



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 06:11 PM JST

PDB ID : 8HSA
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

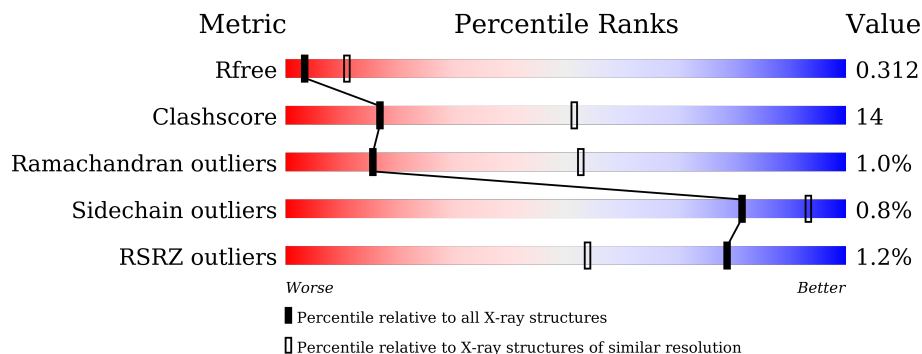
1 Overall quality at a glance

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.



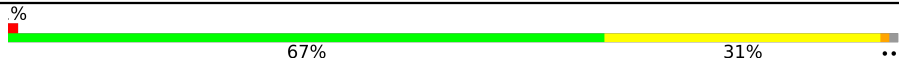

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	73% 27%
1	B	248	1% 72% 27%
1	C	248	71% 29%
1	D	248	1% 75% 25%
1	E	248	2% 67% 30% .
1	F	248	75% 24% .

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Mol	Chain	Length	Quality of chain
1	G	248	 <p>% 67% 31% ..</p>
1	H	248	 <p>5% 57% 35% • 5%</p>

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

There are 16 discrepancies between the modelled and reference sequences:

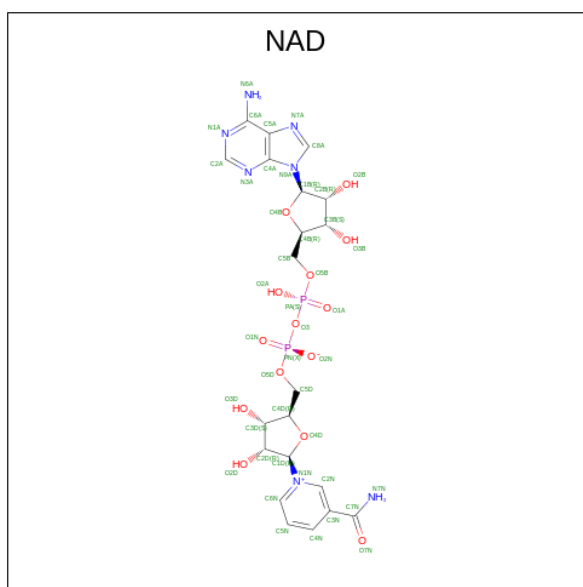
Chain	Residue	Modelled	Actual	Comment	Reference
G	196	ILE	MET	engineered mutation	UNP Q8YIN7
G	241	MET	ILE	conflict	UNP Q8YIN7
A	196	ILE	MET	engineered mutation	UNP Q8YIN7
A	241	MET	ILE	conflict	UNP Q8YIN7
B	196	ILE	MET	engineered mutation	UNP Q8YIN7
B	241	MET	ILE	conflict	UNP Q8YIN7
C	196	ILE	MET	engineered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

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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 (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

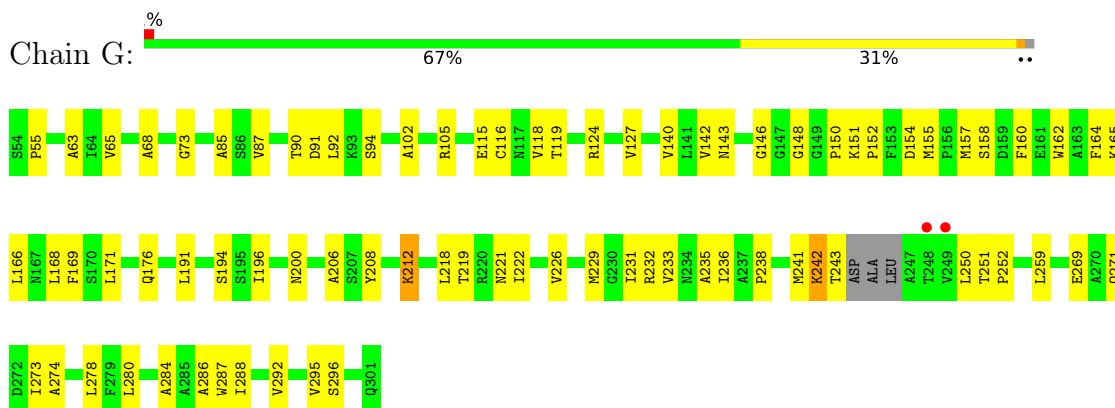


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
		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

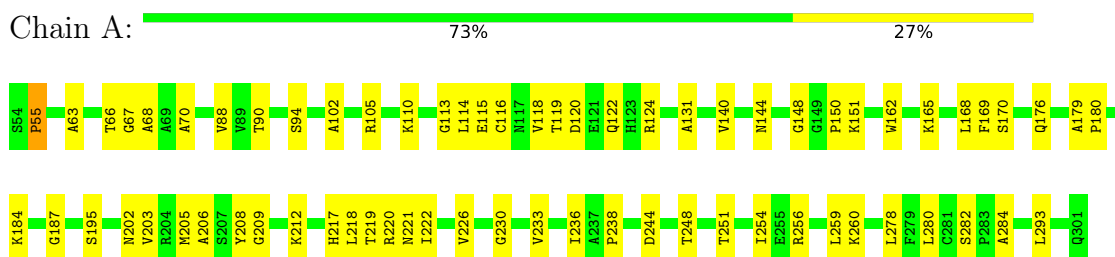
3 Residue-property plots

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.

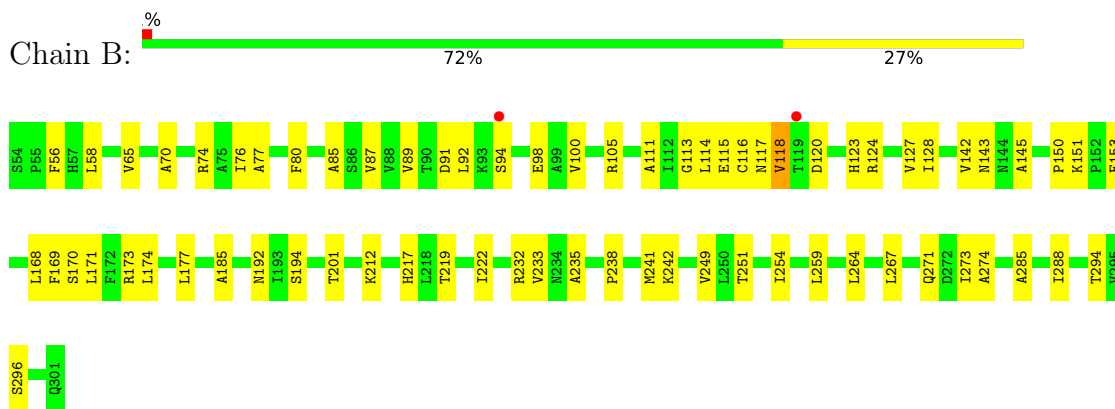
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



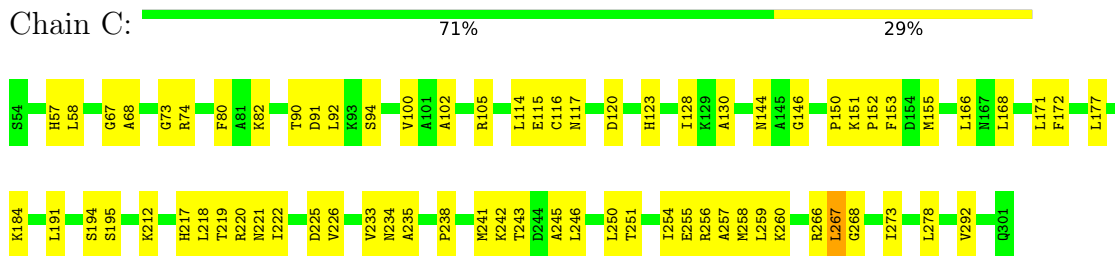
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



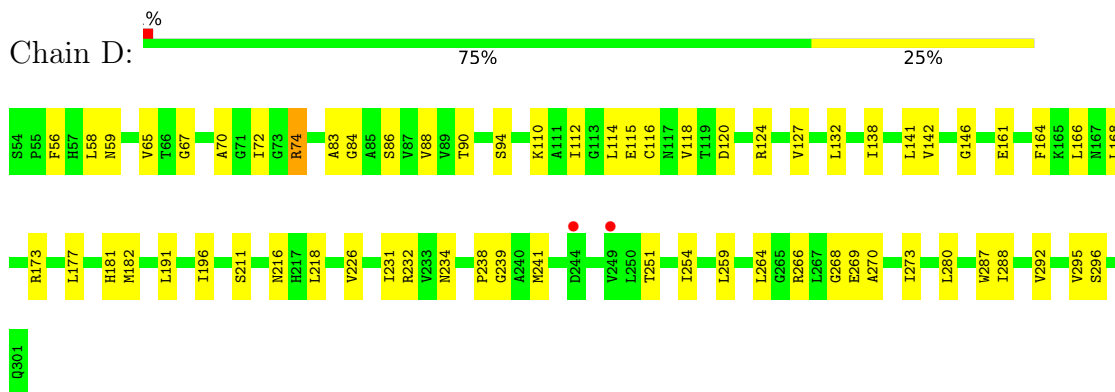
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



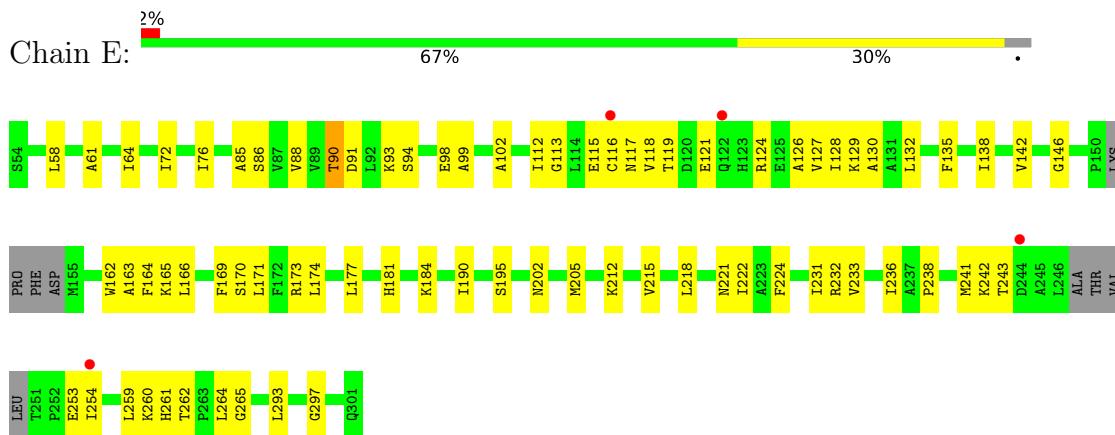
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



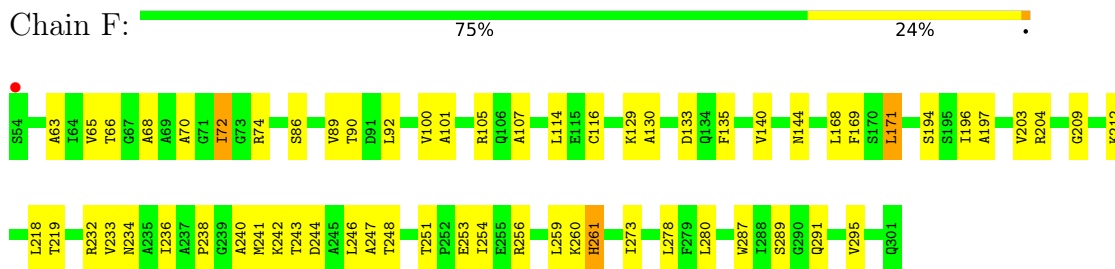
- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase

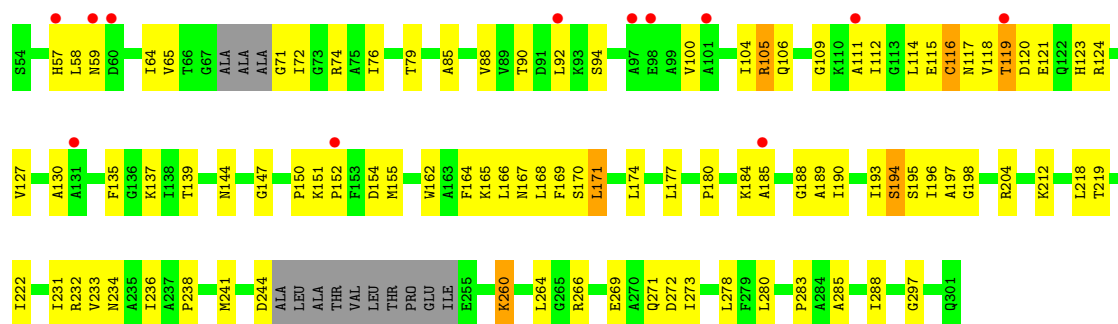


- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase



- Molecule 1: 7-alpha-hydroxysteroid dehydrogenase





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 22.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (23.84-3.00) 86.8 (22.85-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.99Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.225 , 0.315 0.227 , 0.312	Depositor DCC
R_{free} test set	1939 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.50	0/1809	0.70	0/2452
1	B	0.45	0/1809	0.68	0/2452
1	C	0.48	0/1809	0.68	0/2452
1	D	0.47	0/1809	0.69	0/2452
1	E	0.48	0/1743	0.71	0/2358
1	F	0.50	0/1809	0.69	0/2452
1	G	0.52	0/1787	0.69	0/2420
1	H	0.44	0/1720	0.68	0/2324
All	All	0.48	0/14295	0.69	0/19362

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1780	0	1804	42	0
1	B	1780	0	1804	58	0
1	C	1780	0	1804	50	0
1	D	1780	0	1804	42	0
1	E	1718	0	1737	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1780	0	1804	43	0
1	G	1759	0	1783	57	0
1	H	1694	0	1708	79	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	408	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 (408) 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:H:241:MET:HE3	1:H:273:ILE:HD11	1.49	0.93
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: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
1:H:174:LEU:HA	1:H:177:LEU:HD12	1.68	0.75
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: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:F:238:PRO:HB3	1:F:241:MET:HE3	1.75	0.68
1:B:242:LYS:HB2	1:B:267:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:243:THR:C	1:C:245:ALA:H	2.08	0.57
1:G:226:VAL:HA	1:G:229:MET:HE3	1.86	0.56
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:E:127:VAL:HA	1:E:130:ALA:HB3	1.87	0.55
1:C:90:THR:HG23	1:C:116:CYS:HB3	1.88	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:B:238:PRO:HB3	1:B:241:MET:HE2	1.91	0.50
1:D:164:PHE:CE1	1:D:211:SER:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:G:150:PRO:C	1:G:151:LYS:HG2	2.34	0.48
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:151:LYS:HD2	1:H:155:MET:HE3	1.95	0.48
1:H:189:ALA:HB2	1:H:232:ARG:HE	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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
2:E:401:NAD:HO3A	2:E:401:NAD:HO2A	1.53	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: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:157:MET:O	1:G:158:SER:C	2.53	0.46
1:G:143:ASN:ND2	1:G:171:LEU:HB2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:O	1:A:248:THR:HG23	2.16	0.46
1:D:191:LEU:HD12	1:D:234:ASN:O	2.15	0.46
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
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:F:246:LEU:O	1:F:247:ALA:C	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:57:HIS:O	1:C:58:LEU:HD23	2.18	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: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:D:259:LEU:HD21	1:D:266:ARG:C	2.38	0.43
1:H:151:LYS:HD2	1:H:155:MET:CE	2.47	0.43
1:A:113:GLY:C	1:A:114:LEU:HD12	2.38	0.43
1:B:173:ARG:O	1:B:177:LEU:HG	2.18	0.43
1:F:247:ALA:O	1:F:248:THR:C	2.57	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: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:B:238:PRO:CB	1:B:241:MET:HE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:264:LEU:HD23	1:E:264:LEU:HA	1.73	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
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:G:94:SER:HB3	1:G:115:GLU:CB	2.47	0.43
1:H:177:LEU:O	1:H:180:PRO:HD2	2.19	0.43
1:E:238:PRO:HB3	1:E:241:MET:HE3	2.01	0.42
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:H:238:PRO:HB3	1:H:241:MET:HE3	2.01	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:F:194:SER:C	1:F:212:LYS:HE2	2.39	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:B:117:ASN:O	1:B:118:VAL:C	2.58	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:118:VAL:HG12	1:H:174:LEU:HD11	2.02	0.41
1:H:196:ILE:C	1:H:198:GLY:H	2.24	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: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:C:241:MET:HE3	1:C:273:ILE:HD11	2.02	0.41
1:B:170:SER:O	1:B:171:LEU:C	2.59	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:H:241:MET:HE3	1:H:273:ILE:CD1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:191:LEU:HA	1:C:234:ASN:O	2.21	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: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:187:GLY:HA2	1:A:230:GLY:O	2.22	0.40
1:C:241:MET:CE	1:C:273:ILE:HD11	2.51	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/248 (99%)	227 (92%)	17 (7%)	2 (1%)	19	57
1	B	246/248 (99%)	220 (89%)	24 (10%)	2 (1%)	19	57
1	C	246/248 (99%)	225 (92%)	19 (8%)	2 (1%)	19	57
1	D	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
1	E	234/248 (94%)	207 (88%)	25 (11%)	2 (1%)	17	55
1	F	246/248 (99%)	223 (91%)	19 (8%)	4 (2%)	9	40
1	G	241/248 (97%)	222 (92%)	16 (7%)	3 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	229/248 (92%)	202 (88%)	22 (10%)	5 (2%)	6	31
All	All	1934/1984 (98%)	1758 (91%)	156 (8%)	20 (1%)	15	53

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/176 (100%)	176 (100%)	0	100	100
1	B	176/176 (100%)	174 (99%)	2 (1%)	73	90
1	C	176/176 (100%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	176/176 (100%)	175 (99%)	1 (1%)	86	95
1	E	169/176 (96%)	168 (99%)	1 (1%)	86	95
1	F	176/176 (100%)	173 (98%)	3 (2%)	60	85
1	G	174/176 (99%)	173 (99%)	1 (1%)	86	95
1	H	168/176 (96%)	165 (98%)	3 (2%)	59	85
All	All	1391/1408 (99%)	1380 (99%)	11 (1%)	81	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	212	LYS
1	B	118	VAL
1	B	232	ARG
1	D	74	ARG
1	E	90	THR
1	F	171	LEU
1	F	232	ARG
1	F	244	ASP
1	H	105	ARG
1	H	171	LEU
1	H	260	LYS

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

Mol	Chain	Res	Type
1	B	123	HIS
1	E	59	ASN
1	E	291	GLN
1	H	106	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F	401	-	42,48,48	0.88	1 (2%)	50,73,73	1.13	4 (8%)
2	NAD	C	401	-	42,48,48	0.87	0	50,73,73	1.21	5 (10%)
2	NAD	E	401	-	42,48,48	0.84	1 (2%)	50,73,73	1.19	4 (8%)
2	NAD	A	401	-	42,48,48	0.86	1 (2%)	50,73,73	1.13	3 (6%)
2	NAD	D	401	-	42,48,48	0.89	1 (2%)	50,73,73	1.11	4 (8%)
2	NAD	H	401	-	42,48,48	0.85	1 (2%)	50,73,73	1.17	3 (6%)
2	NAD	G	401	-	42,48,48	0.83	1 (2%)	50,73,73	1.13	2 (4%)
2	NAD	B	401	-	42,48,48	0.88	1 (2%)	50,73,73	1.17	3 (6%)

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	F	401	-	-	4/26/62/62	0/5/5/5
2	NAD	C	401	-	-	8/26/62/62	0/5/5/5
2	NAD	E	401	-	-	8/26/62/62	0/5/5/5
2	NAD	A	401	-	-	5/26/62/62	0/5/5/5
2	NAD	D	401	-	-	11/26/62/62	0/5/5/5
2	NAD	H	401	-	-	6/26/62/62	0/5/5/5
2	NAD	G	401	-	-	10/26/62/62	0/5/5/5
2	NAD	B	401	-	-	10/26/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	NAD	C5A-C4A	2.22	1.46	1.40
2	D	401	NAD	C5A-C4A	2.21	1.46	1.40
2	F	401	NAD	C5A-C4A	2.20	1.46	1.40
2	G	401	NAD	C5A-C4A	2.15	1.46	1.40
2	E	401	NAD	C5A-C4A	2.05	1.46	1.40
2	B	401	NAD	C5A-C4A	2.05	1.46	1.40
2	A	401	NAD	C5A-C4A	2.04	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	NAD	PN-O3-PA	-3.45	121.00	132.83
2	A	401	NAD	PN-O3-PA	-3.38	121.22	132.83
2	E	401	NAD	N3A-C2A-N1A	-3.36	123.43	128.68
2	B	401	NAD	N3A-C2A-N1A	-3.25	123.60	128.68
2	E	401	NAD	PN-O3-PA	-3.21	121.79	132.83
2	G	401	NAD	N3A-C2A-N1A	-3.21	123.66	128.68
2	D	401	NAD	C4A-C5A-N7A	-3.16	106.10	109.40
2	B	401	NAD	C4A-C5A-N7A	-3.16	106.10	109.40
2	H	401	NAD	N3A-C2A-N1A	-3.15	123.75	128.68
2	A	401	NAD	C4A-C5A-N7A	-3.07	106.20	109.40
2	C	401	NAD	C4A-C5A-N7A	-3.03	106.24	109.40
2	G	401	NAD	C4A-C5A-N7A	-3.01	106.26	109.40
2	F	401	NAD	N3A-C2A-N1A	-3.00	123.98	128.68
2	F	401	NAD	C4A-C5A-N7A	-2.90	106.37	109.40
2	B	401	NAD	PN-O3-PA	-2.82	123.13	132.83
2	C	401	NAD	PN-O3-PA	-2.82	123.16	132.83
2	D	401	NAD	N3A-C2A-N1A	-2.80	124.31	128.68
2	C	401	NAD	N3A-C2A-N1A	-2.70	124.45	128.68
2	A	401	NAD	N3A-C2A-N1A	-2.62	124.58	128.68
2	H	401	NAD	C4A-C5A-N7A	-2.48	106.81	109.40
2	F	401	NAD	PN-O3-PA	-2.38	124.67	132.83
2	E	401	NAD	C4A-C5A-N7A	-2.36	106.94	109.40
2	C	401	NAD	C6N-N1N-C2N	-2.30	119.87	121.97
2	F	401	NAD	C3B-C2B-C1B	2.27	104.39	100.98
2	D	401	NAD	C3B-C2B-C1B	2.23	104.33	100.98
2	E	401	NAD	O4B-C1B-C2B	-2.21	103.69	106.93
2	D	401	NAD	O4B-C1B-C2B	-2.14	103.80	106.93
2	C	401	NAD	O4B-C1B-C2B	-2.13	103.81	106.93

There are no chirality outliers.

All (62) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	G	401	NAD	C5D-O5D-PN-O1N
2	G	401	NAD	C5D-O5D-PN-O2N
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	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
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	E	401	NAD	C4B-C5B-O5B-PA
2	C	401	NAD	C4D-C5D-O5D-PN
2	C	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	C5D-O5D-PN-O3
2	F	401	NAD	O4B-C4B-C5B-O5B

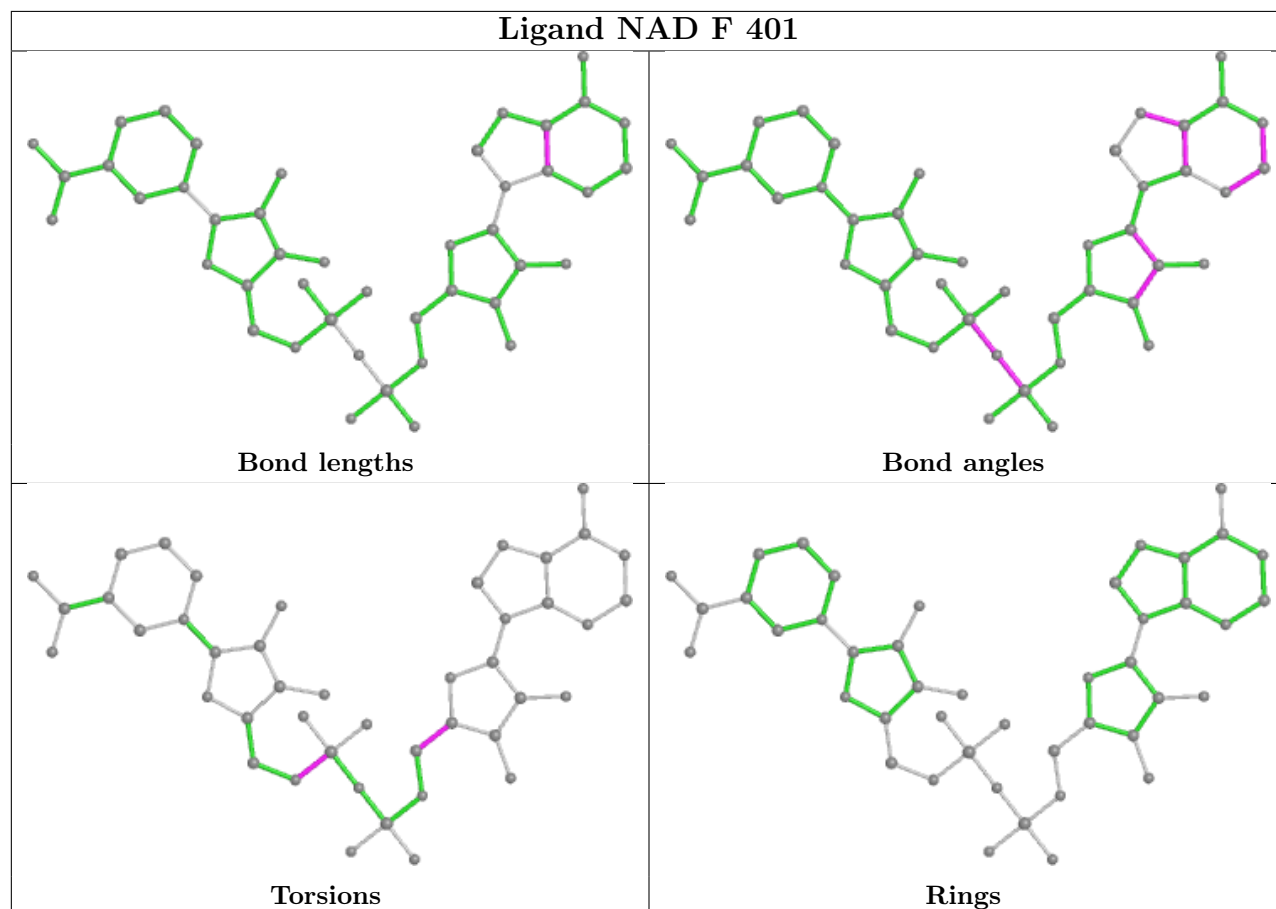
There are no ring outliers.

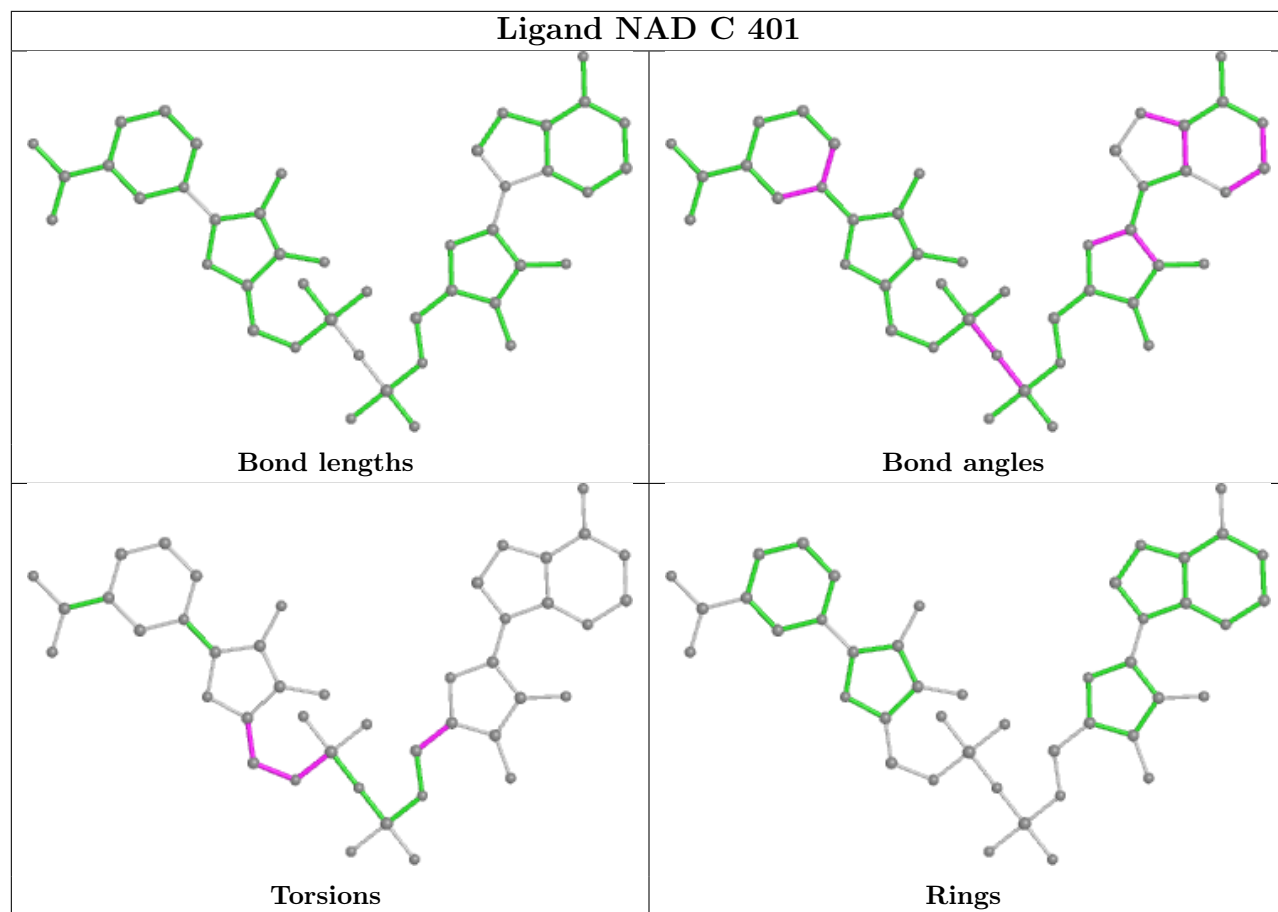
7 monomers are involved in 14 short contacts:

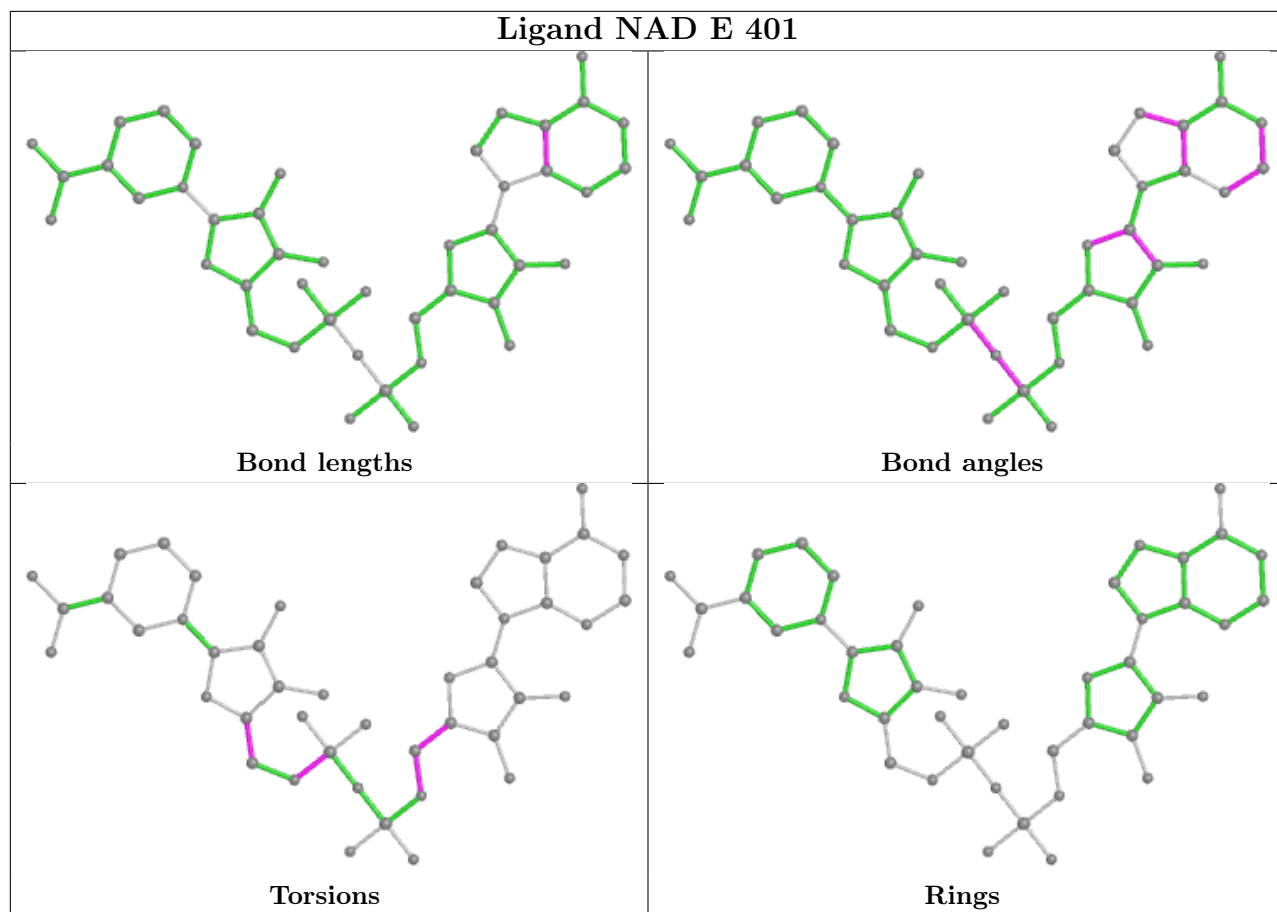
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	NAD	2	0
2	C	401	NAD	3	0
2	E	401	NAD	3	0
2	A	401	NAD	1	0
2	D	401	NAD	1	0
2	H	401	NAD	2	0
2	B	401	NAD	2	0

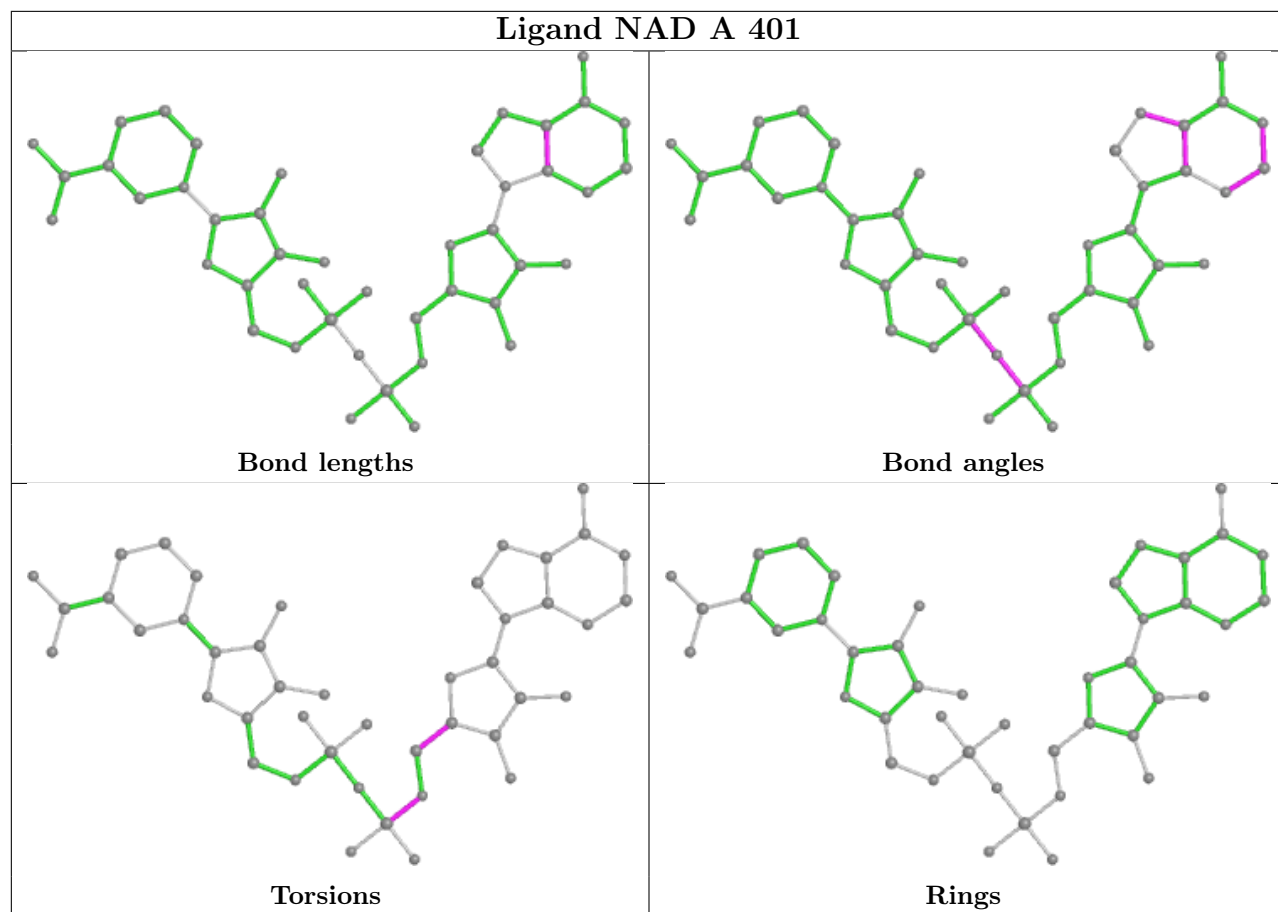
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

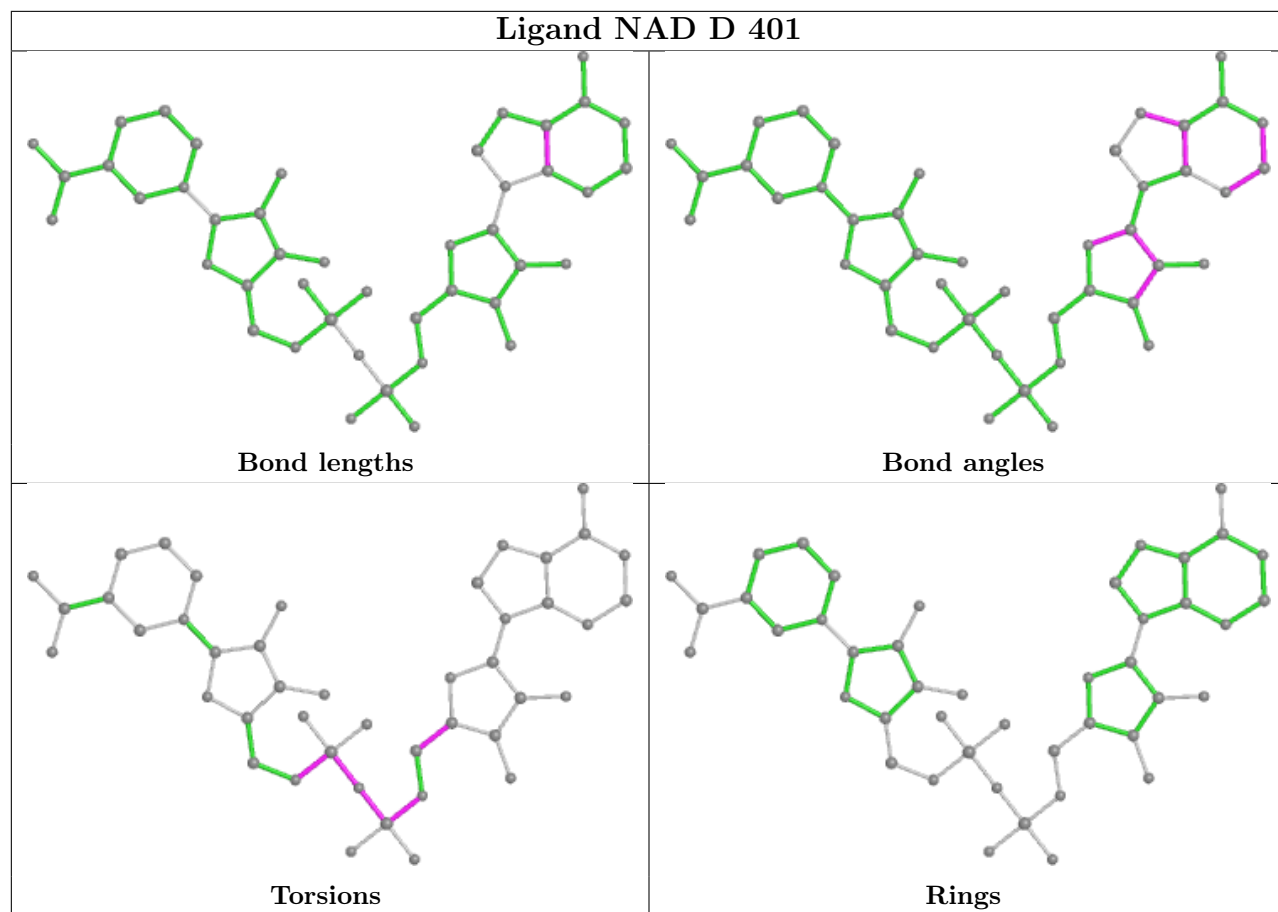
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

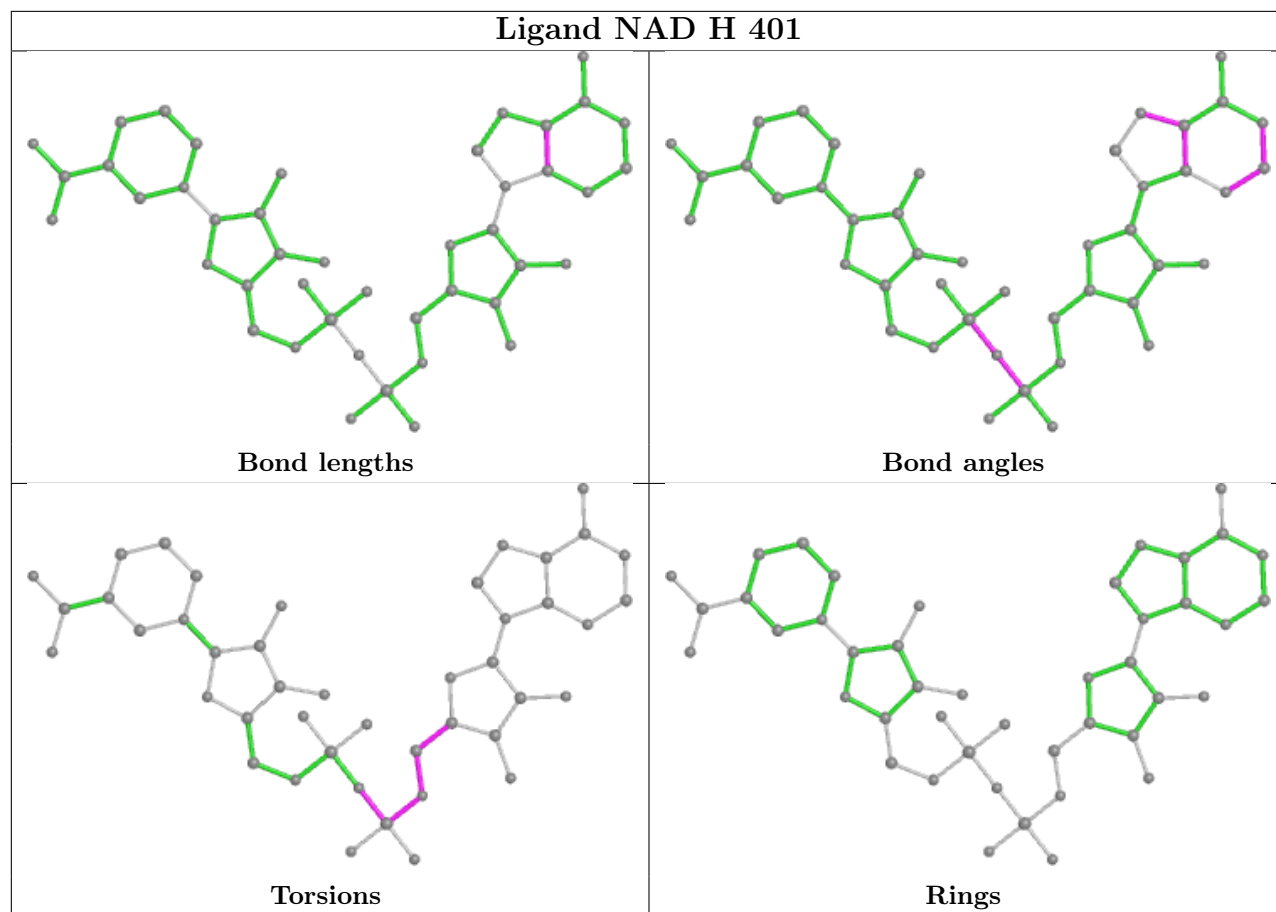


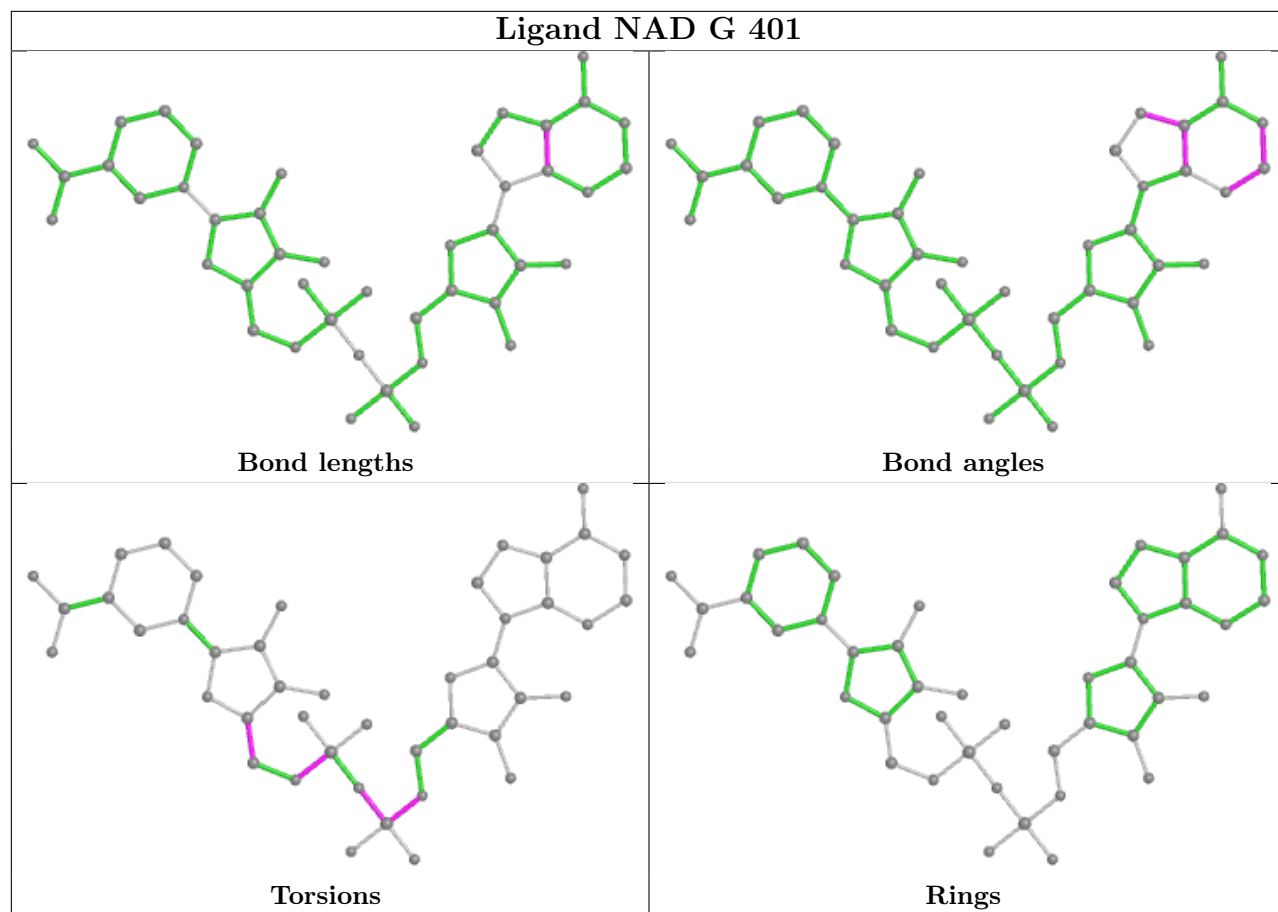


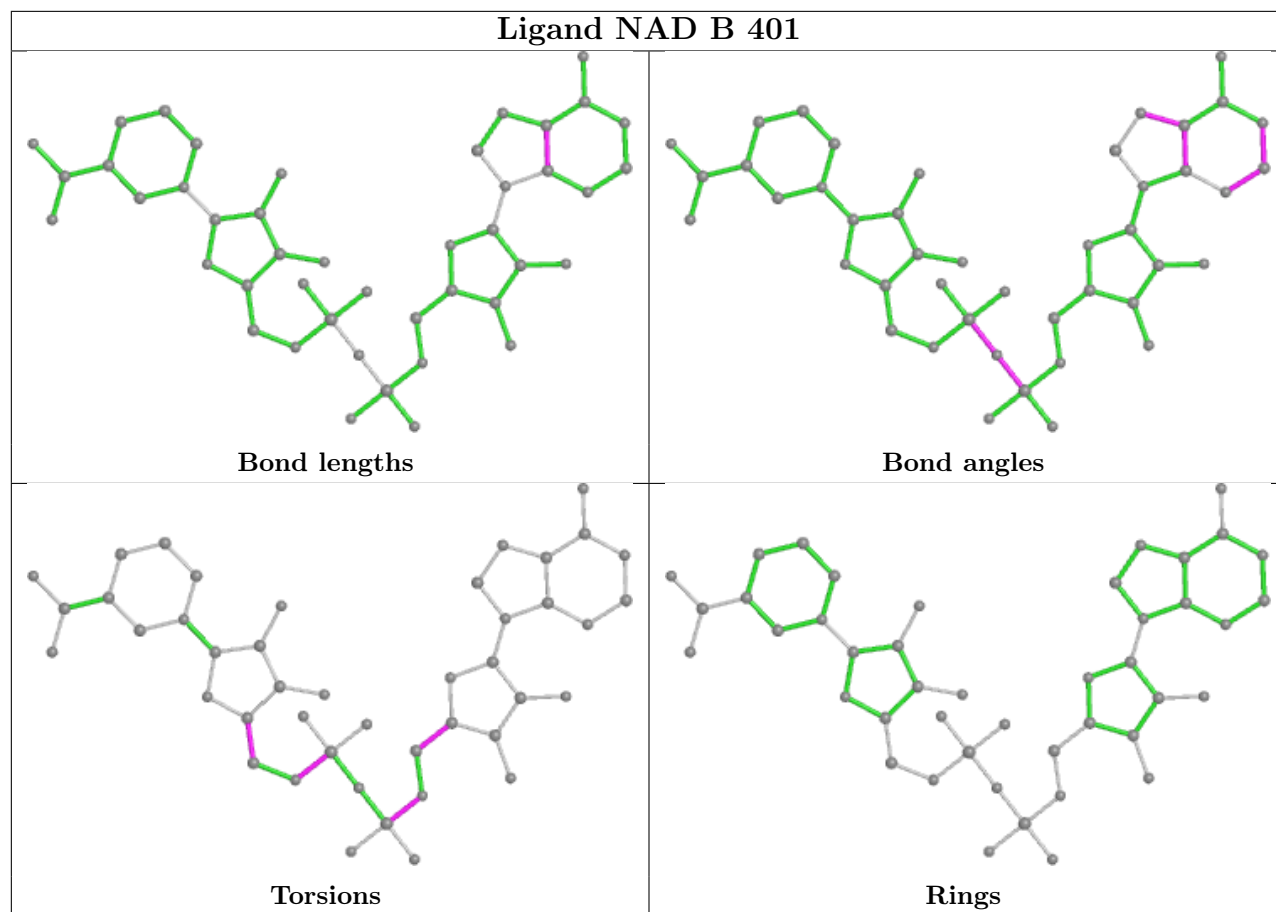












5.7 Other polymers [i](#)

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%)	-0.51	0 100 100	10, 21, 44, 67	0
1	B	248/248 (100%)	-0.07	2 (0%) 86 65	15, 40, 63, 71	0
1	C	248/248 (100%)	-0.34	0 100 100	13, 27, 57, 68	0
1	D	248/248 (100%)	-0.36	2 (0%) 86 65	10, 25, 46, 76	0
1	E	240/248 (96%)	0.06	4 (1%) 70 41	11, 40, 72, 94	0
1	F	248/248 (100%)	-0.37	1 (0%) 92 79	12, 27, 51, 74	0
1	G	245/248 (98%)	-0.29	2 (0%) 86 65	12, 27, 56, 80	0
1	H	235/248 (94%)	0.46	12 (5%) 28 10	18, 56, 75, 93	0
All	All	1960/1984 (98%)	-0.18	23 (1%) 79 54	10, 30, 66, 94	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	ASP	3.5
1	H	59	ASN	3.5
1	E	244	ASP	3.2
1	H	92	LEU	3.0
1	H	131	ALA	2.9
1	E	254	ILE	2.8
1	H	57	HIS	2.8
1	H	111	ALA	2.8
1	E	122	GLN	2.6
1	B	94	SER	2.6
1	G	249	VAL	2.5
1	D	244	ASP	2.5
1	H	97	ALA	2.4
1	E	116	CYS	2.3
1	G	248	THR	2.3
1	H	101	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	54	SER	2.1
1	H	119	THR	2.1
1	H	152	PRO	2.1
1	H	98	GLU	2.1
1	H	185	ALA	2.0
1	D	249	VAL	2.0
1	B	119	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

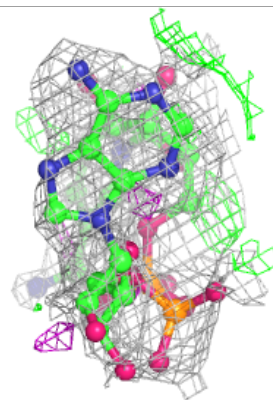
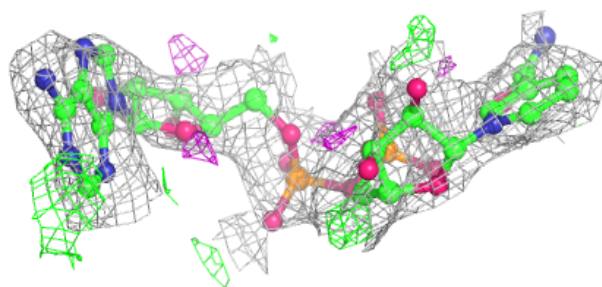
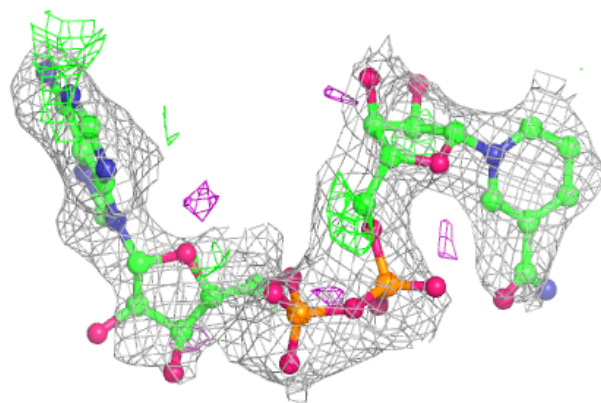
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	H	401	44/44	0.72	0.35	43,62,85,106	0
2	NAD	B	401	44/44	0.84	0.25	27,42,56,78	0
2	NAD	E	401	44/44	0.87	0.21	33,47,64,79	0
2	NAD	G	401	44/44	0.91	0.17	26,33,47,56	0
2	NAD	C	401	44/44	0.91	0.21	27,33,49,51	0
2	NAD	F	401	44/44	0.92	0.18	17,25,33,39	0
2	NAD	D	401	44/44	0.93	0.16	16,24,36,46	0
2	NAD	A	401	44/44	0.94	0.14	14,21,33,38	0

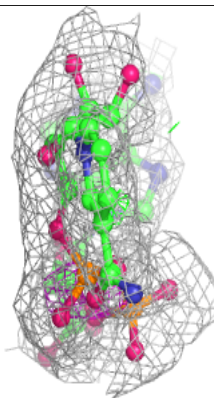
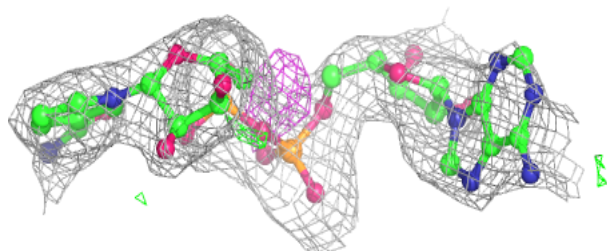
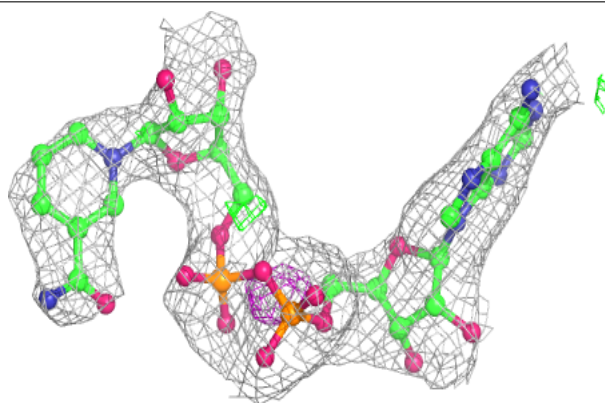
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

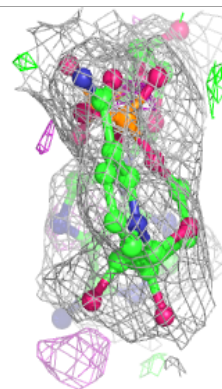
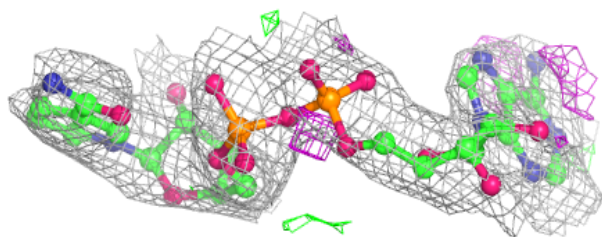
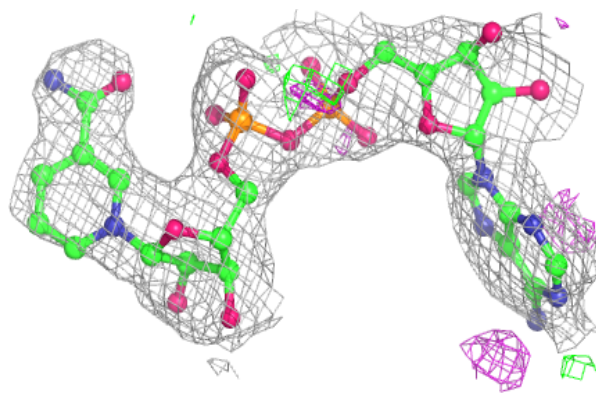
**Electron density around NAD B 401:**

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

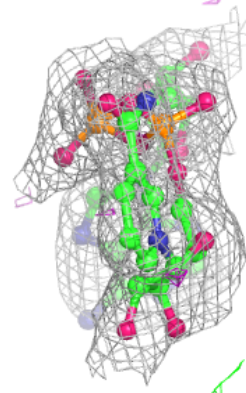
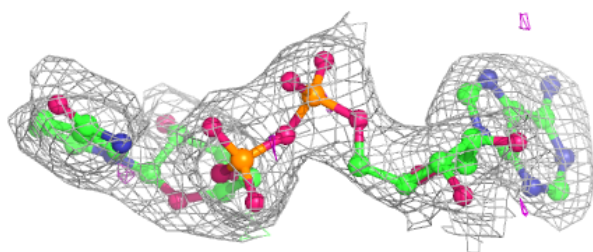
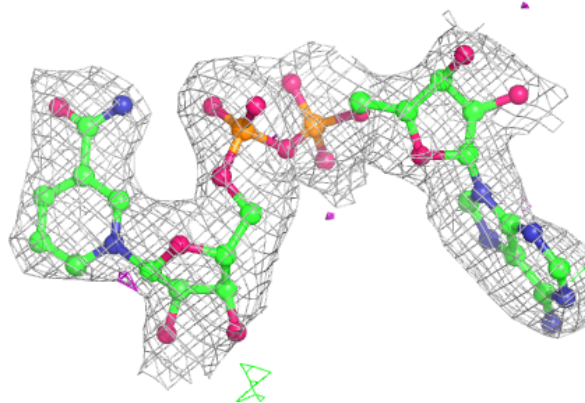


Electron density around NAD E 401:

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

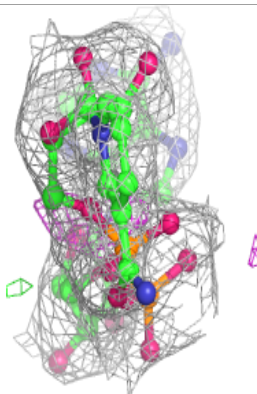
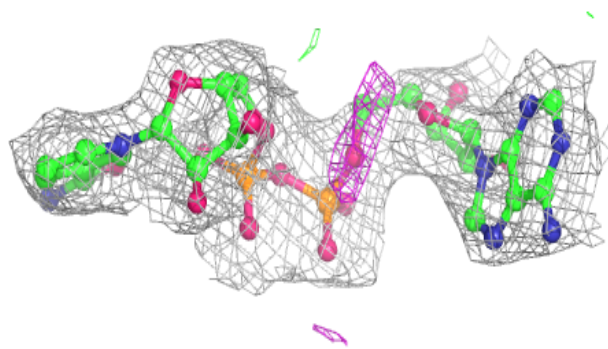
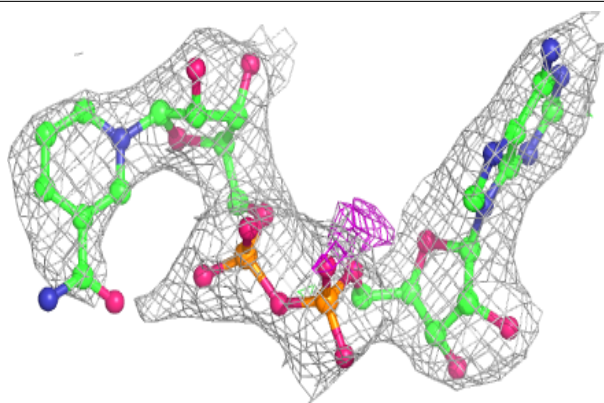
**Electron density around NAD G 401:**

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

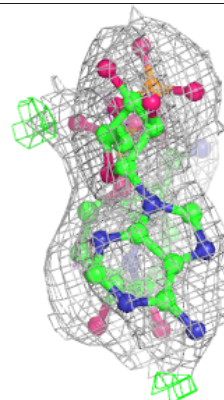
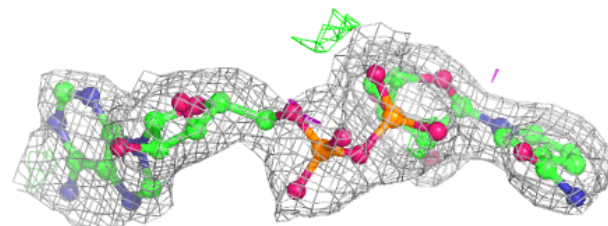
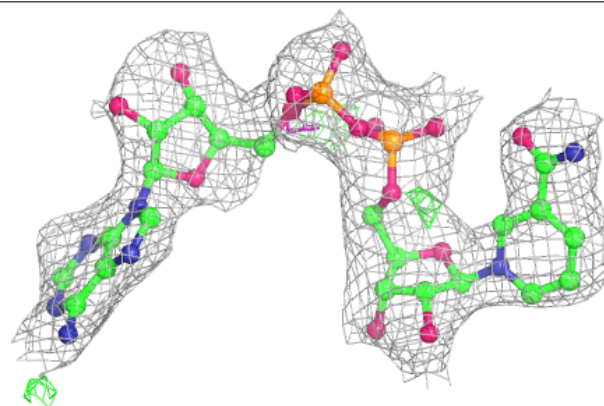


Electron density around NAD C 401:

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

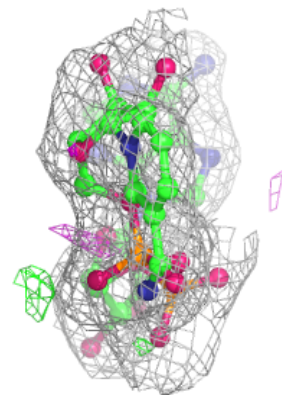
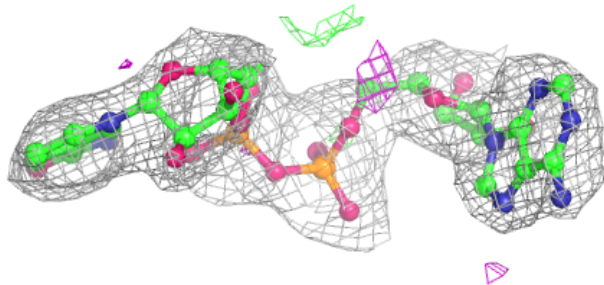
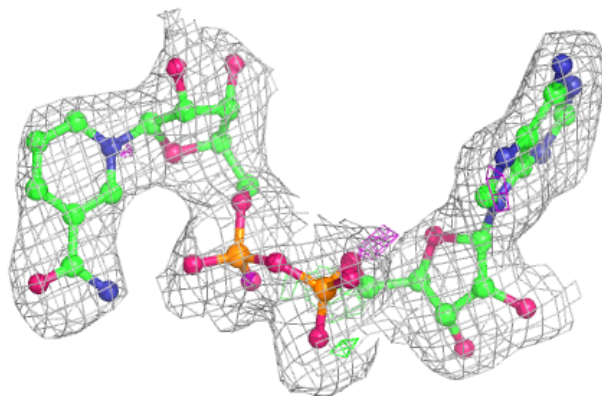
**Electron density around NAD F 401:**

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

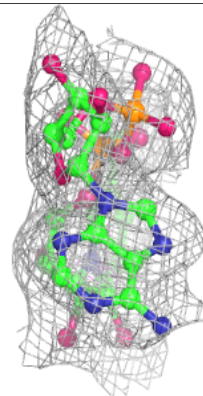
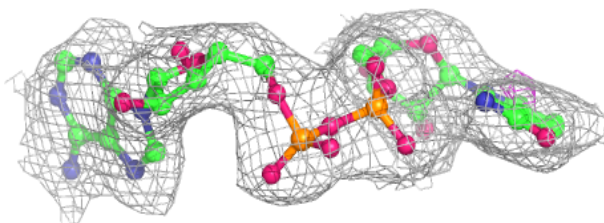
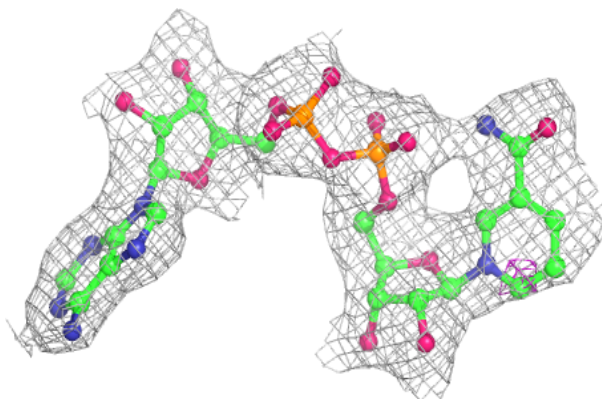


Electron density around NAD D 401:

$2mF_o-DF_c$ (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.