



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:36 PM UTC

PDB ID : 2X06 / pdb_00002x06
Title : SULFOLACTATE DEHYDROGENASE FROM METHANOCALDOCOC-
CUS JANNASCHII
Authors : Irimia, A.; Madern, D.; Zaccai, G.; Vellieux, F.M.D.
Deposited on : 2009-12-07
Resolution : 2.50 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

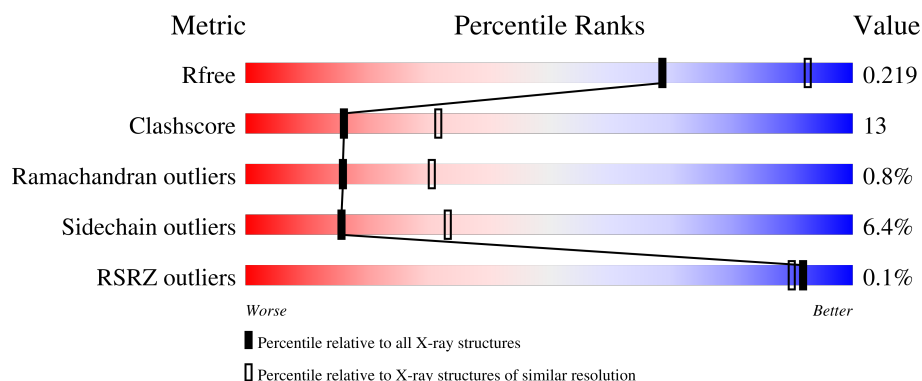
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	344	74% 22% • •
1	B	344	72% 24% •
1	C	344	71% 24% 5%
1	D	344	78% 20% •
1	E	344	72% 25% •

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Mol	Chain	Length	Quality of chain
1	F	344	 72%24%.
1	G	344	 73%24%.
1	H	344	 74%24%.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21878 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 L-SULFOLACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	Se	0	2	0
			2635	1686	436	500	4	9			
1	B	344	Total	C	N	O	S	Se	0	1	0
			2631	1682	438	498	4	9			
1	C	344	Total	C	N	O	S	Se	0	1	0
			2628	1680	436	499	4	9			
1	D	344	Total	C	N	O	S	Se	0	2	0
			2635	1687	437	498	4	9			
1	E	344	Total	C	N	O	S	Se	0	0	0
			2623	1677	435	498	4	9			
1	F	344	Total	C	N	O	S	Se	0	0	0
			2623	1677	435	498	4	9			
1	G	344	Total	C	N	O	S	Se	0	1	0
			2628	1680	435	500	4	9			
1	H	344	Total	C	N	O	S	Se	0	0	0
			2623	1677	435	498	4	9			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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		
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	80	Total	O	0	0
			80	80		
3	B	68	Total	O	0	0
			68	68		
3	C	53	Total	O	0	0
			53	53		
3	D	60	Total	O	0	0
			60	60		

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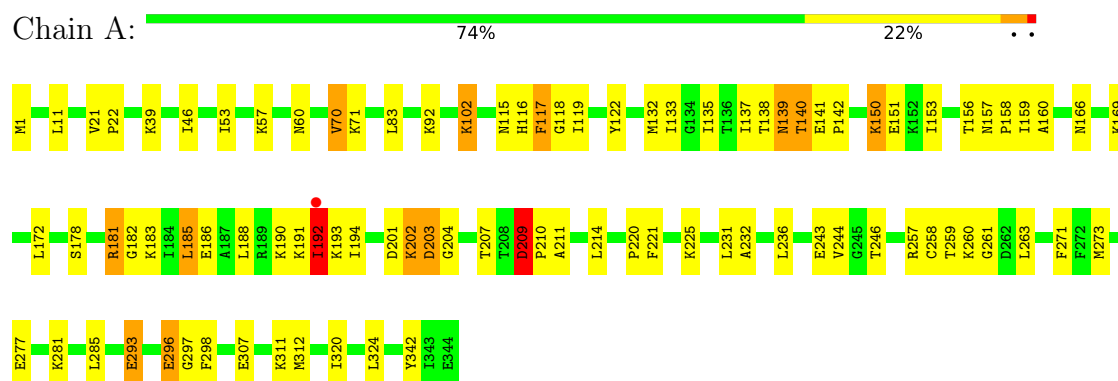
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	65	Total 65	O 65	0	0
3	F	53	Total 53	O 53	0	0
3	G	69	Total 69	O 69	0	0
3	H	52	Total 52	O 52	0	0

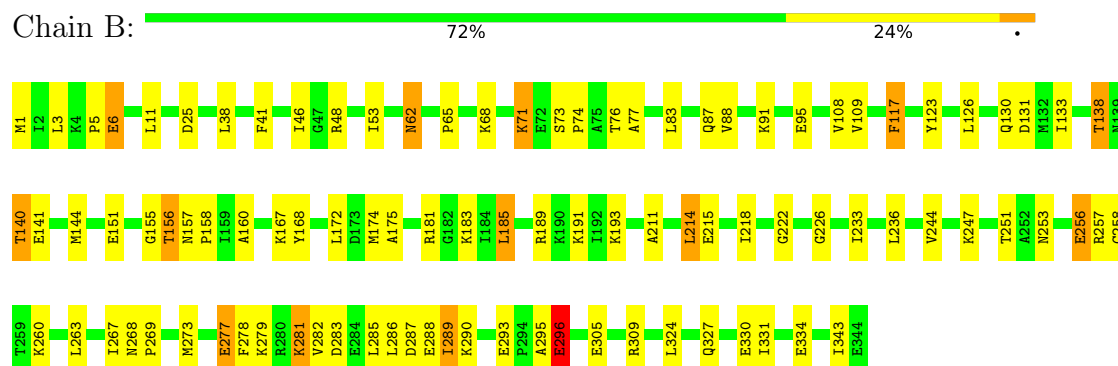
3 Residue-property plots

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

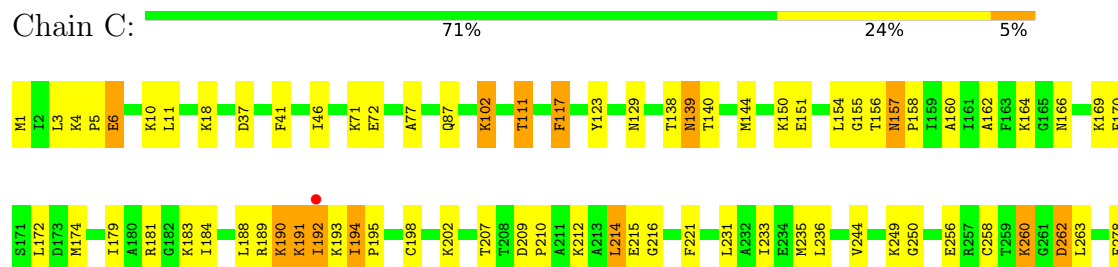
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE



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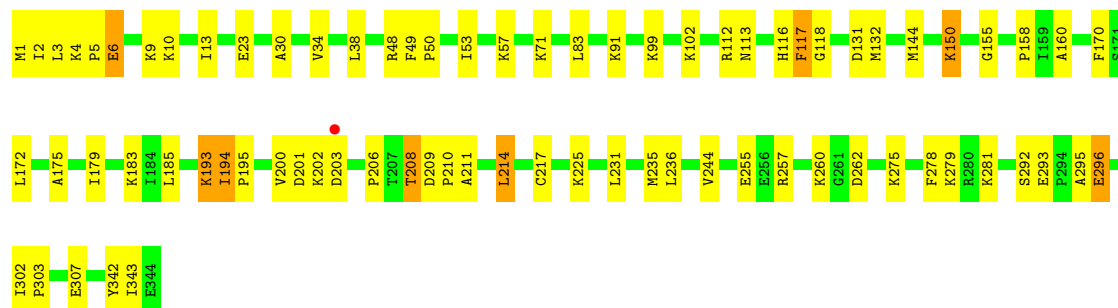
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE





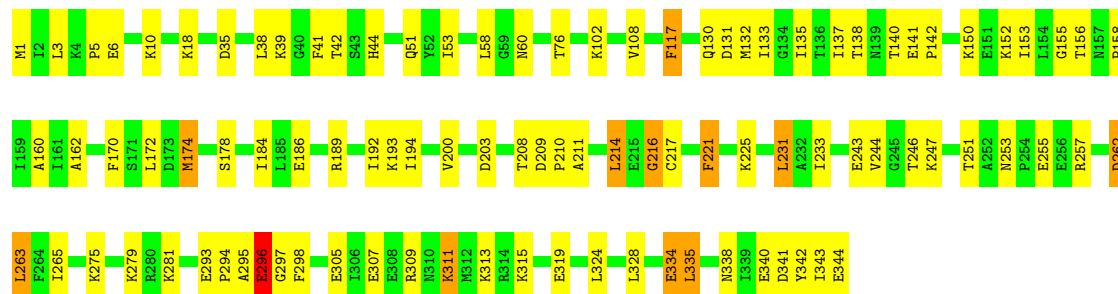
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE

Chain D: 78% 20%



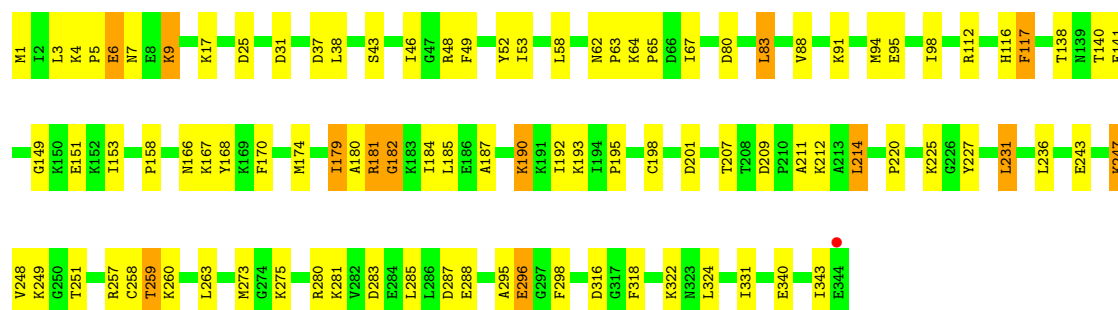
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE

Chain E: 72% 25%



• Molecule 1: L-SULFOLACTATE DEHYDROGENASE

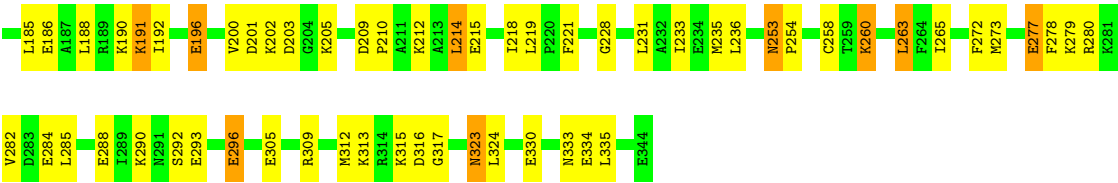
Chain F: 72% 24%



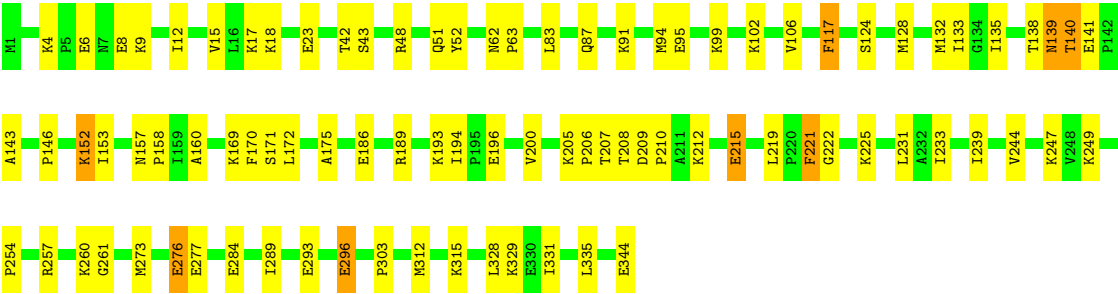
• Molecule 1: L-SULFOLACTATE DEHYDROGENASE

Chain G: 73% 24%





• Molecule 1: L-SULFOLACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.93Å 203.71Å 100.05Å 90.00° 112.05° 90.00°	Depositor
Resolution (Å)	32.83 – 2.50 32.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (32.83-2.50) 96.0 (32.83-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.153 , 0.224 0.150 , 0.219	Depositor DCC
R_{free} test set	4958 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21878	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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	0.52	0/2674	0.88	4/3577 (0.1%)
1	B	0.50	0/2667	0.84	4/3568 (0.1%)
1	C	0.51	0/2664	0.88	5/3565 (0.1%)
1	D	0.51	0/2674	0.83	0/3576
1	E	0.50	0/2656	0.84	4/3554 (0.1%)
1	F	0.48	0/2656	0.84	1/3554 (0.0%)
1	G	0.51	0/2664	0.87	3/3565 (0.1%)
1	H	0.47	0/2656	0.83	0/3554
All	All	0.50	0/21311	0.85	21/28513 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ASN	CA-C-N	6.44	126.36	119.28
1	B	62	ASN	C-N-CA	6.44	126.36	119.28
1	G	221	PHE	N-CA-C	5.96	117.86	111.36
1	C	221	PHE	N-CA-C	5.88	118.64	111.82
1	E	221	PHE	N-CA-C	5.86	117.67	111.28
1	E	217	CYS	N-CA-C	5.84	116.27	108.38
1	C	4	LYS	CA-C-N	5.81	127.11	119.84
1	C	4	LYS	C-N-CA	5.81	127.11	119.84
1	E	335	LEU	N-CA-C	-5.61	106.10	113.17
1	A	209	ASP	CA-C-N	5.47	125.14	119.56
1	A	209	ASP	C-N-CA	5.47	125.14	119.56
1	B	268	ASN	CA-C-N	5.44	126.64	119.84
1	B	268	ASN	C-N-CA	5.44	126.64	119.84
1	C	209	ASP	CA-C-N	5.35	125.17	119.28
1	C	209	ASP	C-N-CA	5.35	125.17	119.28
1	E	311	LYS	N-CA-C	-5.32	105.48	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLU	CA-C-N	5.20	125.67	120.52
1	A	293	GLU	C-N-CA	5.20	125.67	120.52
1	G	253	ASN	CA-C-N	5.06	125.74	120.12
1	G	253	ASN	C-N-CA	5.06	125.74	120.12
1	F	179	ILE	N-CA-C	5.05	113.86	107.70

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	2635	0	2734	73	0
1	B	2631	0	2728	90	0
1	C	2628	0	2721	94	0
1	D	2635	0	2741	53	0
1	E	2623	0	2715	85	0
1	F	2623	0	2715	90	0
1	G	2628	0	2719	73	0
1	H	2623	0	2715	67	0
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	3	0
2	D	44	0	26	0	0
2	E	44	0	26	2	0
2	F	44	0	25	1	0
2	G	44	0	26	3	0
2	H	44	0	26	1	0
3	A	80	0	0	4	0
3	B	68	0	0	2	0
3	C	53	0	0	1	0
3	D	60	0	0	2	0
3	E	65	0	0	2	0
3	F	53	0	0	4	0
3	G	69	0	0	3	0
3	H	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21878	0	21995	570	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 13.

All (570) 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:E:172:LEU:HD11	1:E:174:MSE:HE3	1.37	1.07
1:C:179:ILE:HG13	1:C:183:LYS:HE3	1.39	1.00
1:B:172:LEU:HD11	1:B:174:MSE:HE3	1.42	0.99
1:B:167:LYS:HE3	1:B:168:TYR:CE1	1.98	0.99
1:C:338:ASN:HD22	1:C:338:ASN:H	1.09	0.94
1:F:187:ALA:HA	1:F:190:LYS:HE2	1.52	0.89
1:D:83:LEU:HD11	1:D:257:ARG:HD3	1.56	0.88
1:C:202:LYS:HE2	1:C:215:GLU:HG2	1.56	0.86
1:D:6:GLU:CD	1:D:6:GLU:H	1.83	0.86
1:D:202:LYS:HG3	3:D:2035:HOH:O	1.74	0.86
1:B:156:THR:CG2	2:B:4002:NAD:H5N	2.06	0.85
1:F:181:ARG:HH11	1:F:214:LEU:HD12	1.43	0.84
1:G:309:ARG:O	1:G:313:LYS:HD3	1.78	0.82
1:D:210:PRO:O	1:D:214:LEU:HD22	1.80	0.81
1:H:139:ASN:HD21	1:H:261:GLY:H	1.27	0.81
1:E:194:ILE:O	1:E:208:THR:HG23	1.81	0.80
1:H:140:THR:HG22	1:H:141:GLU:O	1.82	0.79
1:H:276:GLU:CD	1:H:276:GLU:H	1.90	0.79
1:B:156:THR:HG22	2:B:4002:NAD:H5N	1.64	0.79
1:C:172:LEU:HD11	1:C:174:MSE:HE3	1.64	0.78
1:C:179:ILE:CG1	1:C:183:LYS:HE3	2.13	0.77
1:G:1:MSE:HG3	1:G:2:ILE:H	1.48	0.77
1:G:201:ASP:HB2	1:G:205:LYS:H	1.49	0.76
1:A:296:GLU:HG3	1:A:297:GLY:H	1.51	0.76
1:F:207:THR:HG21	1:F:212:LYS:HB2	1.67	0.76
1:G:186:GLU:O	1:G:190:LYS:HB2	1.86	0.75
1:C:338:ASN:H	1:C:338:ASN:ND2	1.85	0.74
1:G:292:SER:HB3	1:H:153:ILE:HD11	1.69	0.73
1:G:1:MSE:CG	1:G:2:ILE:H	2.00	0.73
1:B:172:LEU:HD11	1:B:174:MSE:CE	2.19	0.73
1:D:102:LYS:HG3	1:D:132:MSE:HE1	1.71	0.73
1:A:181:ARG:HH22	1:A:214:LEU:HA	1.52	0.73
1:C:140:THR:HG21	2:C:4003:NAD:H4N	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:MSE:HE2	1:F:225:LYS:HA	1.71	0.72
1:C:181:ARG:HH21	1:C:214:LEU:HD11	1.55	0.71
1:E:315:LYS:HE2	1:G:280:ARG:HG2	1.72	0.71
1:A:204:GLY:HA3	1:B:295:ALA:HB1	1.73	0.71
1:H:6:GLU:CD	1:H:6:GLU:H	1.99	0.71
1:A:166:ASN:O	1:C:169:LYS:HE3	1.90	0.70
1:C:193:LYS:HE3	1:C:194:ILE:H	1.56	0.70
1:F:167:LYS:HE3	1:F:168:TYR:CE2	2.26	0.70
1:C:166:ASN:ND2	1:C:279:LYS:HD3	2.07	0.70
1:E:140:THR:HG22	1:E:141:GLU:O	1.92	0.70
1:G:288:GLU:HG2	1:H:153:ILE:HD13	1.74	0.70
1:F:187:ALA:CA	1:F:190:LYS:HE2	2.21	0.69
1:G:5:PRO:HG3	1:G:38:LEU:HD21	1.73	0.69
1:H:193:LYS:HB3	1:H:208:THR:CG2	2.22	0.69
1:C:285:LEU:HB2	1:D:244:VAL:HG21	1.74	0.69
1:C:166:ASN:HD21	1:C:279:LYS:HD3	1.57	0.69
1:B:167:LYS:HE3	1:B:168:TYR:HE1	1.55	0.69
1:C:174:MSE:HE1	1:D:225:LYS:O	1.93	0.69
1:E:343:ILE:HA	1:E:344:GLU:HB3	1.75	0.69
1:C:338:ASN:HD22	1:C:338:ASN:N	1.79	0.69
1:A:211:ALA:O	1:A:214:LEU:HG	1.93	0.68
1:H:51:GLN:HG3	1:H:254:PRO:HG3	1.74	0.68
1:C:172:LEU:HD11	1:C:174:MSE:CE	2.24	0.68
1:E:193:LYS:HB3	1:E:208:THR:CG2	2.23	0.68
1:E:172:LEU:HD11	1:E:174:MSE:CE	2.21	0.68
1:E:3:LEU:HD13	1:E:343:ILE:HD11	1.75	0.67
1:G:210:PRO:O	1:G:214:LEU:HD22	1.94	0.67
1:F:182:GLY:HA2	1:F:185:LEU:HD11	1.78	0.66
1:H:207:THR:OG1	1:H:212:LYS:HE3	1.94	0.66
1:F:180:ALA:O	1:F:184:ILE:HG13	1.96	0.66
1:E:193:LYS:HB3	1:E:208:THR:HG22	1.76	0.66
1:D:170:PHE:CE1	1:D:303:PRO:HG2	2.30	0.65
1:G:200:VAL:HG13	1:G:219:LEU:HD11	1.77	0.65
1:G:258:CYS:SG	1:G:260:LYS:HG3	2.37	0.65
1:E:193:LYS:HD2	1:E:208:THR:HG22	1.78	0.65
1:G:201:ASP:HB3	1:G:203:ASP:H	1.61	0.65
1:B:327:GLN:O	1:B:331:ILE:HG13	1.96	0.65
1:E:102:LYS:HG3	1:E:132:MSE:HE1	1.78	0.65
1:F:190:LYS:O	1:F:192:ILE:HG23	1.97	0.64
1:B:156:THR:HG21	2:B:4002:NAD:H5N	1.78	0.64
1:C:184:ILE:HG12	1:C:194:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:PHE:HD1	1:G:117:PHE:C	2.05	0.64
1:E:60:ASN:ND2	1:E:257:ARG:HD2	2.12	0.64
1:E:275:LYS:O	1:E:279:LYS:HG3	1.99	0.63
1:C:179:ILE:HG13	1:C:183:LYS:CE	2.23	0.63
1:E:1:MSE:O	1:E:319:GLU:HA	1.99	0.63
1:F:17:LYS:HG3	3:F:2002:HOH:O	1.98	0.63
1:E:1:MSE:SE	1:E:1:MSE:H3	2.31	0.62
1:E:150:LYS:HD3	1:E:203:ASP:O	1.99	0.62
1:B:140:THR:HG22	1:B:141:GLU:O	1.99	0.62
1:B:283:ASP:O	1:B:287:ASP:HB2	1.99	0.62
1:B:258:CYS:SG	1:B:260:LYS:HG2	2.40	0.62
1:F:243:GLU:HB2	1:F:259:THR:CG2	2.29	0.62
1:G:117:PHE:C	1:G:117:PHE:CD1	2.77	0.62
1:C:172:LEU:HD21	1:C:174:MSE:HE3	1.81	0.62
1:E:160:ALA:HA	1:E:172:LEU:O	2.00	0.62
1:A:83:LEU:HD11	1:A:257:ARG:HD3	1.80	0.61
1:H:194:ILE:O	1:H:208:THR:HG23	2.00	0.61
1:B:48:ARG:NH2	1:B:251:THR:O	2.33	0.61
1:C:329:LYS:HB3	1:C:329:LYS:NZ	2.14	0.61
1:C:193:LYS:CG	1:C:194:ILE:H	2.14	0.61
1:E:178:SER:HB3	1:E:221:PHE:HA	1.83	0.61
1:A:158:PRO:HG3	2:A:4001:NAD:C4N	2.30	0.61
1:E:281:LYS:HD2	3:F:2039:HOH:O	2.00	0.61
1:A:293:GLU:CG	1:B:151:GLU:HB2	2.30	0.61
1:A:312:MSE:HE3	3:A:2070:HOH:O	2.00	0.60
1:C:162:ALA:HA	1:C:170:PHE:O	2.01	0.60
1:C:194:ILE:HG12	1:C:195:PRO:HD2	1.82	0.60
1:D:275:LYS:HG3	3:D:2025:HOH:O	2.00	0.60
1:F:187:ALA:HA	1:F:190:LYS:HG2	1.84	0.60
1:F:62:ASN:HD22	1:F:63:PRO:HD2	1.66	0.60
1:A:60:ASN:OD1	1:A:257:ARG:HG2	2.02	0.60
3:E:2052:HOH:O	1:G:315:LYS:HE2	2.02	0.60
1:F:184:ILE:HG22	1:F:214:LEU:HD22	1.84	0.59
1:C:129:ASN:HA	1:C:164:LYS:NZ	2.17	0.59
1:E:1:MSE:SE	1:E:1:MSE:N	2.85	0.59
1:B:172:LEU:CD1	1:B:174:MSE:HE3	2.26	0.59
1:G:1:MSE:HG3	1:G:2:ILE:N	2.16	0.59
1:A:201:ASP:O	1:A:202:LYS:CB	2.51	0.59
1:B:273:MSE:HE1	1:B:281:LYS:HD3	1.85	0.59
1:A:178:SER:HB3	1:A:221:PHE:HA	1.85	0.59
1:C:193:LYS:HG2	1:C:194:ILE:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:PRO:HG3	1:D:38:LEU:HD21	1.84	0.59
1:F:5:PRO:HG3	1:F:38:LEU:HD21	1.85	0.59
1:A:53:ILE:HG22	1:A:57:LYS:HE2	1.84	0.59
1:G:188:LEU:HD22	1:G:214:LEU:HD23	1.85	0.59
1:A:140:THR:HG22	1:A:141:GLU:O	2.02	0.58
1:A:11:LEU:HD13	1:A:342:TYR:CD1	2.38	0.58
1:D:144:MSE:HE2	1:D:155:GLY:O	2.04	0.58
1:C:156:THR:OG1	2:C:4003:NAD:H5N	2.03	0.58
1:D:9[B]:LYS:HG3	1:D:34:VAL:HG21	1.85	0.58
1:E:186:GLU:HG2	1:E:189:ARG:HH12	1.68	0.58
1:B:281:LYS:NZ	1:B:281:LYS:HB3	2.19	0.58
1:G:152:LYS:O	1:G:153:ILE:HD13	2.04	0.58
1:H:219:LEU:HD23	3:H:2030:HOH:O	2.03	0.57
1:A:201:ASP:O	1:A:202:LYS:HB2	2.04	0.57
1:D:260:LYS:HD2	1:D:260:LYS:C	2.29	0.57
1:F:181:ARG:HH11	1:F:214:LEU:CD1	2.16	0.57
1:E:117:PHE:CD1	1:E:117:PHE:C	2.83	0.57
1:G:24:GLU:O	1:G:28:ILE:HG13	2.05	0.57
1:E:324:LEU:O	1:E:328:LEU:HG	2.05	0.57
1:E:117:PHE:C	1:E:117:PHE:HD1	2.13	0.57
1:B:160:ALA:HA	1:B:172:LEU:O	2.05	0.57
1:C:111:THR:OG1	1:C:262:ASP:OD1	2.18	0.57
1:C:138:THR:HG22	1:C:158:PRO:CG	2.35	0.57
1:C:293:GLU:HB3	1:D:150:LYS:HD2	1.87	0.57
1:F:248:VAL:HA	1:F:259:THR:HG22	1.86	0.57
1:H:99:LYS:O	1:H:102:LYS:HG2	2.05	0.56
1:A:225:LYS:O	1:B:174:MSE:HE1	2.04	0.56
1:B:138:THR:CG2	1:B:158:PRO:HG2	2.35	0.56
1:A:220:PRO:HB2	3:A:2050:HOH:O	2.06	0.56
1:C:189:ARG:HB3	1:C:190:LYS:HE3	1.87	0.56
1:C:193:LYS:HE3	1:C:194:ILE:N	2.20	0.56
1:E:133:ILE:HD13	1:F:236:LEU:HD22	1.87	0.56
1:F:243:GLU:OE1	3:F:2040:HOH:O	2.16	0.56
1:G:5:PRO:HD3	1:G:317:GLY:HA2	1.88	0.56
1:B:330:GLU:O	1:B:334:GLU:HG3	2.05	0.56
1:B:77:ALA:HB3	1:B:109:VAL:HG22	1.87	0.56
1:E:18:LYS:HE2	1:E:335:LEU:O	2.06	0.56
1:G:156:THR:OG1	2:G:4007:NAD:H5N	2.05	0.56
1:C:18:LYS:HE3	1:C:335:LEU:O	2.06	0.56
1:D:4:LYS:HB3	1:D:6:GLU:OE1	2.05	0.56
1:E:18:LYS:HG2	1:E:335:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LYS:N	1:C:190:LYS:HD2	2.21	0.55
1:G:202:LYS:HD3	1:G:215:GLU:O	2.07	0.55
1:H:139:ASN:ND2	1:H:261:GLY:H	2.01	0.55
1:E:192:ILE:HG22	1:E:193:LYS:N	2.19	0.55
1:F:9:LYS:HE2	1:F:31:ASP:OD1	2.07	0.55
1:G:196:GLU:CD	1:G:196:GLU:H	2.14	0.55
1:F:179:ILE:HG12	1:F:180:ALA:N	2.22	0.55
1:H:193:LYS:HB3	1:H:208:THR:HG22	1.88	0.55
1:A:153:ILE:HG21	1:B:289:ILE:HG12	1.88	0.55
1:A:181:ARG:HH22	1:A:214:LEU:CA	2.18	0.55
1:E:210:PRO:O	1:E:214:LEU:HD22	2.06	0.55
1:B:11:LEU:HD12	1:B:11:LEU:O	2.07	0.55
1:G:290:LYS:HE2	1:G:305:GLU:OE2	2.07	0.55
1:G:330:GLU:O	1:G:334:GLU:HG2	2.07	0.55
1:B:138:THR:HG23	1:B:158:PRO:HG2	1.87	0.55
1:A:116:HIS:CE1	1:A:118:GLY:HA2	2.42	0.54
1:F:3:LEU:HD13	1:F:343:ILE:HG12	1.89	0.54
1:B:91:LYS:O	1:B:95:GLU:HG2	2.07	0.54
1:F:192:ILE:HG13	1:F:193:LYS:O	2.08	0.54
1:C:192:ILE:HD12	1:C:192:ILE:N	2.22	0.54
1:D:160:ALA:HA	1:D:172:LEU:O	2.07	0.54
1:F:179:ILE:HD13	1:F:184:ILE:HG12	1.89	0.54
1:A:273:MSE:HE2	1:A:277:GLU:HB3	1.90	0.54
1:A:281:LYS:HE3	3:B:2050:HOH:O	2.07	0.54
1:A:160:ALA:HA	1:A:172:LEU:O	2.07	0.54
1:F:195:PRO:HB2	1:F:198:CYS:SG	2.48	0.54
1:G:8:GLU:HG3	1:G:46:ILE:HD12	1.90	0.53
1:H:209:ASP:HB3	1:H:212:LYS:HE2	1.90	0.53
1:A:258:CYS:SG	1:A:260:LYS:HG2	2.48	0.53
1:A:293:GLU:HG2	1:B:151:GLU:HB2	1.90	0.53
1:E:51:GLN:HG3	3:E:2005:HOH:O	2.07	0.53
1:F:83:LEU:HD11	1:F:257:ARG:CD	2.39	0.53
1:G:1:MSE:CG	1:G:2:ILE:N	2.66	0.53
1:A:117:PHE:HD1	1:A:117:PHE:C	2.16	0.53
1:E:295:ALA:O	1:E:297:GLY:N	2.42	0.53
1:A:117:PHE:C	1:A:117:PHE:CD1	2.87	0.53
1:C:193:LYS:HG2	1:C:194:ILE:N	2.24	0.53
1:D:117:PHE:HD1	1:D:117:PHE:C	2.17	0.53
1:E:305:GLU:O	1:E:309:ARG:HG3	2.08	0.53
1:F:243:GLU:CG	1:F:259:THR:HG23	2.39	0.53
1:H:200:VAL:HA	1:H:207:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASN:O	1:B:65:PRO:HD3	2.07	0.53
1:C:157:ASN:HB3	1:C:233:ILE:HG21	1.90	0.53
1:F:209:ASP:OD2	1:F:211:ALA:HB3	2.09	0.53
1:D:194:ILE:O	1:D:208:THR:HG22	2.09	0.53
1:F:207:THR:HG22	1:F:209:ASP:H	1.74	0.53
1:G:284:GLU:OE2	1:H:247:LYS:HE3	2.09	0.53
1:C:192:ILE:O	1:C:192:ILE:HG22	2.09	0.52
1:D:117:PHE:C	1:D:117:PHE:CD1	2.88	0.52
1:G:131:ASP:OD1	1:G:279:LYS:HE2	2.10	0.52
1:C:144:MSE:HE2	1:C:155:GLY:O	2.09	0.52
1:D:158:PRO:HA	1:D:175:ALA:HA	1.92	0.52
1:C:320:ILE:HB	1:C:324:LEU:HD23	1.91	0.52
1:E:35:ASP:OD2	1:E:311:LYS:NZ	2.40	0.52
1:G:13:ILE:O	1:G:17:LYS:HG3	2.09	0.52
1:H:4:LYS:HB3	1:H:6:GLU:OE1	2.10	0.52
1:B:131:ASP:OD2	1:B:279:LYS:CE	2.58	0.52
1:B:156:THR:HG23	1:B:175:ALA:HB1	1.92	0.52
1:F:181:ARG:NH1	1:F:214:LEU:HD12	2.19	0.52
1:A:236:LEU:HD22	1:B:133:ILE:HD13	1.90	0.52
1:C:172:LEU:HD11	1:C:174:MSE:HG2	1.91	0.52
1:H:94:MSE:HE3	1:H:124:SER:HA	1.91	0.52
1:D:194:ILE:HG22	1:D:208:THR:HA	1.92	0.51
1:C:326:ASN:HA	1:C:329:LYS:HZ2	1.75	0.51
1:E:6:GLU:CD	1:E:6:GLU:H	2.18	0.51
1:F:138:THR:HG22	1:F:158:PRO:HG2	1.91	0.51
1:B:1:MSE:SE	1:B:1:MSE:N	2.93	0.51
1:E:5:PRO:HG3	1:E:38:LEU:HD21	1.92	0.51
1:E:231:LEU:HD13	1:F:170:PHE:HE1	1.76	0.51
1:F:181:ARG:O	1:F:181:ARG:HG3	2.10	0.51
1:A:260:LYS:HE2	3:A:2080:HOH:O	2.09	0.51
1:E:184:ILE:HG22	1:E:214:LEU:HD22	1.92	0.51
1:C:157:ASN:HB3	1:C:233:ILE:CG2	2.40	0.51
1:C:189:ARG:NH1	1:C:190:LYS:HE3	2.25	0.51
1:A:244:VAL:HG13	1:B:281:LYS:NZ	2.26	0.51
1:E:44:HIS:CE1	2:E:4005:NAD:C2N	2.93	0.51
1:G:209:ASP:OD2	1:G:212:LYS:HG2	2.10	0.51
1:C:172:LEU:CD1	1:C:174:MSE:HE3	2.39	0.51
1:D:193:LYS:HG2	1:D:208:THR:HB	1.92	0.51
1:H:273:MSE:HE2	1:H:277:GLU:HB3	1.92	0.51
1:B:140:THR:HG21	1:B:156:THR:H	1.75	0.51
1:G:151:GLU:OE1	1:H:293:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:GLU:O	1:B:309[B]:ARG:HD2	2.11	0.51
1:C:117:PHE:CD1	1:C:117:PHE:C	2.89	0.51
1:C:138:THR:HG22	1:C:158:PRO:HG2	1.93	0.51
1:F:179:ILE:CD1	1:F:184:ILE:HG12	2.41	0.51
1:A:296:GLU:HG2	1:A:298:PHE:HD1	1.76	0.51
1:B:25:ASP:HB3	1:B:88:VAL:HG21	1.92	0.51
1:A:1:MSE:HG2	1:A:320:ILE:HG13	1.91	0.50
1:F:80:ASP:OD1	1:F:112:ARG:HD2	2.12	0.50
1:A:243:GLU:HG2	1:A:259:THR:HB	1.91	0.50
1:D:255:GLU:O	1:D:255:GLU:HG3	2.10	0.50
1:E:174:MSE:HE1	1:F:225:LYS:O	2.11	0.50
1:D:131:ASP:OD1	1:D:279:LYS:HE2	2.11	0.50
1:H:175:ALA:HB2	2:H:4008:NAD:H6N	1.93	0.50
1:B:3:LEU:HD13	1:B:343:ILE:HG12	1.93	0.50
1:E:307:GLU:H	1:E:307:GLU:CD	2.19	0.50
1:F:151:GLU:O	1:F:153:ILE:HD12	2.12	0.50
1:F:167:LYS:HE3	1:F:168:TYR:HE2	1.75	0.50
1:A:119:ILE:HD12	1:A:122:TYR:H	1.77	0.50
1:B:138:THR:HG23	1:B:158:PRO:CG	2.42	0.50
1:C:338:ASN:ND2	1:C:338:ASN:N	2.45	0.50
1:D:209:ASP:OD2	1:D:211:ALA:HB3	2.11	0.50
1:B:189:ARG:C	1:B:191:LYS:H	2.18	0.50
1:C:322:LYS:O	1:C:325:TYR:HB3	2.12	0.50
1:E:192:ILE:CG2	1:E:193:LYS:N	2.74	0.49
1:A:133:ILE:HD13	1:B:236:LEU:HD22	1.94	0.49
1:B:156:THR:CG2	1:B:175:ALA:HB1	2.42	0.49
1:E:253:ASN:OD1	1:E:255:GLU:HG2	2.12	0.49
1:G:174:MSE:HB3	2:G:4007:NAD:H52A	1.94	0.49
1:H:51:GLN:CG	1:H:254:PRO:HG3	2.41	0.49
1:B:172:LEU:HD21	1:B:174:MSE:HE3	1.94	0.49
1:B:5:PRO:HG3	1:B:38:LEU:HD21	1.94	0.49
1:E:60:ASN:HD22	1:E:257:ARG:HD2	1.77	0.49
1:E:343:ILE:HA	1:E:344:GLU:CB	2.40	0.49
1:F:83:LEU:HD11	1:F:257:ARG:HD3	1.93	0.49
1:F:117:PHE:HD1	1:F:117:PHE:C	2.20	0.49
1:A:201:ASP:HB3	1:A:207:THR:HG21	1.93	0.49
1:E:142:PRO:HG3	1:E:246:THR:HA	1.95	0.49
1:F:117:PHE:C	1:F:117:PHE:CD1	2.91	0.49
1:G:292:SER:HB3	1:H:153:ILE:CD1	2.41	0.49
1:C:179:ILE:HD11	1:C:183:LYS:HG2	1.94	0.49
1:C:191:LYS:O	1:C:193:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:THR:HG22	1:E:208:THR:O	2.12	0.49
1:B:87:GLN:HA	1:B:123:TYR:OH	2.13	0.49
1:G:273:MSE:O	1:G:277:GLU:HG3	2.13	0.49
1:D:6:GLU:CD	1:D:6:GLU:N	2.62	0.49
1:F:179:ILE:HG21	1:F:198:CYS:HB3	1.95	0.49
1:B:157:ASN:HB3	1:B:233:ILE:CG2	2.42	0.48
1:C:327:GLN:O	1:C:331:ILE:HG13	2.13	0.48
1:A:137:ILE:CG2	1:A:159:ILE:HG13	2.43	0.48
1:A:138:THR:HG22	1:A:158:PRO:HD2	1.96	0.48
1:G:312:MSE:O	1:G:315:LYS:HE3	2.13	0.48
1:A:320:ILE:HB	1:A:324:LEU:HD23	1.93	0.48
1:E:296:GLU:OE1	1:E:297:GLY:N	2.45	0.48
1:F:258:CYS:SG	1:F:260:LYS:HG3	2.53	0.48
1:G:176:THR:HG21	1:G:233:ILE:HD12	1.95	0.48
1:A:244:VAL:HG13	1:B:281:LYS:HZ1	1.77	0.48
1:B:156:THR:CG2	1:B:156:THR:O	2.61	0.48
1:C:293:GLU:HA	1:C:294:PRO:HD3	1.68	0.48
1:C:329:LYS:HB3	1:C:329:LYS:HZ2	1.77	0.48
1:F:193:LYS:NZ	1:F:193:LYS:HB3	2.29	0.48
1:G:138:THR:HG22	1:G:158:PRO:HG2	1.95	0.48
1:B:278:PHE:O	1:B:282:VAL:HG23	2.14	0.48
1:C:193:LYS:CE	1:C:194:ILE:H	2.23	0.48
1:C:329:LYS:NZ	1:C:329:LYS:CB	2.76	0.48
1:D:194:ILE:HG13	1:D:195:PRO:HD2	1.96	0.48
1:H:117:PHE:C	1:H:117:PHE:HD1	2.21	0.48
1:F:273:MSE:HE1	1:F:281:LYS:HE2	1.96	0.48
1:A:139:ASN:HB2	1:A:261:GLY:H	1.79	0.48
1:A:203:ASP:OD2	1:A:203:ASP:N	2.46	0.48
1:C:193:LYS:HE2	1:C:193:LYS:HB3	1.66	0.48
1:C:278:PHE:CD1	1:D:235:MSE:HE2	2.49	0.48
1:F:179:ILE:CG2	1:F:198:CYS:HB3	2.44	0.48
1:G:285:LEU:HB2	1:H:244:VAL:HG21	1.96	0.48
1:E:140:THR:HB	1:E:155:GLY:HA3	1.94	0.48
1:F:220:PRO:HG2	1:F:227:TYR:HB2	1.96	0.48
1:F:296:GLU:HB2	1:F:298:PHE:HD2	1.78	0.48
1:H:8:GLU:O	1:H:12:ILE:HD12	2.14	0.48
1:B:273:MSE:HE2	1:B:277:GLU:HB2	1.96	0.47
1:H:117:PHE:C	1:H:117:PHE:CD1	2.91	0.47
1:C:278:PHE:CE1	1:D:235:MSE:HE2	2.49	0.47
1:B:6:GLU:CD	1:B:6:GLU:H	2.22	0.47
1:H:141:GLU:HG2	1:H:249:LYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:PRO:HB2	1:F:67:ILE:HG13	1.95	0.47
1:F:259:THR:CG2	1:F:259:THR:O	2.62	0.47
1:A:183:LYS:HD2	1:A:186:GLU:OE2	2.14	0.47
1:D:102:LYS:CG	1:D:132:MSE:HE1	2.41	0.47
1:F:190:LYS:HE3	1:F:192:ILE:HD11	1.97	0.47
1:B:76:THR:HA	1:B:108:VAL:O	2.15	0.47
1:B:295:ALA:O	1:B:296:GLU:C	2.58	0.47
1:C:5:PRO:HD3	1:C:317:GLY:HA2	1.95	0.47
1:A:192:ILE:O	1:A:193:LYS:HD3	2.15	0.47
1:A:296:GLU:CG	1:A:297:GLY:H	2.22	0.47
1:B:73:SER:HB2	1:B:74:PRO:HD2	1.95	0.47
1:C:214:LEU:C	1:C:216:GLY:H	2.22	0.47
1:E:338:ASN:HB3	1:E:341:ASP:OD1	2.15	0.47
1:C:11:LEU:HD13	1:C:342:TYR:CD1	2.50	0.47
1:E:162:ALA:HA	1:E:170:PHE:O	2.14	0.47
1:B:141:GLU:HG3	1:B:251:THR:OG1	2.15	0.47
1:E:141:GLU:HG3	1:E:251:THR:OG1	2.15	0.47
1:C:191:LYS:C	1:C:193:LYS:H	2.22	0.47
1:D:307:GLU:N	1:D:307:GLU:CD	2.73	0.47
1:F:140:THR:HG21	2:F:4006:NAD:H4N	1.97	0.47
1:G:87:GLN:HA	1:G:123:TYR:OH	2.15	0.47
1:H:186:GLU:HA	1:H:189:ARG:NH1	2.30	0.47
1:B:46:ILE:HG23	1:B:324:LEU:HD21	1.97	0.46
1:A:46:ILE:HG23	1:A:324:LEU:HD21	1.96	0.46
1:A:190:LYS:HB3	1:A:192:ILE:HG12	1.97	0.46
1:F:166:ASN:HB2	1:F:283:ASP:OD2	2.16	0.46
1:F:243:GLU:HB2	1:F:259:THR:HG23	1.97	0.46
1:C:244:VAL:HG22	1:D:281:LYS:HD2	1.98	0.46
1:G:48:ARG:NH1	3:G:2012:HOH:O	2.46	0.46
1:G:138:THR:CG2	1:G:158:PRO:HG2	2.45	0.46
1:E:76:THR:HA	1:E:108:VAL:O	2.16	0.46
1:G:190:LYS:HD3	1:G:192:ILE:HD13	1.97	0.46
1:A:209:ASP:HA	1:A:210:PRO:HD3	1.71	0.46
1:E:246:THR:HG23	1:F:288:GLU:OE1	2.16	0.46
1:G:201:ASP:C	1:G:203:ASP:H	2.22	0.46
1:H:17:LYS:HD2	1:H:23:GLU:HG3	1.98	0.46
1:H:128:MSE:HE3	1:H:169:LYS:HE3	1.97	0.46
1:C:329:LYS:HZ2	1:C:329:LYS:CB	2.29	0.46
1:D:307:GLU:CD	1:D:307:GLU:H	2.24	0.46
1:E:225:LYS:HE2	1:F:174:MSE:HB2	1.97	0.46
1:E:243:GLU:HB3	1:E:247:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:O	1:B:130:GLN:HG2	2.15	0.46
1:E:231:LEU:HD13	1:F:170:PHE:CE1	2.51	0.46
3:G:2063:HOH:O	1:H:146:PRO:HD2	2.16	0.46
1:B:222:GLY:H	1:B:226:GLY:HA3	1.80	0.46
1:C:250:GLY:HA2	1:C:256:GLU:HB2	1.98	0.46
1:C:295:ALA:O	1:C:296:GLU:C	2.58	0.46
1:E:137:ILE:HB	1:E:233:ILE:HG23	1.98	0.46
1:F:4:LYS:HB2	1:F:7:ASN:HD22	1.81	0.46
1:H:276:GLU:CD	1:H:276:GLU:N	2.66	0.46
1:B:83:LEU:HD11	1:B:257:ARG:HD2	1.98	0.46
1:D:9[A]:LYS:HE2	1:D:13:ILE:HD11	1.98	0.46
1:E:192:ILE:HG22	1:E:193:LYS:O	2.16	0.45
1:F:62:ASN:ND2	1:F:64:LYS:H	2.15	0.45
1:A:137:ILE:HG22	1:A:159:ILE:HG13	1.98	0.45
1:A:236:LEU:CD2	1:B:133:ILE:HD13	2.47	0.45
1:D:200:VAL:CG2	1:D:217:CYS:HB2	2.46	0.45
1:A:135:ILE:HA	1:A:160:ALA:O	2.16	0.45
1:E:296:GLU:OE1	1:E:298:PHE:CD1	2.69	0.45
1:H:157:ASN:HB3	1:H:233:ILE:CG2	2.47	0.45
1:F:201:ASP:HB3	1:F:207:THR:OG1	2.16	0.45
1:H:138:THR:O	1:H:158:PRO:HD2	2.17	0.45
1:B:117:PHE:CD1	1:B:117:PHE:C	2.94	0.45
1:E:152:LYS:O	1:E:153:ILE:HD13	2.17	0.45
1:G:296:GLU:OE2	1:H:205:LYS:HG2	2.16	0.45
1:C:3:LEU:HD13	1:C:343:ILE:HG12	1.98	0.45
1:D:201:ASP:O	1:D:202:LYS:C	2.60	0.45
1:E:172:LEU:CD1	1:E:174:MSE:HE3	2.26	0.45
1:E:244:VAL:HG21	1:F:285:LEU:HB2	1.97	0.45
1:F:260:LYS:HD2	1:F:260:LYS:C	2.42	0.45
1:G:167:LYS:HD3	1:G:168:TYR:CE2	2.51	0.45
1:A:232:ALA:O	1:A:236:LEU:HG	2.16	0.45
1:C:117:PHE:C	1:C:117:PHE:HD1	2.25	0.45
1:F:247:LYS:O	1:F:259:THR:HG21	2.16	0.45
1:H:221:PHE:CG	1:H:222:GLY:N	2.85	0.45
1:A:244:VAL:HG21	1:B:285:LEU:HB2	1.99	0.45
1:F:46:ILE:HG23	1:F:324:LEU:HD21	1.98	0.45
1:B:11:LEU:HD12	1:B:11:LEU:C	2.43	0.45
1:C:139:ASN:HD22	1:C:139:ASN:HA	1.54	0.45
1:E:170:PHE:CE1	1:F:231:LEU:HD13	2.52	0.45
1:G:253:ASN:HA	1:G:254:PRO:HD2	1.77	0.45
1:H:328:LEU:O	1:H:329:LYS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:LEU:C	1:C:190:LYS:H	2.24	0.44
1:E:174:MSE:HE2	1:F:225:LYS:CA	2.43	0.44
1:H:331:ILE:O	1:H:335:LEU:HG	2.17	0.44
1:A:293:GLU:OE2	1:B:151:GLU:HB2	2.16	0.44
1:E:140:THR:HG21	1:E:156:THR:H	1.82	0.44
1:B:140:THR:CG2	1:B:156:THR:H	2.30	0.44
1:C:258:CYS:SG	1:C:260:LYS:HG3	2.58	0.44
1:H:135:ILE:HA	1:H:160:ALA:O	2.18	0.44
1:C:188:LEU:C	1:C:190:LYS:N	2.75	0.44
1:D:71:LYS:HE2	1:D:71:LYS:HB3	1.69	0.44
1:E:294:PRO:HA	1:F:149:GLY:HA2	1.99	0.44
1:F:62:ASN:HD22	1:F:63:PRO:CD	2.30	0.44
1:H:260:LYS:HD2	1:H:260:LYS:C	2.43	0.44
1:C:193:LYS:CG	1:C:194:ILE:N	2.79	0.44
1:D:48:ARG:O	1:D:48:ARG:HG3	2.18	0.44
1:G:46:ILE:HG23	1:G:324:LEU:HD21	1.99	0.44
1:A:150:LYS:HG3	1:B:293:GLU:HG3	1.99	0.44
1:H:102:LYS:HB3	1:H:132:MSE:HE1	1.99	0.44
1:H:200:VAL:HG12	1:H:206:PRO:HA	1.98	0.44
1:G:158:PRO:HD3	2:G:4007:NAD:C5N	2.48	0.44
1:G:236:LEU:HD22	1:H:133:ILE:HD13	1.99	0.44
1:B:157:ASN:HB3	1:B:233:ILE:HG21	2.00	0.44
1:C:150:LYS:HG2	1:D:293:GLU:HB3	2.00	0.44
1:C:195:PRO:HB2	1:C:198:CYS:SG	2.57	0.44
1:D:179:ILE:HD11	1:D:183:LYS:HD3	1.99	0.44
1:A:39:LYS:HG2	1:A:307:GLU:HB3	1.99	0.43
1:B:189:ARG:C	1:B:191:LYS:N	2.74	0.43
1:E:1:MSE:HE3	1:E:1:MSE:H1	1.82	0.43
1:E:263:LEU:HD23	1:E:263:LEU:HA	1.86	0.43
1:A:182:GLY:HA2	1:A:185:LEU:HD21	1.99	0.43
1:D:53:ILE:HG22	1:D:57:LYS:HE3	2.00	0.43
1:E:315:LYS:HD3	1:E:315:LYS:HA	1.71	0.43
1:D:116:HIS:CD2	1:D:118:GLY:H	2.36	0.43
1:G:272:PHE:HB3	1:H:239:ILE:O	2.19	0.43
1:G:323:ASN:HB2	3:G:2066:HOH:O	2.18	0.43
1:B:144:MSE:HE2	1:B:155:GLY:O	2.18	0.43
1:B:168:TYR:HB3	1:B:286:LEU:HD12	2.00	0.43
1:H:209:ASP:HA	1:H:210:PRO:HD3	1.85	0.43
1:C:207:THR:OG1	1:C:212:LYS:HD2	2.18	0.43
1:H:128:MSE:CE	1:H:169:LYS:HE3	2.48	0.43
1:B:87:GLN:H	1:B:87:GLN:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:HG2	1:B:185:LEU:CD2	2.49	0.43
1:B:214:LEU:HD12	1:B:214:LEU:HA	1.89	0.43
1:E:313:LYS:HD3	1:E:313:LYS:HA	1.72	0.43
1:G:28:ILE:HG23	1:G:91:LYS:HD3	2.01	0.43
1:G:157:ASN:O	1:G:176:THR:HG23	2.19	0.43
1:H:62:ASN:HA	1:H:63:PRO:HD3	1.86	0.43
1:H:157:ASN:HB3	1:H:233:ILE:HG21	2.00	0.43
1:B:267:ILE:O	1:B:269:PRO:HD3	2.19	0.43
1:F:53:ILE:HG13	1:F:331:ILE:HD13	2.00	0.43
1:G:205:LYS:HG2	1:H:296:GLU:CD	2.44	0.43
1:F:4:LYS:HB3	1:F:6:GLU:OE2	2.19	0.43
1:F:141:GLU:HG2	1:F:251:THR:OG1	2.17	0.43
1:F:243:GLU:HB2	1:F:259:THR:HG22	1.99	0.43
1:F:283:ASP:O	1:F:287:ASP:HB2	2.18	0.43
1:B:117:PHE:C	1:B:117:PHE:HD1	2.27	0.43
1:D:194:ILE:HD12	1:D:194:ILE:HA	1.94	0.43
1:H:48:ARG:HD3	1:H:52:TYR:HE1	1.84	0.43
1:G:228:GLY:HA3	1:H:172:LEU:HD13	2.01	0.42
1:G:278:PHE:O	1:G:282:VAL:HG23	2.19	0.42
1:H:83:LEU:HD23	1:H:83:LEU:HA	1.90	0.42
1:B:253:ASN:ND2	1:B:256:GLU:OE1	2.51	0.42
1:C:281:LYS:HE2	1:C:284:GLU:OE1	2.19	0.42
1:F:49:PHE:O	1:F:52:TYR:HB2	2.19	0.42
1:A:285:LEU:HB2	1:B:244:VAL:HG21	2.01	0.42
1:B:83:LEU:HD21	1:B:257:ARG:HG2	2.02	0.42
1:E:184:ILE:HG22	1:E:214:LEU:CD2	2.49	0.42
1:E:209:ASP:OD2	1:E:211:ALA:HB3	2.19	0.42
1:E:262:ASP:OD1	1:E:262:ASP:N	2.52	0.42
1:F:340:GLU:CD	1:F:340:GLU:H	2.26	0.42
1:G:1:MSE:SE	1:G:2:ILE:H	2.51	0.42
1:C:6:GLU:CD	1:C:6:GLU:H	2.28	0.42
1:C:170:PHE:CE1	1:C:303:PRO:HG2	2.54	0.42
1:G:263:LEU:HD23	1:G:263:LEU:HA	1.73	0.42
1:H:193:LYS:CD	1:H:208:THR:HG22	2.50	0.42
1:A:70:VAL:HG12	1:A:71:LYS:HG3	2.01	0.42
1:B:273:MSE:O	1:B:277:GLU:HG3	2.19	0.42
1:C:172:LEU:CD1	1:C:174:MSE:HG2	2.49	0.42
1:E:138:THR:HG22	1:E:158:PRO:HG2	2.01	0.42
1:E:307:GLU:CD	1:E:307:GLU:N	2.78	0.42
1:H:212:LYS:O	1:H:215:GLU:HG3	2.19	0.42
1:A:102:LYS:HG3	1:A:132:MSE:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:C	1:A:260:LYS:HE3	2.44	0.42
1:B:211:ALA:O	1:B:215:GLU:HG2	2.20	0.42
1:E:338:ASN:OD1	1:E:340:GLU:HG2	2.19	0.42
1:A:246:THR:HG23	1:B:288:GLU:OE1	2.19	0.42
1:B:83:LEU:HD11	1:B:257:ARG:HG3	2.01	0.42
1:C:37:ASP:OD2	1:C:46:ILE:N	2.50	0.42
1:C:71:LYS:O	1:C:77:ALA:HA	2.18	0.42
1:F:25:ASP:HB3	1:F:88:VAL:HG21	2.01	0.42
1:G:174:MSE:SE	1:H:225:LYS:HG2	2.68	0.42
1:G:218:ILE:HG22	1:G:219:LEU:N	2.35	0.42
1:H:87:GLN:H	1:H:87:GLN:CD	2.27	0.42
1:H:200:VAL:CA	1:H:207:THR:HG22	2.49	0.42
1:B:131:ASP:OD2	1:B:279:LYS:HE3	2.20	0.42
1:F:62:ASN:ND2	1:F:62:ASN:C	2.76	0.42
1:F:295:ALA:O	1:F:296:GLU:C	2.63	0.42
1:G:235:MSE:HE3	1:G:235:MSE:O	2.19	0.42
1:H:143:ALA:HA	1:H:152:LYS:HD2	2.02	0.42
1:C:102:LYS:NZ	3:C:2015:HOH:O	2.53	0.42
1:C:150:LYS:HG2	1:D:293:GLU:CB	2.49	0.42
1:D:170:PHE:HE1	1:D:303:PRO:HG2	1.80	0.42
1:E:142:PRO:CG	1:E:246:THR:HA	2.50	0.42
1:A:151:GLU:OE1	1:B:293:GLU:HG2	2.20	0.41
1:B:260:LYS:HE2	3:B:2030:HOH:O	2.20	0.41
1:C:160:ALA:HA	1:C:172:LEU:O	2.19	0.41
1:E:342:TYR:C	1:E:343:ILE:HG13	2.44	0.41
1:F:187:ALA:HA	1:F:190:LYS:CG	2.49	0.41
1:H:139:ASN:ND2	1:H:139:ASN:H	2.18	0.41
1:H:312:MSE:O	1:H:315:LYS:HG2	2.19	0.41
1:A:271:PHE:O	1:B:71:LYS:HD3	2.20	0.41
1:B:290:LYS:HE2	1:B:305:GLU:OE2	2.20	0.41
1:C:151:GLU:HG2	1:D:292:SER:HB2	2.02	0.41
1:C:235:MSE:HE2	1:D:278:PHE:CE1	2.55	0.41
1:A:225:LYS:HA	1:B:174:MSE:CE	2.50	0.41
1:F:91:LYS:O	1:F:95:GLU:HG2	2.20	0.41
1:B:131:ASP:OD2	1:B:279:LYS:HE2	2.21	0.41
1:E:41:PHE:CE2	2:E:4005:NAD:H52N	2.55	0.41
1:E:200:VAL:O	1:E:216:GLY:HA3	2.21	0.41
1:D:49:PHE:HB3	1:D:50:PRO:HD3	2.02	0.41
1:F:179:ILE:CG1	1:F:180:ALA:N	2.83	0.41
1:A:293:GLU:HG2	1:A:293:GLU:H	1.70	0.41
1:C:10:LYS:HG2	1:C:342:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LEU:HD13	1:D:343:ILE:HG12	2.02	0.41
1:F:151:GLU:HG3	1:F:153:ILE:HD11	2.02	0.41
1:G:18:LYS:HG2	1:G:335:LEU:HB3	2.03	0.41
1:H:170:PHE:CE1	1:H:303:PRO:HG2	2.55	0.41
1:A:21:VAL:HA	1:A:22:PRO:HD2	1.93	0.41
1:E:130:GLN:O	1:E:131:ASP:HB2	2.20	0.41
1:E:293:GLU:HG2	1:F:151:GLU:HG2	2.01	0.41
1:G:128:MSE:HG3	1:G:164:LYS:HG2	2.03	0.41
1:G:154:LEU:HD21	1:H:289:ILE:HD11	2.02	0.41
1:H:15:VAL:O	1:H:18:LYS:HB2	2.21	0.41
1:A:92:LYS:HE3	3:A:2019:HOH:O	2.21	0.41
1:B:41:PHE:CE1	2:B:4002:NAD:H52N	2.56	0.41
1:C:249:LYS:HD3	1:C:256:GLU:OE1	2.21	0.41
1:D:9[A]:LYS:HD2	1:D:30:ALA:CB	2.51	0.41
1:D:10[B]:LYS:HG2	1:D:342:TYR:HE2	1.86	0.41
1:D:302:ILE:HG23	1:D:303:PRO:HD2	2.01	0.41
1:F:280:ARG:NE	3:F:2046:HOH:O	2.52	0.41
1:G:273:MSE:HE2	1:G:277:GLU:HB2	2.02	0.41
1:C:188:LEU:O	1:C:190:LYS:N	2.54	0.41
1:C:262:ASP:OD1	1:C:262:ASP:N	2.54	0.41
1:A:1:MSE:HB3	1:A:320:ILE:O	2.21	0.40
1:A:142:PRO:CG	1:A:246:THR:HA	2.50	0.40
1:C:41:PHE:CE2	2:C:4003:NAD:H52N	2.56	0.40
1:C:188:LEU:HB2	1:C:210:PRO:HB2	2.03	0.40
1:D:302:ILE:O	1:D:303:PRO:C	2.63	0.40
1:F:94:MSE:O	1:F:98:ILE:HG13	2.21	0.40
1:F:249:LYS:H	1:F:259:THR:HB	1.86	0.40
1:G:108:VAL:HG22	1:G:265:ILE:HG12	2.02	0.40
1:G:28:ILE:CG2	1:G:91:LYS:HD3	2.52	0.40
1:A:296:GLU:HG2	1:A:298:PHE:CD1	2.57	0.40
1:B:156:THR:HG22	1:B:156:THR:O	2.22	0.40
1:C:87:GLN:HA	1:C:123:TYR:OH	2.21	0.40
1:E:39:LYS:HG2	1:E:307:GLU:HB3	2.03	0.40
1:E:135:ILE:HB	1:E:265:ILE:HB	2.02	0.40
1:F:187:ALA:HA	1:F:190:LYS:CE	2.38	0.40
1:H:83:LEU:HD11	1:H:257:ARG:HD2	2.03	0.40
1:A:140:THR:HG21	1:A:156:THR:H	1.85	0.40
1:F:37:ASP:HB3	1:F:318:PHE:CZ	2.56	0.40
1:F:138:THR:O	1:F:158:PRO:HD2	2.22	0.40
1:F:296:GLU:HB2	1:F:298:PHE:CD2	2.57	0.40
1:G:71:LYS:O	1:G:77:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:ASP:N	1:G:205:LYS:O	2.54	0.40
1:H:91:LYS:O	1:H:95:GLU:HG2	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	344/344 (100%)	329 (96%)	11 (3%)	4 (1%)	10	20
1	B	343/344 (100%)	327 (95%)	15 (4%)	1 (0%)	36	55
1	C	343/344 (100%)	321 (94%)	18 (5%)	4 (1%)	10	20
1	D	344/344 (100%)	320 (93%)	20 (6%)	4 (1%)	10	20
1	E	342/344 (99%)	329 (96%)	10 (3%)	3 (1%)	14	27
1	F	342/344 (99%)	321 (94%)	18 (5%)	3 (1%)	14	27
1	G	343/344 (100%)	331 (96%)	10 (3%)	2 (1%)	21	38
1	H	342/344 (99%)	327 (96%)	13 (4%)	2 (1%)	21	38
All	All	2743/2752 (100%)	2605 (95%)	115 (4%)	23 (1%)	16	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	GLU
1	C	296	GLU
1	D	296	GLU
1	E	296	GLU
1	E	334	GLU
1	G	296	GLU
1	A	192	ILE
1	A	202	LYS

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Mol	Chain	Res	Type
1	C	191	LYS
1	C	192	ILE
1	E	216	GLY
1	F	190	LYS
1	G	191	LYS
1	H	296	GLU
1	D	203	ASP
1	F	296	GLU
1	H	221	PHE
1	A	296	GLU
1	D	295	ALA
1	C	157	ASN
1	D	206	PRO
1	F	182	GLY
1	A	157	ASN

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	279/268 (104%)	260 (93%)	19 (7%)	14	31
1	B	278/268 (104%)	258 (93%)	20 (7%)	13	28
1	C	278/268 (104%)	254 (91%)	24 (9%)	10	21
1	D	279/268 (104%)	260 (93%)	19 (7%)	14	31
1	E	277/268 (103%)	265 (96%)	12 (4%)	26	51
1	F	277/268 (103%)	259 (94%)	18 (6%)	15	32
1	G	278/268 (104%)	263 (95%)	15 (5%)	20	41
1	H	277/268 (103%)	262 (95%)	15 (5%)	20	41
All	All	2223/2144 (104%)	2081 (94%)	142 (6%)	16	33

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	102	LYS
1	A	117	PHE
1	A	139	ASN
1	A	140	THR
1	A	150	LYS
1	A	169[A]	LYS
1	A	169[B]	LYS
1	A	181	ARG
1	A	185	LEU
1	A	188	LEU
1	A	191	LYS
1	A	192	ILE
1	A	194	ILE
1	A	203	ASP
1	A	209	ASP
1	A	231	LEU
1	A	263	LEU
1	A	311	LYS
1	B	6	GLU
1	B	53	ILE
1	B	68	LYS
1	B	71	LYS
1	B	117	PHE
1	B	138	THR
1	B	140	THR
1	B	156	THR
1	B	183	LYS
1	B	185	LEU
1	B	193	LYS
1	B	214	LEU
1	B	218	ILE
1	B	247	LYS
1	B	256	GLU
1	B	263	LEU
1	B	277	GLU
1	B	281	LYS
1	B	289	ILE
1	B	296	GLU
1	C	1	MSE
1	C	6	GLU
1	C	72	GLU
1	C	102	LYS

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Mol	Chain	Res	Type
1	C	111	THR
1	C	117	PHE
1	C	139	ASN
1	C	154	LEU
1	C	190	LYS
1	C	194	ILE
1	C	214	LEU
1	C	231	LEU
1	C	236	LEU
1	C	260	LYS
1	C	262	ASP
1	C	263	LEU
1	C	281	LYS
1	C	289	ILE
1	C	293	GLU
1	C	313	LYS
1	C	329	LYS
1	C	330	GLU
1	C	338	ASN
1	C	344	GLU
1	D	1	MSE
1	D	2	ILE
1	D	6	GLU
1	D	23	GLU
1	D	91	LYS
1	D	99	LYS
1	D	112	ARG
1	D	113	ASN
1	D	117	PHE
1	D	150	LYS
1	D	185	LEU
1	D	193	LYS
1	D	194	ILE
1	D	208	THR
1	D	214	LEU
1	D	231	LEU
1	D	236	LEU
1	D	262	ASP
1	D	296	GLU
1	E	10	LYS
1	E	42	THR
1	E	53	ILE

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Mol	Chain	Res	Type
1	E	58	LEU
1	E	117	PHE
1	E	174	MSE
1	E	214	LEU
1	E	231	LEU
1	E	262	ASP
1	E	263	LEU
1	E	296	GLU
1	E	334	GLU
1	F	1	MSE
1	F	6	GLU
1	F	9	LYS
1	F	43	SER
1	F	48	ARG
1	F	58	LEU
1	F	83	LEU
1	F	116	HIS
1	F	117	PHE
1	F	181	ARG
1	F	214	LEU
1	F	231	LEU
1	F	247	LYS
1	F	259	THR
1	F	263	LEU
1	F	275	LYS
1	F	316	ASP
1	F	322	LYS
1	G	2	ILE
1	G	24	GLU
1	G	117	PHE
1	G	169	LYS
1	G	185	LEU
1	G	191	LYS
1	G	196	GLU
1	G	214	LEU
1	G	231	LEU
1	G	260	LYS
1	G	263	LEU
1	G	277	GLU
1	G	293	GLU
1	G	323	ASN
1	G	333	ASN

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Mol	Chain	Res	Type
1	H	9	LYS
1	H	42	THR
1	H	43	SER
1	H	106	VAL
1	H	117	PHE
1	H	139	ASN
1	H	140	THR
1	H	152	LYS
1	H	171	SER
1	H	196	GLU
1	H	215	GLU
1	H	231	LEU
1	H	276	GLU
1	H	284	GLU
1	H	344	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	166	ASN
1	A	291	ASN
1	A	333	ASN
1	B	338	ASN
1	C	7	ASN
1	C	139	ASN
1	C	166	ASN
1	C	268	ASN
1	C	338	ASN
1	D	51	GLN
1	D	327	GLN
1	E	60	ASN
1	E	129	ASN
1	E	327	GLN
1	E	333	ASN
1	F	51	GLN
1	F	62	ASN
1	F	113	ASN
1	F	327	GLN
1	G	129	ASN
1	G	166	ASN
1	H	103	ASN

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Mol	Chain	Res	Type
1	H	129	ASN
1	H	139	ASN
1	H	166	ASN
1	H	323	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	4001	-	46,48,48	1.91	8 (17%)	64,73,73	2.23	16 (25%)
2	NAD	C	4003	-	46,48,48	1.82	8 (17%)	64,73,73	2.35	16 (25%)
2	NAD	B	4002	-	46,48,48	1.81	8 (17%)	64,73,73	2.25	17 (26%)
2	NAD	E	4005	-	46,48,48	1.85	7 (15%)	64,73,73	2.25	18 (28%)
2	NAD	D	4004	-	46,48,48	1.83	9 (19%)	64,73,73	2.24	16 (25%)
2	NAD	H	4008	-	46,48,48	1.88	7 (15%)	64,73,73	2.19	16 (25%)
2	NAD	G	4007	-	46,48,48	1.79	8 (17%)	64,73,73	2.30	16 (25%)
2	NAD	F	4006	-	46,48,48	1.82	7 (15%)	64,73,73	2.13	16 (25%)

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	4001	-	-	4/30/62/62	0/5/5/5
2	NAD	C	4003	-	-	1/30/62/62	0/5/5/5
2	NAD	B	4002	-	-	3/30/62/62	0/5/5/5
2	NAD	E	4005	-	-	1/30/62/62	0/5/5/5
2	NAD	D	4004	-	-	10/30/62/62	0/5/5/5
2	NAD	H	4008	-	-	1/30/62/62	0/5/5/5
2	NAD	G	4007	-	-	7/30/62/62	0/5/5/5
2	NAD	F	4006	-	-	3/30/62/62	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	NAD	O4D-C1D	6.88	1.49	1.40
2	H	4008	NAD	O4D-C1D	6.47	1.49	1.40
2	E	4005	NAD	O4D-C1D	6.34	1.49	1.40
2	A	4001	NAD	C7N-N7N	6.16	1.44	1.33
2	B	4002	NAD	C7N-N7N	6.15	1.44	1.33
2	E	4005	NAD	C7N-N7N	6.10	1.44	1.33
2	H	4008	NAD	C7N-N7N	6.01	1.44	1.33
2	F	4006	NAD	C7N-N7N	6.01	1.44	1.33
2	D	4004	NAD	C7N-N7N	6.01	1.44	1.33
2	C	4003	NAD	O4D-C1D	5.97	1.48	1.40
2	C	4003	NAD	C7N-N7N	5.94	1.43	1.33
2	G	4007	NAD	C7N-N7N	5.91	1.43	1.33
2	F	4006	NAD	O4D-C1D	5.81	1.48	1.40
2	B	4002	NAD	O4D-C1D	5.65	1.48	1.40
2	D	4004	NAD	O4D-C1D	5.58	1.48	1.40
2	G	4007	NAD	O4D-C1D	5.39	1.48	1.40
2	D	4004	NAD	C6A-N6A	3.85	1.44	1.34
2	C	4003	NAD	C6A-N6A	3.77	1.43	1.34
2	B	4002	NAD	C6A-N6A	3.76	1.43	1.34
2	A	4001	NAD	C6A-N6A	3.75	1.43	1.34
2	G	4007	NAD	C6A-N6A	3.75	1.43	1.34
2	H	4008	NAD	C6A-N6A	3.74	1.43	1.34
2	E	4005	NAD	C6A-N6A	3.68	1.43	1.34
2	F	4006	NAD	C6A-N6A	3.67	1.43	1.34
2	D	4004	NAD	O4D-C4D	-3.31	1.37	1.45
2	C	4003	NAD	O4D-C4D	-3.11	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4006	NAD	O4D-C4D	-3.09	1.38	1.45
2	B	4002	NAD	O4D-C4D	-3.07	1.38	1.45
2	G	4007	NAD	O4D-C4D	-3.05	1.38	1.45
2	A	4001	NAD	O4D-C4D	-2.95	1.38	1.45
2	H	4008	NAD	C5A-N7A	-2.84	1.33	1.39
2	E	4005	NAD	O4D-C4D	-2.78	1.38	1.45
2	H	4008	NAD	C2B-C3B	-2.73	1.46	1.53
2	A	4001	NAD	C5A-N7A	-2.70	1.34	1.39
2	H	4008	NAD	O4D-C4D	-2.64	1.39	1.45
2	F	4006	NAD	C5A-N7A	-2.63	1.34	1.39
2	B	4002	NAD	C2B-C3B	-2.62	1.46	1.53
2	C	4003	NAD	C2B-C3B	-2.59	1.46	1.53
2	G	4007	NAD	C5A-N7A	-2.50	1.34	1.39
2	F	4006	NAD	O3D-C3D	-2.50	1.36	1.43
2	F	4006	NAD	C2B-C3B	-2.49	1.46	1.53
2	E	4005	NAD	C2B-C3B	-2.46	1.46	1.53
2	D	4004	NAD	O3D-C3D	-2.45	1.36	1.43
2	H	4008	NAD	O3D-C3D	-2.44	1.36	1.43
2	D	4004	NAD	C2B-C3B	-2.42	1.46	1.53
2	E	4005	NAD	C5A-N7A	-2.41	1.34	1.39
2	D	4004	NAD	C2D-C3D	-2.35	1.47	1.53
2	A	4001	NAD	O3D-C3D	-2.34	1.37	1.43
2	G	4007	NAD	C2B-C3B	-2.32	1.47	1.53
2	C	4003	NAD	C5A-N7A	-2.30	1.34	1.39
2	D	4004	NAD	C5A-N7A	-2.30	1.34	1.39
2	G	4007	NAD	C2D-C3D	-2.28	1.47	1.53
2	B	4002	NAD	C5A-N7A	-2.26	1.35	1.39
2	D	4004	NAD	O2D-C2D	-2.23	1.37	1.43
2	G	4007	NAD	O3D-C3D	-2.21	1.37	1.43
2	B	4002	NAD	O3D-C3D	-2.17	1.37	1.43
2	A	4001	NAD	C2B-C3B	-2.16	1.47	1.53
2	E	4005	NAD	O3D-C3D	-2.11	1.37	1.43
2	C	4003	NAD	O3D-C3D	-2.11	1.37	1.43
2	B	4002	NAD	O2D-C2D	-2.10	1.37	1.43
2	C	4003	NAD	O2D-C2D	-2.04	1.37	1.43
2	A	4001	NAD	O2D-C2D	-2.00	1.38	1.43

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	NAD	O2A-PA-O3	-9.07	82.76	107.27
2	C	4003	NAD	O2A-PA-O3	-8.94	83.11	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4007	NAD	O2A-PA-O3	-8.81	83.46	107.27
2	H	4008	NAD	O2A-PA-O3	-8.64	83.92	107.27
2	D	4004	NAD	O2A-PA-O3	-8.63	83.96	107.27
2	E	4005	NAD	O2A-PA-O3	-8.38	84.62	107.27
2	F	4006	NAD	O2A-PA-O3	-8.28	84.89	107.27
2	B	4002	NAD	O2A-PA-O3	-8.23	85.02	107.27
2	B	4002	NAD	O3-PA-O1A	-8.18	86.11	110.70
2	C	4003	NAD	O3-PA-O1A	-8.08	86.39	110.70
2	G	4007	NAD	O3-PA-O1A	-8.07	86.43	110.70
2	E	4005	NAD	O3-PA-O1A	-8.00	86.64	110.70
2	D	4004	NAD	O3-PA-O1A	-7.73	87.44	110.70
2	H	4008	NAD	O3-PA-O1A	-7.63	87.76	110.70
2	A	4001	NAD	O3-PA-O1A	-6.71	90.51	110.70
2	F	4006	NAD	O3-PA-O1A	-6.30	91.76	110.70
2	C	4003	NAD	C4D-O4D-C1D	-5.91	104.51	109.92
2	A	4001	NAD	N3A-C2A-N1A	-4.68	121.50	128.58
2	F	4006	NAD	C5A-C4A-N3A	-4.56	120.44	126.72
2	E	4005	NAD	C4A-N9A-C8A	4.55	110.51	105.74
2	F	4006	NAD	N3A-C2A-N1A	-4.54	121.72	128.58
2	E	4005	NAD	N3A-C2A-N1A	-4.47	121.82	128.58
2	G	4007	NAD	N9A-C8A-N7A	-4.37	107.74	113.94
2	C	4003	NAD	N3A-C2A-N1A	-4.29	122.08	128.58
2	B	4002	NAD	C4D-O4D-C1D	-4.29	106.00	109.92
2	D	4004	NAD	C5A-C4A-N3A	-4.29	120.81	126.72
2	C	4003	NAD	C5A-C4A-N3A	-4.22	120.90	126.72
2	G	4007	NAD	C5A-C4A-N3A	-4.21	120.92	126.72
2	E	4005	NAD	N9A-C8A-N7A	-4.21	107.97	113.94
2	D	4004	NAD	N3A-C2A-N1A	-4.20	122.23	128.58
2	A	4001	NAD	C5A-C4A-N3A	-4.18	120.96	126.72
2	B	4002	NAD	N9A-C8A-N7A	-4.14	108.07	113.94
2	H	4008	NAD	C5A-C4A-N3A	-4.13	121.03	126.72
2	F	4006	NAD	N3A-C4A-N9A	4.10	134.14	127.17
2	B	4002	NAD	N3A-C2A-N1A	-4.09	122.39	128.58
2	B	4002	NAD	C4A-N9A-C8A	4.08	110.03	105.74
2	G	4007	NAD	C4A-N9A-C8A	4.05	109.99	105.74
2	D	4004	NAD	N9A-C8A-N7A	-3.97	108.30	113.94
2	G	4007	NAD	N3A-C2A-N1A	-3.95	122.61	128.58
2	F	4006	NAD	N9A-C8A-N7A	-3.91	108.39	113.94
2	E	4005	NAD	N3A-C4A-N9A	3.90	133.80	127.17
2	E	4005	NAD	C5A-C4A-N3A	-3.89	121.36	126.72
2	D	4004	NAD	C4A-N9A-C8A	3.88	109.81	105.74
2	C	4003	NAD	N9A-C8A-N7A	-3.86	108.46	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	H	4008	NAD	N9A-C8A-N7A	-3.78	108.58	113.94
2	H	4008	NAD	N3A-C2A-N1A	-3.73	122.93	128.58
2	D	4004	NAD	N3A-C4A-N9A	3.73	133.51	127.17
2	H	4008	NAD	N3A-C4A-N9A	3.68	133.42	127.17
2	H	4008	NAD	C4A-N9A-C8A	3.67	109.59	105.74
2	A	4001	NAD	N3A-C4A-N9A	3.62	133.33	127.17
2	F	4006	NAD	C4A-N9A-C8A	3.61	109.53	105.74
2	C	4003	NAD	C4A-N9A-C8A	3.57	109.49	105.74
2	A	4001	NAD	C4A-N9A-C8A	3.56	109.47	105.74
2	C	4003	NAD	N3A-C4A-N9A	3.55	133.20	127.17
2	G	4007	NAD	C5A-N7A-C8A	3.49	108.94	103.45
2	G	4007	NAD	N3A-C4A-N9A	3.48	133.09	127.17
2	A	4001	NAD	O5D-C5D-C4D	3.48	120.85	108.99
2	B	4002	NAD	C5A-C4A-N3A	-3.46	121.95	126.72
2	H	4008	NAD	C3N-C7N-N7N	3.36	121.87	117.74
2	C	4003	NAD	O4B-C1B-N9A	3.32	114.47	108.09
2	F	4006	NAD	C2A-N3A-C4A	3.29	119.86	111.83
2	D	4004	NAD	C5A-N7A-C8A	3.22	108.52	103.45
2	B	4002	NAD	C5A-N7A-C8A	3.20	108.48	103.45
2	B	4002	NAD	O5B-PA-O1A	3.17	121.50	108.94
2	D	4004	NAD	C2A-N3A-C4A	3.15	119.53	111.83
2	A	4001	NAD	C2A-N3A-C4A	3.15	119.52	111.83
2	C	4003	NAD	C2A-N3A-C4A	3.12	119.46	111.83
2	C	4003	NAD	C5A-N7A-C8A	3.12	108.35	103.45
2	A	4001	NAD	C5A-N7A-C8A	3.09	108.31	103.45
2	G	4007	NAD	O5B-PA-O1A	3.09	121.19	108.94
2	H	4008	NAD	C5A-N7A-C8A	3.09	108.31	103.45
2	B	4002	NAD	N3A-C4A-N9A	3.08	132.40	127.17
2	F	4006	NAD	C5A-N7A-C8A	3.01	108.18	103.45
2	A	4001	NAD	O2A-PA-O5B	3.01	121.19	107.57
2	E	4005	NAD	C2A-N3A-C4A	3.00	119.17	111.83
2	G	4007	NAD	C2A-N3A-C4A	3.00	119.16	111.83
2	F	4006	NAD	O5B-PA-O1A	3.00	120.81	108.94
2	G	4007	NAD	C4D-O4D-C1D	-2.98	107.20	109.92
2	E	4005	NAD	C5A-N7A-C8A	2.95	108.09	103.45
2	C	4003	NAD	O5B-PA-O1A	2.95	120.61	108.94
2	D	4004	NAD	O4B-C1B-N9A	2.90	113.67	108.09
2	H	4008	NAD	O5B-PA-O1A	2.90	120.43	108.94
2	E	4005	NAD	O5B-C5B-C4B	2.88	118.79	108.99
2	E	4005	NAD	O5B-PA-O1A	2.87	120.30	108.94
2	G	4007	NAD	C4A-C5A-N7A	-2.86	107.31	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	NAD	O5B-C5B-C4B	2.83	118.62	108.99
2	H	4008	NAD	C2D-C3D-C4D	2.82	108.05	102.61
2	D	4004	NAD	O5B-PA-O1A	2.80	120.03	108.94
2	B	4002	NAD	O5B-C5B-C4B	2.78	118.45	108.99
2	G	4007	NAD	O7N-C7N-N7N	-2.74	118.66	122.62
2	H	4008	NAD	C2A-N3A-C4A	2.71	118.46	111.83
2	H	4008	NAD	O7N-C7N-N7N	-2.71	118.70	122.62
2	F	4006	NAD	O2A-PA-O5B	2.66	119.63	107.57
2	B	4002	NAD	C2A-N3A-C4A	2.66	118.32	111.83
2	G	4007	NAD	C3N-C7N-N7N	2.60	120.94	117.74
2	E	4005	NAD	O2A-PA-O5B	2.54	119.09	107.57
2	F	4006	NAD	C2D-C3D-C4D	2.54	107.52	102.61
2	D	4004	NAD	C4A-C5A-N7A	-2.53	107.69	110.58
2	B	4002	NAD	C3N-C7N-N7N	2.52	120.84	117.74
2	D	4004	NAD	O7N-C7N-N7N	-2.51	118.99	122.62
2	H	4008	NAD	O2A-PA-O5B	2.48	118.80	107.57
2	F	4006	NAD	C4D-O4D-C1D	-2.47	107.66	109.92
2	B	4002	NAD	C4A-C5A-N7A	-2.46	107.77	110.58
2	D	4004	NAD	O2A-PA-O5B	2.46	118.72	107.57
2	C	4003	NAD	C4A-C5A-N7A	-2.44	107.79	110.58
2	E	4005	NAD	O5D-C5D-C4D	2.44	117.29	108.99
2	F	4006	NAD	O5D-C5D-C4D	2.43	117.28	108.99
2	B	4002	NAD	O4B-C1B-N9A	2.40	112.70	108.09
2	A	4001	NAD	C3N-C7N-N7N	2.39	120.69	117.74
2	G	4007	NAD	O5D-C5D-C4D	2.38	117.11	108.99
2	A	4001	NAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	D	4004	NAD	O5B-C5B-C4B	2.34	116.95	108.99
2	H	4008	NAD	O5B-C5B-C4B	2.31	116.87	108.99
2	F	4006	NAD	O5B-C5B-C4B	2.30	116.82	108.99
2	D	4004	NAD	C2D-C3D-C4D	2.30	107.05	102.61
2	H	4008	NAD	C4A-C5A-N7A	-2.29	107.96	110.58
2	C	4003	NAD	O5D-C5D-C4D	2.28	116.77	108.99
2	E	4005	NAD	C4D-O4D-C1D	-2.26	107.86	109.92
2	A	4001	NAD	O5B-PA-O1A	2.22	117.75	108.94
2	C	4003	NAD	O2A-PA-O5B	2.20	117.55	107.57
2	B	4002	NAD	O2A-PA-O5B	2.17	117.40	107.57
2	E	4005	NAD	C3N-C7N-N7N	2.17	120.41	117.74
2	E	4005	NAD	O7N-C7N-N7N	-2.12	119.55	122.62
2	G	4007	NAD	O2A-PA-O5B	2.11	117.14	107.57
2	E	4005	NAD	C2D-C3D-C4D	2.10	106.66	102.61
2	E	4005	NAD	C5A-C6A-N6A	-2.09	118.12	123.29
2	A	4001	NAD	C5D-C4D-C3D	-2.08	107.72	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4002	NAD	C2D-C3D-C4D	2.07	106.61	102.61
2	C	4003	NAD	O5B-C5B-C4B	2.06	116.02	108.99
2	F	4006	NAD	C5A-C6A-N6A	-2.03	118.27	123.29

There are no chirality outliers.

All (30) torsion outliers are listed below:

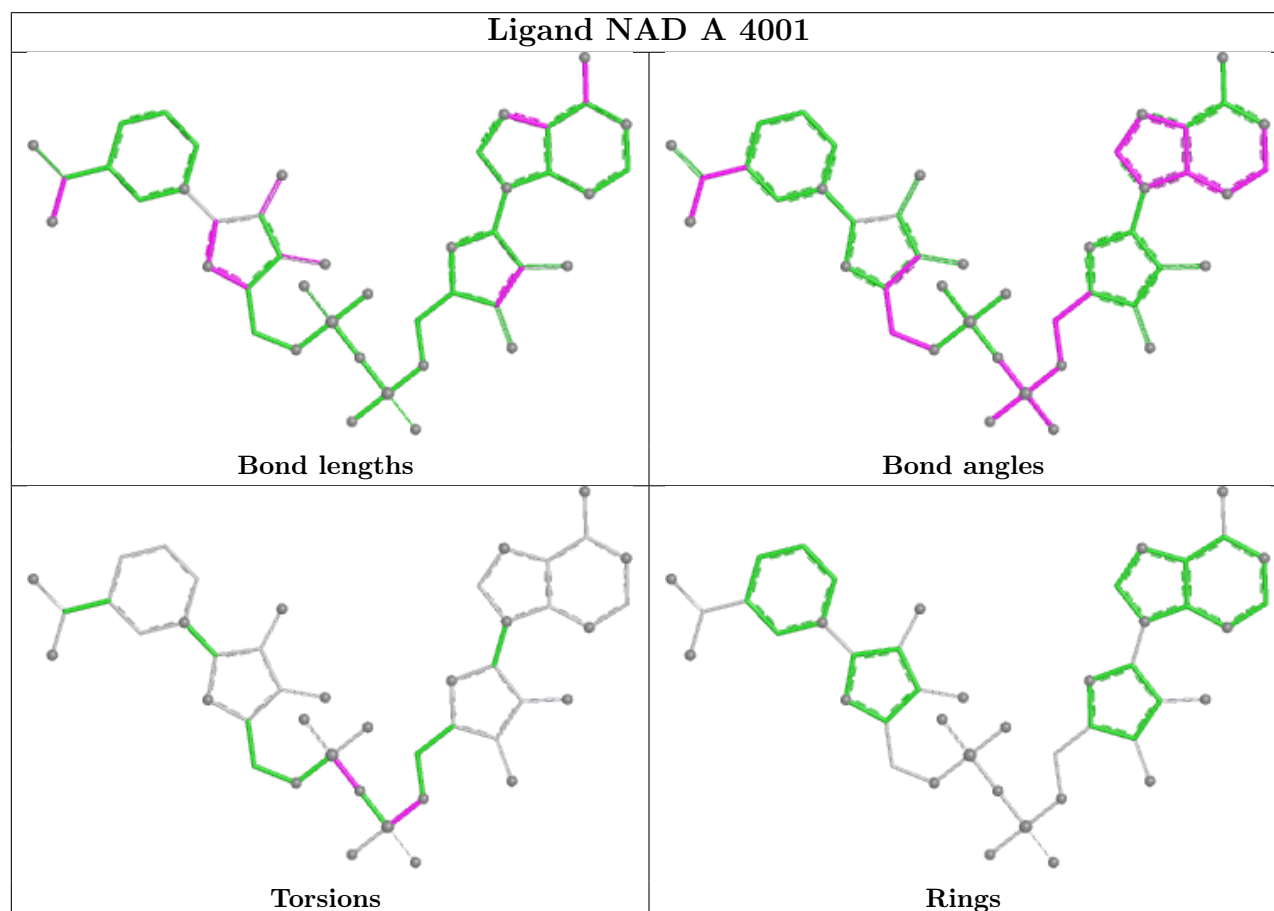
Mol	Chain	Res	Type	Atoms
2	A	4001	NAD	C5B-O5B-PA-O1A
2	B	4002	NAD	C5B-O5B-PA-O1A
2	C	4003	NAD	C5B-O5B-PA-O1A
2	D	4004	NAD	C5B-O5B-PA-O1A
2	D	4004	NAD	C5D-O5D-PN-O3
2	D	4004	NAD	C5D-O5D-PN-O1N
2	D	4004	NAD	C5D-O5D-PN-O2N
2	D	4004	NAD	O4D-C1D-N1N-C6N
2	E	4005	NAD	C5B-O5B-PA-O1A
2	F	4006	NAD	C5B-O5B-PA-O1A
2	G	4007	NAD	C5B-O5B-PA-O3
2	H	4008	NAD	C5B-O5B-PA-O1A
2	G	4007	NAD	C3D-C4D-C5D-O5D
2	D	4004	NAD	O4D-C4D-C5D-O5D
2	D	4004	NAD	C3D-C4D-C5D-O5D
2	G	4007	NAD	O4D-C4D-C5D-O5D
2	G	4007	NAD	C3B-C4B-C5B-O5B
2	G	4007	NAD	O4B-C4B-C5B-O5B
2	F	4006	NAD	O4B-C4B-C5B-O5B
2	F	4006	NAD	C3B-C4B-C5B-O5B
2	D	4004	NAD	O4B-C4B-C5B-O5B
2	B	4002	NAD	O4B-C4B-C5B-O5B
2	A	4001	NAD	C5B-O5B-PA-O2A
2	B	4002	NAD	C5B-O5B-PA-O3
2	G	4007	NAD	C5D-O5D-PN-O1N
2	A	4001	NAD	PA-O3-PN-O2N
2	D	4004	NAD	C3B-C4B-C5B-O5B
2	D	4004	NAD	O4D-C1D-N1N-C2N
2	A	4001	NAD	PA-O3-PN-O1N
2	G	4007	NAD	PN-O3-PA-O2A

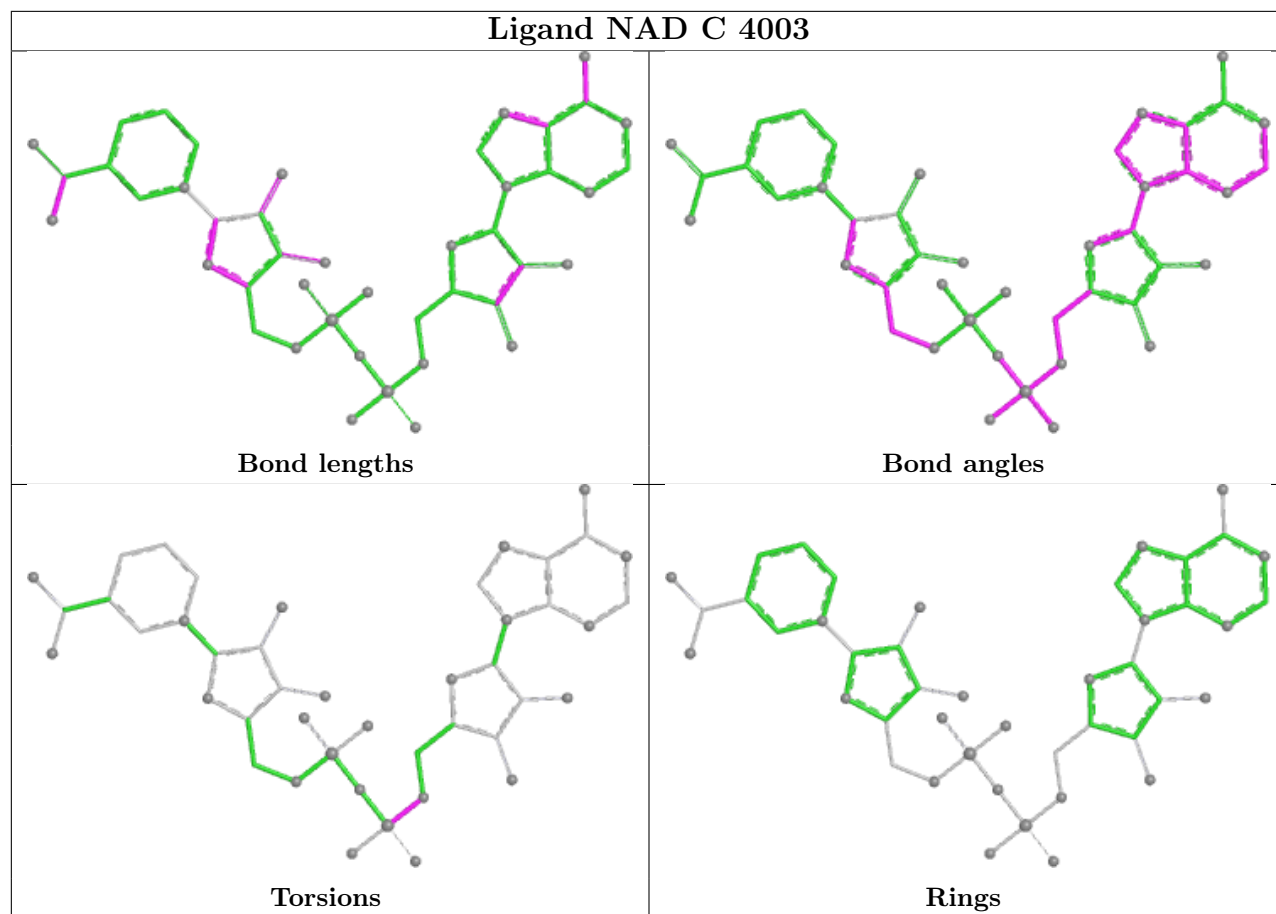
There are no ring outliers.

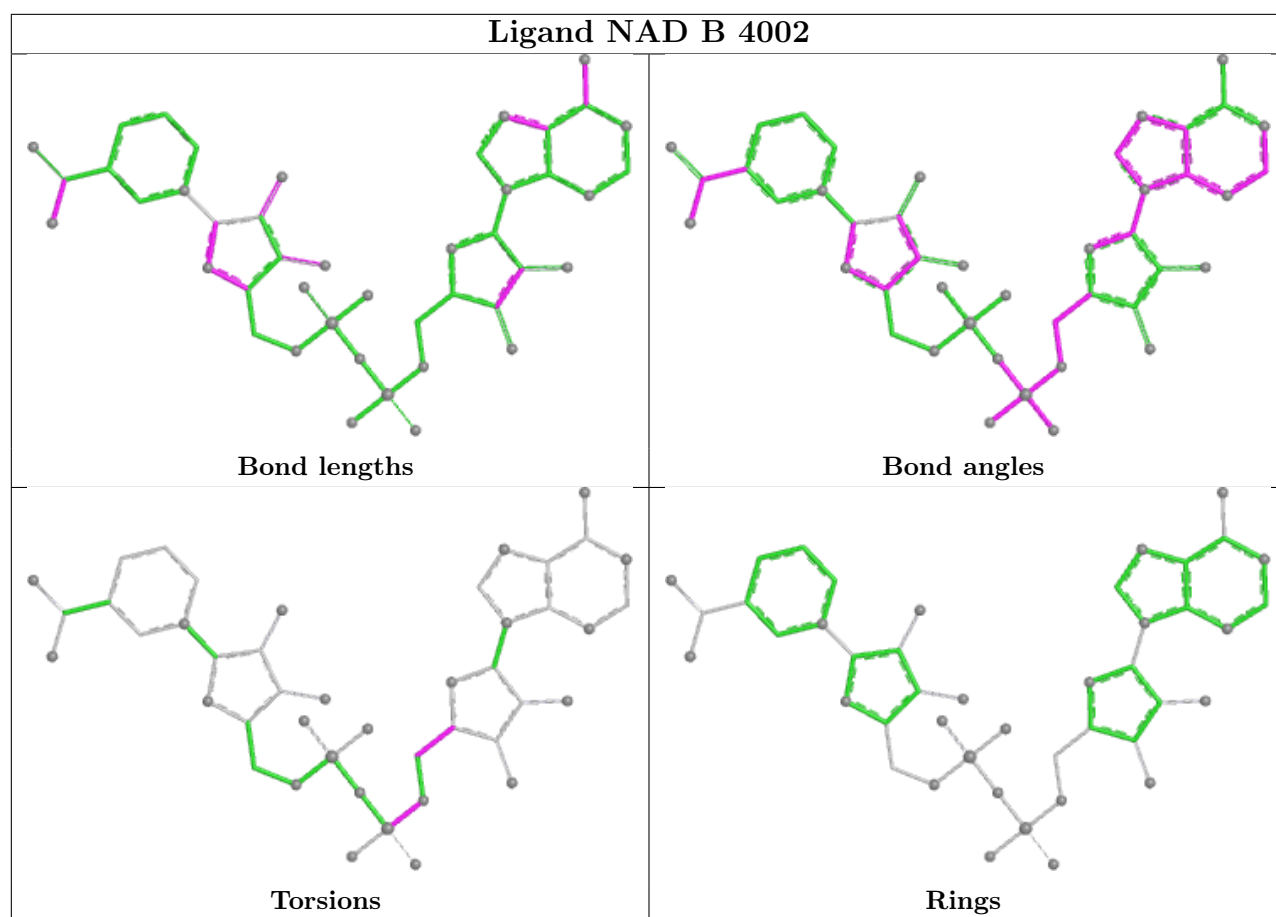
7 monomers are involved in 15 short contacts:

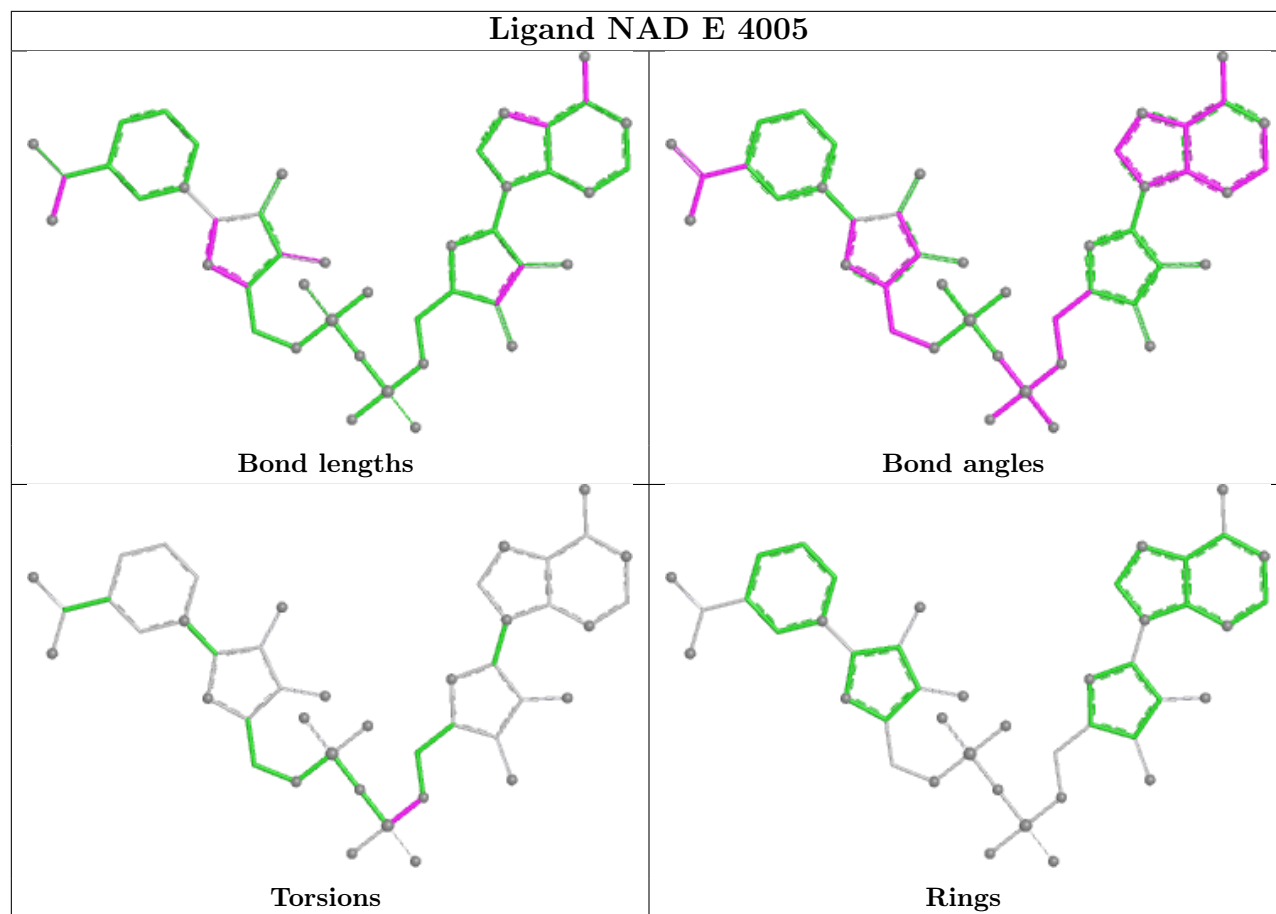
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	NAD	1	0
2	C	4003	NAD	3	0
2	B	4002	NAD	4	0
2	E	4005	NAD	2	0
2	H	4008	NAD	1	0
2	G	4007	NAD	3	0
2	F	4006	NAD	1	0

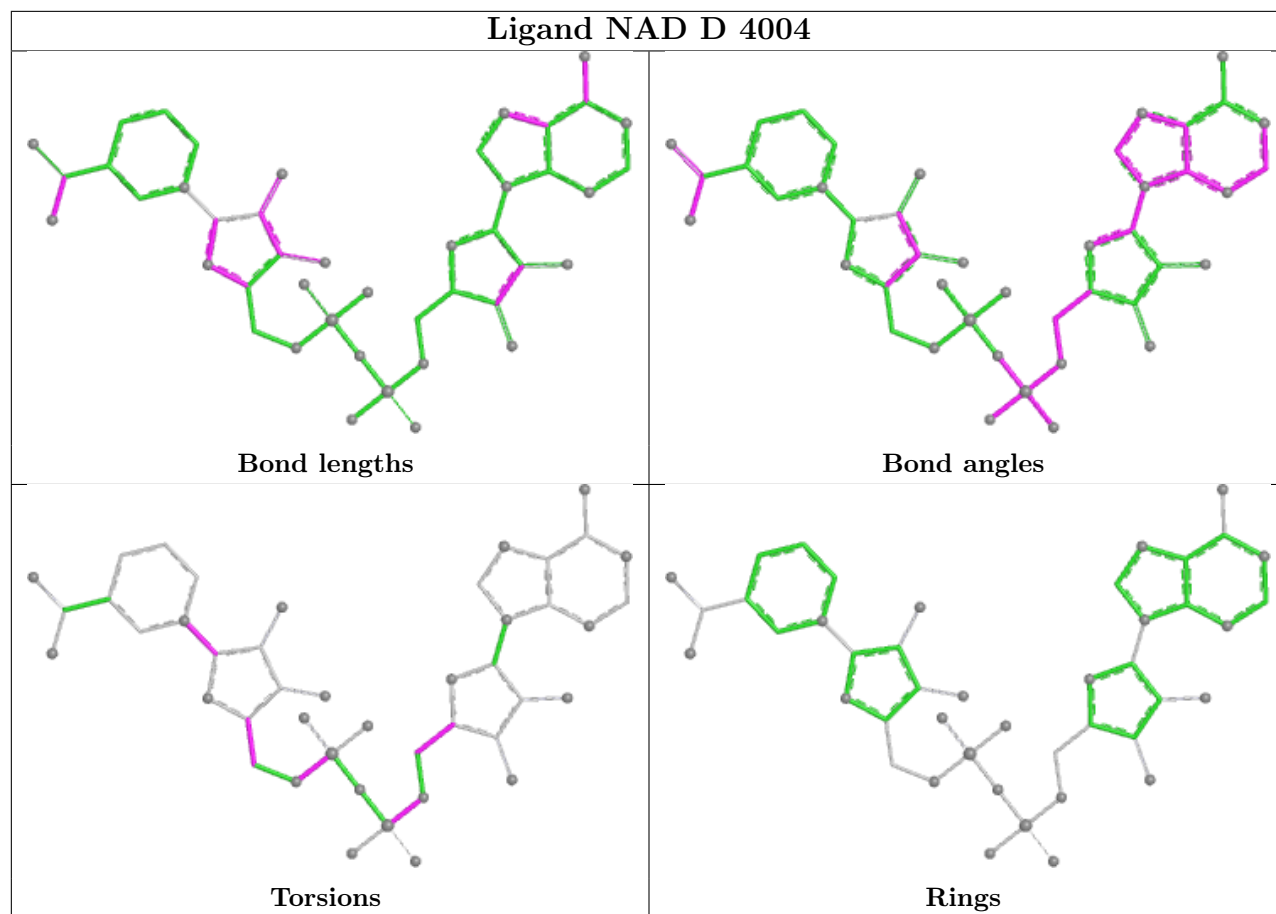
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

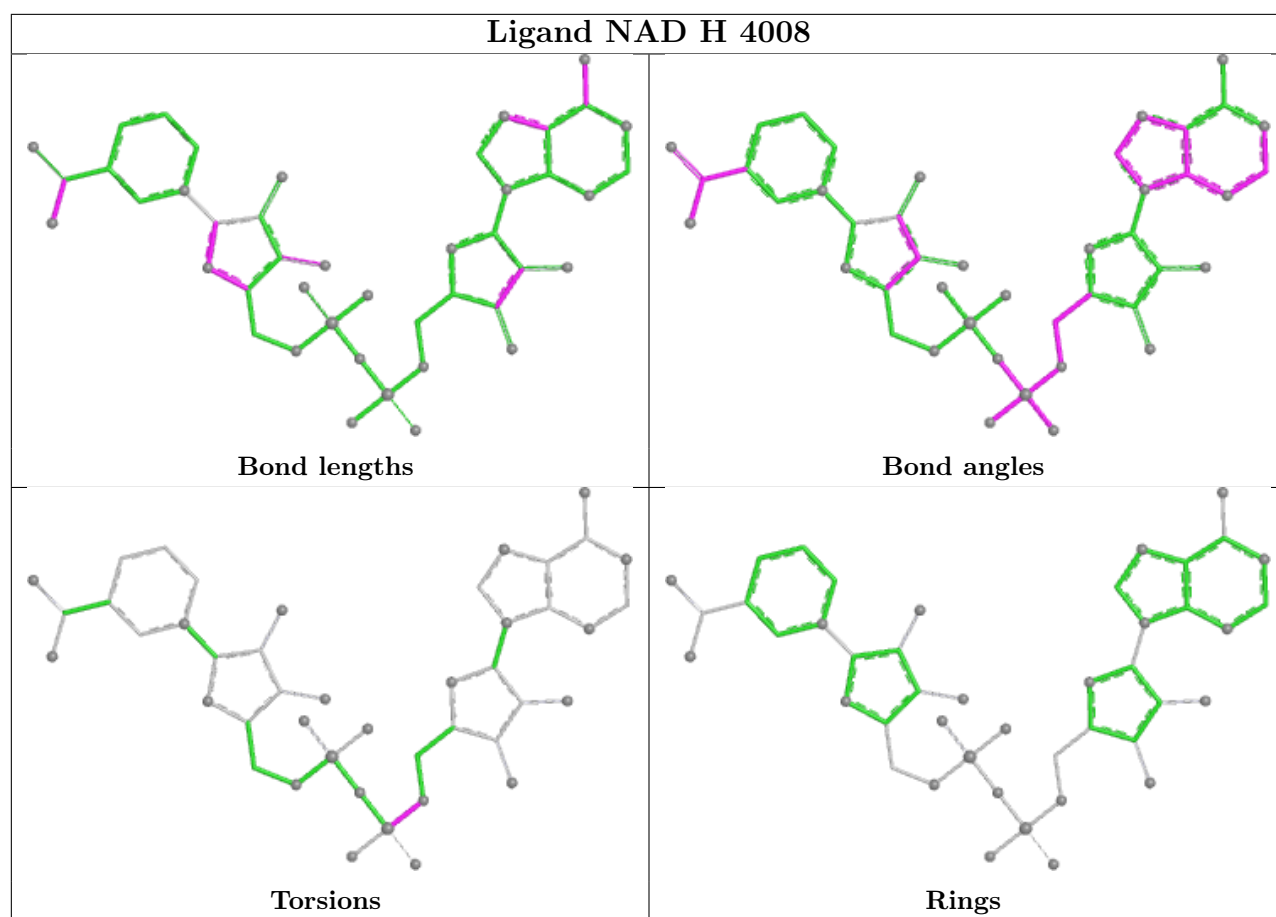


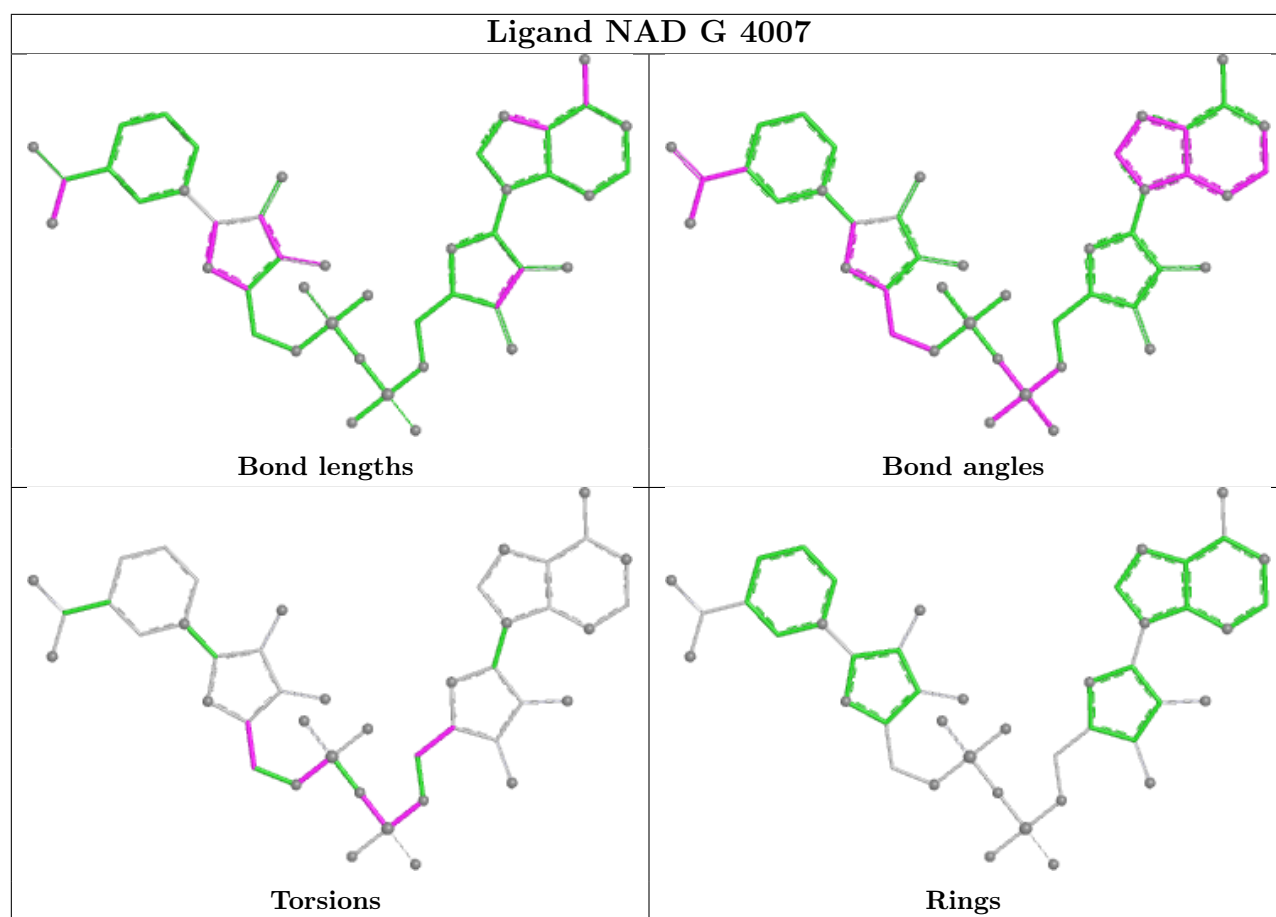


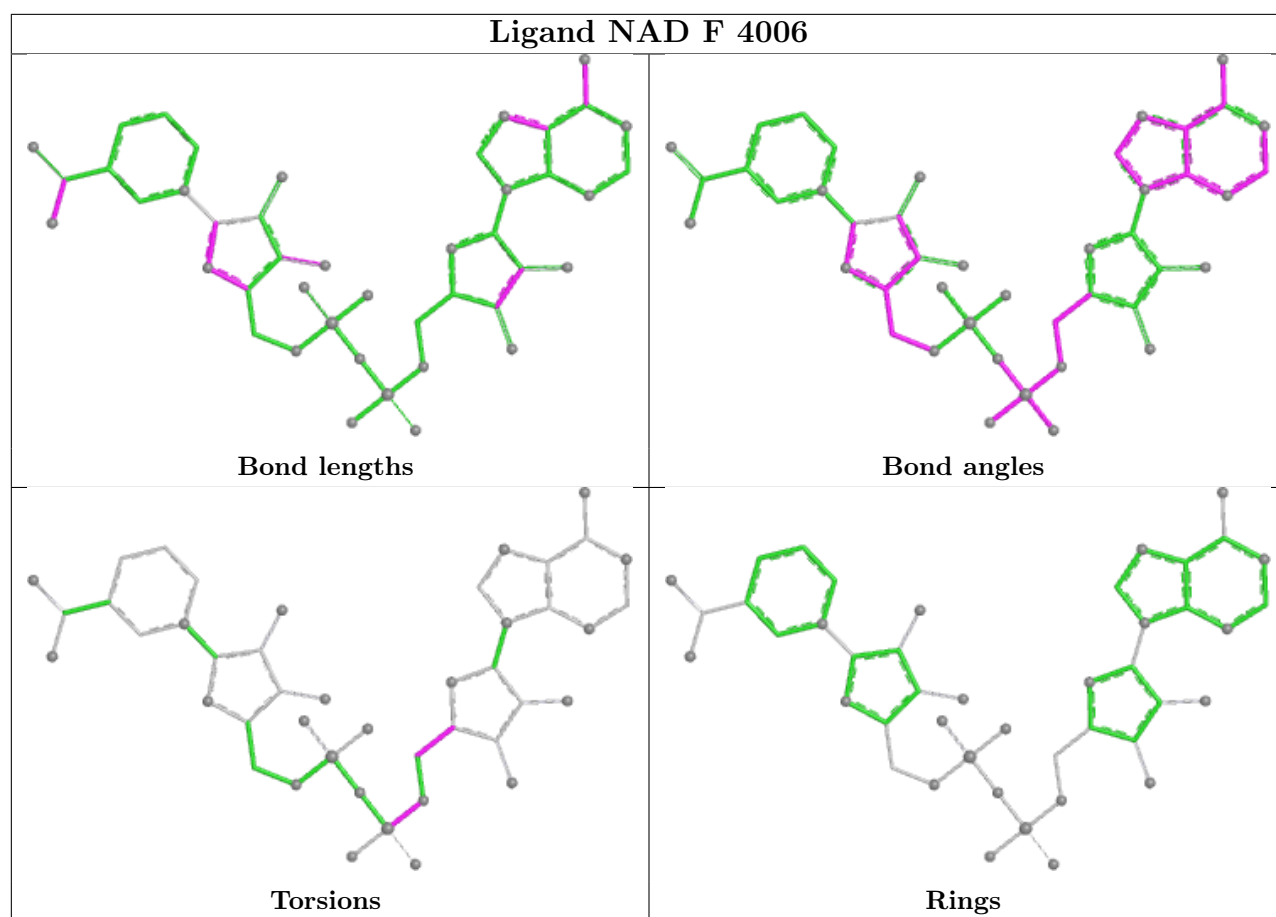












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	335/344 (97%)	-0.70	1 (0%) 90 87	15, 30, 85, 112	2 (0%)
1	B	335/344 (97%)	-0.80	0 100 100	12, 31, 57, 86	1 (0%)
1	C	335/344 (97%)	-0.69	1 (0%) 90 87	15, 33, 86, 125	1 (0%)
1	D	335/344 (97%)	-0.79	1 (0%) 90 87	14, 31, 63, 89	2 (0%)
1	E	335/344 (97%)	-0.71	0 100 100	14, 35, 63, 87	0
1	F	335/344 (97%)	-0.63	1 (0%) 90 87	16, 36, 81, 121	0
1	G	335/344 (97%)	-0.73	0 100 100	16, 33, 63, 91	1 (0%)
1	H	335/344 (97%)	-0.68	0 100 100	16, 37, 67, 98	0
All	All	2680/2752 (97%)	-0.72	4 (0%) 92 90	12, 33, 71, 125	7 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	ILE	2.6
1	A	192	ILE	2.4
1	D	203	ASP	2.1
1	F	344	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

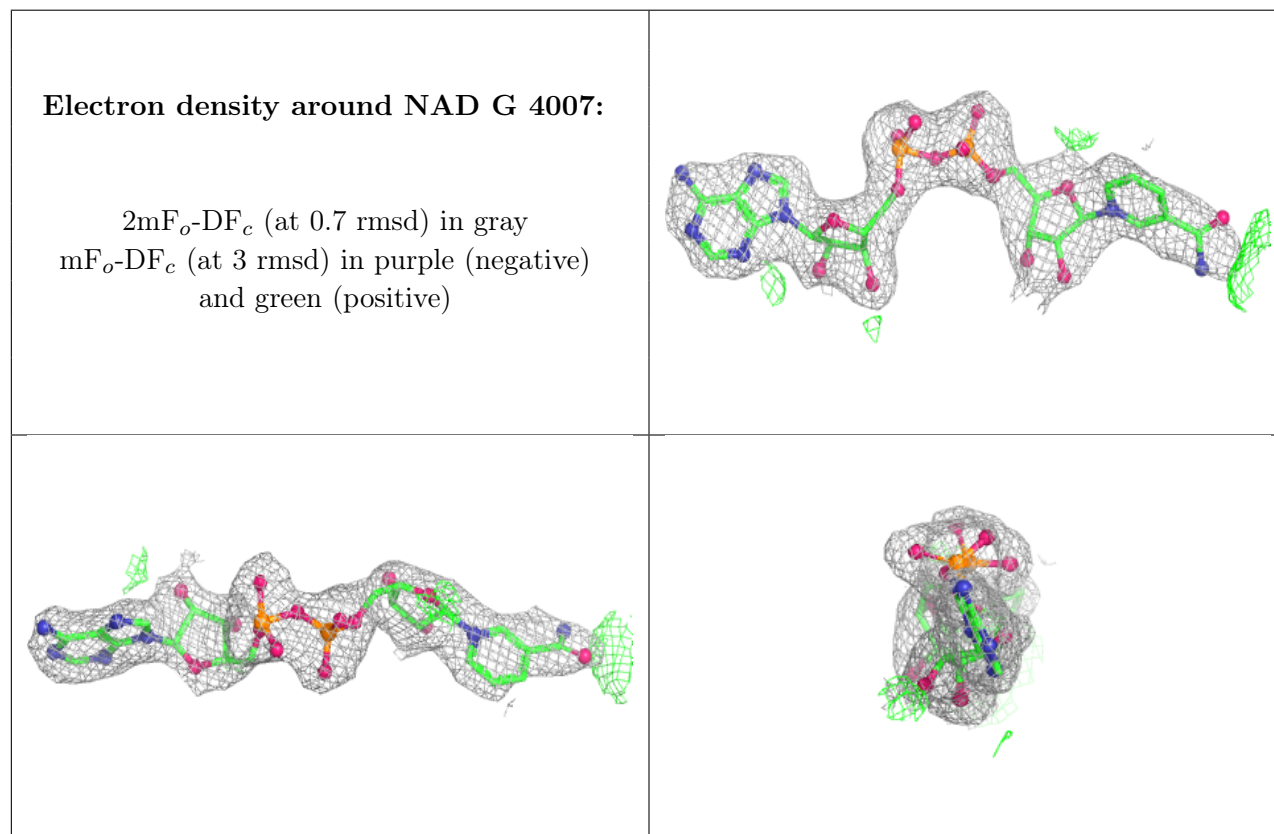
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

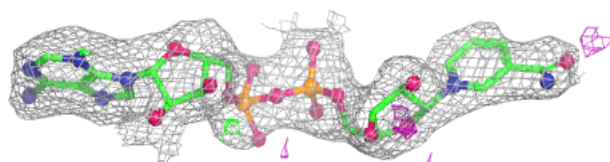
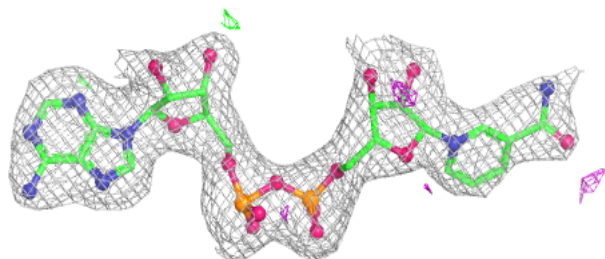
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	G	4007	44/44	0.94	0.08	48,56,71,275	0
2	NAD	E	4005	44/44	0.95	0.08	34,50,54,275	0
2	NAD	B	4002	44/44	0.96	0.08	36,47,59,256	0
2	NAD	F	4006	44/44	0.96	0.07	32,49,69,79	0
2	NAD	C	4003	44/44	0.96	0.07	35,51,59,87	0
2	NAD	H	4008	44/44	0.96	0.08	36,50,63,276	0
2	NAD	A	4001	44/44	0.97	0.07	23,39,52,189	0
2	NAD	D	4004	44/44	0.97	0.06	33,44,56,179	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.

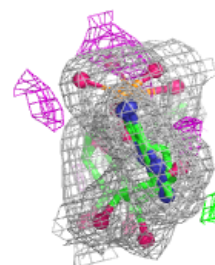
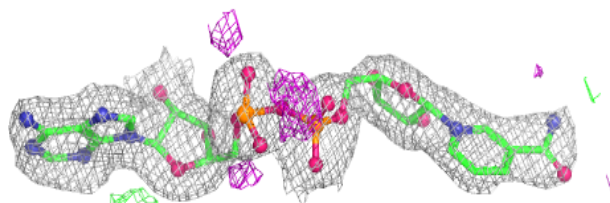
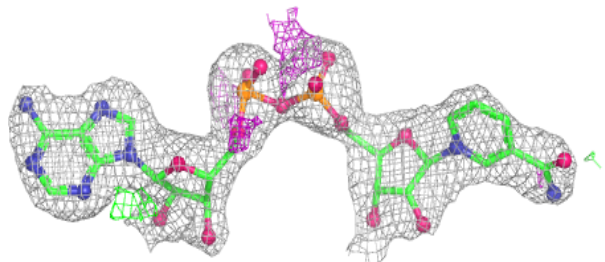


Electron density around NAD E 4005:

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

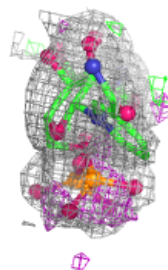
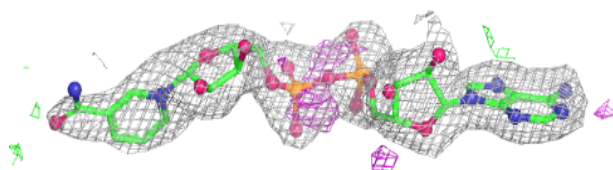
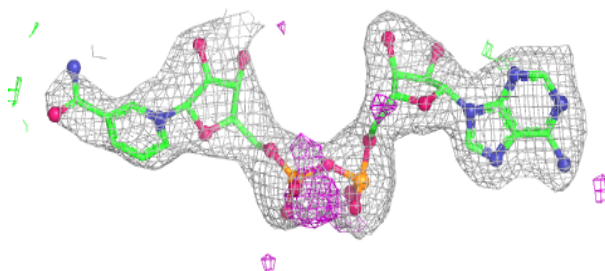
**Electron density around NAD B 4002:**

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

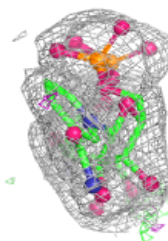
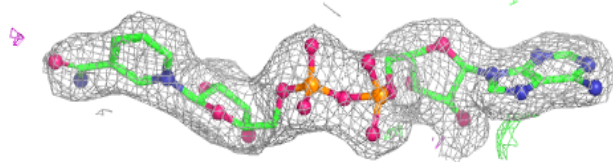
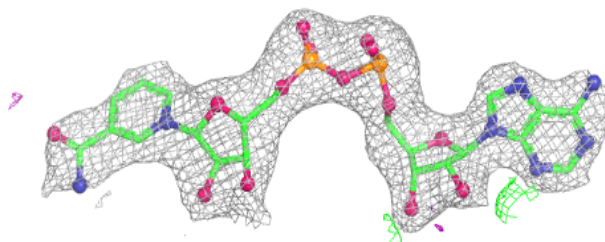


Electron density around NAD F 4006:

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

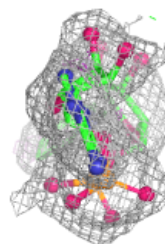
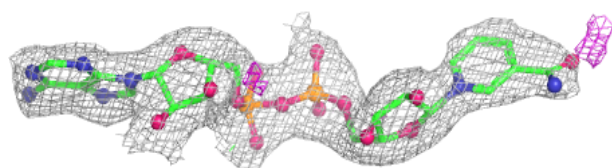
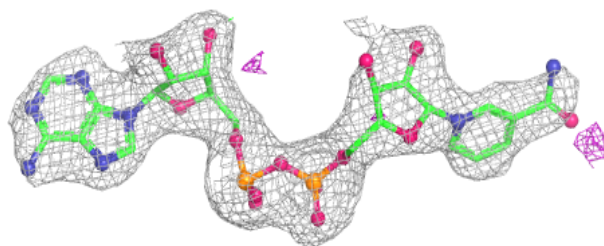
**Electron density around NAD C 4003:**

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

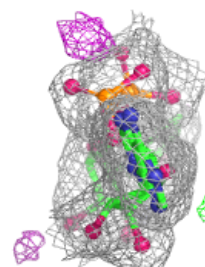
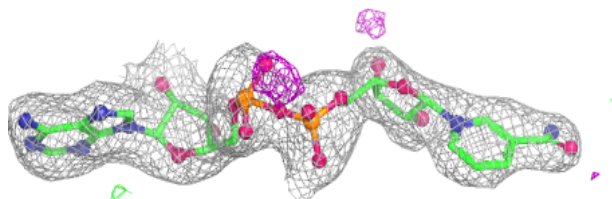
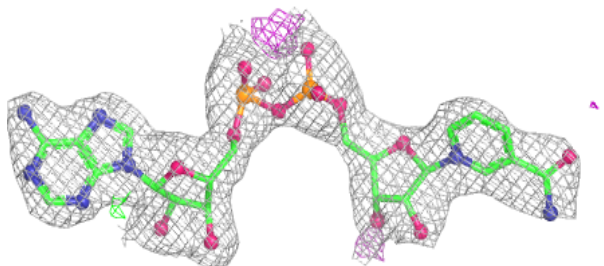


Electron density around NAD H 4008:

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

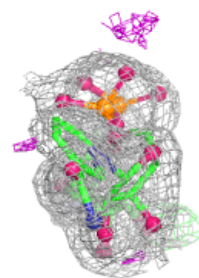
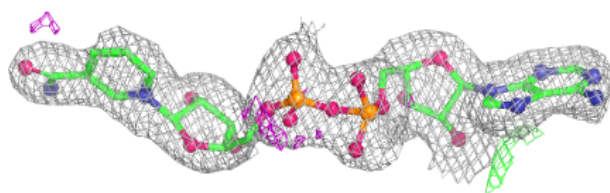
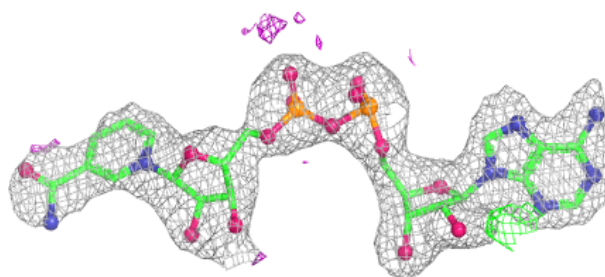
**Electron density around NAD A 4001:**

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



Electron density around NAD D 4004:

$2mF_o-DF_c$ (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.