



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 AM UTC

PDB ID : 3OET / pdb_00003oet
Title : D-Erythronate-4-Phosphate Dehydrogenase complexed with NAD
Authors : Filippova, E.V.; Wawrzak, Z.; Onopriyenko, O.; Savchenko, A.; Edwards, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2010-08-13
Resolution : 2.36 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:

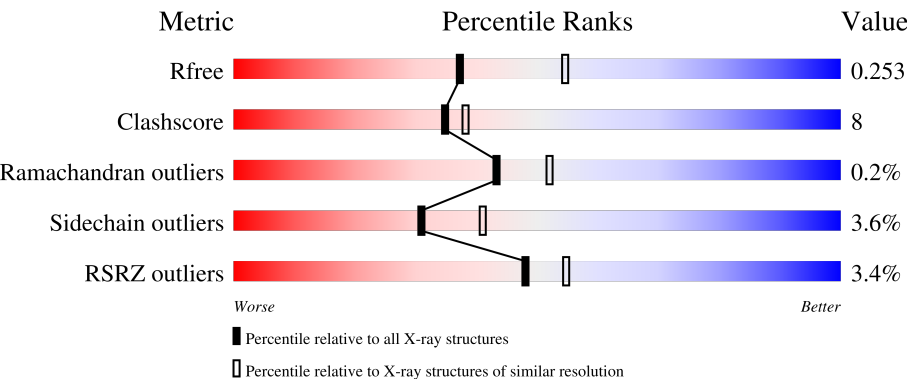
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	381	0% 82%14%..
1	B	381	4% 80%18%..
1	C	381	8% 75%20%..
1	D	381	2% 84%14%..

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Mol	Chain	Length	Quality of chain
1	E	381	% 86% 12% ..
1	F	381	7% 81% 14% ..
1	G	381	2% 73% 21% ..
1	H	381	% 83% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23835 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 Erythronate-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	Se	0	1	0
			2888	1827	514	537	5	5			
1	B	377	Total	C	N	O	S	Se	0	1	0
			2894	1831	511	542	5	5			
1	C	372	Total	C	N	O	S	Se	0	3	0
			2865	1811	506	538	5	5			
1	D	375	Total	C	N	O	S	Se	0	0	0
			2867	1817	506	534	5	5			
1	E	375	Total	C	N	O	S	Se	0	0	0
			2880	1826	507	537	5	5			
1	F	365	Total	C	N	O	S	Se	0	0	0
			2791	1773	489	519	5	5			
1	G	370	Total	C	N	O	S	Se	0	0	0
			2843	1801	501	531	5	5			
1	H	378	Total	C	N	O	S	Se	0	0	0
			2897	1836	516	535	5	5			

There are 24 discrepancies between the modelled and reference sequences:

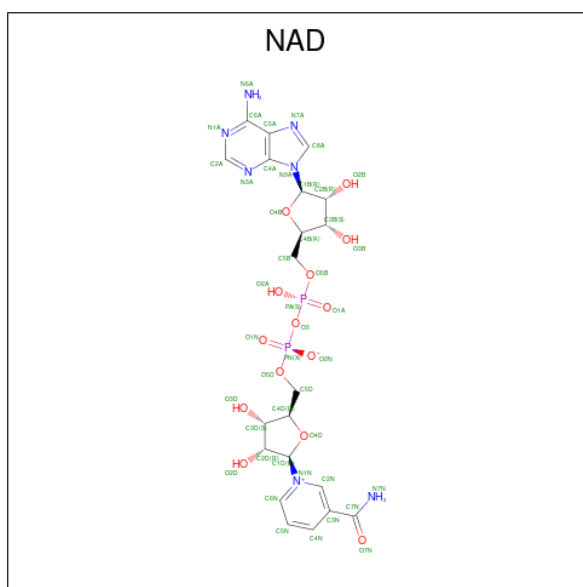
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P60802
A	-1	ASN	-	expression tag	UNP P60802
A	0	ALA	-	expression tag	UNP P60802
B	-2	SER	-	expression tag	UNP P60802
B	-1	ASN	-	expression tag	UNP P60802
B	0	ALA	-	expression tag	UNP P60802
C	-2	SER	-	expression tag	UNP P60802
C	-1	ASN	-	expression tag	UNP P60802
C	0	ALA	-	expression tag	UNP P60802
D	-2	SER	-	expression tag	UNP P60802
D	-1	ASN	-	expression tag	UNP P60802
D	0	ALA	-	expression tag	UNP P60802
E	-2	SER	-	expression tag	UNP P60802

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP P60802
E	0	ALA	-	expression tag	UNP P60802
F	-2	SER	-	expression tag	UNP P60802
F	-1	ASN	-	expression tag	UNP P60802
F	0	ALA	-	expression tag	UNP P60802
G	-2	SER	-	expression tag	UNP P60802
G	-1	ASN	-	expression tag	UNP P60802
G	0	ALA	-	expression tag	UNP P60802
H	-2	SER	-	expression tag	UNP P60802
H	-1	ASN	-	expression tag	UNP P60802
H	0	ALA	-	expression tag	UNP P60802

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

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

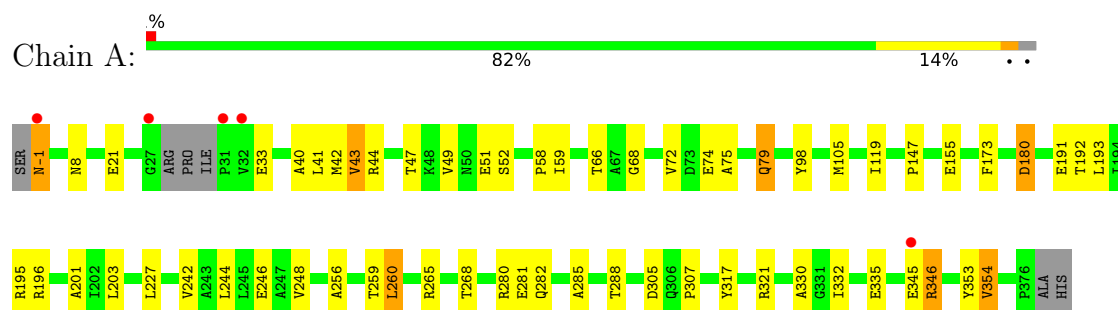
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	79	Total	O	0	3
			79	79		
3	C	78	Total	O	0	0
			78	78		
3	D	62	Total	O	0	0
			62	62		
3	E	91	Total	O	0	1
			91	91		
3	F	84	Total	O	0	1
			85	85		
3	G	47	Total	O	0	1
			48	48		
3	H	36	Total	O	0	0
			36	36		

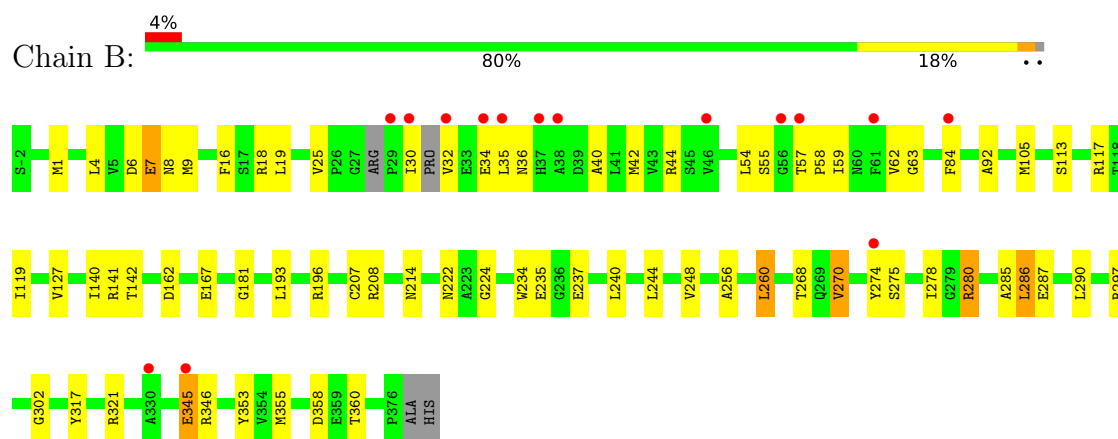
3 Residue-property plots [i](#)

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.

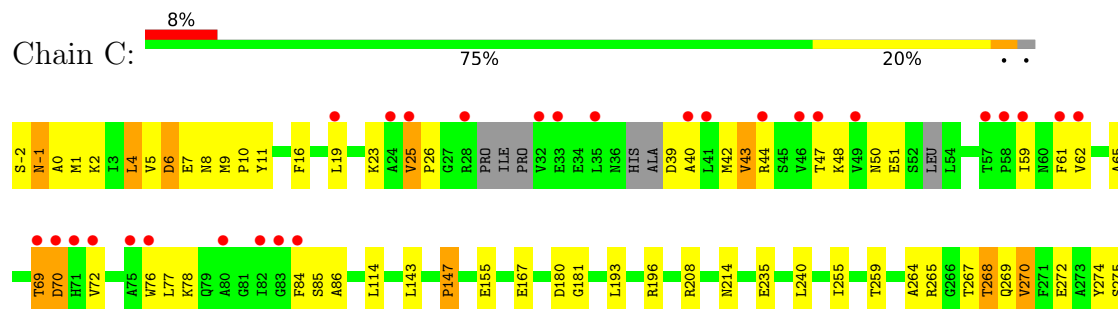
- Molecule 1: Erythronate-4-phosphate dehydrogenase



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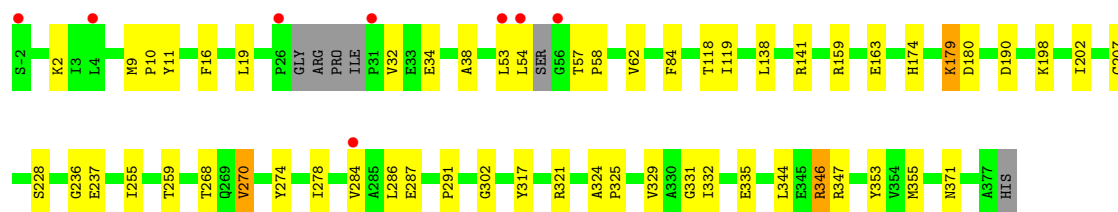
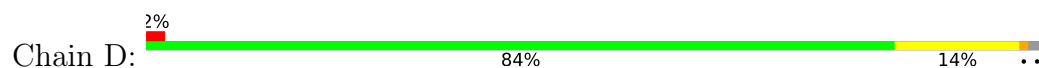


- Molecule 1: Erythronate-4-phosphate dehydrogenase

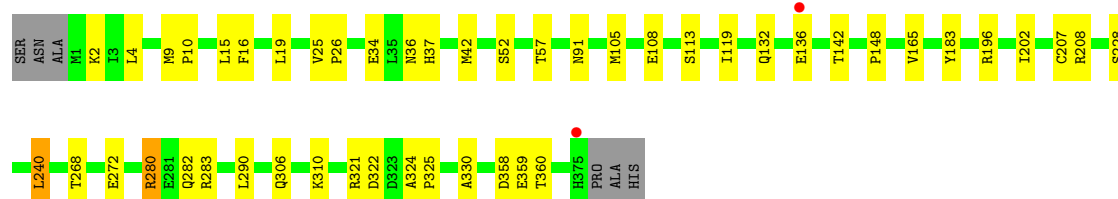
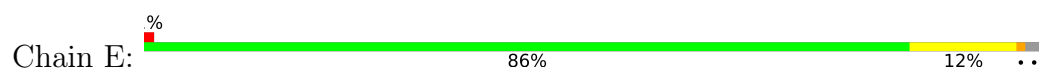




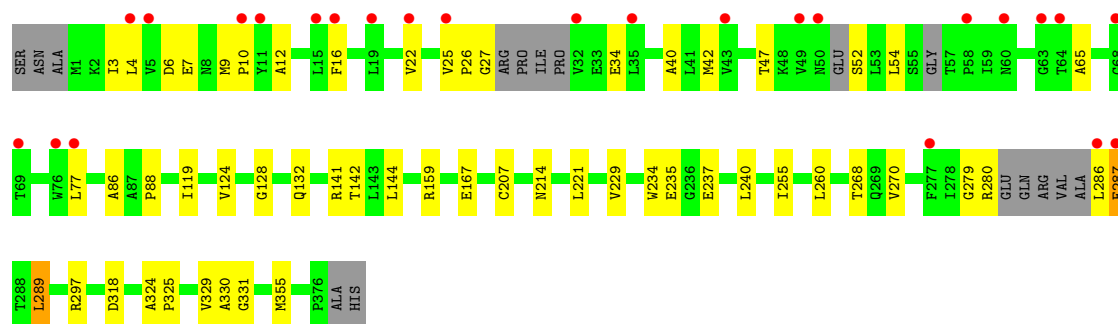
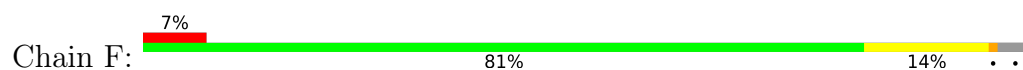
- Molecule 1: Erythronate-4-phosphate dehydrogenase



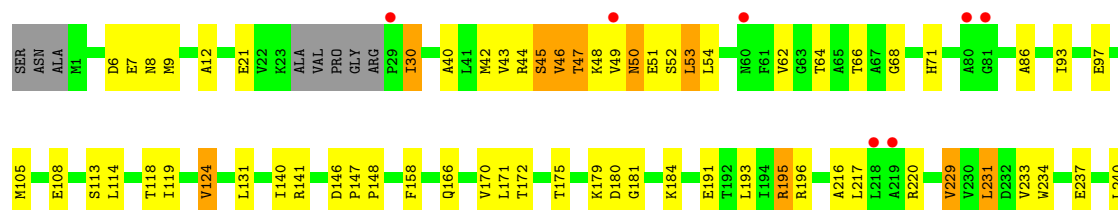
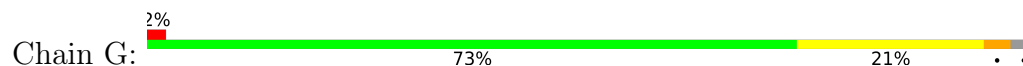
- Molecule 1: Erythronate-4-phosphate dehydrogenase



- Molecule 1: Erythronate-4-phosphate dehydrogenase

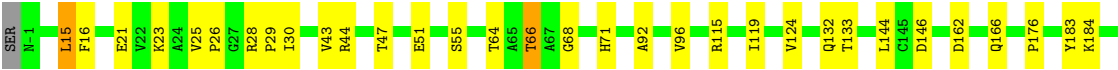
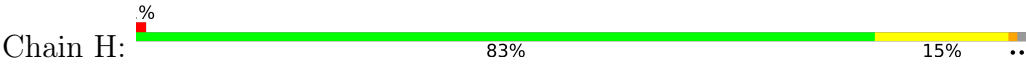


- Molecule 1: Erythronate-4-phosphate dehydrogenase





• Molecule 1: Erythronate-4-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.28Å 167.76Å 103.95Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	30.19 – 2.36 30.19 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.19-2.36) 98.6 (30.19-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.253 0.190 , 0.253	Depositor DCC
R_{free} test set	6469 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23835	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% 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	0.78	0/2937	0.98	5/3981 (0.1%)
1	B	0.81	0/2942	1.02	4/3989 (0.1%)
1	C	0.82	0/2910	1.01	8/3942 (0.2%)
1	D	0.80	0/2915	1.00	10/3953 (0.3%)
1	E	0.83	1/2931 (0.0%)	0.99	5/3977 (0.1%)
1	F	0.81	0/2837	0.96	5/3846 (0.1%)
1	G	0.73	0/2891	0.98	4/3919 (0.1%)
1	H	0.69	0/2948	0.94	2/4000 (0.1%)
All	All	0.79	1/23311 (0.0%)	0.98	43/31607 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	306	GLN	C-O	-5.36	1.19	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	VAL	N-CA-C	8.84	120.63	111.00
1	G	30	ILE	N-CA-C	7.91	115.38	107.55
1	C	302	GLY	CA-C-N	7.33	127.26	119.85
1	C	302	GLY	C-N-CA	7.33	127.26	119.85
1	C	180	ASP	N-CA-C	7.17	119.07	108.60
1	C	332	ILE	N-CA-C	6.89	113.83	107.56
1	E	290	LEU	CA-C-N	-6.89	113.55	120.31
1	E	290	LEU	C-N-CA	-6.89	113.55	120.31
1	G	229	VAL	N-CA-C	6.68	117.42	108.27
1	C	181	GLY	CA-C-N	6.58	126.51	119.28
1	C	181	GLY	C-N-CA	6.58	126.51	119.28
1	D	302	GLY	CA-C-N	6.48	126.45	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	302	GLY	C-N-CA	6.48	126.45	120.03
1	E	306	GLN	CA-C-N	-6.43	113.07	119.56
1	E	306	GLN	C-N-CA	-6.43	113.07	119.56
1	B	181	GLY	CA-C-N	6.11	125.81	119.64
1	B	181	GLY	C-N-CA	6.11	125.81	119.64
1	D	198	LYS	N-CA-C	5.77	116.24	109.60
1	D	286	LEU	N-CA-C	5.77	117.56	111.28
1	A	79	GLN	N-CA-C	-5.70	105.07	111.28
1	F	22	VAL	N-CA-C	5.62	116.19	107.99
1	B	302	GLY	CA-C-N	5.59	125.56	120.03
1	B	302	GLY	C-N-CA	5.59	125.56	120.03
1	D	331	GLY	CA-C-N	-5.58	117.91	123.04
1	D	331	GLY	C-N-CA	-5.58	117.91	123.04
1	D	324	ALA	CA-C-N	-5.56	114.03	119.64
1	D	324	ALA	C-N-CA	-5.56	114.03	119.64
1	A	147	PRO	N-CA-C	5.45	117.35	110.70
1	A	98	TYR	N-CA-C	-5.43	105.28	111.14
1	H	329	VAL	N-CA-C	5.42	117.41	112.43
1	A	354	VAL	N-CA-C	5.40	115.62	107.80
1	A	330	ALA	N-CA-C	5.38	117.14	111.28
1	F	330	ALA	N-CA-C	5.38	117.84	111.33
1	E	330	ALA	N-CA-C	5.37	117.83	111.33
1	C	147	PRO	N-CA-C	5.36	117.24	110.70
1	G	324	ALA	CA-C-N	-5.33	113.04	118.85
1	G	324	ALA	C-N-CA	-5.33	113.04	118.85
1	D	180	ASP	N-CA-C	5.20	114.69	107.73
1	F	331	GLY	CA-C-N	-5.20	118.85	122.59
1	F	331	GLY	C-N-CA	-5.20	118.85	122.59
1	C	86	ALA	N-CA-C	-5.18	101.91	109.63
1	F	329	VAL	N-CA-C	5.09	118.03	113.10
1	H	330	ALA	N-CA-C	5.07	116.80	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	2914	42	0
1	B	2894	0	2904	46	0
1	C	2865	0	2863	72	0
1	D	2867	0	2883	26	0
1	E	2880	0	2906	27	0
1	F	2791	0	2803	33	0
1	G	2843	0	2864	65	0
1	H	2897	0	2929	42	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	3	0
2	F	44	0	26	1	0
2	G	44	0	26	2	0
2	H	44	0	26	2	0
3	A	79	0	0	1	0
3	B	79	0	0	2	0
3	C	78	0	0	5	0
3	D	62	0	0	2	0
3	E	91	0	0	1	0
3	F	85	0	0	3	0
3	G	48	0	0	1	0
3	H	36	0	0	1	0
All	All	23835	0	23274	349	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 8.

All (349) 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:43:VAL:HG22	1:C:44:ARG:H	1.07	1.17
1:H:43:VAL:HG21	1:H:47:THR:HB	1.28	1.15
1:C:4:LEU:HD22	1:C:23:LYS:HB3	1.40	1.02
1:C:9:MSE:HE3	1:C:65:ALA:HB2	1.44	0.97
1:C:265:ARG:HG2	1:C:269:GLN:HE21	1.33	0.92
1:A:43:VAL:HG21	1:A:47:THR:HB	1.52	0.90
1:G:64:THR:OG1	1:G:66:THR:HG22	1.73	0.89
1:G:43:VAL:HG22	1:G:44:ARG:O	1.72	0.88
1:F:16:PHE:HZ	1:F:270:VAL:HG12	1.38	0.88
1:C:43:VAL:HG22	1:C:44:ARG:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HA	1:B:35:LEU:HD12	1.62	0.82
1:G:344:LEU:HG	1:G:345:GLU:N	1.94	0.81
1:A:259:THR:HG22	1:A:346[A]:ARG:HG2	1.64	0.79
1:G:118:THR:HG23	1:G:141:ARG:HG2	1.63	0.78
1:H:25:VAL:HG11	1:H:30:ILE:HG23	1.67	0.77
1:A:66:THR:HG22	1:A:68:GLY:H	1.48	0.76
1:D:274:TYR:CZ	1:D:278:ILE:HD11	2.20	0.76
1:B:140:ILE:O	1:B:142:THR:HG23	1.85	0.76
1:G:43:VAL:HG23	1:G:47:THR:HG23	1.66	0.75
1:B:280:ARG:HH21	1:B:280:ARG:HG3	1.52	0.74
1:A:43:VAL:HG21	1:A:47:THR:CB	2.18	0.74
1:B:317:TYR:CD1	1:B:346[B]:ARG:HD2	2.23	0.73
1:C:43:VAL:CG2	1:C:44:ARG:H	1.88	0.73
1:C:2:LYS:O	1:C:39:ASP:HB3	1.88	0.73
1:H:43:VAL:CG2	1:H:47:THR:HB	2.13	0.73
1:H:43:VAL:HG22	1:H:44:ARG:O	1.89	0.73
1:A:256:ALA:O	1:A:346[B]:ARG:NH2	2.20	0.73
1:B:285:ALA:HB1	1:B:287:GLU:OE2	1.88	0.72
1:C:259:THR:HG22	1:C:346:ARG:HG2	1.70	0.72
1:C:9:MSE:HE2	1:C:267:THR:HG23	1.69	0.72
1:C:240:LEU:C	1:C:240:LEU:HD12	2.15	0.72
1:H:43:VAL:HG21	1:H:47:THR:CB	2.15	0.71
1:G:259:THR:HG22	1:G:346:ARG:HG2	1.74	0.70
1:C:9:MSE:HE3	1:C:65:ALA:CB	2.20	0.69
1:A:317:TYR:CD1	1:A:346[A]:ARG:HD3	2.28	0.69
1:E:105:MSE:HE2	3:E:425:HOH:O	1.91	0.68
1:G:317:TYR:CD1	1:G:346:ARG:HD3	2.28	0.68
1:B:317:TYR:CD1	1:B:346[A]:ARG:HD3	2.30	0.67
1:G:240:LEU:C	1:G:240:LEU:HD12	2.21	0.66
1:F:324:ALA:HB3	1:F:325:PRO:HD3	1.77	0.66
1:D:291:PRO:O	1:D:347:ARG:NH2	2.29	0.65
1:C:69[B]:THR:O	1:C:70[B]:ASP:C	2.38	0.65
1:B:280:ARG:HG3	1:B:280:ARG:NH2	2.11	0.65
1:C:306:GLN:HB3	1:C:307:PRO:HD3	1.78	0.65
3:C:398:HOH:O	1:F:318:ASP:HB3	1.97	0.65
1:H:43:VAL:HG22	1:H:44:ARG:N	2.12	0.65
1:C:4:LEU:CD2	1:C:23:LYS:HB3	2.21	0.65
1:G:43:VAL:CG2	1:G:47:THR:HG23	2.27	0.65
1:C:301:HIS:ND1	1:C:357:ASP:OD2	2.22	0.64
1:F:4:LEU:HD11	1:F:34:GLU:HB3	1.79	0.64
1:G:240:LEU:HD12	1:G:240:LEU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ILE:O	1:G:97:GLU:HG3	1.98	0.64
1:C:317:TYR:CG	1:C:346:ARG:HD2	2.33	0.64
1:A:75:ALA:O	1:A:79:GLN:HG3	1.97	0.63
1:D:259:THR:HG22	1:D:346:ARG:HG2	1.80	0.63
1:B:162:ASP:OD1	1:B:196:ARG:NH1	2.31	0.63
1:A:285:ALA:HB3	1:A:288:THR:HG23	1.81	0.62
1:A:180:ASP:HB3	3:A:418:HOH:O	1.98	0.62
1:E:202:ILE:HG12	1:E:228:SER:HB2	1.82	0.62
1:A:201:ALA:O	1:A:227:LEU:HD12	2.00	0.62
1:B:141:ARG:NH2	1:B:167:GLU:OE1	2.27	0.62
1:C:43:VAL:HG21	1:C:47:THR:OG1	2.00	0.61
1:G:64:THR:OG1	1:G:66:THR:CG2	2.47	0.61
1:A:191:GLU:OE2	1:A:195:ARG:NH2	2.23	0.61
1:A:353:TYR:HH	1:B:353:TYR:HH	1.49	0.61
1:A:244:LEU:O	1:A:248:VAL:HG13	2.01	0.60
1:E:280:ARG:O	1:E:282:GLN:HG3	2.03	0.59
1:G:50:ASN:N	1:G:50:ASN:HD22	2.00	0.59
1:G:9:MSE:HG3	1:G:12:ALA:HB2	1.84	0.58
1:F:9:MSE:HB3	1:F:12:ALA:HB2	1.85	0.58
1:C:39:ASP:O	1:C:59:ILE:HA	2.03	0.58
1:A:49:VAL:HB	1:A:72:VAL:HG13	1.85	0.58
1:H:234:TRP:O	1:H:237:GLU:HG3	2.04	0.58
1:C:193:LEU:HD23	1:C:193:LEU:C	2.29	0.58
1:C:275:SER:O	1:C:281:GLU:N	2.37	0.58
1:B:287:GLU:CD	1:B:287:GLU:H	2.12	0.58
1:C:51:GLU:HG3	1:C:76:TRP:CE2	2.39	0.58
1:E:240:LEU:C	1:E:240:LEU:HD12	2.29	0.57
1:B:42:MSE:HA	1:B:63:GLY:O	2.05	0.57
1:G:326:LEU:O	1:G:330:ALA:HB2	2.04	0.57
1:C:61:PHE:HB3	1:C:274:TYR:HE1	1.69	0.57
1:C:277:PHE:C	1:C:277:PHE:CD2	2.83	0.57
1:D:16:PHE:HZ	1:D:270:VAL:HG12	1.68	0.57
1:E:4:LEU:HD21	1:E:34:GLU:HG3	1.87	0.57
1:G:217:LEU:HD21	1:G:229:VAL:HG11	1.85	0.57
1:F:279:GLY:O	1:F:280:ARG:HG3	2.05	0.56
1:G:6:ASP:OD2	1:G:8:ASN:HB2	2.05	0.56
1:C:290:LEU:HB3	1:C:291:PRO:HD2	1.87	0.56
1:G:234:TRP:O	1:G:237:GLU:HG3	2.06	0.56
1:A:317:TYR:CD1	1:A:346[B]:ARG:HD2	2.41	0.56
1:G:166:GLN:HE21	1:G:196:ARG:HH22	1.53	0.56
1:C:7:GLU:N	1:C:25:VAL:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:GLU:OE2	1:H:23:LYS:HD3	2.06	0.56
1:B:16:PHE:HZ	1:B:270:VAL:HG12	1.71	0.55
1:H:16:PHE:HZ	1:H:270:VAL:HG12	1.72	0.55
1:H:306:GLN:HB3	1:H:307:PRO:HD3	1.89	0.55
1:E:16:PHE:CE1	1:E:42:MSE:HE3	2.41	0.55
1:H:92:ALA:O	1:H:96:VAL:HG23	2.07	0.55
1:F:287:GLU:O	1:F:287:GLU:HG2	2.07	0.55
1:G:166:GLN:HE21	1:G:196:ARG:NH2	2.04	0.55
1:G:231:LEU:HD22	1:G:248:VAL:HG11	1.89	0.55
1:F:286:LEU:HD23	1:F:289:LEU:HD12	1.87	0.55
1:A:-1:ASN:OD1	1:A:-1:ASN:N	2.39	0.55
1:C:9:MSE:CE	1:C:65:ALA:HB2	2.28	0.55
1:F:6:ASP:OD2	1:F:27:GLY:HA3	2.08	0.54
1:E:19:LEU:C	1:E:19:LEU:HD12	2.33	0.54
1:C:196:ARG:HD3	3:C:428:HOH:O	2.06	0.54
1:F:9:MSE:HE2	1:F:65:ALA:HB3	1.90	0.54
1:F:40:ALA:HB1	1:F:42:MSE:HE2	1.89	0.54
1:C:72:VAL:HG11	1:C:84:PHE:CE1	2.43	0.54
1:E:165:VAL:HG11	1:E:196:ARG:NH1	2.23	0.54
1:H:183:TYR:O	1:H:184:LYS:C	2.51	0.54
1:A:317:TYR:CE1	1:A:346[B]:ARG:HD2	2.43	0.54
1:A:242:VAL:O	1:A:246:GLU:HG2	2.07	0.53
1:B:62:VAL:O	1:B:84:PHE:HA	2.08	0.53
1:D:53:LEU:O	1:D:54:LEU:HG	2.08	0.53
1:C:332:ILE:HB	1:C:335:GLU:HG3	1.90	0.53
1:G:332:ILE:HG22	1:G:335:GLU:HG2	1.91	0.53
1:G:66:THR:HG23	1:G:68:GLY:O	2.09	0.53
1:G:51:GLU:C	1:G:53:LEU:H	2.17	0.53
1:B:286:LEU:HD13	1:B:290:LEU:HD11	1.90	0.52
1:G:119:ILE:HG12	1:G:170:VAL:HB	1.91	0.52
1:C:48:LYS:HG3	3:C:419:HOH:O	2.08	0.52
1:H:304:LEU:HD23	1:H:364:LEU:HD23	1.91	0.52
1:F:4:LEU:CD1	1:F:34:GLU:HB3	2.39	0.52
1:C:51:GLU:HG3	1:C:76:TRP:NE1	2.24	0.52
1:A:41:LEU:C	1:A:41:LEU:HD23	2.34	0.52
1:E:240:LEU:HD12	1:E:240:LEU:O	2.10	0.52
1:G:48:LYS:O	1:G:50:ASN:ND2	2.42	0.52
1:H:25:VAL:HG12	1:H:26:PRO:O	2.09	0.52
1:A:285:ALA:CB	1:A:288:THR:HG23	2.40	0.52
1:G:105:MSE:HE2	1:G:320:ARG:HD3	1.91	0.52
1:B:260:LEU:HD13	1:B:345:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HD23	1:C:84:PHE:HB2	1.92	0.52
1:E:324:ALA:HB3	1:E:325:PRO:HD3	1.92	0.52
1:B:4:LEU:HD21	1:B:34:GLU:CG	2.40	0.51
1:B:40:ALA:HB2	1:B:274:TYR:OH	2.09	0.51
1:G:43:VAL:HG22	1:G:44:ARG:N	2.24	0.51
1:E:108:GLU:OE2	1:E:310:LYS:HE3	2.10	0.51
1:H:191:GLU:HG3	1:H:192:THR:N	2.25	0.51
1:B:54:LEU:O	1:B:55:SER:C	2.54	0.51
1:B:297:ARG:HB3	1:B:355:MSE:HE2	1.91	0.51
1:B:260:LEU:HD13	1:B:345:GLU:CB	2.40	0.51
1:D:2:LYS:HB3	1:D:38:ALA:HA	1.92	0.51
1:C:143:LEU:HD23	1:H:333:PRO:HG2	1.92	0.51
1:G:166:GLN:NE2	1:G:196:ARG:HH22	2.09	0.51
1:F:16:PHE:CZ	1:F:270:VAL:HG12	2.30	0.50
1:C:279:GLY:C	1:C:281:GLU:N	2.70	0.50
1:B:7:GLU:HB3	1:B:25:VAL:O	2.11	0.50
1:C:61:PHE:CD1	1:C:61:PHE:C	2.89	0.50
1:G:54:LEU:HD11	1:G:62:VAL:HG21	1.94	0.50
1:F:240:LEU:HD12	1:F:240:LEU:C	2.37	0.50
1:H:244:LEU:O	1:H:248:VAL:HG13	2.12	0.50
1:G:280:ARG:O	1:G:281:GLU:C	2.55	0.50
1:G:49:VAL:HG21	1:G:62:VAL:HG11	1.93	0.50
1:D:57:THR:HB	1:D:58:PRO:CD	2.42	0.49
1:B:244:LEU:O	1:B:248:VAL:HG13	2.12	0.49
1:C:40:ALA:HB2	1:C:274:TYR:OH	2.12	0.49
1:H:162:ASP:O	1:H:166:GLN:HG3	2.12	0.49
1:G:216:ALA:O	1:G:220:ARG:HG2	2.12	0.49
1:H:25:VAL:HG13	1:H:26:PRO:HD2	1.94	0.49
1:H:146:ASP:OD2	2:H:379:NAD:H1B	2.13	0.49
1:G:45:SER:HA	1:G:71:HIS:CE1	2.48	0.49
1:H:64:THR:HG23	1:H:66:THR:HG22	1.95	0.49
1:C:317:TYR:CD1	1:C:346:ARG:CD	2.96	0.49
1:G:30:ILE:HD11	1:G:47:THR:HG21	1.95	0.49
1:H:280:ARG:O	1:H:281:GLU:C	2.55	0.49
1:A:8:ASN:HB2	1:A:44:ARG:NH1	2.28	0.48
1:C:-1:ASN:N	1:C:-1:ASN:OD1	2.45	0.48
1:C:355:MSE:HE1	3:F:386:HOH:O	2.13	0.48
1:H:66:THR:HG23	1:H:68:GLY:O	2.13	0.48
1:H:43:VAL:CG2	1:H:44:ARG:N	2.76	0.48
1:A:285:ALA:HB3	1:A:288:THR:CG2	2.43	0.48
1:F:279:GLY:C	1:F:280:ARG:HG3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASN:HB2	1:B:44:ARG:NH1	2.29	0.48
1:C:324:ALA:HB3	1:C:325:PRO:HD3	1.95	0.48
1:E:36:ASN:OD1	1:E:57:THR:HG22	2.14	0.48
1:G:124:VAL:HG23	1:G:146:ASP:HB2	1.96	0.48
1:C:240:LEU:HD12	1:C:240:LEU:O	2.12	0.48
1:G:147:PRO:HB2	1:G:148:PRO:HD3	1.96	0.48
1:G:193:LEU:C	1:G:193:LEU:HD23	2.39	0.48
1:B:4:LEU:HD21	1:B:34:GLU:HG3	1.95	0.48
1:F:7:GLU:CD	1:F:26:PRO:HA	2.39	0.48
1:C:16:PHE:HZ	1:C:270:VAL:HG12	1.79	0.47
1:G:240:LEU:C	1:G:240:LEU:CD1	2.86	0.47
1:C:61:PHE:HD2	1:C:277:PHE:CD1	2.32	0.47
1:C:317:TYR:CD1	1:C:346:ARG:HD3	2.48	0.47
1:D:332:ILE:HB	1:D:335:GLU:HG3	1.96	0.47
1:A:43:VAL:CG2	1:A:47:THR:HB	2.36	0.47
1:H:214:ASN:ND2	3:H:385:HOH:O	2.33	0.47
1:B:317:TYR:CE1	1:B:346[B]:ARG:HD2	2.49	0.47
1:C:48:LYS:HE3	3:C:419:HOH:O	2.13	0.47
1:C:277:PHE:HD2	1:C:278:ILE:HG23	1.80	0.47
1:D:62:VAL:O	1:D:84:PHE:HA	2.15	0.47
1:E:25:VAL:HG22	1:E:26:PRO:HD2	1.95	0.47
1:A:40:ALA:HB1	1:A:42:MSE:HE2	1.96	0.47
1:C:0:ALA:C	1:C:1:MSE:HE2	2.40	0.47
1:C:345:GLU:HA	3:C:436:HOH:O	2.15	0.47
1:F:9:MSE:HE2	1:F:65:ALA:CB	2.45	0.47
1:G:233:VAL:HA	1:G:237:GLU:OE2	2.15	0.47
1:B:193:LEU:C	1:B:193:LEU:HD23	2.40	0.47
1:C:305:ASP:OD1	1:C:307:PRO:HD2	2.15	0.47
1:C:6:ASP:OD1	1:C:8:ASN:N	2.43	0.46
1:D:274:TYR:CE2	1:D:278:ILE:HD11	2.50	0.46
1:D:317:TYR:CD1	1:D:346:ARG:HD3	2.50	0.46
1:G:305:ASP:CG	1:G:307:PRO:HD2	2.40	0.46
1:G:131:LEU:HD21	1:G:172:THR:HG21	1.97	0.46
1:G:317:TYR:CD1	1:G:346:ARG:CD	2.97	0.46
1:D:57:THR:HB	1:D:58:PRO:HD2	1.98	0.46
1:E:358:ASP:OD1	1:E:360:THR:OG1	2.30	0.46
1:B:18:ARG:O	1:B:19:LEU:HD23	2.16	0.46
1:B:358:ASP:OD1	1:B:360:THR:OG1	2.26	0.46
1:G:44:ARG:O	1:G:46:VAL:N	2.49	0.46
1:H:43:VAL:CG2	1:H:47:THR:CB	2.86	0.46
1:A:193:LEU:C	1:A:193:LEU:HD23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ALA:HB2	1:C:290:LEU:HD21	1.98	0.46
1:G:336:PHE:C	1:G:336:PHE:CD2	2.94	0.46
1:A:260:LEU:HD13	1:A:345:GLU:HG3	1.96	0.46
1:C:10:PRO:HB2	1:C:11:TYR:CD2	2.50	0.46
1:G:7:GLU:O	1:G:7:GLU:CG	2.64	0.46
1:A:332:ILE:HB	1:A:335:GLU:HG3	1.97	0.46
1:B:207:CYS:SG	1:B:208:ARG:N	2.89	0.45
1:C:5:VAL:HG12	1:C:42:MSE:HB2	1.98	0.45
1:E:2:LYS:HD2	1:E:37:HIS:O	2.15	0.45
1:G:329:VAL:HA	1:G:332:ILE:HD12	1.98	0.45
1:B:40:ALA:HB1	1:B:42:MSE:HE2	1.98	0.45
1:C:50:ASN:O	1:C:51:GLU:C	2.57	0.45
1:G:40:ALA:HB1	1:G:42:MSE:HE2	1.98	0.45
1:H:124:VAL:HG21	1:H:144:LEU:HB3	1.98	0.45
1:H:245:LEU:HD23	1:H:330:ALA:CB	2.46	0.45
1:E:207:CYS:HB2	2:E:379:NAD:H4D	1.99	0.45
1:H:66:THR:HG21	1:H:71:HIS:HE1	1.82	0.45
1:H:324:ALA:HB3	1:H:325:PRO:HD3	1.98	0.45
1:B:1:MSE:HE3	3:B:457:HOH:O	2.15	0.44
1:B:105:MSE:SE	1:B:105:MSE:C	3.11	0.44
1:E:119:ILE:O	1:E:142:THR:HA	2.17	0.44
1:F:297:ARG:NH1	3:F:386:HOH:O	2.50	0.44
1:G:147:PRO:HD2	2:G:379:NAD:C2A	2.48	0.44
1:G:191:GLU:O	1:G:195:ARG:HB3	2.16	0.44
1:A:41:LEU:HD23	1:A:42:MSE:N	2.33	0.44
1:B:117:ARG:NH1	3:B:385:HOH:O	2.28	0.44
1:B:275:SER:O	1:B:280:ARG:N	2.51	0.44
1:E:132:GLN:O	1:E:136:GLU:HG3	2.17	0.44
1:F:119:ILE:O	1:F:142:THR:HA	2.17	0.44
1:E:207:CYS:SG	1:E:208:ARG:N	2.89	0.44
1:A:43:VAL:CG2	1:A:47:THR:CB	2.94	0.44
1:F:355:MSE:HE1	3:F:386:HOH:O	2.18	0.44
1:D:118:THR:HG23	1:D:141:ARG:HG2	2.00	0.44
1:F:4:LEU:HD11	1:F:34:GLU:CB	2.47	0.44
1:B:317:TYR:CG	1:B:346[A]:ARG:HD3	2.52	0.43
1:D:10:PRO:O	1:D:11:TYR:HB2	2.18	0.43
1:F:214:ASN:ND2	1:F:235:GLU:H	2.16	0.43
1:C:51:GLU:CG	1:C:76:TRP:CE2	3.01	0.43
1:D:174:HIS:HA	1:D:207:CYS:HB3	1.99	0.43
1:B:92:ALA:HA	1:B:127:VAL:HG22	2.00	0.43
1:C:214:ASN:ND2	1:C:235:GLU:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:LEU:HD23	1:G:364:LEU:HD23	2.00	0.43
1:C:268:THR:O	1:C:272:GLU:HG3	2.19	0.43
1:C:317:TYR:CD1	1:C:346:ARG:HD2	2.53	0.43
1:D:325:PRO:O	1:D:329:VAL:HG22	2.19	0.43
1:F:234:TRP:HB2	1:F:237:GLU:HG3	2.00	0.43
1:A:265:ARG:HA	1:A:268:THR:HB	2.01	0.43
1:B:214:ASN:HB2	1:B:235:GLU:OE1	2.19	0.43
1:B:256:ALA:O	1:B:346[B]:ARG:NH1	2.45	0.43
1:D:9:MSE:HA	1:D:10:PRO:HD3	1.85	0.43
1:D:190:ASP:HB2	3:D:419:HOH:O	2.19	0.43
1:E:321:ARG:HD2	1:E:322:ASP:OD1	2.19	0.43
1:A:66:THR:HG22	1:A:68:GLY:N	2.27	0.43
1:D:353:TYR:HA	1:D:371:ASN:O	2.19	0.43
1:E:15:LEU:HD23	1:E:15:LEU:HA	1.89	0.43
1:G:296:GLY:C	1:G:297:ARG:HG3	2.43	0.43
1:E:108:GLU:CD	1:E:310:LYS:HE3	2.44	0.42
1:H:245:LEU:CD2	1:H:330:ALA:CB	2.97	0.42
1:A:192:THR:O	1:A:196:ARG:HG3	2.19	0.42
1:C:155:GLU:OE1	1:H:341:LYS:NZ	2.52	0.42
1:F:86:ALA:C	1:F:88:PRO:HD3	2.43	0.42
1:G:114:LEU:HB3	1:G:140:ILE:HD11	2.00	0.42
1:A:51:GLU:O	1:A:52:SER:C	2.63	0.42
1:F:54:LEU:HD12	1:F:77:LEU:HD21	2.01	0.42
1:G:7:GLU:O	1:G:7:GLU:HG3	2.20	0.42
1:G:175:THR:HG22	2:G:379:NAD:C4A	2.49	0.42
1:B:234:TRP:HB2	1:B:237:GLU:HG3	2.01	0.42
1:C:240:LEU:C	1:C:240:LEU:CD1	2.88	0.42
1:G:158:PHE:HB3	3:G:498:HOH:O	2.19	0.42
1:G:317:TYR:CG	1:G:346:ARG:HD2	2.54	0.42
1:B:30:ILE:HG21	1:B:35:LEU:HD21	2.01	0.42
1:E:9:MSE:HA	1:E:10:PRO:HD3	1.94	0.42
1:A:33:GLU:OE1	1:A:33:GLU:HA	2.19	0.42
1:A:58:PRO:O	1:A:59:ILE:C	2.62	0.42
1:C:-2:SER:C	1:C:-1:ASN:OD1	2.63	0.42
1:C:274:TYR:O	1:C:278:ILE:HG12	2.19	0.42
1:F:207:CYS:HB2	2:F:379:NAD:H4D	2.02	0.42
1:H:194:ILE:CG2	1:H:220:ARG:HG3	2.49	0.42
1:A:280:ARG:O	1:A:282:GLN:HG3	2.20	0.42
1:B:222:ASN:C	1:B:224:GLY:N	2.76	0.42
1:E:207:CYS:HA	2:E:379:NAD:H1D	2.01	0.42
1:C:255:ILE:HD12	1:C:255:ILE:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:ASP:HB2	1:G:181:GLY:H	1.73	0.42
1:A:173:PHE:HE1	1:A:203:LEU:HD11	1.85	0.42
1:G:179:LYS:O	1:G:184:LYS:HG3	2.20	0.42
1:D:255:ILE:C	1:D:255:ILE:HD12	2.44	0.41
1:F:159:ARG:HE	1:F:159:ARG:HB3	1.73	0.41
1:A:259:THR:HG22	1:A:346[B]:ARG:HG2	2.03	0.41
1:B:58:PRO:O	1:B:59:ILE:C	2.62	0.41
1:F:9:MSE:HA	1:F:10:PRO:HD3	1.90	0.41
1:H:51:GLU:O	1:H:55:SER:HB2	2.20	0.41
1:H:214:ASN:ND2	1:H:235:GLU:H	2.18	0.41
1:E:148:PRO:HG3	1:E:183:TYR:CG	2.55	0.41
1:F:141:ARG:NH2	1:F:167:GLU:OE1	2.47	0.41
1:A:40:ALA:HB1	1:A:42:MSE:CE	2.50	0.41
1:B:6:ASP:HB3	1:B:9:MSE:HE3	2.00	0.41
1:C:296:GLY:C	1:C:297:ARG:HG3	2.45	0.41
1:G:321:ARG:NH1	1:G:322:ASP:OD1	2.53	0.41
1:H:359:GLU:HB2	1:H:374:HIS:CE1	2.56	0.41
1:A:256:ALA:C	1:A:346[B]:ARG:HH22	2.23	0.41
1:B:36:ASN:HA	1:B:57:THR:HG22	2.01	0.41
1:C:61:PHE:HB3	1:C:274:TYR:CE1	2.53	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.93	0.41
1:E:91:ASN:OD1	2:E:379:NAD:H5N	2.21	0.41
1:H:132:GLN:O	1:H:133:THR:C	2.64	0.41
1:F:124:VAL:HA	1:F:128:GLY:HA3	2.02	0.41
1:A:317:TYR:CG	1:A:346[A]:ARG:CD	3.04	0.41
1:C:25:VAL:HG12	1:C:26:PRO:O	2.21	0.41
1:C:353:TYR:HE2	1:C:355:MSE:SE	2.53	0.41
1:H:15:LEU:HD12	1:H:15:LEU:HA	1.86	0.41
1:H:176:PRO:HD3	2:H:379:NAD:H52A	2.03	0.41
1:C:69[B]:THR:O	1:C:69[B]:THR:OG1	2.38	0.41
1:D:236:GLY:O	1:D:237:GLU:C	2.64	0.41
1:F:255:ILE:HD12	1:F:255:ILE:C	2.46	0.41
1:D:159:ARG:HE	1:D:163:GLU:CD	2.29	0.40
1:F:132:GLN:NE2	1:F:144:LEU:HD11	2.36	0.40
1:F:221:LEU:HD11	1:F:229:VAL:HG21	2.02	0.40
1:A:305:ASP:OD1	1:A:307:PRO:HD2	2.21	0.40
1:C:264:ALA:CB	1:C:290:LEU:HD21	2.52	0.40
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.92	0.40
1:G:171:LEU:HD12	1:G:171:LEU:HA	1.91	0.40
1:G:234:TRP:CD2	1:G:240:LEU:HD22	2.56	0.40
1:H:245:LEU:CD2	1:H:330:ALA:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:PRO:HD2	2:C:379:NAD:C2A	2.52	0.40
1:D:179:LYS:NZ	3:D:409:HOH:O	2.54	0.40
1:G:64:THR:HG23	1:G:86:ALA:HA	2.03	0.40
1:G:108:GLU:CD	1:G:310:LYS:HE3	2.46	0.40
1:H:231:LEU:O	1:H:251:GLY:HA2	2.20	0.40
1:C:61:PHE:CD1	1:C:62:VAL:N	2.90	0.40
1:D:202:ILE:HG12	1:D:228:SER:HB2	2.02	0.40
1:D:353:TYR:CE2	1:D:355:MSE:HG2	2.56	0.40
1:E:272:GLU:OE2	1:E:283:ARG:HG3	2.20	0.40
1:H:28:ARG:HA	1:H:29:PRO:HA	1.85	0.40
1:B:240:LEU:HD12	1:B:240:LEU:O	2.21	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	372/381 (98%)	360 (97%)	12 (3%)	0	100	100
1	B	372/381 (98%)	352 (95%)	20 (5%)	0	100	100
1	C	365/381 (96%)	341 (93%)	21 (6%)	3 (1%)	16	17
1	D	369/381 (97%)	352 (95%)	17 (5%)	0	100	100
1	E	373/381 (98%)	358 (96%)	15 (4%)	0	100	100
1	F	355/381 (93%)	339 (96%)	16 (4%)	0	100	100
1	G	366/381 (96%)	341 (93%)	22 (6%)	3 (1%)	16	17
1	H	376/381 (99%)	354 (94%)	22 (6%)	0	100	100
All	All	2948/3048 (97%)	2797 (95%)	145 (5%)	6 (0%)	43	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	45	SER
1	C	70[A]	ASP
1	C	70[B]	ASP
1	G	52	SER
1	G	281	GLU
1	C	43	VAL

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	303/303 (100%)	289 (95%)	14 (5%)	24	31
1	B	303/303 (100%)	292 (96%)	11 (4%)	31	41
1	C	299/303 (99%)	285 (95%)	14 (5%)	23	30
1	D	299/303 (99%)	288 (96%)	11 (4%)	30	40
1	E	303/303 (100%)	297 (98%)	6 (2%)	48	63
1	F	291/303 (96%)	283 (97%)	8 (3%)	39	52
1	G	298/303 (98%)	285 (96%)	13 (4%)	25	33
1	H	303/303 (100%)	293 (97%)	10 (3%)	33	44
All	All	2399/2424 (99%)	2312 (96%)	87 (4%)	31	41

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	21	GLU
1	A	43	VAL
1	A	74	GLU
1	A	105	MSE
1	A	119	ILE
1	A	155	GLU
1	A	180	ASP
1	A	260	LEU
1	A	281	GLU

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Mol	Chain	Res	Type
1	A	321	ARG
1	A	346[A]	ARG
1	A	346[B]	ARG
1	A	354	VAL
1	B	7	GLU
1	B	113	SER
1	B	119	ILE
1	B	260	LEU
1	B	268	THR
1	B	270	VAL
1	B	278	ILE
1	B	280	ARG
1	B	286	LEU
1	B	321	ARG
1	B	345	GLU
1	C	-1	ASN
1	C	4	LEU
1	C	6	ASP
1	C	19	LEU
1	C	25	VAL
1	C	69[A]	THR
1	C	69[B]	THR
1	C	78	LYS
1	C	85	SER
1	C	167	GLU
1	C	208	ARG
1	C	268	THR
1	C	270	VAL
1	C	321	ARG
1	D	19	LEU
1	D	34	GLU
1	D	119	ILE
1	D	179	LYS
1	D	268	THR
1	D	270	VAL
1	D	284	VAL
1	D	287	GLU
1	D	321	ARG
1	D	344	LEU
1	D	346	ARG
1	E	52	SER
1	E	113	SER

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Mol	Chain	Res	Type
1	E	240	LEU
1	E	268	THR
1	E	280	ARG
1	E	359	GLU
1	F	3	ILE
1	F	25	VAL
1	F	47	THR
1	F	52	SER
1	F	260	LEU
1	F	268	THR
1	F	287	GLU
1	F	289	LEU
1	G	46	VAL
1	G	47	THR
1	G	50	ASN
1	G	53	LEU
1	G	113	SER
1	G	124	VAL
1	G	195	ARG
1	G	231	LEU
1	G	260	LEU
1	G	268	THR
1	G	280	ARG
1	G	284	VAL
1	G	346	ARG
1	H	15	LEU
1	H	21	GLU
1	H	66	THR
1	H	115	ARG
1	H	119	ILE
1	H	191	GLU
1	H	192	THR
1	H	288	THR
1	H	321	ARG
1	H	360	THR

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

Mol	Chain	Res	Type
1	A	79	GLN
1	B	60	ASN
1	B	166	GLN

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Mol	Chain	Res	Type
1	C	269	GLN
1	D	282	GLN
1	E	37	HIS
1	F	132	GLN
1	F	214	ASN
1	F	375	HIS
1	G	50	ASN
1	G	166	GLN
1	G	214	ASN
1	H	132	GLN
1	H	166	GLN
1	H	214	ASN
1	H	374	HIS

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	379	-	46,48,48	1.77	5 (10%)	64,73,73	1.52	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	F	379	-	46,48,48	1.67	4 (8%)	64,73,73	1.72	13 (20%)
2	NAD	E	379	-	46,48,48	1.86	7 (15%)	64,73,73	1.64	12 (18%)
2	NAD	G	379	-	46,48,48	1.92	7 (15%)	64,73,73	1.64	11 (17%)
2	NAD	B	379	-	46,48,48	1.72	6 (13%)	64,73,73	1.53	9 (14%)
2	NAD	H	379	-	46,48,48	1.78	6 (13%)	64,73,73	1.63	8 (12%)
2	NAD	C	379	-	46,48,48	1.81	6 (13%)	64,73,73	1.64	12 (18%)
2	NAD	D	379	-	46,48,48	1.75	7 (15%)	64,73,73	1.67	11 (17%)

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	A	379	-	-	7/30/62/62	0/5/5/5
2	NAD	F	379	-	-	2/30/62/62	0/5/5/5
2	NAD	E	379	-	-	9/30/62/62	0/5/5/5
2	NAD	G	379	-	-	7/30/62/62	0/5/5/5
2	NAD	B	379	-	-	11/30/62/62	0/5/5/5
2	NAD	H	379	-	-	10/30/62/62	0/5/5/5
2	NAD	C	379	-	-	7/30/62/62	0/5/5/5
2	NAD	D	379	-	-	4/30/62/62	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	379	NAD	O7N-C7N	10.34	1.43	1.24
2	C	379	NAD	O7N-C7N	9.58	1.42	1.24
2	E	379	NAD	O7N-C7N	9.47	1.41	1.24
2	A	379	NAD	O7N-C7N	9.42	1.41	1.24
2	H	379	NAD	O7N-C7N	9.28	1.41	1.24
2	B	379	NAD	O7N-C7N	9.17	1.41	1.24
2	D	379	NAD	O7N-C7N	8.93	1.40	1.24
2	F	379	NAD	O7N-C7N	8.63	1.40	1.24
2	E	379	NAD	PN-O3	3.47	1.63	1.59
2	F	379	NAD	C2N-N1N	3.14	1.38	1.35
2	H	379	NAD	C2A-N3A	2.99	1.39	1.33
2	E	379	NAD	C2N-N1N	2.93	1.38	1.35
2	B	379	NAD	C2A-N1A	2.84	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	379	NAD	PN-O3	2.79	1.62	1.59
2	C	379	NAD	C2A-N1A	2.77	1.38	1.33
2	G	379	NAD	C2A-N1A	2.72	1.38	1.33
2	F	379	NAD	C2A-N1A	2.67	1.38	1.33
2	A	379	NAD	C2A-N3A	2.63	1.38	1.33
2	G	379	NAD	C2A-N3A	2.63	1.38	1.33
2	D	379	NAD	C8A-N7A	2.61	1.36	1.31
2	D	379	NAD	C2A-N1A	2.61	1.38	1.33
2	C	379	NAD	C8A-N7A	2.60	1.36	1.31
2	C	379	NAD	C5A-N7A	-2.58	1.34	1.39
2	G	379	NAD	PN-O3	2.57	1.62	1.59
2	E	379	NAD	C2A-N1A	2.54	1.38	1.33
2	F	379	NAD	C2A-N3A	2.52	1.38	1.33
2	C	379	NAD	C2N-N1N	2.50	1.37	1.35
2	C	379	NAD	C2A-N3A	2.48	1.38	1.33
2	D	379	NAD	PN-O3	2.47	1.62	1.59
2	H	379	NAD	C2A-N1A	2.44	1.38	1.33
2	D	379	NAD	C2A-N3A	2.36	1.38	1.33
2	B	379	NAD	C2A-N3A	2.36	1.38	1.33
2	A	379	NAD	C2N-N1N	2.32	1.37	1.35
2	E	379	NAD	C2A-N3A	2.29	1.38	1.33
2	A	379	NAD	C2A-N1A	2.29	1.38	1.33
2	D	379	NAD	O4D-C1D	2.27	1.43	1.40
2	B	379	NAD	PN-O3	2.25	1.61	1.59
2	G	379	NAD	C8A-N7A	2.25	1.36	1.31
2	E	379	NAD	C8A-N7A	2.23	1.36	1.31
2	A	379	NAD	O4D-C1D	2.20	1.43	1.40
2	G	379	NAD	C2N-N1N	2.18	1.37	1.35
2	E	379	NAD	C5A-N7A	-2.18	1.35	1.39
2	G	379	NAD	PA-O3	2.17	1.61	1.59
2	H	379	NAD	C2N-N1N	2.12	1.37	1.35
2	B	379	NAD	C8A-N7A	2.07	1.35	1.31
2	B	379	NAD	C5A-N7A	-2.04	1.35	1.39
2	H	379	NAD	C8A-N7A	2.04	1.35	1.31
2	D	379	NAD	C5A-N7A	-2.00	1.35	1.39

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	379	NAD	N3A-C2A-N1A	-5.97	119.54	128.58
2	B	379	NAD	N3A-C2A-N1A	-5.85	119.73	128.58
2	F	379	NAD	N3A-C2A-N1A	-5.82	119.77	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	379	NAD	N3A-C2A-N1A	-5.74	119.89	128.58
2	H	379	NAD	N3A-C2A-N1A	-5.32	120.53	128.58
2	D	379	NAD	N3A-C2A-N1A	-5.18	120.75	128.58
2	C	379	NAD	N3A-C2A-N1A	-5.08	120.89	128.58
2	A	379	NAD	N3A-C2A-N1A	-4.80	121.32	128.58
2	D	379	NAD	C5A-C4A-N3A	-4.80	120.11	126.72
2	H	379	NAD	C5A-C4A-N3A	-4.67	120.29	126.72
2	G	379	NAD	N9A-C8A-N7A	-4.57	107.45	113.94
2	H	379	NAD	N9A-C8A-N7A	-4.49	107.57	113.94
2	A	379	NAD	C5A-C4A-N3A	-4.47	120.56	126.72
2	E	379	NAD	N9A-C8A-N7A	-4.37	107.74	113.94
2	C	379	NAD	N9A-C8A-N7A	-4.31	107.83	113.94
2	C	379	NAD	C5A-N7A-C8A	4.30	110.20	103.45
2	F	379	NAD	N9A-C8A-N7A	-4.19	107.99	113.94
2	C	379	NAD	C5A-C4A-N3A	-4.05	121.13	126.72
2	G	379	NAD	C5A-C4A-N3A	-3.98	121.24	126.72
2	H	379	NAD	C5A-N7A-C8A	3.97	109.69	103.45
2	D	379	NAD	C5A-N7A-C8A	3.94	109.64	103.45
2	A	379	NAD	N9A-C8A-N7A	-3.93	108.37	113.94
2	F	379	NAD	C3N-C7N-N7N	3.81	122.43	117.74
2	B	379	NAD	N9A-C8A-N7A	-3.80	108.54	113.94
2	D	379	NAD	N9A-C8A-N7A	-3.79	108.56	113.94
2	E	379	NAD	C5A-C4A-N3A	-3.77	121.53	126.72
2	G	379	NAD	C5A-N7A-C8A	3.64	109.17	103.45
2	A	379	NAD	C5A-N7A-C8A	3.64	109.17	103.45
2	H	379	NAD	C2A-N3A-C4A	3.61	120.64	111.83
2	D	379	NAD	C4A-C5A-N7A	-3.58	106.48	110.58
2	F	379	NAD	C5A-C4A-N3A	-3.57	121.81	126.72
2	G	379	NAD	C2A-N3A-C4A	3.57	120.54	111.83
2	D	379	NAD	C2A-N3A-C4A	3.49	120.36	111.83
2	F	379	NAD	O7N-C7N-C3N	-3.49	115.33	119.60
2	C	379	NAD	C4A-C5A-N7A	-3.46	106.63	110.58
2	B	379	NAD	C5A-C4A-N3A	-3.40	122.04	126.72
2	E	379	NAD	C5A-N7A-C8A	3.38	108.77	103.45
2	F	379	NAD	C2A-N3A-C4A	3.31	119.91	111.83
2	H	379	NAD	C4A-C5A-N7A	-3.28	106.83	110.58
2	E	379	NAD	C2A-N3A-C4A	3.26	119.79	111.83
2	A	379	NAD	C2A-N3A-C4A	3.25	119.76	111.83
2	F	379	NAD	C5A-N7A-C8A	3.01	108.18	103.45
2	D	379	NAD	O2A-PA-O3	2.98	115.34	107.27
2	E	379	NAD	O7N-C7N-C3N	-2.96	115.98	119.60
2	B	379	NAD	C2A-N3A-C4A	2.95	119.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	379	NAD	O3D-C3D-C4D	-2.94	102.63	111.08
2	B	379	NAD	C5A-N7A-C8A	2.92	108.04	103.45
2	H	379	NAD	N3A-C4A-N9A	2.91	132.11	127.17
2	A	379	NAD	C4A-C5A-N7A	-2.83	107.35	110.58
2	A	379	NAD	N3A-C4A-N9A	2.82	131.96	127.17
2	E	379	NAD	C3N-C7N-N7N	2.81	121.20	117.74
2	D	379	NAD	C3N-C7N-N7N	2.81	121.20	117.74
2	C	379	NAD	C2A-N3A-C4A	2.78	118.61	111.83
2	G	379	NAD	C4A-C5A-N7A	-2.65	107.56	110.58
2	G	379	NAD	O3D-C3D-C4D	-2.61	103.59	111.08
2	A	379	NAD	O4B-C1B-N9A	2.59	113.07	108.09
2	C	379	NAD	C3N-C7N-N7N	2.59	120.93	117.74
2	G	379	NAD	C4A-N9A-C8A	2.58	108.44	105.74
2	B	379	NAD	N3A-C4A-N9A	2.54	131.49	127.17
2	D	379	NAD	C5A-C4A-N9A	2.53	108.57	105.81
2	E	379	NAD	C4A-C5A-N7A	-2.52	107.70	110.58
2	B	379	NAD	C4A-N9A-C8A	2.51	108.38	105.74
2	E	379	NAD	O2A-PA-O3	2.51	114.05	107.27
2	F	379	NAD	C4A-N9A-C8A	2.48	108.34	105.74
2	G	379	NAD	N3A-C4A-N9A	2.48	131.38	127.17
2	H	379	NAD	C4A-N9A-C8A	2.46	108.32	105.74
2	E	379	NAD	C4A-N9A-C8A	2.45	108.31	105.74
2	D	379	NAD	N3A-C4A-N9A	2.43	131.30	127.17
2	C	379	NAD	C6A-C5A-C4A	2.43	120.50	117.18
2	C	379	NAD	N3A-C4A-N9A	2.36	131.19	127.17
2	B	379	NAD	O2A-PA-O3	2.35	113.62	107.27
2	F	379	NAD	C4N-C3N-C7N	-2.29	114.82	121.06
2	F	379	NAD	C4A-C5A-N7A	-2.26	108.00	110.58
2	E	379	NAD	O4B-C1B-N9A	2.26	112.42	108.09
2	C	379	NAD	O2A-PA-O3	2.25	113.34	107.27
2	E	379	NAD	N3A-C4A-N9A	2.24	130.98	127.17
2	C	379	NAD	O2N-PN-O1N	2.21	122.74	112.44
2	B	379	NAD	O3D-C3D-C4D	-2.16	104.89	111.08
2	A	379	NAD	C3N-C7N-N7N	2.14	120.38	117.74
2	C	379	NAD	O7N-C7N-C3N	-2.11	117.02	119.60
2	F	379	NAD	O2N-PN-O1N	2.10	122.20	112.44
2	G	379	NAD	O2N-PN-O1N	2.09	122.14	112.44
2	F	379	NAD	N3A-C4A-N9A	2.08	130.70	127.17
2	D	379	NAD	O3-PA-O1A	-2.08	104.46	110.70
2	G	379	NAD	C4A-N9A-C1B	-2.00	121.94	126.63

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	379	NAD	O4D-C1D-N1N-C2N
2	A	379	NAD	O4D-C1D-N1N-C6N
2	B	379	NAD	O4D-C1D-N1N-C2N
2	B	379	NAD	O4D-C1D-N1N-C6N
2	B	379	NAD	C2D-C1D-N1N-C2N
2	C	379	NAD	O4D-C1D-N1N-C2N
2	C	379	NAD	O4D-C1D-N1N-C6N
2	C	379	NAD	C2D-C1D-N1N-C2N
2	D	379	NAD	O4D-C1D-N1N-C6N
2	E	379	NAD	O4D-C1D-N1N-C6N
2	F	379	NAD	O4D-C1D-N1N-C6N
2	G	379	NAD	O4D-C1D-N1N-C2N
2	G	379	NAD	O4D-C1D-N1N-C6N
2	G	379	NAD	C2D-C1D-N1N-C2N
2	G	379	NAD	C2D-C1D-N1N-C6N
2	H	379	NAD	C5B-O5B-PA-O1A
2	H	379	NAD	O4D-C1D-N1N-C2N
2	H	379	NAD	O4D-C1D-N1N-C6N
2	H	379	NAD	O4B-C4B-C5B-O5B
2	E	379	NAD	C4N-C3N-C7N-O7N
2	E	379	NAD	C4N-C3N-C7N-N7N
2	H	379	NAD	C3B-C4B-C5B-O5B
2	E	379	NAD	O4B-C4B-C5B-O5B
2	A	379	NAD	C4N-C3N-C7N-N7N
2	A	379	NAD	C4N-C3N-C7N-O7N
2	E	379	NAD	C3B-C4B-C5B-O5B
2	G	379	NAD	C4N-C3N-C7N-N7N
2	G	379	NAD	C4N-C3N-C7N-O7N
2	A	379	NAD	C2B-C1B-N9A-C8A
2	E	379	NAD	O4D-C4D-C5D-O5D
2	H	379	NAD	C5B-O5B-PA-O2A
2	H	379	NAD	C5B-O5B-PA-O3
2	B	379	NAD	O4B-C4B-C5B-O5B
2	B	379	NAD	C4N-C3N-C7N-N7N
2	B	379	NAD	O4D-C4D-C5D-O5D
2	B	379	NAD	C3D-C4D-C5D-O5D
2	A	379	NAD	C2D-C1D-N1N-C2N
2	B	379	NAD	C2D-C1D-N1N-C6N
2	C	379	NAD	C2D-C1D-N1N-C6N
2	H	379	NAD	C2D-C1D-N1N-C2N
2	H	379	NAD	C2D-C1D-N1N-C6N
2	C	379	NAD	C2B-C1B-N9A-C8A

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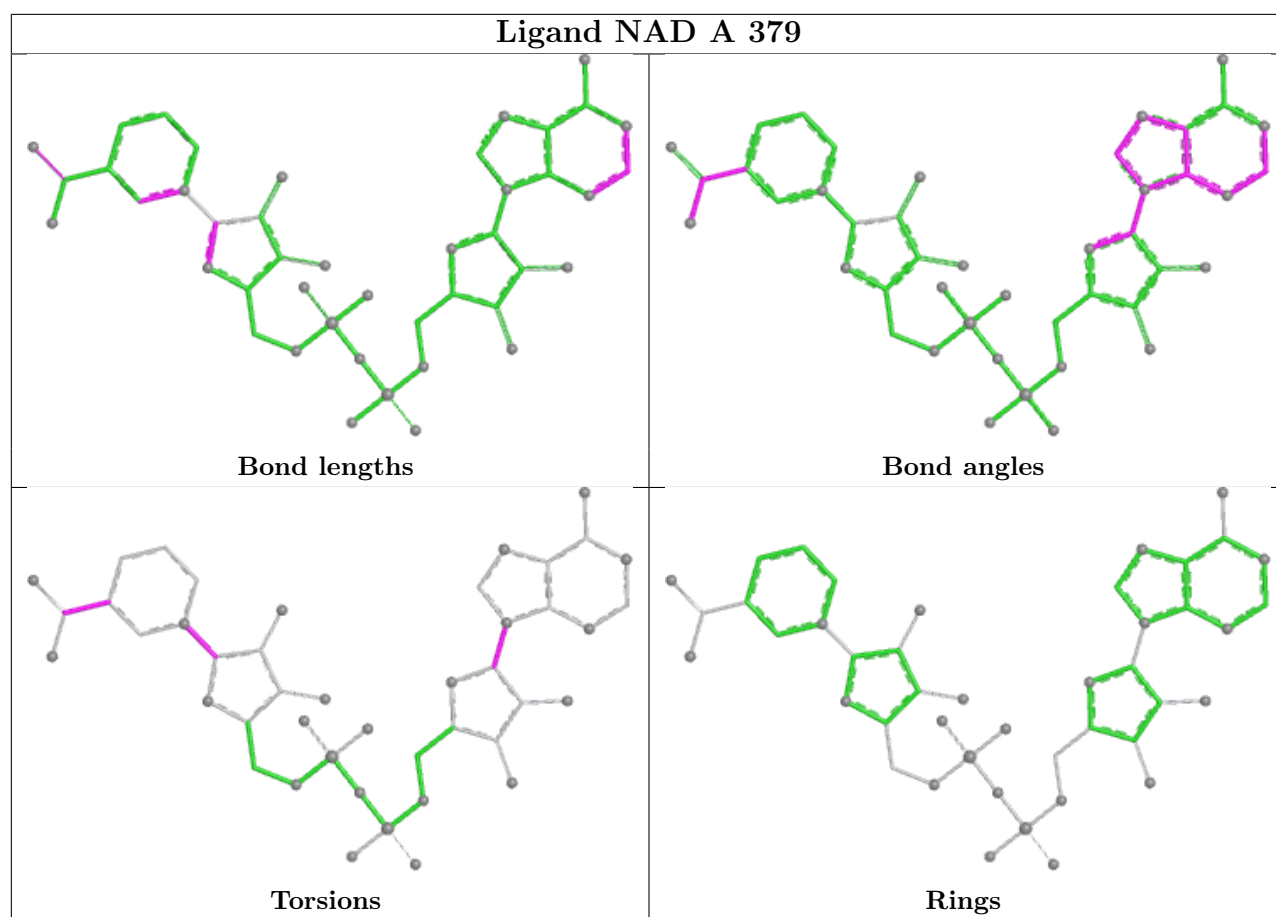
Mol	Chain	Res	Type	Atoms
2	H	379	NAD	C2B-C1B-N9A-C8A
2	B	379	NAD	C4N-C3N-C7N-O7N
2	D	379	NAD	O4D-C1D-N1N-C2N
2	E	379	NAD	O4D-C1D-N1N-C2N
2	F	379	NAD	O4D-C1D-N1N-C2N
2	C	379	NAD	PN-O3-PA-O1A
2	A	379	NAD	O4B-C1B-N9A-C8A
2	D	379	NAD	O4B-C4B-C5B-O5B
2	B	379	NAD	C2B-C1B-N9A-C8A
2	E	379	NAD	C3D-C4D-C5D-O5D
2	G	379	NAD	O4B-C4B-C5B-O5B
2	D	379	NAD	C2B-C1B-N9A-C8A
2	E	379	NAD	C2B-C1B-N9A-C8A
2	C	379	NAD	O4B-C4B-C5B-O5B
2	B	379	NAD	C3B-C4B-C5B-O5B

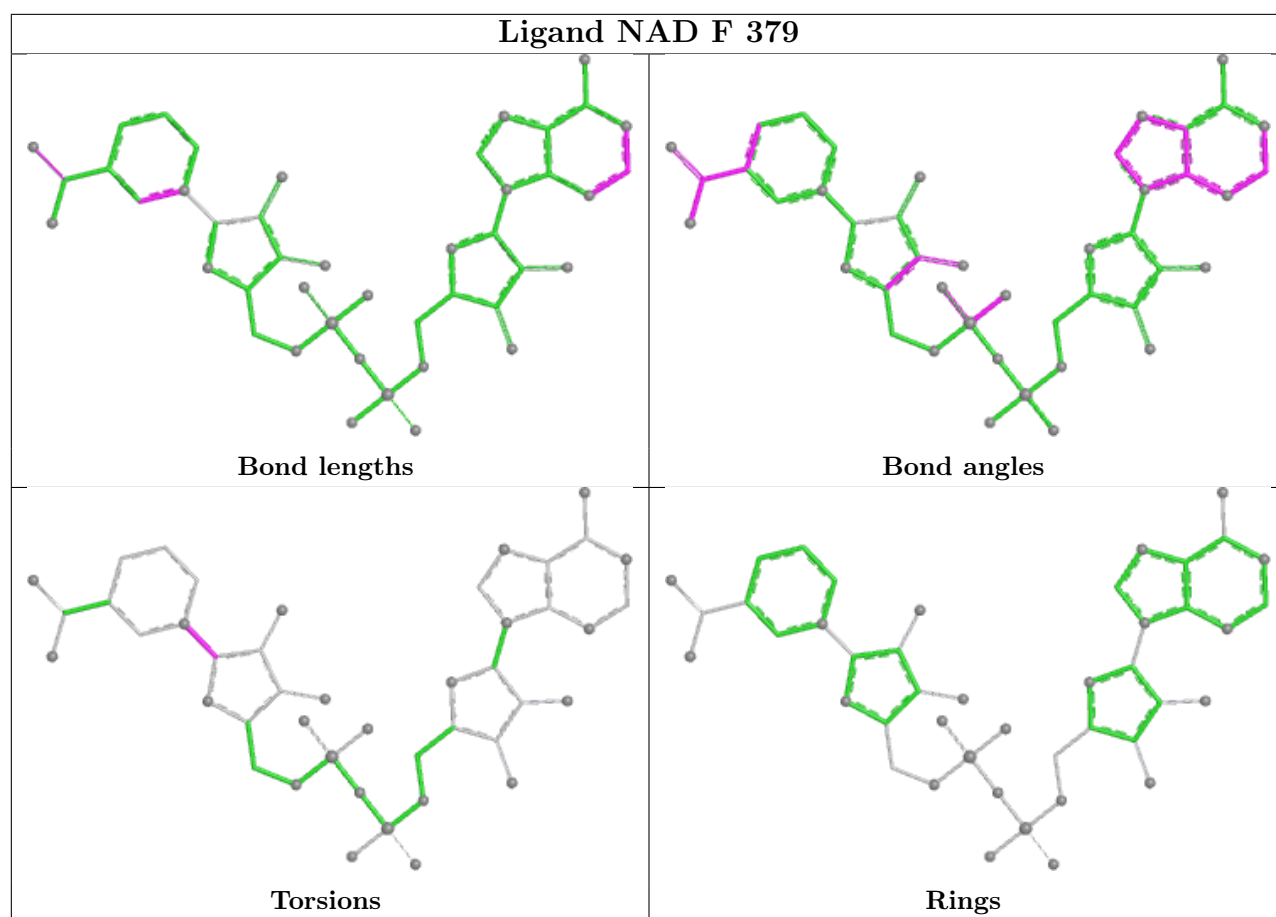
There are no ring outliers.

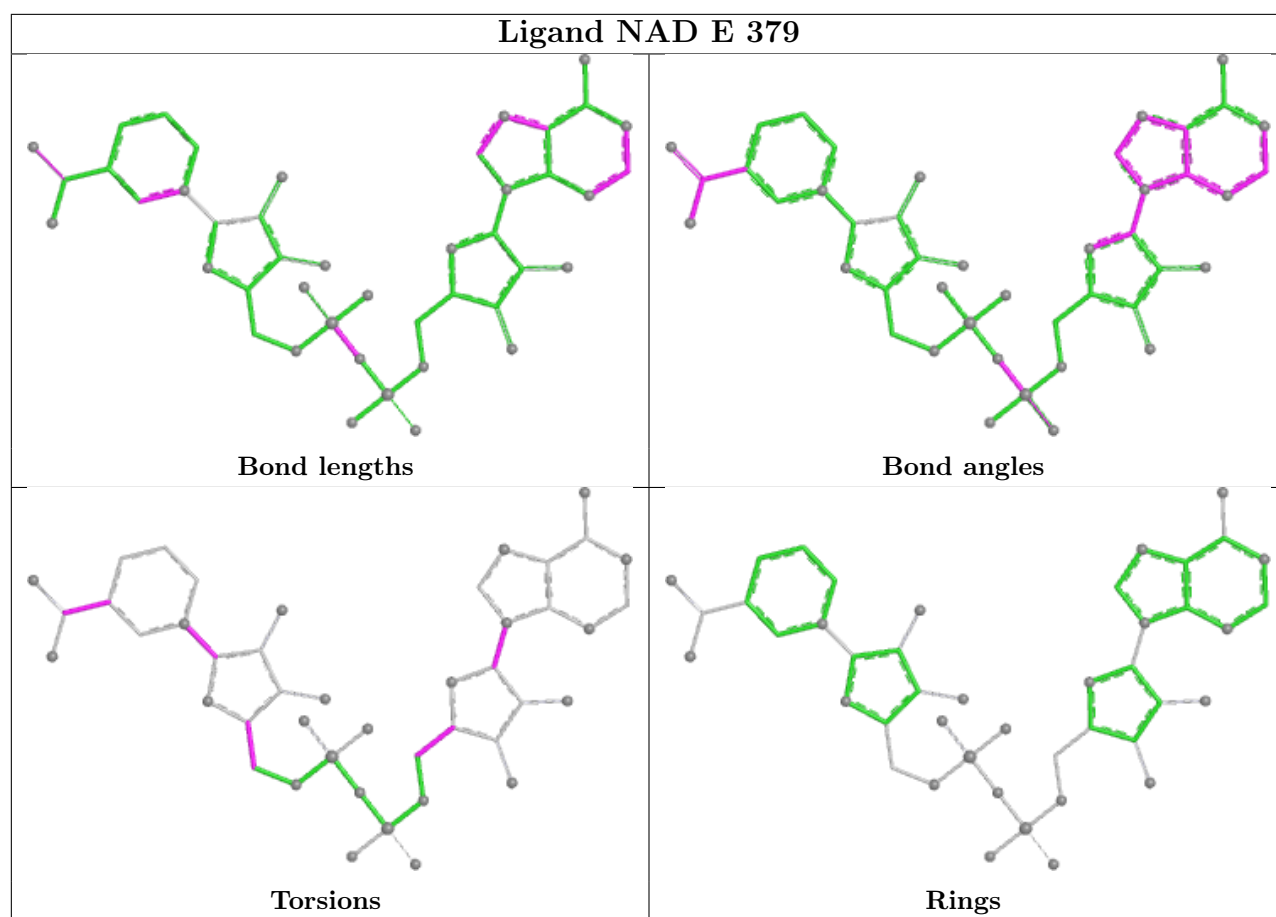
5 monomers are involved in 9 short contacts:

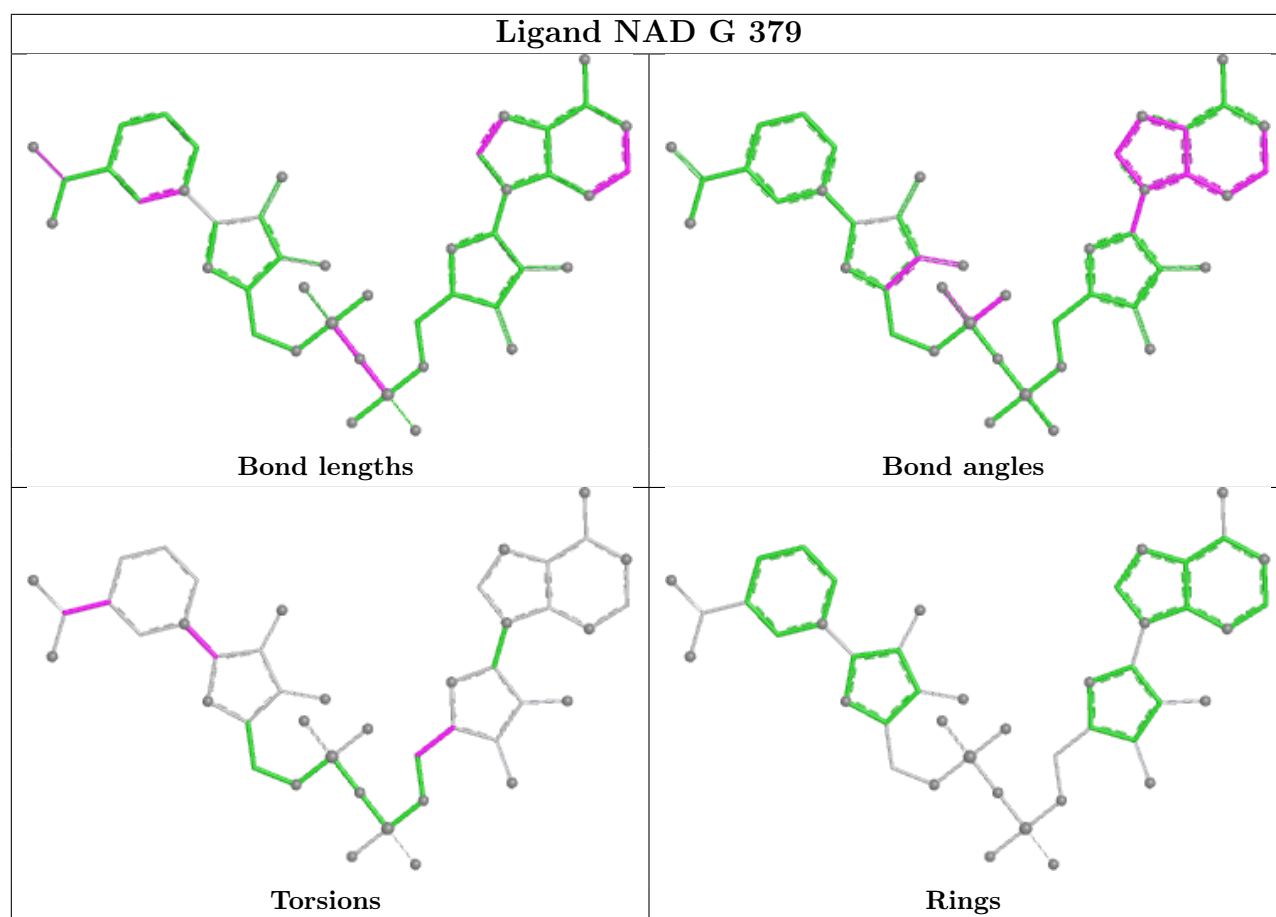
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	379	NAD	1	0
2	E	379	NAD	3	0
2	G	379	NAD	2	0
2	H	379	NAD	2	0
2	C	379	NAD	1	0

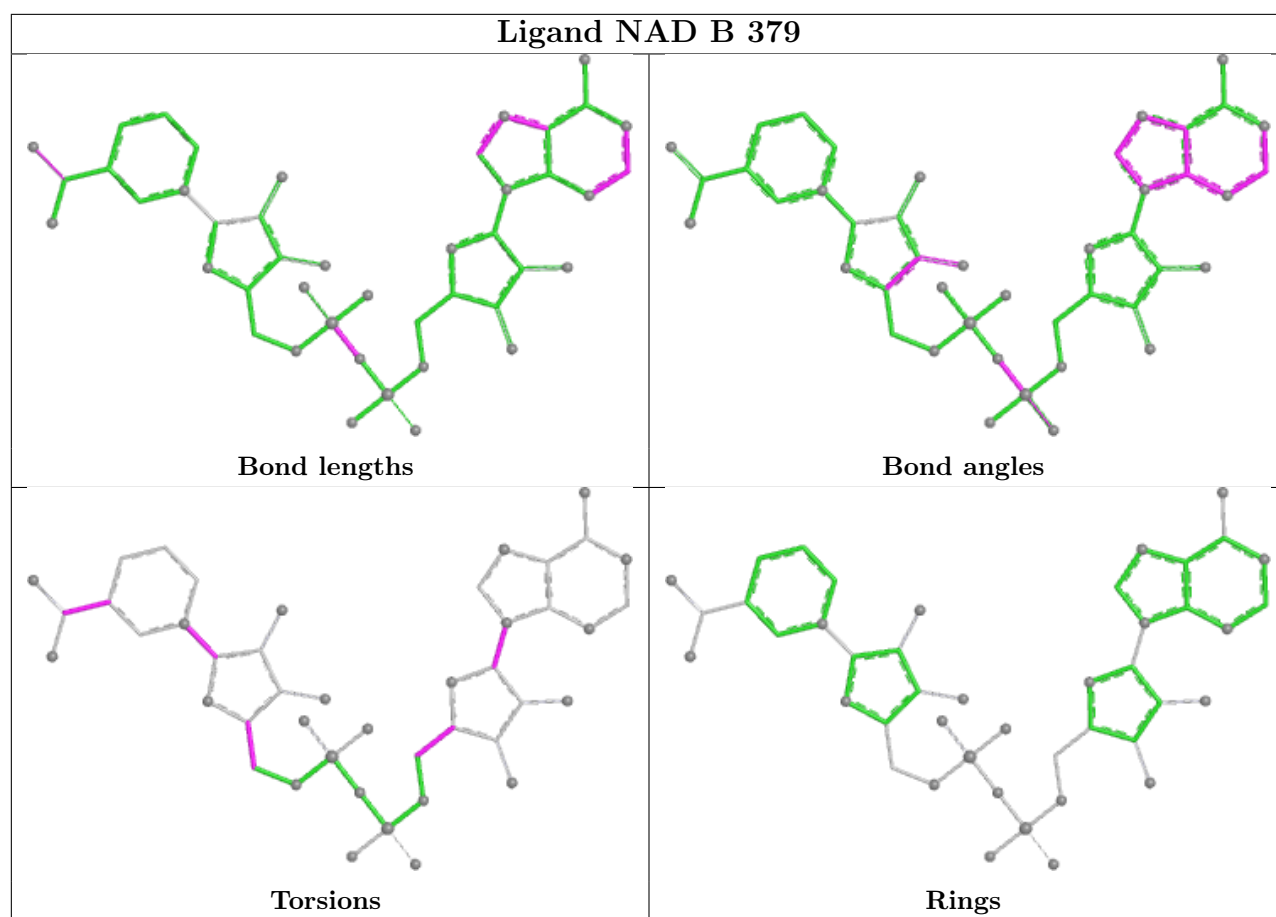
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

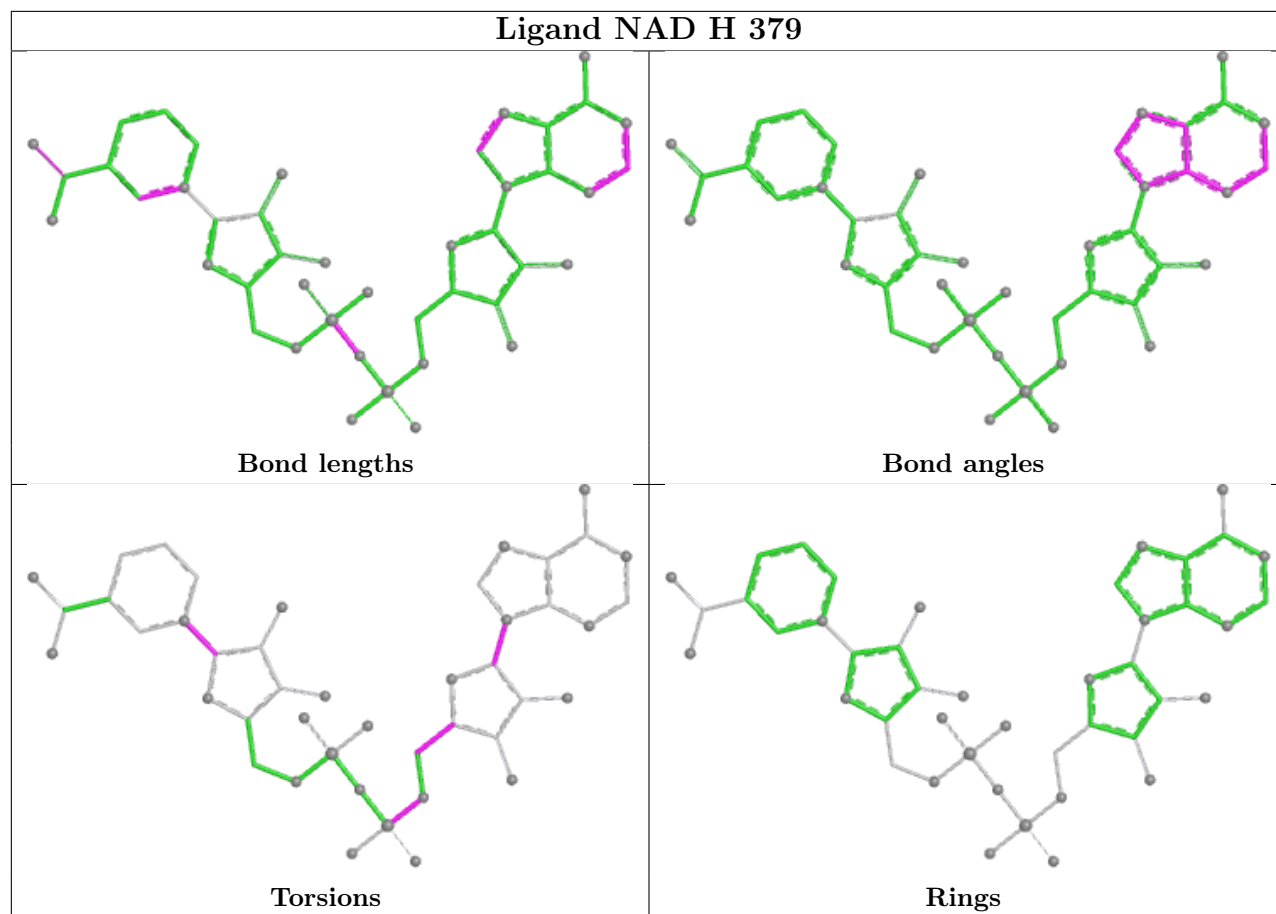


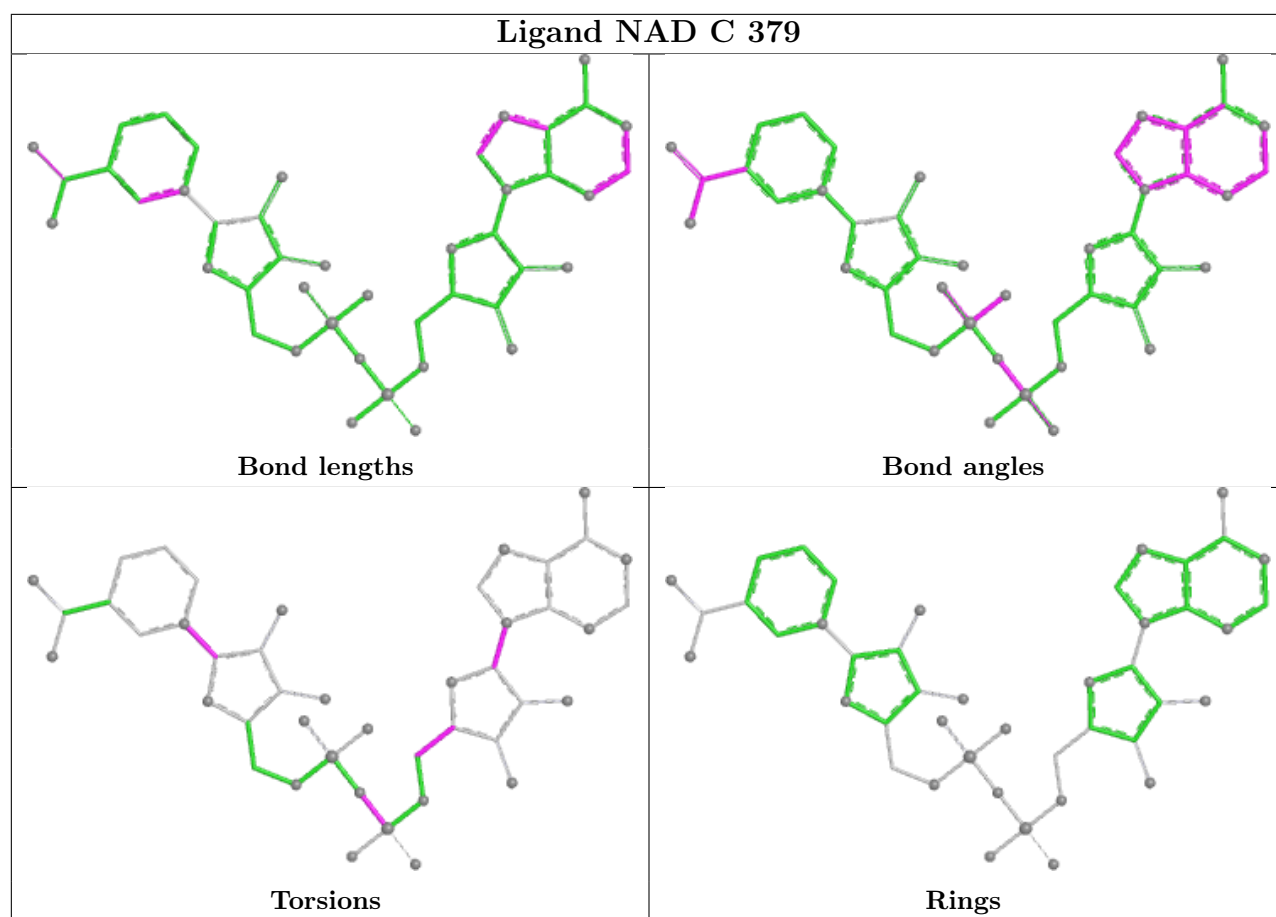


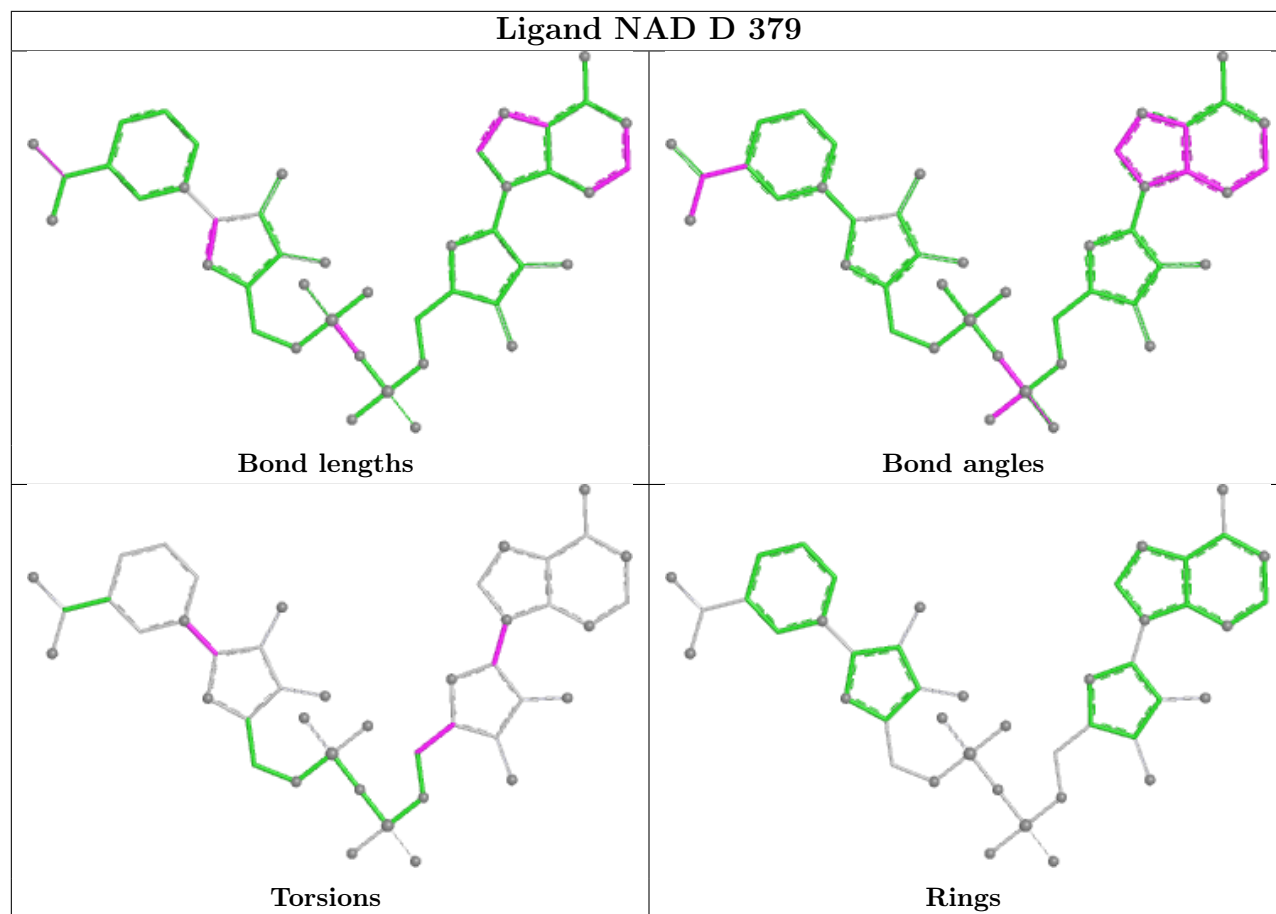












5.7 Other polymers [i](#)

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	370/381 (97%)	-0.09	5 (1%) 73 78	16, 41, 83, 116	1 (0%)
1	B	372/381 (97%)	-0.03	15 (4%) 42 48	15, 37, 86, 118	1 (0%)
1	C	367/381 (96%)	0.10	32 (8%) 16 18	22, 37, 84, 99	3 (0%)
1	D	370/381 (97%)	-0.07	8 (2%) 62 67	23, 37, 91, 121	0
1	E	370/381 (97%)	-0.33	2 (0%) 87 90	23, 38, 59, 73	0
1	F	360/381 (94%)	0.12	25 (6%) 23 26	23, 39, 79, 112	0
1	G	365/381 (95%)	0.33	9 (2%) 58 64	29, 50, 76, 98	0
1	H	373/381 (97%)	0.08	3 (0%) 82 86	28, 51, 76, 95	0
All	All	2947/3048 (96%)	0.01	99 (3%) 48 55	15, 42, 80, 121	5 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	PRO	5.7
1	F	32	VAL	5.4
1	C	49	VAL	4.4
1	C	35	LEU	4.2
1	C	32	VAL	4.2
1	C	46	VAL	4.2
1	D	56	GLY	4.1
1	B	30	ILE	4.0
1	A	31	PRO	3.9
1	F	63	GLY	3.8
1	G	29	PRO	3.8
1	G	49	VAL	3.7
1	G	375	HIS	3.6
1	C	62	VAL	3.5
1	C	70[A]	ASP	3.5
1	C	28	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	29	PRO	3.4
1	C	25	VAL	3.3
1	G	80	ALA	3.3
1	A	27	GLY	3.2
1	C	71[A]	HIS	3.2
1	D	26	PRO	3.2
1	F	4	LEU	3.1
1	F	77	LEU	3.1
1	B	57	THR	3.0
1	F	50	ASN	3.0
1	H	333	PRO	3.0
1	C	59	ILE	3.0
1	C	33	GLU	3.0
1	A	345	GLU	3.0
1	F	19	LEU	3.0
1	C	82	ILE	3.0
1	A	32	VAL	2.9
1	F	43	VAL	2.9
1	F	64	THR	2.9
1	F	76	TRP	2.8
1	F	35	LEU	2.8
1	B	32	VAL	2.8
1	B	35	LEU	2.8
1	B	37	HIS	2.7
1	F	15	LEU	2.7
1	E	375	HIS	2.7
1	C	277	PHE	2.7
1	F	16	PHE	2.7
1	D	53	LEU	2.7
1	F	5	VAL	2.6
1	B	345	GLU	2.6
1	C	57	THR	2.6
1	C	61	PHE	2.6
1	C	76	TRP	2.5
1	F	49	VAL	2.5
1	C	24	ALA	2.4
1	A	-1	ASN	2.4
1	F	10	PRO	2.4
1	C	41	LEU	2.4
1	F	286	LEU	2.4
1	F	58	PRO	2.4
1	C	276	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	81	GLY	2.4
1	H	332	ILE	2.4
1	C	47	THR	2.3
1	B	38	ALA	2.3
1	G	219	ALA	2.3
1	C	19	LEU	2.3
1	F	60	ASN	2.3
1	F	11	TYR	2.3
1	F	69	THR	2.3
1	G	218	LEU	2.2
1	G	330	ALA	2.2
1	B	84	PHE	2.2
1	G	60	ASN	2.2
1	C	279	GLY	2.2
1	D	4	LEU	2.2
1	D	54	LEU	2.2
1	B	46	VAL	2.2
1	C	72	VAL	2.2
1	C	58	PRO	2.2
1	C	44	ARG	2.1
1	E	136	GLU	2.1
1	F	68	GLY	2.1
1	B	34	GLU	2.1
1	F	287	GLU	2.1
1	F	22	VAL	2.1
1	C	84	PHE	2.1
1	B	56	GLY	2.1
1	B	330	ALA	2.1
1	B	274	TYR	2.1
1	H	376	PRO	2.1
1	C	284	VAL	2.1
1	F	25	VAL	2.1
1	C	83	GLY	2.1
1	F	277	PHE	2.1
1	C	69[A]	THR	2.0
1	D	-2	SER	2.0
1	C	75	ALA	2.0
1	C	80	ALA	2.0
1	D	284	VAL	2.0
1	B	61	PHE	2.0
1	C	40	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

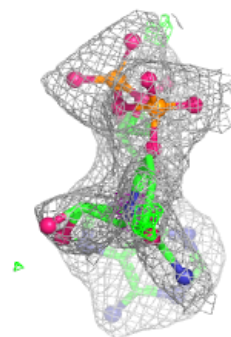
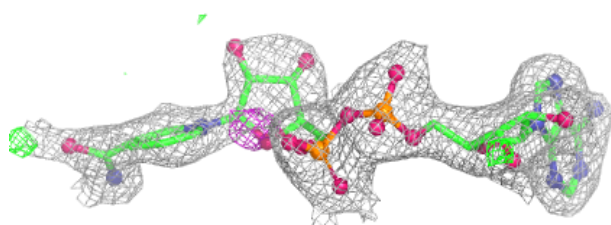
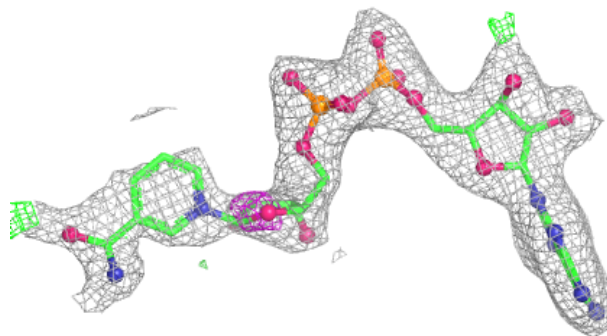
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	379	44/44	0.92	0.10	40,52,68,69	0
2	NAD	G	379	44/44	0.94	0.08	42,49,55,57	0
2	NAD	H	379	44/44	0.94	0.09	49,52,61,64	0
2	NAD	F	379	44/44	0.95	0.07	38,43,50,55	0
2	NAD	C	379	44/44	0.96	0.06	32,41,46,48	0
2	NAD	A	379	44/44	0.97	0.06	33,39,45,47	0
2	NAD	D	379	44/44	0.97	0.07	29,37,47,47	0
2	NAD	B	379	44/44	0.97	0.06	36,39,51,51	0

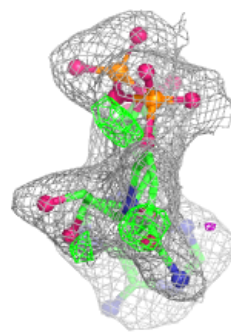
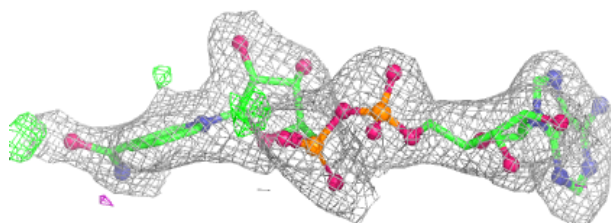
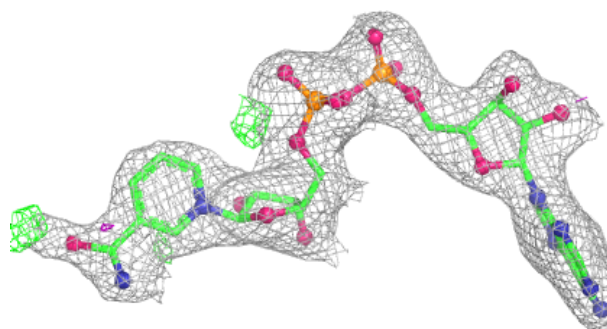
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD E 379:

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

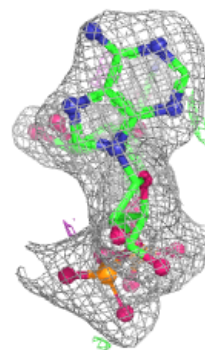
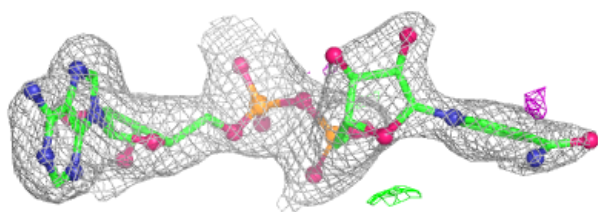
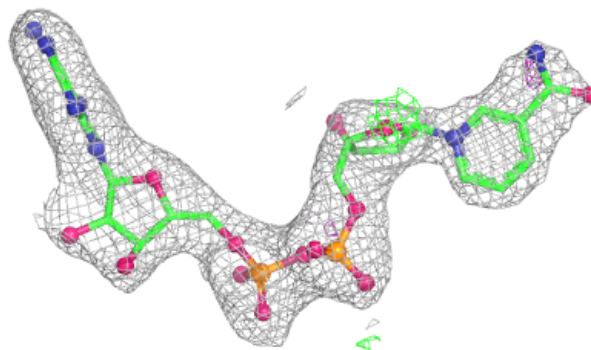
**Electron density around NAD G 379:**

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

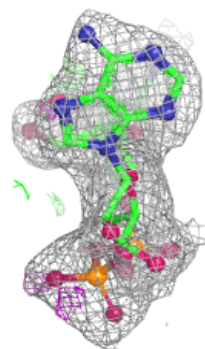
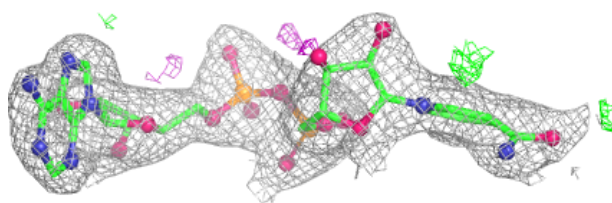
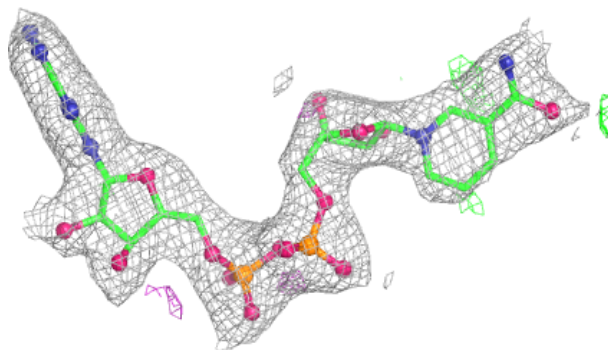


Electron density around NAD H 379:

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

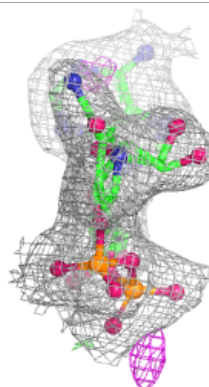
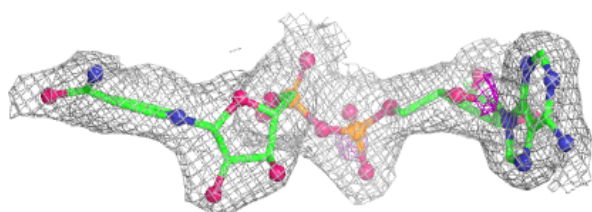
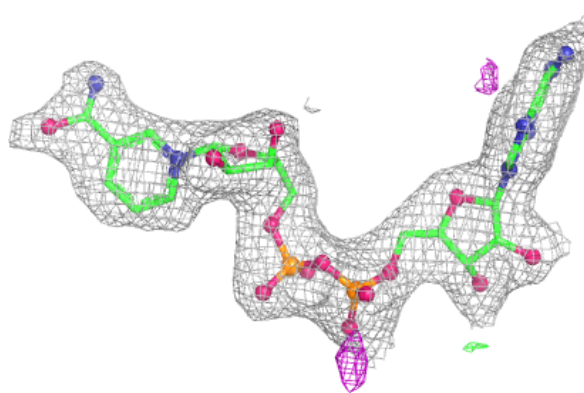
**Electron density around NAD F 379:**

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

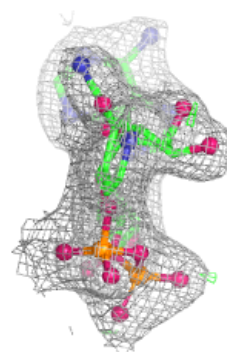
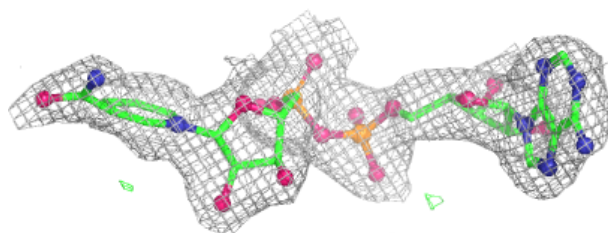
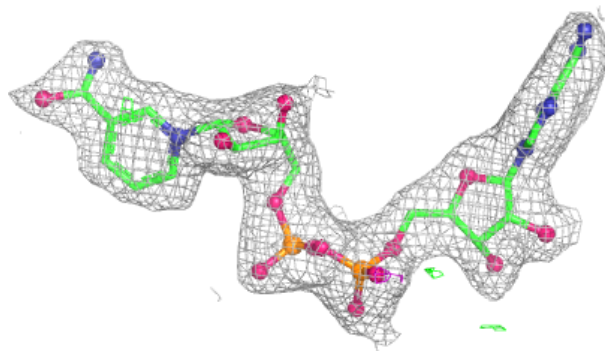


Electron density around NAD C 379:

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

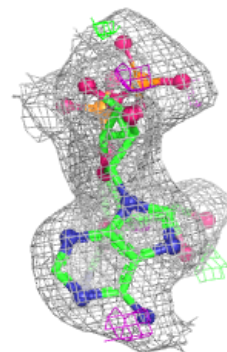
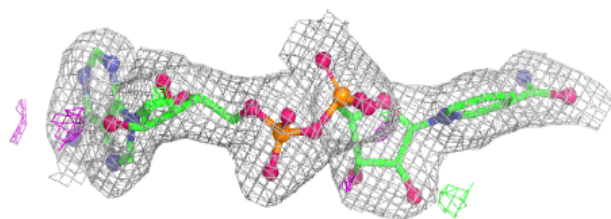
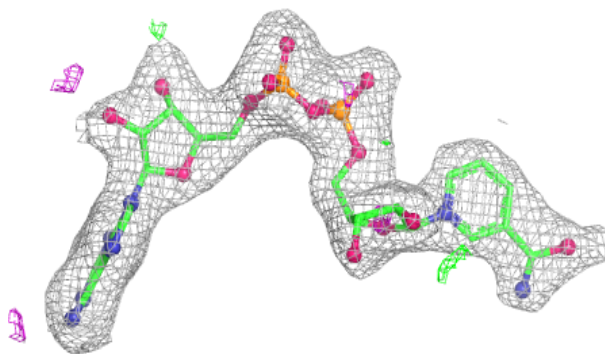
**Electron density around NAD A 379:**

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

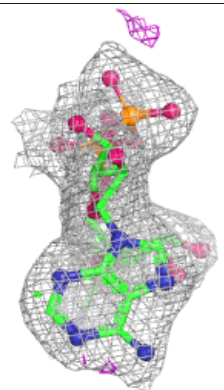
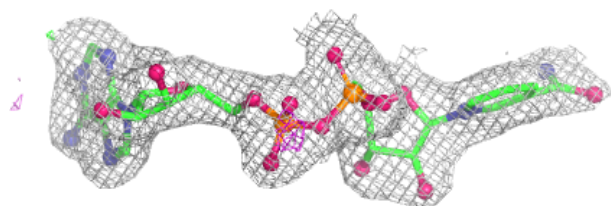
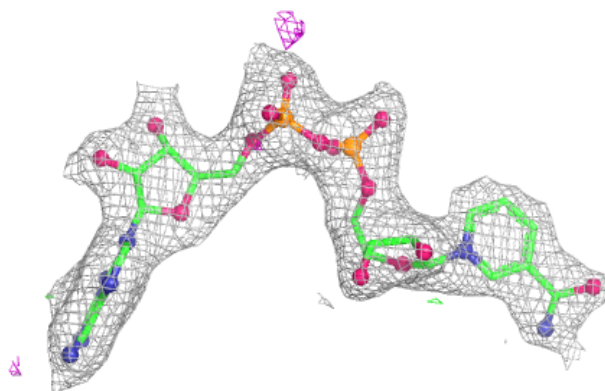


Electron density around NAD D 379:

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

**Electron density around NAD B 379:**

$2mF_o-DF_c$ (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.