



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:56 AM UTC

PDB ID : 8PUT / pdb\_00008put  
Title : IF5A in complex with Deoxyhypusine synthase  
Authors : Ennifar, E.; D'agostino, M.  
Deposited on : 2023-07-17  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Xtrriage (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

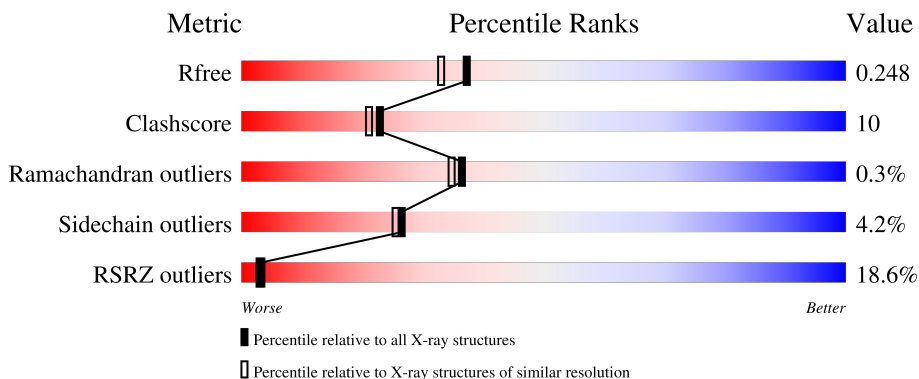
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



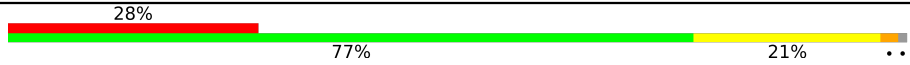

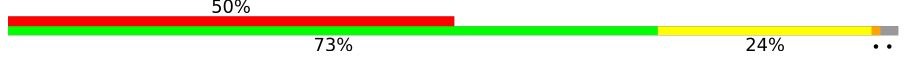
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	312	
1	B	312	
1	C	312	
1	D	312	
2	E	131	

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Mol	Chain	Length	Quality of chain
2	F	131	
2	G	131	
2	H	131	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14257 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 Probable deoxyhypusine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	312	2476	1605	411	455	5	0	0	0
1	B	312	2476	1605	411	455	5	0	0	0
1	C	312	2476	1605	411	455	5	0	0	0
1	D	312	2476	1605	411	455	5	0	0	0

- Molecule 2 is a protein called Translation initiation factor 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	129	1000	637	167	191	5	0	0	0
2	F	130	1006	640	168	193	5	0	0	0
2	G	129	1000	637	167	191	5	0	0	0
2	H	129	1000	637	167	191	5	0	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

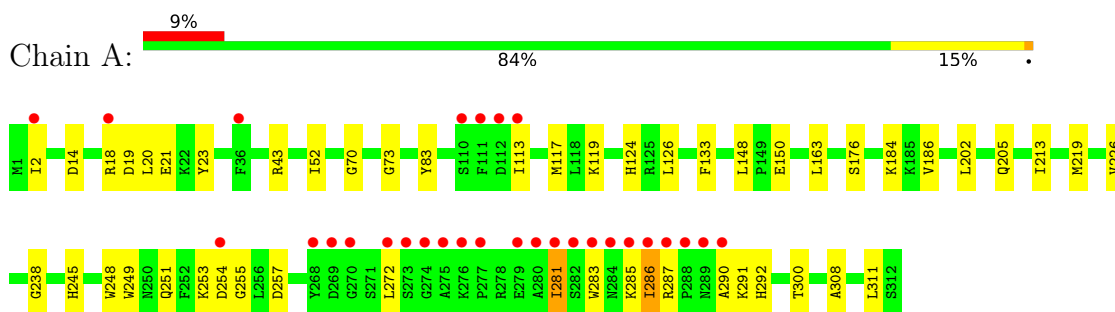
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	82	Total O 82 82	0	0
5	B	48	Total O 48 48	0	0
5	C	5	Total O 5 5	0	0
5	D	9	Total O 9 9	0	0
5	E	1	Total O 1 1	0	0
5	F	5	Total O 5 5	0	0

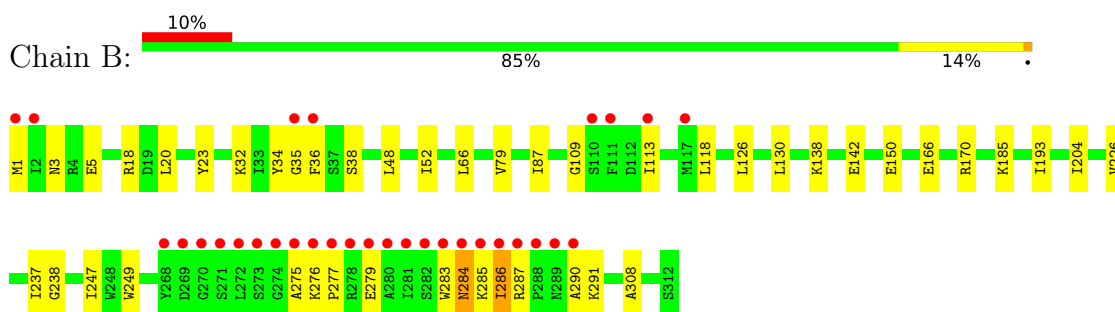
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

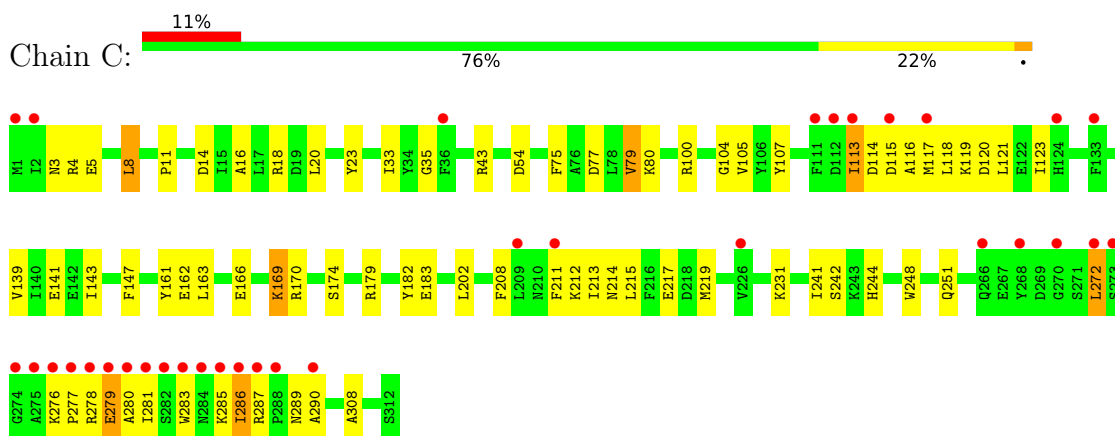
- Molecule 1: Probable deoxyhypusine synthase



- Molecule 1: Probable deoxyhypusine synthase

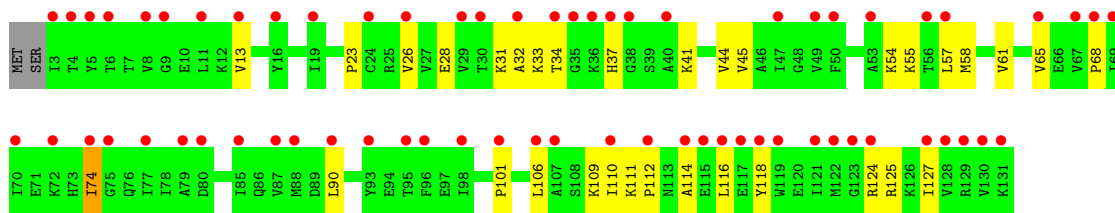


- Molecule 1: Probable deoxyhypusine synthase



- Molecule 1: Probable deoxyhypusine synthase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.37Å 136.76Å 144.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.00 29.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	57.3 (29.83-2.00) 53.2 (29.83-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.06 (at 1.87Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.190 , 0.247 0.190 , 0.248	Depositor DCC
$R_{free}$ test set	4493 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 70.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.010 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	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 20.07 % 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 9.4175e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, 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	0.14	0/2527	0.34	0/3409
1	B	0.15	0/2527	0.37	0/3409
1	C	0.14	0/2527	0.36	0/3409
1	D	0.19	0/2527	0.51	2/3409 (0.1%)
2	E	0.17	0/1014	0.39	0/1367
2	F	0.15	0/1020	0.47	0/1375
2	G	0.18	0/1014	0.52	0/1367
2	H	0.32	0/1014	0.54	0/1367
All	All	0.17	0/14170	0.43	2/19112 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	GLU	N-CA-C	-14.30	95.83	113.28
1	D	280	ALA	N-CA-C	-9.08	101.33	111.14

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	2476	0	2521	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2476	0	2521	31	0
1	C	2476	0	2521	61	0
1	D	2476	0	2521	69	0
2	E	1000	0	1039	33	0
2	F	1006	0	1044	16	0
2	G	1000	0	1039	53	0
2	H	1000	0	1039	27	0
3	A	44	0	25	2	0
3	B	44	0	25	2	0
3	C	88	0	50	2	0
4	A	7	0	10	0	0
4	B	14	0	20	0	0
5	A	82	0	0	0	0
5	B	48	0	0	0	0
5	C	5	0	0	0	0
5	D	9	0	0	0	0
5	E	1	0	0	0	0
5	F	5	0	0	0	0
All	All	14257	0	14375	296	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 10.

All (296) 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:C:251:GLN:HE22	2:G:36:LYS:HB2	1.27	0.96
1:D:284:ASN:HD21	2:H:34:THR:HB	1.35	0.92
1:D:251:GLN:HB3	1:D:285:LYS:HG2	1.58	0.86
1:D:171:ILE:HB	1:D:179:ARG:HG2	1.64	0.80
1:A:287:ARG:HB2	1:A:290:ALA:HB2	1.61	0.80
2:H:111:LYS:HG2	2:H:114:ALA:HB2	1.67	0.76
1:D:276:LYS:O	1:D:279:GLU:HG3	1.85	0.76
1:B:247:ILE:HG22	1:B:285:LYS:HD3	1.68	0.75
1:A:285:LYS:HZ3	2:F:36:LYS:HD3	1.51	0.75
2:G:87:VAL:HG12	2:G:88:MET:H	1.51	0.75
1:B:275:ALA:HB1	1:B:279:GLU:HG2	1.69	0.75
2:G:78:ILE:H	2:G:87:VAL:HG21	1.53	0.74
2:E:36:LYS:H	2:E:36:LYS:HD2	1.54	0.73
2:E:23:PRO:HB3	2:E:68:PRO:HG3	1.71	0.73
2:H:37:HIS:HD1	2:H:41:LYS:HE3	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:THR:HG23	2:F:67:VAL:HB	1.72	0.72
2:G:116:LEU:HD23	2:G:127:ILE:HG23	1.70	0.71
2:G:29:VAL:HG22	2:G:44:VAL:HG12	1.73	0.70
2:G:116:LEU:HA	2:G:130:VAL:HA	1.72	0.70
1:B:138:LYS:NZ	1:B:142:GLU:OE2	2.26	0.69
2:F:80:ASP:O	2:F:82:GLY:N	2.26	0.69
2:E:77:ILE:HD13	2:E:85:ILE:HG23	1.75	0.69
1:B:35:GLY:HA3	1:D:300:THR:HG21	1.75	0.68
2:E:115:GLU:HG3	2:E:131:LYS:HB2	1.76	0.68
1:D:105:VAL:HG23	1:D:107:TYR:HE1	1.59	0.67
1:D:287:ARG:HB2	1:D:290:ALA:HB2	1.77	0.67
2:F:78:ILE:HD11	2:F:88:MET:HB2	1.75	0.67
2:G:104:ASP:O	2:G:105:GLU:HG3	1.94	0.67
1:B:287:ARG:HB2	1:B:290:ALA:HB2	1.78	0.66
1:D:119:LYS:O	1:D:120:ASP:HB2	1.94	0.66
1:A:21:GLU:HG3	1:A:311:LEU:HD13	1.77	0.66
1:A:238:GLY:HA2	3:A:401:NAD:H1B	1.77	0.66
1:D:122:GLU:HG2	1:D:133:PHE:HE2	1.61	0.66
1:D:124:HIS:NE2	1:D:133:PHE:HD1	1.94	0.65
2:E:85:ILE:HD13	2:E:100:LYS:HG3	1.79	0.65
1:B:66:LEU:HD21	1:B:237:ILE:HG21	1.79	0.64
1:C:113:ILE:HG23	1:C:115:ASP:H	1.62	0.64
1:C:244:HIS:HB2	1:C:272:LEU:HD21	1.79	0.64
1:D:4:ARG:NH2	1:D:122:GLU:O	2.31	0.64
2:G:83:ASN:OD1	2:G:84:LYS:N	2.30	0.63
1:C:287:ARG:HB2	1:C:290:ALA:HB2	1.80	0.63
1:A:43:ARG:NH2	1:A:292:HIS:O	2.32	0.63
2:H:34:THR:OG1	2:H:37:HIS:NE2	2.32	0.62
1:C:169:LYS:HG2	1:C:182:TYR:CZ	2.35	0.62
2:G:101:PRO:HG2	2:G:106:LEU:HD13	1.81	0.61
1:C:117:MET:SD	1:C:117:MET:N	2.71	0.61
2:E:81:MET:HE2	2:E:84:LYS:HE2	1.82	0.61
1:D:122:GLU:HA	1:D:133:PHE:CE2	2.35	0.61
2:F:103:GLU:O	2:F:104:ASP:HB2	2.01	0.61
1:B:284:ASN:HB2	2:E:36:LYS:CE	2.31	0.61
1:B:3:ASN:ND2	1:B:5:GLU:OE1	2.35	0.60
2:H:101:PRO:HD2	2:H:110:ILE:HD11	1.84	0.59
2:G:103:GLU:H	2:G:106:LEU:HD11	1.68	0.59
1:A:300:THR:HG21	1:C:35:GLY:HA3	1.84	0.59
1:D:124:HIS:HE2	1:D:133:PHE:HD1	1.50	0.59
2:E:116:LEU:HD22	2:E:127:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:63:GLN:OE1	2:G:64:GLN:NE2	2.35	0.59
2:G:98:ILE:HD12	2:G:125:ARG:HG3	1.85	0.59
1:A:248:TRP:HA	1:A:285:LYS:HE3	1.84	0.59
1:C:14:ASP:OD1	1:C:100:ARG:NH2	2.36	0.59
1:C:166:GLU:O	1:C:170:ARG:HD2	2.02	0.59
1:D:124:HIS:CE1	1:D:133:PHE:HA	2.38	0.58
1:C:278:ARG:HD2	1:D:115:ASP:HB2	1.86	0.58
2:G:74:ILE:HB	2:G:131:LYS:HZ1	1.68	0.58
1:D:205:GLN:HB3	1:D:209:LEU:HD22	1.84	0.58
1:D:283:TRP:HE3	1:D:285:LYS:H	1.52	0.58
1:D:8:LEU:HD21	1:D:123:ILE:HD11	1.86	0.57
1:D:251:GLN:CB	1:D:285:LYS:HG2	2.32	0.57
2:G:101:PRO:HG3	2:G:127:ILE:HB	1.86	0.57
1:D:219:MET:HE1	1:D:245:HIS:CE1	2.39	0.57
1:C:105:VAL:HG13	1:C:107:TYR:HE1	1.68	0.57
1:D:102:PHE:CD2	1:D:143:ILE:HG12	2.40	0.57
2:G:126:LYS:HD3	2:G:127:ILE:H	1.68	0.56
1:C:113:ILE:HD12	1:C:118:LEU:HG	1.86	0.56
1:B:238:GLY:HA2	3:B:401:NAD:H1B	1.86	0.56
2:H:28:GLU:HB3	2:H:45:VAL:HB	1.88	0.56
2:E:16:TYR:CE1	2:E:25:ARG:HG3	2.41	0.56
1:A:283:TRP:HB3	1:A:285:LYS:HD2	1.86	0.56
2:E:4:THR:HG23	2:E:67:VAL:HB	1.87	0.56
3:C:402:NAD:H8A	1:D:271:SER:HB3	1.86	0.56
2:G:119:TRP:HZ3	2:G:128:VAL:HB	1.71	0.55
1:C:161:TYR:CE1	1:C:162:GLU:HG3	2.41	0.55
2:H:23:PRO:HB3	2:H:68:PRO:HG3	1.87	0.55
1:C:147:PHE:HD2	1:C:170:ARG:HE	1.53	0.55
1:D:124:HIS:CD2	2:G:36:LYS:HG2	2.41	0.55
1:D:166:GLU:O	1:D:170:ARG:HD2	2.07	0.55
1:D:181:ALA:HA	1:D:186:VAL:HG22	1.89	0.55
2:F:104:ASP:O	2:F:108:SER:OG	2.22	0.55
2:G:100:LYS:HE3	2:G:110:ILE:HG13	1.88	0.55
2:H:106:LEU:HD13	2:H:127:ILE:HG22	1.87	0.55
2:H:32:ALA:O	2:H:33:LYS:HG2	2.07	0.55
1:C:8:LEU:HD21	1:C:123:ILE:HD11	1.88	0.54
1:C:251:GLN:NE2	2:G:35:GLY:O	2.40	0.54
1:D:147:PHE:HD2	1:D:170:ARG:HE	1.54	0.54
2:F:70:ILE:HD13	2:F:70:ILE:H	1.73	0.54
2:H:74:ILE:HG23	2:H:90:LEU:HB2	1.90	0.53
1:C:251:GLN:HB2	1:C:285:LYS:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASP:OD2	1:D:258:TYR:OH	2.27	0.53
2:F:3:ILE:HG13	2:F:66:GLU:HB3	1.91	0.53
2:G:77:ILE:HA	2:G:87:VAL:HB	1.90	0.53
1:A:18:ARG:HG3	1:A:19:ASP:H	1.75	0.52
1:B:1:MET:N	1:B:1:MET:SD	2.80	0.52
1:A:126:LEU:HD11	3:A:401:NAD:N7N	2.24	0.52
1:D:163:LEU:HD21	1:D:202:LEU:HD21	1.90	0.52
1:D:147:PHE:O	1:D:151:ILE:HG13	2.08	0.52
1:D:253:LYS:NZ	1:D:255:GLY:O	2.43	0.52
2:G:88:MET:HA	2:G:94:GLU:O	2.09	0.52
1:D:214:ASN:HD21	1:D:216:PHE:HD2	1.58	0.52
1:D:110:SER:OG	1:D:112:ASP:OD1	2.25	0.52
1:D:4:ARG:HH21	1:D:122:GLU:HB3	1.75	0.52
1:B:283:TRP:O	2:E:36:LYS:HE2	2.10	0.52
2:E:77:ILE:HD12	2:E:86:GLN:O	2.10	0.52
1:C:277:PRO:C	1:C:279:GLU:H	2.18	0.52
1:A:219:MET:HE1	1:A:245:HIS:NE2	2.25	0.51
1:B:18:ARG:HD2	1:B:18:ARG:N	2.26	0.51
1:C:100:ARG:HA	1:C:104:GLY:O	2.10	0.51
1:C:163:LEU:HD21	1:C:202:LEU:HD11	1.92	0.51
2:E:6:THR:OG1	2:E:7:THR:N	2.43	0.51
1:C:119:LYS:HD2	1:C:119:LYS:C	2.34	0.51
1:D:114:ASP:OD1	1:D:117:MET:HG2	2.10	0.51
1:D:122:GLU:HG2	1:D:133:PHE:CE2	2.42	0.51
1:A:281:ILE:HD13	1:A:286:ILE:HG12	1.92	0.51
2:G:81:MET:HE3	2:G:82:GLY:N	2.25	0.51
2:G:72:LYS:HG3	2:G:119:TRP:NE1	2.26	0.51
2:H:111:LYS:O	2:H:112:PRO:C	2.53	0.51
1:B:109:GLY:HA3	1:B:130:LEU:HD13	1.92	0.50
2:E:84:LYS:HG2	2:E:99:GLU:OE2	2.12	0.50
1:C:117:MET:O	1:C:121:LEU:HD12	2.11	0.50
1:A:18:ARG:HG3	1:A:19:ASP:N	2.26	0.50
2:G:78:ILE:HG12	2:G:87:VAL:HG21	1.92	0.50
1:B:204:ILE:HG12	2:F:58:MET:HE3	1.93	0.49
1:D:141:GLU:HG3	1:D:201:ASN:OD1	2.11	0.49
1:D:141:GLU:OE1	2:G:38:GLY:HA3	2.12	0.49
2:G:78:ILE:HG23	2:G:87:VAL:HG11	1.93	0.49
1:A:23:TYR:HD1	1:C:23:TYR:HD1	1.60	0.49
1:C:276:LYS:HD2	1:C:277:PRO:HD2	1.94	0.49
1:B:113:ILE:HD11	1:B:118:LEU:HD11	1.93	0.49
1:C:139:VAL:O	1:C:143:ILE:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:SER:HB3	1:D:171:ILE:HG23	1.94	0.49
2:E:84:LYS:O	2:E:85:ILE:HD12	2.13	0.49
1:C:116:ALA:O	1:C:119:LYS:HG3	2.13	0.49
2:G:77:ILE:O	2:G:113:ASN:N	2.41	0.49
1:C:119:LYS:HD2	1:C:120:ASP:N	2.28	0.48
1:C:166:GLU:OE1	1:C:170:ARG:NH1	2.46	0.48
2:E:45:VAL:HG11	2:E:54:LYS:HE2	1.95	0.48
2:G:87:VAL:HG12	2:G:88:MET:N	2.24	0.48
1:A:52:ILE:HD12	1:A:83:TYR:HD1	1.78	0.48
2:H:34:THR:HG1	2:H:37:HIS:CE1	2.29	0.48
1:A:20:LEU:HB3	1:A:308:ALA:HB2	1.95	0.48
1:B:32:LYS:HE2	1:D:15:ILE:HG22	1.95	0.48
1:D:100:ARG:HA	1:D:104:GLY:O	2.14	0.47
1:D:151:ILE:HD13	1:D:166:GLU:HB3	1.96	0.47
1:B:284:ASN:HB2	2:E:36:LYS:HE3	1.96	0.47
1:C:280:ALA:HA	1:C:283:TRP:CE3	2.50	0.47
1:D:14:ASP:HB3	1:D:73:GLY:HA3	1.97	0.47
2:G:110:ILE:H	2:G:110:ILE:HD13	1.79	0.47
2:H:118:TYR:CE2	2:H:125:ARG:HD3	2.49	0.47
1:A:257:ASP:OD1	1:A:287:ARG:NE	2.46	0.47
2:H:34:THR:OG1	2:H:37:HIS:CE1	2.68	0.47
1:B:34:TYR:HA	1:B:38:SER:HB2	1.97	0.47
1:C:3:ASN:HD22	1:C:5:GLU:CD	2.22	0.46
1:C:20:LEU:HB3	1:C:308:ALA:HB2	1.97	0.46
1:C:179:ARG:NE	1:C:183:GLU:OE2	2.48	0.46
1:D:11:PRO:HA	1:D:107:TYR:HA	1.96	0.46
1:B:20:LEU:HB3	1:B:308:ALA:HB2	1.98	0.46
1:B:48:LEU:O	1:B:52:ILE:HG12	2.15	0.46
2:E:98:ILE:HD11	2:E:127:ILE:HD11	1.97	0.46
2:G:86:GLN:C	2:G:87:VAL:HG23	2.39	0.46
2:H:37:HIS:ND1	2:H:41:LYS:HE3	2.27	0.46
1:C:283:TRP:HB2	1:C:285:LYS:HD2	1.98	0.46
2:E:78:ILE:HG13	2:E:79:ALA:H	1.81	0.46
2:E:103:GLU:OE1	2:E:105:GLU:N	2.48	0.46
1:D:223:LYS:HB2	1:D:249:TRP:CZ3	2.51	0.46
1:C:241:ILE:HA	3:C:401:NAD:H4D	1.98	0.46
1:D:141:GLU:OE2	2:G:41:LYS:NZ	2.45	0.46
1:C:113:ILE:HD13	1:C:113:ILE:O	2.16	0.46
1:C:278:ARG:O	1:D:125:ARG:NH2	2.49	0.46
1:D:161:TYR:CE2	1:D:221:LEU:HD22	2.50	0.46
1:A:163:LEU:HD22	1:A:213:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:HIS:HB2	1:C:272:LEU:CD2	2.43	0.46
1:D:236:ILE:HG21	1:D:243:LYS:HG3	1.97	0.46
2:H:74:ILE:HD12	2:H:90:LEU:HD22	1.97	0.46
1:A:163:LEU:HD21	1:A:202:LEU:HD21	1.97	0.45
1:D:55:ALA:O	1:D:58:ARG:NH1	2.46	0.45
1:D:124:HIS:NE2	1:D:133:PHE:CD1	2.82	0.45
1:C:11:PRO:HA	1:C:107:TYR:HA	1.99	0.45
2:G:28:GLU:HB2	2:G:45:VAL:HB	1.97	0.45
2:G:77:ILE:CD1	2:G:85:ILE:HG12	2.46	0.45
2:G:106:LEU:HA	2:G:109:LYS:HE2	1.98	0.45
1:C:3:ASN:ND2	1:C:5:GLU:OE2	2.42	0.45
1:C:289:ASN:OD1	1:C:289:ASN:N	2.48	0.45
2:F:37:HIS:CE1	2:F:41:LYS:HD2	2.52	0.45
1:A:18:ARG:NH1	1:A:19:ASP:OD1	2.50	0.45
1:C:163:LEU:HD22	1:C:211:PHE:HZ	1.81	0.45
2:E:87:VAL:O	2:E:95:THR:HA	2.17	0.45
1:C:80:LYS:NZ	1:C:174:SER:O	2.30	0.45
1:C:166:GLU:O	1:C:169:LYS:HB2	2.17	0.45
1:D:61:SER:HA	1:D:88:VAL:O	2.17	0.45
1:D:276:LYS:HB3	1:D:277:PRO:CD	2.47	0.45
1:A:283:TRP:CB	1:A:285:LYS:HD2	2.47	0.44
1:D:176:SER:HB3	1:D:179:ARG:HB2	1.98	0.44
1:B:226:VAL:HG11	1:B:249:TRP:O	2.17	0.44
2:G:9:GLY:HA3	2:G:61:VAL:HG22	2.00	0.44
1:B:23:TYR:HD1	1:D:23:TYR:HD1	1.65	0.44
2:E:18:VAL:HG23	2:E:68:PRO:HD3	1.99	0.44
2:G:110:ILE:O	2:G:110:ILE:HG12	2.18	0.44
2:E:3:ILE:HG13	2:E:66:GLU:HB3	2.00	0.44
2:E:36:LYS:H	2:E:36:LYS:CD	2.15	0.44
1:D:159:PRO:HB3	1:D:217:GLU:HB2	1.99	0.44
2:E:83:ASN:HD22	2:E:83:ASN:H	1.65	0.44
2:G:87:VAL:CG1	2:G:88:MET:H	2.25	0.44
1:A:254:ASP:OD1	1:A:287:ARG:HA	2.18	0.44
1:D:124:HIS:NE2	2:G:36:LYS:HG2	2.32	0.44
2:G:22:GLU:OE1	2:G:50:PHE:HB2	2.17	0.44
2:H:31:LYS:HE3	2:H:61:VAL:HG11	2.00	0.44
1:D:279:GLU:C	1:D:279:GLU:CD	2.86	0.44
2:G:117:GLU:HB3	2:G:131:LYS:HD2	2.00	0.44
1:A:14:ASP:HB3	1:A:73:GLY:HA3	1.99	0.43
1:A:119:LYS:HG3	1:B:284:ASN:ND2	2.33	0.43
2:G:86:GLN:HG2	2:G:97:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:VAL:HG22	2:H:57:LEU:HB3	2.00	0.43
1:B:286:ILE:HG12	1:B:287:ARG:N	2.31	0.43
2:G:126:LYS:HD3	2:G:127:ILE:N	2.32	0.43
1:A:253:LYS:NZ	1:A:255:GLY:O	2.51	0.43
1:C:214:ASN:ND2	1:C:217:GLU:HG2	2.34	0.43
2:E:70:ILE:HG22	2:E:72:LYS:HG2	2.00	0.43
1:A:124:HIS:CE1	1:A:133:PHE:HA	2.53	0.43
1:C:211:PHE:O	1:C:212:LYS:HD3	2.19	0.43
2:E:94:GLU:O	2:E:96:PHE:HD1	2.01	0.43
2:H:54:LYS:HE2	2:H:54:LYS:HB2	1.83	0.43
1:C:281:ILE:HG13	1:C:286:ILE:HD11	2.00	0.43
1:D:244:HIS:O	1:D:248:TRP:N	2.45	0.43
2:F:49:VAL:HG11	2:F:121:ILE:HD11	2.01	0.43
2:F:122:MET:HE3	2:F:122:MET:HB3	1.85	0.43
1:A:226:VAL:HG11	1:A:249:TRP:O	2.18	0.43
2:E:78:ILE:HG13	2:E:79:ALA:N	2.34	0.43
1:C:141:GLU:OE1	2:H:41:LYS:NZ	2.33	0.43
2:E:8:VAL:HG21	2:E:59:ALA:HB3	2.00	0.43
2:E:68:PRO:HB2	2:E:121:ILE:CG2	2.49	0.43
1:A:113:ILE:HG23	1:A:117:MET:HE3	2.00	0.42
2:G:23:PRO:HB3	2:G:68:PRO:HG3	2.00	0.42
1:C:213:ILE:HD12	1:C:215:LEU:HG	2.01	0.42
2:G:72:LYS:HG3	2:G:119:TRP:HE1	1.84	0.42
2:E:44:VAL:HG22	2:E:57:LEU:HB3	2.00	0.42
1:A:133:PHE:CD2	2:E:35:GLY:HA2	2.54	0.42
1:C:114:ASP:OD1	1:C:114:ASP:C	2.62	0.42
2:G:89:ASP:OD1	2:G:90:LEU:N	2.53	0.42
1:C:75:PHE:O	1:C:79:VAL:HG12	2.19	0.42
1:D:169:LYS:HA	1:D:182:TYR:CD2	2.54	0.42
1:B:166:GLU:O	1:B:170:ARG:NH1	2.48	0.42
1:B:126:LEU:HD21	3:B:401:NAD:H72N	1.84	0.42
2:G:81:MET:HE3	2:G:83:ASN:H	1.85	0.42
2:G:97:GLU:O	2:G:125:ARG:NH2	2.52	0.42
1:B:185:LYS:HD2	1:B:185:LYS:HA	1.88	0.42
1:D:48:LEU:O	1:D:52:ILE:HG12	2.20	0.42
1:B:79:VAL:HG21	1:B:87:ILE:HD11	2.02	0.42
1:B:277:PRO:C	1:B:279:GLU:H	2.27	0.42
2:G:78:ILE:N	2:G:87:VAL:HG21	2.29	0.42
1:C:211:PHE:C	1:C:212:LYS:HD3	2.45	0.42
1:D:286:ILE:HG13	1:D:292:HIS:CE1	2.55	0.42
2:G:8:VAL:HA	2:G:11:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:81:MET:HE3	2:G:82:GLY:H	1.85	0.41
1:C:215:LEU:O	1:C:219:MET:HG2	2.19	0.41
1:C:277:PRO:O	1:C:281:ILE:HD12	2.19	0.41
1:D:286:ILE:HG13	1:D:292:HIS:NE2	2.34	0.41
1:B:276:LYS:O	1:B:279:GLU:HB3	2.20	0.41
1:D:284:ASN:ND2	2:H:34:THR:HB	2.18	0.41
2:G:85:ILE:N	2:G:98:ILE:O	2.48	0.41
2:H:13:VAL:HA	2:H:26:VAL:HG23	2.01	0.41
2:E:118:TYR:CE2	2:E:125:ARG:HD3	2.54	0.41
1:A:251:GLN:OE1	2:F:36:LYS:HB3	2.20	0.41
1:C:251:GLN:HB2	1:C:285:LYS:CG	2.50	0.41
1:D:215:LEU:O	1:D:219:MET:HG2	2.19	0.41
1:C:16:ALA:HB1	1:C:77:ASP:OD2	2.21	0.41
1:C:248:TRP:O	1:C:251:GLN:HB3	2.21	0.41
1:D:159:PRO:HB2	1:D:161:TYR:CE1	2.56	0.41
1:D:252:PHE:CE1	2:H:37:HIS:CE1	3.08	0.41
2:F:2:SER:HB3	2:F:69:ILE:H	1.86	0.41
2:F:33:LYS:HE3	2:F:33:LYS:HB2	1.77	0.41
2:H:109:LYS:HE2	2:H:109:LYS:HB3	1.90	0.41
1:C:248:TRP:HA	1:C:285:LYS:HE2	2.02	0.41
1:D:148:LEU:HD23	1:D:205:GLN:HB2	2.03	0.41
1:A:184:LYS:HB2	1:A:186:VAL:HG23	2.03	0.41
1:C:4:ARG:HG2	1:C:8:LEU:HD23	2.02	0.41
1:C:54:ASP:OD1	1:C:231:LYS:HD2	2.21	0.41
1:D:276:LYS:HB3	1:D:277:PRO:HD2	2.03	0.41
2:G:103:GLU:N	2:G:106:LEU:HD11	2.33	0.41
2:H:58:MET:HE3	2:H:58:MET:HB3	1.82	0.40
1:B:284:ASN:OD1	1:B:284:ASN:N	2.54	0.40
1:D:71:LEU:HD11	1:D:300:THR:HA	2.02	0.40
1:A:70:GLY:HA3	1:C:33:ILE:HA	2.02	0.40
1:A:148:LEU:HD23	1:A:205:GLN:HB2	2.04	0.40
1:C:208:PHE:HE1	2:H:65:VAL:HG23	1.86	0.40
2:G:77:ILE:HD12	2:G:78:ILE:H	1.86	0.40
2:F:106:LEU:C	2:F:108:SER:H	2.29	0.40
2:H:55:LYS:HA	2:H:55:LYS:HD2	1.76	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	310/312 (99%)	306 (99%)	4 (1%)	0	100	100
1	B	310/312 (99%)	302 (97%)	8 (3%)	0	100	100
1	C	310/312 (99%)	305 (98%)	5 (2%)	0	100	100
1	D	310/312 (99%)	300 (97%)	9 (3%)	1 (0%)	36	35
2	E	127/131 (97%)	119 (94%)	8 (6%)	0	100	100
2	F	128/131 (98%)	114 (89%)	12 (9%)	2 (2%)	7	3
2	G	127/131 (97%)	116 (91%)	8 (6%)	3 (2%)	4	2
2	H	127/131 (97%)	120 (94%)	7 (6%)	0	100	100
All	All	1749/1772 (99%)	1682 (96%)	61 (4%)	6 (0%)	36	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	120	ASP
2	F	81	MET
2	G	87	VAL
2	F	104	ASP
2	G	122	MET
2	G	130	VAL

### 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	267/267 (100%)	260 (97%)	7 (3%)	40	44
1	B	267/267 (100%)	261 (98%)	6 (2%)	45	50
1	C	267/267 (100%)	257 (96%)	10 (4%)	30	30
1	D	267/267 (100%)	260 (97%)	7 (3%)	40	44
2	E	110/112 (98%)	99 (90%)	11 (10%)	7	4
2	F	111/112 (99%)	105 (95%)	6 (5%)	20	17
2	G	110/112 (98%)	97 (88%)	13 (12%)	5	3
2	H	110/112 (98%)	107 (97%)	3 (3%)	39	42
All	All	1509/1516 (100%)	1446 (96%)	63 (4%)	26	25

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	150	GLU
1	A	176	SER
1	A	272	LEU
1	A	281	ILE
1	A	286	ILE
1	A	291	LYS
1	B	36	PHE
1	B	150	GLU
1	B	193	ILE
1	B	284	ASN
1	B	286	ILE
1	B	291	LYS
1	C	8	LEU
1	C	18	ARG
1	C	43	ARG
1	C	79	VAL
1	C	113	ILE
1	C	169	LYS
1	C	242	SER
1	C	272	LEU
1	C	279	GLU
1	C	286	ILE
1	D	2	ILE
1	D	8	LEU
1	D	150	GLU
1	D	194	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	272	LEU
1	D	278	ARG
1	D	283	TRP
2	E	4	THR
2	E	15	SER
2	E	36	LYS
2	E	64	GLN
2	E	72	LYS
2	E	77	ILE
2	E	83	ASN
2	E	85	ILE
2	E	95	THR
2	E	121	ILE
2	E	130	VAL
2	F	15	SER
2	F	44	VAL
2	F	70	ILE
2	F	77	ILE
2	F	90	LEU
2	F	110	ILE
2	G	4	THR
2	G	5	TYR
2	G	22	GLU
2	G	49	VAL
2	G	61	VAL
2	G	78	ILE
2	G	85	ILE
2	G	105	GLU
2	G	110	ILE
2	G	116	LEU
2	G	117	GLU
2	G	121	ILE
2	G	131	LYS
2	H	74	ILE
2	H	116	LEU
2	H	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	10	ASN
1	A	124	HIS

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Mol	Chain	Res	Type
1	A	284	ASN
1	B	244	HIS
1	C	201	ASN
1	C	210	ASN
1	C	250	ASN
1	C	251	GLN
1	D	205	GLN
1	D	214	ASN
1	D	250	ASN
1	D	284	ASN
2	F	113	ASN
2	G	63	GLN
2	G	64	GLN
2	H	83	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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
3	NAD	C	402	-	46,48,48	3.83	17 (36%)	64,73,73	1.72	12 (18%)
3	NAD	C	401	-	46,48,48	3.83	18 (39%)	64,73,73	1.73	11 (17%)
4	PEG	B	403	-	6,6,6	0.51	0	5,5,5	0.45	0
3	NAD	B	401	-	46,48,48	3.82	17 (36%)	64,73,73	1.72	11 (17%)
3	NAD	A	401	-	46,48,48	3.84	17 (36%)	64,73,73	1.64	11 (17%)
4	PEG	A	402	-	6,6,6	0.49	0	5,5,5	0.46	0
4	PEG	B	402	-	6,6,6	0.50	0	5,5,5	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	402	-	-	10/30/62/62	0/5/5/5
3	NAD	C	401	-	-	5/30/62/62	0/5/5/5
4	PEG	B	403	-	-	3/4/4/4	-
3	NAD	B	401	-	-	9/30/62/62	0/5/5/5
3	NAD	A	401	-	-	15/30/62/62	0/5/5/5
4	PEG	A	402	-	-	3/4/4/4	-
4	PEG	B	402	-	-	3/4/4/4	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	O4D-C1D	14.28	1.59	1.40
3	C	402	NAD	O4D-C1D	14.22	1.59	1.40
3	B	401	NAD	O4D-C1D	14.19	1.59	1.40
3	C	401	NAD	O4D-C1D	14.10	1.59	1.40
3	C	401	NAD	C2B-C3B	-11.02	1.23	1.53
3	A	401	NAD	C2B-C3B	-10.98	1.23	1.53
3	B	401	NAD	C2B-C3B	-10.94	1.23	1.53
3	C	402	NAD	C2B-C3B	-10.91	1.23	1.53
3	A	401	NAD	PN-O3	8.18	1.68	1.59
3	C	402	NAD	PN-O3	8.16	1.68	1.59
3	C	401	NAD	PN-O3	8.14	1.68	1.59
3	B	401	NAD	PN-O3	8.07	1.68	1.59
3	C	402	NAD	C7N-N7N	6.88	1.45	1.33
3	C	401	NAD	C7N-N7N	6.87	1.45	1.33
3	A	401	NAD	C7N-N7N	6.86	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	C7N-N7N	6.86	1.45	1.33
3	C	401	NAD	O4D-C4D	-6.70	1.30	1.45
3	B	401	NAD	O4D-C4D	-6.57	1.30	1.45
3	A	401	NAD	O4D-C4D	-6.51	1.30	1.45
3	C	402	NAD	O4D-C4D	-6.51	1.30	1.45
3	A	401	NAD	PA-O3	6.46	1.66	1.59
3	C	402	NAD	PA-O3	6.30	1.66	1.59
3	C	401	NAD	PA-O3	6.24	1.66	1.59
3	B	401	NAD	PA-O3	6.21	1.66	1.59
3	A	401	NAD	C6A-N6A	4.82	1.46	1.34
3	B	401	NAD	C6A-N6A	4.81	1.46	1.34
3	C	401	NAD	C6A-N6A	4.80	1.46	1.34
3	C	402	NAD	C6A-N6A	4.78	1.46	1.34
3	C	402	NAD	O4B-C1B	-4.61	1.31	1.42
3	B	401	NAD	O4B-C1B	-4.53	1.31	1.42
3	C	401	NAD	O4B-C1B	-4.51	1.31	1.42
3	A	401	NAD	O4B-C1B	-4.51	1.31	1.42
3	C	402	NAD	C2B-C1B	4.06	1.66	1.53
3	C	401	NAD	C2B-C1B	3.98	1.66	1.53
3	B	401	NAD	C2B-C1B	3.96	1.65	1.53
3	A	401	NAD	C2B-C1B	3.95	1.65	1.53
3	C	401	NAD	C3N-C7N	3.56	1.55	1.50
3	B	401	NAD	C3N-C7N	3.49	1.55	1.50
3	A	401	NAD	C3N-C7N	3.48	1.55	1.50
3	C	402	NAD	C3N-C7N	3.46	1.55	1.50
3	B	401	NAD	C3B-C4B	3.15	1.61	1.53
3	C	401	NAD	C3B-C4B	3.13	1.60	1.53
3	C	402	NAD	O2B-C2B	3.13	1.50	1.43
3	C	402	NAD	C3B-C4B	3.10	1.60	1.53
3	A	401	NAD	C3B-C4B	3.09	1.60	1.53
3	B	401	NAD	O2B-C2B	3.05	1.50	1.43
3	C	401	NAD	O2B-C2B	3.05	1.50	1.43
3	A	401	NAD	O2B-C2B	3.02	1.50	1.43
3	A	401	NAD	C5B-C4B	-3.02	1.42	1.51
3	B	401	NAD	C5B-C4B	-3.01	1.42	1.51
3	B	401	NAD	O2D-C2D	3.01	1.50	1.43
3	C	401	NAD	C5B-C4B	-3.00	1.42	1.51
3	C	402	NAD	O2D-C2D	3.00	1.50	1.43
3	C	401	NAD	O2D-C2D	2.99	1.50	1.43
3	A	401	NAD	O2D-C2D	2.95	1.50	1.43
3	C	402	NAD	C5B-C4B	-2.94	1.42	1.51
3	A	401	NAD	PA-O5B	2.55	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAD	PA-O5B	2.55	1.69	1.59
3	B	401	NAD	PA-O5B	2.54	1.69	1.59
3	C	402	NAD	PA-O5B	2.54	1.69	1.59
3	B	401	NAD	O3B-C3B	2.50	1.49	1.43
3	C	402	NAD	O3B-C3B	2.50	1.49	1.43
3	C	401	NAD	O3B-C3B	2.48	1.49	1.43
3	A	401	NAD	O3B-C3B	2.48	1.49	1.43
3	A	401	NAD	C8A-N9A	-2.37	1.33	1.37
3	C	401	NAD	C8A-N9A	-2.36	1.33	1.37
3	B	401	NAD	C8A-N9A	-2.32	1.33	1.37
3	C	402	NAD	C8A-N9A	-2.30	1.33	1.37
3	C	401	NAD	O4B-C4B	2.00	1.49	1.45

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAD	C5A-C4A-N3A	-5.56	119.06	126.72
3	B	401	NAD	C5A-C4A-N3A	-5.53	119.10	126.72
3	C	401	NAD	C5A-C4A-N3A	-5.42	119.25	126.72
3	C	402	NAD	C5A-C4A-N3A	-5.42	119.26	126.72
3	C	401	NAD	C4D-O4D-C1D	-5.05	105.30	109.92
3	B	401	NAD	C4D-O4D-C1D	-4.60	105.71	109.92
3	C	401	NAD	N3A-C2A-N1A	-4.31	122.06	128.58
3	C	402	NAD	N3A-C2A-N1A	-4.30	122.07	128.58
3	A	401	NAD	N3A-C2A-N1A	-4.25	122.15	128.58
3	C	402	NAD	C4D-O4D-C1D	-4.18	106.09	109.92
3	B	401	NAD	N3A-C2A-N1A	-4.18	122.25	128.58
3	B	401	NAD	N3A-C4A-N9A	4.04	134.04	127.17
3	A	401	NAD	N3A-C4A-N9A	4.02	134.01	127.17
3	C	401	NAD	N3A-C4A-N9A	3.89	133.79	127.17
3	C	402	NAD	N3A-C4A-N9A	3.86	133.74	127.17
3	A	401	NAD	C2A-N3A-C4A	3.65	120.74	111.83
3	B	401	NAD	C2A-N3A-C4A	3.62	120.68	111.83
3	C	402	NAD	C2A-N3A-C4A	3.61	120.66	111.83
3	C	401	NAD	C2A-N3A-C4A	3.60	120.61	111.83
3	C	402	NAD	C4A-C5A-N7A	-3.29	106.82	110.58
3	A	401	NAD	C4A-C5A-N7A	-3.27	106.84	110.58
3	C	401	NAD	C4A-C5A-N7A	-3.27	106.84	110.58
3	B	401	NAD	C4A-C5A-N7A	-3.19	106.94	110.58
3	B	401	NAD	C3B-C2B-C1B	3.14	107.41	101.46
3	C	402	NAD	N9A-C8A-N7A	-3.14	109.49	113.94
3	C	401	NAD	N9A-C8A-N7A	-3.12	109.50	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NAD	C5A-N7A-C8A	3.12	108.36	103.45
3	C	401	NAD	C5A-N7A-C8A	3.12	108.35	103.45
3	A	401	NAD	C5A-N7A-C8A	3.11	108.34	103.45
3	B	401	NAD	C5A-N7A-C8A	3.10	108.32	103.45
3	B	401	NAD	N9A-C8A-N7A	-3.06	109.59	113.94
3	A	401	NAD	N9A-C8A-N7A	-3.03	109.64	113.94
3	C	402	NAD	C3B-C2B-C1B	2.98	107.10	101.46
3	A	401	NAD	C3B-C2B-C1B	2.83	106.81	101.46
3	C	401	NAD	C3B-C2B-C1B	2.70	106.56	101.46
3	A	401	NAD	C4D-O4D-C1D	-2.67	107.48	109.92
3	C	402	NAD	C4B-O4B-C1B	-2.57	103.80	109.47
3	C	401	NAD	C4A-N9A-C8A	2.48	108.34	105.74
3	C	402	NAD	C4A-N9A-C8A	2.47	108.33	105.74
3	B	401	NAD	C4A-N9A-C8A	2.43	108.29	105.74
3	A	401	NAD	C4A-N9A-C8A	2.39	108.25	105.74
3	C	402	NAD	C5N-C4N-C3N	-2.18	118.22	120.36
3	B	401	NAD	C5N-C4N-C3N	-2.14	118.27	120.36
3	A	401	NAD	C5N-C4N-C3N	-2.09	118.31	120.36
3	C	401	NAD	C5N-C4N-C3N	-2.05	118.35	120.36

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAD	C5B-O5B-PA-O2A
3	A	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	C5D-O5D-PN-O1N
3	B	401	NAD	C2N-C3N-C7N-O7N
3	B	401	NAD	C2N-C3N-C7N-N7N
3	C	401	NAD	C5D-O5D-PN-O3
3	C	401	NAD	C5D-O5D-PN-O1N
3	C	401	NAD	C5D-O5D-PN-O2N
3	C	402	NAD	C5D-O5D-PN-O3
3	C	402	NAD	C5D-O5D-PN-O1N
3	C	402	NAD	C2N-C3N-C7N-O7N
3	C	402	NAD	C2N-C3N-C7N-N7N
3	C	402	NAD	C4N-C3N-C7N-O7N
3	C	402	NAD	C4N-C3N-C7N-N7N
3	B	401	NAD	C4N-C3N-C7N-N7N
3	B	401	NAD	C4N-C3N-C7N-O7N
3	B	401	NAD	O4D-C4D-C5D-O5D
3	A	401	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	C	402	NAD	O4D-C4D-C5D-O5D
4	A	402	PEG	O2-C3-C4-O4
4	A	402	PEG	O1-C1-C2-O2
4	B	402	PEG	O2-C3-C4-O4
4	B	403	PEG	O2-C3-C4-O4
3	B	401	NAD	PN-O3-PA-O1A
3	B	401	NAD	C3D-C4D-C5D-O5D
4	B	402	PEG	O1-C1-C2-O2
4	B	402	PEG	C4-C3-O2-C2
3	A	401	NAD	O4D-C4D-C5D-O5D
3	C	402	NAD	C3D-C4D-C5D-O5D
3	C	401	NAD	PN-O3-PA-O2A
3	C	402	NAD	PN-O3-PA-O2A
3	A	401	NAD	C5B-O5B-PA-O1A
3	A	401	NAD	C5B-O5B-PA-O3
3	A	401	NAD	C5D-O5D-PN-O3
3	A	401	NAD	C5D-O5D-PN-O1N
3	A	401	NAD	C5D-O5D-PN-O2N
4	B	403	PEG	C4-C3-O2-C2
4	B	403	PEG	O1-C1-C2-O2
3	A	401	NAD	C2N-C3N-C7N-N7N
3	A	401	NAD	C2N-C3N-C7N-O7N
3	A	401	NAD	C4N-C3N-C7N-N7N
4	A	402	PEG	C1-C2-O2-C3
3	A	401	NAD	PA-O3-PN-O1N
3	C	401	NAD	PN-O3-PA-O1A
3	A	401	NAD	C4N-C3N-C7N-O7N
3	A	401	NAD	PA-O3-PN-O2N
3	B	401	NAD	PA-O3-PN-O2N
3	C	402	NAD	PA-O3-PN-O2N

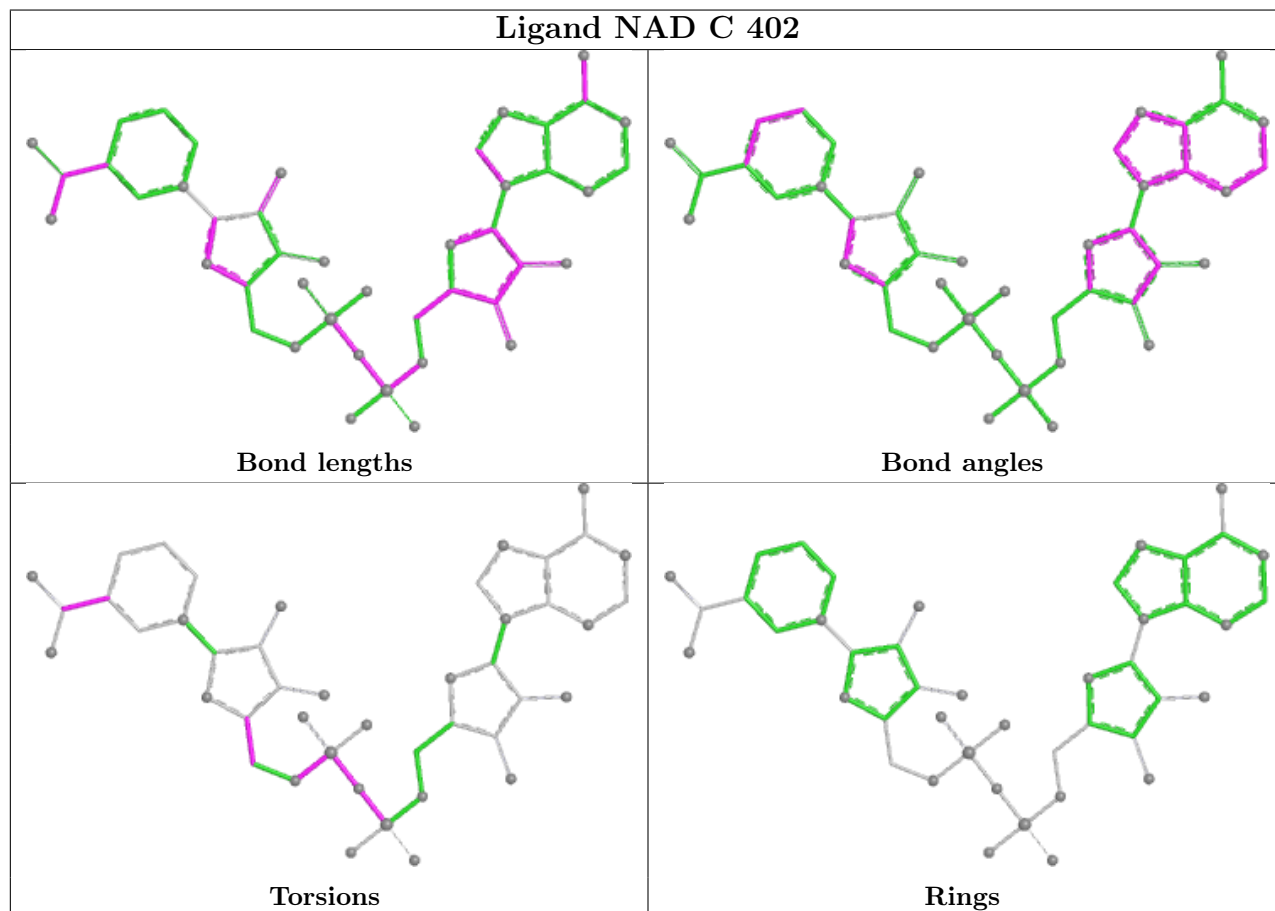
There are no ring outliers.

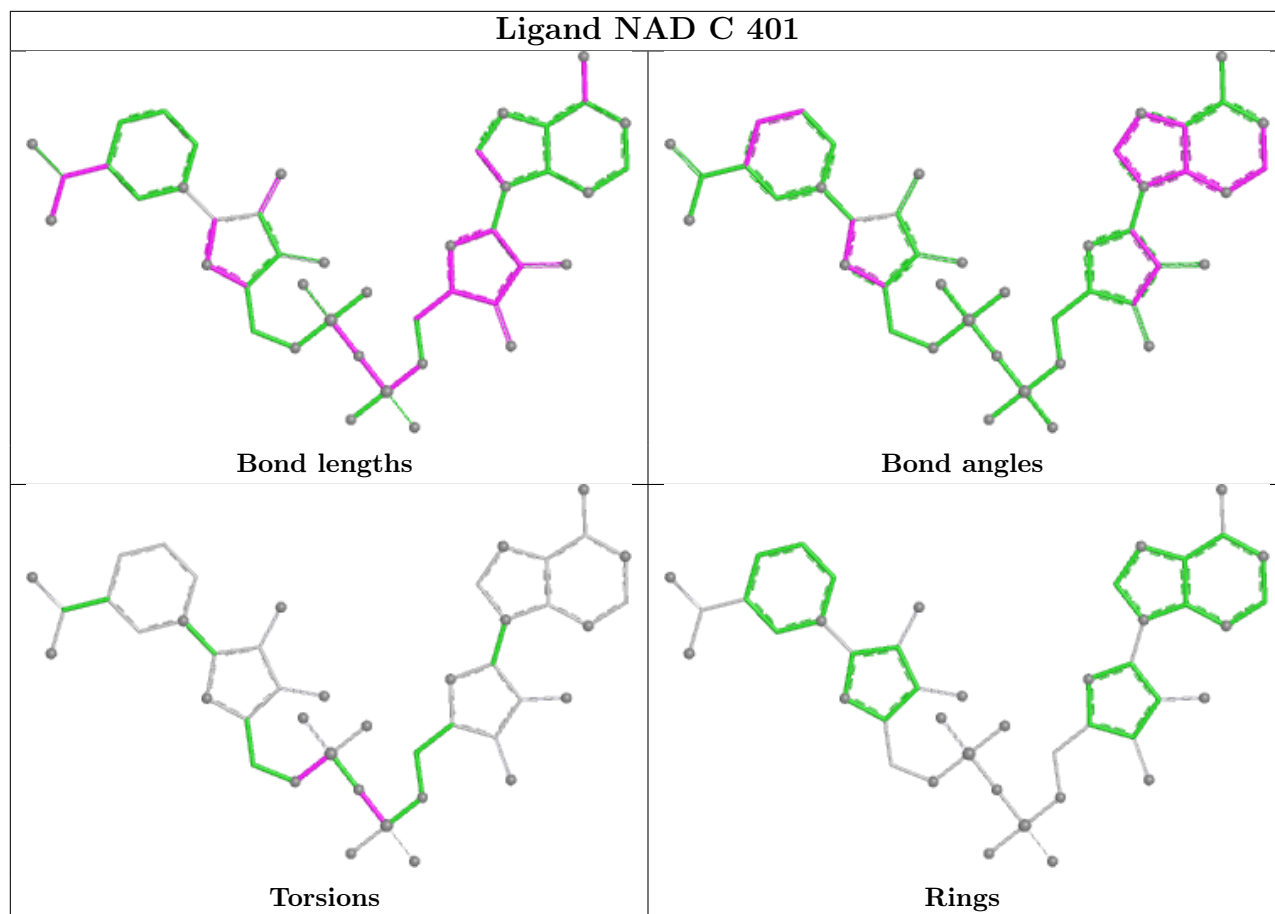
4 monomers are involved in 6 short contacts:

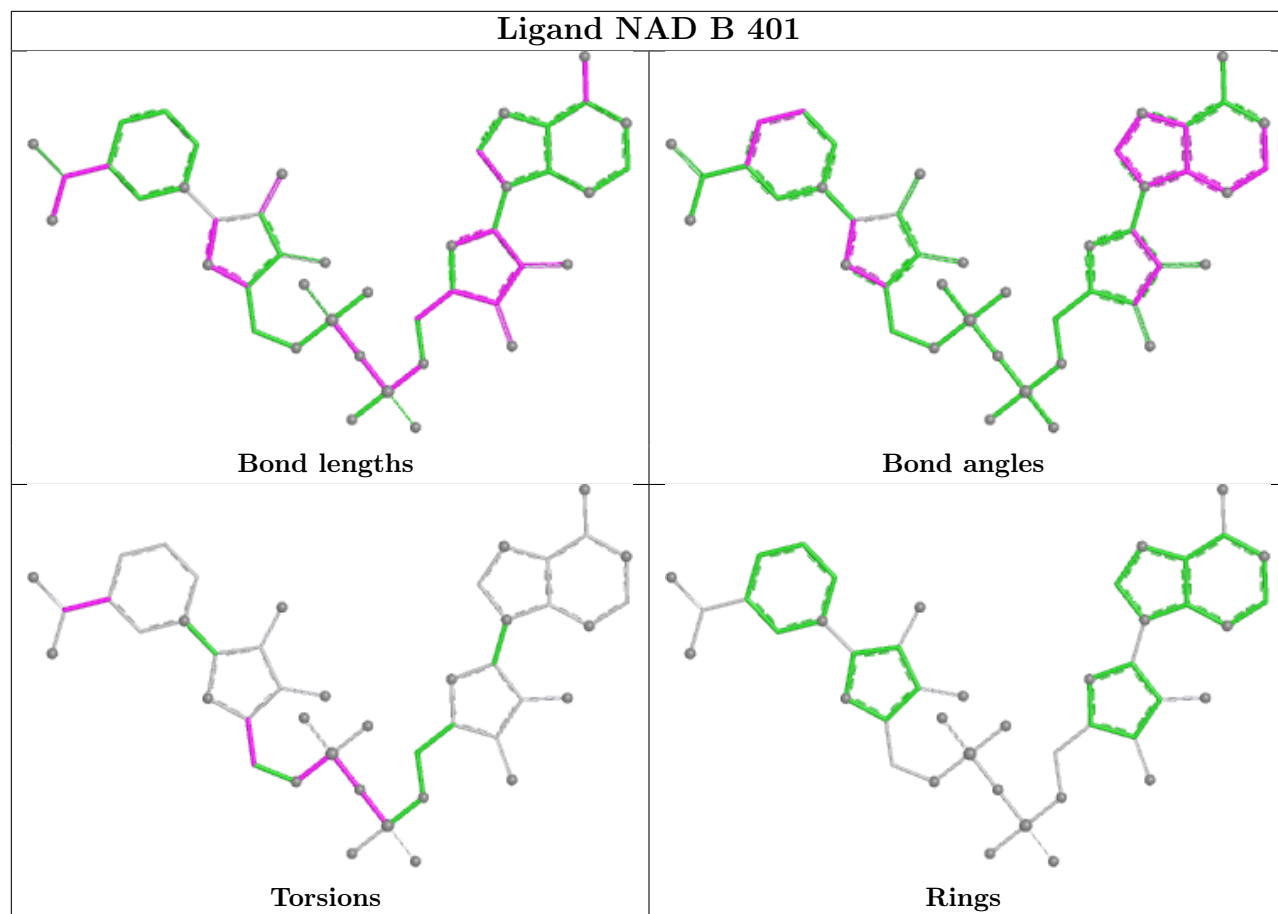
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	NAD	1	0
3	C	401	NAD	1	0
3	B	401	NAD	2	0
3	A	401	NAD	2	0

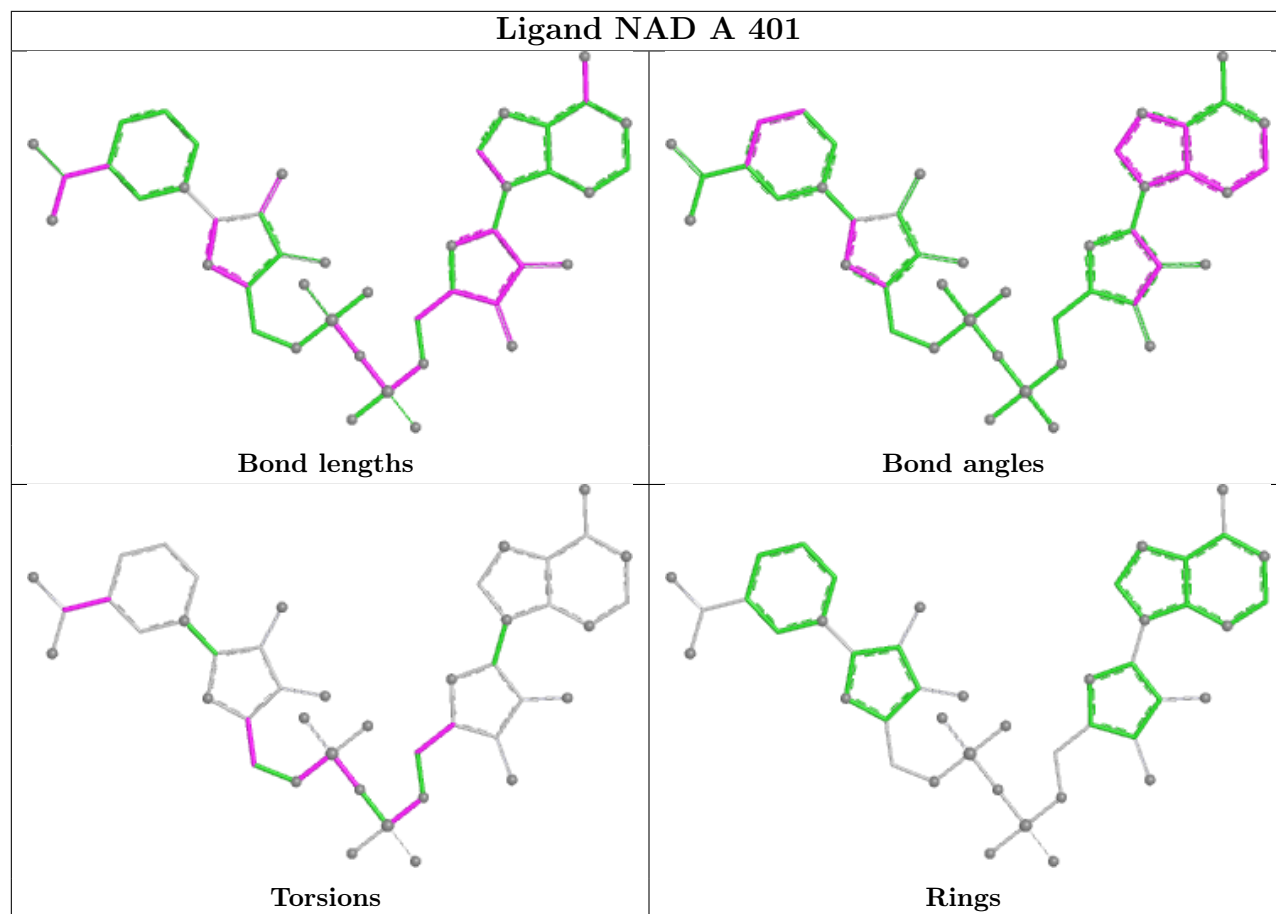
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	312/312 (100%)	-0.10	29 (9%) 14 13	13, 30, 129, 290	0
1	B	312/312 (100%)	0.04	31 (9%) 13 11	13, 33, 140, 291	0
1	C	312/312 (100%)	0.67	34 (10%) 10 9	28, 65, 141, 310	0
1	D	312/312 (100%)	0.66	31 (9%) 13 11	22, 66, 158, 369	0
2	E	129/131 (98%)	1.38	35 (27%) 1 1	36, 104, 172, 189	0
2	F	130/131 (99%)	1.31	37 (28%) 1 1	32, 108, 175, 203	0
2	G	129/131 (98%)	2.17	66 (51%) 0 0	75, 145, 205, 217	0
2	H	129/131 (98%)	2.10	66 (51%) 0 0	80, 118, 145, 179	0
All	All	1765/1772 (99%)	0.73	329 (18%) 3 3	13, 65, 175, 369	0

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	SER	9.8
1	B	285	LYS	9.4
1	B	280	ALA	9.2
1	B	281	ILE	8.6
1	B	277	PRO	8.1
1	B	282	SER	8.0
1	B	283	TRP	8.0
1	A	283	TRP	7.9
1	C	283	TRP	7.5
1	B	284	ASN	7.5
1	C	280	ALA	7.4
1	A	277	PRO	7.2
2	G	3	ILE	7.1
1	A	284	ASN	7.0
1	C	281	ILE	7.0
1	A	281	ILE	7.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	277	PRO	6.9
1	C	285	LYS	6.7
1	D	282	SER	6.6
1	D	283	TRP	6.6
1	D	285	LYS	6.5
1	A	286	ILE	6.4
1	A	280	ALA	6.4
1	D	281	ILE	6.3
1	B	111	PHE	6.3
1	B	286	ILE	6.2
2	H	74	ILE	6.1
2	F	85	ILE	6.0
1	C	282	SER	5.8
2	G	110	ILE	5.7
2	G	85	ILE	5.6
2	H	116	LEU	5.6
1	A	279	GLU	5.5
1	C	286	ILE	5.4
1	D	277	PRO	5.4
1	A	285	LYS	5.4
1	C	284	ASN	5.3
1	B	279	GLU	5.3
1	D	284	ASN	5.3
2	H	3	ILE	5.1
1	A	290	ALA	5.0
2	E	98	ILE	5.0
2	G	98	ILE	4.9
1	A	272	LEU	4.9
1	A	270	GLY	4.8
2	E	3	ILE	4.8
2	F	110	ILE	4.7
2	E	69	ILE	4.7
1	D	286	ILE	4.7
2	H	130	VAL	4.7
2	F	35	GLY	4.7
2	F	98	ILE	4.7
2	G	74	ILE	4.6
2	F	90	LEU	4.6
1	B	2	ILE	4.6
1	D	116	ALA	4.6
2	E	85	ILE	4.6
1	A	268	TYR	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	49	VAL	4.5
1	A	275	ALA	4.4
2	G	127	ILE	4.4
2	H	68	PRO	4.3
1	B	268	TYR	4.3
1	D	275	ALA	4.3
1	D	280	ALA	4.3
2	F	130	VAL	4.3
1	B	270	GLY	4.3
2	E	79	ALA	4.3
2	H	90	LEU	4.3
2	G	69	ILE	4.3
2	E	116	LEU	4.2
2	G	67	VAL	4.2
2	E	74	ILE	4.2
1	A	111	PHE	4.2
2	H	114	ALA	4.2
1	B	110	SER	4.2
2	F	127	ILE	4.2
2	H	36	LYS	4.2
2	G	65	VAL	4.2
1	D	124	HIS	4.1
2	G	119	TRP	4.1
2	H	121	ILE	4.1
2	F	34	THR	4.0
2	H	34	THR	4.0
2	G	68	PRO	4.0
2	E	110	ILE	4.0
1	B	275	ALA	4.0
2	E	90	LEU	4.0
2	E	87	VAL	4.0
1	D	288	PRO	4.0
2	F	70	ILE	3.9
1	B	1	MET	3.9
1	C	270	GLY	3.9
1	C	113	ILE	3.8
2	G	4	THR	3.8
1	D	113	ILE	3.8
1	D	268	TYR	3.8
2	G	5	TYR	3.8
1	C	273	SER	3.8
2	H	4	THR	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	70	ILE	3.7
1	B	36	PHE	3.7
1	C	36	PHE	3.7
1	B	113	ILE	3.7
2	G	125	ARG	3.7
2	H	110	ILE	3.7
2	H	67	VAL	3.7
2	G	19	ILE	3.6
1	D	290	ALA	3.6
2	H	93	TYR	3.6
2	E	119	TRP	3.6
2	F	119	TRP	3.6
2	E	78	ILE	3.6
2	G	90	LEU	3.6
2	G	87	VAL	3.6
2	G	121	ILE	3.6
2	E	114	ALA	3.6
1	A	288	PRO	3.6
1	B	288	PRO	3.6
2	H	87	VAL	3.5
1	B	272	LEU	3.5
1	C	272	LEU	3.5
1	D	36	PHE	3.5
2	E	35	GLY	3.5
2	E	36	LYS	3.5
1	A	287	ARG	3.5
1	D	111	PHE	3.4
2	G	96	PHE	3.4
1	B	278	ARG	3.4
2	H	13	VAL	3.4
2	H	106	LEU	3.4
2	E	112	PRO	3.4
2	G	49	VAL	3.4
1	A	269	ASP	3.4
2	F	93	TYR	3.3
2	G	93	TYR	3.3
2	G	92	SER	3.3
2	G	78	ILE	3.3
1	A	18	ARG	3.2
2	H	5	TYR	3.2
2	F	74	ILE	3.2
1	D	276	LYS	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	112	ASP	3.2
1	B	276	LYS	3.2
2	F	78	ILE	3.2
2	H	50	PHE	3.2
1	C	2	ILE	3.2
2	F	118	TYR	3.2
2	G	118	TYR	3.2
1	C	278	ARG	3.2
1	D	270	GLY	3.2
2	G	128	VAL	3.1
1	A	113	ILE	3.1
1	C	111	PHE	3.1
1	A	276	LYS	3.1
2	H	119	TRP	3.1
2	F	121	ILE	3.1
2	H	35	GLY	3.1
2	H	65	VAL	3.1
1	C	124	HIS	3.1
1	D	117	MET	3.1
2	F	37	HIS	3.1
2	E	88	MET	3.1
2	G	81	MET	3.1
1	B	273	SER	3.1
2	H	96	PHE	3.0
2	H	69	ILE	3.0
2	H	118	TYR	3.0
2	G	8	VAL	3.0
2	G	106	LEU	3.0
2	G	91	GLU	3.0
1	C	211	PHE	3.0
2	G	79	ALA	3.0
2	F	77	ILE	3.0
2	G	38	GLY	3.0
2	G	77	ILE	3.0
1	C	288	PRO	3.0
2	G	114	ALA	2.9
2	H	8	VAL	2.9
1	C	274	GLY	2.9
1	C	209	LEU	2.9
2	G	101	PRO	2.9
1	D	118	LEU	2.9
2	F	106	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	112	PRO	2.9
1	C	276	LYS	2.9
2	H	122	MET	2.8
1	A	273	SER	2.8
2	G	50	PHE	2.8
2	H	129	ARG	2.8
1	C	279	GLU	2.8
2	G	34	THR	2.8
2	G	83	ASN	2.8
1	A	274	GLY	2.8
2	G	75	GLY	2.8
2	E	68	PRO	2.8
2	H	37	HIS	2.8
2	F	96	PHE	2.8
1	B	290	ALA	2.8
1	C	268	TYR	2.8
2	G	116	LEU	2.8
2	G	130	VAL	2.8
2	H	128	VAL	2.8
2	F	95	THR	2.7
1	A	289	ASN	2.7
2	H	75	GLY	2.7
1	B	117	MET	2.7
2	H	70	ILE	2.7
2	E	84	LYS	2.7
2	G	33	LYS	2.7
2	F	107	ALA	2.7
2	F	101	PRO	2.7
2	E	93	TYR	2.7
2	H	29	VAL	2.7
2	E	96	PHE	2.6
1	D	272	LEU	2.6
2	G	6	THR	2.6
2	G	122	MET	2.6
2	H	101	PRO	2.6
1	A	2	ILE	2.6
2	E	130	VAL	2.6
2	F	3	ILE	2.6
2	H	123	GLY	2.6
2	H	32	ALA	2.6
1	D	8	LEU	2.6
2	F	72	LYS	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	70	ILE	2.6
2	H	85	ILE	2.6
2	G	72	LYS	2.6
2	G	86	GLN	2.5
1	D	279	GLU	2.5
2	H	53	ALA	2.5
1	D	273	SER	2.5
2	G	11	LEU	2.5
2	F	88	MET	2.5
2	H	19	ILE	2.5
1	C	112	ASP	2.5
2	G	88	MET	2.5
1	D	274	GLY	2.5
2	H	38	GLY	2.5
2	H	127	ILE	2.5
2	E	118	TYR	2.5
1	B	271	SER	2.5
2	E	83	ASN	2.5
1	A	254	ASP	2.4
2	E	4	THR	2.4
1	C	1	MET	2.4
1	C	117	MET	2.4
2	F	81	MET	2.4
2	H	88	MET	2.4
2	H	57	LEU	2.4
2	H	131	LYS	2.4
2	F	113	ASN	2.4
2	F	87	VAL	2.4
2	H	6	THR	2.4
2	F	114	ALA	2.4
2	G	46	ALA	2.4
2	G	107	ALA	2.4
1	C	133	PHE	2.4
1	A	110	SER	2.4
1	C	275	ALA	2.4
2	F	79	ALA	2.4
2	H	9	GLY	2.4
2	H	80	ASP	2.4
2	H	16	TYR	2.3
2	H	11	LEU	2.3
2	E	82	GLY	2.3
2	G	82	GLY	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	47	ILE	2.3
2	F	128	VAL	2.3
2	G	60	PRO	2.3
2	E	107	ALA	2.3
1	B	287	ARG	2.3
1	C	115	ASP	2.3
2	G	109	LYS	2.3
2	G	73	HIS	2.3
1	C	226	VAL	2.3
2	F	83	ASN	2.3
2	H	72	LYS	2.3
2	G	37	HIS	2.2
1	A	36	PHE	2.2
2	H	98	ILE	2.2
2	F	84	LYS	2.2
1	D	278	ARG	2.2
2	H	95	THR	2.2
2	G	18	VAL	2.2
1	B	269	ASP	2.2
2	H	24	CYS	2.2
2	E	100	LYS	2.2
2	G	100	LYS	2.2
2	G	112	PRO	2.2
1	B	274	GLY	2.2
2	H	56	THR	2.2
1	D	2	ILE	2.1
2	F	50	PHE	2.1
2	G	120	GLU	2.1
2	H	117	GLU	2.1
1	C	290	ALA	2.1
2	G	131	LYS	2.1
1	C	266	GLN	2.1
2	H	77	ILE	2.1
1	B	35	GLY	2.1
2	F	129	ARG	2.1
2	H	107	ALA	2.1
2	E	131	LYS	2.1
2	G	80	ASP	2.1
2	G	64	GLN	2.1
2	H	30	THR	2.1
2	H	26	VAL	2.1
2	H	40	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	79	ALA	2.1
2	E	106	LEU	2.1
1	D	54	ASP	2.1
2	G	89	ASP	2.1
1	C	287	ARG	2.1
1	D	287	ARG	2.1
2	E	73	HIS	2.1
2	H	124	ARG	2.1
2	E	72	LYS	2.1
1	B	289	ASN	2.0
2	E	34	THR	2.0
2	G	61	VAL	2.0
2	H	115	GLU	2.0
1	D	152	ALA	2.0
2	F	86	GLN	2.0
2	E	125	ARG	2.0
2	G	36	LYS	2.0
2	G	84	LYS	2.0
2	F	112	PRO	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, 95<sup>th</sup> 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.

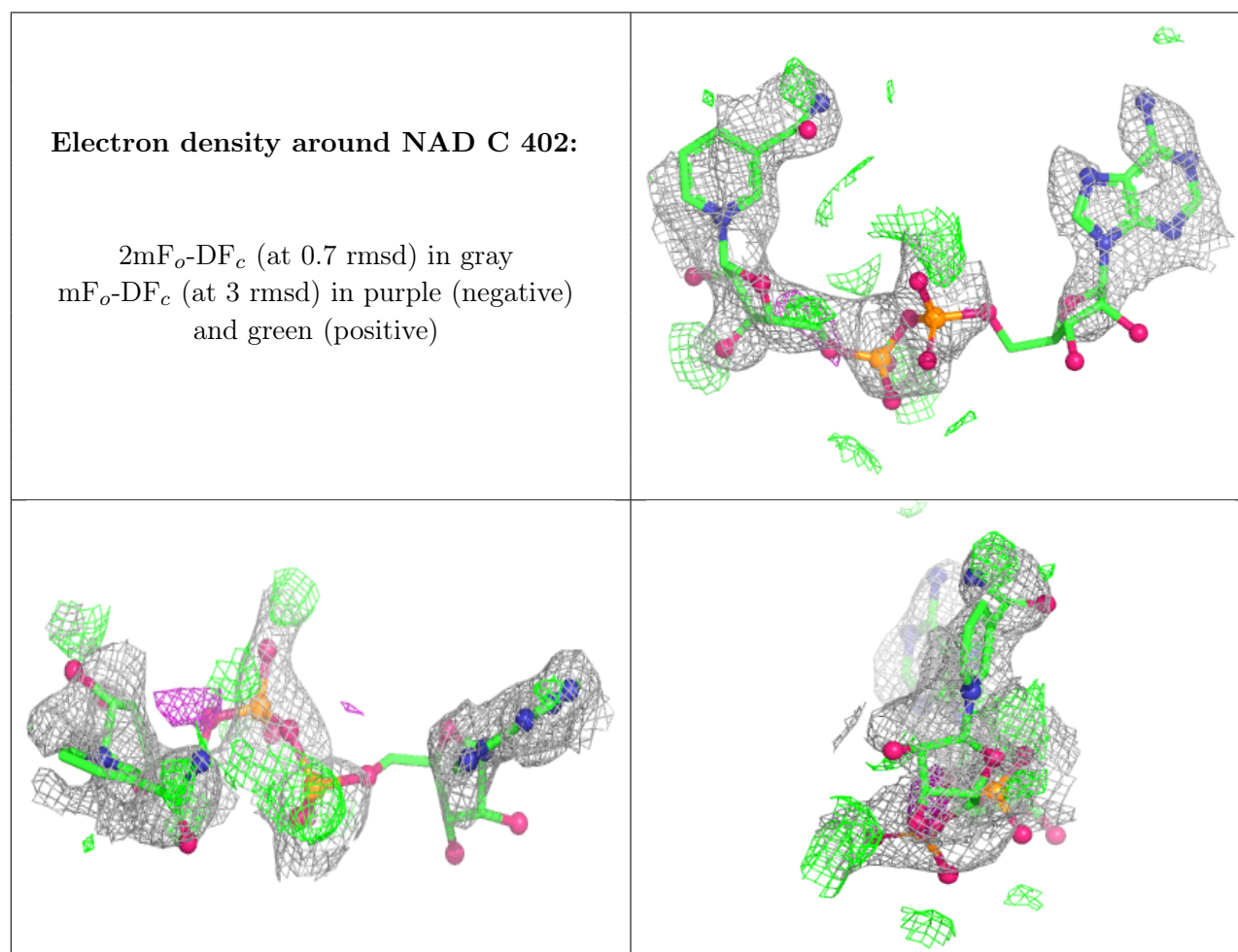
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	C	402	44/44	0.68	0.25	143,164,174,175	0
3	NAD	C	401	44/44	0.80	0.17	112,119,126,129	0
3	NAD	B	401	44/44	0.81	0.21	100,109,122,129	0
3	NAD	A	401	44/44	0.85	0.17	75,94,116,122	0

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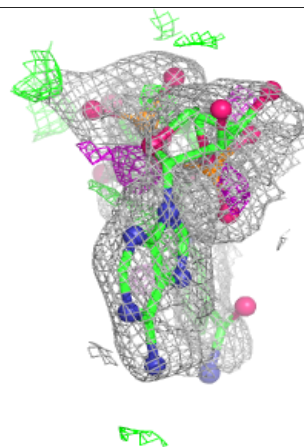
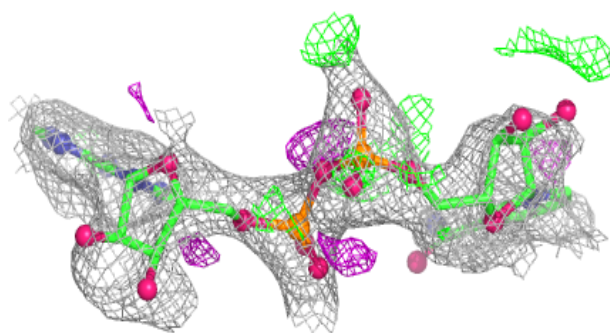
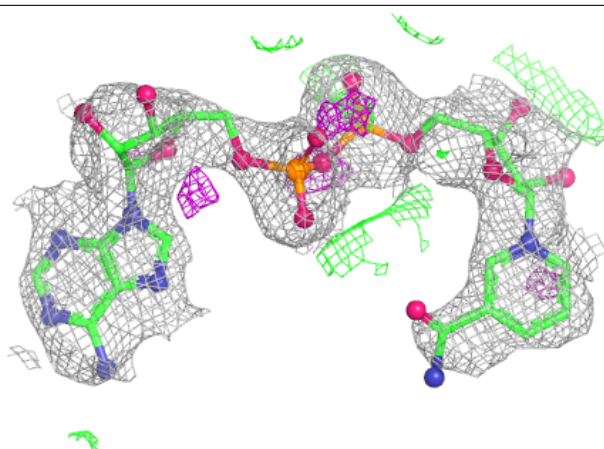
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	402	7/7	0.89	0.10	50,51,55,56	0
4	PEG	B	402	7/7	0.91	0.12	52,57,67,69	0
4	PEG	B	403	7/7	0.93	0.10	52,52,68,71	0

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



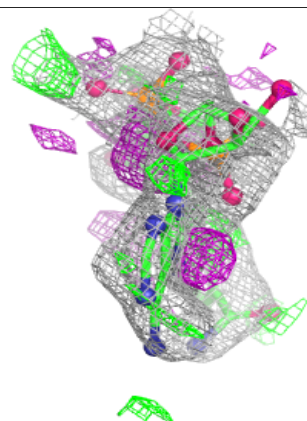
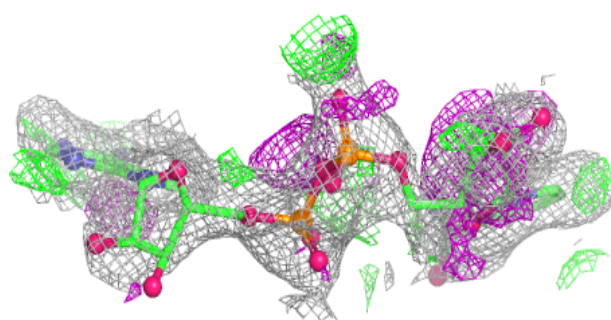
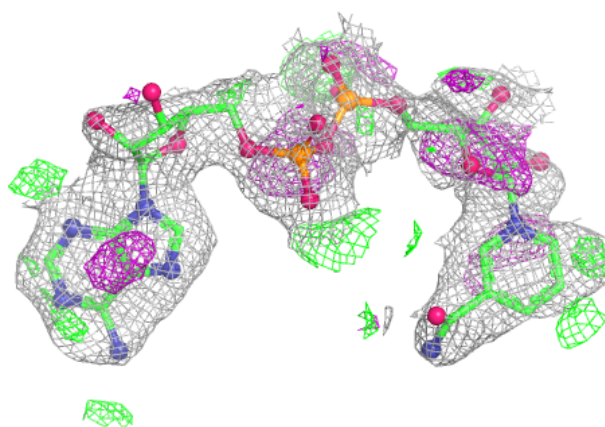
**Electron density around NAD C 401:**

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

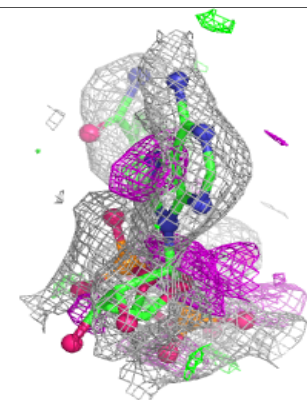
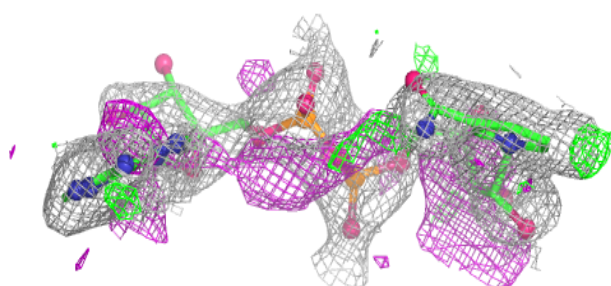
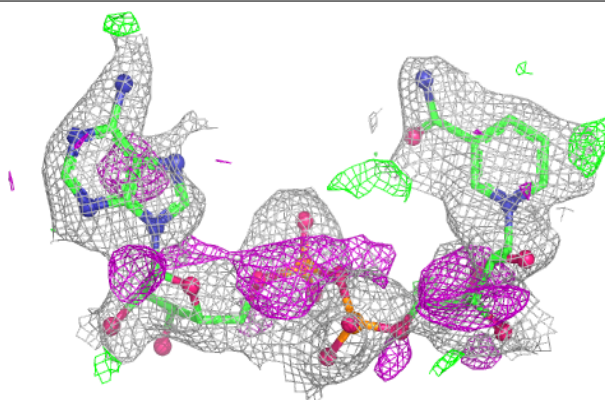


**Electron density around NAD B 401:**

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

**Electron density around NAD 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.