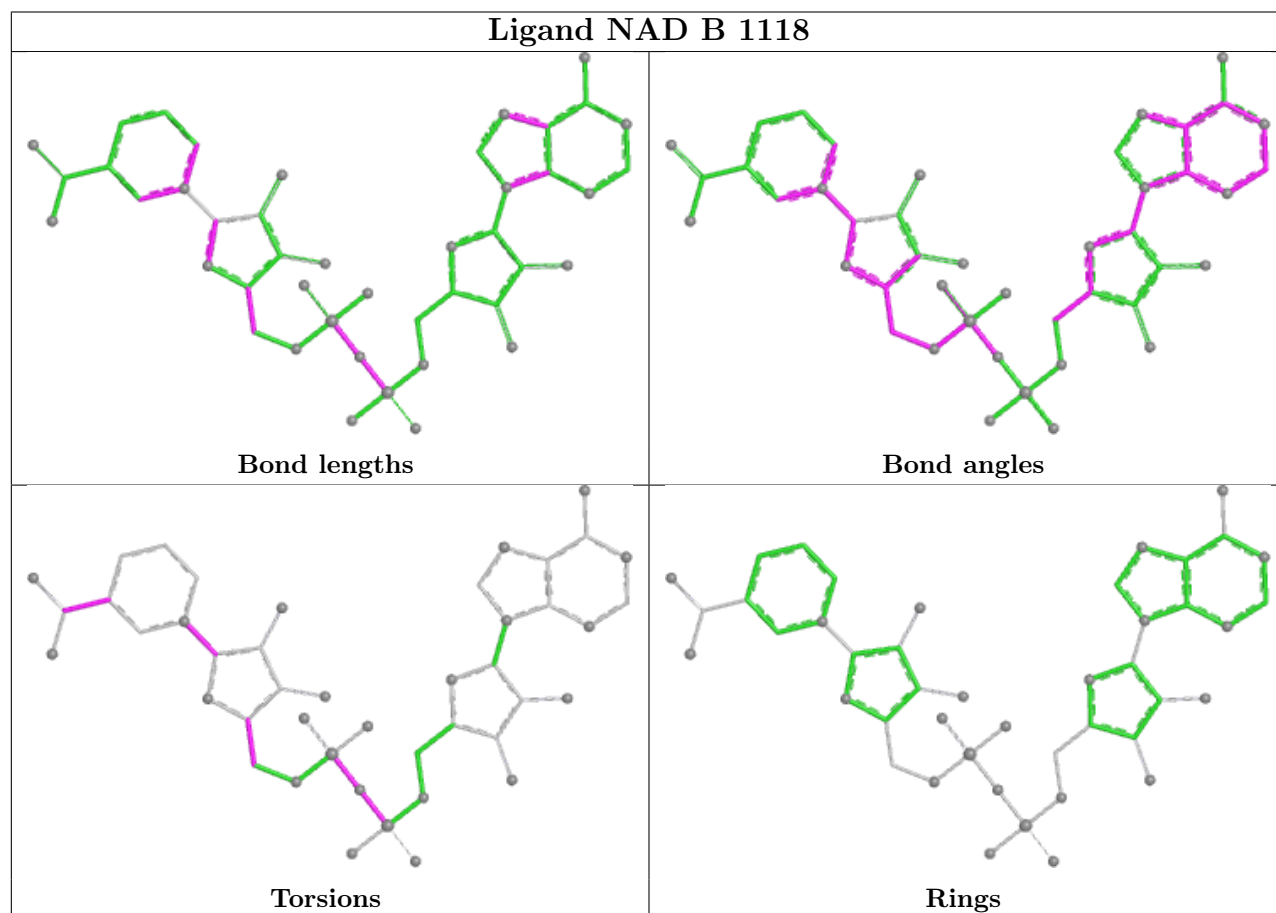
There are no ring outliers.

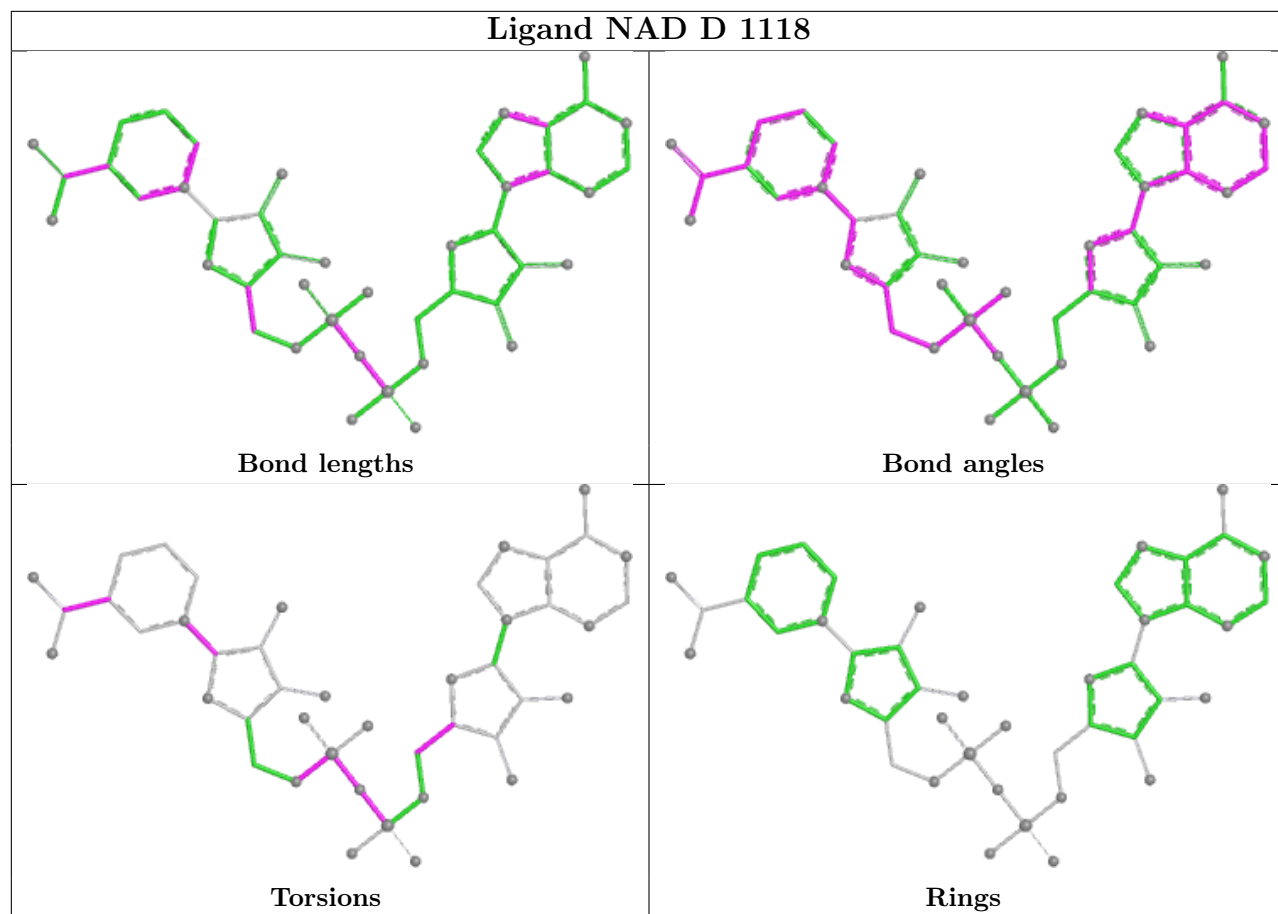
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1118	NAD	3	0
2	D	1118	NAD	3	0
2	A	1118	NAD	3	0
2	C	1118	NAD	1	0

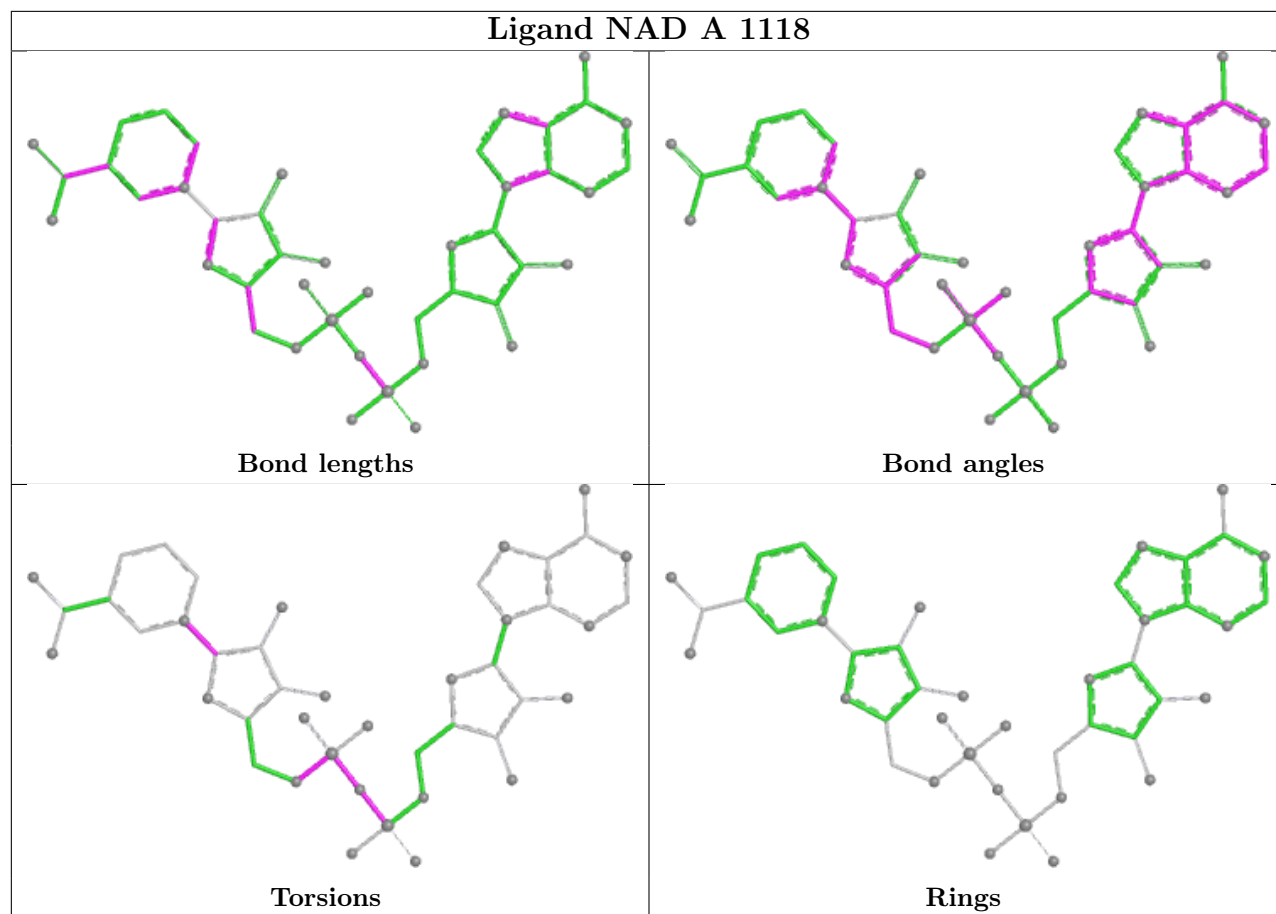
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

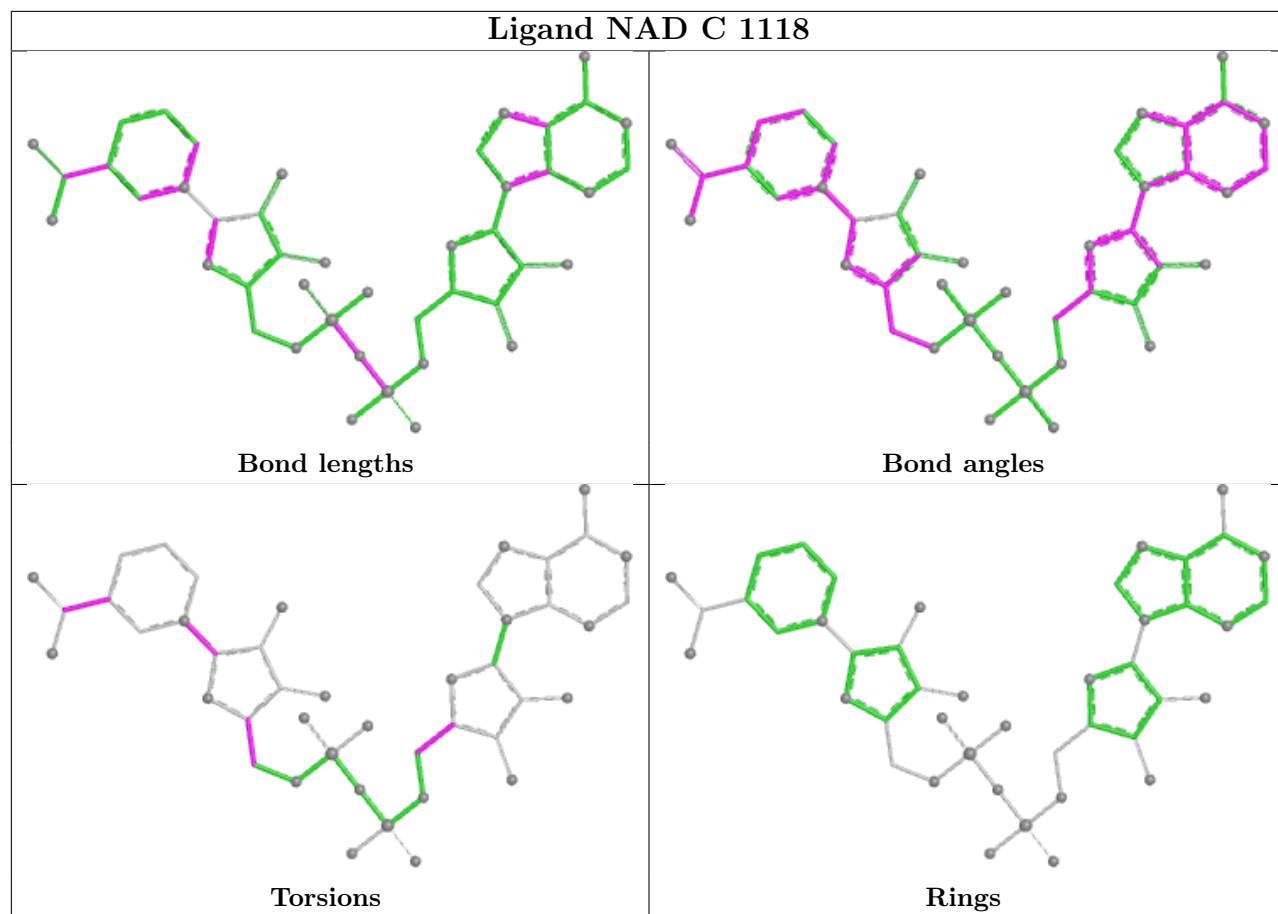
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand NAD A 1118





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/311 (100%)	0.34	24 (7%) 19 18	9, 21, 42, 80	0
1	B	311/311 (100%)	0.59	44 (14%) 6 5	13, 24, 65, 89	0
1	C	311/311 (100%)	0.72	39 (12%) 8 7	14, 28, 50, 67	0
1	D	311/311 (100%)	0.18	19 (6%) 27 26	8, 21, 40, 60	0
All	All	1244/1244 (100%)	0.46	126 (10%) 12 11	8, 23, 51, 89	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	ALA	12.7
1	B	311	VAL	11.6
1	A	180	PRO	10.9
1	A	311	VAL	9.6
1	C	180	PRO	8.8
1	D	311	VAL	8.6
1	C	311	VAL	8.5
1	A	183	GLU	7.6
1	A	181	HIS	7.4
1	A	182	GLY	6.9
1	A	44	GLY	6.8
1	B	310	ALA	6.4
1	A	179	ASP	6.3
1	A	310	ALA	5.7
1	B	262	ALA	5.6
1	C	183	GLU	5.2
1	C	182	GLY	5.2
1	B	272	PRO	4.9
1	C	184	ALA	4.7
1	A	77	ALA	4.5
1	B	180	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	309	GLY	4.4
1	C	179	ASP	4.3
1	C	181	HIS	4.1
1	D	208	PRO	4.1
1	D	209	GLY	4.0
1	D	35	THR	3.9
1	C	45	VAL	3.9
1	C	291	ARG	3.9
1	A	185	GLY	3.9
1	B	200	VAL	3.8
1	D	310	ALA	3.8
1	B	207	THR	3.7
1	B	263	PRO	3.7
1	A	257	GLU	3.6
1	B	273	GLY	3.6
1	D	272	PRO	3.6
1	B	198	LEU	3.5
1	A	211	GLU	3.5
1	B	264	GLU	3.5
1	C	257	GLU	3.4
1	B	208	PRO	3.3
1	B	205	ARG	3.3
1	C	56	GLU	3.3
1	B	195	LEU	3.3
1	B	271	ARG	3.2
1	B	274	ASP	3.2
1	C	35	THR	3.2
1	D	273	GLY	3.1
1	C	310	ALA	3.1
1	C	63	ARG	3.1
1	B	261	LYS	3.1
1	B	269	PRO	3.0
1	C	27	VAL	3.0
1	C	6	THR	3.0
1	A	154	LEU	3.0
1	A	56	GLU	3.0
1	B	265	VAL	3.0
1	A	291	ARG	2.9
1	B	258	ALA	2.9
1	B	257	GLU	2.9
1	A	309	GLY	2.9
1	C	5	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	59	GLU	2.9
1	C	7	GLY	2.8
1	B	193	ARG	2.8
1	B	268	ALA	2.8
1	B	260	GLY	2.8
1	C	106	GLN	2.8
1	C	107	TYR	2.8
1	D	56	GLU	2.8
1	B	242	THR	2.8
1	D	180	PRO	2.8
1	C	66	ARG	2.8
1	B	201	THR	2.7
1	A	178	GLN	2.7
1	B	192	GLU	2.7
1	B	267	PRO	2.7
1	B	206	LYS	2.6
1	A	63	ARG	2.6
1	B	154	LEU	2.5
1	B	266	GLN	2.5
1	B	259	ALA	2.5
1	D	207	THR	2.4
1	D	58	VAL	2.4
1	B	297	GLN	2.4
1	C	271	ARG	2.4
1	D	64	GLU	2.4
1	D	43	LYS	2.4
1	C	39	GLU	2.4
1	B	253	MET	2.4
1	B	209	GLY	2.4
1	B	196	LYS	2.4
1	B	305	ASP	2.3
1	C	189	ILE	2.3
1	D	121	ILE	2.3
1	A	110	GLU	2.3
1	D	257	GLU	2.3
1	A	43	LYS	2.3
1	B	182	GLY	2.3
1	C	25	LEU	2.2
1	D	262	ALA	2.2
1	C	47	PHE	2.2
1	C	232	PHE	2.2
1	A	60	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	263	PRO	2.2
1	C	43	LYS	2.2
1	C	70	VAL	2.2
1	D	179	ASP	2.2
1	B	210	ASP	2.1
1	B	199	PRO	2.1
1	B	211	GLU	2.1
1	C	59	GLU	2.1
1	B	181	HIS	2.1
1	C	108	GLY	2.1
1	A	39	GLU	2.1
1	C	244	GLU	2.1
1	C	2	ARG	2.1
1	C	18	GLU	2.1
1	C	69	HIS	2.1
1	B	194	VAL	2.1
1	C	60	ARG	2.1
1	A	18	GLU	2.1
1	D	211	GLU	2.0
1	C	49	ARG	2.0
1	C	21	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	1118	44/44	0.82	0.50	56,96,130,134	0
2	NAD	B	1118	44/44	0.84	0.49	51,102,136,141	0

Continued on next page...

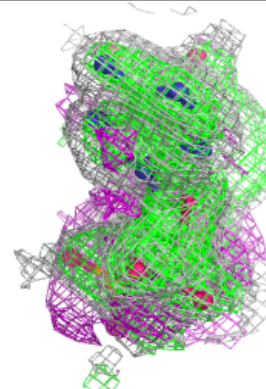
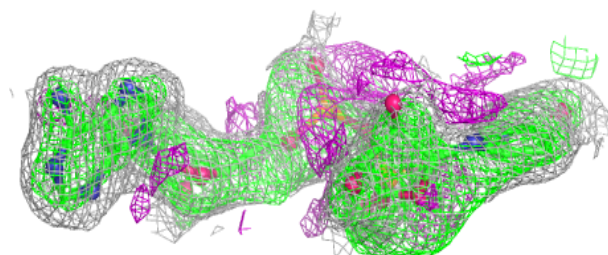
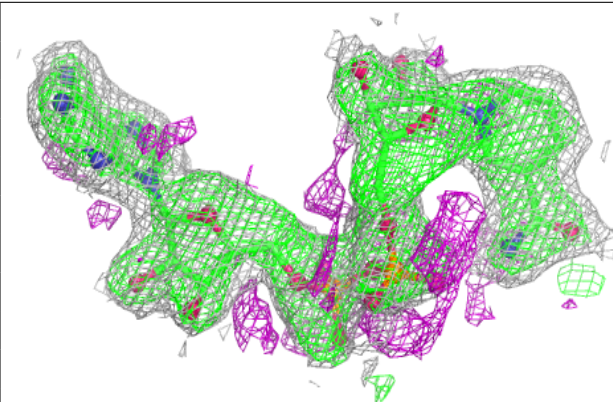
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	1118	44/44	0.84	0.51	52,98,136,140	0
2	NAD	C	1118	44/44	0.85	0.51	80,112,144,149	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.

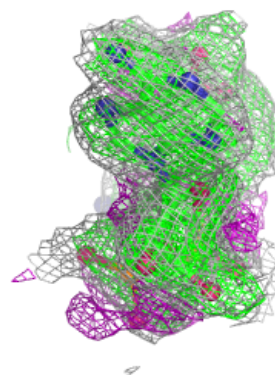
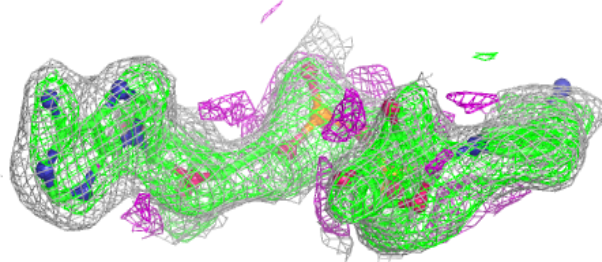
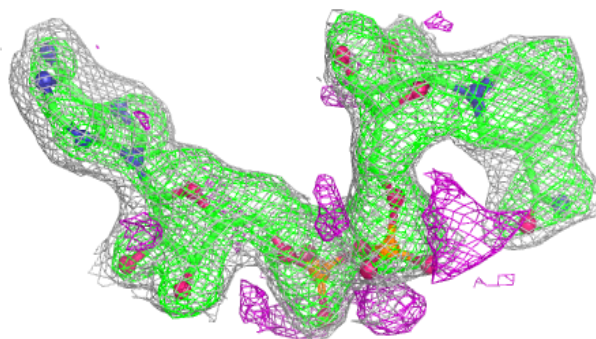
Electron density around NAD A 1118:

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

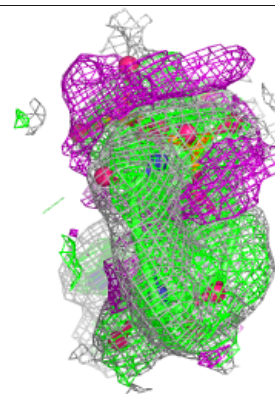
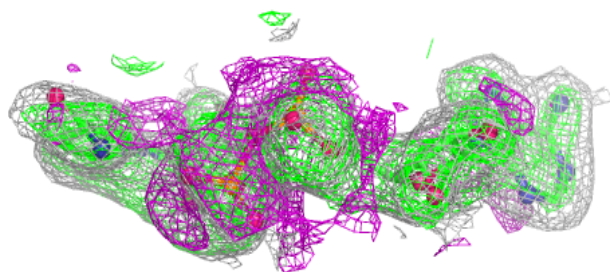
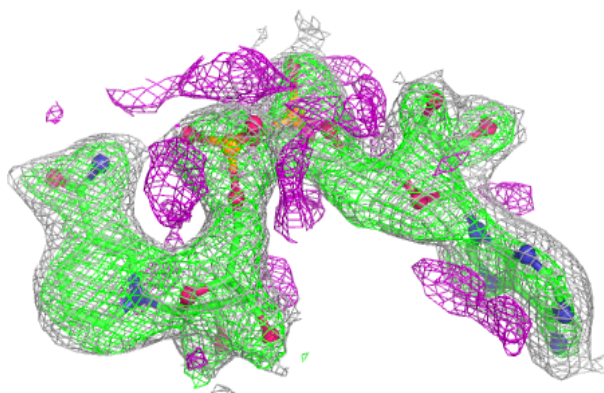


Electron density around NAD B 1118:

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

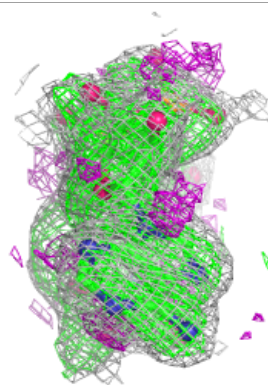
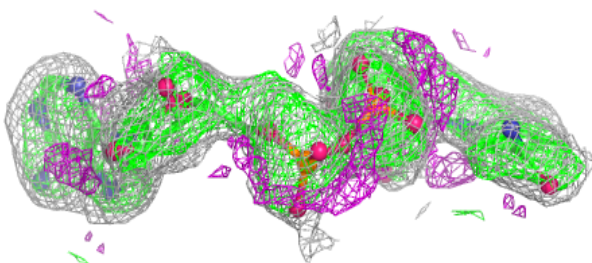
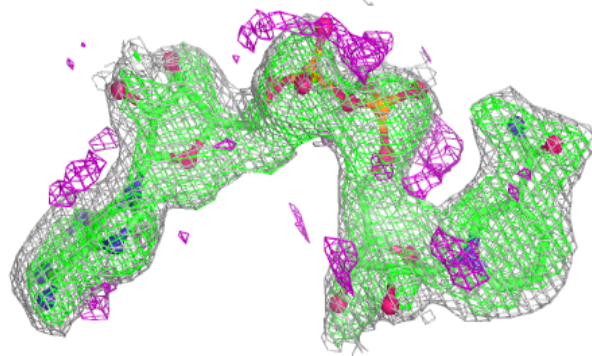
**Electron density around NAD D 1118:**

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



Electron density around NAD C 1118:

$2mF_o-DF_c$ (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.