



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:55 AM UTC

PDB ID : 8HSA / pdb_00008hsa
Title : Brucella melitensis 7-alpha-Hydroxysteroid Dehydrogenase mutant: 1-53 truncation/M196I/I258M/K262T-NAD+
Authors : Liu, Z.Y.; Zhang, R.Z.
Deposited on : 2022-12-18
Resolution : 3.00 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

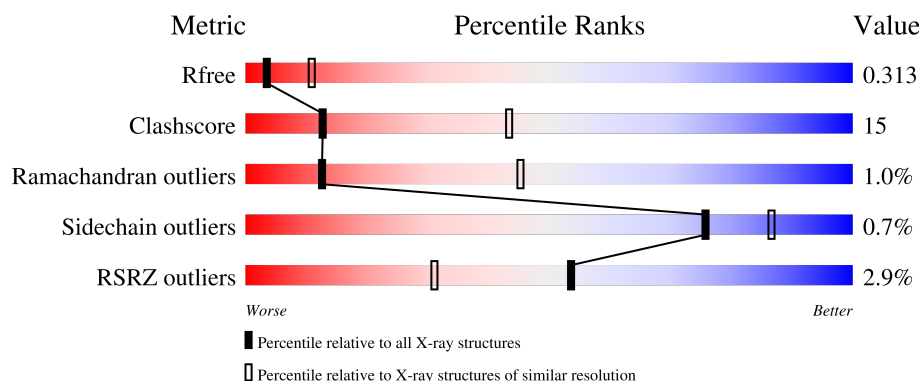
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	248	71%28%.
1	B	248	3% 72%28%
1	C	248	70%30%
1	D	248	% 73%27%
1	E	248	5% 66%29%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	248	% 71% 27%
1	G	248	66% 32% ••
1	H	248	13% 54% 39% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14423 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 7-alpha-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	245	Total	C	N	O	S	0	0	0
			1759	1107	315	328	9			
1	A	248	Total	C	N	O	S	0	0	0
			1780	1120	318	333	9			
1	B	248	Total	C	N	O	S	0	0	0
			1780	1120	318	333	9			
1	C	248	Total	C	N	O	S	0	0	0
			1780	1120	318	333	9			
1	D	248	Total	C	N	O	S	0	0	0
			1780	1120	318	333	9			
1	E	240	Total	C	N	O	S	0	0	0
			1718	1078	309	322	9			
1	F	248	Total	C	N	O	S	0	0	0
			1780	1120	318	333	9			
1	H	235	Total	C	N	O	S	0	0	0
			1694	1064	305	316	9			

There are 16 discrepancies between the modelled and reference sequences:

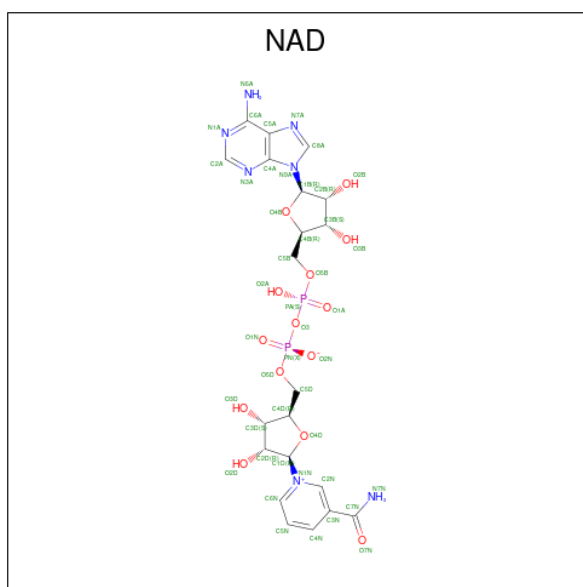
Chain	Residue	Modelled	Actual	Comment	Reference
G	196	ILE	MET	engineered mutation	UNP Q8YIN7
G	241	MET	ILE	conflict	UNP Q8YIN7
A	196	ILE	MET	engineered mutation	UNP Q8YIN7
A	241	MET	ILE	conflict	UNP Q8YIN7
B	196	ILE	MET	engineered mutation	UNP Q8YIN7
B	241	MET	ILE	conflict	UNP Q8YIN7
C	196	ILE	MET	engineered mutation	UNP Q8YIN7
C	241	MET	ILE	conflict	UNP Q8YIN7
D	196	ILE	MET	engineered mutation	UNP Q8YIN7
D	241	MET	ILE	conflict	UNP Q8YIN7
E	196	ILE	MET	engineered mutation	UNP Q8YIN7
E	241	MET	ILE	conflict	UNP Q8YIN7
F	196	ILE	MET	engineered mutation	UNP Q8YIN7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	241	MET	ILE	conflict	UNP Q8YIN7
H	196	ILE	MET	engineered mutation	UNP Q8YIN7
H	241	MET	ILE	conflict	UNP Q8YIN7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

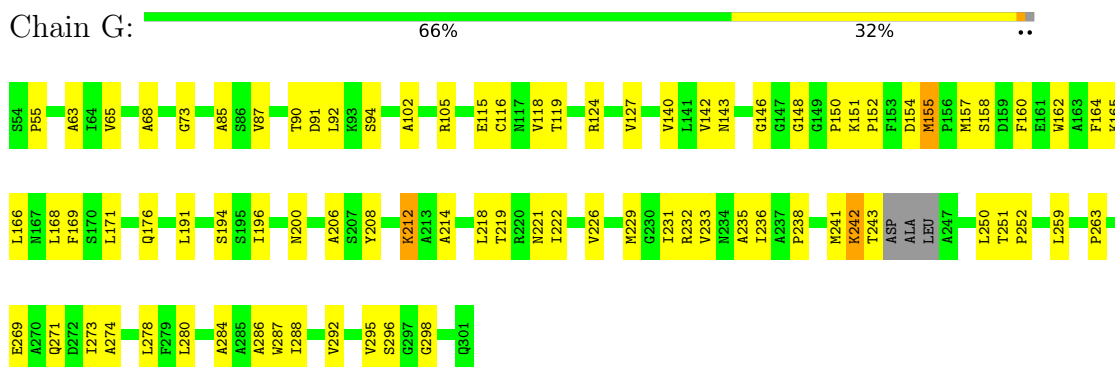


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	G	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	F	1	Total 44	C 21	N 7	O 14	P 2	0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

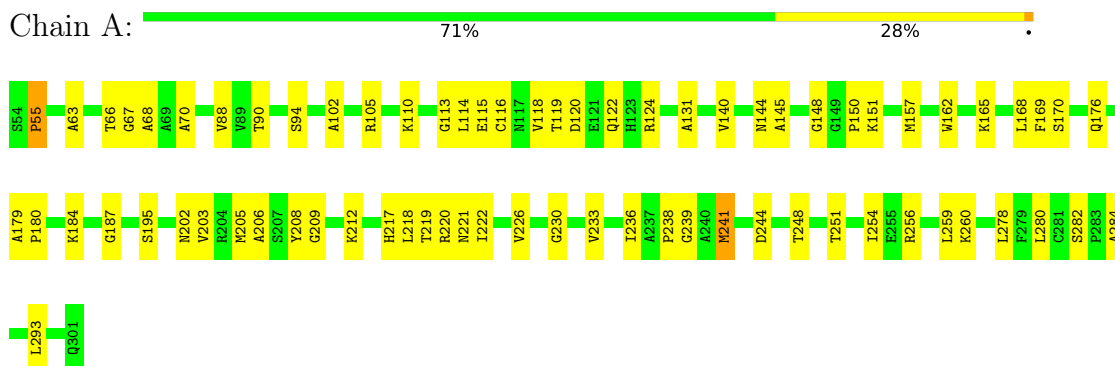
3 Residue-property plots

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.

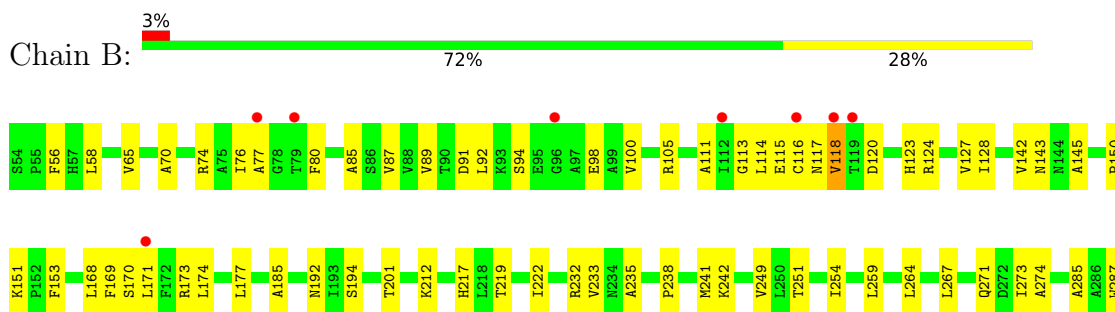
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



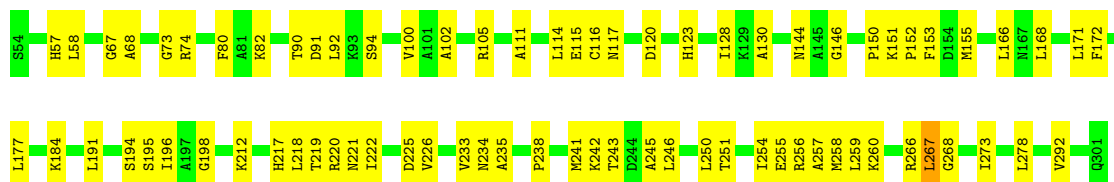
• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase





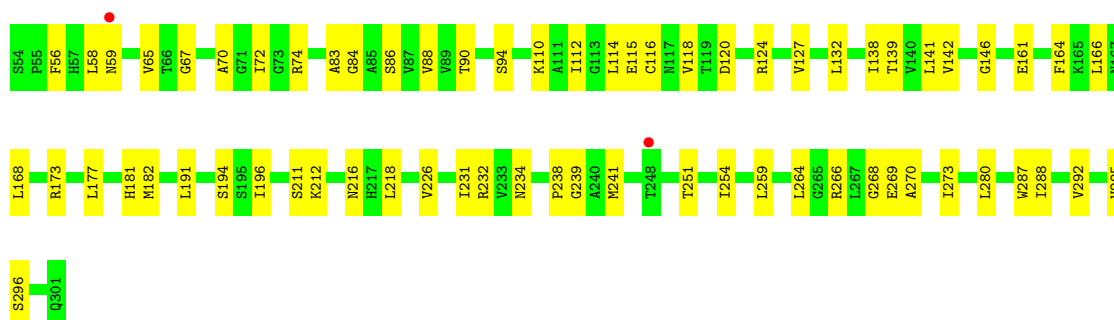
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain C: 70% 30%



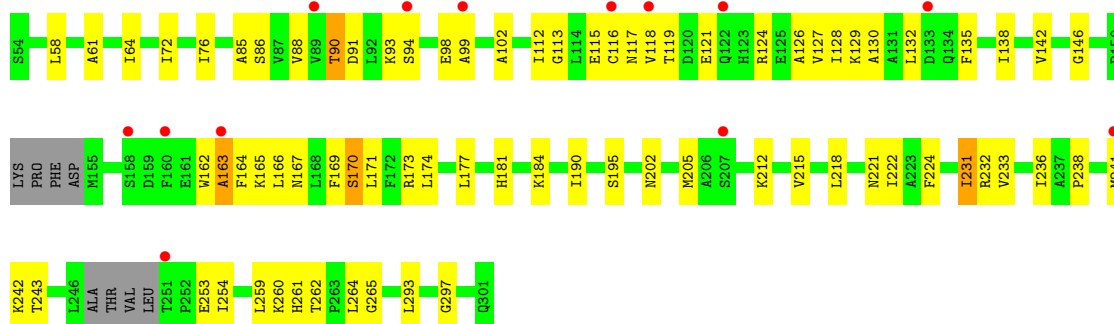
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain D: 73% 27%



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

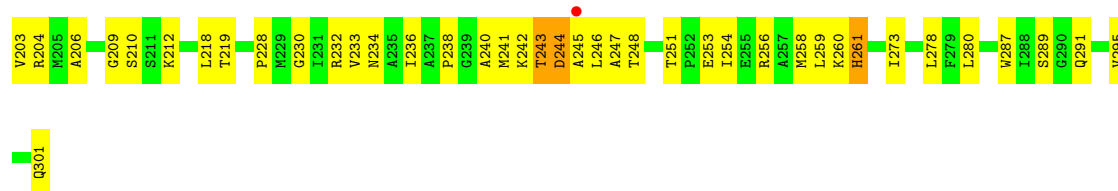
Chain E: 5% 66% 29%



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

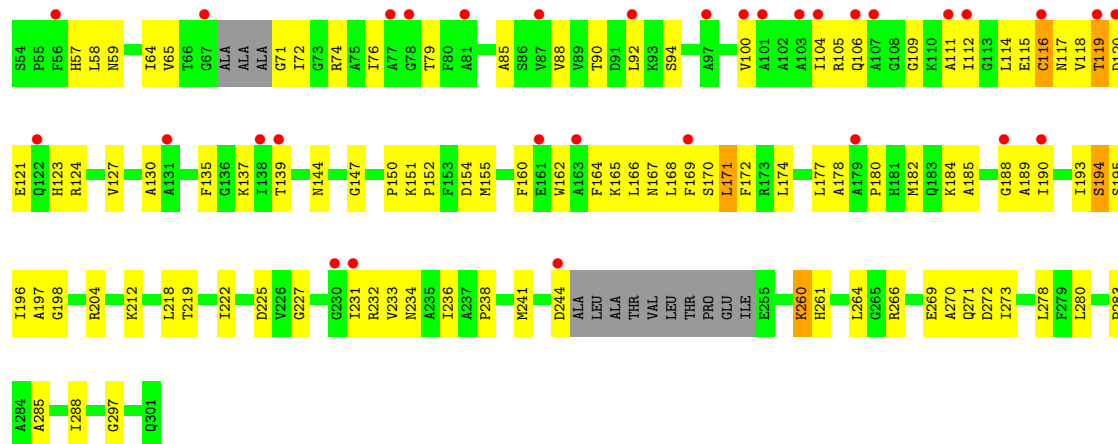
Chain F: 71% 27%





• Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

Chain H: 13% 54% 39% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.93Å 108.65Å 130.88Å 90.00° 96.61° 90.00°	Depositor
Resolution (Å)	23.84 – 3.00 23.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (23.84-3.00) 86.5 (23.84-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.99Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.225 , 0.315 0.227 , 0.313	Depositor DCC
R_{free} test set	1939 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14423	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8593e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.47	0/1809	0.71	0/2452
1	B	0.43	0/1809	0.69	0/2452
1	C	0.47	0/1809	0.69	1/2452 (0.0%)
1	D	0.45	0/1809	0.70	0/2452
1	E	0.52	0/1743	0.77	3/2358 (0.1%)
1	F	0.48	0/1809	0.69	2/2452 (0.1%)
1	G	0.55	0/1787	0.73	3/2420 (0.1%)
1	H	0.44	0/1720	0.70	1/2324 (0.0%)
All	All	0.48	0/14295	0.71	10/19362 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	261	HIS	N-CA-C	-6.97	102.82	112.30
1	E	167	ASN	N-CA-C	6.67	118.20	111.07
1	G	155	MET	CA-C-N	-6.41	113.35	120.14
1	G	155	MET	C-N-CA	-6.41	113.35	120.14
1	C	111	ALA	N-CA-C	6.02	118.20	108.32
1	F	243	THR	N-CA-C	-6.00	99.60	109.80
1	F	172	PHE	N-CA-C	-5.90	104.77	111.14
1	E	231	ILE	N-CA-C	5.62	117.83	109.17
1	E	170	SER	N-CA-C	5.26	116.69	111.07
1	G	214	ALA	N-CA-C	-5.02	105.91	112.23

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	1780	0	1804	45	0
1	B	1780	0	1804	60	0
1	C	1780	0	1804	52	0
1	D	1780	0	1804	45	0
1	E	1718	0	1737	60	0
1	F	1780	0	1804	52	0
1	G	1759	0	1783	60	0
1	H	1694	0	1708	86	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	3	0
2	D	44	0	26	1	0
2	E	44	0	26	3	0
2	F	44	0	26	2	0
2	G	44	0	26	0	0
2	H	44	0	26	2	0
All	All	14423	0	14456	438	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 (438) 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:F:90:THR:HG23	1:F:116:CYS:HB3	1.43	0.97
1:H:94:SER:HB3	1:H:115:GLU:HB2	1.50	0.94
1:D:94:SER:HB3	1:D:115:GLU:HB2	1.59	0.83
1:D:65:VAL:O	1:D:90:THR:HB	1.79	0.81
1:C:241:MET:HE3	1:C:273:ILE:HD11	1.62	0.80
1:C:94:SER:HB3	1:C:115:GLU:HB2	1.63	0.80
1:A:90:THR:HG23	1:A:116:CYS:HB3	1.63	0.78
1:A:94:SER:HB3	1:A:115:GLU:HB2	1.65	0.77
1:D:90:THR:HG23	1:D:116:CYS:HB3	1.66	0.75
1:B:222:ILE:HG13	1:B:233:VAL:HG21	1.67	0.75
1:E:146:GLY:HA2	1:E:166:LEU:HG	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:LEU:HA	1:H:177:LEU:HD12	1.68	0.75
1:H:238:PRO:HB3	1:H:241:MET:HE3	1.68	0.74
1:H:118:VAL:HB	1:H:170:SER:HB2	1.70	0.74
1:A:66:THR:O	1:A:144:ASN:HB3	1.87	0.74
1:F:238:PRO:HB3	1:F:241:MET:HE3	1.71	0.72
1:H:137:LYS:HD2	1:H:185:ALA:HB1	1.71	0.72
1:G:250:LEU:O	1:E:93:LYS:NZ	2.21	0.71
1:B:76:ILE:HG21	1:B:142:VAL:HG11	1.73	0.70
1:G:219:THR:HG23	1:G:233:VAL:HG12	1.73	0.70
1:F:65:VAL:O	1:F:90:THR:HB	1.93	0.69
1:H:190:ILE:HD12	1:H:233:VAL:HG22	1.73	0.69
1:B:242:LYS:HB2	1:B:267:LEU:HD23	1.76	0.68
1:B:70:ALA:HA	1:B:74:ARG:HD2	1.76	0.67
1:G:296:SER:HA	1:D:287:TRP:CZ3	2.29	0.67
1:A:251:THR:HG23	1:A:254:ILE:HD12	1.77	0.67
1:B:241:MET:HE3	1:B:273:ILE:HD11	1.77	0.66
1:E:162:TRP:HE3	1:E:165:LYS:HD2	1.60	0.65
1:C:90:THR:CG2	1:C:116:CYS:HB3	2.26	0.65
1:H:232:ARG:NH1	1:H:285:ALA:O	2.29	0.65
1:G:236:ILE:HG21	1:G:273:ILE:HG23	1.78	0.65
1:H:234:ASN:ND2	1:H:288:ILE:O	2.26	0.64
1:G:168:LEU:HD11	1:G:218:LEU:HD22	1.77	0.64
1:D:70:ALA:HA	1:D:74:ARG:HD2	1.78	0.64
1:H:114:LEU:HD13	1:H:127:VAL:HG22	1.80	0.64
1:G:118:VAL:O	1:G:124:ARG:NH1	2.28	0.64
1:E:162:TRP:O	1:E:165:LYS:N	2.25	0.63
1:D:90:THR:CG2	1:D:116:CYS:HB3	2.28	0.62
1:C:102:ALA:HA	1:C:105:ARG:NH1	2.15	0.61
1:C:243:THR:C	1:C:245:ALA:H	2.08	0.61
1:G:94:SER:HB3	1:G:115:GLU:HB2	1.81	0.61
1:F:219:THR:HG23	1:F:233:VAL:HG12	1.81	0.61
1:A:118:VAL:O	1:A:124:ARG:NH1	2.33	0.61
1:E:90:THR:HG23	1:E:116:CYS:HB3	1.83	0.61
1:H:194:SER:O	2:H:401:NAD:H6N	2.01	0.61
1:B:296:SER:HA	1:F:287:TRP:CZ3	2.36	0.61
1:H:236:ILE:O	1:H:238:PRO:HD3	2.01	0.61
1:C:146:GLY:HA2	1:C:166:LEU:HG	1.82	0.60
1:G:226:VAL:HA	1:G:229:MET:HE3	1.82	0.60
1:B:219:THR:HG23	1:B:233:VAL:HG12	1.83	0.60
1:G:232:ARG:HG2	1:D:264:LEU:HD11	1.84	0.60
1:B:77:ALA:HB1	1:B:87:VAL:HG11	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG13	1:B:177:LEU:HB3	1.82	0.59
1:C:257:ALA:O	1:C:260:LYS:HG2	2.02	0.59
1:E:128:ILE:O	1:E:132:LEU:HD12	2.03	0.59
1:F:114:LEU:HD11	1:F:130:ALA:HB3	1.84	0.59
1:B:98:GLU:HA	1:B:113:GLY:HA3	1.85	0.59
1:G:90:THR:HG23	1:G:116:CYS:HB3	1.85	0.58
1:F:203:VAL:HG22	1:F:204:ARG:HG3	1.84	0.58
1:G:191:LEU:HD21	1:G:236:ILE:HD12	1.85	0.58
1:F:196:ILE:HG23	1:F:238:PRO:O	2.03	0.58
1:H:139:THR:O	1:H:188:GLY:HA2	2.04	0.58
1:G:251:THR:OG1	1:H:106:GLN:NE2	2.37	0.58
1:H:219:THR:HG23	1:H:233:VAL:HG12	1.84	0.58
1:E:236:ILE:O	1:E:238:PRO:HD3	2.04	0.57
1:H:194:SER:HA	1:H:212:LYS:HD2	1.86	0.57
1:H:92:LEU:HG	1:H:117:ASN:HB2	1.87	0.57
1:C:217:HIS:ND1	1:C:220:ARG:HD2	2.19	0.57
1:E:58:LEU:HB3	1:E:85:ALA:HB2	1.86	0.57
1:A:90:THR:CG2	1:A:116:CYS:HB3	2.32	0.57
1:H:119:THR:OG1	1:H:120:ASP:N	2.38	0.57
1:B:120:ASP:O	1:B:124:ARG:HG3	2.05	0.56
1:C:219:THR:HG23	1:C:233:VAL:HG12	1.87	0.56
1:F:89:VAL:HG11	1:F:100:VAL:HB	1.87	0.56
1:F:234:ASN:HD21	1:F:289:SER:HA	1.71	0.56
1:F:240:ALA:HB1	1:F:246:LEU:HD21	1.88	0.56
1:B:56:PHE:CE2	1:F:278:LEU:HD23	2.41	0.55
1:C:68:ALA:HA	1:C:73:GLY:HA3	1.87	0.55
1:H:121:GLU:OE1	1:H:124:ARG:NH2	2.33	0.55
1:A:55:PRO:HG2	1:A:284:ALA:HB2	1.88	0.55
1:E:128:ILE:HG13	1:E:177:LEU:HB3	1.87	0.55
1:G:176:GLN:NE2	1:B:153:PHE:O	2.36	0.55
1:H:232:ARG:NH2	1:H:280:LEU:O	2.39	0.55
1:B:287:TRP:HZ3	1:F:241:MET:HE1	1.72	0.55
1:E:127:VAL:HA	1:E:130:ALA:HB3	1.87	0.55
1:F:241:MET:HE3	1:F:273:ILE:HD11	1.89	0.55
1:C:90:THR:HG23	1:C:116:CYS:HB3	1.88	0.55
1:F:258:MET:HE2	1:F:301:GLN:HB3	1.87	0.55
1:H:266:ARG:NH2	1:H:272:ASP:OD2	2.40	0.55
1:A:217:HIS:HA	1:A:220:ARG:HH11	1.71	0.55
1:D:251:THR:HG23	1:D:254:ILE:H	1.71	0.55
1:C:251:THR:HG22	1:C:254:ILE:HD12	1.89	0.54
1:G:295:VAL:HG22	1:D:288:ILE:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:O	1:A:151:LYS:HG2	2.07	0.54
1:C:150:PRO:O	1:C:151:LYS:HG2	2.08	0.54
1:H:241:MET:CE	1:H:273:ILE:HD11	2.36	0.54
1:A:102:ALA:HA	1:A:105:ARG:NH1	2.23	0.54
1:B:251:THR:HG23	1:B:254:ILE:H	1.72	0.54
1:C:120:ASP:HB3	1:C:123:HIS:HB2	1.90	0.54
1:A:219:THR:HG23	1:A:233:VAL:HG12	1.90	0.54
1:F:236:ILE:O	1:F:238:PRO:HD3	2.08	0.54
1:H:174:LEU:HD23	1:H:177:LEU:HD12	1.90	0.54
1:B:171:LEU:HD11	1:B:192:ASN:HB3	1.90	0.53
1:H:168:LEU:CD1	1:H:218:LEU:HD22	2.37	0.53
1:H:90:THR:CG2	1:H:116:CYS:HB3	2.38	0.53
1:G:150:PRO:C	1:G:151:LYS:HG2	2.34	0.53
1:C:116:CYS:O	2:C:401:NAD:H2A	2.08	0.53
1:B:117:ASN:HD22	1:B:120:ASP:HB2	1.74	0.53
1:C:255:GLU:HG3	1:C:267:LEU:HD13	1.91	0.53
1:B:91:ASP:OD1	1:B:92:LEU:N	2.42	0.53
1:C:217:HIS:CD2	1:C:221:ASN:HD21	2.27	0.53
1:G:287:TRP:CZ3	1:D:296:SER:HA	2.44	0.53
1:A:116:CYS:O	2:A:401:NAD:H2A	2.09	0.53
1:H:194:SER:OG	1:H:195:SER:N	2.42	0.53
1:B:238:PRO:HB3	1:B:273:ILE:HD11	1.90	0.53
1:H:189:ALA:CB	1:H:232:ARG:HE	2.21	0.53
1:H:115:GLU:O	1:H:116:CYS:HB2	2.10	0.52
1:B:56:PHE:HE2	1:F:278:LEU:HD23	1.74	0.52
1:H:114:LEU:HD11	1:H:130:ALA:HB3	1.90	0.52
1:G:241:MET:HB2	1:G:243:THR:HG23	1.91	0.52
1:E:162:TRP:O	1:E:164:PHE:N	2.43	0.52
1:B:117:ASN:ND2	1:B:120:ASP:HB2	2.24	0.52
1:C:90:THR:HG21	1:C:116:CYS:HB3	1.91	0.52
1:A:239:GLY:H	1:A:241:MET:HE3	1.75	0.52
1:H:90:THR:HG23	1:H:116:CYS:HB3	1.92	0.52
1:H:65:VAL:O	1:H:90:THR:HB	2.10	0.52
1:H:168:LEU:HD12	1:H:218:LEU:HD22	1.91	0.52
1:G:196:ILE:HG23	1:G:238:PRO:O	2.10	0.52
1:B:89:VAL:HG11	1:B:100:VAL:HB	1.92	0.52
1:D:120:ASP:O	1:D:124:ARG:HG3	2.09	0.52
1:E:212:LYS:O	1:E:215:VAL:HB	2.10	0.52
1:E:91:ASP:OD1	2:E:401:NAD:H1B	2.09	0.52
1:E:221:ASN:O	1:E:224:PHE:N	2.40	0.52
1:G:146:GLY:HA2	1:G:166:LEU:HG	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:HG2	1:F:169:PHE:CE2	2.46	0.51
1:E:117:ASN:OD1	1:E:119:THR:HG23	2.10	0.51
1:G:68:ALA:HA	1:G:73:GLY:HA3	1.91	0.51
1:G:235:ALA:HB3	1:G:292:VAL:HG22	1.91	0.51
1:H:104:ILE:HG21	1:H:111:ALA:HB2	1.92	0.51
1:G:63:ALA:HA	1:G:140:VAL:O	2.10	0.51
1:C:74:ARG:HG3	1:C:100:VAL:HG22	1.92	0.51
1:C:222:ILE:O	1:C:226:VAL:HG22	2.11	0.51
1:G:232:ARG:HD2	1:G:286:ALA:O	2.10	0.51
1:B:114:LEU:HD23	1:B:115:GLU:N	2.26	0.51
1:E:165:LYS:HA	1:E:169:PHE:CD2	2.45	0.51
1:A:165:LYS:HA	1:A:169:PHE:CD2	2.46	0.51
1:G:65:VAL:HG22	1:G:142:VAL:HB	1.92	0.51
1:G:91:ASP:OD1	1:G:92:LEU:N	2.43	0.51
1:C:266:ARG:NH1	1:C:268:GLY:HA2	2.25	0.51
1:G:157:MET:O	1:G:158:SER:C	2.53	0.50
1:B:105:ARG:NE	1:B:111:ALA:O	2.42	0.50
1:B:123:HIS:O	1:B:127:VAL:HG23	2.11	0.50
1:D:164:PHE:CE1	1:D:211:SER:HB3	2.46	0.50
1:F:90:THR:CG2	1:F:116:CYS:HB3	2.30	0.50
1:B:118:VAL:O	1:B:124:ARG:NH1	2.43	0.50
1:C:194:SER:O	2:C:401:NAD:H6N	2.11	0.50
1:E:118:VAL:HG12	1:E:174:LEU:HD11	1.93	0.50
1:H:155:MET:HE2	1:H:160:PHE:N	2.27	0.50
1:A:195:SER:HB3	1:A:212:LYS:HG3	1.94	0.50
1:E:61:ALA:O	1:E:86:SER:N	2.43	0.50
1:H:165:LYS:HA	1:H:169:PHE:HB2	1.93	0.50
1:F:246:LEU:O	1:F:247:ALA:C	2.55	0.50
1:H:105:ARG:HA	1:H:109:GLY:H	1.76	0.50
1:E:90:THR:CG2	1:E:116:CYS:HB3	2.41	0.50
1:A:119:THR:HG21	1:A:162:TRP:CH2	2.47	0.49
1:B:114:LEU:HD22	1:B:127:VAL:HG22	1.95	0.49
1:E:169:PHE:CD1	1:E:169:PHE:N	2.78	0.49
1:F:168:LEU:HD11	1:F:218:LEU:HD22	1.95	0.49
1:C:246:LEU:HG	1:C:250:LEU:HD13	1.94	0.49
1:E:64:ILE:HD11	1:E:138:ILE:HD13	1.94	0.49
1:G:242:LYS:NZ	1:G:269:GLU:OE2	2.36	0.49
1:E:99:ALA:O	1:E:102:ALA:HB3	2.12	0.49
1:G:164:PHE:CZ	1:B:168:LEU:HD21	2.48	0.49
1:G:238:PRO:HB3	1:G:273:ILE:HD11	1.95	0.49
1:G:200:ASN:O	1:B:217:HIS:CE1	2.65	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:O	1:B:111:ALA:HA	2.12	0.49
1:C:243:THR:HG23	1:C:246:LEU:H	1.78	0.49
1:D:259:LEU:HD21	1:D:266:ARG:C	2.38	0.49
1:H:162:TRP:HA	1:H:165:LYS:HD2	1.95	0.49
1:B:65:VAL:HG22	1:B:142:VAL:HB	1.95	0.49
1:H:285:ALA:HA	1:H:288:ILE:HD12	1.95	0.49
1:H:64:ILE:HA	1:H:88:VAL:HB	1.95	0.48
1:F:65:VAL:HG12	1:F:68:ALA:HB2	1.95	0.48
1:C:235:ALA:O	1:C:292:VAL:HA	2.13	0.48
1:H:189:ALA:HB2	1:H:232:ARG:HE	1.78	0.48
1:A:113:GLY:C	1:A:114:LEU:HD12	2.38	0.48
1:F:247:ALA:O	1:F:248:THR:C	2.57	0.48
1:H:72:ILE:HD11	1:H:241:MET:HG3	1.95	0.48
1:C:168:LEU:HD11	1:C:218:LEU:HD22	1.96	0.48
1:H:164:PHE:O	1:H:169:PHE:N	2.27	0.48
1:A:205:MET:O	1:A:209:GLY:N	2.37	0.48
1:E:260:LYS:HG3	1:E:261:HIS:ND1	2.29	0.48
1:G:232:ARG:NH2	1:G:280:LEU:O	2.45	0.48
1:D:88:VAL:HG13	1:D:112:ILE:HG23	1.96	0.48
1:F:260:LYS:O	1:F:261:HIS:ND1	2.47	0.48
1:D:259:LEU:HD11	1:D:266:ARG:HA	1.96	0.47
1:F:241:MET:O	1:F:246:LEU:HB2	2.14	0.47
1:H:72:ILE:O	1:H:76:ILE:HG13	2.14	0.47
1:B:94:SER:HB3	1:B:115:GLU:HB2	1.96	0.47
1:D:226:VAL:HB	1:D:231:ILE:HB	1.96	0.47
1:H:244:ASP:O	2:H:401:NAD:H51A	2.14	0.47
1:D:238:PRO:HB3	1:D:241:MET:HE3	1.95	0.47
1:H:151:LYS:HD2	1:H:155:MET:HE1	1.95	0.47
1:F:194:SER:C	1:F:212:LYS:HE2	2.39	0.47
1:F:251:THR:HG23	1:F:254:ILE:HD12	1.96	0.47
1:G:259:LEU:HD23	1:G:259:LEU:HA	1.58	0.47
1:A:176:GLN:HA	1:C:153:PHE:CE1	2.50	0.47
1:B:117:ASN:O	1:B:118:VAL:C	2.58	0.47
1:C:128:ILE:HG13	1:C:177:LEU:HB3	1.97	0.47
1:D:67:GLY:O	2:D:401:NAD:H4B	2.15	0.47
1:E:94:SER:HB3	1:E:115:GLU:HB2	1.97	0.47
1:D:59:ASN:HA	1:D:84:GLY:O	2.14	0.47
1:D:146:GLY:HA2	1:D:166:LEU:HG	1.96	0.47
1:E:262:THR:HG22	1:E:265:GLY:H	1.78	0.47
1:F:86:SER:HB3	1:F:135:PHE:CE1	2.50	0.47
1:D:72:ILE:HA	1:D:270:ALA:HB1	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:MET:O	1:E:243:THR:N	2.42	0.47
1:G:278:LEU:HD23	1:D:56:PHE:CZ	2.50	0.47
1:C:195:SER:HB3	1:C:212:LYS:HG3	1.97	0.47
2:E:401:NAD:HO3A	2:E:401:NAD:HO2A	1.55	0.46
1:H:184:LYS:HD3	1:H:184:LYS:N	2.30	0.46
1:A:148:GLY:HA3	1:A:208:TYR:CD1	2.50	0.46
1:H:105:ARG:HD2	1:H:111:ALA:H	1.80	0.46
1:G:287:TRP:CH2	1:D:296:SER:HA	2.50	0.46
1:C:82:LYS:HB3	1:C:82:LYS:HE2	1.49	0.46
1:D:232:ARG:NH2	1:D:280:LEU:O	2.48	0.46
1:H:57:HIS:HB2	1:H:59:ASN:OD1	2.15	0.46
1:H:264:LEU:HD12	1:H:297:GLY:HA2	1.98	0.46
1:E:58:LEU:HD23	1:E:58:LEU:HA	1.67	0.46
1:F:92:LEU:HD12	2:F:401:NAD:C6A	2.45	0.46
1:B:114:LEU:HD23	1:B:115:GLU:H	1.80	0.46
1:F:86:SER:HB3	1:F:135:PHE:CZ	2.51	0.46
1:H:196:ILE:C	1:H:198:GLY:H	2.24	0.46
1:G:148:GLY:HA3	1:G:208:TYR:CD1	2.51	0.46
1:G:221:ASN:OD1	1:B:201:THR:HA	2.15	0.46
1:H:58:LEU:HD13	1:H:85:ALA:HB2	1.96	0.46
1:H:112:ILE:HG22	1:H:135:PHE:HE2	1.81	0.46
1:H:152:PRO:O	1:H:155:MET:HB3	2.16	0.46
1:G:143:ASN:ND2	1:G:171:LEU:HB2	2.31	0.46
1:G:241:MET:HE3	1:G:241:MET:HB3	1.52	0.46
1:B:288:ILE:HG12	1:F:295:VAL:HG13	1.97	0.46
1:E:72:ILE:HD11	1:E:241:MET:HG3	1.96	0.46
1:A:88:VAL:HG21	1:A:131:ALA:CB	2.46	0.46
1:A:244:ASP:O	1:A:248:THR:HG23	2.16	0.46
1:B:170:SER:O	1:B:171:LEU:C	2.59	0.46
1:D:139:THR:C	1:D:182:MET:HE2	2.41	0.46
1:D:191:LEU:HD12	1:D:234:ASN:O	2.15	0.46
1:H:241:MET:HE3	1:H:273:ILE:HD11	1.98	0.45
1:C:171:LEU:HD12	1:C:172:PHE:N	2.31	0.45
1:E:259:LEU:HA	1:E:259:LEU:HD23	1.61	0.45
1:H:114:LEU:HD11	1:H:130:ALA:CB	2.46	0.45
1:H:116:CYS:SG	1:H:123:HIS:HB3	2.57	0.45
1:H:144:ASN:HA	1:H:193:ILE:CG1	2.46	0.45
1:G:165:LYS:HA	1:G:169:PHE:HB2	1.97	0.45
1:A:67:GLY:O	1:A:144:ASN:ND2	2.50	0.45
1:A:168:LEU:HD11	1:A:218:LEU:HD22	1.97	0.45
1:B:249:VAL:HG12	1:B:249:VAL:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:GLY:O	1:H:74:ARG:HB3	2.16	0.45
1:G:55:PRO:HG2	1:G:284:ALA:HB2	1.99	0.45
1:C:91:ASP:OD1	1:C:92:LEU:N	2.49	0.45
1:B:194:SER:HA	1:B:212:LYS:HD2	1.99	0.45
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.83	0.45
1:E:253:GLU:OE2	1:E:254:ILE:HG13	2.17	0.45
1:F:241:MET:CE	1:F:273:ILE:HD11	2.47	0.45
1:A:202:ASN:OD1	1:A:203:VAL:N	2.49	0.45
1:B:118:VAL:HG22	2:B:401:NAD:N1A	2.31	0.45
1:D:173:ARG:NH2	1:D:177:LEU:HD21	2.32	0.45
1:E:86:SER:HB3	1:E:135:PHE:CE1	2.50	0.45
1:E:195:SER:HB3	1:E:212:LYS:HG3	1.98	0.45
1:E:202:ASN:O	1:E:205:MET:HB2	2.16	0.45
1:G:90:THR:CG2	1:G:116:CYS:HB3	2.46	0.45
1:G:119:THR:HG21	1:G:162:TRP:CH2	2.52	0.45
1:B:91:ASP:OD2	2:B:401:NAD:H1B	2.16	0.45
1:C:114:LEU:HD11	1:C:130:ALA:CB	2.47	0.45
1:E:124:ARG:HB3	1:E:177:LEU:HD12	1.98	0.45
1:A:195:SER:HA	1:A:238:PRO:HD2	1.98	0.45
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.81	0.45
1:C:238:PRO:HB3	1:C:273:ILE:HD11	1.99	0.45
1:D:114:LEU:HD22	1:D:127:VAL:HG22	1.98	0.45
1:E:121:GLU:OE1	1:E:173:ARG:HG2	2.17	0.45
1:E:164:PHE:HB3	1:E:169:PHE:CZ	2.52	0.45
1:H:196:ILE:C	1:H:198:GLY:N	2.75	0.45
1:G:65:VAL:HG12	1:G:68:ALA:HB2	1.98	0.45
1:E:181:HIS:O	1:E:184:LYS:HB2	2.17	0.45
1:H:190:ILE:HB	1:H:233:VAL:HG13	1.97	0.45
1:G:238:PRO:HB3	1:G:273:ILE:CD1	2.47	0.45
1:A:88:VAL:HG21	1:A:131:ALA:HB2	1.99	0.45
1:E:190:ILE:O	1:E:233:VAL:HA	2.17	0.45
1:F:197:ALA:HB1	1:F:209:GLY:HA2	1.98	0.45
1:F:228:PRO:C	1:F:230:GLY:H	2.25	0.45
1:H:222:ILE:HG13	1:H:233:VAL:HG21	1.99	0.45
1:H:231:ILE:HG22	1:H:232:ARG:H	1.81	0.45
1:D:118:VAL:O	1:D:124:ARG:HD3	2.17	0.44
1:G:152:PRO:O	1:G:155:MET:HB3	2.17	0.44
1:B:150:PRO:O	1:B:151:LYS:HG2	2.17	0.44
1:B:294:THR:HB	1:F:291:GLN:OE1	2.18	0.44
1:E:94:SER:HB3	1:E:115:GLU:HG3	2.00	0.44
1:H:147:GLY:O	1:H:167:ASN:ND2	2.40	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:O	1:A:145:ALA:C	2.61	0.44
1:D:268:GLY:O	1:D:269:GLU:HG3	2.18	0.44
1:F:259:LEU:HA	1:F:259:LEU:HD23	1.73	0.44
1:A:203:VAL:HG23	1:C:225:ASP:HA	1.98	0.44
1:B:171:LEU:HD11	1:B:192:ASN:CG	2.42	0.44
1:C:57:HIS:O	1:C:58:LEU:HD23	2.18	0.44
1:C:196:ILE:C	1:C:198:GLY:H	2.25	0.44
1:E:231:ILE:HG22	1:E:232:ARG:N	2.32	0.44
1:D:72:ILE:HD11	1:D:241:MET:HG3	1.98	0.44
1:G:252:PRO:HD2	1:H:106:GLN:HE22	1.81	0.44
1:E:76:ILE:HG21	1:E:142:VAL:HG11	2.00	0.44
1:F:244:ASP:O	1:F:245:ALA:C	2.61	0.44
1:C:150:PRO:C	1:C:151:LYS:HG2	2.43	0.44
1:F:171:LEU:H	1:F:171:LEU:HG	1.65	0.44
1:H:112:ILE:HG22	1:H:135:PHE:CE2	2.53	0.44
1:H:269:GLU:O	1:H:271:GLN:N	2.50	0.44
1:B:285:ALA:HB1	1:B:288:ILE:HB	2.00	0.43
1:D:238:PRO:HB3	1:D:273:ILE:HD11	1.99	0.43
1:H:151:LYS:HD2	1:H:155:MET:CE	2.47	0.43
1:B:173:ARG:O	1:B:177:LEU:HG	2.18	0.43
1:C:243:THR:C	1:C:245:ALA:N	2.73	0.43
1:C:251:THR:HG23	1:C:254:ILE:H	1.83	0.43
1:E:170:SER:OG	1:E:171:LEU:N	2.49	0.43
1:G:263:PRO:HD2	1:G:298:GLY:C	2.42	0.43
1:B:192:ASN:O	1:B:235:ALA:HA	2.18	0.43
1:C:256:ARG:HA	1:C:259:LEU:HB2	1.99	0.43
1:E:94:SER:CB	1:E:115:GLU:HB2	2.49	0.43
1:E:218:LEU:HG	1:E:222:ILE:HG23	2.00	0.43
1:A:222:ILE:O	1:A:226:VAL:HG22	2.18	0.43
1:A:278:LEU:O	1:A:282:SER:HB3	2.18	0.43
1:B:143:ASN:ND2	1:B:171:LEU:HG	2.32	0.43
1:B:80:PHE:O	1:B:85:ALA:HB3	2.17	0.43
1:D:264:LEU:HD23	1:D:264:LEU:HA	1.83	0.43
1:H:124:ARG:HB3	1:H:177:LEU:HD11	2.01	0.43
1:C:80:PHE:CE1	1:C:278:LEU:HA	2.53	0.43
1:C:242:LYS:HB2	1:C:268:GLY:O	2.18	0.43
1:E:238:PRO:HB3	1:E:241:MET:HE3	2.01	0.43
1:E:264:LEU:HD23	1:E:264:LEU:HA	1.73	0.43
1:D:194:SER:C	1:D:212:LYS:HE3	2.43	0.43
1:H:260:LYS:HD3	1:H:260:LYS:HA	1.71	0.43
1:A:118:VAL:HB	1:A:170:SER:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:O	1:D:182:MET:HG2	2.19	0.43
1:F:116:CYS:O	2:F:401:NAD:H2A	2.19	0.43
1:F:280:LEU:HD23	1:F:280:LEU:HA	1.78	0.43
1:H:100:VAL:O	1:H:104:ILE:HG13	2.19	0.43
1:H:269:GLU:O	1:H:270:ALA:C	2.61	0.43
1:G:94:SER:HB3	1:G:115:GLU:CB	2.47	0.43
1:G:157:MET:HB3	1:G:157:MET:HE3	1.73	0.43
1:B:287:TRP:CZ3	1:F:241:MET:HE1	2.53	0.43
1:F:206:ALA:O	1:F:210:SER:OG	2.36	0.43
1:H:177:LEU:O	1:H:180:PRO:HD2	2.19	0.43
1:F:66:THR:O	1:F:144:ASN:HB3	2.19	0.42
1:H:162:TRP:NE1	1:H:166:LEU:HD22	2.35	0.42
1:E:88:VAL:HA	1:E:112:ILE:HG23	2.00	0.42
1:E:164:PHE:HB3	1:E:169:PHE:CE1	2.54	0.42
1:G:85:ALA:O	1:G:87:VAL:HG23	2.19	0.42
1:G:288:ILE:HG12	1:D:295:VAL:HG22	2.01	0.42
1:B:118:VAL:HG11	1:B:145:ALA:HB3	2.01	0.42
1:G:116:CYS:HB2	1:G:127:VAL:HG21	2.01	0.42
1:A:63:ALA:HA	1:A:140:VAL:O	2.20	0.42
1:B:238:PRO:HB3	1:B:273:ILE:CD1	2.50	0.42
1:C:184:LYS:HE2	1:C:184:LYS:HA	2.00	0.42
1:C:67:GLY:O	1:C:144:ASN:ND2	2.52	0.42
1:C:152:PRO:O	1:C:155:MET:HB3	2.20	0.42
1:D:86:SER:HA	1:D:110:LYS:O	2.20	0.42
1:H:171:LEU:O	1:H:172:PHE:C	2.61	0.42
1:A:184:LYS:HE2	1:A:184:LYS:HA	2.01	0.42
1:C:74:ARG:HG3	1:C:100:VAL:CG2	2.49	0.42
1:G:208:TYR:O	1:G:212:LYS:HG3	2.20	0.42
1:A:236:ILE:HA	1:A:293:LEU:O	2.20	0.42
1:B:116:CYS:HA	1:B:123:HIS:HB3	2.00	0.42
1:C:242:LYS:N	1:C:268:GLY:O	2.47	0.42
1:E:166:LEU:O	1:E:170:SER:OG	2.28	0.42
1:G:92:LEU:O	1:G:92:LEU:HD23	2.19	0.42
1:G:102:ALA:HA	1:G:105:ARG:NH1	2.35	0.42
1:A:68:ALA:O	1:A:70:ALA:N	2.45	0.42
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.68	0.42
1:D:58:LEU:HD12	1:D:83:ALA:HB3	2.02	0.42
1:D:141:LEU:HD12	1:D:142:VAL:N	2.35	0.42
1:D:196:ILE:HD13	1:D:239:GLY:HA2	2.02	0.42
1:D:259:LEU:HD23	1:D:259:LEU:HA	1.72	0.42
1:E:124:ARG:HB3	1:E:177:LEU:CD1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ALA:O	1:E:129:LYS:N	2.53	0.42
1:C:243:THR:O	1:C:245:ALA:N	2.50	0.41
1:H:105:ARG:HG3	1:H:109:GLY:O	2.20	0.41
1:H:137:LYS:HD2	1:H:185:ALA:CB	2.45	0.41
1:H:236:ILE:C	1:H:238:PRO:HD3	2.45	0.41
1:B:171:LEU:HD11	1:B:192:ASN:CB	2.50	0.41
1:F:253:GLU:HA	1:F:256:ARG:CZ	2.50	0.41
1:H:57:HIS:CE1	1:H:283:PRO:HG2	2.55	0.41
1:H:225:ASP:C	1:H:227:GLY:H	2.29	0.41
1:H:118:VAL:HG12	1:H:174:LEU:HD11	2.02	0.41
1:C:117:ASN:HA	2:C:401:NAD:N1A	2.34	0.41
1:B:264:LEU:HA	1:B:264:LEU:HD23	1.64	0.41
1:E:236:ILE:HA	1:E:293:LEU:O	2.21	0.41
1:F:63:ALA:HA	1:F:140:VAL:O	2.20	0.41
1:F:129:LYS:HG2	1:F:133:ASP:OD2	2.21	0.41
1:H:79:THR:CG2	1:H:278:LEU:HD22	2.51	0.41
1:H:178:ALA:HB1	1:H:182:MET:HE3	2.01	0.41
1:A:179:ALA:N	1:A:180:PRO:HD2	2.35	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.84	0.41
1:F:241:MET:O	1:F:243:THR:N	2.53	0.41
1:H:118:VAL:H	1:H:118:VAL:HG22	1.56	0.41
1:A:120:ASP:OD1	1:A:122:GLN:N	2.53	0.41
1:A:256:ARG:O	1:A:260:LYS:HG2	2.20	0.41
1:G:152:PRO:HB2	1:G:154:ASP:OD1	2.21	0.41
1:G:226:VAL:HG23	1:G:231:ILE:HB	2.03	0.41
1:G:271:GLN:HA	1:G:274:ALA:HB3	2.03	0.41
1:B:251:THR:HG22	1:B:254:ILE:HD12	2.03	0.41
1:B:271:GLN:O	1:B:274:ALA:N	2.54	0.41
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.84	0.41
1:E:112:ILE:HG22	1:E:135:PHE:HE2	1.86	0.41
1:E:264:LEU:HD12	1:E:297:GLY:HA2	2.01	0.41
1:F:72:ILE:HD11	1:F:241:MET:HG3	2.03	0.41
1:F:101:ALA:O	1:F:105:ARG:HG3	2.21	0.41
1:A:110:LYS:HE3	1:A:110:LYS:HB2	1.76	0.41
1:E:98:GLU:HG3	1:E:113:GLY:HA3	2.03	0.41
1:E:118:VAL:H	1:E:118:VAL:HG22	1.57	0.41
2:E:401:NAD:H2N	2:E:401:NAD:O5D	2.21	0.41
1:F:137:LYS:C	1:F:138:ILE:HG13	2.46	0.41
1:F:241:MET:C	1:F:246:LEU:HD22	2.46	0.41
1:A:217:HIS:CD2	1:A:221:ASN:HD21	2.39	0.40
1:B:174:LEU:HD23	1:B:177:LEU:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LEU:HA	1:C:234:ASN:O	2.21	0.40
1:E:162:TRP:O	1:E:163:ALA:C	2.64	0.40
1:E:162:TRP:HA	1:E:165:LYS:HD2	2.03	0.40
1:H:196:ILE:O	1:H:198:GLY:N	2.54	0.40
1:G:222:ILE:HD13	1:G:222:ILE:HG21	1.83	0.40
1:E:162:TRP:C	1:E:164:PHE:N	2.80	0.40
1:H:150:PRO:HB3	1:H:204:ARG:NH1	2.37	0.40
1:D:168:LEU:HD11	1:D:218:LEU:HD22	2.03	0.40
1:H:167:ASN:O	1:H:171:LEU:HD21	2.22	0.40
1:G:157:MET:O	1:G:160:PHE:N	2.54	0.40
1:A:157:MET:HE3	1:A:157:MET:HB3	1.81	0.40
1:A:187:GLY:HA2	1:A:230:GLY:O	2.22	0.40
1:D:132:LEU:HD11	1:D:181:HIS:ND1	2.37	0.40
1:D:216:ASN:HB3	1:D:292:VAL:HG21	2.04	0.40
1:E:118:VAL:O	1:E:124:ARG:NH1	2.52	0.40
1:F:70:ALA:HA	1:F:74:ARG:HD2	2.03	0.40
1:H:196:ILE:HG23	1:H:238:PRO:O	2.22	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	246/248 (99%)	227 (92%)	17 (7%)	2 (1%)	16	50
1	B	246/248 (99%)	220 (89%)	24 (10%)	2 (1%)	16	50
1	C	246/248 (99%)	225 (92%)	19 (8%)	2 (1%)	16	50
1	D	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
1	E	234/248 (94%)	207 (88%)	25 (11%)	2 (1%)	14	48
1	F	246/248 (99%)	223 (91%)	19 (8%)	4 (2%)	7	34
1	G	241/248 (97%)	222 (92%)	16 (7%)	3 (1%)	10	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	229/248 (92%)	202 (88%)	22 (10%)	5 (2%)	5	26
All	All	1934/1984 (98%)	1758 (91%)	156 (8%)	20 (1%)	12	45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	163	ALA
1	F	107	ALA
1	H	194	SER
1	G	242	LYS
1	C	258	MET
1	H	154	ASP
1	E	242	LYS
1	F	242	LYS
1	H	116	CYS
1	B	169	PHE
1	B	185	ALA
1	F	261	HIS
1	H	197	ALA
1	G	194	SER
1	A	206	ALA
1	C	267	LEU
1	G	206	ALA
1	A	55	PRO
1	H	119	THR
1	F	72	ILE

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	176/176 (100%)	175 (99%)	1 (1%)	78	88
1	B	176/176 (100%)	174 (99%)	2 (1%)	65	83
1	C	176/176 (100%)	176 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	176/176 (100%)	176 (100%)	0	100	100
1	E	169/176 (96%)	168 (99%)	1 (1%)	78	88
1	F	176/176 (100%)	173 (98%)	3 (2%)	53	78
1	G	174/176 (99%)	173 (99%)	1 (1%)	78	88
1	H	168/176 (96%)	166 (99%)	2 (1%)	63	82
All	All	1391/1408 (99%)	1381 (99%)	10 (1%)	76	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	212	LYS
1	A	241	MET
1	B	118	VAL
1	B	232	ARG
1	E	90	THR
1	F	171	LEU
1	F	232	ARG
1	F	244	ASP
1	H	171	LEU
1	H	260	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	143	ASN
1	G	192	ASN
1	G	271	GLN
1	A	144	ASN
1	A	221	ASN
1	A	271	GLN
1	A	275	ASN
1	B	123	HIS
1	B	192	ASN
1	C	192	ASN
1	C	271	GLN
1	C	275	ASN
1	D	176	GLN
1	D	271	GLN
1	E	59	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	291	GLN
1	F	144	ASN
1	H	57	HIS
1	H	59	ASN
1	H	106	GLN
1	H	271	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	D	401	-	46,48,48	1.26	7 (15%)	64,73,73	1.57	8 (12%)
2	NAD	G	401	-	46,48,48	1.21	6 (13%)	64,73,73	1.60	10 (15%)
2	NAD	H	401	-	46,48,48	1.17	5 (10%)	64,73,73	1.52	9 (14%)
2	NAD	A	401	-	46,48,48	1.16	6 (13%)	64,73,73	1.52	9 (14%)
2	NAD	B	401	-	46,48,48	1.27	8 (17%)	64,73,73	1.59	9 (14%)
2	NAD	E	401	-	46,48,48	1.17	6 (13%)	64,73,73	1.67	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	401	-	46,48,48	1.19	6 (13%)	64,73,73	1.55	11 (17%)
2	NAD	F	401	-	46,48,48	1.20	5 (10%)	64,73,73	1.50	8 (12%)

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	D	401	-	-	11/30/62/62	0/5/5/5
2	NAD	G	401	-	-	10/30/62/62	0/5/5/5
2	NAD	H	401	-	-	10/30/62/62	0/5/5/5
2	NAD	A	401	-	-	5/30/62/62	0/5/5/5
2	NAD	B	401	-	-	11/30/62/62	0/5/5/5
2	NAD	E	401	-	-	8/30/62/62	0/5/5/5
2	NAD	C	401	-	-	9/30/62/62	0/5/5/5
2	NAD	F	401	-	-	3/30/62/62	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	NAD	C5A-C4A	4.32	1.46	1.39
2	D	401	NAD	C5A-C4A	4.32	1.46	1.39
2	F	401	NAD	C5A-C4A	4.30	1.46	1.39
2	G	401	NAD	C5A-C4A	4.22	1.46	1.39
2	E	401	NAD	C5A-C4A	4.08	1.46	1.39
2	B	401	NAD	C5A-C4A	4.07	1.46	1.39
2	A	401	NAD	C5A-C4A	4.05	1.46	1.39
2	C	401	NAD	C5A-C4A	3.98	1.46	1.39
2	G	401	NAD	C5A-N7A	-2.72	1.34	1.39
2	D	401	NAD	C5A-C6A	2.70	1.48	1.41
2	C	401	NAD	C5A-N7A	-2.70	1.34	1.39
2	A	401	NAD	C5A-C6A	2.62	1.48	1.41
2	D	401	NAD	C5A-N7A	-2.57	1.34	1.39
2	E	401	NAD	C5A-N7A	-2.57	1.34	1.39
2	C	401	NAD	C4A-N9A	-2.56	1.32	1.37
2	F	401	NAD	C5A-C6A	2.55	1.48	1.41
2	B	401	NAD	C5A-C6A	2.55	1.48	1.41
2	B	401	NAD	C5A-N7A	-2.51	1.34	1.39
2	A	401	NAD	C5A-N7A	-2.48	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C4A-N9A	-2.48	1.32	1.37
2	F	401	NAD	C5A-N7A	-2.48	1.34	1.39
2	H	401	NAD	C5A-C6A	2.45	1.47	1.41
2	G	401	NAD	C5A-C6A	2.44	1.47	1.41
2	C	401	NAD	C5A-C6A	2.43	1.47	1.41
2	H	401	NAD	C5A-N7A	-2.37	1.34	1.39
2	D	401	NAD	PA-O3	2.36	1.62	1.59
2	B	401	NAD	PN-O3	2.35	1.62	1.59
2	B	401	NAD	C4A-N9A	-2.33	1.32	1.37
2	F	401	NAD	C8A-N7A	2.31	1.36	1.31
2	B	401	NAD	C8A-N9A	-2.28	1.33	1.37
2	B	401	NAD	C8A-N7A	2.27	1.36	1.31
2	E	401	NAD	C5A-C6A	2.26	1.47	1.41
2	B	401	NAD	PA-O3	2.24	1.61	1.59
2	E	401	NAD	C4A-N9A	-2.22	1.33	1.37
2	D	401	NAD	C4A-N9A	-2.20	1.33	1.37
2	C	401	NAD	C8A-N7A	2.20	1.35	1.31
2	D	401	NAD	C8A-N7A	2.16	1.35	1.31
2	E	401	NAD	PA-O3	2.15	1.61	1.59
2	F	401	NAD	C4A-N9A	-2.15	1.33	1.37
2	G	401	NAD	C4A-N9A	-2.14	1.33	1.37
2	D	401	NAD	PN-O3	2.14	1.61	1.59
2	H	401	NAD	C8A-N7A	2.12	1.35	1.31
2	G	401	NAD	C8A-N7A	2.11	1.35	1.31
2	C	401	NAD	C8A-N9A	-2.11	1.34	1.37
2	E	401	NAD	C8A-N7A	2.09	1.35	1.31
2	A	401	NAD	C8A-N9A	-2.08	1.34	1.37
2	H	401	NAD	C4A-N9A	-2.05	1.33	1.37
2	A	401	NAD	C8A-N7A	2.03	1.35	1.31
2	G	401	NAD	PN-O3	2.03	1.61	1.59

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	C5A-C4A-N3A	-6.04	118.40	126.72
2	G	401	NAD	C5A-C4A-N3A	-5.87	118.64	126.72
2	F	401	NAD	C5A-C4A-N3A	-5.76	118.78	126.72
2	B	401	NAD	C5A-C4A-N3A	-5.74	118.81	126.72
2	A	401	NAD	C5A-C4A-N3A	-5.69	118.88	126.72
2	E	401	NAD	C5A-C4A-N3A	-5.57	119.05	126.72
2	C	401	NAD	C5A-C4A-N3A	-5.49	119.16	126.72
2	H	401	NAD	C5A-C4A-N3A	-5.39	119.30	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	NAD	N3A-C4A-N9A	4.59	134.97	127.17
2	H	401	NAD	N3A-C4A-N9A	4.54	134.90	127.17
2	G	401	NAD	N3A-C4A-N9A	4.45	134.74	127.17
2	B	401	NAD	N3A-C4A-N9A	4.39	134.63	127.17
2	D	401	NAD	N3A-C4A-N9A	4.37	134.60	127.17
2	F	401	NAD	N3A-C4A-N9A	4.33	134.54	127.17
2	A	401	NAD	N3A-C4A-N9A	4.29	134.47	127.17
2	E	401	NAD	O4B-C1B-N9A	4.15	116.05	108.09
2	C	401	NAD	N3A-C4A-N9A	3.95	133.88	127.17
2	D	401	NAD	C4A-C5A-N7A	-3.92	106.10	110.58
2	B	401	NAD	C4A-C5A-N7A	-3.92	106.10	110.58
2	A	401	NAD	C4A-C5A-N7A	-3.83	106.20	110.58
2	C	401	NAD	C4A-C5A-N7A	-3.80	106.24	110.58
2	G	401	NAD	C4A-C5A-N7A	-3.78	106.26	110.58
2	B	401	NAD	C2A-N3A-C4A	3.74	120.96	111.83
2	G	401	NAD	C2A-N3A-C4A	3.73	120.93	111.83
2	F	401	NAD	C4A-C5A-N7A	-3.68	106.37	110.58
2	D	401	NAD	C2A-N3A-C4A	3.68	120.82	111.83
2	E	401	NAD	C2A-N3A-C4A	3.66	120.77	111.83
2	F	401	NAD	C2A-N3A-C4A	3.63	120.69	111.83
2	A	401	NAD	C2A-N3A-C4A	3.52	120.42	111.83
2	H	401	NAD	C2A-N3A-C4A	3.47	120.30	111.83
2	C	401	NAD	C2A-N3A-C4A	3.41	120.15	111.83
2	E	401	NAD	N3A-C2A-N1A	-3.40	123.43	128.58
2	H	401	NAD	C4A-N9A-C8A	3.34	109.24	105.74
2	H	401	NAD	C4A-C5A-N7A	-3.30	106.81	110.58
2	B	401	NAD	N3A-C2A-N1A	-3.29	123.60	128.58
2	G	401	NAD	N3A-C2A-N1A	-3.25	123.66	128.58
2	H	401	NAD	N3A-C2A-N1A	-3.19	123.75	128.58
2	E	401	NAD	C4A-C5A-N7A	-3.19	106.94	110.58
2	B	401	NAD	C4A-N9A-C8A	3.16	109.05	105.74
2	E	401	NAD	C4A-N9A-C8A	3.15	109.04	105.74
2	F	401	NAD	N3A-C2A-N1A	-3.04	123.98	128.58
2	A	401	NAD	C4A-N9A-C8A	2.89	108.77	105.74
2	D	401	NAD	N3A-C2A-N1A	-2.83	124.31	128.58
2	B	401	NAD	C5A-N7A-C8A	2.79	107.83	103.45
2	G	401	NAD	C5A-N7A-C8A	2.76	107.79	103.45
2	C	401	NAD	N3A-C2A-N1A	-2.73	124.45	128.58
2	E	401	NAD	C2B-C1B-N9A	-2.65	106.71	113.30
2	A	401	NAD	N3A-C2A-N1A	-2.64	124.58	128.58
2	A	401	NAD	C5A-N7A-C8A	2.64	107.60	103.45
2	G	401	NAD	O4B-C1B-N9A	2.61	113.11	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	NAD	C5A-N7A-C8A	2.59	107.52	103.45
2	D	401	NAD	C5A-N7A-C8A	2.59	107.51	103.45
2	G	401	NAD	C4A-N9A-C8A	2.58	108.44	105.74
2	C	401	NAD	C4A-N9A-C8A	2.56	108.43	105.74
2	F	401	NAD	C4A-N9A-C8A	2.55	108.42	105.74
2	C	401	NAD	C5A-N7A-C8A	2.54	107.44	103.45
2	F	401	NAD	C5A-N7A-C8A	2.52	107.41	103.45
2	E	401	NAD	C5A-N7A-C8A	2.51	107.39	103.45
2	B	401	NAD	C6A-C5A-N7A	2.47	136.85	132.09
2	B	401	NAD	N9A-C8A-N7A	-2.45	110.46	113.94
2	A	401	NAD	C6A-C5A-N7A	2.37	136.66	132.09
2	C	401	NAD	C6N-N1N-C2N	-2.36	119.87	121.88
2	H	401	NAD	N9A-C8A-N7A	-2.33	110.62	113.94
2	E	401	NAD	N9A-C8A-N7A	-2.32	110.65	113.94
2	G	401	NAD	C6A-C5A-N7A	2.29	136.51	132.09
2	C	401	NAD	C5N-C4N-C3N	-2.29	118.11	120.36
2	C	401	NAD	C6A-C5A-N7A	2.28	136.50	132.09
2	F	401	NAD	C6A-C5A-N7A	2.27	136.46	132.09
2	D	401	NAD	C6A-C5A-N7A	2.26	136.44	132.09
2	A	401	NAD	N9A-C8A-N7A	-2.23	110.78	113.94
2	D	401	NAD	C4A-N9A-C8A	2.18	108.02	105.74
2	G	401	NAD	N9A-C8A-N7A	-2.15	110.89	113.94
2	C	401	NAD	N9A-C8A-N7A	-2.11	110.95	113.94
2	H	401	NAD	C6A-C5A-N7A	2.02	135.99	132.09

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	NAD	C5B-O5B-PA-O2A
2	G	401	NAD	C5D-O5D-PN-O2N
2	G	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	C5B-O5B-PA-O3
2	B	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4D-C4D-C5D-O5D
2	C	401	NAD	C5D-O5D-PN-O3
2	C	401	NAD	C5D-O5D-PN-O1N
2	C	401	NAD	C5D-O5D-PN-O2N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	D	401	NAD	C5B-O5B-PA-O1A
2	D	401	NAD	C5B-O5B-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5D-O5D-PN-O2N
2	E	401	NAD	C5D-O5D-PN-O3
2	E	401	NAD	C5D-O5D-PN-O1N
2	F	401	NAD	C5D-O5D-PN-O3
2	F	401	NAD	C5D-O5D-PN-O1N
2	H	401	NAD	C5B-O5B-PA-O2A
2	H	401	NAD	C5B-O5B-PA-O3
2	H	401	NAD	C4B-C5B-O5B-PA
2	G	401	NAD	C3D-C4D-C5D-O5D
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	C3D-C4D-C5D-O5D
2	H	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	O4D-C4D-C5D-O5D
2	H	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C3B-C4B-C5B-O5B
2	H	401	NAD	C2B-C1B-N9A-C8A
2	C	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	PN-O3-PA-O5B
2	H	401	NAD	PN-O3-PA-O5B
2	E	401	NAD	C3B-C4B-C5B-O5B
2	G	401	NAD	PN-O3-PA-O2A
2	G	401	NAD	C5B-O5B-PA-O1A
2	G	401	NAD	C5B-O5B-PA-O3
2	G	401	NAD	C5D-O5D-PN-O3
2	G	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	C5B-O5B-PA-O2A
2	B	401	NAD	C5B-O5B-PA-O1A
2	B	401	NAD	C5B-O5B-PA-O2A
2	B	401	NAD	C5B-O5B-PA-O3
2	B	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O2N
2	E	401	NAD	C5D-O5D-PN-O2N
2	F	401	NAD	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

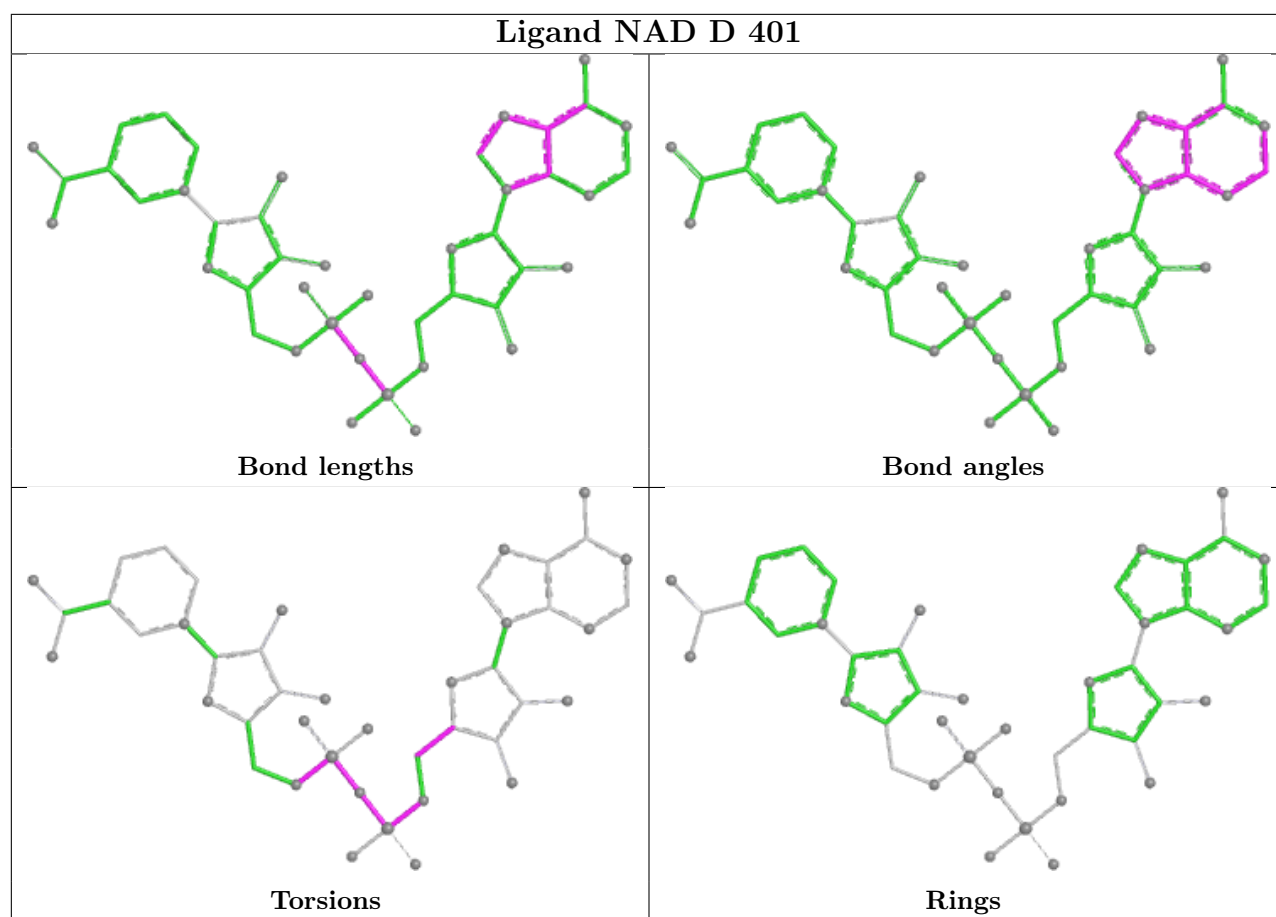
Mol	Chain	Res	Type	Atoms
2	E	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	PN-O3-PA-O1A
2	D	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O2N
2	H	401	NAD	C2B-C1B-N9A-C4A
2	C	401	NAD	C4D-C5D-O5D-PN
2	E	401	NAD	C4B-C5B-O5B-PA
2	H	401	NAD	O4B-C1B-N9A-C8A
2	B	401	NAD	C2B-C1B-N9A-C8A
2	C	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	C2B-C1B-N9A-C8A
2	H	401	NAD	PN-O3-PA-O1A

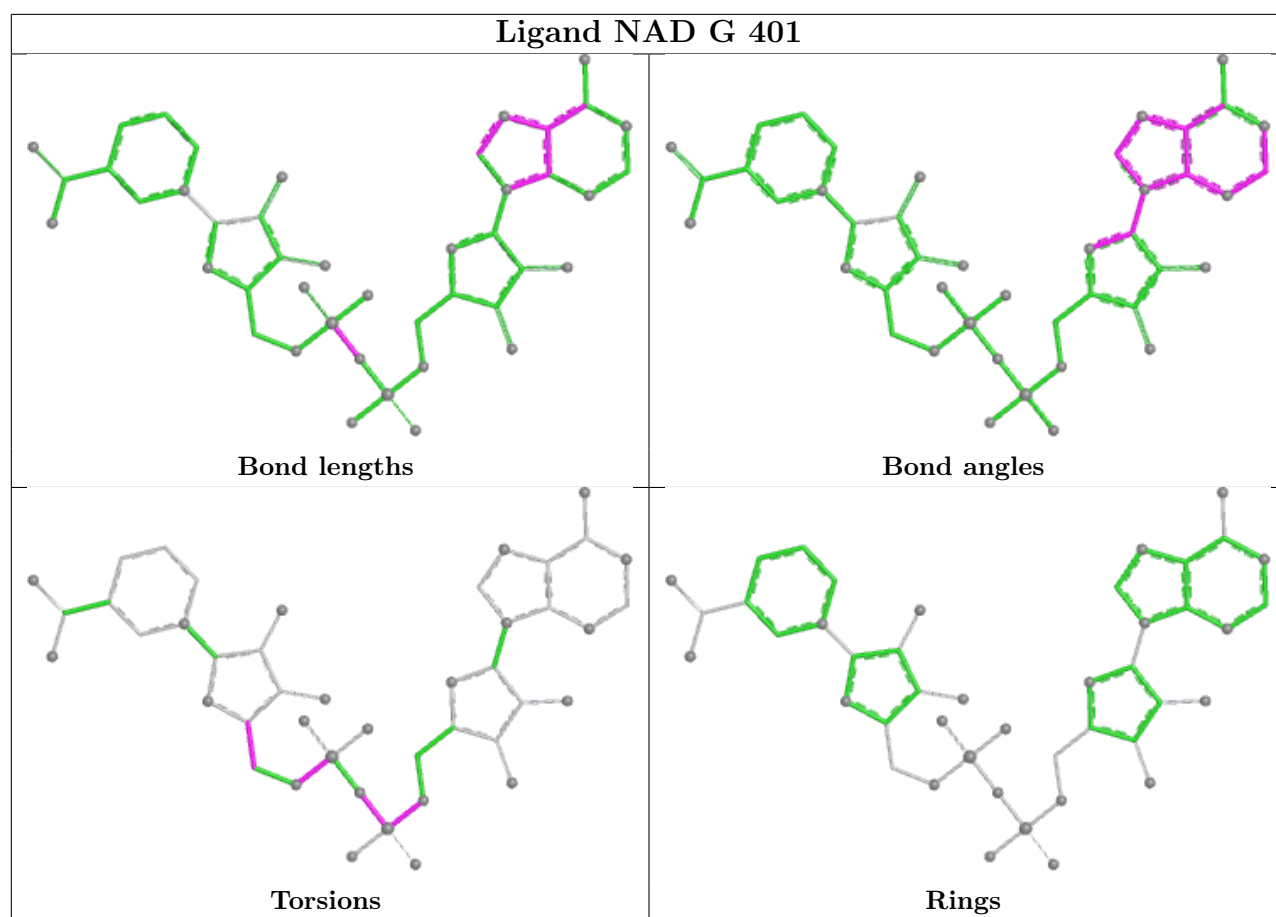
There are no ring outliers.

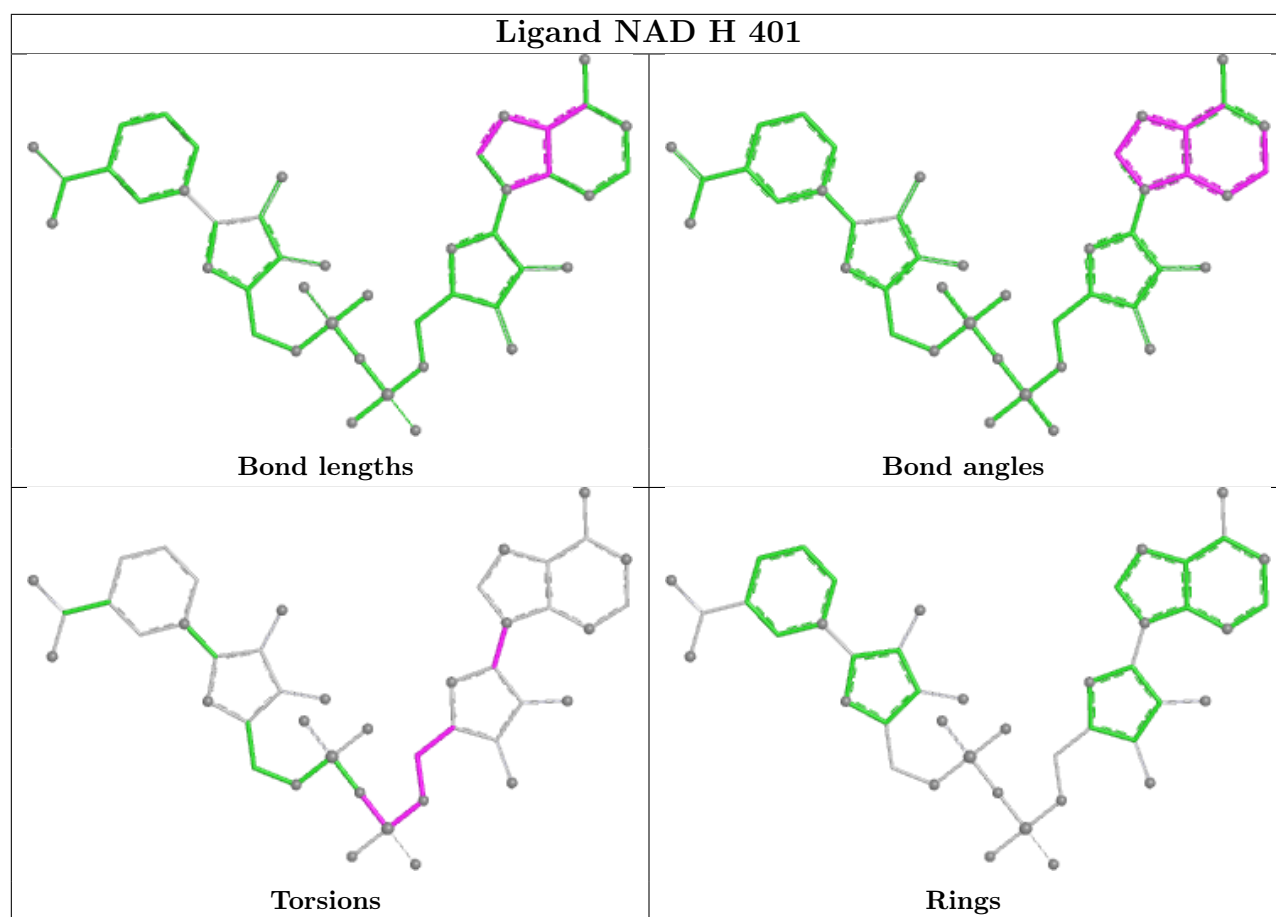
7 monomers are involved in 14 short contacts:

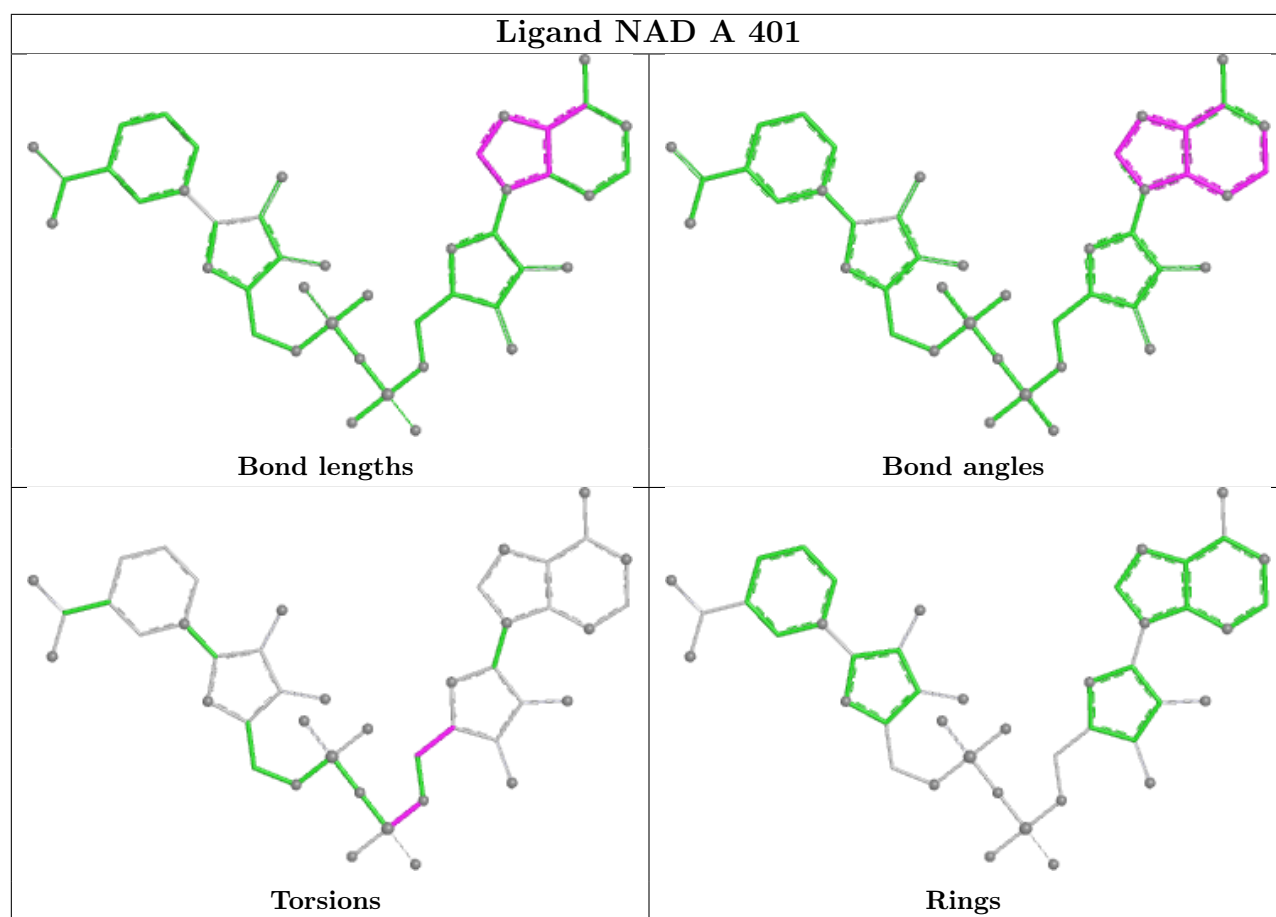
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAD	1	0
2	H	401	NAD	2	0
2	A	401	NAD	1	0
2	B	401	NAD	2	0
2	E	401	NAD	3	0
2	C	401	NAD	3	0
2	F	401	NAD	2	0

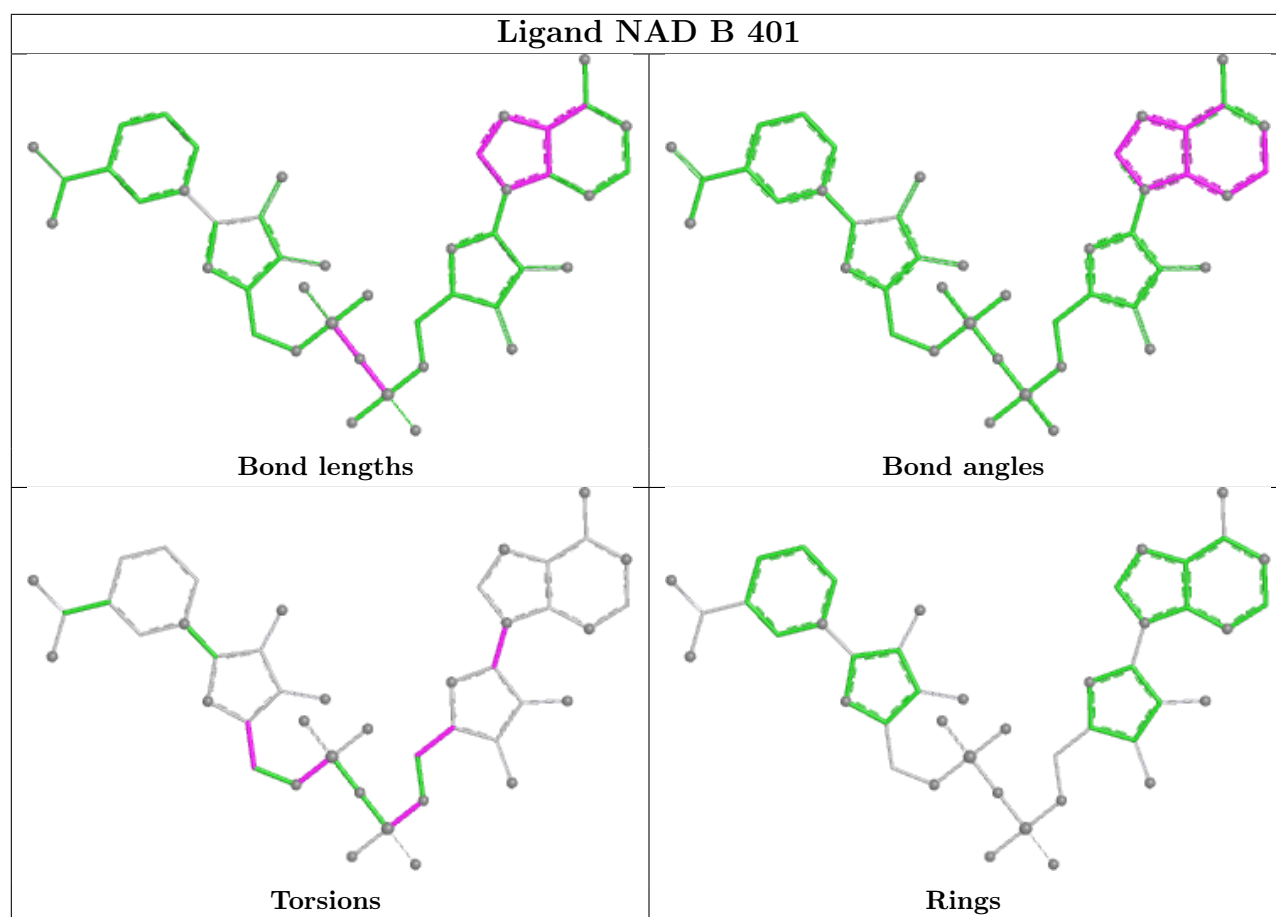
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

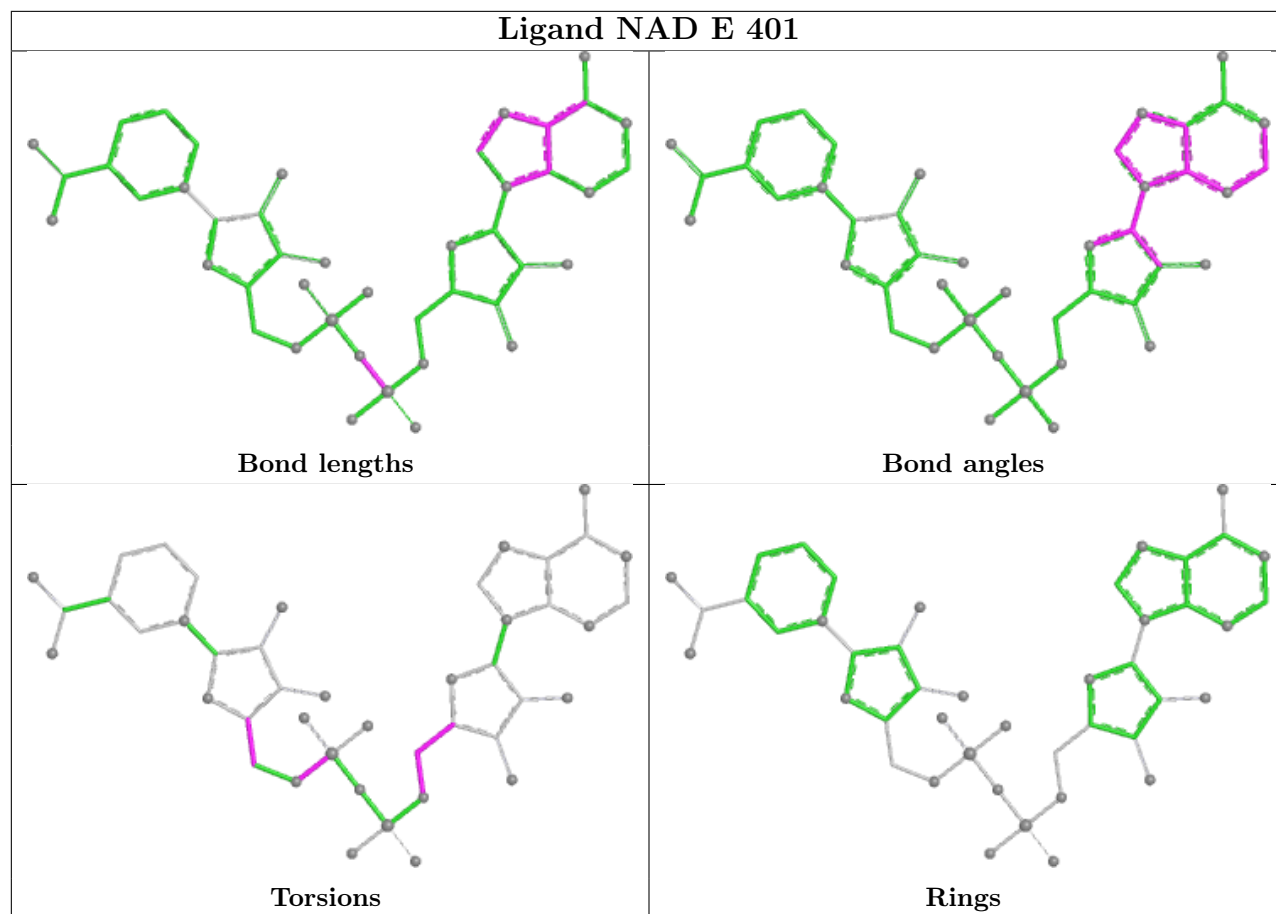


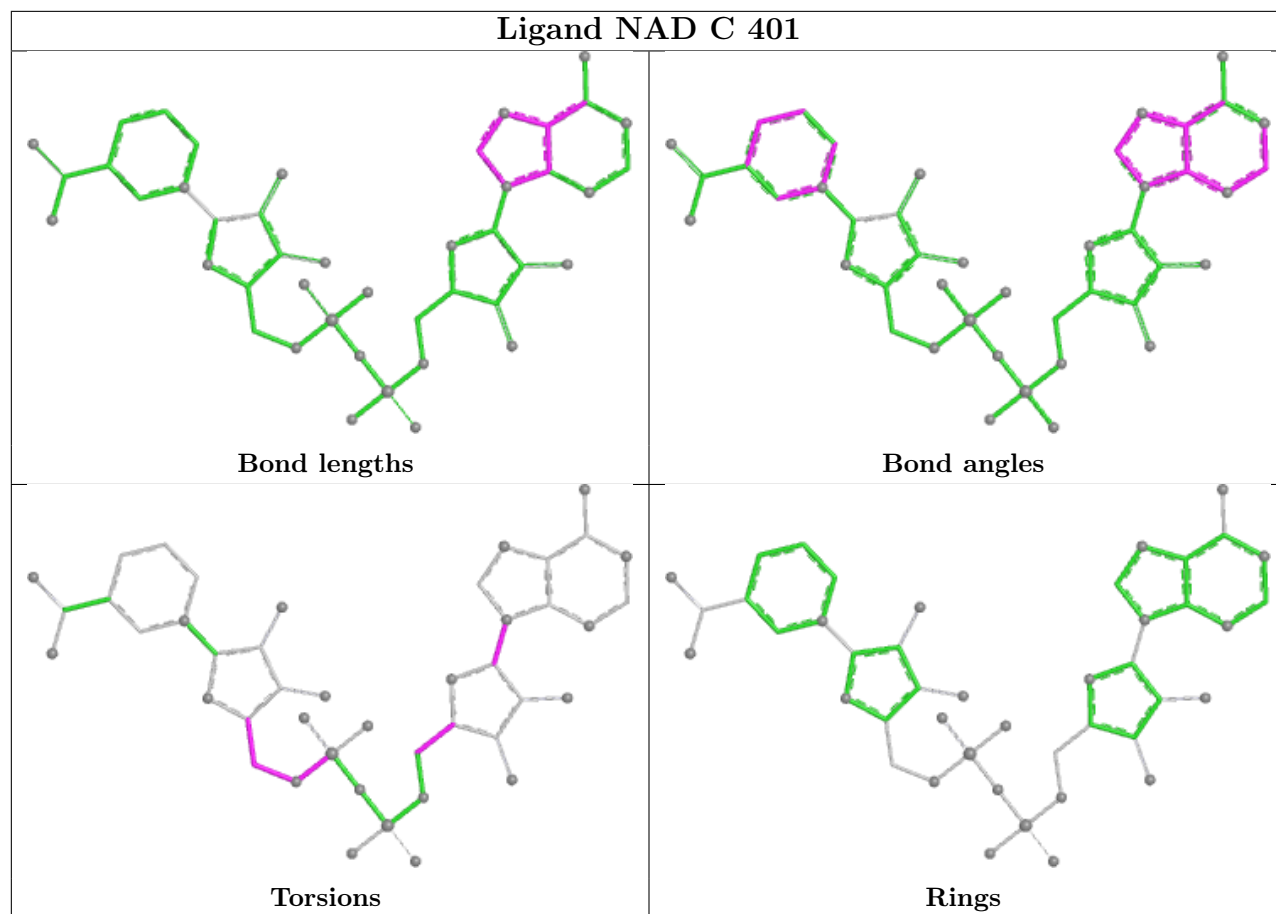


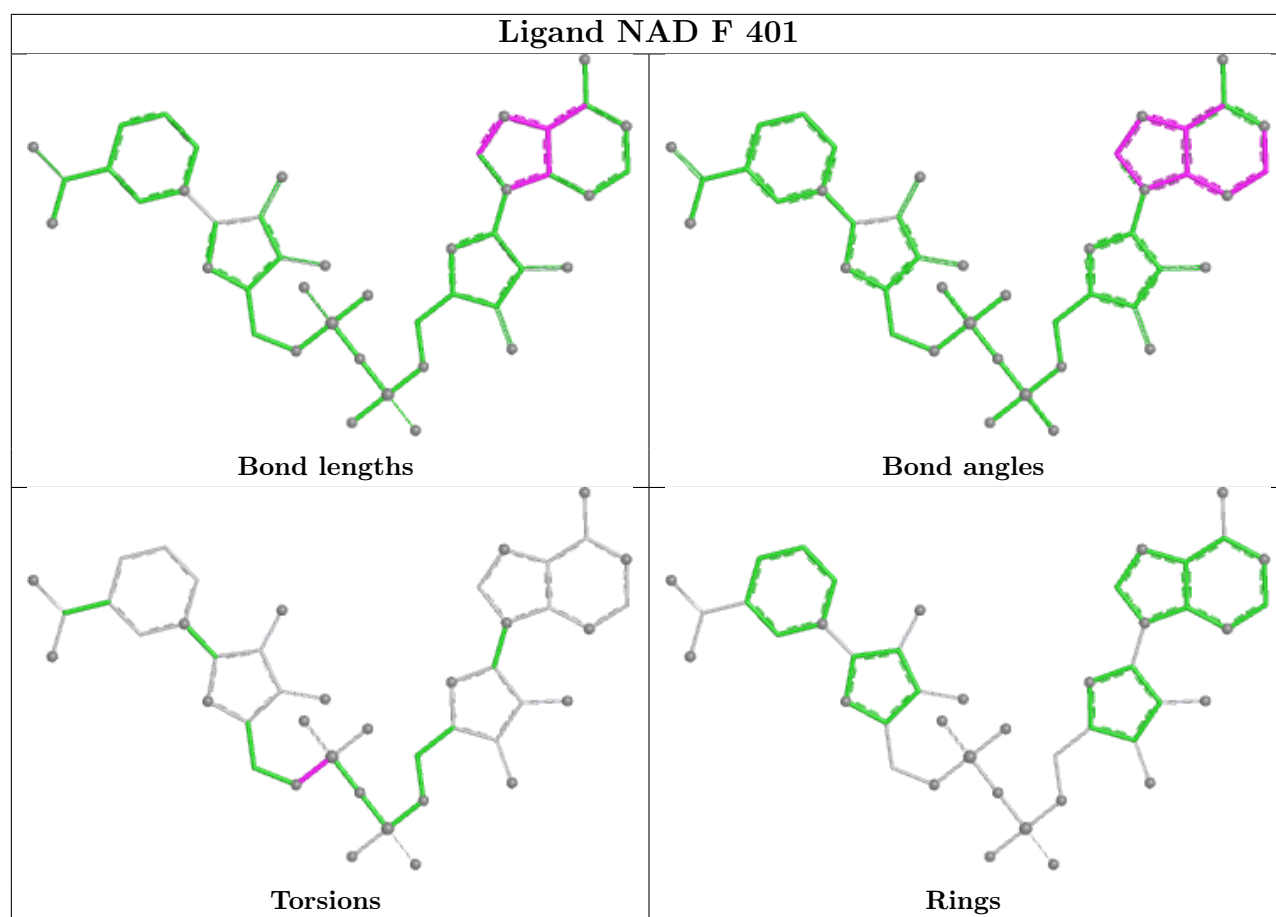












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	248/248 (100%)	-0.16	0 100 100	10, 21, 44, 67	0
1	B	248/248 (100%)	0.48	8 (3%) 50 29	15, 40, 63, 71	0
1	C	248/248 (100%)	0.03	0 100 100	13, 27, 57, 68	0
1	D	248/248 (100%)	-0.06	2 (0%) 82 64	10, 25, 46, 76	0
1	E	240/248 (96%)	0.53	13 (5%) 31 16	11, 40, 72, 94	0
1	F	248/248 (100%)	-0.07	2 (0%) 82 64	12, 27, 51, 74	0
1	G	245/248 (98%)	0.05	0 100 100	12, 27, 56, 80	0
1	H	235/248 (94%)	1.10	32 (13%) 7 4	18, 56, 75, 93	0
All	All	1960/1984 (98%)	0.23	57 (2%) 53 31	10, 30, 66, 94	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	231	ILE	4.7
1	H	111	ALA	4.0
1	H	131	ALA	3.6
1	H	119	THR	3.6
1	E	160	PHE	3.6
1	H	116	CYS	3.5
1	H	78	GLY	3.3
1	H	138	ILE	3.3
1	H	92	LEU	3.2
1	H	112	ILE	3.0
1	H	97	ALA	2.9
1	E	118	VAL	2.9
1	B	112	ILE	2.9
1	H	161	GLU	2.9
1	B	118	VAL	2.9
1	E	116	CYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	245	ALA	2.8
1	E	207	SER	2.7
1	H	67	GLY	2.6
1	B	116	CYS	2.6
1	H	163	ALA	2.6
1	B	96	GLY	2.5
1	B	119	THR	2.5
1	H	106	GLN	2.5
1	B	171	LEU	2.5
1	H	244	ASP	2.4
1	H	179	ALA	2.3
1	E	89	VAL	2.3
1	E	251	THR	2.3
1	E	133	ASP	2.3
1	H	100	VAL	2.3
1	H	188	GLY	2.3
1	E	94	SER	2.3
1	D	59	ASN	2.3
1	H	139	THR	2.3
1	H	56	PHE	2.3
1	B	77	ALA	2.2
1	E	99	ALA	2.2
1	H	81	ALA	2.2
1	H	77	ALA	2.2
1	H	101	ALA	2.2
1	H	107	ALA	2.2
1	H	169	PHE	2.2
1	D	248	THR	2.2
1	H	190	ILE	2.2
1	H	104	ILE	2.1
1	E	122	GLN	2.1
1	E	163	ALA	2.1
1	H	230	GLY	2.1
1	E	241	MET	2.1
1	B	79	THR	2.1
1	H	87	VAL	2.0
1	H	120	ASP	2.0
1	H	122	GLN	2.0
1	E	158	SER	2.0
1	H	103	ALA	2.0
1	F	122	GLN	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](#)

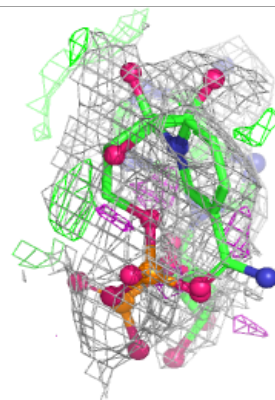
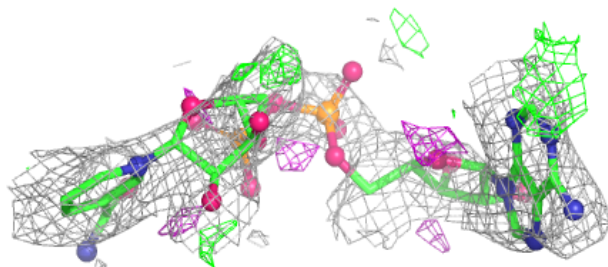
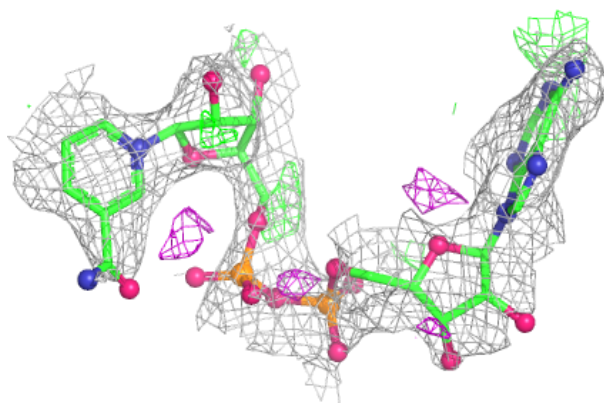
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	H	401	44/44	0.63	0.17	43,62,85,106	0
2	NAD	E	401	44/44	0.81	0.13	33,47,64,79	0
2	NAD	B	401	44/44	0.84	0.13	27,42,56,78	0
2	NAD	G	401	44/44	0.89	0.11	26,33,47,56	0
2	NAD	C	401	44/44	0.91	0.10	27,33,49,51	0
2	NAD	F	401	44/44	0.91	0.11	17,25,33,39	0
2	NAD	D	401	44/44	0.91	0.10	16,24,36,46	0
2	NAD	A	401	44/44	0.92	0.09	14,21,33,38	0

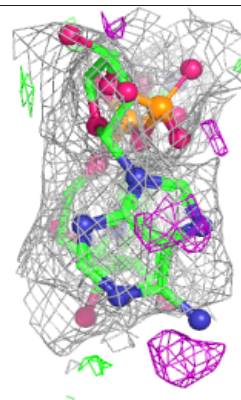
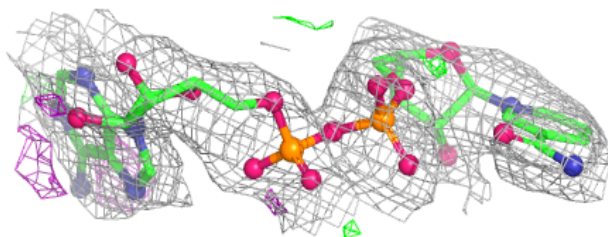
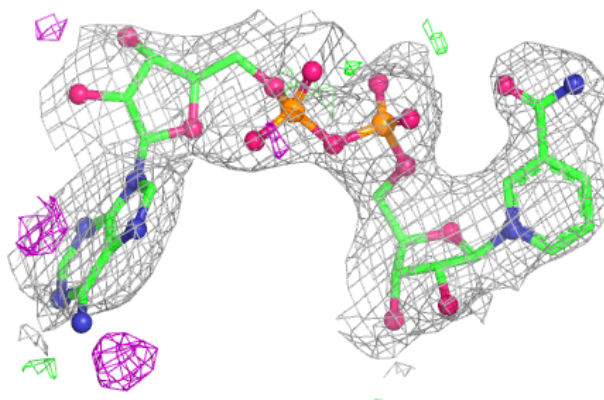
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD H 401:

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

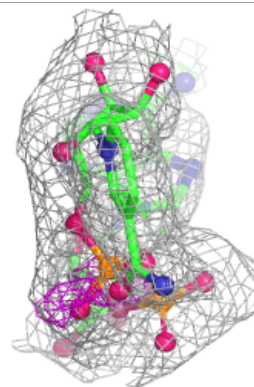
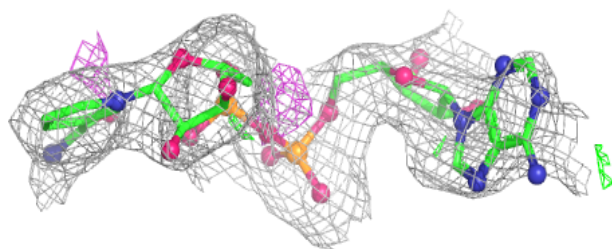
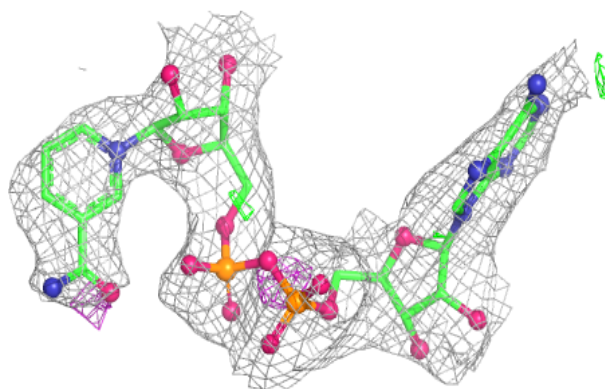
**Electron density around NAD E 401:**

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

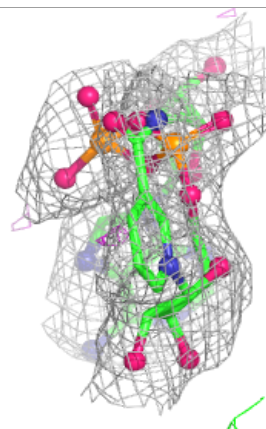
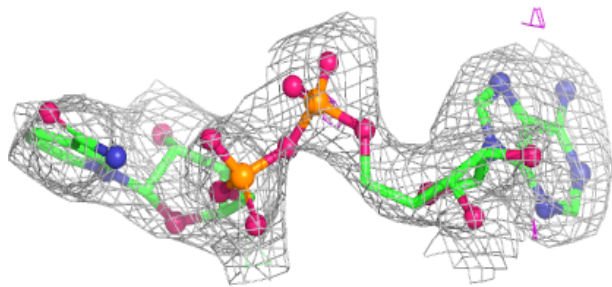
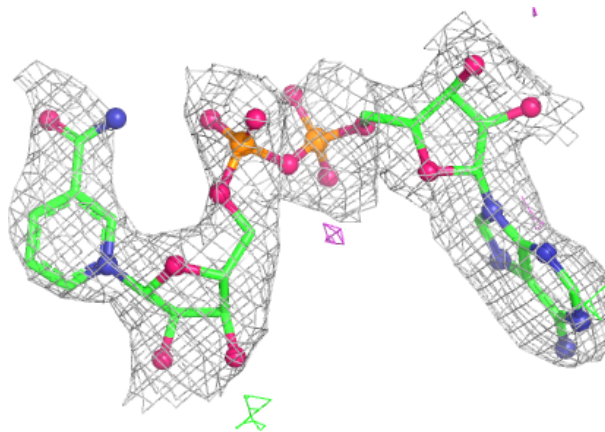


Electron density around NAD B 401:

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

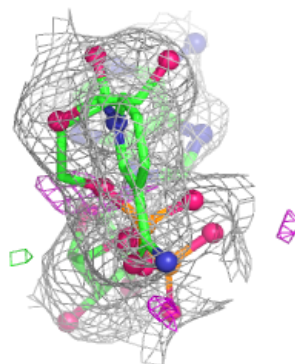
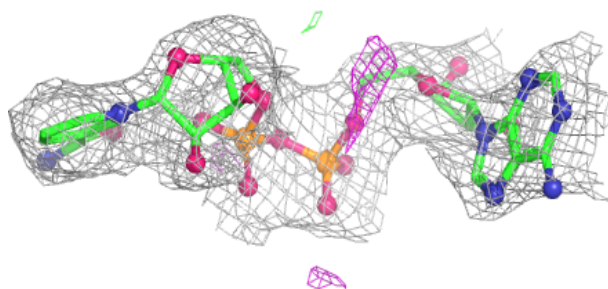
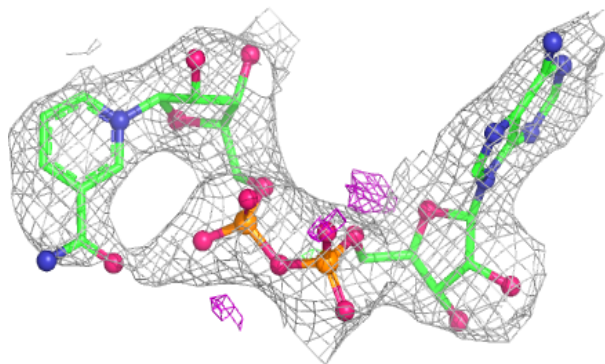
**Electron density around NAD G 401:**

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

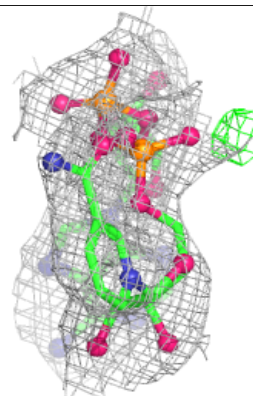
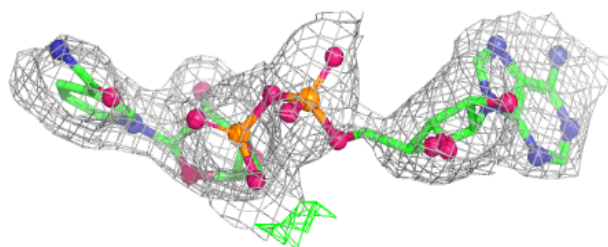
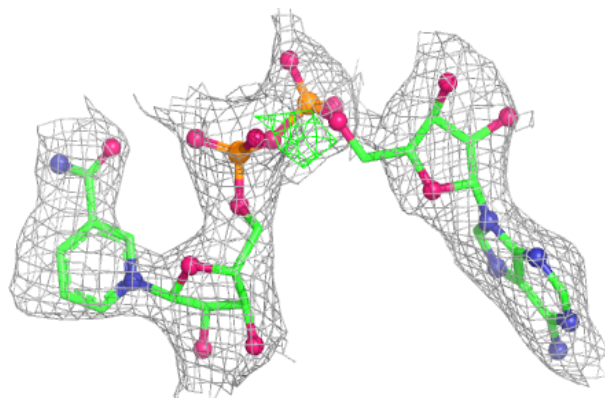


Electron density around NAD C 401:

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

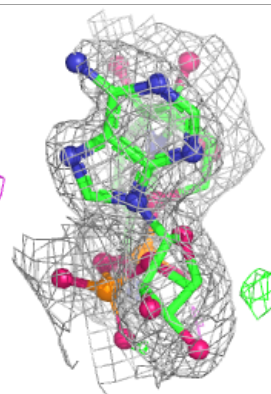
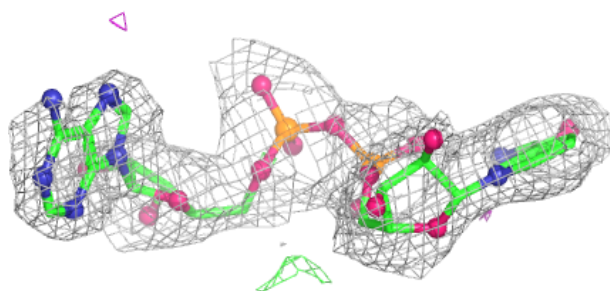
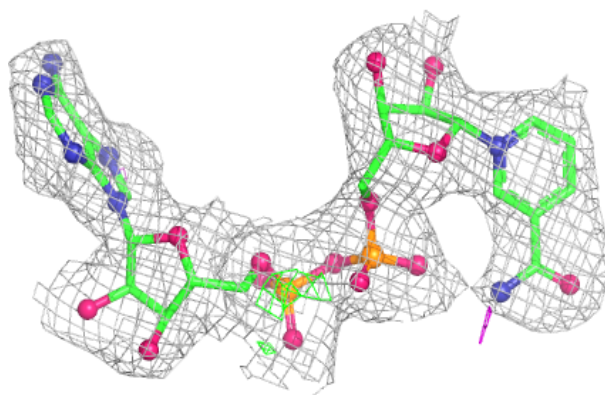
**Electron density around NAD F 401:**

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

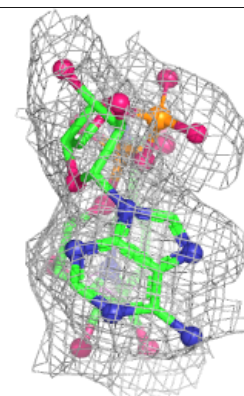
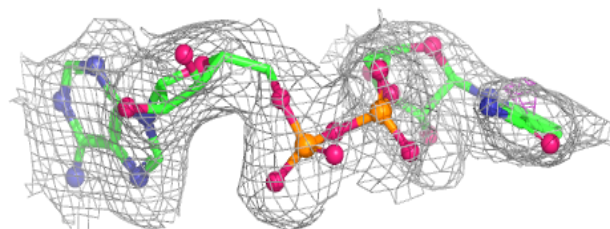
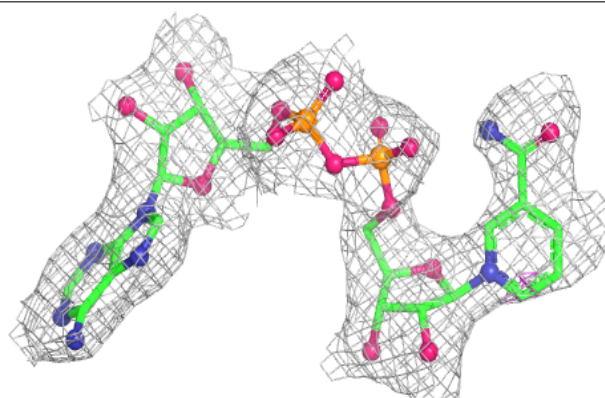


Electron density around NAD D 401:

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

**Electron density around NAD A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.