



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:43 AM UTC

PDB ID : 7XRE / pdb_00007xre
Title : Crystal structure of DgpA
Authors : Ma, W.; He, P.
Deposited on : 2022-05-10
Resolution : 2.76 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

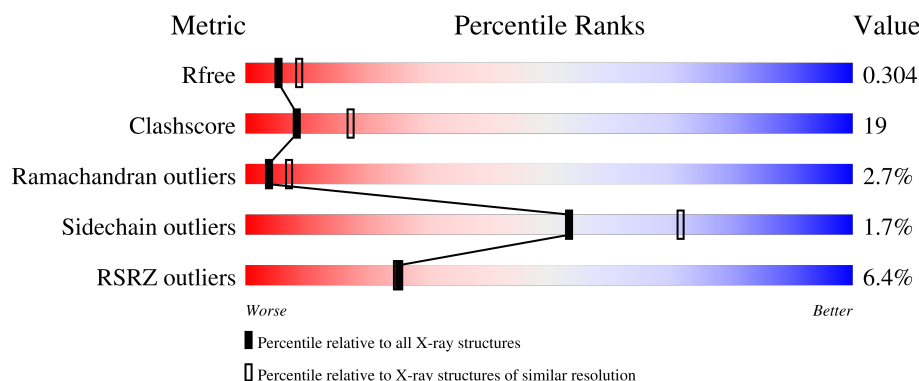
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	367	13% 58% 32% 5% ..
1	B	367	% 71% 26% .
1	C	367	6% 64% 32% ..
1	D	367	7% 66% 31% ..
1	E	367	2% 74% 24% .

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Mol	Chain	Length	Quality of chain
1	F	367	8% 62% 33% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16550 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 DgpA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2662	1666	463	518	6	9			
1	B	357	Total	C	N	O	S	Se	0	0	0
			2702	1695	466	524	7	10			
1	C	363	Total	C	N	O	S	Se	0	0	0
			2742	1723	472	530	7	10			
1	D	361	Total	C	N	O	S	Se	0	0	0
			2734	1718	469	530	7	10			
1	E	360	Total	C	N	O	S	Se	0	0	0
			2717	1704	469	527	7	10			
1	F	355	Total	C	N	O	S	Se	0	0	0
			2691	1691	463	520	7	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A3Q9WWX8
A	?	-	GLU	deletion	UNP A0A3Q9WWX8
B	0	GLY	-	expression tag	UNP A0A3Q9WWX8
B	?	-	GLU	deletion	UNP A0A3Q9WWX8
C	0	GLY	-	expression tag	UNP A0A3Q9WWX8
C	?	-	GLU	deletion	UNP A0A3Q9WWX8
D	0	GLY	-	expression tag	UNP A0A3Q9WWX8
D	?	-	GLU	deletion	UNP A0A3Q9WWX8
E	0	GLY	-	expression tag	UNP A0A3Q9WWX8
E	?	-	GLU	deletion	UNP A0A3Q9WWX8
F	0	GLY	-	expression tag	UNP A0A3Q9WWX8
F	?	-	GLU	deletion	UNP A0A3Q9WWX8

- Molecule 2 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
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		

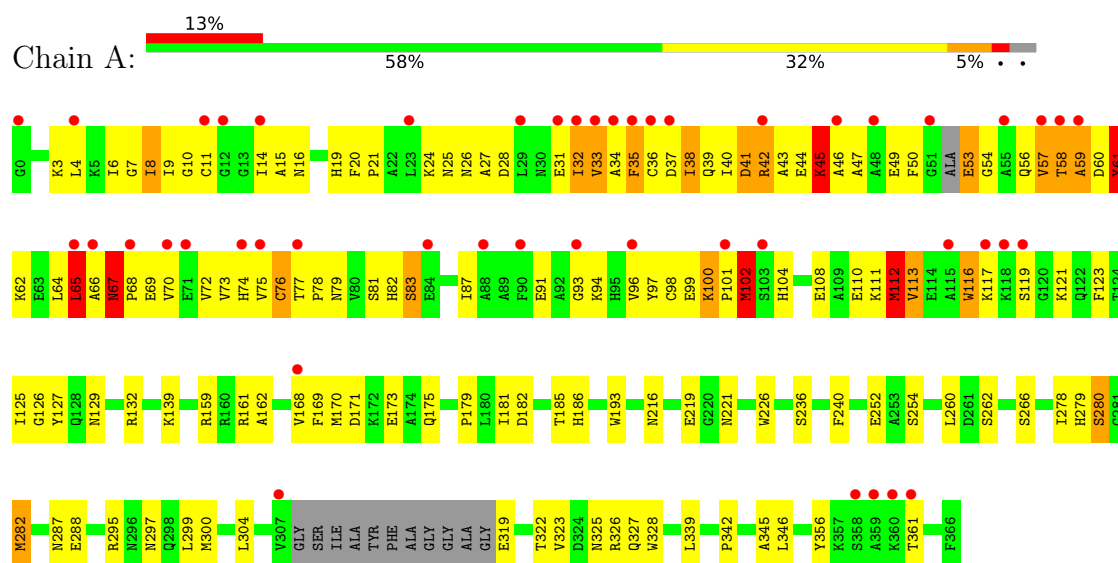
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	11	Total	O	0	0
			11	11		
3	C	4	Total	O	0	0
			4	4		
3	D	3	Total	O	0	0
			3	3		
3	E	4	Total	O	0	0
			4	4		
3	F	6	Total	O	0	0
			6	6		

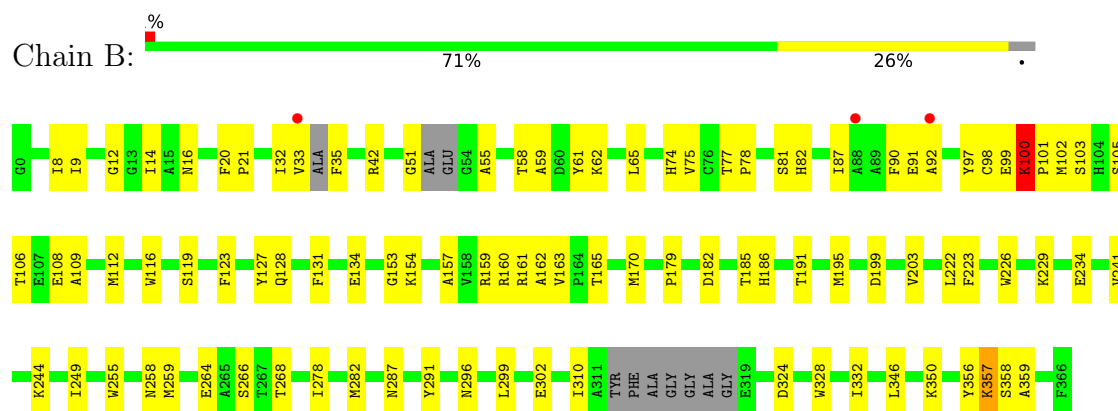
3 Residue-property plots [i](#)

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.

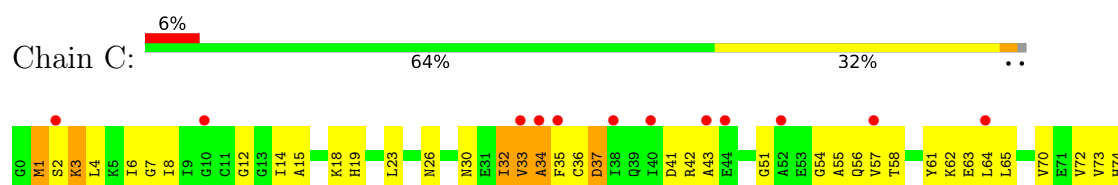
• Molecule 1: DgpA

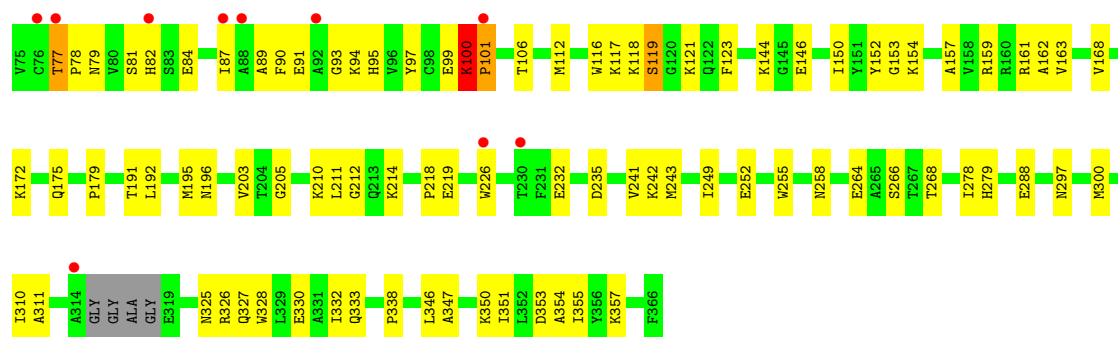


• Molecule 1: DgpA

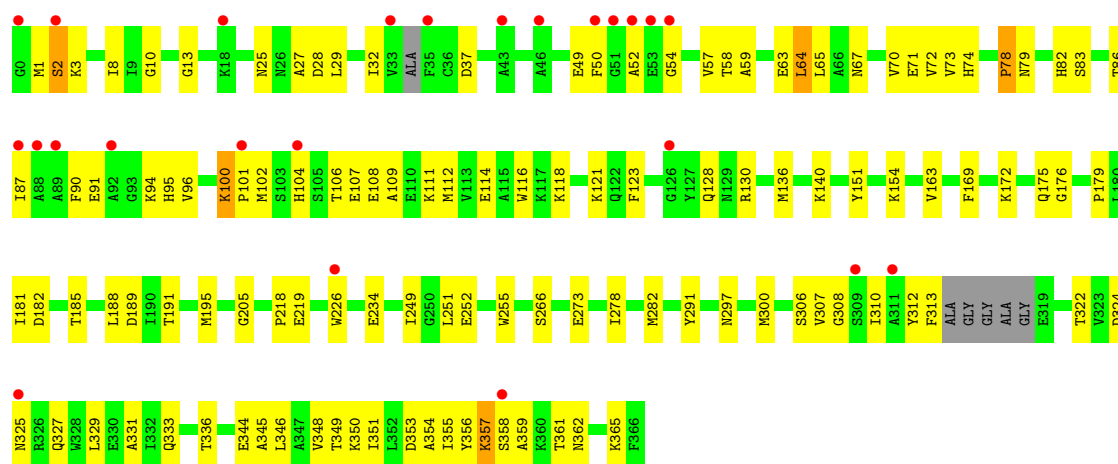


• Molecule 1: DgpA

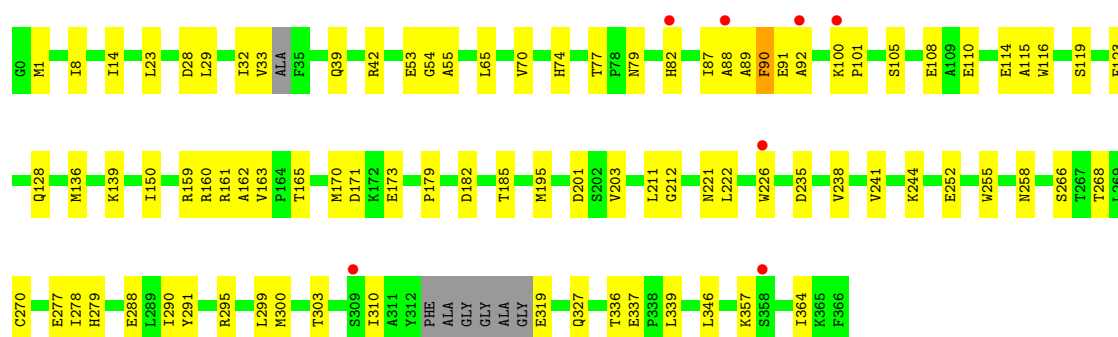
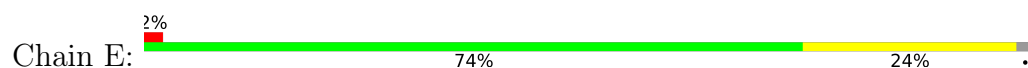




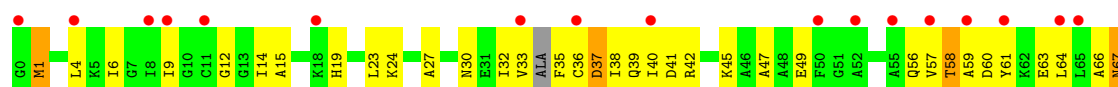
• Molecule 1: DgpA

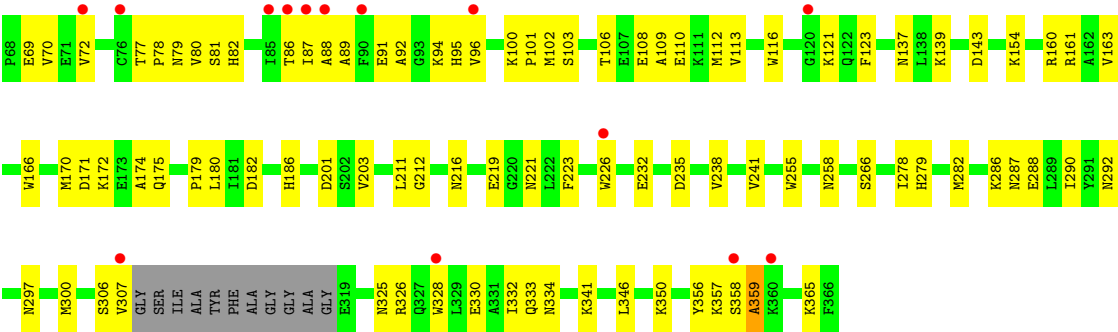


• Molecule 1: DgpA



• Molecule 1: DgpA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.79Å 130.76Å 206.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.08 – 2.76 17.08 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.5 (17.08-2.76) 93.6 (17.08-2.76)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.235 , 0.294 0.254 , 0.304	Depositor DCC
R_{free} test set	3318 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16550	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0/2701	0.90	12/3638 (0.3%)
1	B	0.26	1/2741 (0.0%)	0.56	6/3687 (0.2%)
1	C	0.28	0/2784	0.56	1/3750 (0.0%)
1	D	0.29	0/2775	0.58	2/3735 (0.1%)
1	E	0.20	0/2757	0.43	0/3711
1	F	0.41	2/2731 (0.1%)	0.62	5/3676 (0.1%)
All	All	0.34	3/16489 (0.0%)	0.62	26/22197 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	67	ASN	C-N	14.21	1.47	1.33
1	B	100	LYS	C-N	6.98	1.50	1.33
1	F	201	ASP	CA-C	5.04	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	ASN	CB-CA-C	-12.71	85.12	110.17
1	B	100	LYS	CA-C-N	11.43	134.13	119.84
1	B	100	LYS	C-N-CA	11.43	134.13	119.84
1	B	359	ALA	N-CA-C	-10.47	100.52	113.18
1	B	99	GLU	O-C-N	8.41	132.91	122.65
1	F	67	ASN	CA-C-N	8.32	129.69	120.45
1	F	67	ASN	C-N-CA	8.32	129.69	120.45
1	A	57	VAL	CA-C-N	7.47	135.81	121.54
1	A	57	VAL	C-N-CA	7.47	135.81	121.54
1	A	65	LEU	N-CA-C	-7.21	102.92	112.72
1	A	59	ALA	N-CA-C	6.80	116.31	108.49
1	F	359	ALA	N-CA-C	-6.79	104.81	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ALA	N-CA-C	6.07	116.26	108.24
1	A	35	PHE	CA-C-N	5.87	132.76	121.54
1	A	35	PHE	C-N-CA	5.87	132.76	121.54
1	D	359	ALA	N-CA-C	-5.86	106.13	113.28
1	A	102	MSE	CG-SE-CE	5.59	111.21	98.92
1	D	64	LEU	N-CA-C	-5.55	105.24	112.23
1	C	101	PRO	N-CA-C	-5.51	101.12	112.47
1	F	358	SER	CB-CA-C	5.46	117.99	111.22
1	B	99	GLU	CA-C-N	5.38	134.92	121.80
1	B	99	GLU	C-N-CA	5.38	134.92	121.80
1	A	33	VAL	CA-C-O	-5.33	114.40	120.26
1	A	57	VAL	N-CA-C	-5.32	105.94	111.58
1	A	112	MSE	CG-SE-CE	5.26	110.50	98.92
1	A	67	ASN	CB-CA-C	5.01	120.05	110.17

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	2662	0	2533	173	0
1	B	2702	0	2603	67	0
1	C	2742	0	2650	134	0
1	D	2734	0	2638	96	0
1	E	2717	0	2613	59	0
1	F	2691	0	2599	111	0
2	A	44	0	26	12	0
2	B	44	0	25	6	0
2	C	44	0	25	4	0
2	D	44	0	25	4	0
2	E	44	0	24	4	0
2	F	44	0	26	4	0
3	A	10	0	0	0	0
3	B	11	0	0	1	0
3	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	3	0	0	0	0
3	E	4	0	0	1	0
3	F	6	0	0	2	0
All	All	16550	0	15787	616	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 19.

All (616) 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:A:110:GLU:HA	1:A:113:VAL:CG1	1.50	1.38
1:C:33:VAL:CG2	1:C:56:GLN:H	1.46	1.29
1:C:100:LYS:HB3	1:C:101:PRO:CD	1.62	1.27
1:A:110:GLU:CA	1:A:113:VAL:CG1	2.18	1.20
1:A:110:GLU:CA	1:A:113:VAL:HG12	1.70	1.18
1:C:7:GLY:HA2	1:C:34:ALA:HB2	1.19	1.17
1:A:25:ASN:HD22	1:A:322:THR:HG21	1.02	1.15
1:A:25:ASN:ND2	1:A:322:THR:HG21	1.66	1.10
1:A:91:GLU:OE1	1:A:116:TRP:HB2	1.51	1.09
1:C:33:VAL:HG23	1:C:55:ALA:CB	1.81	1.09
1:A:82:HIS:O	1:A:112:MSE:HE2	1.51	1.09
1:C:100:LYS:HB3	1:C:101:PRO:HD3	1.33	1.07
1:C:33:VAL:CG2	1:C:55:ALA:HB1	1.84	1.07
1:C:8:ILE:H	1:C:34:ALA:HB1	1.07	1.06
1:A:110:GLU:HA	1:A:113:VAL:HG12	1.10	1.06
1:C:8:ILE:H	1:C:34:ALA:CB	1.69	1.05
1:C:33:VAL:HG23	1:C:55:ALA:HB1	1.08	1.05
1:A:56:GLN:HB2	1:A:58:THR:HG22	1.39	1.03
1:A:110:GLU:HA	1:A:113:VAL:HG11	1.37	1.02
1:C:33:VAL:CG2	1:C:56:GLN:N	2.20	1.02
1:C:33:VAL:HG21	1:C:56:GLN:H	1.25	1.00
1:A:100:LYS:HB3	1:A:101:PRO:HD3	1.43	1.00
1:D:70:VAL:HG13	1:D:94:LYS:HE2	1.45	0.99
1:A:110:GLU:O	1:A:113:VAL:HG13	1.61	0.99
1:B:100:LYS:HB3	1:B:101:PRO:HD3	1.43	0.98
1:F:40:ILE:CD1	1:F:58:THR:O	2.11	0.98
1:A:119:SER:HB3	1:A:121:LYS:NZ	1.79	0.98
1:A:110:GLU:C	1:A:113:VAL:HG12	1.89	0.97
1:A:56:GLN:HB2	1:A:58:THR:CG2	1.96	0.94
1:A:7:GLY:O	1:A:73:VAL:HA	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:O	1:A:113:VAL:CG1	2.17	0.91
1:A:116:TRP:CD1	1:A:123:PHE:HB2	2.05	0.91
1:C:33:VAL:HG23	1:C:56:GLN:N	1.86	0.91
1:C:100:LYS:HB3	1:C:101:PRO:HD2	1.51	0.90
1:A:82:HIS:C	1:A:112:MSE:CE	2.43	0.90
1:C:79:ASN:HB2	1:C:175:GLN:HA	1.54	0.90
1:A:91:GLU:OE1	1:A:116:TRP:CB	2.19	0.89
1:D:70:VAL:HG13	1:D:94:LYS:CE	2.01	0.89
1:B:100:LYS:HE2	2:B:401:NAD:C2N	2.03	0.89
1:F:100:LYS:NZ	1:F:182:ASP:O	2.05	0.88
1:C:35:PHE:O	1:C:43:ALA:HB1	1.73	0.88
1:D:70:VAL:O	1:D:94:LYS:HE3	1.74	0.88
1:C:100:LYS:CB	1:C:101:PRO:CD	2.49	0.87
1:A:20:PHE:HB2	1:A:21:PRO:HD3	1.57	0.87
1:A:110:GLU:C	1:A:113:VAL:CG1	2.45	0.86
1:B:8:ILE:HD13	1:B:20:PHE:HE1	1.40	0.86
1:D:100:LYS:HB3	1:D:101:PRO:HD3	1.58	0.86
1:A:82:HIS:C	1:A:112:MSE:HE2	2.01	0.85
1:C:6:ILE:HB	1:C:32:ILE:HG22	1.60	0.84
1:A:32:ILE:H	1:A:32:ILE:HD12	1.40	0.84
1:A:119:SER:HB3	1:A:121:LYS:HZ2	1.43	0.84
1:A:119:SER:CB	1:A:121:LYS:NZ	2.41	0.84
1:A:119:SER:CB	1:A:121:LYS:HZ1	1.91	0.83
1:C:310:ILE:HG22	1:C:311:ALA:H	1.45	0.81
1:A:56:GLN:CB	1:A:58:THR:HG22	2.11	0.81
1:C:7:GLY:CA	1:C:34:ALA:HB2	2.08	0.80
1:C:8:ILE:N	1:C:34:ALA:HB1	1.91	0.80
1:E:100:LYS:HB2	2:E:401:NAD:H2N	1.64	0.80
1:F:72:VAL:HG22	1:F:95:HIS:HB2	1.64	0.80
1:C:32:ILE:O	1:C:51:GLY:HA2	1.83	0.78
1:A:110:GLU:CA	1:A:113:VAL:HG11	2.03	0.78
1:F:14:ILE:HD12	2:F:401:NAD:C2N	2.14	0.78
1:C:8:ILE:N	1:C:34:ALA:CB	2.47	0.78
1:A:60:ASP:O	1:A:62:LYS:N	2.17	0.77
1:C:195:MSE:HE1	1:C:249:ILE:HG12	1.66	0.77
1:A:82:HIS:O	1:A:112:MSE:CE	2.30	0.77
1:C:211:LEU:N	1:C:235:ASP:OD2	2.17	0.76
1:F:15:ALA:HA	1:F:19:HIS:HB2	1.65	0.76
1:A:25:ASN:HD22	1:A:322:THR:CG2	1.92	0.76
1:C:58:THR:HG21	1:C:64:LEU:HB2	1.67	0.76
1:D:70:VAL:CG1	1:D:94:LYS:HE2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ALA:HA	1:F:112:MSE:HE3	1.68	0.75
1:F:108:GLU:OE2	3:F:502:HOH:O	2.04	0.75
1:B:191:THR:HG22	1:B:195:MSE:HE2	1.69	0.74
1:C:33:VAL:HG23	1:C:55:ALA:CA	2.17	0.74
1:F:14:ILE:HD12	2:F:401:NAD:C3N	2.16	0.74
1:F:40:ILE:HD11	1:F:58:THR:O	1.86	0.74
1:A:94:LYS:O	1:A:121:LYS:HD2	1.86	0.74
1:B:100:LYS:CE	2:B:401:NAD:C2N	2.66	0.74
1:D:82:HIS:O	1:D:86:THR:OG1	2.06	0.74
1:A:6:ILE:HA	1:A:72:VAL:HB	1.69	0.73
1:A:38:ILE:HG21	2:A:401:NAD:C8A	2.18	0.73
1:F:292:ASN:OD1	3:F:501:HOH:O	2.04	0.73
1:C:79:ASN:OD1	1:C:101:PRO:HG2	1.89	0.73
1:F:106:THR:HG23	1:F:350:LYS:HG2	1.69	0.73
1:A:83:SER:HA	1:A:112:MSE:HE3	1.70	0.73
1:E:100:LYS:HB3	1:E:101:PRO:HD3	1.69	0.73
1:D:64:LEU:C	1:D:64:LEU:HD23	2.13	0.72
1:C:354:ALA:HA	1:C:357:LYS:HE2	1.71	0.72
1:A:62:LYS:O	1:A:65:LEU:HG	1.90	0.72
1:B:170:MSE:HE1	1:B:226:TRP:HB2	1.70	0.72
1:C:23:LEU:O	1:C:30:ASN:ND2	2.21	0.72
1:A:32:ILE:HD12	1:A:32:ILE:N	2.05	0.72
1:A:42:ARG:CG	1:A:42:ARG:HH21	2.02	0.72
1:B:102:MSE:HE3	1:B:109:ALA:HB1	1.72	0.71
1:F:33:VAL:HG21	1:F:70:VAL:HG12	1.72	0.71
1:B:109:ALA:HA	1:B:112:MSE:HE3	1.73	0.71
1:D:3:LYS:NZ	1:D:27:ALA:O	2.23	0.71
1:A:42:ARG:HB3	1:A:42:ARG:NH2	2.05	0.71
1:A:42:ARG:HH21	1:A:42:ARG:HB3	1.53	0.71
1:D:130:ARG:NH2	1:D:189:ASP:OD1	2.22	0.71
1:A:38:ILE:CG2	2:A:401:NAD:N9A	2.54	0.70
1:F:102:MSE:HE3	1:F:109:ALA:HB1	1.73	0.70
1:A:60:ASP:C	1:A:62:LYS:H	1.99	0.70
1:B:100:LYS:HD3	1:B:182:ASP:O	1.90	0.70
1:C:191:THR:HG22	1:C:195:MSE:HE2	1.73	0.70
1:C:79:ASN:HA	1:C:82:HIS:CD2	2.27	0.70
1:A:39:GLN:H	1:A:42:ARG:HD2	1.56	0.70
1:A:83:SER:N	1:A:112:MSE:HE3	2.06	0.69
1:C:33:VAL:CB	1:C:55:ALA:HB1	2.21	0.69
1:C:243:MSE:HE3	1:C:249:ILE:HD12	1.75	0.69
1:F:40:ILE:HD13	1:F:58:THR:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG23	2:A:401:NAD:C1B	2.23	0.68
1:F:91:GLU:OE2	1:F:116:TRP:HA	1.92	0.68
1:E:65:LEU:HD13	1:E:89:ALA:HB1	1.75	0.68
1:E:201:ASP:HB2	1:E:244:LYS:HG2	1.76	0.68
1:D:28:ASP:HB2	1:D:29:LEU:HD22	1.75	0.68
1:D:313:PHE:HA	1:F:223:PHE:HE1	1.57	0.68
1:F:88:ALA:O	1:F:92:ALA:N	2.25	0.68
1:F:332:ILE:HG13	1:F:333:GLN:H	1.58	0.68
1:C:90:PHE:O	1:C:94:LYS:HG2	1.94	0.68
1:A:83:SER:CA	1:A:112:MSE:HE3	2.25	0.67
1:A:56:GLN:CB	1:A:58:THR:CG2	2.71	0.67
1:A:78:PRO:HG3	1:A:168:VAL:HG11	1.77	0.67
1:C:26:ASN:HD22	1:C:326:ARG:HH11	1.41	0.66
1:A:45:LYS:HA	1:A:49:GLU:HG3	1.77	0.66
1:E:77:THR:O	1:E:82:HIS:HE1	1.78	0.66
1:D:100:LYS:HB2	2:D:401:NAD:H2N	1.77	0.65
1:F:332:ILE:HG13	1:F:333:GLN:N	2.11	0.65
1:A:100:LYS:CB	1:A:101:PRO:HD3	2.21	0.65
1:E:87:ILE:O	1:E:89:ALA:N	2.30	0.65
1:A:3:LYS:HG2	1:A:31:GLU:HG3	1.76	0.65
1:C:7:GLY:HA2	1:C:34:ALA:CB	2.11	0.65
1:F:116:TRP:CD1	1:F:123:PHE:HB2	2.31	0.65
1:A:38:ILE:O	1:A:38:ILE:HG12	1.96	0.65
1:E:268:THR:HG23	1:E:277:GLU:HB3	1.78	0.65
1:A:119:SER:HB2	1:A:121:LYS:HZ1	1.60	0.65
1:A:252:GLU:OE2	1:F:154:LYS:NZ	2.30	0.65
1:E:8:ILE:HD13	1:E:74:HIS:HB2	1.79	0.65
1:D:128:GLN:HE22	2:D:401:NAD:H72N	1.43	0.65
1:F:6:ILE:HD12	1:F:72:VAL:HB	1.79	0.65
1:B:100:LYS:CB	1:B:101:PRO:HD3	2.15	0.64
1:C:214:LYS:HE3	1:D:273:GLU:OE2	1.98	0.64
1:F:58:THR:HG22	1:F:60:ASP:H	1.61	0.64
1:A:42:ARG:HH21	1:A:42:ARG:CB	2.09	0.64
1:A:65:LEU:HD23	1:A:65:LEU:N	2.13	0.64
1:E:105:SER:HB3	1:E:108:GLU:HB2	1.80	0.64
1:C:161:ARG:NH2	1:C:258:ASN:OD1	2.23	0.63
1:D:37:ASP:OD1	2:D:401:NAD:O2B	2.15	0.63
1:B:356:TYR:C	1:B:358:SER:H	2.06	0.63
1:D:29:LEU:HD12	1:D:333:GLN:HE22	1.62	0.63
1:D:95:HIS:CE1	1:D:121:LYS:HD3	2.32	0.63
1:A:15:ALA:HA	1:A:19:HIS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:VAL:HG23	1:D:123:PHE:CD1	2.33	0.63
1:D:100:LYS:HE3	1:D:101:PRO:HD3	1.81	0.62
2:F:401:NAD:O1N	2:F:401:NAD:H6N	1.99	0.62
1:E:212:GLY:O	1:E:226:TRP:HZ3	1.82	0.62
1:A:110:GLU:CB	1:A:113:VAL:HG11	2.29	0.62
1:A:20:PHE:HB3	1:A:50:PHE:CE1	2.34	0.62
1:A:82:HIS:C	1:A:112:MSE:HE3	2.23	0.62
1:B:8:ILE:HD13	1:B:20:PHE:CE1	2.29	0.62
1:A:56:GLN:OE1	1:A:56:GLN:N	2.20	0.62
1:A:25:ASN:ND2	1:A:322:THR:CG2	2.56	0.62
1:B:100:LYS:HE2	2:B:401:NAD:H2N	1.82	0.62
1:C:152:TYR:OH	1:D:252:GLU:OE2	2.16	0.62
1:A:16:ASN:HA	1:A:20:PHE:CD2	2.35	0.61
1:A:38:ILE:HG21	2:A:401:NAD:N9A	2.15	0.61
1:E:161:ARG:HG2	1:E:221:ASN:HA	1.82	0.61
1:A:38:ILE:HG23	2:A:401:NAD:H1B	1.82	0.61
1:A:170:MSE:HE1	1:A:226:TRP:HB2	1.81	0.61
1:A:42:ARG:HH21	1:A:42:ARG:HG2	1.65	0.61
1:A:116:TRP:NE1	1:A:123:PHE:HB2	2.16	0.61
1:B:154:LYS:HB2	1:B:268:THR:HB	1.83	0.61
1:D:73:VAL:HG23	1:D:96:VAL:HG12	1.83	0.61
1:D:205:GLY:HA3	1:D:355:ILE:HG23	1.81	0.61
1:A:6:ILE:N	1:A:31:GLU:O	2.22	0.61
1:B:90:PHE:C	1:B:92:ALA:H	2.09	0.60
1:F:38:ILE:HG13	1:F:39:GLN:N	2.15	0.60
1:F:58:THR:HG22	1:F:60:ASP:N	2.17	0.60
1:A:56:GLN:CG	1:A:58:THR:CG2	2.80	0.60
1:C:100:LYS:HD2	1:C:101:PRO:HD3	1.84	0.60
1:F:78:PRO:O	1:F:81:SER:OG	2.16	0.60
1:C:100:LYS:HB2	2:C:401:NAD:H2N	1.83	0.60
1:A:96:VAL:HG13	1:A:123:PHE:CD1	2.37	0.59
1:C:33:VAL:HG23	1:C:55:ALA:C	2.27	0.59
1:A:56:GLN:HB2	1:A:58:THR:HG21	1.84	0.59
1:F:103:SER:HB3	1:F:112:MSE:HE1	1.83	0.59
1:A:113:VAL:HG23	1:A:117:LYS:HE3	1.83	0.59
1:E:179:PRO:HB3	1:E:255:TRP:CD1	2.38	0.59
1:E:279:HIS:HB2	1:E:288:GLU:HB2	1.84	0.59
1:E:89:ALA:O	1:E:91:GLU:N	2.36	0.59
1:F:47:ALA:CB	1:F:57:VAL:HG11	2.33	0.59
1:A:3:LYS:HG2	1:A:31:GLU:CG	2.32	0.59
1:D:188:LEU:HG	1:D:251:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:HG2	1:D:297:ASN:HA	1.85	0.58
1:F:56:GLN:HG2	1:F:56:GLN:O	2.03	0.58
1:B:33:VAL:HA	1:B:55:ALA:HB1	1.85	0.58
1:A:56:GLN:HG3	1:A:58:THR:CG2	2.32	0.58
1:A:169:PHE:HA	1:A:175:GLN:HG3	1.84	0.58
1:C:100:LYS:CD	1:C:101:PRO:HD3	2.34	0.58
1:A:102:MSE:HE3	1:A:345:ALA:HB3	1.85	0.58
1:D:107:GLU:O	1:D:111:LYS:HG2	2.04	0.58
1:E:33:VAL:HG23	1:E:70:VAL:HG12	1.85	0.58
1:F:100:LYS:HB3	1:F:101:PRO:HD3	1.85	0.58
1:D:361:THR:O	1:D:361:THR:HG22	2.02	0.57
1:A:75:VAL:HG22	1:A:98:CYS:HA	1.85	0.57
1:A:297:ASN:HA	1:F:219:GLU:HG2	1.86	0.57
1:A:91:GLU:CD	1:A:116:TRP:HB2	2.29	0.57
1:E:77:THR:O	2:E:401:NAD:H4D	2.04	0.57
1:B:75:VAL:HG22	1:B:98:CYS:HA	1.87	0.57
1:C:26:ASN:ND2	1:C:326:ARG:HD2	2.19	0.57
1:D:114:GLU:OE1	1:D:118:LYS:NZ	2.34	0.57
1:A:279:HIS:HB2	1:A:288:GLU:HB2	1.86	0.57
1:C:252:GLU:OE2	1:D:154:LYS:HE3	2.04	0.57
1:A:127:TYR:OH	1:A:185:THR:OG1	2.23	0.57
1:C:3:LYS:HG3	1:C:4:LEU:H	1.69	0.57
1:C:100:LYS:CB	1:C:101:PRO:HD3	2.19	0.57
1:C:72:VAL:HG13	1:C:95:HIS:HB2	1.86	0.56
1:D:64:LEU:HD23	1:D:64:LEU:O	2.05	0.56
1:C:65:LEU:HD23	1:C:90:PHE:HA	1.87	0.56
1:C:300:MSE:HE1	1:E:291:TYR:CE2	2.40	0.56
1:A:26:ASN:OD1	1:A:326:ARG:HB2	2.05	0.56
1:A:60:ASP:C	1:A:62:LYS:N	2.64	0.56
1:B:159:ARG:HD3	1:B:162:ALA:HB3	1.88	0.56
1:A:74:HIS:CD2	1:A:97:TYR:HB3	2.40	0.56
1:C:7:GLY:O	1:C:73:VAL:HA	2.06	0.56
1:C:327:GLN:OE1	1:C:338:PRO:HA	2.05	0.56
1:C:87:ILE:O	1:C:89:ALA:N	2.33	0.55
1:C:23:LEU:HD13	1:C:32:ILE:HG21	1.87	0.55
1:A:93:GLY:H	1:A:121:LYS:HE3	1.71	0.55
1:A:3:LYS:CG	1:A:31:GLU:HG3	2.36	0.55
1:C:279:HIS:HB2	1:C:288:GLU:HB2	1.88	0.55
1:D:195:MSE:HE1	1:D:249:ILE:HG13	1.88	0.55
1:E:161:ARG:NH2	1:E:258:ASN:OD1	2.38	0.55
1:F:47:ALA:HB2	1:F:57:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ALA:HA	1:C:19:HIS:HB2	1.89	0.55
1:C:70:VAL:HG12	1:C:94:LYS:NZ	2.22	0.55
1:D:218:PRO:HG3	1:D:226:TRP:CD2	2.42	0.55
1:A:304:LEU:HD23	1:D:300:MSE:HG2	1.88	0.54
1:F:171:ASP:HB3	1:F:174:ALA:HB3	1.89	0.54
1:C:23:LEU:C	1:C:30:ASN:HD21	2.13	0.54
1:A:3:LYS:HB3	1:A:31:GLU:HG3	1.89	0.54
1:A:91:GLU:OE1	1:A:116:TRP:CA	2.56	0.54
1:B:77:THR:OG1	1:B:81:SER:OG	2.22	0.54
1:E:100:LYS:NZ	1:E:182:ASP:O	2.37	0.54
1:A:159:ARG:HD3	1:A:162:ALA:HB3	1.90	0.54
1:A:280:SER:OG	1:A:287:ASN:OD1	2.24	0.54
1:B:12:GLY:O	1:B:16:ASN:ND2	2.36	0.54
1:D:91:GLU:OE2	1:D:116:TRP:HA	2.07	0.54
1:D:351:ILE:O	1:D:355:ILE:HG13	2.07	0.54
1:C:203:VAL:HG22	1:C:241:VAL:HG13	1.90	0.54
1:B:163:VAL:HG22	1:B:255:TRP:HB3	1.90	0.54
1:C:65:LEU:CD2	1:C:90:PHE:HA	2.38	0.54
1:C:242:LYS:NZ	1:D:205:GLY:O	2.41	0.54
1:C:159:ARG:HD3	1:C:162:ALA:HB3	1.90	0.54
1:D:71:GLU:O	1:D:94:LYS:HB3	2.07	0.54
1:A:127:TYR:HH	1:A:185:THR:HG1	1.55	0.54
1:F:266:SER:HB3	1:F:278:ILE:O	2.08	0.54
1:A:37:ASP:CB	1:A:43:ALA:HB2	2.38	0.54
1:A:100:LYS:HG3	1:A:186:HIS:CE1	2.43	0.54
1:C:70:VAL:HG12	1:C:94:LYS:HZ1	1.73	0.53
1:C:195:MSE:HE1	1:C:249:ILE:CG1	2.37	0.53
1:A:61:TYR:CD1	1:A:61:TYR:C	2.86	0.53
1:A:38:ILE:CG2	2:A:401:NAD:C4A	2.86	0.53
1:F:67:ASN:OD1	1:F:69:GLU:N	2.29	0.53
1:C:72:VAL:HG21	1:C:332:ILE:HD12	1.90	0.53
1:F:80:VAL:HG23	1:F:175:GLN:HA	1.90	0.53
1:A:171:ASP:OD2	1:A:173:GLU:HG2	2.07	0.53
1:E:77:THR:O	1:E:82:HIS:CE1	2.62	0.53
1:B:90:PHE:O	1:B:92:ALA:N	2.41	0.53
1:C:179:PRO:HB3	1:C:255:TRP:CD1	2.44	0.53
1:B:179:PRO:HD2	1:B:234:GLU:HG2	1.89	0.53
1:D:106:THR:HG23	1:D:353:ASP:OD2	2.09	0.53
1:A:91:GLU:OE1	1:A:116:TRP:HA	2.09	0.53
1:C:61:TYR:O	1:C:64:LEU:N	2.42	0.53
1:C:346:LEU:O	1:C:350:LYS:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ASP:O	1:C:357:LYS:HG3	2.09	0.53
1:C:297:ASN:HA	1:D:219:GLU:HG2	1.90	0.52
1:F:45:LYS:HE3	1:F:45:LYS:HA	1.91	0.52
1:C:1:MSE:SE	1:C:1:MSE:C	3.02	0.52
1:C:3:LYS:HG3	1:C:4:LEU:N	2.24	0.52
1:E:336:THR:HG22	1:E:337:GLU:H	1.71	0.52
1:A:8:ILE:HD11	1:A:11:CYS:SG	2.48	0.52
1:E:357:LYS:HB3	1:E:364:ILE:HD11	1.90	0.52
1:F:172:LYS:H	1:F:232:GLU:HG3	1.74	0.52
1:F:58:THR:CG2	1:F:60:ASP:H	2.22	0.52
1:C:347:ALA:O	1:C:351:ILE:HG13	2.09	0.52
1:D:188:LEU:HG	1:D:251:LEU:HD12	1.92	0.52
1:D:331:ALA:HA	1:D:336:THR:OG1	2.10	0.52
1:D:100:LYS:NZ	1:D:181:ILE:O	2.41	0.52
1:C:266:SER:HB3	1:C:278:ILE:O	2.09	0.52
1:E:150:ILE:HD12	1:E:195:MSE:HA	1.92	0.52
1:B:259:MSE:HG2	1:E:270:CYS:SG	2.50	0.52
1:C:74:HIS:CD2	1:C:97:TYR:HB3	2.45	0.51
1:F:64:LEU:O	1:F:64:LEU:HD23	2.10	0.51
1:A:100:LYS:HB3	1:A:101:PRO:CD	2.30	0.51
1:C:32:ILE:C	1:C:32:ILE:HD12	2.34	0.51
1:E:39:GLN:HG2	1:E:42:ARG:HE	1.76	0.51
1:C:191:THR:HG22	1:C:195:MSE:CE	2.39	0.51
1:F:113:VAL:HG23	1:F:116:TRP:HE3	1.75	0.51
1:F:326:ARG:NH1	1:F:330:GLU:OE2	2.43	0.51
1:F:235:ASP:OD1	1:F:235:ASP:N	2.44	0.51
1:A:38:ILE:CG2	2:A:401:NAD:C1B	2.87	0.51
1:F:330:GLU:O	1:F:334:ASN:HB2	2.11	0.51
1:A:76:CYS:O	2:A:401:NAD:H51N	2.10	0.51
1:B:160:ARG:HD3	1:E:299:LEU:HD13	1.92	0.51
1:E:32:ILE:HG12	3:E:502:HOH:O	2.11	0.51
1:F:36:CYS:O	1:F:37:ASP:HB2	2.10	0.51
1:F:139:LYS:HE2	1:F:143:ASP:OD2	2.10	0.51
1:B:9:ILE:HD13	1:B:61:TYR:HB2	1.93	0.51
1:B:100:LYS:HG3	1:B:186:HIS:NE2	2.26	0.51
1:C:36:CYS:O	1:C:37:ASP:HB2	2.10	0.50
1:C:58:THR:CG2	1:C:64:LEU:HB2	2.39	0.50
1:F:79:ASN:H	1:F:175:GLN:HG3	1.75	0.50
1:A:161:ARG:HG3	1:A:221:ASN:HA	1.93	0.50
1:C:163:VAL:HG22	1:C:255:TRP:HB3	1.93	0.50
1:D:324:ASP:O	1:D:327:GLN:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLU:C	1:C:93:GLY:H	2.19	0.50
1:D:179:PRO:HB3	1:D:255:TRP:CD1	2.46	0.50
1:D:356:TYR:C	1:D:358:SER:H	2.17	0.50
1:F:23:LEU:O	1:F:30:ASN:ND2	2.26	0.50
1:D:70:VAL:O	1:D:94:LYS:CE	2.53	0.50
1:D:266:SER:HB3	1:D:278:ILE:O	2.11	0.50
1:A:99:GLU:OE2	1:A:99:GLU:HA	2.11	0.50
1:E:235:ASP:OD1	1:E:235:ASP:N	2.41	0.50
1:E:266:SER:HB3	1:E:278:ILE:O	2.12	0.50
1:F:70:VAL:O	1:F:94:LYS:HD2	2.12	0.50
1:A:240:PHE:HZ	1:F:238:VAL:HG23	1.77	0.50
1:B:116:TRP:O	1:B:119:SER:OG	2.23	0.50
1:F:58:THR:HG21	1:F:63:GLU:HB3	1.93	0.50
1:A:119:SER:HB3	1:A:121:LYS:HZ1	1.51	0.49
1:A:266:SER:HB3	1:A:278:ILE:O	2.12	0.49
1:C:61:TYR:O	1:C:63:GLU:N	2.45	0.49
1:A:260:LEU:HD21	1:F:290:ILE:HG21	1.95	0.49
1:B:296:ASN:ND2	1:F:137:ASN:O	2.45	0.49
1:D:25:ASN:HD22	1:D:322:THR:HG21	1.77	0.49
1:D:169:PHE:HA	1:D:175:GLN:HG3	1.95	0.49
1:D:310:ILE:C	1:D:312:TYR:H	2.19	0.49
1:A:20:PHE:HB3	1:A:50:PHE:CZ	2.46	0.49
1:A:104:HIS:ND1	1:A:104:HIS:N	2.60	0.49
1:A:179:PRO:HA	1:A:182:ASP:HB3	1.94	0.49
1:B:291:TYR:HE1	1:F:300:MSE:HE1	1.76	0.49
1:D:108:GLU:O	1:D:112:MSE:HG3	2.12	0.49
1:F:38:ILE:HG13	1:F:39:GLN:H	1.76	0.49
1:C:36:CYS:SG	1:C:37:ASP:N	2.82	0.49
1:C:116:TRP:CD1	1:C:123:PHE:HB2	2.48	0.49
1:A:56:GLN:CG	1:A:58:THR:HG22	2.41	0.49
1:E:165:THR:HA	1:E:170:MSE:HE2	1.95	0.49
1:E:171:ASP:OD1	1:E:173:GLU:HB2	2.13	0.49
1:A:67:ASN:C	1:A:69:GLU:H	2.20	0.49
1:A:116:TRP:CZ2	1:A:342:PRO:HG2	2.48	0.49
1:D:79:ASN:HB2	1:D:175:GLN:HA	1.94	0.49
1:B:222:LEU:HD22	1:B:282:MSE:SE	2.63	0.49
1:B:328:TRP:CZ2	1:B:332:ILE:HD11	2.47	0.49
1:D:102:MSE:HE2	1:D:109:ALA:HB1	1.95	0.49
1:E:79:ASN:HA	1:E:82:HIS:CG	2.48	0.49
1:A:327:GLN:HE22	1:A:339:LEU:N	2.10	0.48
1:C:172:LYS:HB2	1:C:232:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:SER:C	1:C:121:LYS:H	2.21	0.48
1:D:346:LEU:O	1:D:350:LYS:HG3	2.13	0.48
1:D:100:LYS:HB3	1:D:101:PRO:CD	2.35	0.48
1:E:211:LEU:N	1:E:235:ASP:OD2	2.46	0.48
1:A:79:ASN:ND2	1:A:175:GLN:OE1	2.47	0.48
1:C:77:THR:OG1	1:C:82:HIS:ND1	2.44	0.48
1:C:93:GLY:C	1:C:94:LYS:HD2	2.38	0.48
1:F:170:MSE:O	1:F:232:GLU:HG2	2.13	0.48
1:C:12:GLY:H	1:C:15:ALA:HB3	1.78	0.48
1:E:79:ASN:HA	1:E:82:HIS:CD2	2.48	0.48
1:F:57:VAL:HG23	1:F:57:VAL:O	2.12	0.48
1:B:42:ARG:NH2	2:B:401:NAD:O3B	2.47	0.48
1:C:77:THR:HB	1:C:81:SER:HB2	1.96	0.48
1:F:91:GLU:CD	1:F:116:TRP:HA	2.39	0.48
1:D:67:ASN:O	1:D:70:VAL:HG12	2.14	0.48
1:D:106:THR:O	1:D:109:ALA:HB3	2.14	0.48
1:F:45:LYS:O	1:F:49:GLU:HG3	2.13	0.48
1:A:39:GLN:HB2	1:A:42:ARG:CD	2.44	0.48
1:E:110:GLU:HG3	1:E:346:LEU:HD11	1.96	0.48
1:D:310:ILE:C	1:D:312:TYR:N	2.72	0.47
1:E:357:LYS:HB3	1:E:364:ILE:CD1	2.43	0.47
1:D:65:LEU:HD22	1:D:90:PHE:HA	1.95	0.47
1:F:33:VAL:CG2	1:F:70:VAL:HG12	2.43	0.47
1:A:42:ARG:NH2	1:A:42:ARG:CB	2.73	0.47
1:A:125:ILE:O	1:A:127:TYR:N	2.43	0.47
1:C:14:ILE:HG13	1:C:18:LYS:HB3	1.95	0.47
1:D:8:ILE:HD13	1:D:74:HIS:HB2	1.95	0.47
1:D:32:ILE:HD12	1:D:50:PHE:O	2.14	0.47
1:F:63:GLU:O	1:F:66:ALA:HB3	2.14	0.47
1:C:205:GLY:HA3	1:C:355:ILE:HG23	1.96	0.47
1:D:104:HIS:HB2	1:D:176:GLY:HA3	1.96	0.47
1:D:310:ILE:HG22	1:D:310:ILE:O	2.13	0.47
1:C:32:ILE:O	1:C:32:ILE:HD12	2.14	0.47
1:A:6:ILE:O	1:A:33:VAL:N	2.32	0.47
1:A:39:GLN:HB2	1:A:42:ARG:HD2	1.96	0.47
1:B:102:MSE:HE1	1:B:346:LEU:HB2	1.97	0.47
1:B:356:TYR:C	1:B:358:SER:N	2.71	0.47
1:D:72:VAL:HG13	1:D:95:HIS:HB2	1.97	0.47
1:A:116:TRP:NE1	1:A:123:PHE:CB	2.78	0.47
1:D:344:GLU:O	1:D:348:VAL:HG23	2.14	0.47
1:D:354:ALA:HA	1:D:357:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:TRP:CD1	1:E:123:PHE:HB2	2.50	0.47
1:F:32:ILE:HG22	1:F:35:PHE:HE1	1.79	0.47
1:F:161:ARG:NH2	1:F:258:ASN:OD1	2.33	0.47
1:A:62:LYS:HA	1:A:65:LEU:HD21	1.97	0.47
1:A:73:VAL:HG23	1:A:96:VAL:HA	1.96	0.47
1:A:110:GLU:HG3	1:A:346:LEU:HD11	1.97	0.47
1:B:103:SER:HB2	1:B:112:MSE:HE1	1.97	0.47
1:C:117:LYS:C	1:C:118:LYS:HD3	2.40	0.47
1:B:199:ASP:HB3	1:B:244:LYS:HE3	1.97	0.47
1:C:42:ARG:NH2	1:C:42:ARG:HA	2.29	0.47
1:D:356:TYR:O	1:D:358:SER:N	2.38	0.47
1:F:9:ILE:HD12	1:F:9:ILE:N	2.29	0.47
1:A:73:VAL:HG23	1:A:96:VAL:HG23	1.97	0.47
1:C:78:PRO:HB3	1:C:168:VAL:HG21	1.96	0.47
1:C:100:LYS:HE2	2:C:401:NAD:C2N	2.45	0.47
1:A:62:LYS:C	1:A:65:LEU:HG	2.39	0.46
1:A:110:GLU:CB	1:A:113:VAL:CG1	2.87	0.46
1:A:20:PHE:HB2	1:A:21:PRO:CD	2.37	0.46
2:A:401:NAD:H8A	2:A:401:NAD:H2B	1.76	0.46
1:B:266:SER:HB3	1:B:278:ILE:O	2.15	0.46
1:A:64:LEU:C	1:A:66:ALA:H	2.24	0.46
1:A:129:ASN:O	1:A:132:ARG:HG3	2.16	0.46
1:A:100:LYS:CB	1:A:101:PRO:CD	2.92	0.46
1:A:102:MSE:HG3	1:A:125:ILE:HD12	1.97	0.46
1:A:53:GLU:HB3	1:A:54:GLY:H	1.64	0.46
1:C:79:ASN:O	1:C:82:HIS:HB2	2.16	0.46
1:E:128:GLN:HE22	2:E:401:NAD:H72N	1.62	0.46
1:A:14:ILE:HG13	2:A:401:NAD:C5N	2.46	0.46
1:B:35:PHE:CE2	1:B:51:GLY:HA2	2.50	0.46
1:D:179:PRO:HA	1:D:182:ASP:HB3	1.96	0.46
1:F:211:LEU:N	1:F:235:ASP:OD2	2.36	0.46
1:E:100:LYS:HD3	1:E:185:THR:OG1	2.15	0.46
1:E:136:MSE:HA	1:E:139:LYS:HB3	1.97	0.46
1:F:86:THR:HG23	1:F:96:VAL:HG21	1.97	0.46
1:A:74:HIS:HE2	1:A:328:TRP:CD1	2.33	0.46
1:A:77:THR:HB	1:A:81:SER:OG	2.16	0.46
1:C:157:ALA:HA	1:C:264:GLU:HA	1.97	0.46
1:D:83:SER:HA	1:D:112:MSE:SE	2.65	0.46
1:D:109:ALA:HA	1:D:112:MSE:HE3	1.98	0.46
1:A:8:ILE:O	1:A:8:ILE:HG13	2.15	0.46
1:A:139:LYS:HG2	1:A:193:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LEU:O	1:C:196:ASN:N	2.49	0.46
1:A:216:ASN:OD1	1:A:216:ASN:N	2.44	0.45
1:B:153:GLY:O	1:B:249:ILE:HA	2.16	0.45
1:D:58:THR:OG1	1:D:59:ALA:N	2.49	0.45
1:D:78:PRO:HD3	2:D:401:NAD:H52A	1.98	0.45
1:B:302:GLU:HG2	1:F:300:MSE:SE	2.66	0.45
1:E:327:GLN:OE1	1:E:339:LEU:N	2.46	0.45
1:F:163:VAL:HG22	1:F:255:TRP:HB3	1.97	0.45
1:F:346:LEU:O	1:F:350:LYS:HG3	2.16	0.45
1:F:139:LYS:HE2	1:F:143:ASP:CG	2.42	0.45
1:A:9:ILE:HG22	1:A:10:GLY:N	2.31	0.45
1:F:100:LYS:HG3	1:F:186:HIS:CE1	2.51	0.45
1:C:150:ILE:HB	1:C:195:MSE:HG2	1.99	0.45
1:E:203:VAL:HG22	1:E:241:VAL:HG13	1.98	0.45
1:A:219:GLU:HG3	1:F:297:ASN:HA	1.99	0.45
1:C:79:ASN:N	1:C:175:GLN:OE1	2.49	0.45
1:D:102:MSE:HE3	1:D:112:MSE:HE3	1.99	0.45
1:A:110:GLU:HB3	1:A:113:VAL:HG11	1.98	0.45
1:A:319:GLU:O	1:A:323:VAL:HG23	2.17	0.45
1:E:14:ILE:HD12	1:E:14:ILE:HA	1.83	0.45
1:B:127:TYR:HH	1:B:185:THR:HG1	1.59	0.45
1:B:203:VAL:HG22	1:B:241:VAL:HG13	1.98	0.45
1:F:36:CYS:SG	1:F:61:TYR:HA	2.57	0.45
1:A:82:HIS:CD2	1:A:82:HIS:H	2.35	0.45
1:B:161:ARG:NH2	1:B:258:ASN:OD1	2.50	0.45
1:C:26:ASN:ND2	1:C:326:ARG:HB2	2.32	0.45
1:C:34:ALA:O	1:C:56:GLN:O	2.35	0.45
1:C:77:THR:HG1	1:C:82:HIS:HD1	1.63	0.45
1:D:195:MSE:HE1	1:D:249:ILE:CG1	2.47	0.45
1:E:159:ARG:HD3	1:E:162:ALA:HB3	1.99	0.45
1:F:40:ILE:HD13	1:F:58:THR:C	2.42	0.45
1:A:119:SER:HB2	1:A:121:LYS:NZ	2.23	0.44
1:F:36:CYS:SG	1:F:37:ASP:N	2.90	0.44
1:A:295:ARG:HB3	1:A:300:MSE:SE	2.68	0.44
1:C:34:ALA:HA	1:C:64:LEU:HD11	1.99	0.44
1:A:82:HIS:HB3	1:A:112:MSE:HE1	2.00	0.44
1:A:70:VAL:HG12	1:A:72:VAL:H	1.83	0.44
1:F:286:LYS:NZ	1:F:287:ASN:H	2.15	0.44
1:A:19:HIS:CE1	1:A:74:HIS:ND1	2.85	0.44
1:F:179:PRO:HB3	1:F:255:TRP:CD1	2.53	0.44
1:D:308:GLY:H	1:F:282:MSE:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:THR:HG22	1:C:350:LYS:HA	2.00	0.44
1:D:163:VAL:HG22	1:D:255:TRP:HB3	2.00	0.44
1:F:40:ILE:HD11	1:F:57:VAL:O	2.17	0.44
1:B:106:THR:CG2	1:B:350:LYS:HA	2.48	0.44
1:B:77:THR:O	1:B:82:HIS:NE2	2.50	0.44
1:E:23:LEU:HD13	1:E:32:ILE:HD11	2.00	0.44
1:C:310:ILE:HG22	1:C:311:ALA:N	2.23	0.43
1:D:136:MSE:O	1:D:140:LYS:HG3	2.18	0.43
1:E:90:PHE:C	1:E:92:ALA:H	2.26	0.43
1:F:40:ILE:HD13	1:F:59:ALA:CA	2.47	0.43
1:F:77:THR:O	1:F:82:HIS:NE2	2.51	0.43
1:C:41:ASP:OD2	1:C:42:ARG:NE	2.51	0.43
1:B:128:GLN:HE22	2:B:401:NAD:H72N	1.67	0.43
1:C:100:LYS:CB	1:C:101:PRO:HD2	2.35	0.43
1:D:63:GLU:HG3	1:D:63:GLU:O	2.18	0.43
1:F:38:ILE:HA	1:F:59:ALA:O	2.18	0.43
1:F:357:LYS:C	1:F:359:ALA:H	2.26	0.43
1:A:39:GLN:O	1:A:41:ASP:N	2.52	0.43
1:B:116:TRP:CD1	1:B:123:PHE:HB2	2.54	0.43
1:D:2:SER:O	1:D:333:GLN:NE2	2.52	0.43
1:D:356:TYR:C	1:D:358:SER:N	2.76	0.43
1:E:115:ALA:O	1:E:119:SER:HB3	2.18	0.43
1:A:300:MSE:HE1	1:D:291:TYR:CE2	2.53	0.43
1:C:93:GLY:O	1:C:94:LYS:HD2	2.19	0.43
1:E:290:ILE:HG12	1:E:303:THR:HG22	2.00	0.43
1:C:6:ILE:CB	1:C:32:ILE:HG22	2.41	0.43
1:D:100:LYS:HZ3	1:D:182:ASP:C	2.26	0.43
1:E:100:LYS:HB2	2:E:401:NAD:C2N	2.42	0.43
1:A:98:CYS:O	1:A:125:ILE:HA	2.19	0.43
1:C:325:ASN:O	1:C:328:TRP:HB3	2.19	0.43
1:E:163:VAL:HG22	1:E:255:TRP:HB3	2.00	0.43
1:F:365:LYS:HE2	1:F:365:LYS:H	1.83	0.43
1:A:38:ILE:HG21	2:A:401:NAD:C4A	2.49	0.43
1:B:14:ILE:HD13	2:B:401:NAD:C4N	2.49	0.43
1:F:95:HIS:ND1	1:F:121:LYS:HB3	2.33	0.43
1:A:325:ASN:HD22	1:A:325:ASN:C	2.27	0.42
1:C:33:VAL:CA	1:C:55:ALA:HB1	2.49	0.42
1:C:72:VAL:HG21	1:C:332:ILE:CD1	2.48	0.42
1:F:279:HIS:HB2	1:F:288:GLU:HB2	2.00	0.42
1:A:3:LYS:CB	1:A:31:GLU:HG3	2.49	0.42
1:C:300:MSE:HE1	1:E:291:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:PRO:HD2	1:D:234:GLU:HG2	2.01	0.42
1:F:24:LYS:O	1:F:27:ALA:N	2.51	0.42
1:F:161:ARG:HG2	1:F:221:ASN:HA	2.01	0.42
1:A:236:SER:HB3	1:A:254:SER:HB2	2.01	0.42
1:A:262:SER:HB3	1:A:282:MSE:HG3	2.00	0.42
1:C:153:GLY:O	1:C:249:ILE:HA	2.19	0.42
1:F:86:THR:O	1:F:89:ALA:N	2.52	0.42
1:B:195:MSE:HE1	1:B:249:ILE:HG12	2.00	0.42
1:B:229:LYS:HA	1:B:229:LYS:HD3	1.82	0.42
1:C:212:GLY:O	1:C:226:TRP:HZ3	2.01	0.42
1:F:341:LYS:HB2	1:F:341:LYS:HE2	1.80	0.42
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.79	0.42
1:A:299:LEU:HB3	1:F:160:ARG:CZ	2.49	0.42
1:F:203:VAL:HG22	1:F:241:VAL:HG13	2.00	0.42
1:B:74:HIS:CD2	1:B:97:TYR:HB3	2.54	0.42
1:D:100:LYS:HZ2	1:D:185:THR:HG21	1.83	0.42
1:D:345:ALA:O	1:D:349:THR:HG23	2.20	0.42
1:A:361:THR:O	1:A:361:THR:HG22	2.20	0.42
1:B:62:LYS:O	3:B:501:HOH:O	2.21	0.42
1:C:326:ARG:O	1:C:330:GLU:HG3	2.20	0.42
1:D:365:LYS:HB2	1:D:365:LYS:HE2	1.68	0.42
1:A:116:TRP:HE3	1:A:117:LYS:HD2	1.85	0.42
1:C:26:ASN:HD22	1:C:326:ARG:HD2	1.83	0.42
1:C:218:PRO:HG3	1:C:226:TRP:CD2	2.54	0.42
1:D:191:THR:HG22	1:D:195:MSE:HE3	2.01	0.42
1:E:53:GLU:O	1:E:55:ALA:N	2.53	0.42
1:F:325:ASN:O	1:F:328:TRP:HB3	2.20	0.42
1:A:116:TRP:CE3	1:A:117:LYS:HD2	2.55	0.42
1:B:58:THR:OG1	1:B:59:ALA:N	2.53	0.42
1:B:131:PHE:CD1	1:B:324:ASP:HB2	2.54	0.42
1:C:41:ASP:HB2	1:C:42:ARG:NH1	2.35	0.42
1:F:56:GLN:OE1	1:F:67:ASN:HB2	2.20	0.42
1:F:58:THR:HG22	1:F:59:ALA:N	2.34	0.42
1:D:218:PRO:HG3	1:D:226:TRP:CE2	2.55	0.41
1:E:28:ASP:OD2	1:E:29:LEU:HD12	2.20	0.41
1:E:238:VAL:HG12	1:E:252:GLU:HG3	2.02	0.41
1:F:79:ASN:OD1	1:F:101:PRO:HG2	2.19	0.41
1:F:106:THR:O	1:F:110:GLU:HG3	2.19	0.41
1:D:191:THR:HG22	1:D:195:MSE:CE	2.50	0.41
1:F:216:ASN:O	1:F:219:GLU:HB2	2.20	0.41
1:A:82:HIS:CB	1:A:112:MSE:HE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:PHE:HB2	1:B:21:PRO:HD3	2.01	0.41
1:B:134:GLU:OE2	1:B:287:ASN:HB3	2.21	0.41
1:B:165:THR:OG1	1:B:223:PHE:O	2.33	0.41
1:B:299:LEU:HD13	1:E:160:ARG:HD3	2.01	0.41
1:B:356:TYR:O	1:B:358:SER:N	2.54	0.41
1:C:112:MSE:H	1:C:112:MSE:HG2	1.71	0.41
1:D:282:MSE:HE2	1:D:282:MSE:HB3	1.94	0.41
1:A:19:HIS:HE1	1:A:74:HIS:ND1	2.18	0.41
1:D:102:MSE:C	1:D:112:MSE:HE1	2.45	0.41
1:D:172:LYS:HE2	1:D:176:GLY:O	2.21	0.41
1:E:295:ARG:HB3	1:E:300:MSE:SE	2.71	0.41
1:C:65:LEU:HD12	1:C:65:LEU:H	1.85	0.41
1:C:172:LYS:O	1:C:172:LYS:HD3	2.21	0.41
1:C:77:THR:O	2:C:401:NAD:H4D	2.20	0.41
1:C:154:LYS:HB2	1:C:268:THR:HB	2.02	0.41
1:D:102:MSE:O	1:D:112:MSE:HE1	2.19	0.41
1:E:114:GLU:HA	1:E:114:GLU:OE2	2.21	0.41
1:F:4:LEU:O	1:F:30:ASN:HA	2.21	0.41
1:F:212:GLY:HA2	1:F:226:TRP:CH2	2.56	0.41
1:A:181:ILE:HG23	1:A:356:TYR:HE2	1.84	0.41
1:B:8:ILE:HD12	1:B:32:ILE:HG21	2.03	0.41
1:C:33:VAL:HG13	1:C:34:ALA:H	1.85	0.41
1:C:99:GLU:OE2	2:C:401:NAD:H2N	2.21	0.41
1:E:222:LEU:HD13	1:F:307:VAL:HG21	2.03	0.41
1:B:102:MSE:CE	1:B:109:ALA:HB1	2.47	0.41
1:F:12:GLY:HA3	2:F:401:NAD:O5B	2.21	0.41
1:A:58:THR:OG1	1:A:59:ALA:N	2.54	0.40
1:A:108:GLU:HA	1:A:111:LYS:HB2	2.02	0.40
2:A:401:NAD:H3B	2:A:401:NAD:O2A	2.21	0.40
1:B:65:LEU:HD13	1:B:90:PHE:HA	2.02	0.40
1:B:157:ALA:HA	1:B:264:GLU:HA	2.02	0.40
1:C:144:LYS:HB2	1:C:146:GLU:HG3	2.03	0.40
1:F:41:ASP:OD1	1:F:42:ARG:HG3	2.22	0.40
1:F:79:ASN:CG	1:F:101:PRO:HG2	2.46	0.40
1:F:100:LYS:HB3	1:F:100:LYS:HE3	1.87	0.40
1:A:10:GLY:O	1:A:76:CYS:HB2	2.21	0.40
1:A:260:LEU:CD1	1:F:292:ASN:HB3	2.52	0.40
1:E:319:GLU:HA	1:E:319:GLU:OE2	2.21	0.40
1:F:33:VAL:O	1:F:35:PHE:HD1	2.03	0.40
1:F:180:LEU:HD23	1:F:356:TYR:CE2	2.56	0.40
1:A:73:VAL:O	1:A:97:TYR:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LYS:HD2	1:D:151:TYR:CD1	2.56	0.40
1:D:73:VAL:HG23	1:D:96:VAL:CG1	2.51	0.40
1:F:32:ILE:HG22	1:F:35:PHE:CE1	2.56	0.40
1:F:161:ARG:HD2	1:F:219:GLU:O	2.21	0.40
1:B:105:SER:HG	1:B:108:GLU:H	1.69	0.40
1:B:106:THR:HG22	1:B:350:LYS:HA	2.01	0.40
1:C:33:VAL:HA	1:C:55:ALA:HB1	2.03	0.40
1:C:168:VAL:HG22	1:C:175:GLN:HG2	2.04	0.40
1:D:325:ASN:O	1:D:329:LEU:HG	2.22	0.40
1:F:166:TRP:HZ3	1:F:223:PHE:CG	2.40	0.40
1:B:179:PRO:HD3	1:B:255:TRP:CE3	2.56	0.40
1:D:310:ILE:O	1:D:312:TYR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/367 (95%)	301 (86%)	30 (9%)	18 (5%)	1	2
1	B	349/367 (95%)	320 (92%)	23 (7%)	6 (2%)	7	14
1	C	359/367 (98%)	311 (87%)	36 (10%)	12 (3%)	3	5
1	D	355/367 (97%)	305 (86%)	38 (11%)	12 (3%)	3	5
1	E	354/367 (96%)	326 (92%)	24 (7%)	4 (1%)	11	22
1	F	349/367 (95%)	311 (89%)	33 (10%)	5 (1%)	9	17
All	All	2115/2202 (96%)	1874 (89%)	184 (9%)	57 (3%)	4	7

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ILE

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Mol	Chain	Res	Type
1	A	44	GLU
1	A	45	LYS
1	A	58	THR
1	A	100	LYS
1	B	87	ILE
1	C	37	ASP
1	C	77	THR
1	C	100	LYS
1	D	57	VAL
1	D	100	LYS
1	D	306	SER
1	F	58	THR
1	A	28	ASP
1	A	35	PHE
1	A	36	CYS
1	A	46	ALA
1	A	61	TYR
1	A	76	CYS
1	A	126	GLY
1	B	357	LYS
1	C	2	SER
1	C	62	LYS
1	C	84	GLU
1	C	119	SER
1	C	333	GLN
1	D	13	GLY
1	D	49	GLU
1	D	78	PRO
1	D	87	ILE
1	D	307	VAL
1	D	357	LYS
1	E	54	GLY
1	E	88	ALA
1	E	90	PHE
1	E	310	ILE
1	F	37	ASP
1	F	87	ILE
1	A	87	ILE
1	A	102	MSE
1	C	3	LYS
1	C	34	ALA
1	B	91	GLU

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Mol	Chain	Res	Type
1	D	52	ALA
1	F	1	MSE
1	F	306	SER
1	A	47	ALA
1	A	83	SER
1	B	100	LYS
1	B	310	ILE
1	A	27	ALA
1	D	10	GLY
1	C	54	GLY
1	A	68	PRO
1	D	54	GLY
1	C	57	VAL
1	B	78	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/284 (94%)	249 (94%)	17 (6%)	16	29
1	B	276/284 (97%)	274 (99%)	2 (1%)	76	86
1	C	279/284 (98%)	275 (99%)	4 (1%)	59	75
1	D	280/284 (99%)	277 (99%)	3 (1%)	65	79
1	E	276/284 (97%)	275 (100%)	1 (0%)	84	91
1	F	275/284 (97%)	274 (100%)	1 (0%)	84	91
All	All	1652/1704 (97%)	1624 (98%)	28 (2%)	53	71

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	24	LYS
1	A	32	ILE
1	A	38	ILE

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Mol	Chain	Res	Type
1	A	41	ASP
1	A	42	ARG
1	A	45	LYS
1	A	53	GLU
1	A	57	VAL
1	A	61	TYR
1	A	65	LEU
1	A	67	ASN
1	A	112	MSE
1	A	113	VAL
1	A	116	TRP
1	A	280	SER
1	A	282	MSE
1	B	100	LYS
1	B	357	LYS
1	C	1	MSE
1	C	32	ILE
1	C	33	VAL
1	C	100	LYS
1	D	1	MSE
1	D	2	SER
1	D	362	ASN
1	E	1	MSE
1	F	1	MSE

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

Mol	Chain	Res	Type
1	A	16	ASN
1	A	19	HIS
1	A	25	ASN
1	A	39	GLN
1	A	213	GLN
1	A	325	ASN
1	A	327	GLN
1	C	17	GLN
1	C	26	ASN
1	C	216	ASN
1	C	333	GLN
1	C	362	ASN
1	D	17	GLN
1	D	26	ASN

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Mol	Chain	Res	Type
1	D	325	ASN
1	D	333	GLN
1	E	129	ASN
1	E	196	ASN
1	E	213	GLN
1	E	333	GLN
1	F	79	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	401	-	46,48,48	4.05	21 (45%)	64,73,73	2.16	16 (25%)
2	NAD	B	401	-	46,48,48	4.34	23 (50%)	64,73,73	2.30	17 (26%)
2	NAD	A	401	-	46,48,48	4.09	20 (43%)	64,73,73	2.25	15 (23%)
2	NAD	E	401	-	46,48,48	4.09	21 (45%)	64,73,73	2.23	17 (26%)
2	NAD	F	401	-	46,48,48	4.07	21 (45%)	64,73,73	2.21	14 (21%)
2	NAD	C	401	-	46,48,48	4.11	21 (45%)	64,73,73	2.28	19 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	401	-	-	11/30/62/62	0/5/5/5
2	NAD	B	401	-	-	17/30/62/62	0/5/5/5
2	NAD	A	401	-	-	16/30/62/62	0/5/5/5
2	NAD	E	401	-	-	9/30/62/62	0/5/5/5
2	NAD	F	401	-	-	14/30/62/62	0/5/5/5
2	NAD	C	401	-	-	13/30/62/62	0/5/5/5

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAD	C7N-N7N	12.44	1.55	1.33
2	B	401	NAD	O4D-C1D	-11.33	1.26	1.40
2	E	401	NAD	O4D-C1D	-10.46	1.27	1.40
2	A	401	NAD	O4D-C1D	-10.31	1.27	1.40
2	D	401	NAD	O4D-C1D	-10.26	1.27	1.40
2	F	401	NAD	PN-O3	10.20	1.70	1.59
2	F	401	NAD	O4D-C1D	-10.13	1.27	1.40
2	C	401	NAD	PN-O3	10.09	1.70	1.59
2	C	401	NAD	O4D-C1D	-10.06	1.27	1.40
2	A	401	NAD	PN-O3	10.01	1.70	1.59
2	E	401	NAD	PN-O3	9.88	1.70	1.59
2	D	401	NAD	PN-O3	9.81	1.70	1.59
2	B	401	NAD	PN-O3	9.72	1.70	1.59
2	D	401	NAD	C3B-C4B	-9.22	1.29	1.53
2	A	401	NAD	C3B-C4B	-9.19	1.29	1.53
2	C	401	NAD	C3B-C4B	-9.08	1.30	1.53
2	B	401	NAD	C3B-C4B	-9.06	1.30	1.53
2	F	401	NAD	C3B-C4B	-9.04	1.30	1.53
2	E	401	NAD	C3B-C4B	-9.02	1.30	1.53
2	C	401	NAD	C7N-N7N	8.86	1.49	1.33
2	F	401	NAD	C7N-N7N	8.83	1.49	1.33
2	A	401	NAD	C7N-N7N	8.83	1.49	1.33
2	D	401	NAD	C7N-N7N	8.82	1.49	1.33
2	E	401	NAD	C7N-N7N	8.77	1.49	1.33
2	A	401	NAD	C3D-C4D	-8.31	1.31	1.53
2	E	401	NAD	C3D-C4D	-8.28	1.32	1.53
2	F	401	NAD	C3D-C4D	-8.24	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAD	C3D-C4D	-8.21	1.32	1.53
2	D	401	NAD	C3D-C4D	-8.18	1.32	1.53
2	B	401	NAD	C3D-C4D	-8.11	1.32	1.53
2	A	401	NAD	O4B-C4B	7.94	1.62	1.45
2	B	401	NAD	O4D-C4D	7.89	1.62	1.45
2	F	401	NAD	O4D-C4D	7.83	1.62	1.45
2	A	401	NAD	O4D-C4D	7.73	1.62	1.45
2	D	401	NAD	O4D-C4D	7.66	1.62	1.45
2	C	401	NAD	O4B-C4B	7.62	1.61	1.45
2	D	401	NAD	O4B-C4B	7.62	1.61	1.45
2	B	401	NAD	O4B-C4B	7.62	1.61	1.45
2	C	401	NAD	O4D-C4D	7.58	1.61	1.45
2	E	401	NAD	O4B-C4B	7.54	1.61	1.45
2	F	401	NAD	O4B-C4B	7.48	1.61	1.45
2	E	401	NAD	O4D-C4D	7.44	1.61	1.45
2	D	401	NAD	C6A-N6A	6.08	1.49	1.34
2	E	401	NAD	C6A-N6A	6.05	1.49	1.34
2	C	401	NAD	C6A-N6A	6.02	1.49	1.34
2	B	401	NAD	C6A-N6A	6.01	1.49	1.34
2	F	401	NAD	C6A-N6A	5.99	1.49	1.34
2	A	401	NAD	C6A-N6A	5.93	1.49	1.34
2	C	401	NAD	O3D-C3D	5.69	1.57	1.43
2	E	401	NAD	O3D-C3D	5.57	1.56	1.43
2	A	401	NAD	PA-O3	5.32	1.65	1.59
2	C	401	NAD	PA-O3	5.24	1.65	1.59
2	C	401	NAD	C3N-C7N	5.24	1.58	1.50
2	E	401	NAD	C3N-C7N	5.19	1.58	1.50
2	E	401	NAD	PA-O3	5.17	1.65	1.59
2	F	401	NAD	PA-O3	5.04	1.64	1.59
2	F	401	NAD	C3N-C7N	4.99	1.58	1.50
2	D	401	NAD	C3N-C7N	4.97	1.58	1.50
2	D	401	NAD	PA-O3	4.73	1.64	1.59
2	B	401	NAD	PA-O3	4.70	1.64	1.59
2	A	401	NAD	C3N-C7N	4.65	1.57	1.50
2	B	401	NAD	O3D-C3D	4.60	1.54	1.43
2	B	401	NAD	O7N-C7N	-4.56	1.15	1.24
2	F	401	NAD	O3D-C3D	4.36	1.53	1.43
2	C	401	NAD	O4B-C1B	-4.34	1.32	1.42
2	D	401	NAD	O3D-C3D	4.34	1.53	1.43
2	B	401	NAD	O4B-C1B	-4.32	1.32	1.42
2	A	401	NAD	O3D-C3D	4.31	1.53	1.43
2	E	401	NAD	O4B-C1B	-4.31	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	NAD	O4B-C1B	-4.25	1.32	1.42
2	D	401	NAD	O4B-C1B	-4.20	1.32	1.42
2	A	401	NAD	O4B-C1B	-4.08	1.32	1.42
2	B	401	NAD	C2N-C3N	3.93	1.45	1.39
2	F	401	NAD	C2N-N1N	3.21	1.38	1.35
2	D	401	NAD	C2N-N1N	3.20	1.38	1.35
2	A	401	NAD	O3B-C3B	3.18	1.50	1.43
2	F	401	NAD	O3B-C3B	3.17	1.50	1.43
2	E	401	NAD	O3B-C3B	3.12	1.50	1.43
2	B	401	NAD	O3B-C3B	3.10	1.50	1.43
2	C	401	NAD	O3B-C3B	3.09	1.50	1.43
2	C	401	NAD	C2N-N1N	3.06	1.38	1.35
2	D	401	NAD	O3B-C3B	3.03	1.50	1.43
2	A	401	NAD	C2A-N1A	2.87	1.39	1.33
2	A	401	NAD	C5A-C4A	-2.80	1.34	1.39
2	E	401	NAD	C2A-N1A	2.79	1.38	1.33
2	A	401	NAD	C2N-N1N	2.79	1.38	1.35
2	B	401	NAD	C2A-N1A	2.75	1.38	1.33
2	D	401	NAD	C2A-N1A	2.75	1.38	1.33
2	C	401	NAD	C2A-N1A	2.75	1.38	1.33
2	F	401	NAD	C5A-C4A	-2.73	1.34	1.39
2	F	401	NAD	C2A-N1A	2.70	1.38	1.33
2	D	401	NAD	O2B-C2B	-2.68	1.36	1.43
2	B	401	NAD	C5A-C4A	-2.68	1.34	1.39
2	E	401	NAD	C8A-N9A	-2.64	1.33	1.37
2	A	401	NAD	C8A-N9A	-2.62	1.33	1.37
2	C	401	NAD	C5A-C4A	-2.60	1.34	1.39
2	E	401	NAD	C2N-N1N	2.58	1.37	1.35
2	E	401	NAD	C5A-C4A	-2.57	1.34	1.39
2	F	401	NAD	C8A-N9A	-2.56	1.33	1.37
2	E	401	NAD	O2B-C2B	-2.55	1.36	1.43
2	B	401	NAD	C8A-N9A	-2.54	1.33	1.37
2	C	401	NAD	C8A-N9A	-2.52	1.33	1.37
2	B	401	NAD	O2B-C2B	-2.50	1.36	1.43
2	D	401	NAD	C8A-N9A	-2.49	1.33	1.37
2	C	401	NAD	O2B-C2B	-2.46	1.36	1.43
2	D	401	NAD	C5A-C4A	-2.40	1.34	1.39
2	F	401	NAD	O2B-C2B	-2.40	1.37	1.43
2	A	401	NAD	O2B-C2B	-2.37	1.37	1.43
2	A	401	NAD	O7N-C7N	-2.36	1.19	1.24
2	D	401	NAD	C8A-N7A	2.35	1.36	1.31
2	C	401	NAD	O7N-C7N	-2.35	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	PA-O5B	2.35	1.68	1.59
2	B	401	NAD	C3N-C7N	2.33	1.54	1.50
2	F	401	NAD	O7N-C7N	-2.32	1.19	1.24
2	B	401	NAD	C8A-N7A	2.30	1.36	1.31
2	D	401	NAD	O7N-C7N	-2.27	1.19	1.24
2	F	401	NAD	C8A-N7A	2.26	1.36	1.31
2	E	401	NAD	O7N-C7N	-2.25	1.19	1.24
2	C	401	NAD	C8A-N7A	2.21	1.35	1.31
2	C	401	NAD	PA-O5B	2.18	1.67	1.59
2	F	401	NAD	PA-O5B	2.16	1.67	1.59
2	B	401	NAD	PA-O5B	2.15	1.67	1.59
2	E	401	NAD	PA-O5B	2.12	1.67	1.59
2	D	401	NAD	PA-O5B	2.11	1.67	1.59
2	E	401	NAD	C8A-N7A	2.07	1.35	1.31
2	B	401	NAD	C2N-N1N	2.07	1.37	1.35
2	B	401	NAD	C4N-C3N	-2.05	1.36	1.39

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAD	C4A-N9A-C1B	-6.97	110.32	126.63
2	B	401	NAD	C4A-N9A-C1B	-6.79	110.76	126.63
2	C	401	NAD	C4A-N9A-C1B	-6.44	111.58	126.63
2	E	401	NAD	C4A-N9A-C1B	-6.41	111.64	126.63
2	D	401	NAD	C4A-N9A-C1B	-6.27	111.97	126.63
2	A	401	NAD	C4A-N9A-C1B	-6.24	112.05	126.63
2	A	401	NAD	N3A-C2A-N1A	-6.09	119.36	128.58
2	F	401	NAD	N3A-C2A-N1A	-5.69	119.97	128.58
2	B	401	NAD	N3A-C2A-N1A	-5.64	120.05	128.58
2	E	401	NAD	N3A-C2A-N1A	-5.63	120.07	128.58
2	A	401	NAD	N9A-C8A-N7A	-5.61	105.97	113.94
2	C	401	NAD	N3A-C2A-N1A	-5.60	120.11	128.58
2	F	401	NAD	C1B-N9A-C8A	5.58	139.47	127.09
2	D	401	NAD	N3A-C2A-N1A	-5.51	120.24	128.58
2	A	401	NAD	C4A-N9A-C8A	5.47	111.48	105.74
2	F	401	NAD	N9A-C8A-N7A	-5.37	106.32	113.94
2	B	401	NAD	C1B-N9A-C8A	5.35	138.97	127.09
2	B	401	NAD	N9A-C8A-N7A	-5.32	106.39	113.94
2	A	401	NAD	C2B-C1B-N9A	-5.26	100.23	113.30
2	C	401	NAD	N9A-C8A-N7A	-5.21	106.54	113.94
2	D	401	NAD	C5A-C4A-N3A	-5.20	119.56	126.72
2	D	401	NAD	C1B-N9A-C8A	5.16	138.55	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAD	C1B-N9A-C8A	5.05	138.30	127.09
2	E	401	NAD	N9A-C8A-N7A	-5.04	106.78	113.94
2	E	401	NAD	C1B-N9A-C8A	5.03	138.27	127.09
2	D	401	NAD	N6A-C6A-N1A	-4.99	107.26	118.38
2	F	401	NAD	N6A-C6A-N1A	-4.98	107.27	118.38
2	D	401	NAD	N9A-C8A-N7A	-4.93	106.94	113.94
2	C	401	NAD	N6A-C6A-N1A	-4.89	107.48	118.38
2	B	401	NAD	N6A-C6A-N1A	-4.86	107.56	118.38
2	E	401	NAD	N6A-C6A-N1A	-4.81	107.66	118.38
2	C	401	NAD	C5A-C4A-N3A	-4.67	120.28	126.72
2	F	401	NAD	C5A-C4A-N3A	-4.65	120.32	126.72
2	E	401	NAD	C5A-C4A-N3A	-4.61	120.37	126.72
2	B	401	NAD	C5A-C4A-N3A	-4.46	120.58	126.72
2	A	401	NAD	N6A-C6A-N1A	-4.38	108.62	118.38
2	B	401	NAD	C4A-N9A-C8A	4.32	110.27	105.74
2	F	401	NAD	C4A-N9A-C8A	4.26	110.21	105.74
2	E	401	NAD	C4D-O4D-C1D	-4.25	106.03	109.92
2	A	401	NAD	C1B-N9A-C8A	4.23	136.47	127.09
2	C	401	NAD	C4A-N9A-C8A	4.18	110.12	105.74
2	B	401	NAD	C6N-N1N-C2N	-4.16	118.34	121.88
2	E	401	NAD	C4A-N9A-C8A	4.14	110.09	105.74
2	C	401	NAD	C4D-O4D-C1D	-4.13	106.14	109.92
2	A	401	NAD	C4D-O4D-C1D	-3.93	106.33	109.92
2	A	401	NAD	C5A-C4A-N3A	-3.90	121.34	126.72
2	D	401	NAD	C5A-C6A-N6A	3.85	132.81	123.29
2	F	401	NAD	C5A-C6A-N6A	3.79	132.68	123.29
2	B	401	NAD	C5A-C6A-N6A	3.77	132.61	123.29
2	D	401	NAD	N3A-C4A-N9A	3.75	133.55	127.17
2	C	401	NAD	C5A-C6A-N6A	3.75	132.56	123.29
2	E	401	NAD	C5A-C6A-N6A	3.74	132.55	123.29
2	A	401	NAD	N3A-C4A-N9A	3.65	133.37	127.17
2	D	401	NAD	C4A-N9A-C8A	3.56	109.47	105.74
2	E	401	NAD	N3A-C4A-N9A	3.55	133.20	127.17
2	C	401	NAD	N3A-C4A-N9A	3.55	133.20	127.17
2	C	401	NAD	C6N-N1N-C2N	-3.53	118.87	121.88
2	B	401	NAD	C3N-C7N-N7N	3.52	122.07	117.74
2	F	401	NAD	N3A-C4A-N9A	3.43	133.00	127.17
2	D	401	NAD	C2A-N3A-C4A	3.38	120.08	111.83
2	A	401	NAD	C5A-C6A-N6A	3.36	131.61	123.29
2	F	401	NAD	C5A-N7A-C8A	3.35	108.71	103.45
2	B	401	NAD	N3A-C4A-N9A	3.34	132.85	127.17
2	D	401	NAD	C5A-N7A-C8A	3.33	108.68	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAD	C2A-N3A-C4A	3.30	119.89	111.83
2	C	401	NAD	C2A-N3A-C4A	3.25	119.76	111.83
2	C	401	NAD	C5A-N7A-C8A	3.23	108.53	103.45
2	E	401	NAD	C2A-N3A-C4A	3.22	119.70	111.83
2	F	401	NAD	C4D-O4D-C1D	-3.21	106.98	109.92
2	B	401	NAD	C5A-N7A-C8A	3.21	108.49	103.45
2	B	401	NAD	C5N-C4N-C3N	3.18	123.49	120.36
2	B	401	NAD	C2A-N3A-C4A	3.16	119.55	111.83
2	E	401	NAD	C5A-N7A-C8A	3.12	108.35	103.45
2	A	401	NAD	C2A-N3A-C4A	3.11	119.42	111.83
2	A	401	NAD	C5A-N7A-C8A	2.91	108.03	103.45
2	E	401	NAD	C6N-N1N-C2N	-2.85	119.45	121.88
2	B	401	NAD	O7N-C7N-N7N	-2.75	118.65	122.62
2	C	401	NAD	C2D-C3D-C4D	-2.72	97.36	102.61
2	C	401	NAD	C3B-C2B-C1B	2.49	106.17	101.46
2	E	401	NAD	C3B-C2B-C1B	2.48	106.16	101.46
2	A	401	NAD	C5B-C4B-C3B	-2.45	106.39	115.21
2	E	401	NAD	C2D-C3D-C4D	-2.44	97.90	102.61
2	C	401	NAD	C3N-C7N-N7N	2.42	120.72	117.74
2	C	401	NAD	C2B-C3B-C4B	2.42	107.29	102.61
2	E	401	NAD	C2B-C3B-C4B	2.37	107.18	102.61
2	F	401	NAD	C6N-N1N-C2N	-2.31	119.91	121.88
2	D	401	NAD	C5B-C4B-C3B	-2.26	107.08	115.21
2	D	401	NAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	D	401	NAD	C6A-C5A-C4A	2.23	120.22	117.18
2	E	401	NAD	C3N-C7N-N7N	2.22	120.47	117.74
2	F	401	NAD	C4A-C5A-N7A	-2.19	108.08	110.58
2	C	401	NAD	O7N-C7N-N7N	-2.17	119.48	122.62
2	B	401	NAD	C2B-C3B-C4B	2.09	106.65	102.61
2	D	401	NAD	C2B-C3B-C4B	2.08	106.62	102.61
2	D	401	NAD	C4D-O4D-C1D	-2.07	108.03	109.92
2	B	401	NAD	C4A-C5A-N7A	-2.02	108.28	110.58
2	A	401	NAD	C2B-C3B-C4B	2.01	106.49	102.61
2	C	401	NAD	C4A-C5A-N7A	-2.01	108.29	110.58

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	C5B-O5B-PA-O2A
2	A	401	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	A	401	NAD	PN-O3-PA-O5B
2	A	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	C5B-O5B-PA-O1A
2	B	401	NAD	C5B-O5B-PA-O2A
2	B	401	NAD	C5B-O5B-PA-O3
2	B	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	C5D-O5D-PN-O3
2	C	401	NAD	C5D-O5D-PN-O1N
2	C	401	NAD	C5D-O5D-PN-O2N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	C5B-O5B-PA-O1A
2	D	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C2N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C5B-O5B-PA-O1A
2	F	401	NAD	C5B-O5B-PA-O2A
2	F	401	NAD	C5B-O5B-PA-O3
2	F	401	NAD	PN-O3-PA-O5B
2	F	401	NAD	C2B-C1B-N9A-C8A
2	F	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	401	NAD	O4D-C4D-C5D-O5D
2	F	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	C2B-C1B-N9A-C4A
2	F	401	NAD	C2B-C1B-N9A-C4A
2	F	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	C3B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C4B-C5B-O5B-PA
2	C	401	NAD	C2B-C1B-N9A-C8A
2	E	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O2N
2	E	401	NAD	PA-O3-PN-O2N
2	C	401	NAD	C2B-C1B-N9A-C4A
2	E	401	NAD	C2D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	E	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	C4B-C5B-O5B-PA
2	F	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	PA-O3-PN-O2N
2	B	401	NAD	PN-O3-PA-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C3D-C4D-C5D-O5D
2	B	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	PA-O3-PN-O2N
2	D	401	NAD	PA-O3-PN-O1N
2	E	401	NAD	PA-O3-PN-O1N
2	C	401	NAD	O4B-C1B-N9A-C8A
2	A	401	NAD	C3B-C4B-C5B-O5B
2	E	401	NAD	C3B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 34 short contacts:

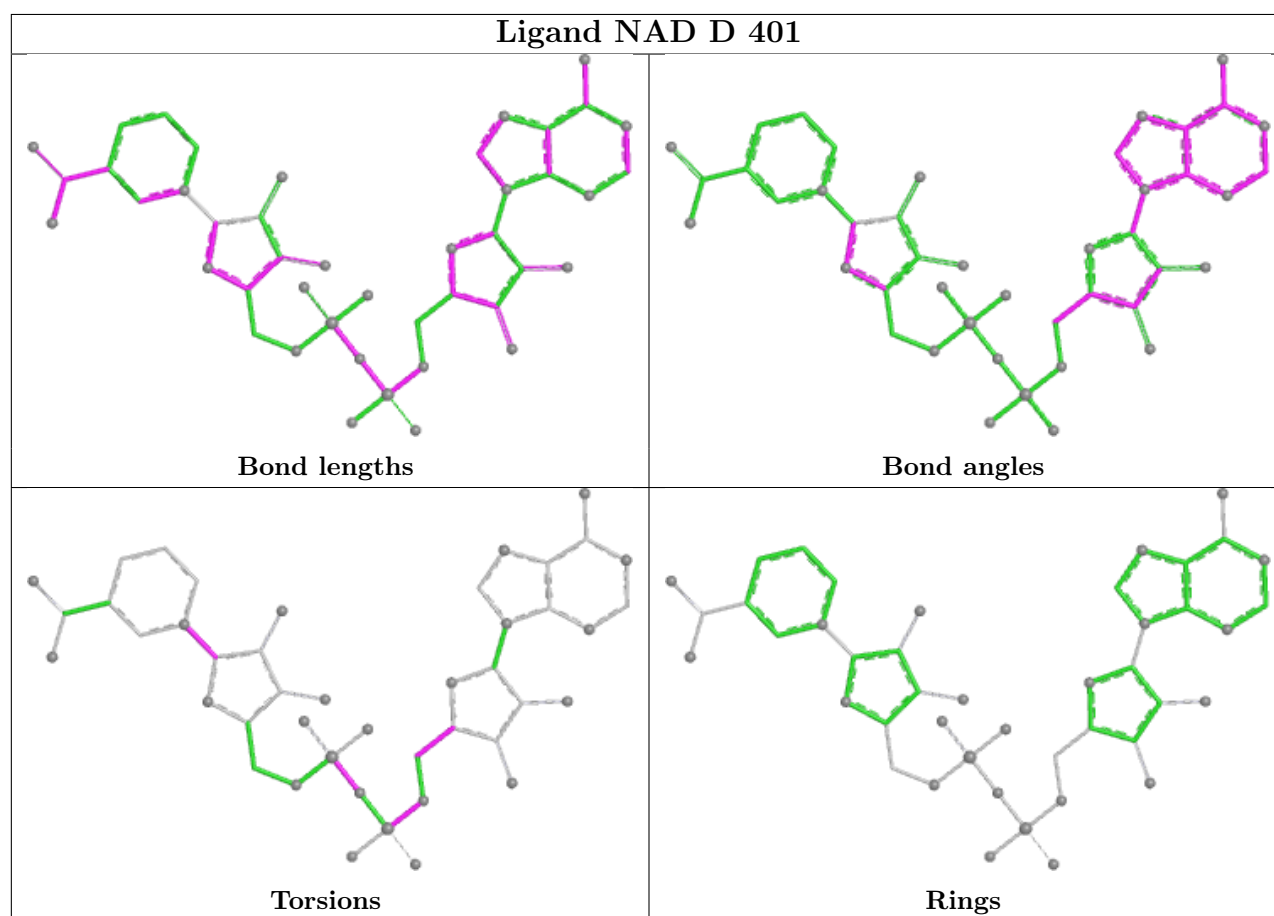
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAD	4	0
2	B	401	NAD	6	0

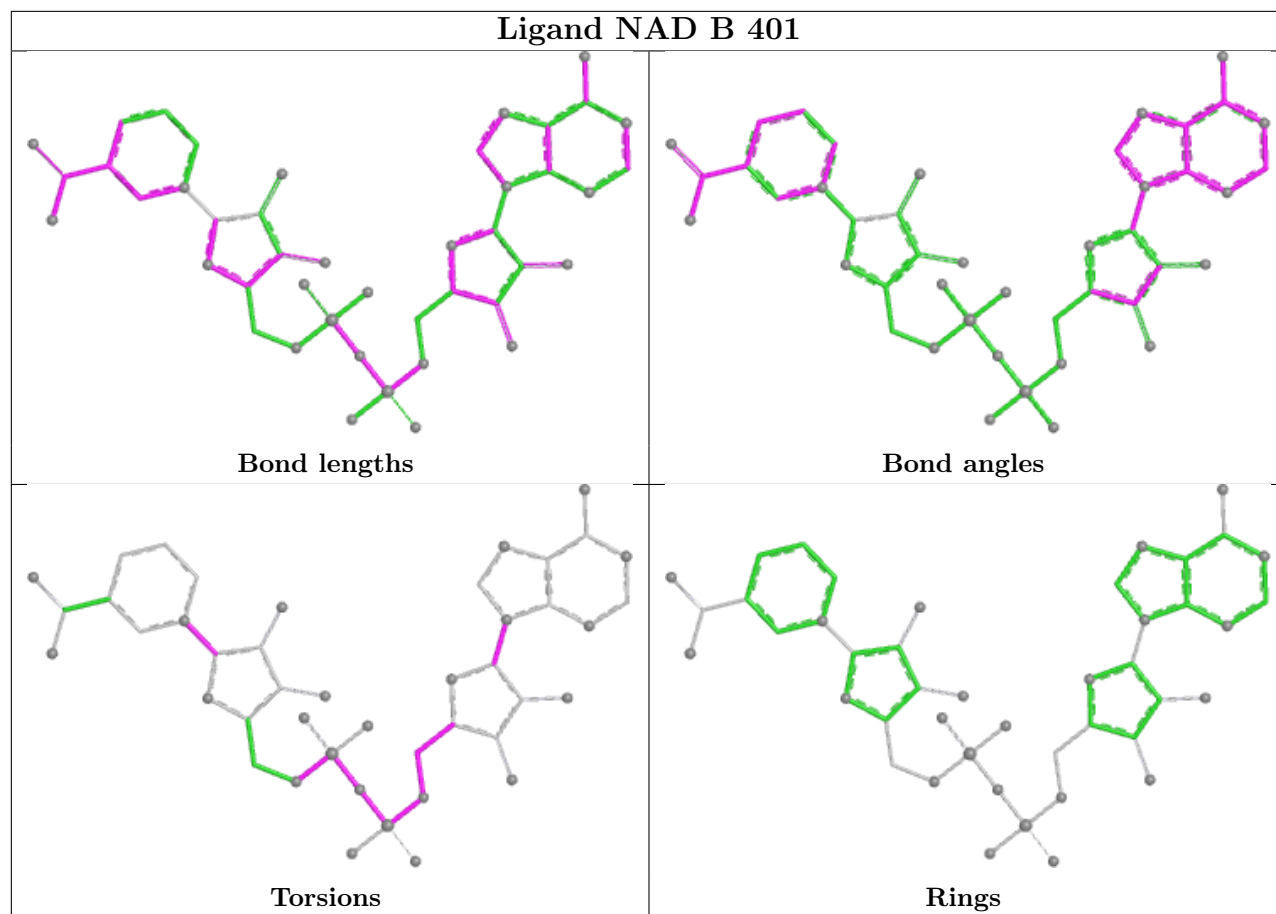
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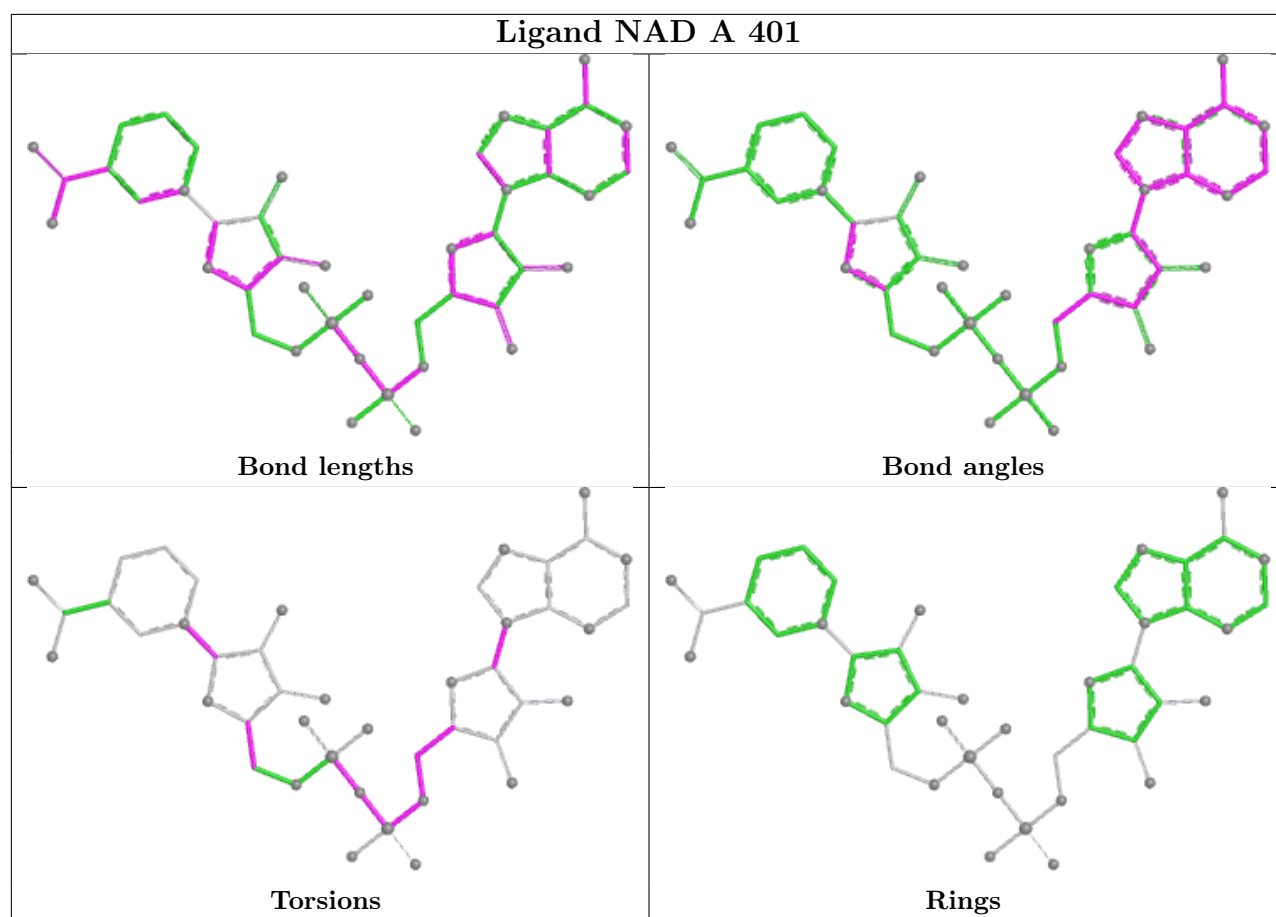
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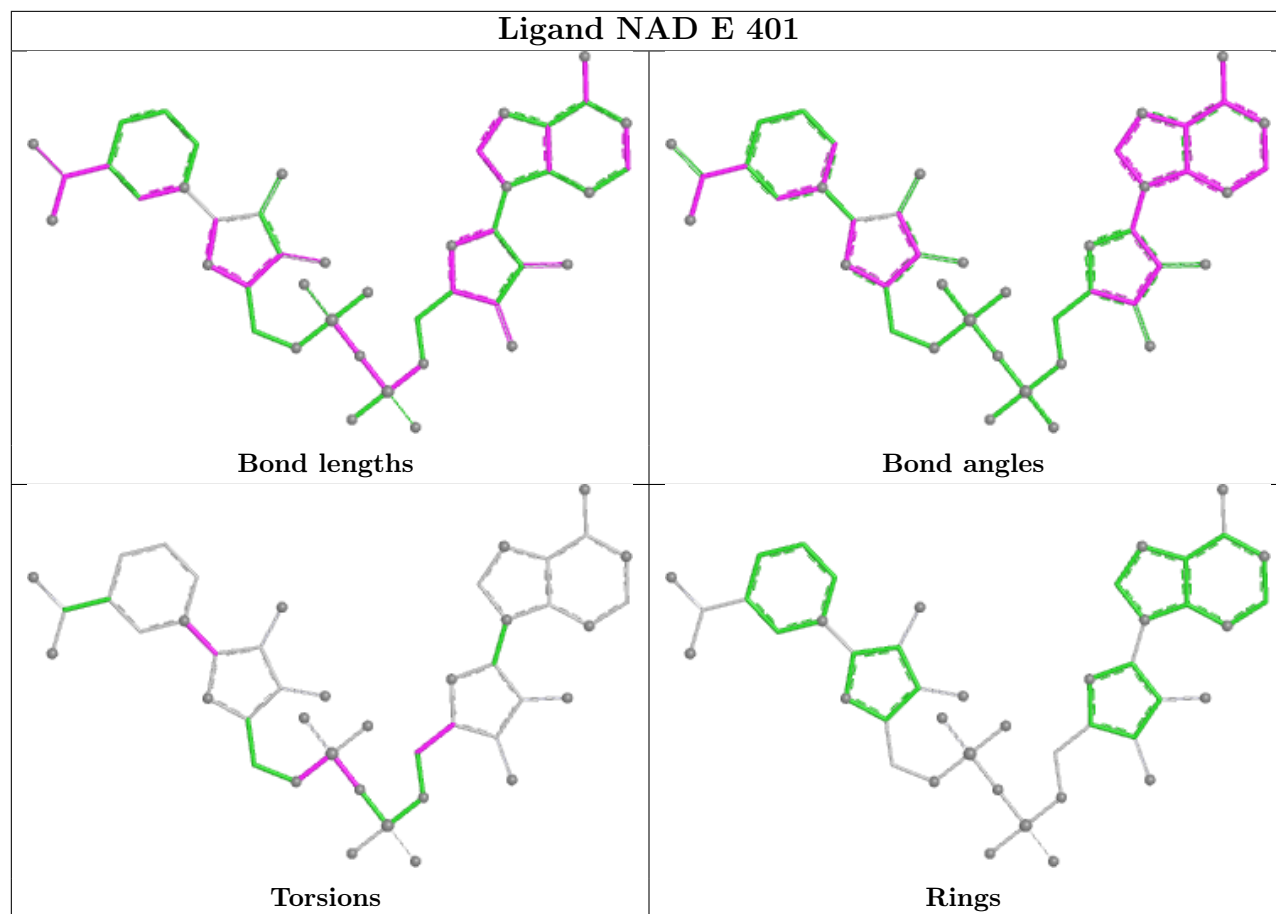
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	12	0
2	E	401	NAD	4	0
2	F	401	NAD	4	0
2	C	401	NAD	4	0

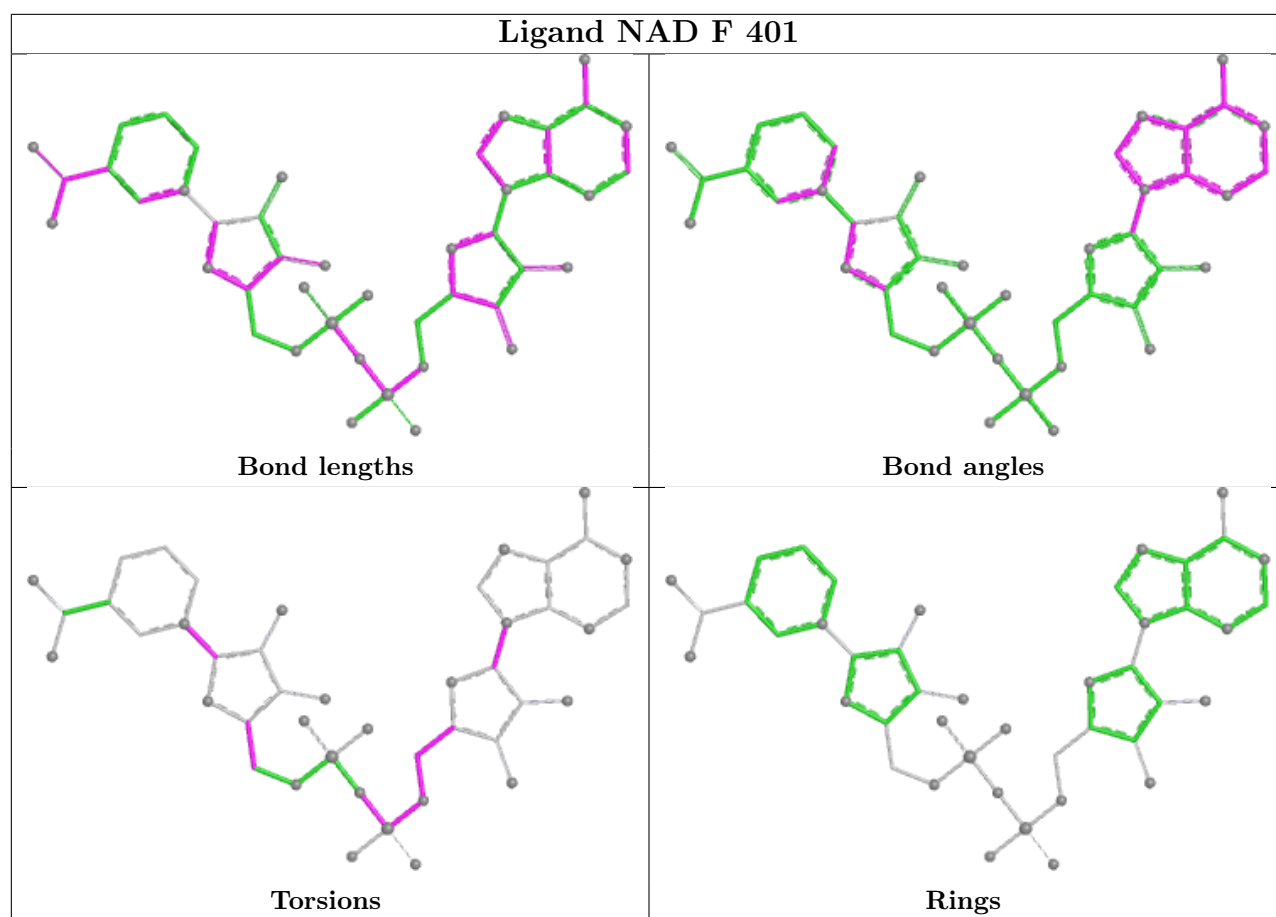
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

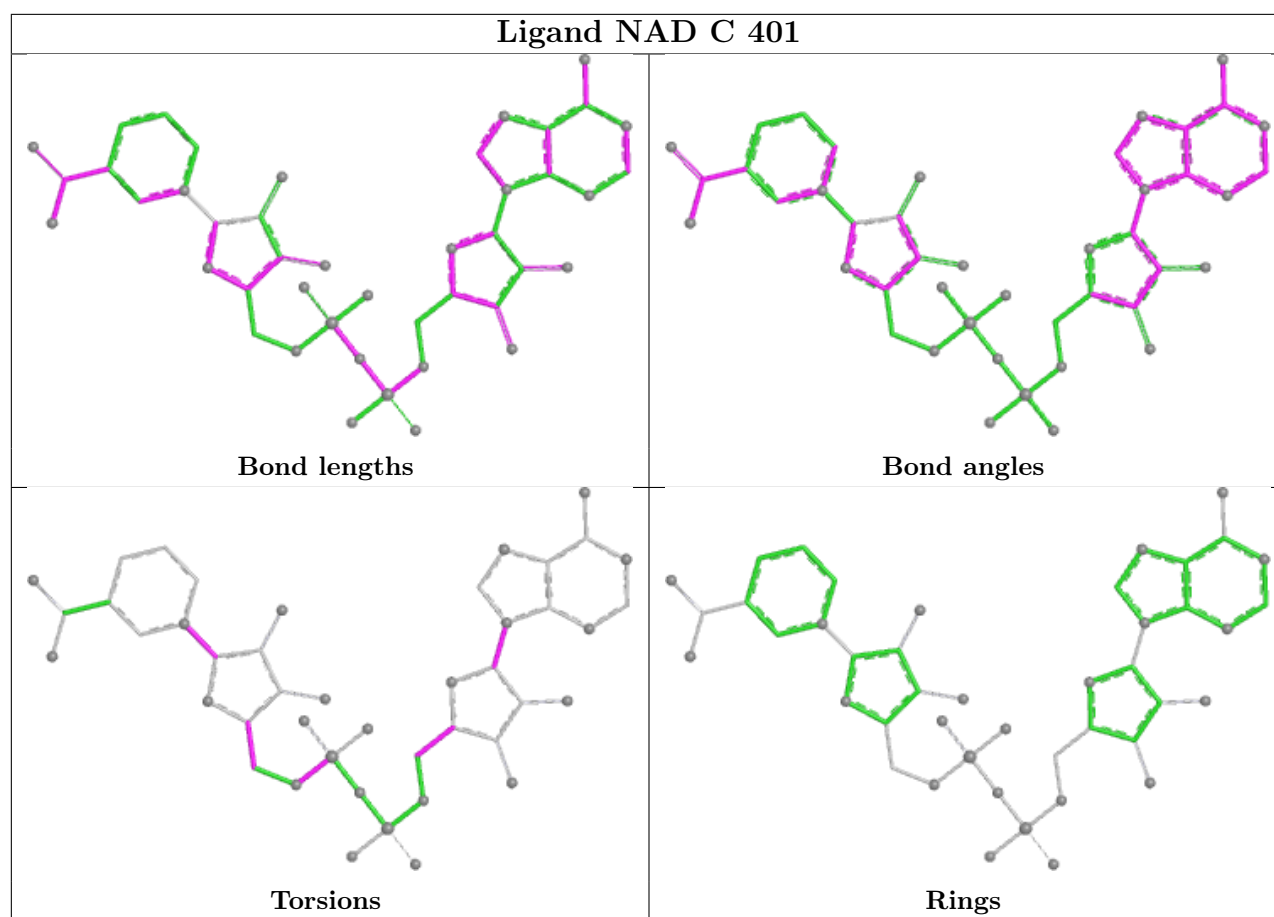












5.7 Other polymers [i](#)

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	345/367 (94%)	0.64	47 (13%) 7 5	30, 69, 127, 134	0
1	B	347/367 (94%)	0.11	3 (0%) 81 81	39, 62, 86, 118	0
1	C	353/367 (96%)	0.52	22 (6%) 26 26	49, 73, 110, 154	0
1	D	351/367 (95%)	0.45	24 (6%) 23 23	30, 71, 104, 125	0
1	E	350/367 (95%)	0.20	7 (2%) 65 63	48, 67, 92, 126	0
1	F	345/367 (94%)	0.46	31 (8%) 15 14	42, 72, 115, 142	0
All	All	2091/2202 (94%)	0.40	134 (6%) 25 25	30, 69, 115, 154	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	CYS	8.2
1	D	52	ALA	5.9
1	A	34	ALA	5.7
1	E	88	ALA	5.6
1	A	35	PHE	5.5
1	D	88	ALA	5.3
1	A	37	ASP	5.1
1	C	40	ILE	4.7
1	C	33	VAL	4.6
1	A	359	ALA	4.5
1	D	53	GLU	4.4
1	A	11	CYS	4.4
1	F	0	GLY	4.1
1	A	32	ILE	4.1
1	B	88	ALA	3.9
1	D	51	GLY	3.8
1	D	35	PHE	3.7
1	F	57	VAL	3.7
1	A	0	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	44	GLU	3.6
1	D	87	ILE	3.6
1	A	33	VAL	3.6
1	C	34	ALA	3.5
1	F	120	GLY	3.5
1	A	168	VAL	3.4
1	A	48	ALA	3.4
1	D	126	GLY	3.3
1	F	11	CYS	3.3
1	A	71	GLU	3.3
1	C	43	ALA	3.2
1	A	14	ILE	3.2
1	E	226	TRP	3.0
1	A	55	ALA	3.0
1	E	309	SER	3.0
1	C	77	THR	3.0
1	C	92	ALA	3.0
1	E	92	ALA	3.0
1	C	82	HIS	3.0
1	D	46	ALA	2.9
1	C	38	ILE	2.9
1	A	46	ALA	2.9
1	F	88	ALA	2.9
1	A	68	PRO	2.9
1	F	36	CYS	2.9
1	A	58	THR	2.9
1	D	101	PRO	2.8
1	A	358	SER	2.8
1	A	4	LEU	2.8
1	A	66	ALA	2.8
1	A	65	LEU	2.8
1	A	57	VAL	2.8
1	F	96	VAL	2.8
1	A	361	THR	2.8
1	F	65	LEU	2.8
1	A	59	ALA	2.8
1	F	61	TYR	2.8
1	A	23	LEU	2.7
1	B	92	ALA	2.7
1	F	55	ALA	2.7
1	C	226	TRP	2.7
1	A	12	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	18	LYS	2.7
1	F	64	LEU	2.6
1	C	52	ALA	2.6
1	A	51	GLY	2.6
1	A	77	THR	2.6
1	C	2	SER	2.6
1	D	33	VAL	2.6
1	F	87	ILE	2.5
1	D	0	GLY	2.5
1	B	33	VAL	2.5
1	A	101	PRO	2.5
1	D	89	ALA	2.5
1	D	92	ALA	2.5
1	C	87	ILE	2.5
1	A	360	LYS	2.4
1	C	57	VAL	2.4
1	A	88	ALA	2.4
1	F	4	LEU	2.4
1	E	358	SER	2.4
1	F	52	ALA	2.4
1	E	82	HIS	2.4
1	A	70	VAL	2.3
1	A	307	VAL	2.3
1	C	35	PHE	2.3
1	D	43	ALA	2.3
1	A	75	VAL	2.3
1	F	50	PHE	2.3
1	A	115	ALA	2.3
1	C	101	PRO	2.3
1	C	314	ALA	2.2
1	A	74	HIS	2.2
1	D	311	ALA	2.2
1	C	76	CYS	2.2
1	F	86	THR	2.2
1	D	226	TRP	2.2
1	D	325	ASN	2.2
1	F	307	VAL	2.2
1	D	50	PHE	2.2
1	A	84	GLU	2.2
1	A	29	LEU	2.2
1	C	64	LEU	2.2
1	F	8	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	33	VAL	2.2
1	A	118	LYS	2.1
1	D	54	GLY	2.1
1	F	40	ILE	2.1
1	F	72	VAL	2.1
1	A	31	GLU	2.1
1	C	10	GLY	2.1
1	D	104	HIS	2.1
1	A	96	VAL	2.1
1	F	9	ILE	2.1
1	C	88	ALA	2.1
1	F	59	ALA	2.1
1	F	85	ILE	2.1
1	A	90	PHE	2.1
1	D	2	SER	2.1
1	D	309	SER	2.1
1	A	117	LYS	2.1
1	F	360	LYS	2.1
1	F	90	PHE	2.1
1	A	119	SER	2.0
1	F	226	TRP	2.0
1	C	230	THR	2.0
1	F	76	CYS	2.0
1	A	42	ARG	2.0
1	D	18	LYS	2.0
1	E	100	LYS	2.0
1	A	103	SER	2.0
1	D	358	SER	2.0
1	F	358	SER	2.0
1	F	328	TRP	2.0
1	A	93	GLY	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](#)

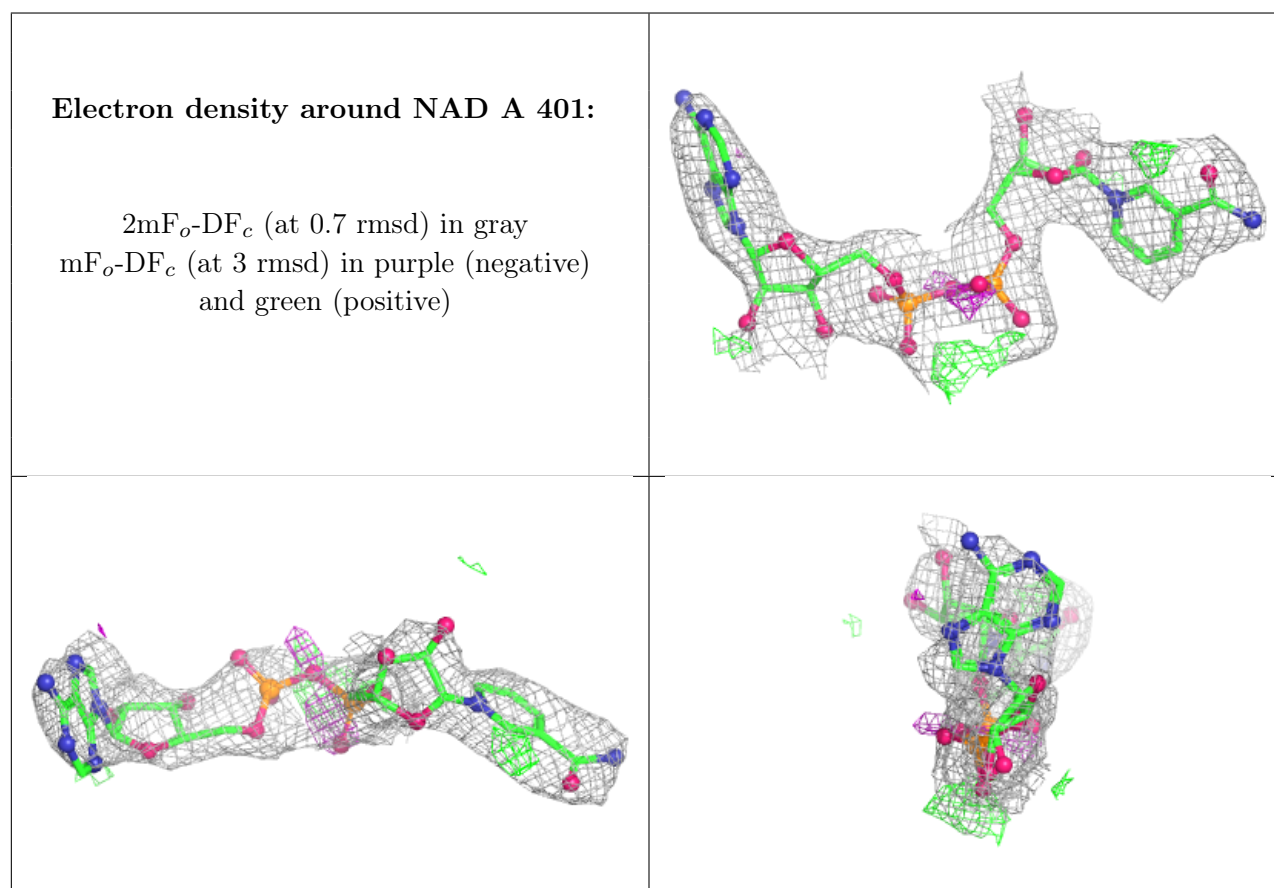
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

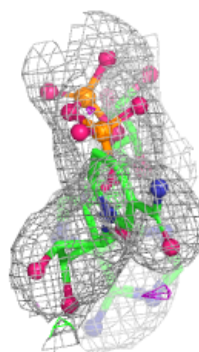
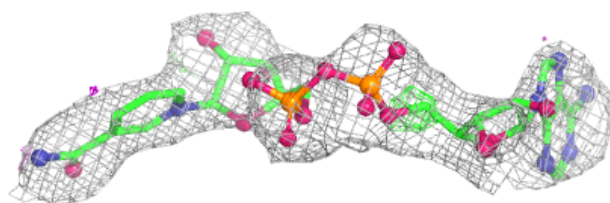
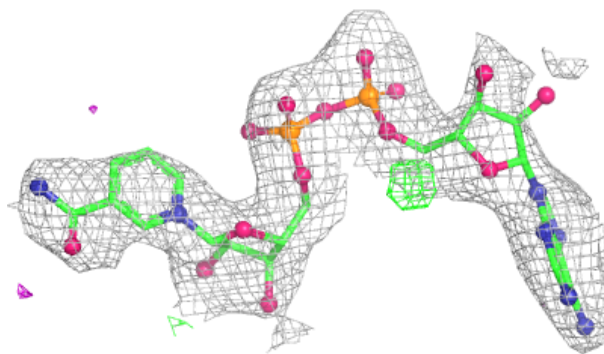
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	401	44/44	0.72	0.14	73,111,120,122	0
2	NAD	F	401	44/44	0.77	0.14	67,98,108,111	0
2	NAD	C	401	44/44	0.88	0.10	71,90,103,106	0
2	NAD	E	401	44/44	0.90	0.10	57,68,74,78	0
2	NAD	D	401	44/44	0.90	0.10	64,79,88,90	0
2	NAD	B	401	44/44	0.93	0.09	63,71,76,78	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.

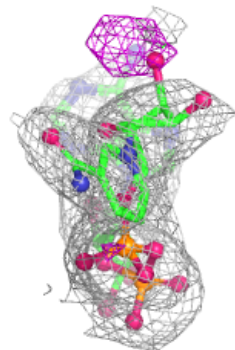
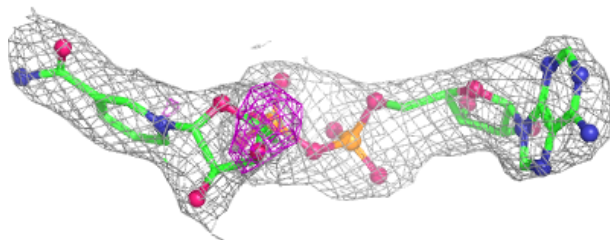
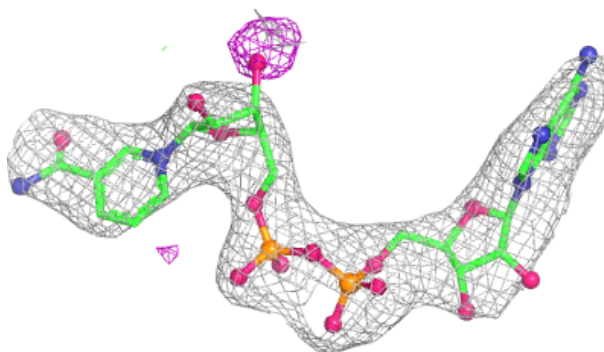


Electron density around NAD F 401:

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

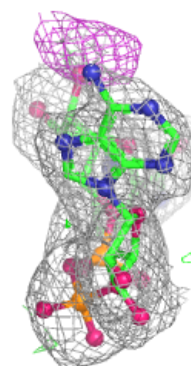
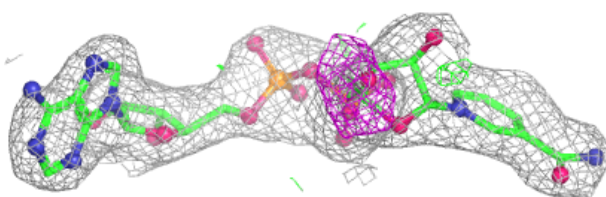
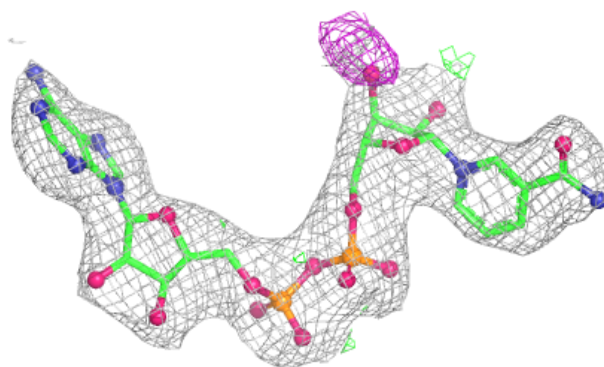
**Electron density around NAD C 401:**

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

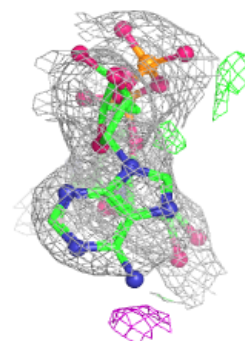
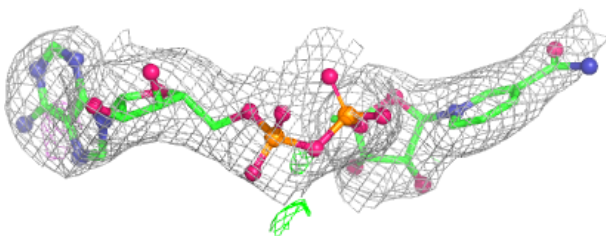
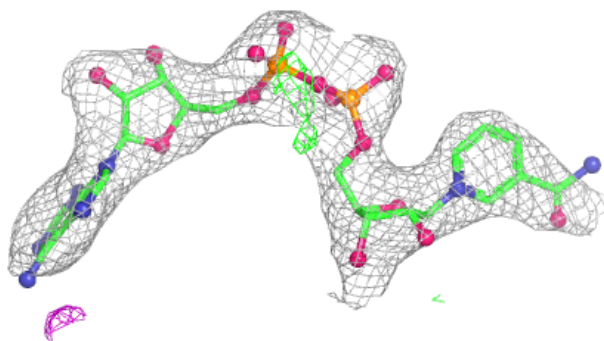


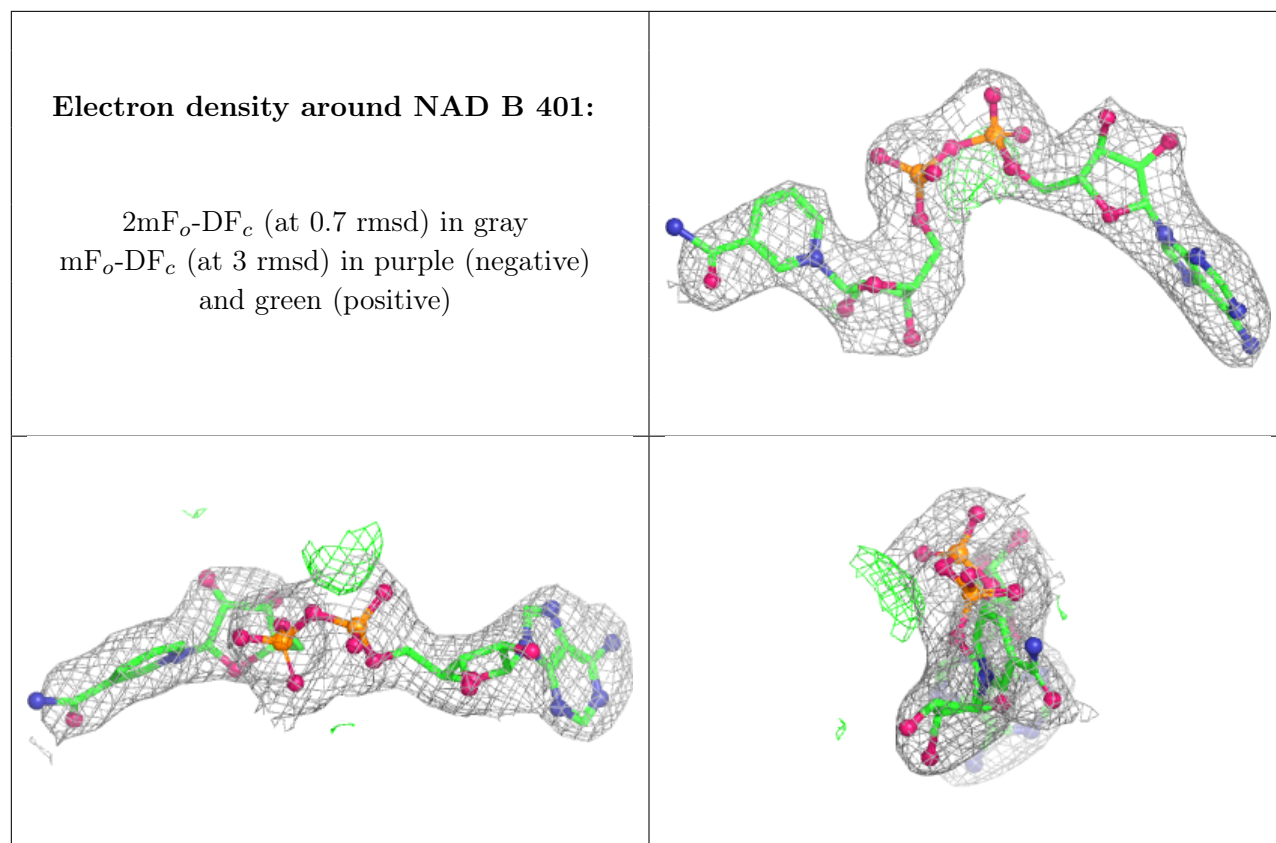
Electron density around NAD E 401:

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

**Electron density around NAD 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.