



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:47 AM UTC

PDB ID : 1P44 / pdb_00001p44
Title : Targeting tuberculosis and malaria through inhibition of enoyl reductase: compound activity and structural data
Authors : Kuo, M.R.; Morbidoni, H.R.; Alland, D.; Sneddon, S.F.; Gourlie, B.B.; Staveski, M.M.; Leonard, M.; Gregory, J.S.; Janjigian, A.D.; Yee, C.; Musser, J.M.; Kreiswirth, B.; Iwamoto, H.; Perozzo, R.; Jacobs Jr, W.R.; Sacchettini, J.C.; Fidock, D.A.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-04-21
Resolution : 2.70 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)

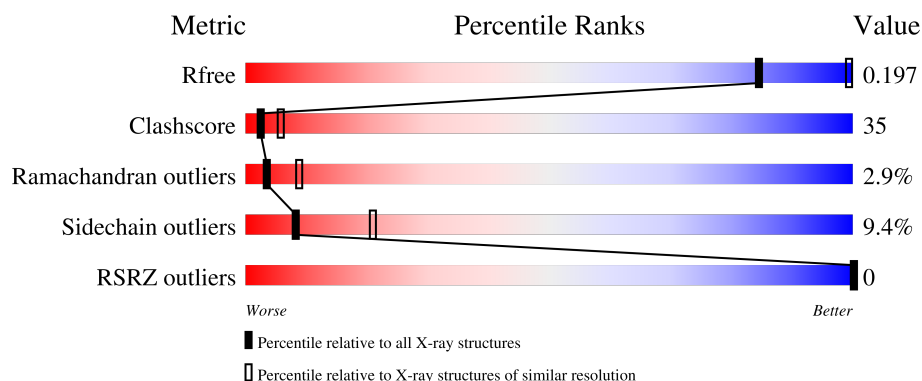
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

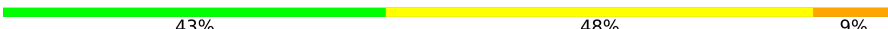
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	269	
1	B	269	
1	C	269	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	269	 38% 52% 10%
1	E	269	 43% 49% 7%
1	F	269	 42% 49% 8%

2 Entry composition [i](#)

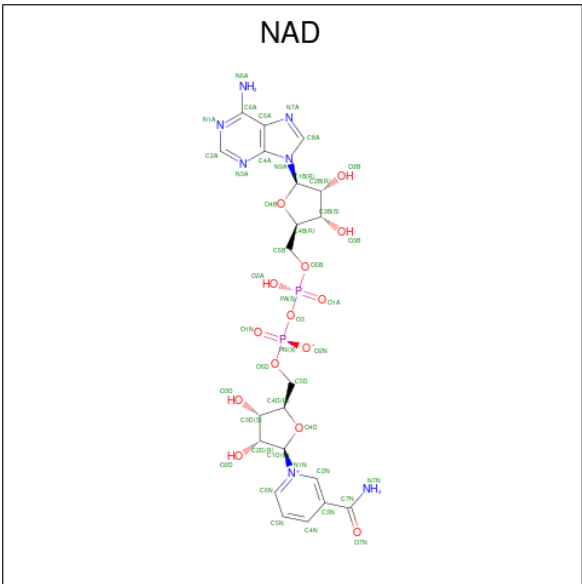
There are 4 unique types of molecules in this entry. The entry contains 12495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-[acyl-carrier-protein] reductase [NADH].

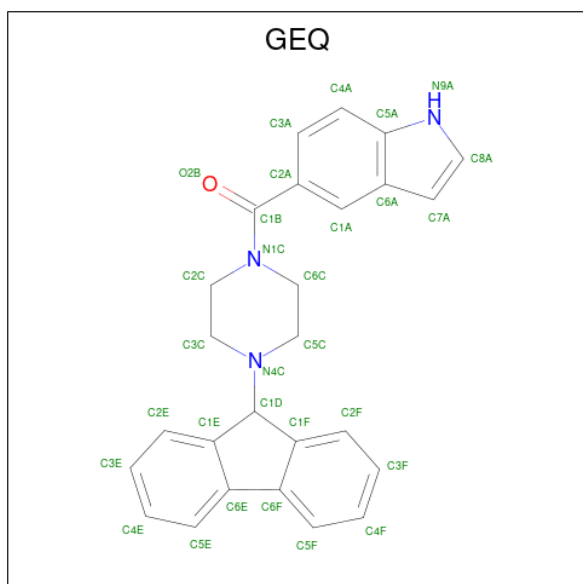
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	B	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	C	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	D	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	E	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	F	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			

- 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		

- Molecule 3 is 5- $\{[4-(9H\text{-FLUOREN-9-YL})\text{PIPERAZIN-1-YL}]\text{CARBONYL}\}$ -1H-INDOLE (CCD ID: GEQ) (formula: $\text{C}_{26}\text{H}_{23}\text{N}_3\text{O}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	26	3	1		
3	B	1	Total	C	N	O	0	0
			30	26	3	1		
3	C	1	Total	C	N	O	0	0
			30	26	3	1		
3	D	1	Total	C	N	O	0	0
			30	26	3	1		

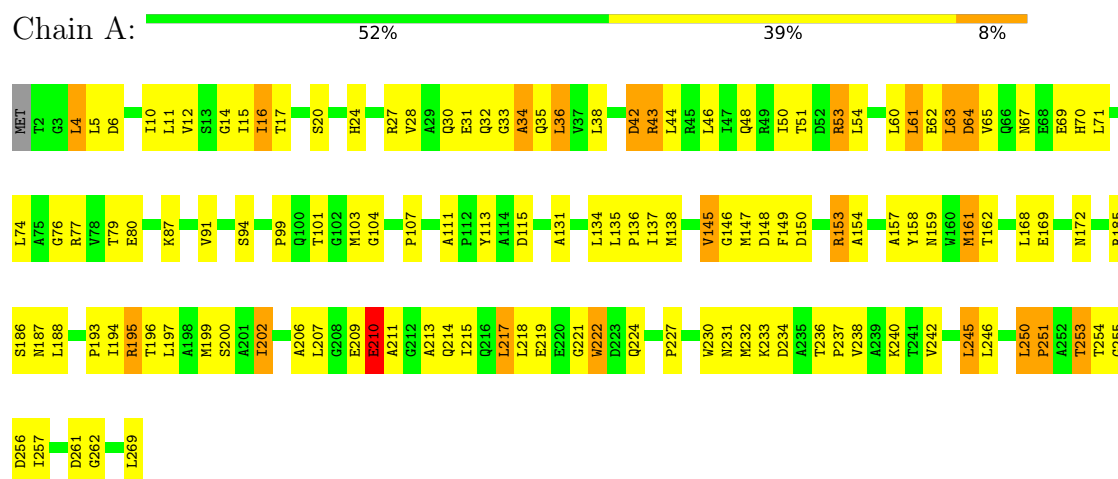
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	36	Total 36	O 36	0	0
4	C	27	Total 27	O 27	0	0
4	D	14	Total 14	O 14	0	0
4	E	21	Total 21	O 21	0	0
4	F	19	Total 19	O 19	0	0

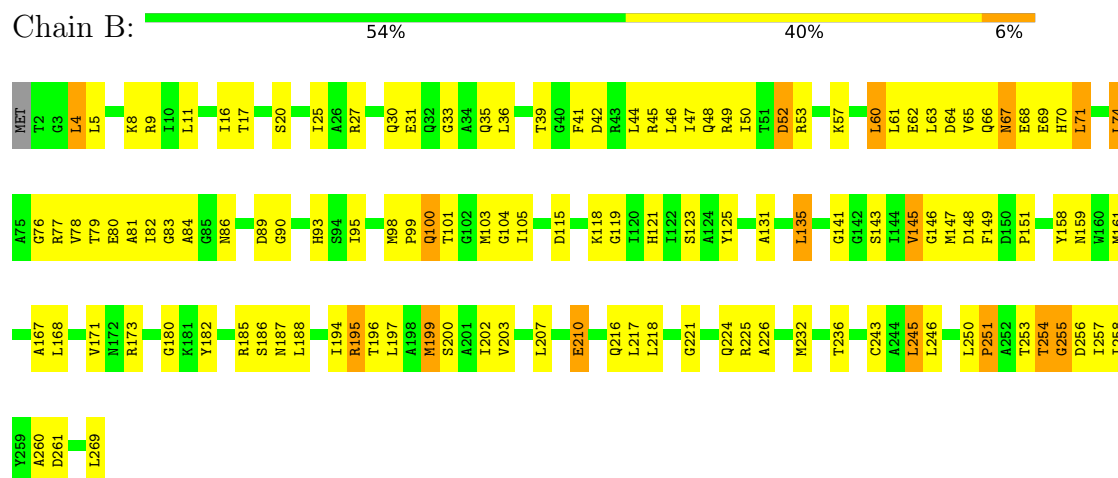
3 Residue-property plots

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: Enoyl-[acyl-carrier-protein] reductase [NADH]

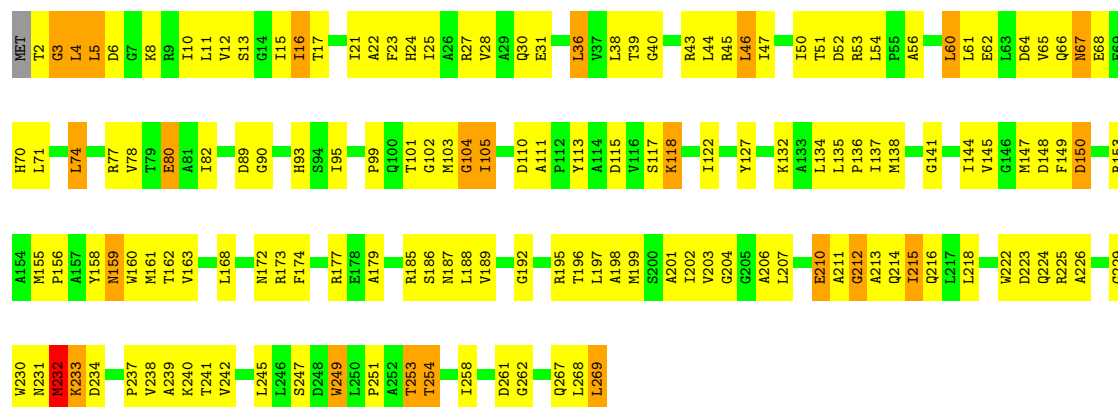


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



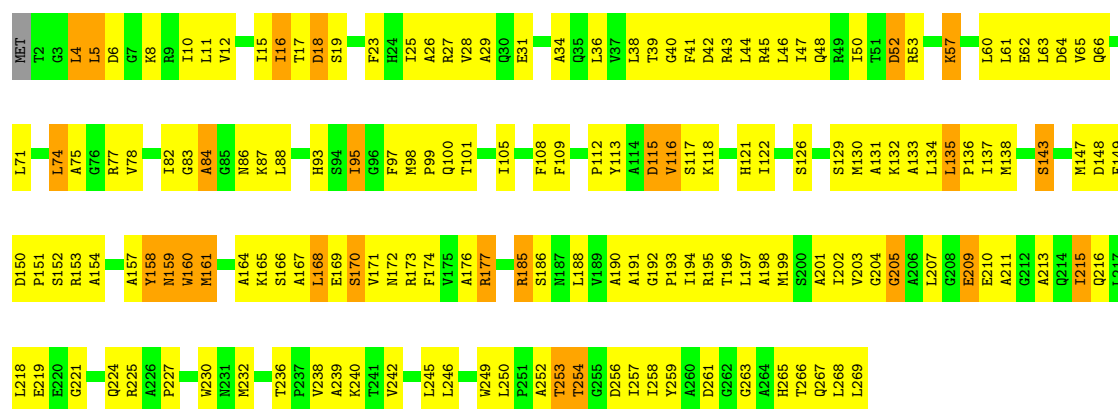
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





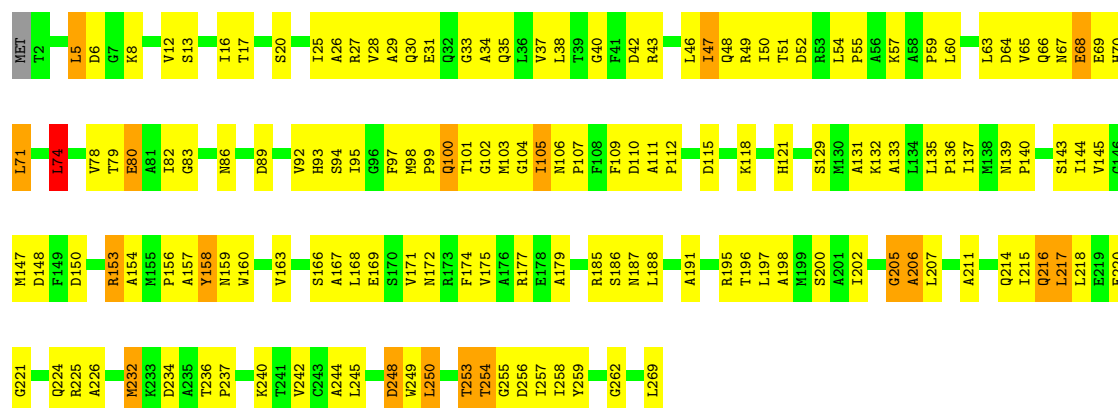
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D: 38% 52% 10%



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E: 43% 49% 7%



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain F: 42% 49% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.62Å 83.22Å 192.97Å 90.00° 94.95° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 67.9 (30.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.288 0.208 , 0.197	Depositor DCC
R_{free} test set	2205 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12495	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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, GEQ

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	0.55	0/2032	1.04	7/2758 (0.3%)
1	B	0.57	0/2032	1.04	9/2758 (0.3%)
1	C	0.46	0/2032	1.04	11/2758 (0.4%)
1	D	0.44	0/2032	1.03	12/2758 (0.4%)
1	E	0.46	0/2032	1.02	7/2758 (0.3%)
1	F	0.48	0/2032	1.05	10/2758 (0.4%)
All	All	0.50	0/12192	1.03	56/16548 (0.3%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LEU	N-CA-C	8.11	122.47	110.46
1	C	141	GLY	N-CA-C	-8.03	104.78	115.21
1	F	166	SER	N-CA-C	-7.79	102.73	111.07
1	C	52	ASP	N-CA-C	-7.15	104.64	113.15
1	A	53	ARG	N-CA-C	-7.00	105.93	114.75
1	B	36	LEU	N-CA-C	6.93	120.89	110.14
1	D	263	GLY	N-CA-C	-6.74	105.93	115.30
1	F	36	LEU	N-CA-C	6.62	119.07	110.53
1	C	192	GLY	N-CA-C	-6.62	103.96	112.10
1	C	36	LEU	N-CA-C	6.60	119.81	110.50
1	E	37	VAL	N-CA-C	-6.46	98.74	108.17
1	C	249	TRP	N-CA-C	6.42	121.12	113.16
1	F	141	GLY	N-CA-C	-6.40	106.25	115.27
1	B	226	ALA	CA-C-N	6.38	126.29	119.28
1	B	226	ALA	C-N-CA	6.38	126.29	119.28
1	D	160	TRP	N-CA-C	6.35	120.12	112.38
1	A	42	ASP	N-CA-C	6.15	118.52	111.02
1	B	260	ALA	N-CA-C	-6.14	100.39	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	MET	N-CA-C	-6.05	104.97	112.90
1	C	223	ASP	N-CA-C	-6.02	106.06	113.41
1	D	52	ASP	N-CA-C	-5.99	105.97	113.28
1	F	10	ILE	N-CA-C	5.98	116.49	108.11
1	B	105	ILE	N-CA-C	5.93	120.74	112.50
1	E	166	SER	N-CA-C	-5.90	104.85	111.28
1	D	161	MET	N-CA-C	-5.88	104.95	111.36
1	F	218	LEU	N-CA-C	-5.87	104.83	112.23
1	A	34	ALA	N-CA-C	-5.84	100.37	109.72
1	A	63	LEU	N-CA-C	5.84	117.13	107.20
1	D	215	ILE	N-CA-C	-5.78	107.35	112.90
1	A	161	MET	N-CA-C	-5.72	105.56	112.54
1	D	18	ASP	N-CA-C	-5.69	106.31	113.20
1	C	161	MET	N-CA-C	-5.56	106.45	113.18
1	E	256	ASP	N-CA-C	5.56	117.69	109.69
1	B	33	GLY	N-CA-C	5.55	123.69	114.48
1	C	110	ASP	N-CA-C	5.51	118.79	112.57
1	B	161	MET	N-CA-C	-5.49	105.46	111.82
1	B	141	GLY	N-CA-C	-5.42	108.17	115.21
1	C	5	LEU	N-CA-C	5.41	119.86	112.88
1	D	95	ILE	N-CA-C	5.40	115.87	107.28
1	E	200	SER	N-CA-C	-5.25	106.13	112.54
1	D	170	SER	N-CA-C	-5.24	105.26	110.97
1	B	25	ILE	N-CA-C	-5.24	105.43	110.72
1	F	134	LEU	N-CA-C	5.23	119.75	112.90
1	C	118	LYS	N-CA-C	-5.22	105.77	111.82
1	F	250	LEU	CA-C-N	5.21	124.87	119.56
1	F	250	LEU	C-N-CA	5.21	124.87	119.56
1	E	205	GLY	N-CA-C	5.20	116.81	111.56
1	A	64	ASP	N-CA-C	-5.17	100.31	108.73
1	F	200	SER	N-CA-C	-5.16	106.98	113.28
1	D	213	ALA	N-CA-C	-5.16	107.50	112.97
1	E	143	SER	N-CA-C	5.15	117.80	108.69
1	D	77	ARG	N-CA-C	-5.12	105.61	111.14
1	C	160	TRP	N-CA-C	5.12	118.62	112.38
1	E	35	GLN	N-CA-C	-5.11	101.37	109.96
1	D	143	SER	N-CA-C	5.02	116.22	107.93
1	D	116	VAL	N-CA-C	-5.02	105.53	111.00

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	1994	0	2008	121	1
1	B	1994	0	2008	115	0
1	C	1994	0	2008	159	0
1	D	1994	0	2008	183	0
1	E	1994	0	2008	152	0
1	F	1994	0	2008	168	0
2	A	44	0	26	8	0
2	B	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	4	0
2	E	44	0	26	4	0
2	F	44	0	26	1	0
3	A	30	0	23	2	0
3	B	30	0	23	5	0
3	C	30	0	23	2	0
3	D	30	0	23	1	0
4	A	30	0	0	2	0
4	B	36	0	0	4	0
4	C	27	0	0	4	0
4	D	14	0	0	2	0
4	E	21	0	0	2	0
4	F	19	0	0	1	0
All	All	12495	0	12296	856	1

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 35.

All (856) 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:B:195:ARG:HH11	1:B:195:ARG:HB2	1.19	1.05
1:F:16:ILE:HG23	1:F:17:THR:HG23	1.33	1.05
1:D:186:SER:H	1:D:254:THR:HG23	1.20	1.03
1:C:245:LEU:HD21	1:C:258:ILE:HD12	1.41	1.00
1:B:186:SER:H	1:B:254:THR:HG22	1.26	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HG23	1:A:17:THR:HG23	1.43	0.98
1:E:16:ILE:HG23	1:E:17:THR:HG23	1.42	0.97
1:F:49:ARG:HB3	1:F:49:ARG:NH1	1.81	0.95
1:C:168:LEU:HD22	1:C:188:LEU:HD21	1.46	0.95
1:B:64:ASP:H	1:B:70:HIS:HD2	1.11	0.93
1:C:196:THR:HG22	1:C:197:LEU:H	1.32	0.93
1:C:77:ARG:O	1:C:80:GLU:HG3	1.70	0.92
1:B:44:LEU:HD21	1:B:62:GLU:HG3	1.51	0.90
1:D:5:LEU:O	1:D:8:LYS:HB2	1.74	0.88
1:D:60:LEU:HD23	1:D:61:LEU:N	1.91	0.86
1:F:9:ARG:HH22	1:F:86:ASN:ND2	1.74	0.86
1:D:143:SER:HB2	1:D:185:ARG:NH1	1.91	0.85
1:A:199:MET:HA	1:A:202:ILE:HD13	1.59	0.85
1:E:135:LEU:HD21	1:E:179:ALA:HA	1.56	0.84
1:D:66:GLN:HG2	1:D:121:HIS:CD2	2.13	0.84
1:A:214:GLN:O	1:A:218:LEU:HD23	1.77	0.84
1:A:231:ASN:HD21	1:A:233:LYS:HG2	1.42	0.84
1:A:99:PRO:HB2	1:A:101:THR:HG22	1.58	0.83
1:D:108:PHE:HB2	1:D:159:ASN:ND2	1.93	0.83
1:F:49:ARG:HB3	1:F:49:ARG:HH11	1.41	0.83
1:E:109:PHE:HB3	1:F:132:LYS:HD2	1.61	0.82
1:A:202:ILE:HD12	1:A:202:ILE:H	1.44	0.82
1:D:57:LYS:O	1:D:57:LYS:HD3	1.78	0.82
1:E:202:ILE:HG13	1:E:207:LEU:HD22	1.62	0.81
1:D:16:ILE:HG13	1:D:43:ARG:HH22	1.45	0.81
1:B:202:ILE:HG23	1:B:207:LEU:HD22	1.62	0.81
1:F:195:ARG:HH12	1:F:203:VAL:HG11	1.46	0.81
1:E:38:LEU:HB2	1:E:60:LEU:HD13	1.60	0.81
1:F:231:ASN:HD21	1:F:233:LYS:NZ	1.78	0.80
1:B:17:THR:HA	1:B:50:ILE:HD13	1.61	0.80
1:F:99:PRO:HG3	1:F:115:ASP:HB3	1.61	0.80
1:D:66:GLN:HG2	1:D:121:HIS:HD2	1.46	0.80
1:F:74:LEU:O	1:F:78:VAL:HG23	1.81	0.79
1:D:27:ARG:O	1:D:31:GLU:HG3	1.83	0.79
1:E:17:THR:HA	1:E:50:ILE:HD13	1.63	0.79
1:B:67:ASN:HD22	1:B:67:ASN:C	1.89	0.78
1:D:186:SER:N	1:D:254:THR:HG23	1.98	0.78
1:C:174:PHE:CE2	1:D:159:ASN:HA	2.18	0.78
1:A:101:THR:HG21	1:A:115:ASP:OD1	1.84	0.78
1:A:186:SER:H	1:A:254:THR:HG23	1.48	0.77
1:D:108:PHE:HB2	1:D:159:ASN:HD22	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:PRO:HG3	1:D:115:ASP:HB2	1.67	0.77
1:C:202:ILE:HA	1:C:207:LEU:HD13	1.67	0.77
1:A:24:HIS:O	1:A:28:VAL:HG23	1.84	0.76
1:E:105:ILE:HG23	1:E:106:ASN:H	1.50	0.76
1:C:177:ARG:HA	1:F:227:PRO:HB3	1.67	0.75
1:F:91:VAL:HG23	1:F:138:MET:HE3	1.68	0.75
1:C:105:ILE:O	1:C:105:ILE:HD13	1.87	0.75
1:F:82:ILE:HG13	1:F:83:GLY:H	1.50	0.75
1:E:27:ARG:O	1:E:31:GLU:HG3	1.87	0.74
1:B:195:ARG:HH11	1:B:195:ARG:CB	1.98	0.74
1:F:231:ASN:ND2	1:F:233:LYS:NZ	2.36	0.74
1:F:231:ASN:ND2	1:F:233:LYS:HG2	2.01	0.74
1:D:168:LEU:HD13	1:D:188:LEU:HD21	1.69	0.74
1:C:186:SER:H	1:C:254:THR:CG2	2.01	0.74
1:A:231:ASN:HD21	1:A:233:LYS:CG	2.01	0.74
1:F:222:TRP:HE1	1:F:261:ASP:HB2	1.51	0.73
1:C:99:PRO:HB2	1:C:101:THR:HG22	1.71	0.73
1:C:137:ILE:HG13	1:C:137:ILE:O	1.89	0.73
1:F:10:ILE:HD13	1:F:246:LEU:HD13	1.70	0.73
1:C:201:ALA:O	1:C:206:ALA:HB3	1.87	0.73
1:D:143:SER:HB2	1:D:185:ARG:HH11	1.53	0.72
1:B:186:SER:H	1:B:254:THR:CG2	2.01	0.72
1:F:18:ASP:H	1:F:50:ILE:HD13	1.52	0.72
1:B:195:ARG:HB2	1:B:195:ARG:NH1	2.01	0.72
1:C:67:ASN:C	1:C:67:ASN:HD22	1.98	0.72
1:C:186:SER:H	1:C:254:THR:HG23	1.53	0.72
1:D:186:SER:H	1:D:254:THR:CG2	2.00	0.72
1:E:47:ILE:O	1:E:51:THR:HG23	1.90	0.72
1:F:228:ILE:HD11	1:F:262:GLY:HA2	1.71	0.71
1:A:135:LEU:HB3	1:A:136:PRO:HD3	1.72	0.71
1:C:8:LYS:HA	1:C:89:ASP:OD2	1.89	0.71
1:A:4:LEU:HB3	1:A:5:LEU:HD12	1.72	0.71
1:A:202:ILE:HA	1:A:206:ALA:HB3	1.73	0.71
1:F:99:PRO:CG	1:F:115:ASP:HB3	2.21	0.70
1:F:231:ASN:ND2	1:F:233:LYS:HZ2	1.89	0.70
1:C:222:TRP:HE1	1:C:261:ASP:HB2	1.56	0.70
1:A:20:SER:HB3	2:A:300:NAD:O2A	1.92	0.70
1:D:249:TRP:HB3	1:E:244:ALA:HB2	1.72	0.70
1:C:199:MET:SD	1:C:215:ILE:HD11	2.32	0.69
1:E:171:VAL:O	1:E:175:VAL:HG23	1.93	0.69
1:D:105:ILE:HG22	1:D:211:ALA:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLN:OE1	1:F:154:ALA:HB3	1.92	0.69
1:A:10:ILE:HD13	1:A:246:LEU:HD13	1.74	0.69
1:C:135:LEU:HD21	1:C:179:ALA:HA	1.74	0.69
1:E:26:ALA:O	1:E:30:GLN:HG3	1.93	0.69
1:E:67:ASN:HD22	1:E:68:GLU:N	1.91	0.68
1:C:196:THR:HG22	1:C:197:LEU:N	2.08	0.68
1:E:168:LEU:HD22	1:E:188:LEU:HD21	1.76	0.68
1:F:11:LEU:HD13	1:F:134:LEU:HD11	1.76	0.68
1:E:269:LEU:OXT	1:E:269:LEU:HD13	1.94	0.67
1:C:218:LEU:HD21	1:E:269:LEU:HB2	1.75	0.67
1:F:231:ASN:HD21	1:F:233:LYS:HG2	1.57	0.67
1:D:157:ALA:HB3	1:D:215:ILE:HD11	1.76	0.67
1:B:167:ALA:O	1:B:171:VAL:HG23	1.94	0.67
1:D:101:THR:HG21	1:D:115:ASP:OD2	1.95	0.67
1:C:64:ASP:H	1:C:70:HIS:CD2	2.12	0.66
1:C:185:ARG:HG3	1:C:185:ARG:HH11	1.60	0.66
1:D:16:ILE:HG13	1:D:43:ARG:NH2	2.09	0.66
1:D:17:THR:HG22	1:D:19:SER:H	1.61	0.66
1:E:103:MET:HB3	1:E:105:ILE:HG22	1.78	0.66
1:E:196:THR:HG21	2:E:700:NAD:O1N	1.95	0.66
1:C:62:GLU:HG2	1:C:70:HIS:NE2	2.10	0.66
1:F:82:ILE:HG13	1:F:83:GLY:N	2.11	0.66
1:D:238:VAL:O	1:D:242:VAL:HG23	1.96	0.66
1:E:78:VAL:O	1:E:82:ILE:HG12	1.96	0.65
1:D:153:ARG:NH2	1:F:153:ARG:HE	1.95	0.65
1:D:174:PHE:O	1:D:177:ARG:HG2	1.96	0.65
1:F:9:ARG:HH22	1:F:86:ASN:HD22	1.43	0.65
1:A:6:ASP:HA	1:A:33:GLY:O	1.97	0.65
1:C:64:ASP:H	1:C:70:HIS:HD2	1.43	0.65
1:C:11:LEU:HD23	1:C:11:LEU:C	2.22	0.65
1:A:131:ALA:O	1:A:135:LEU:HB2	1.96	0.64
1:A:236:THR:O	1:A:240:LYS:HG3	1.97	0.64
1:B:17:THR:HA	1:B:50:ILE:CD1	2.27	0.64
1:A:202:ILE:HD12	1:A:202:ILE:N	2.13	0.64
1:D:60:LEU:HD23	1:D:61:LEU:H	1.60	0.64
1:D:172:ASN:CG	1:D:188:LEU:HD13	2.22	0.64
1:F:268:LEU:O	1:F:269:LEU:HB3	1.97	0.64
1:D:108:PHE:HD2	1:D:159:ASN:HB3	1.62	0.64
1:B:99:PRO:HB2	1:B:101:THR:HG22	1.79	0.64
1:D:267:GLN:CD	1:F:154:ALA:HB3	2.23	0.64
1:A:209:GLU:C	1:A:211:ALA:H	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASN:HD21	1:B:69:GLU:HB2	1.63	0.64
1:A:64:ASP:H	1:A:70:HIS:HD2	1.46	0.63
1:B:145:VAL:HA	1:B:187:ASN:O	1.98	0.63
1:C:78:VAL:O	1:C:82:ILE:HG12	1.98	0.63
1:A:11:LEU:HD13	1:A:134:LEU:HD13	1.81	0.63
1:B:64:ASP:H	1:B:70:HIS:CD2	2.03	0.63
1:C:21:ILE:O	1:C:25:ILE:HG13	1.98	0.63
1:F:174:PHE:O	1:F:177:ARG:HG3	1.99	0.63
1:F:215:ILE:HG22	1:F:219:GLU:OE2	1.97	0.63
1:C:25:ILE:HA	1:C:239:ALA:HB1	1.79	0.63
1:D:16:ILE:CG1	1:D:43:ARG:HH22	2.12	0.63
1:A:218:LEU:HD12	3:A:350:GEQ:H4E	1.81	0.63
1:F:30:GLN:NE2	1:F:56:ALA:HB3	2.14	0.63
1:A:5:LEU:HD12	1:A:5:LEU:N	2.14	0.63
1:F:199:MET:HE1	1:F:215:ILE:HG21	1.81	0.63
1:F:9:ARG:NH2	1:F:86:ASN:HD22	1.97	0.63
1:F:201:ALA:O	1:F:206:ALA:HB3	1.99	0.63
1:C:39:THR:HG22	1:C:61:LEU:HB2	1.80	0.62
1:B:44:LEU:CD2	1:B:62:GLU:HG3	2.24	0.62
1:B:221:GLY:O	1:B:225:ARG:HD3	1.99	0.62
1:D:39:THR:HB	1:D:63:LEU:HB3	1.81	0.62
1:E:186:SER:H	1:E:254:THR:HG22	1.64	0.62
1:D:43:ARG:HB3	1:D:46:LEU:HB2	1.81	0.62
1:F:146:GLY:C	1:F:147:MET:HE2	2.24	0.62
1:B:103:MET:HE1	3:B:450:GEQ:H1A	1.79	0.62
1:B:27:ARG:O	1:B:31:GLU:HG3	1.99	0.62
1:E:157:ALA:O	1:E:158:TYR:HB2	1.99	0.62
1:F:145:VAL:HA	1:F:187:ASN:O	2.00	0.62
1:D:218:LEU:HD12	1:F:269:LEU:HD21	1.81	0.62
1:A:197:LEU:HD22	1:A:200:SER:HB2	1.82	0.61
1:B:39:THR:HB	1:B:63:LEU:HB3	1.82	0.61
1:B:61:LEU:HD13	1:B:77:ARG:HB3	1.82	0.61
1:C:210:GLU:H	1:C:210:GLU:CD	2.06	0.61
1:C:225:ARG:HG3	1:C:225:ARG:HH11	1.66	0.61
1:D:134:LEU:O	1:D:138:MET:HG3	2.00	0.61
1:C:95:ILE:HG12	2:C:500:NAD:H1B	1.81	0.61
1:C:24:HIS:O	1:C:28:VAL:HG23	2.01	0.61
1:C:132:LYS:HD2	1:D:109:PHE:HB3	1.82	0.61
1:F:39:THR:HA	1:F:61:LEU:O	2.01	0.61
1:C:269:LEU:HD11	1:E:218:LEU:HA	1.83	0.61
1:F:146:GLY:O	1:F:147:MET:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:SER:HB3	2:E:700:NAD:O2A	2.01	0.61
1:E:202:ILE:CG1	1:E:207:LEU:HD22	2.29	0.61
1:F:230:TRP:CZ3	1:F:261:ASP:HA	2.35	0.61
1:A:197:LEU:HA	1:A:200:SER:OG	2.01	0.61
1:C:103:MET:O	1:C:104:GLY:O	2.19	0.60
1:F:135:LEU:HG	1:F:182:TYR:CD1	2.35	0.60
1:C:10:ILE:HG23	1:C:90:GLY:HA3	1.83	0.60
1:C:198:ALA:O	1:C:202:ILE:HD13	1.99	0.60
1:E:6:ASP:HA	1:E:33:GLY:O	2.01	0.60
1:C:27:ARG:O	1:C:31:GLU:HG3	2.00	0.60
1:E:101:THR:HG21	1:E:112:PRO:HD2	1.84	0.60
1:D:25:ILE:O	1:D:29:ALA:HB2	2.02	0.60
1:E:172:ASN:CG	1:E:188:LEU:HD13	2.27	0.60
1:F:199:MET:HE2	1:F:219:GLU:OE2	2.01	0.60
1:D:195:ARG:N	1:D:232:MET:O	2.29	0.60
1:E:104:GLY:HA3	1:E:157:ALA:HA	1.82	0.60
1:B:67:ASN:ND2	1:B:69:GLU:H	2.00	0.60
1:D:218:LEU:CD1	1:F:269:LEU:HD21	2.32	0.60
1:F:21:ILE:O	1:F:25:ILE:HG13	2.01	0.60
1:A:250:LEU:N	1:A:251:PRO:HD3	2.16	0.60
1:D:168:LEU:HD13	1:D:188:LEU:CD2	2.31	0.60
1:C:40:GLY:HA3	1:C:47:ILE:CD1	2.32	0.60
1:E:13:SER:O	1:E:94:SER:HB2	2.01	0.60
1:B:103:MET:HE3	1:B:158:TYR:CE2	2.36	0.59
1:D:65:VAL:HB	1:D:126:SER:HB2	1.82	0.59
1:A:65:VAL:HG22	2:A:300:NAD:N1A	2.17	0.59
1:C:127:TYR:OH	1:C:144:ILE:HG22	2.01	0.59
1:A:211:ALA:HA	1:A:214:GLN:HE21	1.67	0.59
1:E:16:ILE:HB	2:E:700:NAD:O3B	2.03	0.59
1:F:62:GLU:O	1:F:77:ARG:NH1	2.35	0.59
1:F:225:ARG:HG2	1:F:269:LEU:HA	1.83	0.59
1:B:131:ALA:O	1:B:135:LEU:HB2	2.02	0.59
1:E:69:GLU:CD	1:E:69:GLU:H	2.10	0.59
1:F:202:ILE:O	1:F:202:ILE:HG22	2.01	0.59
1:A:217:LEU:HD12	1:A:217:LEU:C	2.28	0.59
1:B:146:GLY:C	1:B:147:MET:HE2	2.27	0.59
1:E:211:ALA:O	1:E:215:ILE:HG12	2.02	0.59
1:F:171:VAL:O	1:F:175:VAL:HG23	2.03	0.59
1:F:253:THR:HG23	1:F:253:THR:O	2.02	0.59
1:E:198:ALA:O	1:E:202:ILE:HD13	2.03	0.59
1:F:176:ALA:HB1	1:F:254:THR:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HG23	1:C:17:THR:HG23	1.84	0.59
1:C:101:THR:HG21	1:C:115:ASP:OD2	2.02	0.59
1:D:209:GLU:C	1:D:211:ALA:H	2.10	0.59
1:F:49:ARG:HH11	1:F:49:ARG:CB	2.13	0.59
1:B:67:ASN:HD22	1:B:68:GLU:N	2.01	0.59
1:D:108:PHE:CB	1:D:159:ASN:HD22	2.15	0.59
1:E:80:GLU:C	1:E:80:GLU:CD	2.70	0.59
1:F:46:LEU:HD23	1:F:46:LEU:O	2.02	0.59
1:B:199:MET:HE3	1:B:199:MET:O	2.02	0.58
1:C:134:LEU:O	1:C:138:MET:HG3	2.02	0.58
1:D:26:ALA:O	1:D:29:ALA:HB3	2.04	0.58
1:E:245:LEU:HD22	1:E:258:ILE:HD12	1.85	0.58
1:C:158:TYR:CD1	1:C:162:THR:OG1	2.56	0.58
1:C:206:ALA:C	1:C:207:LEU:HD12	2.29	0.58
1:B:67:ASN:ND2	1:B:69:GLU:N	2.52	0.58
1:E:236:THR:O	1:E:240:LYS:HG2	2.03	0.58
1:F:186:SER:H	1:F:254:THR:HG23	1.69	0.58
1:B:16:ILE:HG23	1:B:17:THR:HG23	1.85	0.58
1:B:93:HIS:CE1	1:B:95:ILE:HB	2.39	0.58
4:C:800:HOH:O	1:E:269:LEU:HD12	2.02	0.58
1:D:253:THR:HB	1:E:259:TYR:O	2.04	0.58
1:B:67:ASN:HD21	1:B:69:GLU:CB	2.16	0.58
1:B:101:THR:HG21	1:B:115:ASP:OD1	2.03	0.58
1:E:107:PRO:HB2	1:E:110:ASP:OD1	2.04	0.58
1:A:27:ARG:HG2	1:A:31:GLU:OE2	2.04	0.57
1:A:87:LYS:HB3	1:A:137:ILE:O	2.03	0.57
1:A:74:LEU:HD13	1:A:134:LEU:HD21	1.87	0.57
1:B:218:LEU:HG	3:B:450:GEQ:H4E	1.86	0.57
1:C:172:ASN:CG	1:C:188:LEU:HD13	2.29	0.57
1:D:48:GLN:HG2	1:D:60:LEU:HD13	1.85	0.57
1:D:254:THR:C	1:D:256:ASP:H	2.13	0.57
1:C:43:ARG:HD2	1:C:46:LEU:CD1	2.34	0.57
1:E:156:PRO:HD3	1:F:177:ARG:HH12	1.68	0.57
1:B:83:GLY:O	1:B:86:ASN:HB2	2.05	0.57
1:F:9:ARG:NH2	1:F:86:ASN:ND2	2.50	0.57
1:F:16:ILE:HG23	1:F:17:THR:CG2	2.22	0.57
1:F:173:ARG:O	1:F:176:ALA:HB3	2.05	0.57
1:F:215:ILE:HA	1:F:218:LEU:CD1	2.35	0.57
1:B:64:ASP:N	1:B:70:HIS:HD2	1.93	0.56
1:D:157:ALA:CB	1:D:215:ILE:HD11	2.35	0.56
1:D:218:LEU:C	1:D:218:LEU:HD23	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:H	1:A:202:ILE:CD1	2.16	0.56
1:C:189:VAL:HG21	1:C:242:VAL:HG22	1.87	0.56
1:C:225:ARG:HD2	1:C:267:GLN:O	2.06	0.56
1:E:157:ALA:CB	1:E:214:GLN:HB3	2.35	0.56
1:F:53:ARG:HH11	1:F:53:ARG:HG2	1.68	0.56
1:C:174:PHE:O	1:C:177:ARG:HG2	2.05	0.56
1:D:27:ARG:HG2	1:D:27:ARG:HH11	1.69	0.56
1:F:6:ASP:HA	1:F:33:GLY:O	2.06	0.56
1:A:231:ASN:ND2	1:A:233:LYS:HG2	2.16	0.56
1:F:195:ARG:NH1	1:F:203:VAL:HG11	2.16	0.56
1:D:202:ILE:HG12	1:D:207:LEU:HB2	1.88	0.56
1:F:231:ASN:HD21	1:F:233:LYS:HZ3	1.53	0.56
1:E:131:ALA:O	1:E:135:LEU:HB2	2.06	0.56
1:E:185:ARG:HA	1:E:254:THR:HG23	1.87	0.55
1:D:42:ASP:OD2	1:D:43:ARG:HG3	2.06	0.55
1:E:5:LEU:CB	1:E:34:ALA:HB2	2.35	0.55
1:C:198:ALA:C	1:C:202:ILE:HD13	2.31	0.55
1:E:167:ALA:O	1:E:171:VAL:HG23	2.06	0.55
1:F:5:LEU:HD23	1:F:32:GLN:CB	2.36	0.55
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.72	0.55
1:E:100:GLN:HA	1:E:103:MET:HB2	1.88	0.55
1:A:169:GLU:OE2	1:A:257:ILE:HD13	2.06	0.55
1:B:98:MET:CE	1:B:119:GLY:HA3	2.35	0.55
1:C:148:ASP:OD2	1:C:149:PHE:N	2.40	0.55
1:F:18:ASP:N	1:F:50:ILE:HD13	2.18	0.55
1:D:161:MET:HE3	1:D:164:ALA:HB3	1.88	0.55
1:E:169:GLU:OE2	1:E:257:ILE:HD13	2.06	0.55
1:F:98:MET:HE3	1:F:160:TRP:O	2.06	0.55
1:A:250:LEU:HD23	1:A:253:THR:HG21	1.89	0.55
1:B:8:LYS:HA	1:B:89:ASP:OD1	2.06	0.55
1:C:153:ARG:NH2	1:E:153:ARG:CZ	2.70	0.55
1:D:47:ILE:HG22	1:D:60:LEU:HD11	1.88	0.55
1:D:245:LEU:HD21	1:D:258:ILE:HG13	1.89	0.55
1:F:17:THR:HA	1:F:50:ILE:HD12	1.89	0.55
1:D:266:THR:HG21	1:E:255:GLY:O	2.07	0.55
1:F:24:HIS:O	1:F:28:VAL:HG23	2.06	0.55
1:B:199:MET:SD	3:B:450:GEQ:H5C2	2.47	0.55
1:D:227:PRO:HB3	1:E:177:ARG:HA	1.89	0.55
1:E:156:PRO:HD3	1:F:177:ARG:NH1	2.21	0.55
1:F:202:ILE:HG22	1:F:215:ILE:HG13	1.87	0.55
1:C:43:ARG:O	1:C:47:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:HG2	1:C:45:ARG:HH11	1.72	0.54
1:A:231:ASN:ND2	1:A:233:LYS:H	2.05	0.54
1:B:64:ASP:HB3	1:B:70:HIS:CD2	2.42	0.54
1:C:231:ASN:OD1	1:C:233:LYS:HG2	2.07	0.54
1:E:30:GLN:OE1	1:E:55:PRO:HG2	2.07	0.54
1:E:186:SER:H	1:E:254:THR:CG2	2.20	0.54
1:D:112:PRO:O	1:D:115:ASP:OD1	2.26	0.54
1:A:12:VAL:HG23	1:A:36:LEU:HD22	1.89	0.54
1:A:194:ILE:HD11	1:A:230:TRP:CZ2	2.43	0.54
1:C:60:LEU:O	1:C:61:LEU:HD23	2.06	0.54
1:F:66:GLN:HE21	1:F:121:HIS:CD2	2.26	0.54
1:A:43:ARG:HD2	1:A:46:LEU:HD13	1.89	0.54
1:B:250:LEU:N	1:B:251:PRO:CD	2.71	0.54
1:D:259:TYR:O	1:E:253:THR:HG22	2.06	0.54
1:E:139:ASN:OD1	1:E:140:PRO:HD2	2.07	0.54
1:D:44:LEU:H	1:D:44:LEU:HD22	1.72	0.54
1:D:47:ILE:HG22	1:D:47:ILE:O	2.06	0.54
1:A:209:GLU:O	1:A:211:ALA:N	2.40	0.54
1:C:201:ALA:C	1:C:206:ALA:HB3	2.32	0.54
1:E:49:ARG:O	1:E:52:ASP:HB3	2.08	0.54
1:E:147:MET:HE1	1:E:242:VAL:CG2	2.38	0.54
1:A:113:TYR:CE2	1:B:121:HIS:HB2	2.42	0.54
1:B:16:ILE:O	1:B:50:ILE:HD12	2.08	0.54
1:D:53:ARG:HE	1:D:53:ARG:CA	2.21	0.54
1:E:42:ASP:OD2	1:E:43:ARG:HG3	2.08	0.54
1:E:234:ASP:OD1	1:E:237:PRO:HD3	2.08	0.54
1:B:67:ASN:C	1:B:67:ASN:ND2	2.62	0.53
1:F:215:ILE:O	1:F:218:LEU:HD13	2.07	0.53
1:A:158:TYR:HD1	1:A:162:THR:HG1	1.52	0.53
1:A:210:GLU:CD	1:A:210:GLU:N	2.66	0.53
1:F:192:GLY:O	1:F:194:ILE:HD12	2.07	0.53
1:F:231:ASN:HD21	1:F:233:LYS:CG	2.19	0.53
1:B:146:GLY:O	1:B:147:MET:HE2	2.07	0.53
1:C:4:LEU:HB3	1:C:5:LEU:HD12	1.89	0.53
1:D:170:SER:HA	1:D:173:ARG:NH1	2.24	0.53
1:B:101:THR:HG21	1:B:115:ASP:CG	2.33	0.53
1:B:103:MET:HE2	3:B:450:GEQ:C3F	2.37	0.53
1:C:268:LEU:HD23	1:C:269:LEU:HD23	1.90	0.53
1:C:47:ILE:O	1:C:50:ILE:HB	2.09	0.53
1:C:153:ARG:CZ	1:E:153:ARG:CZ	2.86	0.53
1:F:5:LEU:HD23	1:F:32:GLN:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ALA:HB3	1:A:215:ILE:HD11	1.91	0.53
1:A:135:LEU:CB	1:A:136:PRO:HD3	2.38	0.53
1:B:46:LEU:HD11	1:B:49:ARG:NH2	2.23	0.53
1:C:2:THR:O	1:C:3:GLY:O	2.26	0.53
1:C:113:TYR:CE2	1:C:117:SER:HB2	2.43	0.53
1:D:95:ILE:HD13	2:D:600:NAD:N3A	2.24	0.53
1:B:41:PHE:HE1	1:B:64:ASP:CG	2.17	0.53
1:C:199:MET:O	1:C:203:VAL:HG23	2.09	0.53
1:D:27:ARG:HH12	1:D:28:VAL:HG22	1.74	0.53
1:E:154:ALA:HB2	1:F:173:ARG:HB3	1.91	0.53
1:D:192:GLY:HA3	1:D:230:TRP:CZ2	2.43	0.53
1:B:195:ARG:HG2	1:B:200:SER:HB3	1.90	0.52
1:C:43:ARG:HD2	1:C:46:LEU:HD13	1.92	0.52
1:D:108:PHE:HD2	1:D:159:ASN:HD22	1.55	0.52
1:F:17:THR:C	1:F:19:SER:H	2.17	0.52
1:A:14:GLY:HA3	1:A:94:SER:O	2.09	0.52
1:C:4:LEU:C	1:C:5:LEU:HD12	2.34	0.52
1:F:71:LEU:C	1:F:73:SER:H	2.18	0.52
1:C:149:PHE:O	1:C:150:ASP:C	2.52	0.52
1:D:47:ILE:O	1:D:47:ILE:CG2	2.57	0.52
1:D:63:LEU:HD22	1:D:74:LEU:HD11	1.91	0.52
1:D:202:ILE:HG22	1:D:215:ILE:HG13	1.90	0.52
1:E:57:LYS:HD3	1:E:57:LYS:N	2.24	0.52
1:F:250:LEU:N	1:F:251:PRO:HD3	2.23	0.52
1:A:67:ASN:ND2	1:A:69:GLU:H	2.07	0.52
1:A:236:THR:HB	1:A:237:PRO:HD3	1.92	0.52
1:B:100:GLN:N	1:B:100:GLN:HE21	2.07	0.52
1:F:71:LEU:CD2	1:F:129:SER:HB3	2.40	0.52
1:A:5:LEU:HD23	1:A:10:ILE:HD12	1.91	0.52
1:D:99:PRO:O	1:D:101:THR:N	2.43	0.52
1:A:91:VAL:HG23	1:A:138:MET:HE3	1.92	0.52
1:E:54:LEU:HB3	1:E:55:PRO:HD2	1.92	0.52
1:F:61:LEU:HD13	1:F:77:ARG:HD2	1.92	0.52
2:A:300:NAD:H71N	3:A:350:GEQ:H3A	1.74	0.52
1:D:44:LEU:HD11	1:D:62:GLU:HG3	1.90	0.52
1:D:93:HIS:HE1	1:D:95:ILE:O	1.92	0.52
1:E:135:LEU:HD21	1:E:179:ALA:CA	2.34	0.52
1:E:145:VAL:HA	1:E:187:ASN:O	2.10	0.52
1:F:199:MET:O	1:F:203:VAL:HB	2.10	0.52
1:A:250:LEU:N	1:A:251:PRO:CD	2.73	0.51
1:C:66:GLN:CD	1:C:122:ILE:HD11	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ASN:HD22	1:E:67:ASN:C	2.17	0.51
1:A:48:GLN:HE21	1:A:60:LEU:HD23	1.75	0.51
1:E:104:GLY:CA	1:E:157:ALA:HA	2.40	0.51
1:A:44:LEU:HD11	1:A:62:GLU:HG3	1.93	0.51
1:A:146:GLY:C	1:A:147:MET:HE2	2.34	0.51
1:B:99:PRO:HB2	1:B:101:THR:CG2	2.40	0.51
1:B:185:ARG:HA	1:B:254:THR:CG2	2.40	0.51
1:D:15:ILE:HD12	1:D:38:LEU:HD13	1.90	0.51
1:A:76:GLY:O	1:A:79:THR:HB	2.11	0.51
1:A:154:ALA:HB2	1:B:173:ARG:HB3	1.91	0.51
1:C:215:ILE:HD13	1:C:215:ILE:C	2.35	0.51
1:F:11:LEU:HD13	1:F:134:LEU:CD1	2.38	0.51
1:F:21:ILE:HD11	1:F:194:ILE:HD13	1.93	0.51
1:F:211:ALA:O	1:F:215:ILE:HG12	2.09	0.51
1:F:218:LEU:HD22	1:F:219:GLU:N	2.25	0.51
1:A:215:ILE:O	1:A:219:GLU:HG3	2.10	0.51
1:C:51:THR:C	1:C:53:ARG:H	2.17	0.51
1:D:265:HIS:CE1	1:D:266:THR:HG23	2.46	0.51
1:F:71:LEU:O	1:F:73:SER:N	2.44	0.51
1:B:243:CYS:HA	1:B:246:LEU:HD12	1.92	0.51
1:C:233:LYS:H	1:C:233:LYS:HD2	1.75	0.51
1:D:201:ALA:HB1	1:D:205:GLY:HA3	1.93	0.51
1:E:5:LEU:HB3	1:E:34:ALA:HB2	1.91	0.51
1:A:16:ILE:HB	2:A:300:NAD:O3B	2.11	0.51
1:B:4:LEU:HD22	1:B:4:LEU:O	2.10	0.51
1:E:80:GLU:HB2	4:E:828:HOH:O	2.11	0.51
1:F:185:ARG:HG3	1:F:185:ARG:HH11	1.76	0.51
1:C:201:ALA:C	1:C:203:VAL:H	2.19	0.51
1:D:48:GLN:C	1:D:50:ILE:H	2.18	0.51
1:F:199:MET:HE3	1:F:203:VAL:HG23	1.93	0.51
1:C:269:LEU:CD1	1:E:218:LEU:HA	2.40	0.51
1:F:57:LYS:NZ	1:F:57:LYS:HB3	2.26	0.51
1:F:254:THR:HG21	4:F:776:HOH:O	2.11	0.51
1:B:103:MET:HE3	1:B:158:TYR:CD2	2.46	0.50
1:D:44:LEU:HD22	1:D:44:LEU:N	2.26	0.50
1:F:43:ARG:HD2	1:F:46:LEU:HD22	1.92	0.50
1:C:201:ALA:C	1:C:203:VAL:N	2.68	0.50
1:A:193:PRO:O	1:A:194:ILE:HD13	2.10	0.50
1:D:176:ALA:HB1	1:D:254:THR:HG22	1.94	0.50
1:E:245:LEU:CD2	1:E:258:ILE:HD12	2.40	0.50
1:F:43:ARG:O	1:F:47:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD13	1:A:134:LEU:CD1	2.40	0.50
1:A:193:PRO:HA	2:A:300:NAD:O7N	2.12	0.50
1:A:238:VAL:O	1:A:242:VAL:HG23	2.11	0.50
1:B:90:GLY:HA2	1:B:143:SER:O	2.11	0.50
1:C:3:GLY:O	1:C:6:ASP:OD1	2.30	0.50
1:C:163:VAL:HA	1:D:170:SER:OG	2.11	0.50
1:C:211:ALA:C	1:C:213:ALA:H	2.19	0.50
1:C:231:ASN:CG	1:C:233:LYS:HD3	2.35	0.50
1:E:97:PHE:CE2	1:E:99:PRO:HD3	2.47	0.50
1:F:4:LEU:HD11	1:F:247:SER:HB3	1.93	0.50
1:C:240:LYS:HG2	1:F:249:TRP:CZ3	2.46	0.50
1:D:16:ILE:CD1	1:D:43:ARG:HH22	2.25	0.50
1:D:74:LEU:HD13	1:D:134:LEU:HD21	1.93	0.50
1:C:231:ASN:C	1:C:233:LYS:H	2.20	0.50
1:C:66:GLN:HE22	1:C:118:LYS:HG3	1.75	0.49
1:E:232:MET:HE3	1:E:232:MET:H	1.77	0.49
1:A:67:ASN:HD21	1:A:69:GLU:HB3	1.77	0.49
1:D:17:THR:HG22	1:D:18:ASP:N	2.27	0.49
1:D:167:ALA:O	1:D:171:VAL:HG23	2.13	0.49
1:E:43:ARG:O	1:E:47:ILE:HG13	2.11	0.49
1:C:30:GLN:NE2	1:C:36:LEU:HD12	2.26	0.49
1:A:61:LEU:N	1:A:61:LEU:HD23	2.26	0.49
1:C:27:ARG:HH11	1:C:27:ARG:HG2	1.77	0.49
1:D:99:PRO:CG	1:D:115:ASP:HB2	2.38	0.49
1:D:53:ARG:HE	1:D:53:ARG:HA	1.78	0.49
1:D:65:VAL:HG21	1:D:122:ILE:HG23	1.94	0.49
1:D:99:PRO:HB2	1:D:101:THR:HG22	1.94	0.49
1:D:147:MET:O	1:D:165:LYS:NZ	2.45	0.49
1:A:254:THR:HG21	4:A:851:HOH:O	2.13	0.49
1:E:25:ILE:O	1:E:29:ALA:HB2	2.12	0.49
1:E:46:LEU:O	1:E:47:ILE:C	2.56	0.49
1:E:196:THR:O	1:E:197:LEU:C	2.55	0.49
1:F:71:LEU:HD21	1:F:129:SER:HB3	1.93	0.49
1:F:103:MET:O	1:F:104:GLY:C	2.56	0.49
1:C:214:GLN:HB3	4:C:800:HOH:O	2.12	0.49
1:F:76:GLY:O	1:F:80:GLU:HG3	2.12	0.49
1:F:195:ARG:HH12	1:F:203:VAL:HG21	1.78	0.49
1:D:25:ILE:HA	1:D:239:ALA:HB1	1.95	0.49
1:D:193:PRO:HA	2:D:600:NAD:O7N	2.13	0.49
1:D:196:THR:O	1:D:197:LEU:HD23	2.13	0.49
1:E:60:LEU:HD22	1:E:60:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:SER:O	1:F:94:SER:HB3	2.12	0.49
1:F:228:ILE:CD1	1:F:262:GLY:HA2	2.42	0.49
1:C:44:LEU:N	1:C:44:LEU:HD22	2.27	0.49
1:C:67:ASN:HD22	1:C:68:GLU:N	2.10	0.49
1:D:221:GLY:HA2	1:D:224:GLN:CD	2.38	0.49
1:B:196:THR:HG21	2:B:400:NAD:O1N	2.12	0.48
1:D:5:LEU:N	1:D:5:LEU:HD22	2.28	0.48
1:D:154:ALA:HB3	1:F:267:GLN:OE1	2.12	0.48
1:E:42:ASP:CG	1:E:43:ARG:N	2.68	0.48
1:E:168:LEU:C	1:E:168:LEU:HD23	2.38	0.48
1:F:219:GLU:C	1:F:221:GLY:H	2.21	0.48
1:D:11:LEU:C	1:D:11:LEU:HD23	2.38	0.48
1:D:135:LEU:N	1:D:136:PRO:CD	2.77	0.48
1:F:49:ARG:HH11	1:F:49:ARG:C	2.21	0.48
1:F:129:SER:O	1:F:132:LYS:HB3	2.14	0.48
1:A:197:LEU:C	1:A:197:LEU:HD13	2.39	0.48
1:B:16:ILE:HG23	1:B:17:THR:N	2.28	0.48
1:D:112:PRO:HB2	1:D:115:ASP:OD1	2.13	0.48
1:E:174:PHE:O	1:E:177:ARG:HG2	2.13	0.48
1:C:60:LEU:HD12	1:C:61:LEU:H	1.78	0.48
1:C:67:ASN:C	1:C:67:ASN:ND2	2.66	0.48
1:C:135:LEU:N	1:C:136:PRO:CD	2.75	0.48
1:F:131:ALA:O	1:F:135:LEU:HB2	2.14	0.48
1:A:51:THR:C	1:A:53:ARG:H	2.22	0.48
1:B:68:GLU:HG3	4:B:866:HOH:O	2.12	0.48
1:C:25:ILE:HA	1:C:239:ALA:CB	2.41	0.48
1:C:153:ARG:CZ	1:E:153:ARG:NH1	2.76	0.48
1:D:10:ILE:HD12	1:D:34:ALA:HB1	1.95	0.48
1:D:63:LEU:HD21	1:D:130:MET:HE3	1.95	0.48
1:D:129:SER:O	1:D:132:LYS:HE2	2.14	0.48
1:D:254:THR:HG21	4:D:833:HOH:O	2.12	0.48
1:C:4:LEU:HD22	1:C:247:SER:HB2	1.96	0.48
1:C:158:TYR:HD1	1:C:162:THR:OG1	1.95	0.48
1:C:226:ALA:HA	1:C:262:GLY:O	2.14	0.48
1:E:216:GLN:HE21	1:E:216:GLN:HB2	1.54	0.48
1:E:214:GLN:O	1:E:218:LEU:HB2	2.13	0.48
1:F:4:LEU:HD21	1:F:249:TRP:CD1	2.48	0.48
1:A:197:LEU:HA	1:A:200:SER:CB	2.44	0.48
1:C:17:THR:HG21	1:C:197:LEU:HD23	1.95	0.48
1:C:102:GLY:O	1:C:159:ASN:HB2	2.14	0.48
1:D:195:ARG:HG3	1:D:232:MET:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:VAL:CG1	1:E:95:ILE:HD13	2.44	0.48
1:A:101:THR:HG21	1:A:115:ASP:CG	2.39	0.48
1:B:200:SER:O	1:B:203:VAL:HG12	2.13	0.48
1:F:67:ASN:HB3	1:F:70:HIS:CD2	2.48	0.48
1:D:40:GLY:N	1:D:61:LEU:O	2.46	0.47
1:E:147:MET:HE1	1:E:242:VAL:HG21	1.96	0.47
1:F:87:LYS:HB2	1:F:139:ASN:ND2	2.29	0.47
1:B:67:ASN:O	1:B:71:LEU:HD22	2.14	0.47
1:B:261:ASP:OD2	1:B:261:ASP:C	2.56	0.47
1:F:28:VAL:O	1:F:31:GLU:HB2	2.14	0.47
1:C:101:THR:O	1:C:111:ALA:HB2	2.14	0.47
1:D:99:PRO:C	1:D:101:THR:N	2.72	0.47
1:C:186:SER:N	1:C:254:THR:HG23	2.25	0.47
1:C:230:TRP:CD1	1:C:232:MET:HB3	2.50	0.47
1:D:75:ALA:HB2	1:D:133:ALA:O	2.14	0.47
1:F:71:LEU:O	1:F:74:LEU:HB2	2.14	0.47
1:F:151:PRO:HB3	1:F:162:THR:CG2	2.44	0.47
1:A:101:THR:HG21	1:A:115:ASP:CB	2.45	0.47
1:B:20:SER:HB3	2:B:400:NAD:O2A	2.13	0.47
1:D:4:LEU:HB3	1:D:5:LEU:HD22	1.96	0.47
1:D:169:GLU:OE2	1:D:257:ILE:HD13	2.15	0.47
1:A:111:ALA:O	1:B:125:TYR:OH	2.26	0.47
1:C:21:ILE:HG22	1:C:25:ILE:HG13	1.96	0.47
1:D:63:LEU:CD2	1:D:130:MET:HE3	2.44	0.47
1:D:65:VAL:HG22	2:D:600:NAD:N1A	2.29	0.47
1:E:248:ASP:OD2	1:E:248:ASP:N	2.47	0.47
1:F:9:ARG:HH12	1:F:86:ASN:CB	2.28	0.47
1:F:67:ASN:C	1:F:67:ASN:HD22	2.21	0.47
1:E:157:ALA:O	1:E:158:TYR:CB	2.61	0.47
1:F:30:GLN:OE1	1:F:55:PRO:HG2	2.14	0.47
1:F:64:ASP:H	1:F:70:HIS:CD2	2.33	0.47
1:F:44:LEU:O	1:F:44:LEU:HD13	2.15	0.47
1:A:254:THR:HG22	1:A:255:GLY:N	2.30	0.47
1:B:79:THR:C	1:B:81:ALA:N	2.68	0.47
1:B:199:MET:HA	1:B:202:ILE:HD13	1.97	0.47
1:F:11:LEU:C	1:F:11:LEU:HD23	2.39	0.47
1:A:210:GLU:CD	1:A:210:GLU:H	2.21	0.46
1:F:165:LYS:HA	1:F:168:LEU:HB2	1.97	0.46
1:B:76:GLY:O	1:B:80:GLU:HG3	2.15	0.46
1:D:41:PHE:HE1	1:D:64:ASP:CG	2.23	0.46
1:E:82:ILE:O	1:E:86:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:ALA:O	1:F:202:ILE:HG13	2.15	0.46
1:C:149:PHE:HD1	1:C:158:TYR:CE1	2.33	0.46
1:C:218:LEU:HD21	1:E:269:LEU:CB	2.45	0.46
1:E:148:ASP:OD1	1:E:169:GLU:OE2	2.33	0.46
1:B:99:PRO:C	1:B:101:THR:H	2.23	0.46
1:B:180:GLY:C	1:B:182:TYR:H	2.22	0.46
1:E:67:ASN:HB3	1:E:70:HIS:HD2	1.80	0.46
1:F:164:ALA:O	1:F:168:LEU:N	2.48	0.46
1:F:195:ARG:NH1	1:F:203:VAL:HG21	2.31	0.46
1:B:256:ASP:OD1	1:B:257:ILE:N	2.46	0.46
1:D:151:PRO:HB2	1:D:166:SER:OG	2.14	0.46
1:F:49:ARG:HH11	1:F:50:ILE:N	2.14	0.46
1:B:216:GLN:HA	4:B:876:HOH:O	2.16	0.46
1:C:11:LEU:HD23	1:C:12:VAL:N	2.30	0.46
1:C:43:ARG:HD2	1:C:46:LEU:HD12	1.98	0.46
1:D:99:PRO:C	1:D:101:THR:H	2.24	0.46
1:D:203:VAL:HG13	1:D:216:GLN:HB2	1.97	0.46
1:E:191:ALA:O	2:E:700:NAD:H5N	2.16	0.46
1:F:4:LEU:HD22	1:F:4:LEU:O	2.15	0.46
1:A:28:VAL:O	1:A:32:GLN:HG2	2.16	0.46
1:E:66:GLN:HE22	1:E:118:LYS:HD2	1.81	0.46
1:F:74:LEU:HD22	1:F:134:LEU:HD21	1.97	0.46
1:E:5:LEU:HB2	1:E:34:ALA:HB2	1.97	0.46
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.81	0.46
1:C:5:LEU:HD12	1:C:5:LEU:N	2.31	0.46
1:D:199:MET:HE2	3:D:650:GEQ:H5C1	1.97	0.46
1:B:42:ASP:O	1:B:44:LEU:HG	2.16	0.46
1:D:15:ILE:HG22	1:D:16:ILE:N	2.31	0.46
1:E:65:VAL:HG11	1:E:95:ILE:HD13	1.98	0.46
1:A:12:VAL:HB	1:A:38:LEU:CD2	2.46	0.45
1:F:248:ASP:O	1:F:251:PRO:HG3	2.16	0.45
1:A:202:ILE:HA	1:A:206:ALA:CB	2.42	0.45
1:B:100:GLN:HE21	1:B:100:GLN:CA	2.29	0.45
1:C:185:ARG:HH11	1:C:185:ARG:CG	2.26	0.45
1:C:195:ARG:HH12	1:C:203:VAL:HG11	1.81	0.45
1:F:201:ALA:HB1	1:F:206:ALA:HB3	1.99	0.45
1:C:225:ARG:O	1:C:267:GLN:HG3	2.17	0.45
1:D:203:VAL:CG1	1:D:216:GLN:HB2	2.47	0.45
1:F:79:THR:HG23	1:F:84:ALA:HA	1.98	0.45
1:A:148:ASP:OD2	1:A:149:PHE:N	2.50	0.45
1:B:60:LEU:C	1:B:60:LEU:HD13	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:O	1:B:74:LEU:HB2	2.16	0.45
1:C:197:LEU:HD22	4:C:830:HOH:O	2.15	0.45
1:A:145:VAL:HA	1:A:187:ASN:O	2.17	0.45
1:A:197:LEU:HD13	1:A:197:LEU:O	2.17	0.45
1:D:203:VAL:HG22	1:D:216:GLN:HB2	1.99	0.45
1:A:227:PRO:HD2	1:A:262:GLY:O	2.16	0.45
1:D:98:MET:HE3	1:D:160:TRP:C	2.41	0.45
1:B:254:THR:HG21	4:B:845:HOH:O	2.16	0.45
1:D:83:GLY:O	1:D:84:ALA:C	2.59	0.45
1:E:5:LEU:HD22	1:E:5:LEU:H	1.80	0.45
1:E:68:GLU:HB3	1:E:69:GLU:OE2	2.17	0.45
1:E:69:GLU:CD	1:E:69:GLU:N	2.75	0.45
1:C:11:LEU:C	1:C:11:LEU:CD2	2.90	0.45
1:C:233:LYS:HD2	1:C:233:LYS:N	2.32	0.45
1:D:18:ASP:HA	1:D:23:PHE:CD2	2.52	0.45
1:D:87:LYS:HB3	1:D:137:ILE:O	2.17	0.45
1:E:103:MET:HE3	1:E:103:MET:HA	1.98	0.45
1:B:119:GLY:O	1:B:123:SER:HB2	2.17	0.45
1:C:269:LEU:HD13	1:E:217:LEU:HD12	1.99	0.45
1:D:66:GLN:HG3	1:D:122:ILE:HG12	1.99	0.45
1:D:203:VAL:CG2	1:D:216:GLN:HB2	2.47	0.45
1:E:249:TRP:O	1:E:250:LEU:HG	2.17	0.45
1:F:135:LEU:HD21	1:F:179:ALA:HA	1.99	0.45
1:A:15:ILE:HG22	1:A:16:ILE:N	2.31	0.45
1:A:67:ASN:C	1:A:67:ASN:HD22	2.25	0.45
1:C:113:TYR:CZ	1:C:117:SER:HB2	2.52	0.45
1:C:196:THR:CG2	1:C:197:LEU:H	2.15	0.45
1:D:112:PRO:O	1:D:116:VAL:HG23	2.17	0.45
1:E:132:LYS:HG3	1:F:109:PHE:HB3	1.99	0.45
1:C:156:PRO:HG3	4:C:800:HOH:O	2.17	0.44
1:C:269:LEU:CD1	1:E:217:LEU:HD12	2.47	0.44
2:C:500:NAD:O3	3:C:550:GEQ:H4A	2.17	0.44
1:D:4:LEU:HD21	1:D:249:TRP:CD1	2.52	0.44
1:E:6:ASP:HA	1:E:33:GLY:C	2.42	0.44
1:A:67:ASN:ND2	1:A:69:GLU:HB3	2.32	0.44
1:B:65:VAL:HG13	2:B:400:NAD:C2A	2.47	0.44
1:D:15:ILE:HG13	4:D:814:HOH:O	2.15	0.44
1:D:45:ARG:HG3	1:D:45:ARG:NH1	2.32	0.44
1:A:11:LEU:C	1:A:11:LEU:HD23	2.42	0.44
1:B:27:ARG:HG2	1:B:27:ARG:HH11	1.81	0.44
1:B:99:PRO:C	1:B:101:THR:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ILE:O	1:D:219:GLU:HB2	2.17	0.44
1:D:83:GLY:HA3	1:D:86:ASN:HD22	1.83	0.44
1:D:252:ALA:O	1:E:262:GLY:N	2.46	0.44
1:F:149:PHE:O	1:F:150:ASP:C	2.58	0.44
1:A:5:LEU:N	1:A:5:LEU:CD1	2.80	0.44
1:C:185:ARG:HB3	1:C:254:THR:HG23	1.99	0.44
1:A:91:VAL:HG23	1:A:138:MET:CE	2.47	0.44
1:A:158:TYR:CZ	1:A:161:MET:HG3	2.53	0.44
1:C:212:GLY:O	1:C:216:GLN:HB2	2.18	0.44
1:D:88:LEU:N	1:D:137:ILE:O	2.50	0.44
1:D:148:ASP:OD1	1:D:169:GLU:OE2	2.35	0.44
1:D:154:ALA:HB3	1:F:267:GLN:CD	2.43	0.44
1:D:209:GLU:C	1:D:211:ALA:N	2.75	0.44
1:D:215:ILE:O	1:D:215:ILE:HG22	2.17	0.44
1:E:137:ILE:O	1:E:137:ILE:HG13	2.17	0.44
1:F:63:LEU:HD12	1:F:64:ASP:N	2.32	0.44
1:F:238:VAL:O	1:F:241:THR:HB	2.17	0.44
1:B:39:THR:HA	1:B:61:LEU:O	2.18	0.44
1:B:254:THR:C	1:B:256:ASP:N	2.74	0.44
1:D:250:LEU:HB3	1:D:253:THR:CG2	2.48	0.44
1:F:53:ARG:HG2	1:F:53:ARG:NH1	2.31	0.44
1:F:65:VAL:HG22	2:F:750:NAD:N1A	2.32	0.44
1:A:113:TYR:CZ	1:B:121:HIS:HB2	2.53	0.44
1:B:9:ARG:HA	1:B:35:GLN:O	2.18	0.44
1:B:66:GLN:HE22	1:B:118:LYS:HG3	1.82	0.44
1:C:44:LEU:HD13	1:C:47:ILE:HD11	1.99	0.44
1:D:48:GLN:C	1:D:50:ILE:N	2.75	0.44
1:D:236:THR:O	1:D:240:LYS:HG3	2.18	0.44
1:E:221:GLY:HA2	1:E:224:GLN:HB3	1.99	0.44
1:D:12:VAL:O	1:D:38:LEU:HA	2.17	0.43
1:D:202:ILE:CG2	1:D:215:ILE:HG13	2.48	0.43
1:A:221:GLY:O	1:A:224:GLN:HB3	2.19	0.43
1:B:60:LEU:C	1:B:61:LEU:HD23	2.43	0.43
1:B:148:ASP:OD2	1:B:149:PHE:N	2.48	0.43
1:C:68:GLU:OE2	1:C:68:GLU:HA	2.17	0.43
1:E:70:HIS:O	1:E:74:LEU:HB2	2.17	0.43
1:E:83:GLY:HA3	1:E:86:ASN:HD22	1.83	0.43
1:A:148:ASP:O	2:A:300:NAD:H5N	2.19	0.43
1:A:193:PRO:O	1:A:232:MET:HB2	2.18	0.43
1:A:194:ILE:O	1:A:196:THR:N	2.52	0.43
1:C:103:MET:HE2	3:C:550:GEQ:C4F	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:MET:HA	1:D:202:ILE:HD12	2.00	0.43
1:A:150:ASP:C	1:A:150:ASP:OD1	2.62	0.43
1:A:211:ALA:C	1:A:213:ALA:H	2.26	0.43
1:B:46:LEU:HD11	1:B:49:ARG:HH22	1.83	0.43
1:C:65:VAL:HA	1:C:71:LEU:HD21	1.99	0.43
1:C:147:MET:HE1	1:C:238:VAL:CG1	2.49	0.43
1:D:199:MET:HA	1:D:202:ILE:HB	2.00	0.43
1:E:38:LEU:HD12	1:E:60:LEU:HD11	2.00	0.43
1:A:4:LEU:HB3	1:A:5:LEU:CD1	2.46	0.43
1:A:30:GLN:OE1	1:A:54:LEU:HB3	2.18	0.43
1:A:135:LEU:HB3	1:A:136:PRO:CD	2.46	0.43
1:B:78:VAL:O	1:B:82:ILE:HG23	2.19	0.43
1:B:79:THR:C	1:B:81:ALA:H	2.26	0.43
1:D:259:TYR:CD2	1:D:265:HIS:CD2	3.06	0.43
1:B:99:PRO:CB	1:B:101:THR:HG22	2.48	0.43
1:C:54:LEU:C	1:C:56:ALA:H	2.25	0.43
1:D:149:PHE:CD1	1:D:158:TYR:CE1	3.06	0.43
1:C:225:ARG:HG3	1:C:225:ARG:NH1	2.32	0.43
1:D:132:LYS:O	1:D:132:LYS:HG2	2.18	0.43
1:D:195:ARG:CG	1:D:232:MET:HG3	2.49	0.43
1:E:93:HIS:CE1	1:E:95:ILE:HB	2.53	0.43
1:E:225:ARG:O	1:E:226:ALA:C	2.62	0.43
1:A:158:TYR:HD1	1:A:162:THR:OG1	2.00	0.43
1:C:4:LEU:HB3	1:C:5:LEU:CD1	2.49	0.43
1:D:15:ILE:CD1	1:D:38:LEU:HD13	2.49	0.43
1:D:256:ASP:C	1:D:257:ILE:HG13	2.44	0.43
1:E:59:PRO:C	1:E:60:LEU:HD22	2.44	0.43
1:B:197:LEU:HD13	1:B:197:LEU:C	2.44	0.43
1:C:145:VAL:HA	1:C:187:ASN:O	2.19	0.43
1:C:249:TRP:C	1:C:251:PRO:HD3	2.44	0.43
1:D:113:TYR:CZ	1:D:117:SER:HB2	2.53	0.43
1:E:28:VAL:HA	1:E:31:GLU:OE1	2.19	0.43
1:E:121:HIS:HB2	1:F:113:TYR:CZ	2.54	0.43
1:F:88:LEU:O	1:F:138:MET:HA	2.19	0.43
1:F:194:ILE:HD12	1:F:194:ILE:N	2.34	0.43
1:B:254:THR:O	1:B:256:ASP:N	2.52	0.43
1:C:16:ILE:HD12	1:C:47:ILE:HG22	2.00	0.43
1:E:79:THR:HG22	1:E:79:THR:O	2.18	0.43
1:E:147:MET:HE1	1:E:242:VAL:HG22	2.00	0.43
1:F:71:LEU:C	1:F:73:SER:N	2.75	0.43
1:F:215:ILE:HA	1:F:218:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:PHE:O	1:B:151:PRO:HD3	2.19	0.42
1:B:245:LEU:HD12	1:B:250:LEU:HD13	2.01	0.42
1:C:253:THR:HG22	1:F:259:TYR:O	2.19	0.42
1:D:148:ASP:CG	1:D:149:PHE:N	2.77	0.42
1:E:205:GLY:O	1:E:206:ALA:HB3	2.18	0.42
1:A:195:ARG:HB2	1:A:232:MET:HG3	2.01	0.42
1:B:199:MET:HG2	3:B:450:GEQ:H5C2	2.00	0.42
1:C:77:ARG:O	1:C:78:VAL:C	2.61	0.42
1:D:4:LEU:O	1:D:5:LEU:HD13	2.19	0.42
1:D:199:MET:C	1:D:201:ALA:H	2.27	0.42
1:E:67:ASN:CB	1:E:70:HIS:HD2	2.31	0.42
1:F:9:ARG:HD3	1:F:35:GLN:HB2	2.01	0.42
1:B:47:ILE:HD11	1:B:60:LEU:HD21	2.01	0.42
1:B:254:THR:O	1:B:256:ASP:HB2	2.19	0.42
1:F:60:LEU:O	1:F:60:LEU:HG	2.19	0.42
1:F:202:ILE:HG23	1:F:207:LEU:HD12	2.01	0.42
1:A:215:ILE:O	1:A:218:LEU:HB2	2.19	0.42
2:A:300:NAD:H52A	2:A:300:NAD:H52N	2.00	0.42
1:D:44:LEU:HD11	1:D:62:GLU:CG	2.49	0.42
1:D:132:LYS:HE2	1:D:132:LYS:HB3	1.90	0.42
1:C:16:ILE:HB	2:C:500:NAD:O3B	2.19	0.42
1:C:153:ARG:NH2	1:E:153:ARG:NE	2.68	0.42
1:C:173:ARG:HB3	1:D:154:ALA:HB2	2.01	0.42
1:C:211:ALA:C	1:C:213:ALA:N	2.78	0.42
1:E:158:TYR:O	1:E:158:TYR:CD1	2.72	0.42
1:E:160:TRP:CE3	1:E:163:VAL:HG21	2.54	0.42
1:A:199:MET:SD	1:A:199:MET:O	2.77	0.42
1:C:241:THR:HG23	1:F:250:LEU:HD23	2.01	0.42
1:D:78:VAL:O	1:D:82:ILE:HG23	2.19	0.42
1:D:221:GLY:CA	1:D:224:GLN:NE2	2.82	0.42
1:E:63:LEU:HD22	1:E:74:LEU:HD11	2.00	0.42
1:C:13:SER:O	1:C:22:ALA:HB1	2.19	0.42
1:D:135:LEU:HD12	1:D:135:LEU:HA	1.80	0.42
1:F:49:ARG:HB3	1:F:49:ARG:CZ	2.45	0.42
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.84	0.42
1:B:245:LEU:CD1	1:B:250:LEU:HD13	2.49	0.42
1:B:254:THR:O	1:B:255:GLY:C	2.62	0.42
1:E:99:PRO:HG2	1:E:115:ASP:HB3	2.00	0.42
1:F:4:LEU:CD1	1:F:247:SER:HB3	2.49	0.42
1:F:197:LEU:O	1:F:197:LEU:HD22	2.19	0.42
1:A:48:GLN:HE21	1:A:60:LEU:CD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ILE:HD11	1:C:23:PHE:HA	2.01	0.42
1:C:66:GLN:HG3	1:C:122:ILE:HG12	2.02	0.42
1:C:230:TRP:CZ3	1:C:261:ASP:HA	2.55	0.42
1:D:191:ALA:HB3	2:D:600:NAD:C5N	2.49	0.42
1:E:66:GLN:NE2	1:E:118:LYS:HD2	2.35	0.42
1:E:105:ILE:HG12	1:E:106:ASN:N	2.35	0.42
1:E:195:ARG:NH1	1:E:195:ARG:HG3	2.35	0.42
1:A:77:ARG:O	1:A:80:GLU:HB2	2.20	0.42
1:D:148:ASP:O	1:D:190:ALA:HA	2.20	0.42
1:D:194:ILE:HD11	1:D:238:VAL:HG21	2.01	0.42
1:E:185:ARG:HA	1:E:254:THR:CG2	2.49	0.42
1:F:17:THR:C	1:F:19:SER:N	2.78	0.42
1:F:201:ALA:HB1	1:F:206:ALA:CB	2.50	0.42
1:F:249:TRP:C	1:F:251:PRO:HD3	2.45	0.42
1:A:63:LEU:HB3	4:A:751:HOH:O	2.20	0.41
1:A:147:MET:HE2	1:A:147:MET:N	2.35	0.41
1:C:27:ARG:HG2	1:C:27:ARG:NH1	2.35	0.41
1:C:105:ILE:O	1:C:105:ILE:CD1	2.65	0.41
1:D:74:LEU:HD22	1:D:78:VAL:HG23	2.03	0.41
1:D:221:GLY:O	1:D:224:GLN:HB2	2.19	0.41
1:D:242:VAL:O	1:D:246:LEU:HG	2.20	0.41
1:E:132:LYS:HB2	1:F:109:PHE:CD1	2.55	0.41
1:F:150:ASP:CG	1:F:152:SER:HG	2.28	0.41
1:A:185:ARG:HD3	1:A:251:PRO:HA	2.01	0.41
1:A:202:ILE:CG1	1:A:207:LEU:HD13	2.50	0.41
1:A:202:ILE:HG13	1:A:207:LEU:HD13	2.02	0.41
1:B:11:LEU:HD21	1:B:39:THR:HG23	2.02	0.41
1:B:143:SER:HB2	4:B:778:HOH:O	2.21	0.41
1:C:71:LEU:HD13	1:C:74:LEU:HD12	2.01	0.41
1:D:221:GLY:HA3	1:D:224:GLN:NE2	2.35	0.41
1:D:254:THR:C	1:D:256:ASP:N	2.75	0.41
1:E:40:GLY:HA2	4:E:812:HOH:O	2.20	0.41
1:E:57:LYS:HD3	1:E:57:LYS:H	1.85	0.41
1:E:217:LEU:HA	1:E:220:GLU:HB3	2.02	0.41
1:B:98:MET:HE1	1:B:119:GLY:HA3	2.02	0.41
1:C:38:LEU:HD13	1:C:51:THR:HG21	2.02	0.41
1:C:231:ASN:OD1	1:C:233:LYS:HD3	2.20	0.41
1:E:102:GLY:HA3	1:E:160:TRP:HB2	2.02	0.41
1:E:186:SER:O	1:E:255:GLY:N	2.51	0.41
1:A:5:LEU:HB2	1:A:34:ALA:HB2	2.02	0.41
1:A:157:ALA:CB	1:A:215:ILE:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.75	0.41
1:B:67:ASN:ND2	1:B:69:GLU:HB2	2.31	0.41
1:B:250:LEU:N	1:B:251:PRO:HD3	2.35	0.41
1:C:185:ARG:CG	1:C:185:ARG:NH1	2.84	0.41
1:C:201:ALA:O	1:C:203:VAL:N	2.53	0.41
1:D:131:ALA:O	1:D:135:LEU:HB2	2.20	0.41
1:D:225:ARG:O	1:D:227:PRO:HD3	2.19	0.41
1:D:267:GLN:NE2	1:F:154:ALA:HB3	2.34	0.41
1:F:17:THR:HA	1:F:50:ILE:CD1	2.51	0.41
1:C:46:LEU:O	1:C:50:ILE:HG12	2.19	0.41
1:F:49:ARG:C	1:F:49:ARG:HD2	2.46	0.41
1:A:42:ASP:OD2	1:A:42:ASP:N	2.52	0.41
1:B:60:LEU:HD13	1:B:61:LEU:N	2.35	0.41
1:D:74:LEU:HD22	1:D:78:VAL:CG2	2.51	0.41
1:E:68:GLU:HA	1:E:68:GLU:OE1	2.19	0.41
1:E:101:THR:HB	1:E:111:ALA:CB	2.50	0.41
1:E:105:ILE:HG23	1:E:106:ASN:N	2.27	0.41
1:E:195:ARG:HG3	1:E:195:ARG:HH11	1.85	0.41
1:F:20:SER:C	1:F:22:ALA:N	2.78	0.41
1:F:91:VAL:HG23	1:F:138:MET:CE	2.45	0.41
1:A:12:VAL:HB	1:A:38:LEU:HD22	2.03	0.41
1:E:71:LEU:HD12	1:E:133:ALA:HB2	2.03	0.41
1:E:129:SER:O	1:E:133:ALA:N	2.54	0.41
1:E:232:MET:H	1:E:232:MET:CE	2.34	0.41
1:F:49:ARG:NH1	1:F:50:ILE:HG13	2.35	0.41
1:B:185:ARG:HA	1:B:254:THR:HG23	2.02	0.41
1:C:45:ARG:HG2	1:C:45:ARG:NH1	2.33	0.41
1:C:103:MET:HE3	1:C:158:TYR:CD2	2.55	0.41
1:C:153:ARG:NH1	1:E:153:ARG:NH2	2.68	0.41
1:E:8:LYS:HA	1:E:89:ASP:OD2	2.20	0.41
1:B:194:ILE:HA	1:B:232:MET:O	2.21	0.41
1:C:135:LEU:HD21	1:C:179:ALA:CA	2.48	0.41
1:D:10:ILE:O	1:D:36:LEU:HA	2.20	0.41
1:D:209:GLU:O	1:D:211:ALA:N	2.54	0.41
1:D:261:ASP:OD1	1:D:265:HIS:CD2	2.74	0.41
1:E:135:LEU:N	1:E:136:PRO:CD	2.83	0.41
1:F:197:LEU:C	1:F:197:LEU:HD13	2.46	0.41
1:D:19:SER:O	1:D:196:THR:HG22	2.20	0.41
1:D:198:ALA:O	1:D:202:ILE:HG13	2.21	0.41
1:E:97:PHE:CG	1:E:98:MET:N	2.89	0.41
1:F:50:ILE:C	1:F:52:ASP:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:VAL:O	1:F:120:ILE:HG13	2.20	0.41
1:F:219:GLU:C	1:F:221:GLY:N	2.79	0.41
1:B:67:ASN:HD22	1:B:69:GLU:H	1.69	0.40
1:C:155:MET:HB2	1:C:156:PRO:HD2	2.04	0.40
1:C:185:ARG:HD3	1:C:251:PRO:O	2.21	0.40
1:D:5:LEU:HB2	1:D:34:ALA:HB2	2.03	0.40
1:E:207:LEU:HD12	1:E:207:LEU:N	2.36	0.40
1:B:84:ALA:C	1:B:86:ASN:H	2.29	0.40
1:C:203:VAL:O	1:C:203:VAL:HG12	2.19	0.40
1:D:97:PHE:HE2	1:D:118:LYS:NZ	2.19	0.40
1:F:49:ARG:O	1:F:52:ASP:HB2	2.21	0.40
1:A:148:ASP:OD1	1:A:169:GLU:OE2	2.40	0.40
1:A:202:ILE:O	1:A:202:ILE:HG22	2.22	0.40
1:B:48:GLN:O	1:B:52:ASP:HB2	2.21	0.40
1:C:234:ASP:O	1:C:237:PRO:HD2	2.22	0.40
1:D:11:LEU:HD23	1:D:12:VAL:N	2.36	0.40
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.84	0.40
1:D:53:ARG:HE	1:D:53:ARG:N	2.20	0.40
1:E:135:LEU:HD13	1:E:144:ILE:HD11	2.03	0.40
1:E:197:LEU:C	1:E:197:LEU:HD23	2.46	0.40
1:F:218:LEU:HD22	1:F:218:LEU:C	2.46	0.40
1:A:46:LEU:HD23	1:A:50:ILE:HD13	2.03	0.40
1:B:66:GLN:NE2	1:B:118:LYS:HG3	2.36	0.40
1:C:93:HIS:CD2	1:C:127:TYR:HA	2.56	0.40
1:D:25:ILE:HG12	1:D:239:ALA:HA	2.03	0.40
1:E:12:VAL:HA	1:E:92:VAL:HB	2.03	0.40
1:E:64:ASP:HB3	1:E:67:ASN:HB2	2.04	0.40
1:E:163:VAL:HA	1:F:170:SER:OG	2.21	0.40
1:F:253:THR:O	1:F:253:THR:CG2	2.68	0.40
1:A:20:SER:CB	2:A:300:NAD:O2A	2.67	0.40
1:F:17:THR:O	1:F:19:SER:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH1	1:A:153:ARG:NH1[2_555]	1.51	0.69

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/269 (99%)	233 (88%)	25 (9%)	8 (3%)	3	8
1	B	266/269 (99%)	233 (88%)	28 (10%)	5 (2%)	6	17
1	C	266/269 (99%)	224 (84%)	32 (12%)	10 (4%)	2	5
1	D	266/269 (99%)	222 (84%)	36 (14%)	8 (3%)	3	8
1	E	266/269 (99%)	234 (88%)	24 (9%)	8 (3%)	3	8
1	F	266/269 (99%)	232 (87%)	27 (10%)	7 (3%)	4	11
All	All	1596/1614 (99%)	1378 (86%)	172 (11%)	46 (3%)	3	9

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLY
1	A	195	ARG
1	A	210	GLU
1	B	210	GLU
1	C	104	GLY
1	E	158	TYR
1	E	159	ASN
1	F	104	GLY
1	A	159	ASN
1	A	234	ASP
1	B	104	GLY
1	C	3	GLY
1	D	16	ILE
1	D	100	GLN
1	D	210	GLU
1	E	105	ILE
1	F	18	ASP
1	F	72	ALA
1	B	159	ASN
1	C	16	ILE

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Mol	Chain	Res	Type
1	C	159	ASN
1	C	232	MET
1	D	84	ALA
1	D	159	ASN
1	E	100	GLN
1	A	43	ARG
1	A	107	PRO
1	B	199	MET
1	B	255	GLY
1	E	206	ALA
1	F	65	VAL
1	A	16	ILE
1	C	46	LEU
1	D	150	ASP
1	E	74	LEU
1	E	150	ASP
1	F	103	MET
1	C	150	ASP
1	C	204	GLY
1	C	212	GLY
1	F	41	PHE
1	D	204	GLY
1	C	229	GLY
1	D	205	GLY
1	F	203	VAL
1	E	47	ILE

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	203/205 (99%)	183 (90%)	20 (10%)	7	19
1	B	203/205 (99%)	176 (87%)	27 (13%)	4	10
1	C	203/205 (99%)	189 (93%)	14 (7%)	14	34
1	D	203/205 (99%)	184 (91%)	19 (9%)	8	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	203/205 (99%)	189 (93%)	14 (7%)	14	34
1	F	203/205 (99%)	183 (90%)	20 (10%)	7	19
All	All	1218/1230 (99%)	1104 (91%)	114 (9%)	8	21

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	35	GLN
1	A	61	LEU
1	A	71	LEU
1	A	103	MET
1	A	145	VAL
1	A	153	ARG
1	A	168	LEU
1	A	172	ASN
1	A	188	LEU
1	A	202	ILE
1	A	210	GLU
1	A	217	LEU
1	A	222	TRP
1	A	245	LEU
1	A	250	LEU
1	A	251	PRO
1	A	253	THR
1	A	256	ASP
1	A	269	LEU
1	B	4	LEU
1	B	5	LEU
1	B	30	GLN
1	B	45	ARG
1	B	52	ASP
1	B	53	ARG
1	B	57	LYS
1	B	60	LEU
1	B	67	ASN
1	B	71	LEU
1	B	74	LEU
1	B	100	GLN
1	B	135	LEU
1	B	145	VAL

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Mol	Chain	Res	Type
1	B	168	LEU
1	B	188	LEU
1	B	195	ARG
1	B	210	GLU
1	B	217	LEU
1	B	224	GLN
1	B	236	THR
1	B	245	LEU
1	B	251	PRO
1	B	253	THR
1	B	254	THR
1	B	258	ILE
1	B	269	LEU
1	C	4	LEU
1	C	60	LEU
1	C	67	ASN
1	C	74	LEU
1	C	80	GLU
1	C	105	ILE
1	C	210	GLU
1	C	215	ILE
1	C	224	GLN
1	C	232	MET
1	C	233	LYS
1	C	253	THR
1	C	254	THR
1	C	269	LEU
1	D	4	LEU
1	D	5	LEU
1	D	6	ASP
1	D	52	ASP
1	D	57	LYS
1	D	71	LEU
1	D	74	LEU
1	D	115	ASP
1	D	135	LEU
1	D	152	SER
1	D	158	TYR
1	D	168	LEU
1	D	177	ARG
1	D	185	ARG
1	D	209	GLU

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Mol	Chain	Res	Type
1	D	253	THR
1	D	254	THR
1	D	268	LEU
1	D	269	LEU
1	E	5	LEU
1	E	48	GLN
1	E	68	GLU
1	E	71	LEU
1	E	74	LEU
1	E	80	GLU
1	E	153	ARG
1	E	216	GLN
1	E	217	LEU
1	E	232	MET
1	E	248	ASP
1	E	250	LEU
1	E	253	THR
1	E	254	THR
1	F	4	LEU
1	F	17	THR
1	F	44	LEU
1	F	45	ARG
1	F	49	ARG
1	F	50	ILE
1	F	57	LYS
1	F	74	LEU
1	F	80	GLU
1	F	105	ILE
1	F	135	LEU
1	F	145	VAL
1	F	158	TYR
1	F	168	LEU
1	F	197	LEU
1	F	210	GLU
1	F	218	LEU
1	F	233	LYS
1	F	245	LEU
1	F	256	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	35	GLN
1	A	48	GLN
1	A	67	ASN
1	A	70	HIS
1	A	86	ASN
1	A	214	GLN
1	A	224	GLN
1	A	231	ASN
1	B	32	GLN
1	B	67	ASN
1	B	70	HIS
1	B	100	GLN
1	C	66	GLN
1	C	67	ASN
1	C	187	ASN
1	C	224	GLN
1	D	30	GLN
1	D	66	GLN
1	D	70	HIS
1	D	86	ASN
1	D	224	GLN
1	D	265	HIS
1	E	67	ASN
1	E	70	HIS
1	E	86	ASN
1	E	159	ASN
1	E	216	GLN
1	E	231	ASN
1	F	35	GLN
1	F	66	GLN
1	F	67	ASN
1	F	70	HIS
1	F	86	ASN
1	F	139	ASN
1	F	224	GLN
1	F	231	ASN

5.3.3 RNA ⓘ

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GEQ	C	550	-	35,35,35	2.11	19 (54%)	51,51,51	1.78	11 (21%)
2	NAD	D	600	-	46,48,48	2.47	12 (26%)	64,73,73	2.14	24 (37%)
2	NAD	A	300	-	46,48,48	2.23	10 (21%)	64,73,73	2.12	21 (32%)
3	GEQ	A	350	-	35,35,35	2.10	20 (57%)	51,51,51	1.77	11 (21%)
2	NAD	F	750	-	46,48,48	2.18	11 (23%)	64,73,73	2.12	22 (34%)
2	NAD	B	400	-	46,48,48	2.15	12 (26%)	64,73,73	2.16	22 (34%)
3	GEQ	D	650	-	35,35,35	2.03	20 (57%)	51,51,51	1.76	12 (23%)
2	NAD	C	500	-	46,48,48	2.23	10 (21%)	64,73,73	2.12	19 (29%)
3	GEQ	B	450	-	35,35,35	2.08	19 (54%)	51,51,51	1.82	12 (23%)
2	NAD	E	700	-	46,48,48	2.26	10 (21%)	64,73,73	2.18	20 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GEQ	C	550	-	-	0/12/34/34	0/6/6/6
2	NAD	D	600	-	-	9/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	300	-	-	8/30/62/62	0/5/5/5
3	GEQ	A	350	-	-	0/12/34/34	0/6/6/6
2	NAD	F	750	-	-	6/30/62/62	0/5/5/5
2	NAD	B	400	-	-	3/30/62/62	0/5/5/5
3	GEQ	D	650	-	-	0/12/34/34	0/6/6/6
2	NAD	C	500	-	-	9/30/62/62	0/5/5/5
3	GEQ	B	450	-	-	0/12/34/34	0/6/6/6
2	NAD	E	700	-	-	11/30/62/62	0/5/5/5

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	NAD	PN-O3	-8.60	1.50	1.59
2	E	700	NAD	PN-O3	-8.30	1.50	1.59
2	A	300	NAD	PN-O3	-8.16	1.50	1.59
2	C	500	NAD	PN-O3	-7.77	1.51	1.59
2	F	750	NAD	PN-O3	-7.43	1.51	1.59
2	D	600	NAD	C2N-N1N	7.11	1.42	1.35
2	B	400	NAD	C2N-N1N	6.33	1.41	1.35
2	B	400	NAD	PN-O3	-6.22	1.52	1.59
2	E	700	NAD	C2N-N1N	6.22	1.41	1.35
2	C	500	NAD	C2N-N1N	5.91	1.41	1.35
2	F	750	NAD	C2N-N1N	5.64	1.41	1.35
2	A	300	NAD	C2N-N1N	5.63	1.41	1.35
2	D	600	NAD	PA-O3	-5.25	1.53	1.59
2	E	700	NAD	C4A-N3A	4.99	1.43	1.34
2	D	600	NAD	C2N-C3N	4.66	1.46	1.39
2	D	600	NAD	C4A-N3A	4.66	1.43	1.34
2	A	300	NAD	C4A-N3A	4.57	1.43	1.34
2	C	500	NAD	C4A-N3A	4.54	1.42	1.34
2	B	400	NAD	C4A-N3A	4.52	1.42	1.34
2	D	600	NAD	C4N-C3N	4.46	1.46	1.39
2	F	750	NAD	C4N-C3N	4.45	1.46	1.39
2	F	750	NAD	C4A-N3A	4.44	1.42	1.34
2	B	400	NAD	C2N-C3N	4.40	1.46	1.39
2	E	700	NAD	PA-O3	-4.34	1.54	1.59
2	B	400	NAD	C4N-C3N	4.26	1.45	1.39
2	A	300	NAD	PA-O3	-4.22	1.54	1.59
2	C	500	NAD	PA-O3	-4.09	1.55	1.59
2	C	500	NAD	C4N-C3N	4.08	1.45	1.39
2	A	300	NAD	C4N-C3N	3.99	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	750	NAD	PA-O3	-3.88	1.55	1.59
2	A	300	NAD	C2N-C3N	3.81	1.45	1.39
2	C	500	NAD	C2N-C3N	3.75	1.44	1.39
2	E	700	NAD	C4N-C3N	3.64	1.44	1.39
3	A	350	GEQ	C2F-C1F	3.60	1.44	1.39
3	B	450	GEQ	C2F-C1F	3.53	1.44	1.39
2	F	750	NAD	C2N-C3N	3.52	1.44	1.39
3	C	550	GEQ	C2F-C1F	3.51	1.44	1.39
2	E	700	NAD	C2N-C3N	3.26	1.44	1.39
3	B	450	GEQ	C1D-N4C	3.23	1.53	1.48
3	C	550	GEQ	C5C-N4C	3.19	1.53	1.47
3	B	450	GEQ	C1F-C1D	3.14	1.57	1.52
3	D	650	GEQ	C3A-C2A	3.10	1.44	1.39
2	B	400	NAD	PA-O3	-3.09	1.56	1.59
3	C	550	GEQ	C1D-N4C	3.02	1.53	1.48
3	A	350	GEQ	C1D-N4C	3.01	1.53	1.48
3	D	650	GEQ	C5C-N4C	2.97	1.52	1.47
3	D	650	GEQ	C1D-N4C	2.96	1.53	1.48
3	C	550	GEQ	C1F-C1D	2.94	1.56	1.52
3	C	550	GEQ	C3A-C2A	2.93	1.43	1.39
3	C	550	GEQ	C1A-C2A	2.90	1.43	1.39
3	A	350	GEQ	C3C-N4C	2.90	1.52	1.47
3	D	650	GEQ	C3C-N4C	2.88	1.52	1.47
3	D	650	GEQ	C2F-C1F	2.88	1.43	1.39
3	B	450	GEQ	C5C-N4C	2.87	1.52	1.47
3	B	450	GEQ	C6F-C6E	-2.81	1.39	1.46
3	B	450	GEQ	C2E-C1E	2.80	1.43	1.39
3	A	350	GEQ	C5C-N4C	2.79	1.52	1.47
3	D	650	GEQ	C1A-C2A	2.78	1.43	1.39
3	A	350	GEQ	C3A-C2A	2.76	1.43	1.39
3	A	350	GEQ	C1F-C1D	2.71	1.56	1.52
2	B	400	NAD	O2B-C2B	2.69	1.49	1.43
2	A	300	NAD	O2B-C2B	2.68	1.49	1.43
2	C	500	NAD	O4B-C4B	-2.67	1.39	1.45
3	A	350	GEQ	C1A-C2A	2.62	1.43	1.39
3	A	350	GEQ	C1B-N1C	2.61	1.40	1.34
2	D	600	NAD	O4B-C4B	-2.60	1.39	1.45
3	C	550	GEQ	C2E-C1E	2.58	1.42	1.39
3	C	550	GEQ	C3C-N4C	2.58	1.51	1.47
2	D	600	NAD	O2B-C2B	2.57	1.49	1.43
3	D	650	GEQ	C8A-C7A	2.56	1.40	1.36
3	D	650	GEQ	C1F-C1D	2.56	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	350	GEQ	C3F-C2F	2.56	1.43	1.38
2	C	500	NAD	O2B-C2B	2.56	1.49	1.43
3	A	350	GEQ	C3E-C2E	2.55	1.43	1.38
3	B	450	GEQ	C3A-C2A	2.55	1.43	1.39
2	E	700	NAD	O2B-C2B	2.54	1.49	1.43
3	C	550	GEQ	C3F-C2F	2.54	1.43	1.38
3	B	450	GEQ	C1A-C2A	2.53	1.43	1.39
3	B	450	GEQ	C4F-C5F	2.53	1.43	1.38
3	A	350	GEQ	C4F-C5F	2.53	1.43	1.38
3	B	450	GEQ	C3C-N4C	2.52	1.51	1.47
2	F	750	NAD	C5A-C4A	2.51	1.43	1.39
3	A	350	GEQ	C2E-C1E	2.51	1.42	1.39
3	D	650	GEQ	C2E-C1E	2.50	1.42	1.39
2	D	600	NAD	C5A-C4A	2.50	1.43	1.39
2	D	600	NAD	O3D-C3D	2.50	1.49	1.43
3	C	550	GEQ	C8A-C7A	2.49	1.40	1.36
3	A	350	GEQ	C8A-C7A	2.49	1.40	1.36
2	F	750	NAD	O4B-C4B	-2.48	1.39	1.45
2	B	400	NAD	O3D-C3D	2.48	1.49	1.43
2	F	750	NAD	O2B-C2B	2.47	1.49	1.43
3	A	350	GEQ	C6F-C6E	-2.47	1.40	1.46
3	C	550	GEQ	C4F-C5F	2.47	1.43	1.38
3	A	350	GEQ	C5F-C6F	2.46	1.43	1.40
3	D	650	GEQ	C5F-C6F	2.46	1.43	1.40
3	C	550	GEQ	C3E-C2E	2.45	1.43	1.38
2	B	400	NAD	O4B-C4B	-2.45	1.39	1.45
3	D	650	GEQ	C3F-C2F	2.41	1.43	1.38
3	C	550	GEQ	C6F-C6E	-2.40	1.40	1.46
2	F	750	NAD	O3D-C3D	2.40	1.48	1.43
2	C	500	NAD	O3D-C3D	2.40	1.48	1.43
3	B	450	GEQ	C4E-C5E	2.40	1.43	1.38
3	D	650	GEQ	C6F-C6E	-2.40	1.40	1.46
3	B	450	GEQ	C8A-C7A	2.37	1.40	1.36
3	B	450	GEQ	C3F-C2F	2.37	1.43	1.38
3	B	450	GEQ	C4E-C3E	2.36	1.43	1.38
3	A	350	GEQ	C4E-C5E	2.36	1.42	1.38
3	B	450	GEQ	C3E-C2E	2.35	1.42	1.38
3	C	550	GEQ	C4E-C3E	2.34	1.43	1.38
2	A	300	NAD	C5A-C4A	2.34	1.43	1.39
3	C	550	GEQ	C5F-C6F	2.33	1.43	1.40
3	D	650	GEQ	C4F-C5F	2.33	1.42	1.38
2	E	700	NAD	C5A-C4A	2.28	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	450	GEQ	C5F-C6F	2.28	1.43	1.40
3	D	650	GEQ	C3E-C2E	2.28	1.42	1.38
3	B	450	GEQ	C4A-C3A	2.26	1.42	1.38
3	C	550	GEQ	C4F-C3F	2.26	1.43	1.38
3	D	650	GEQ	C4A-C3A	2.24	1.42	1.38
3	A	350	GEQ	C4E-C3E	2.24	1.43	1.38
2	A	300	NAD	O3D-C3D	2.23	1.48	1.43
2	E	700	NAD	C2B-C1B	2.21	1.60	1.53
3	B	450	GEQ	C4F-C3F	2.21	1.43	1.38
3	D	650	GEQ	C4E-C5E	2.21	1.42	1.38
3	D	650	GEQ	C2A-C1B	2.20	1.53	1.50
3	C	550	GEQ	C4E-C5E	2.18	1.42	1.38
3	A	350	GEQ	C4F-C3F	2.17	1.43	1.38
2	A	300	NAD	C2B-C1B	2.17	1.60	1.53
3	C	550	GEQ	C4A-C3A	2.16	1.42	1.38
3	D	650	GEQ	C4E-C3E	2.14	1.42	1.38
3	D	650	GEQ	C4F-C3F	2.14	1.42	1.38
3	A	350	GEQ	C5E-C6E	2.12	1.43	1.40
2	B	400	NAD	C5A-C4A	2.10	1.42	1.39
2	B	400	NAD	C2B-C1B	2.10	1.60	1.53
3	A	350	GEQ	C5A-N9A	-2.07	1.34	1.37
2	C	500	NAD	C5A-C4A	2.07	1.42	1.39
2	E	700	NAD	C5N-C4N	2.07	1.42	1.38
2	D	600	NAD	C5N-C4N	2.07	1.42	1.38
2	D	600	NAD	C2B-C1B	2.06	1.60	1.53
3	D	650	GEQ	C5E-C6E	2.05	1.43	1.40
3	B	450	GEQ	C5A-N9A	-2.03	1.34	1.37
2	F	750	NAD	C2B-C1B	2.03	1.59	1.53
3	C	550	GEQ	C5E-C6E	2.03	1.43	1.40
2	B	400	NAD	C6A-N6A	-2.01	1.29	1.34

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	450	GEQ	C1F-C1D-C1E	-6.45	97.25	102.06
3	D	650	GEQ	C1F-C1D-C1E	-6.27	97.38	102.06
3	C	550	GEQ	C1F-C1D-C1E	-6.07	97.53	102.06
3	A	350	GEQ	C1F-C1D-C1E	-6.05	97.54	102.06
2	C	500	NAD	C6A-C5A-C4A	-5.37	109.84	117.18
2	D	600	NAD	C6A-C5A-C4A	-5.36	109.86	117.18
2	E	700	NAD	O7N-C7N-N7N	-5.33	114.91	122.62
2	F	750	NAD	C6A-C5A-C4A	-5.29	109.96	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NAD	C6A-C5A-C4A	-5.27	109.98	117.18
2	B	400	NAD	C6A-C5A-C4A	-5.24	110.02	117.18
2	E	700	NAD	C6A-C5A-C4A	-5.24	110.03	117.18
2	D	600	NAD	O7N-C7N-N7N	-5.19	115.11	122.62
2	B	400	NAD	O7N-C7N-N7N	-5.12	115.21	122.62
2	A	300	NAD	O7N-C7N-N7N	-5.11	115.23	122.62
2	C	500	NAD	O3B-C3B-C4B	5.02	125.50	111.08
2	F	750	NAD	O7N-C7N-N7N	-5.00	115.39	122.62
2	C	500	NAD	O7N-C7N-N7N	-4.96	115.45	122.62
2	A	300	NAD	O3B-C3B-C4B	4.82	124.93	111.08
2	D	600	NAD	O3B-C3B-C4B	4.79	124.84	111.08
2	E	700	NAD	O3B-C3B-C4B	4.70	124.58	111.08
2	B	400	NAD	O3B-C3B-C4B	4.67	124.49	111.08
2	F	750	NAD	O3B-C3B-C4B	4.65	124.44	111.08
2	E	700	NAD	O7N-C7N-C3N	4.61	125.23	119.60
3	C	550	GEQ	C2A-C1B-N1C	4.61	124.41	118.66
3	A	350	GEQ	C2A-C1B-N1C	4.34	124.08	118.66
3	B	450	GEQ	C2A-C1B-N1C	4.29	124.02	118.66
3	D	650	GEQ	C2A-C1B-N1C	4.25	123.97	118.66
2	A	300	NAD	O7N-C7N-C3N	4.14	124.66	119.60
2	B	400	NAD	O7N-C7N-C3N	4.13	124.65	119.60
2	D	600	NAD	O7N-C7N-C3N	4.12	124.64	119.60
2	F	750	NAD	O7N-C7N-C3N	4.12	124.64	119.60
2	E	700	NAD	C6A-C5A-N7A	4.08	139.95	132.09
2	D	600	NAD	C6A-C5A-N7A	4.05	139.90	132.09
2	C	500	NAD	C6A-C5A-N7A	4.05	139.89	132.09
2	F	750	NAD	C6A-C5A-N7A	4.00	139.80	132.09
2	A	300	NAD	C6A-C5A-N7A	4.00	139.79	132.09
2	C	500	NAD	O7N-C7N-C3N	3.90	124.37	119.60
2	B	400	NAD	C6A-C5A-N7A	3.86	139.54	132.09
3	D	650	GEQ	C6C-N1C-C2C	3.68	120.18	112.68
2	C	500	NAD	N3A-C2A-N1A	-3.64	123.07	128.58
2	B	400	NAD	N3A-C2A-N1A	-3.60	123.13	128.58
2	D	600	NAD	N6A-C6A-N1A	-3.60	110.36	118.38
2	E	700	NAD	N6A-C6A-N1A	-3.59	110.38	118.38
2	E	700	NAD	N3A-C2A-N1A	-3.59	123.15	128.58
2	B	400	NAD	C6N-N1N-C2N	-3.58	118.83	121.88
2	F	750	NAD	N3A-C2A-N1A	-3.57	123.18	128.58
2	A	300	NAD	N6A-C6A-N1A	-3.54	110.48	118.38
2	F	750	NAD	N6A-C6A-N1A	-3.53	110.52	118.38
2	D	600	NAD	C6N-N1N-C2N	-3.50	118.90	121.88
2	A	300	NAD	N3A-C2A-N1A	-3.48	123.31	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	NAD	N3A-C2A-N1A	-3.48	123.31	128.58
2	C	500	NAD	N6A-C6A-N1A	-3.41	110.78	118.38
3	C	550	GEQ	C5C-N4C-C3C	3.41	115.63	109.13
2	A	300	NAD	C6N-N1N-C2N	-3.41	118.98	121.88
2	B	400	NAD	N6A-C6A-N1A	-3.40	110.81	118.38
3	B	450	GEQ	C6C-N1C-C2C	3.39	119.59	112.68
2	B	400	NAD	O2N-PN-O3	3.38	116.42	107.27
2	C	500	NAD	C4A-N9A-C8A	3.35	109.25	105.74
2	E	700	NAD	O2N-PN-O3	3.34	116.30	107.27
2	F	750	NAD	O2B-C2B-C3B	3.33	122.50	111.82
3	C	550	GEQ	C6C-N1C-C2C	3.32	119.45	112.68
2	B	400	NAD	O2B-C2B-C3B	3.31	122.42	111.82
2	B	400	NAD	C4A-N9A-C8A	3.30	109.20	105.74
2	A	300	NAD	O2N-PN-O3	3.29	116.18	107.27
2	C	500	NAD	C6N-N1N-C2N	-3.29	119.08	121.88
2	C	500	NAD	O2B-C2B-C3B	3.29	122.35	111.82
2	E	700	NAD	O3-PN-O1N	-3.26	100.90	110.70
2	E	700	NAD	C6N-N1N-C2N	-3.26	119.11	121.88
3	A	350	GEQ	C6C-N1C-C2C	3.25	119.31	112.68
2	E	700	NAD	C4A-N9A-C8A	3.24	109.14	105.74
2	B	400	NAD	C5A-C6A-N1A	3.24	125.73	117.51
2	D	600	NAD	O2B-C2B-C3B	3.22	122.13	111.82
2	F	750	NAD	O2N-PN-O3	3.20	115.92	107.27
2	C	500	NAD	O2N-PN-O3	3.18	115.87	107.27
2	A	300	NAD	C4A-N9A-C8A	3.16	109.06	105.74
2	E	700	NAD	C5A-C6A-N1A	3.16	125.53	117.51
3	B	450	GEQ	C5C-N4C-C3C	3.15	115.14	109.13
2	F	750	NAD	C5A-C6A-N1A	3.14	125.49	117.51
2	A	300	NAD	C5A-C6A-N1A	3.13	125.46	117.51
2	E	700	NAD	O5D-PN-O1N	-3.13	96.55	108.94
2	D	600	NAD	C5A-C6A-N1A	3.12	125.43	117.51
2	D	600	NAD	C4A-N9A-C8A	3.09	108.99	105.74
2	F	750	NAD	C6N-N1N-C2N	-3.09	119.25	121.88
2	C	500	NAD	C5A-C6A-N1A	3.08	125.34	117.51
3	A	350	GEQ	O2B-C1B-C2A	-3.05	114.23	120.29
3	D	650	GEQ	C6E-C1E-C1D	3.01	112.62	110.18
3	A	350	GEQ	C1E-C1D-N4C	-3.00	110.80	117.64
3	D	650	GEQ	C1E-C1D-N4C	-2.98	110.84	117.64
2	B	400	NAD	O3-PN-O1N	-2.96	101.79	110.70
2	A	300	NAD	O2B-C2B-C3B	2.96	121.31	111.82
2	E	700	NAD	C4B-O4B-C1B	-2.95	102.95	109.47
3	B	450	GEQ	C6E-C1E-C1D	2.91	112.54	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	NAD	O2N-PN-O3	2.89	115.09	107.27
2	F	750	NAD	C4A-N9A-C8A	2.89	108.77	105.74
3	D	650	GEQ	C5C-N4C-C3C	2.88	114.63	109.13
3	B	450	GEQ	O2B-C1B-C2A	-2.88	114.58	120.29
3	A	350	GEQ	C1A-C6A-C5A	2.87	120.91	119.13
3	C	550	GEQ	O2B-C1B-C2A	-2.86	114.62	120.29
3	A	350	GEQ	C5C-N4C-C3C	2.86	114.57	109.13
3	B	450	GEQ	C1E-C1D-N4C	-2.84	111.17	117.64
3	A	350	GEQ	C6E-C1E-C1D	2.84	112.48	110.18
2	B	400	NAD	O5D-PN-O1N	-2.82	97.74	108.94
2	D	600	NAD	C2N-N1N-C1D	2.82	125.36	119.13
2	B	400	NAD	C2N-N1N-C1D	2.79	125.29	119.13
2	A	300	NAD	O3-PA-O1A	-2.78	102.35	110.70
2	C	500	NAD	O3-PN-O1N	-2.78	102.36	110.70
3	C	550	GEQ	C6E-C1E-C1D	2.77	112.43	110.18
2	E	700	NAD	O2B-C2B-C3B	2.76	120.67	111.82
2	E	700	NAD	O3-PA-O1A	-2.73	102.50	110.70
2	F	750	NAD	O3-PA-O1A	-2.72	102.51	110.70
3	D	650	GEQ	C1A-C6A-C5A	2.69	120.79	119.13
3	A	350	GEQ	C6A-C5A-N9A	2.69	109.69	107.53
2	A	300	NAD	C4B-O4B-C1B	-2.67	103.56	109.47
2	F	750	NAD	O2D-C2D-C3D	2.66	120.36	111.82
2	B	400	NAD	C4B-O4B-C1B	-2.64	103.63	109.47
2	D	600	NAD	O3-PN-O1N	-2.64	102.76	110.70
2	D	600	NAD	C4B-O4B-C1B	-2.59	103.75	109.47
3	D	650	GEQ	O2B-C1B-C2A	-2.59	115.16	120.29
2	C	500	NAD	C4B-O4B-C1B	-2.57	103.78	109.47
2	C	500	NAD	C2N-N1N-C1D	2.55	124.76	119.13
3	C	550	GEQ	C1E-C1D-N4C	-2.53	111.88	117.64
2	A	300	NAD	O5D-PN-O1N	-2.52	98.95	108.94
2	A	300	NAD	C2N-N1N-C1D	2.51	124.67	119.13
2	F	750	NAD	O4B-C4B-C3B	-2.50	100.19	105.15
2	D	600	NAD	O3-PA-O1A	-2.50	103.19	110.70
3	C	550	GEQ	C6C-C5C-N4C	2.49	115.00	110.61
2	C	500	NAD	O5D-PN-O1N	-2.49	99.07	108.94
3	B	450	GEQ	C1A-C6A-C5A	2.46	120.65	119.13
2	F	750	NAD	O3D-C3D-C2D	2.44	119.65	111.82
2	B	400	NAD	O2D-C2D-C3D	2.43	119.62	111.82
2	E	700	NAD	O2D-C2D-C3D	2.43	119.60	111.82
3	C	550	GEQ	C1A-C6A-C5A	2.41	120.62	119.13
2	F	750	NAD	O3-PN-O1N	-2.41	103.46	110.70
2	F	750	NAD	C2N-N1N-C1D	2.41	124.44	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAD	O4B-C4B-C3B	-2.38	100.42	105.15
2	F	750	NAD	C4B-O4B-C1B	-2.37	104.23	109.47
2	A	300	NAD	O3-PN-O1N	-2.36	103.61	110.70
3	C	550	GEQ	C6A-C5A-N9A	2.36	109.42	107.53
2	D	600	NAD	O4B-C4B-C3B	-2.33	100.53	105.15
2	D	600	NAD	O5D-PN-O1N	-2.33	99.71	108.94
3	B	450	GEQ	C6C-C5C-N4C	2.32	114.70	110.61
3	D	650	GEQ	C6A-C5A-N9A	2.31	109.38	107.53
2	F	750	NAD	O5D-PN-O1N	-2.28	99.90	108.94
2	A	300	NAD	O4B-C4B-C3B	-2.28	100.63	105.15
2	A	300	NAD	O2D-C2D-C3D	2.26	119.07	111.82
3	B	450	GEQ	C6A-C5A-N9A	2.25	109.33	107.53
2	B	400	NAD	C5N-C6N-N1N	2.24	123.44	120.38
2	E	700	NAD	O4B-C4B-C3B	-2.24	100.71	105.15
2	B	400	NAD	O3-PA-O1A	-2.23	104.00	110.70
2	C	500	NAD	O4B-C4B-C3B	-2.21	100.76	105.15
3	A	350	GEQ	C6A-C1A-C2A	-2.18	117.88	121.32
2	D	600	NAD	O3D-C3D-C2D	2.18	118.82	111.82
2	C	500	NAD	O3-PA-O1A	-2.17	104.16	110.70
2	D	600	NAD	O2D-C2D-C3D	2.17	118.78	111.82
2	D	600	NAD	C5N-C6N-N1N	2.17	123.34	120.38
2	B	400	NAD	O3D-C3D-C2D	2.15	118.71	111.82
3	D	650	GEQ	C6F-C1F-C1D	2.14	111.92	110.18
2	E	700	NAD	O2B-C2B-C1B	2.13	117.43	110.10
2	E	700	NAD	C2N-N1N-C1D	2.12	123.81	119.13
3	D	650	GEQ	C6A-C1A-C2A	-2.10	118.01	121.32
2	F	750	NAD	C5N-C6N-N1N	2.10	123.25	120.38
2	B	400	NAD	O2B-C2B-C1B	2.10	117.33	110.10
2	F	750	NAD	C2D-C3D-C4D	-2.07	98.60	102.61
3	B	450	GEQ	C3E-C2E-C1E	-2.06	118.52	120.99
2	A	300	NAD	O2B-C2B-C1B	2.06	117.19	110.10
3	D	650	GEQ	C6C-C5C-N4C	2.05	114.22	110.61
2	D	600	NAD	O2B-C2B-C1B	2.05	117.16	110.10
3	B	450	GEQ	C6F-C1F-C1D	2.05	111.84	110.18
2	A	300	NAD	C5N-C6N-N1N	2.04	123.17	120.38
2	D	600	NAD	C3N-C7N-N7N	2.04	120.25	117.74
2	D	600	NAD	C6N-N1N-C1D	-2.03	115.73	119.73
3	A	350	GEQ	C6F-C1F-C1D	2.03	111.83	110.18
3	C	550	GEQ	C3E-C2E-C1E	-2.01	118.58	120.99
2	C	500	NAD	C5N-C6N-N1N	2.01	123.12	120.38

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAD	O4D-C1D-N1N-C2N
2	A	300	NAD	O4D-C1D-N1N-C6N
2	A	300	NAD	C2D-C1D-N1N-C2N
2	A	300	NAD	C2D-C1D-N1N-C6N
2	C	500	NAD	C5D-O5D-PN-O3
2	C	500	NAD	O4D-C1D-N1N-C2N
2	C	500	NAD	O4D-C1D-N1N-C6N
2	D	600	NAD	O4D-C4D-C5D-O5D
2	D	600	NAD	O4D-C1D-N1N-C2N
2	D	600	NAD	O4D-C1D-N1N-C6N
2	D	600	NAD	C2D-C1D-N1N-C2N
2	D	600	NAD	C2D-C1D-N1N-C6N
2	E	700	NAD	C5D-O5D-PN-O3
2	E	700	NAD	C5D-O5D-PN-O2N
2	E	700	NAD	O4D-C1D-N1N-C2N
2	E	700	NAD	O4D-C1D-N1N-C6N
2	E	700	NAD	C2D-C1D-N1N-C2N
2	E	700	NAD	C2D-C1D-N1N-C6N
2	F	750	NAD	O4D-C4D-C5D-O5D
2	F	750	NAD	O4D-C1D-N1N-C2N
2	A	300	NAD	O4D-C4D-C5D-O5D
2	F	750	NAD	C3D-C4D-C5D-O5D
2	D	600	NAD	C3D-C4D-C5D-O5D
2	E	700	NAD	O4D-C4D-C5D-O5D
2	A	300	NAD	C3D-C4D-C5D-O5D
2	E	700	NAD	C3D-C4D-C5D-O5D
2	A	300	NAD	PA-O3-PN-O1N
2	E	700	NAD	PA-O3-PN-O1N
2	F	750	NAD	PA-O3-PN-O1N
2	C	500	NAD	C5D-O5D-PN-O1N
2	E	700	NAD	C5D-O5D-PN-O1N
2	C	500	NAD	PA-O3-PN-O2N
2	C	500	NAD	C2D-C1D-N1N-C2N
2	C	500	NAD	C2D-C1D-N1N-C6N
2	B	400	NAD	O4D-C1D-N1N-C2N
2	B	400	NAD	O4D-C1D-N1N-C6N
2	F	750	NAD	O4D-C1D-N1N-C6N
2	D	600	NAD	O4B-C4B-C5B-O5B
2	A	300	NAD	O4B-C4B-C5B-O5B
2	E	700	NAD	O4B-C4B-C5B-O5B
2	C	500	NAD	PA-O3-PN-O1N
2	D	600	NAD	PA-O3-PN-O2N

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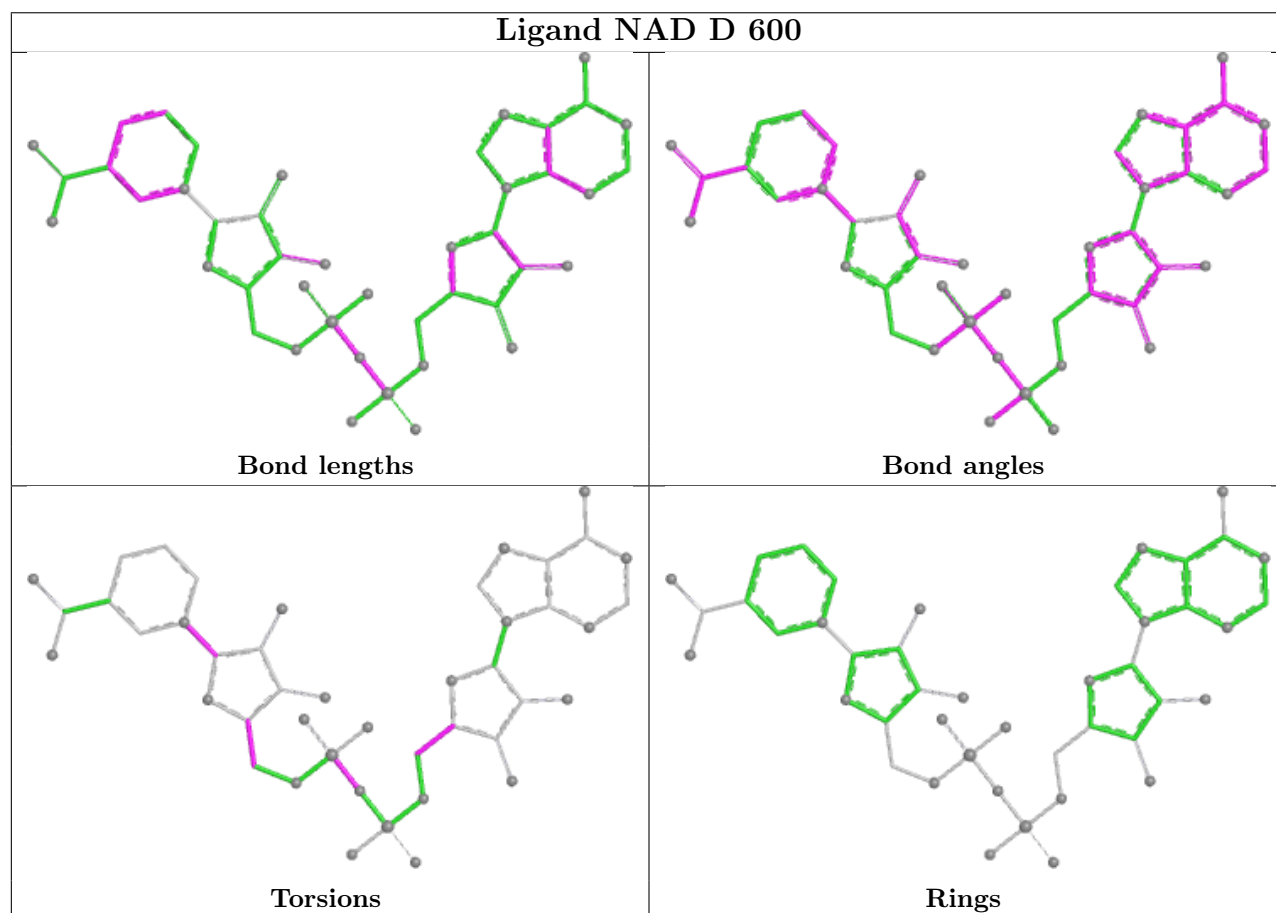
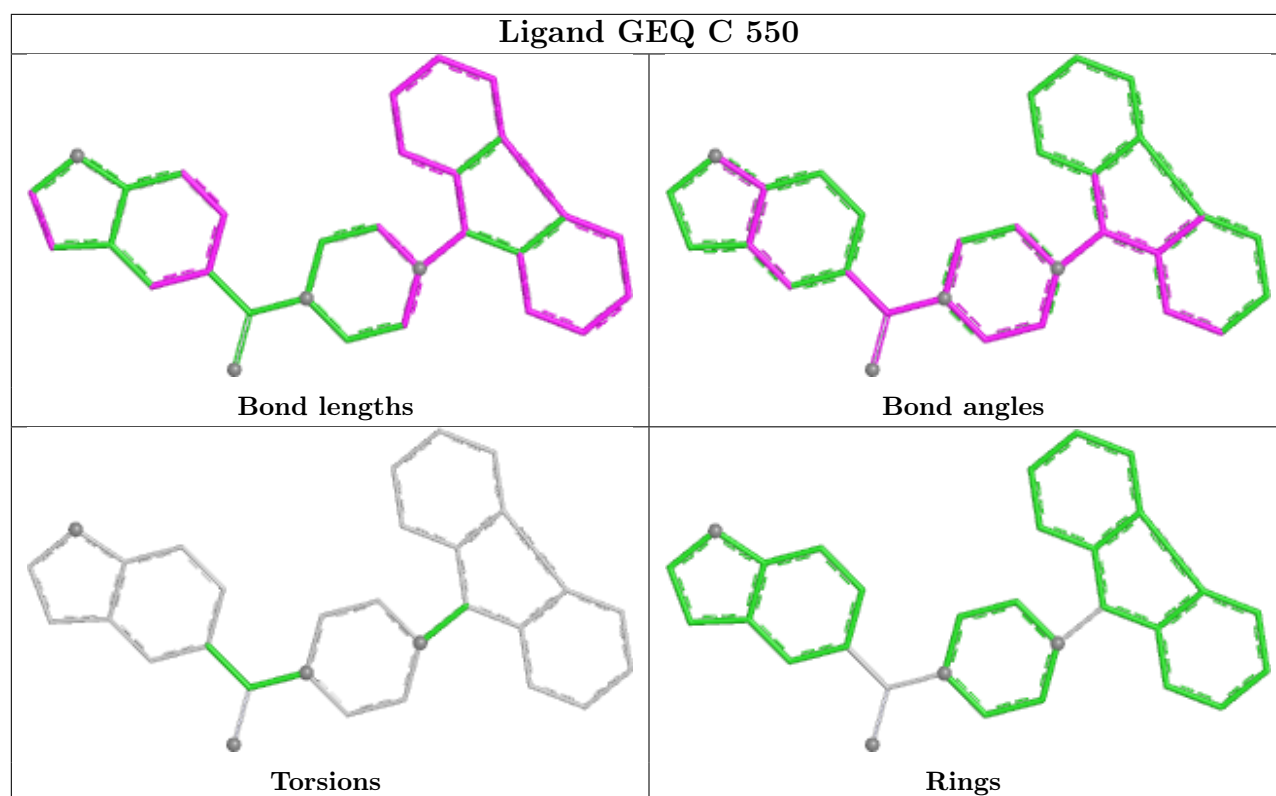
Mol	Chain	Res	Type	Atoms
2	B	400	NAD	O4B-C4B-C5B-O5B
2	C	500	NAD	O4B-C4B-C5B-O5B
2	F	750	NAD	O4B-C4B-C5B-O5B
2	D	600	NAD	PA-O3-PN-O1N

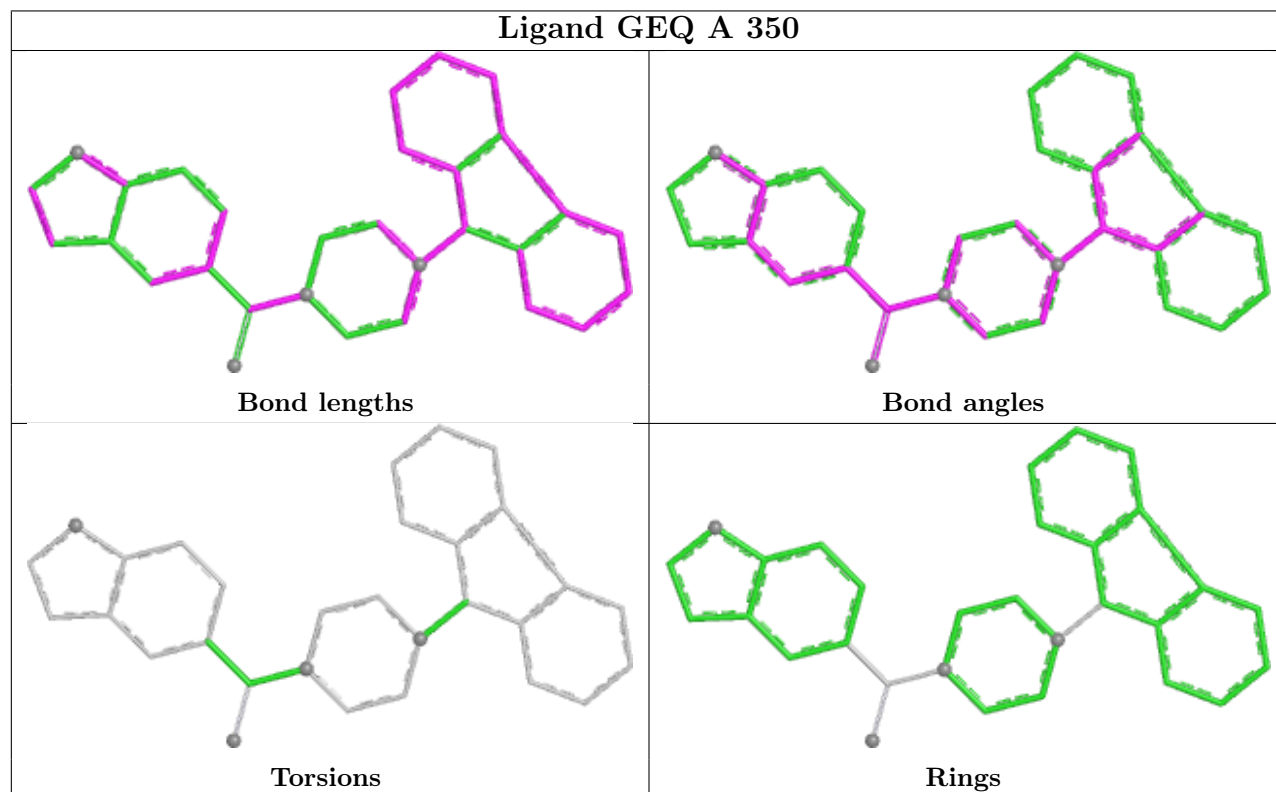
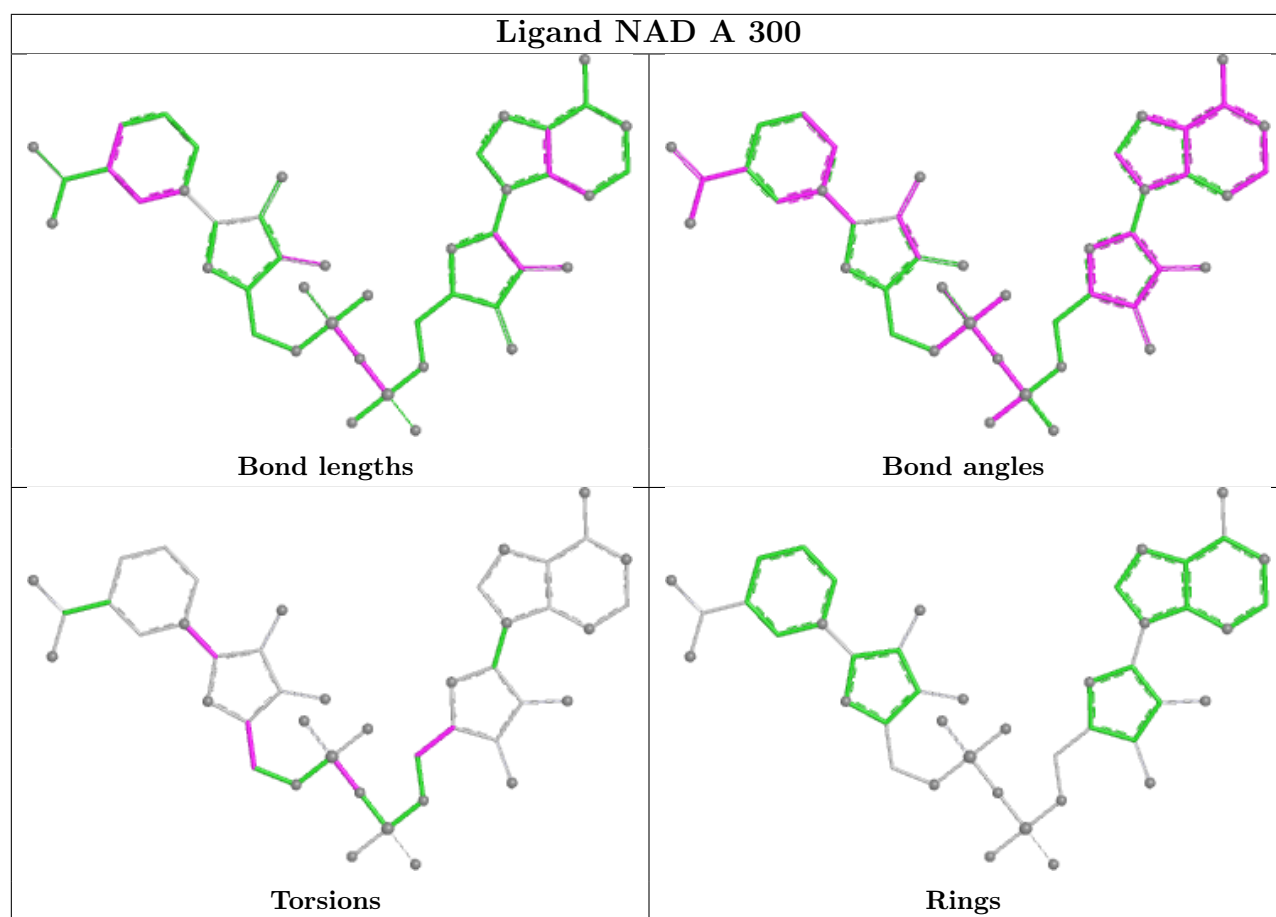
There are no ring outliers.

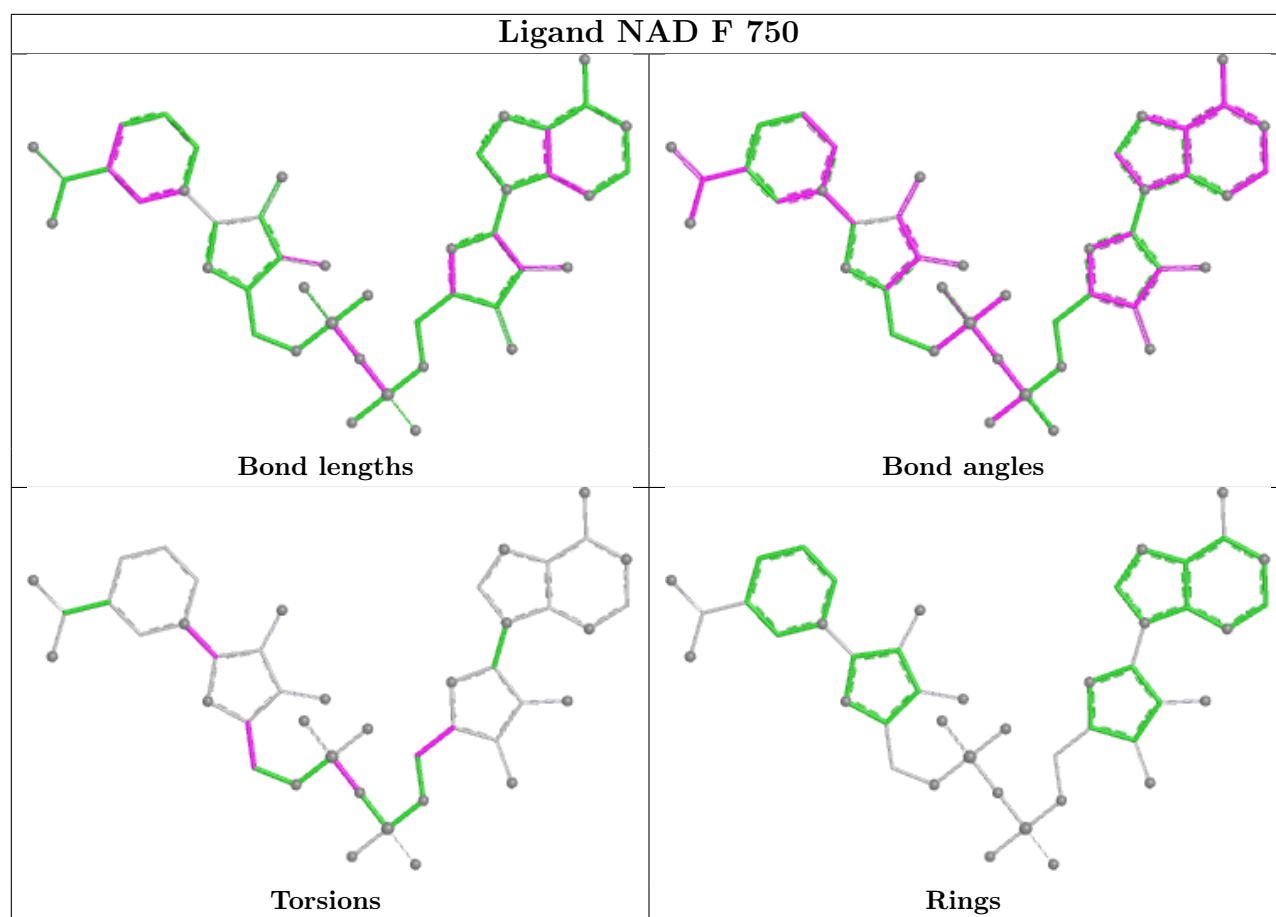
10 monomers are involved in 31 short contacts:

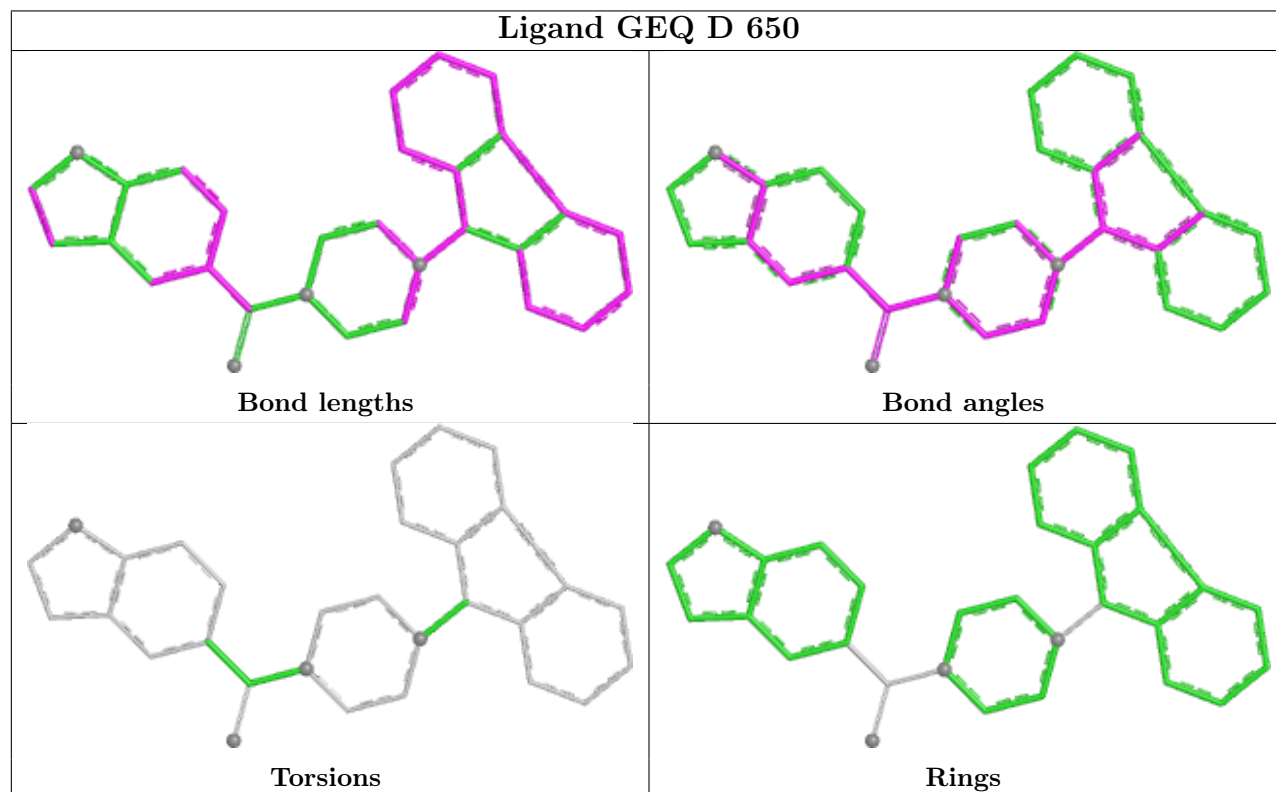
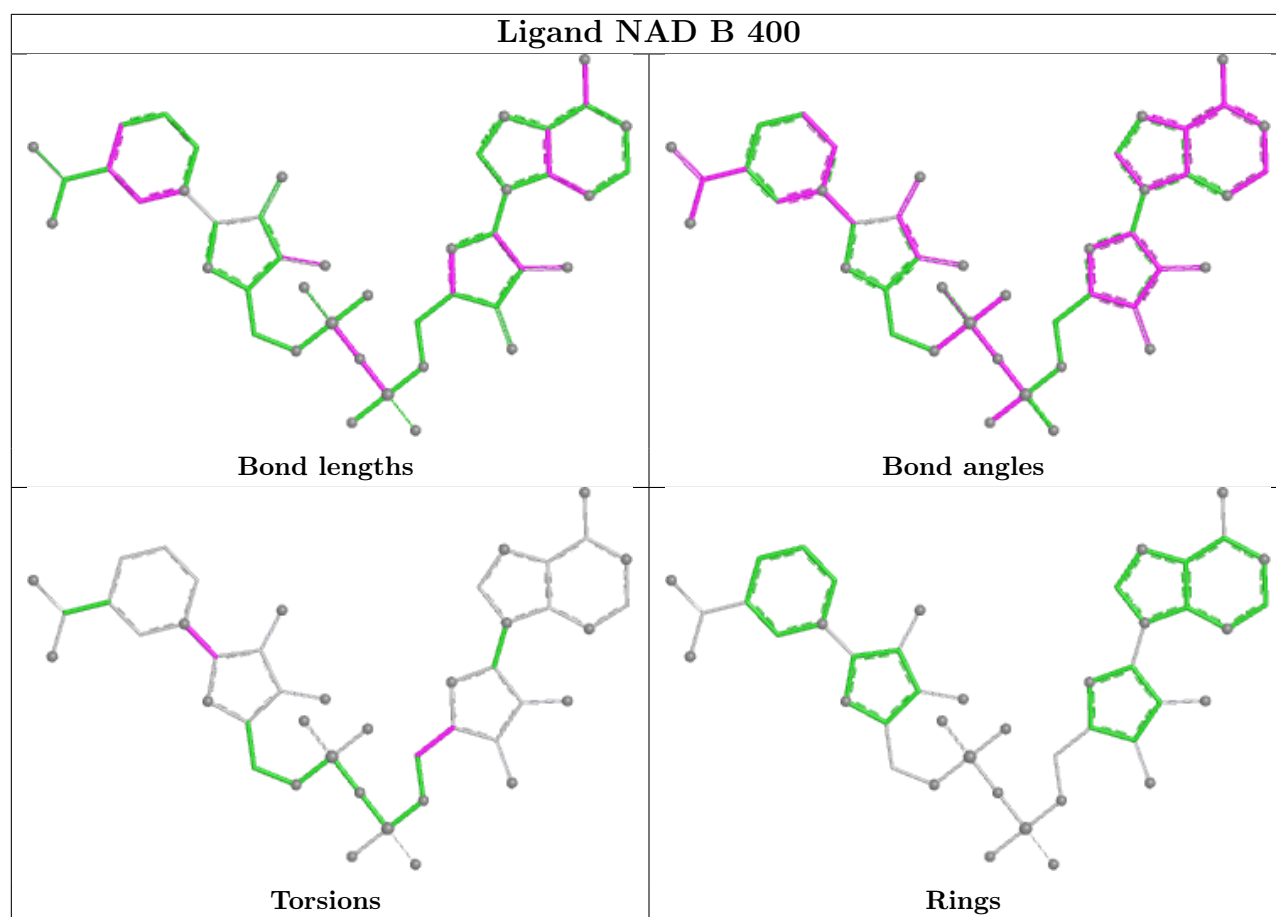
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	550	GEQ	2	0
2	D	600	NAD	4	0
2	A	300	NAD	8	0
3	A	350	GEQ	2	0
2	F	750	NAD	1	0
2	B	400	NAD	3	0
3	D	650	GEQ	1	0
2	C	500	NAD	3	0
3	B	450	GEQ	5	0
2	E	700	NAD	4	0

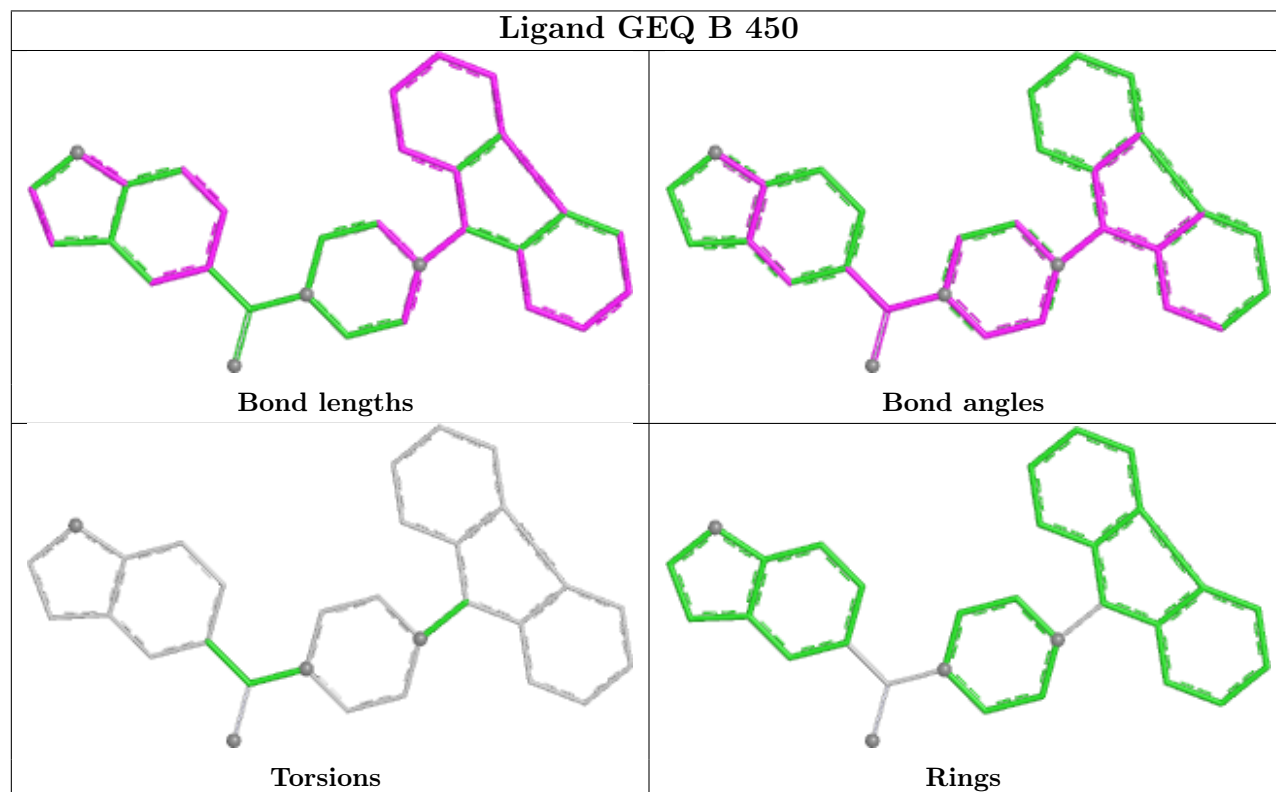
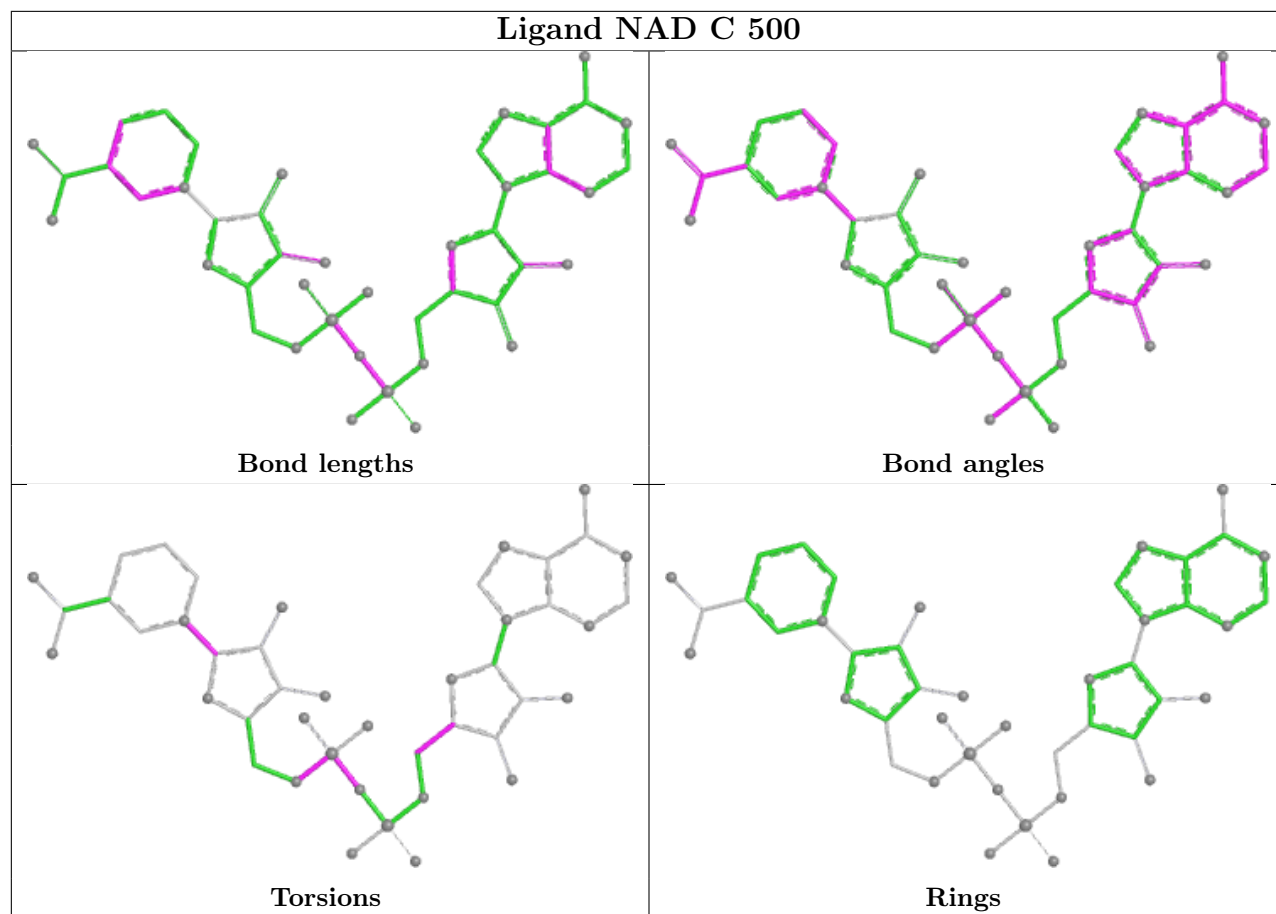
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

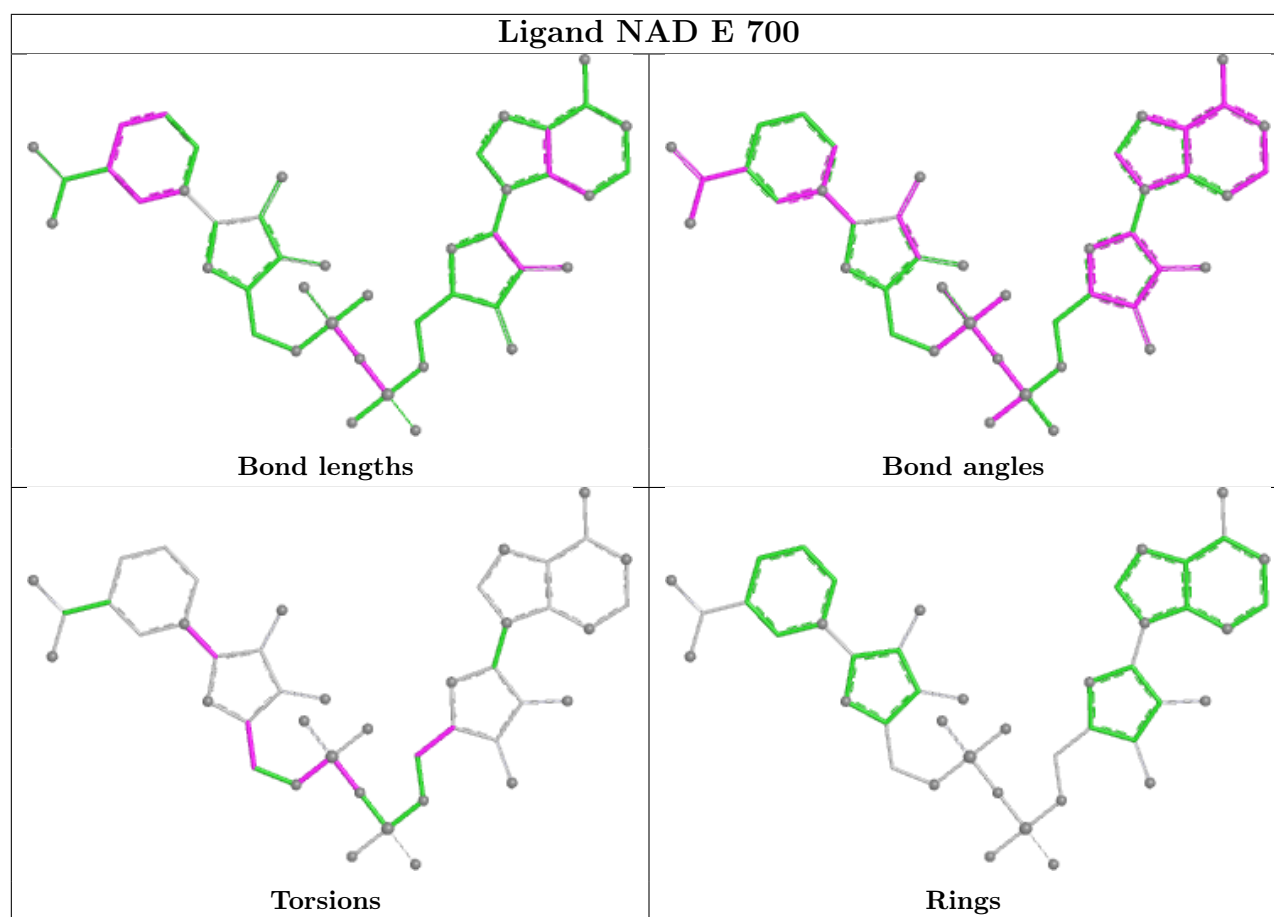












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	268/269 (99%)	-1.78	0 100 100	3, 12, 54, 87	0
1	B	268/269 (99%)	-1.79	0 100 100	3, 13, 53, 80	0
1	C	268/269 (99%)	-1.68	0 100 100	9, 30, 61, 70	0
1	D	268/269 (99%)	-1.64	0 100 100	13, 34, 82, 102	0
1	E	268/269 (99%)	-1.70	0 100 100	8, 28, 55, 68	0
1	F	268/269 (99%)	-1.69	0 100 100	6, 26, 59, 88	0
All	All	1608/1614 (99%)	-1.71	0 100 100	3, 25, 61, 102	0

There are no RSRZ outliers to report.

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.

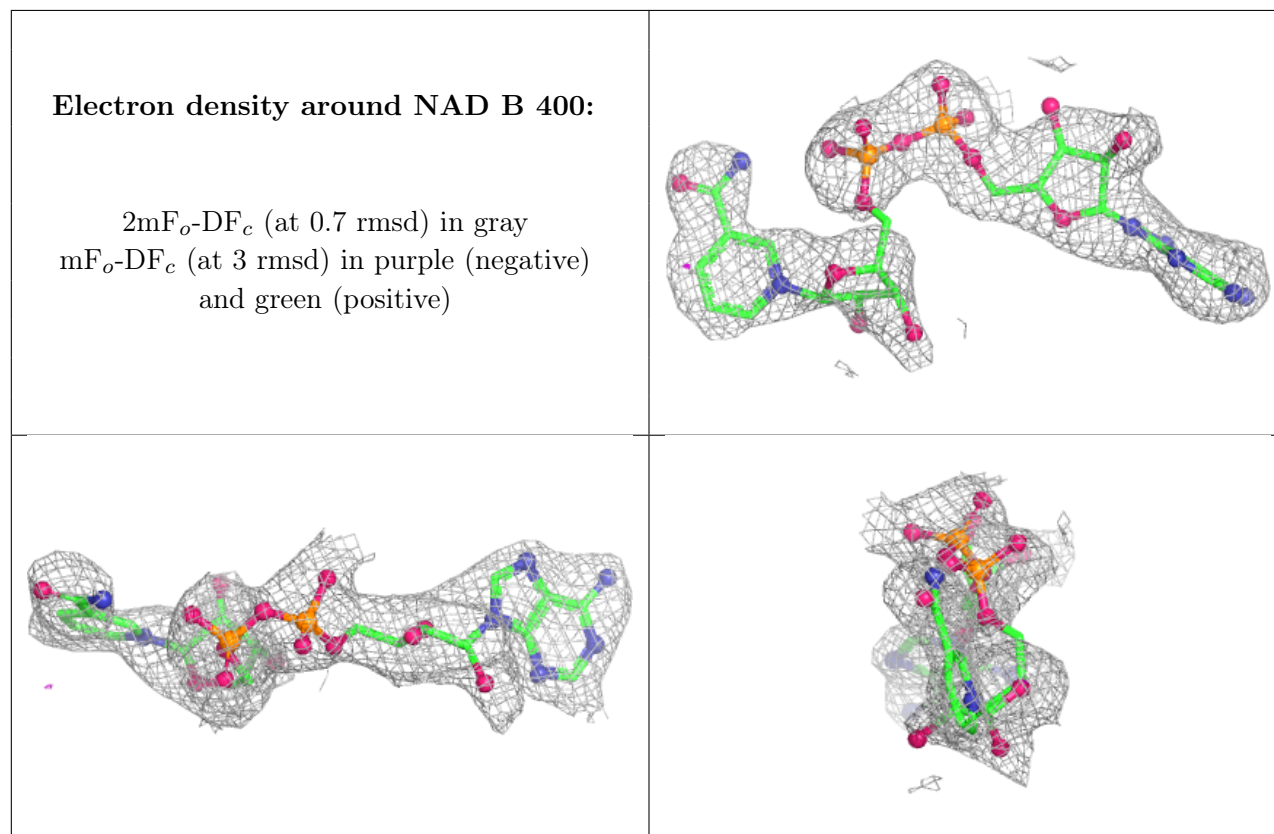
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	B	400	44/44	0.99	0.03	34,42,45,45	0

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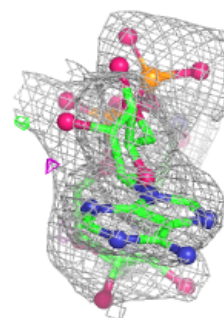
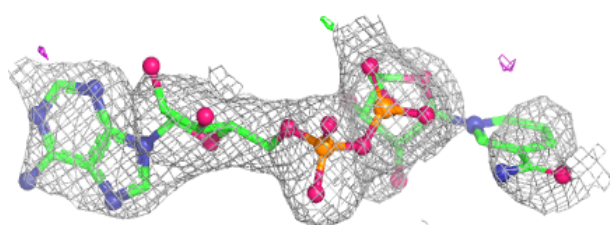
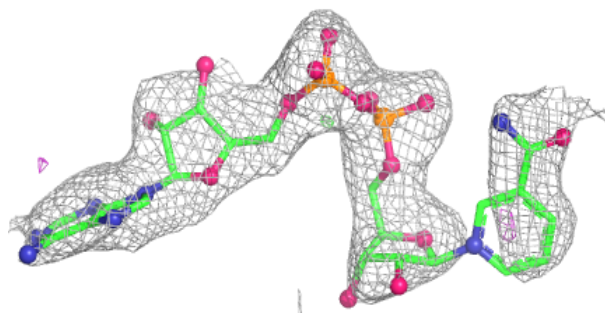
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	C	500	44/44	0.99	0.03	47,53,56,57	0
2	NAD	D	600	44/44	0.99	0.04	54,64,72,73	0
2	NAD	E	700	44/44	0.99	0.03	19,34,39,41	0
2	NAD	F	750	44/44	0.99	0.03	43,47,49,51	0
3	GEQ	A	350	30/30	0.99	0.04	42,52,56,56	0
3	GEQ	B	450	30/30	0.99	0.04	46,51,57,58	0
3	GEQ	C	550	30/30	0.99	0.04	57,61,64,64	0
3	GEQ	D	650	30/30	0.99	0.04	58,62,71,72	0
2	NAD	A	300	44/44	1.00	0.02	29,37,47,48	0

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

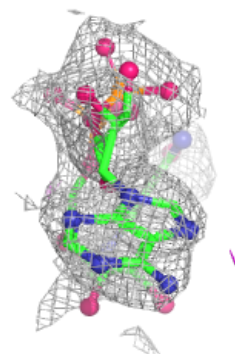
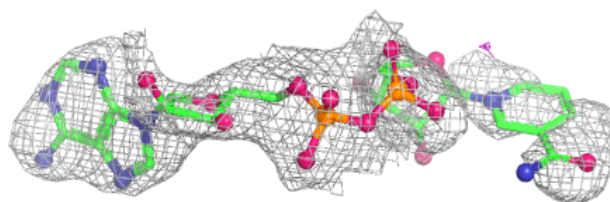
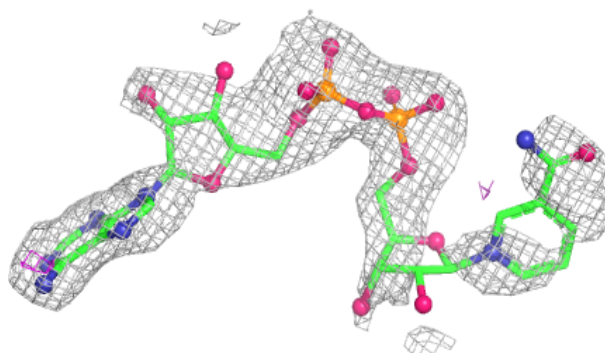


Electron density around NAD C 500:

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

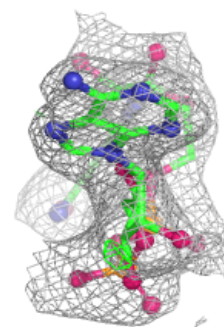
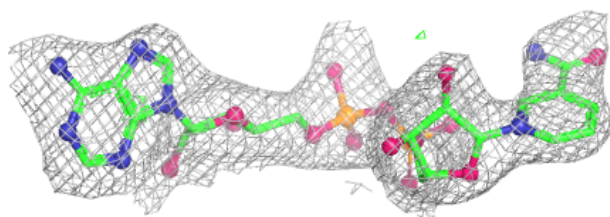
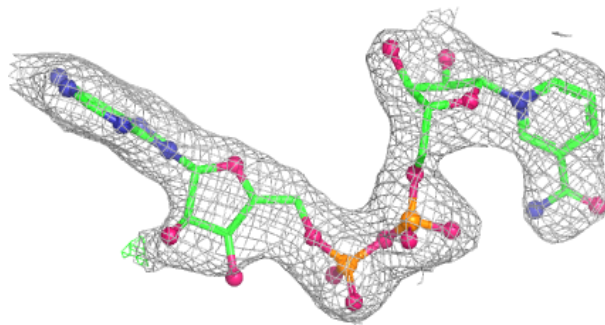
**Electron density around NAD D 600:**

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

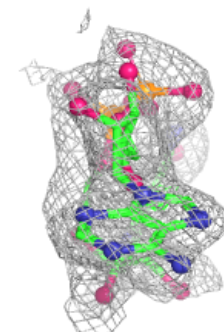
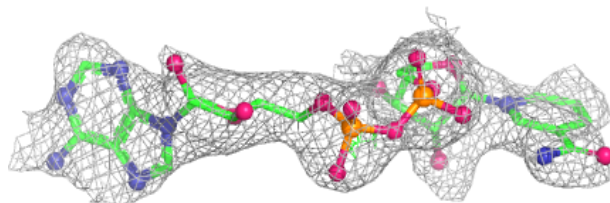
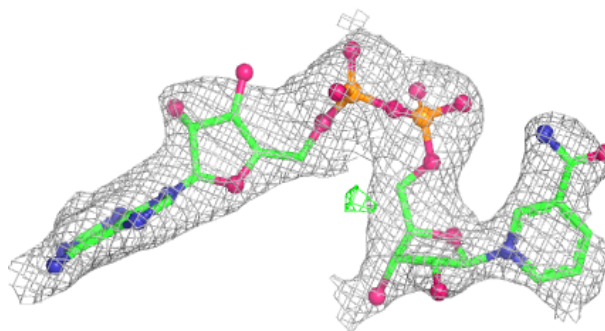


Electron density around NAD E 700:

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

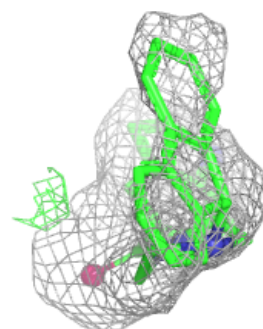
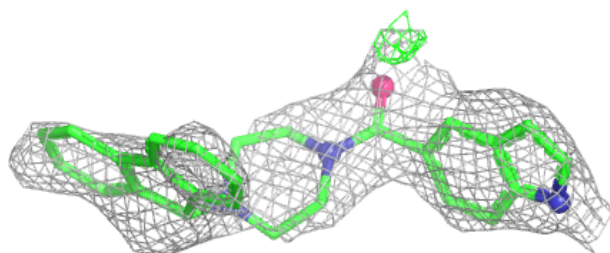
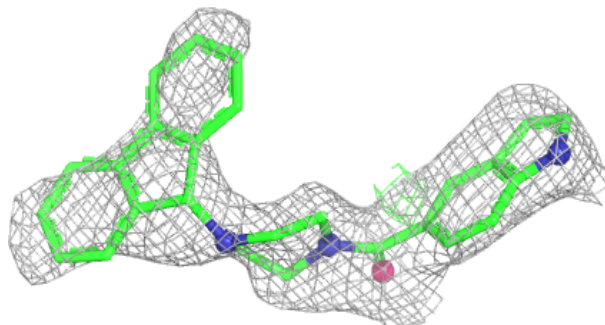
**Electron density around NAD F 750:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

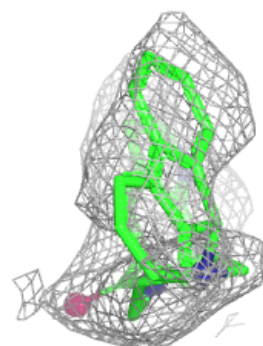
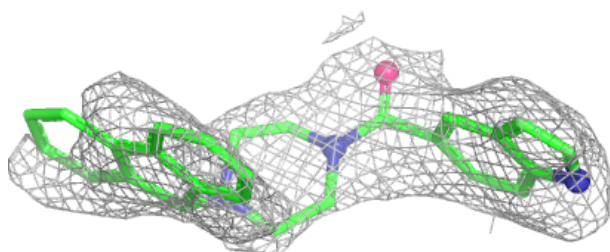
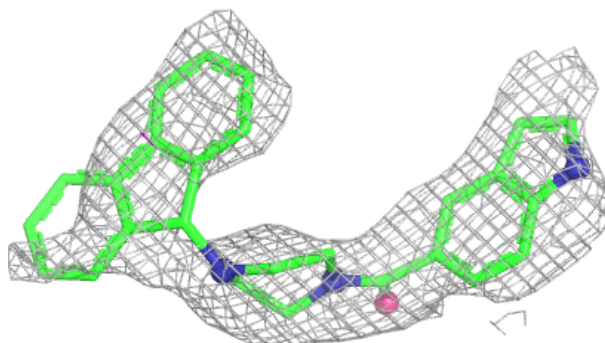


Electron density around GEQ A 350:

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

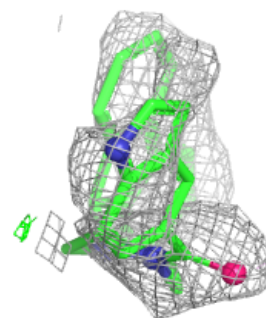
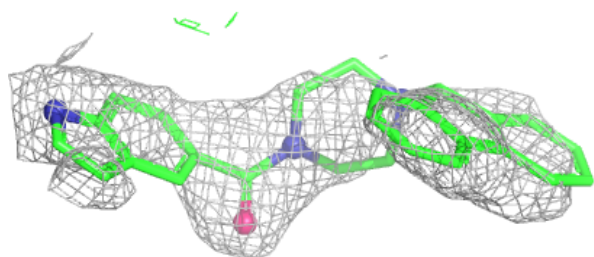
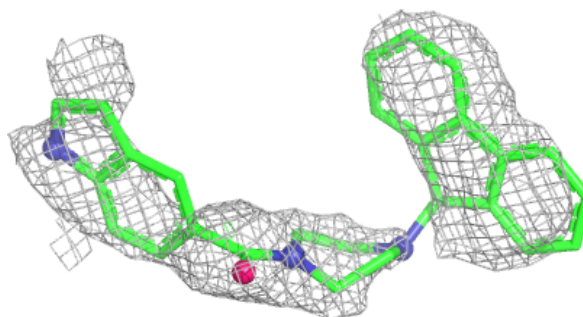
**Electron density around GEQ B 450:**

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

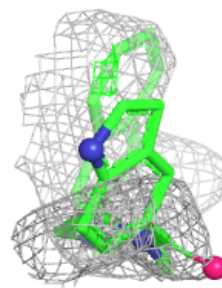
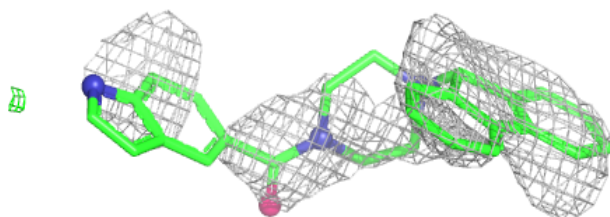
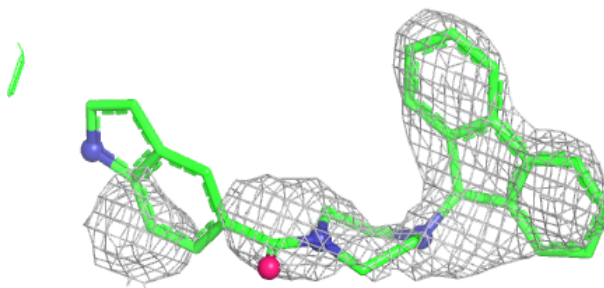


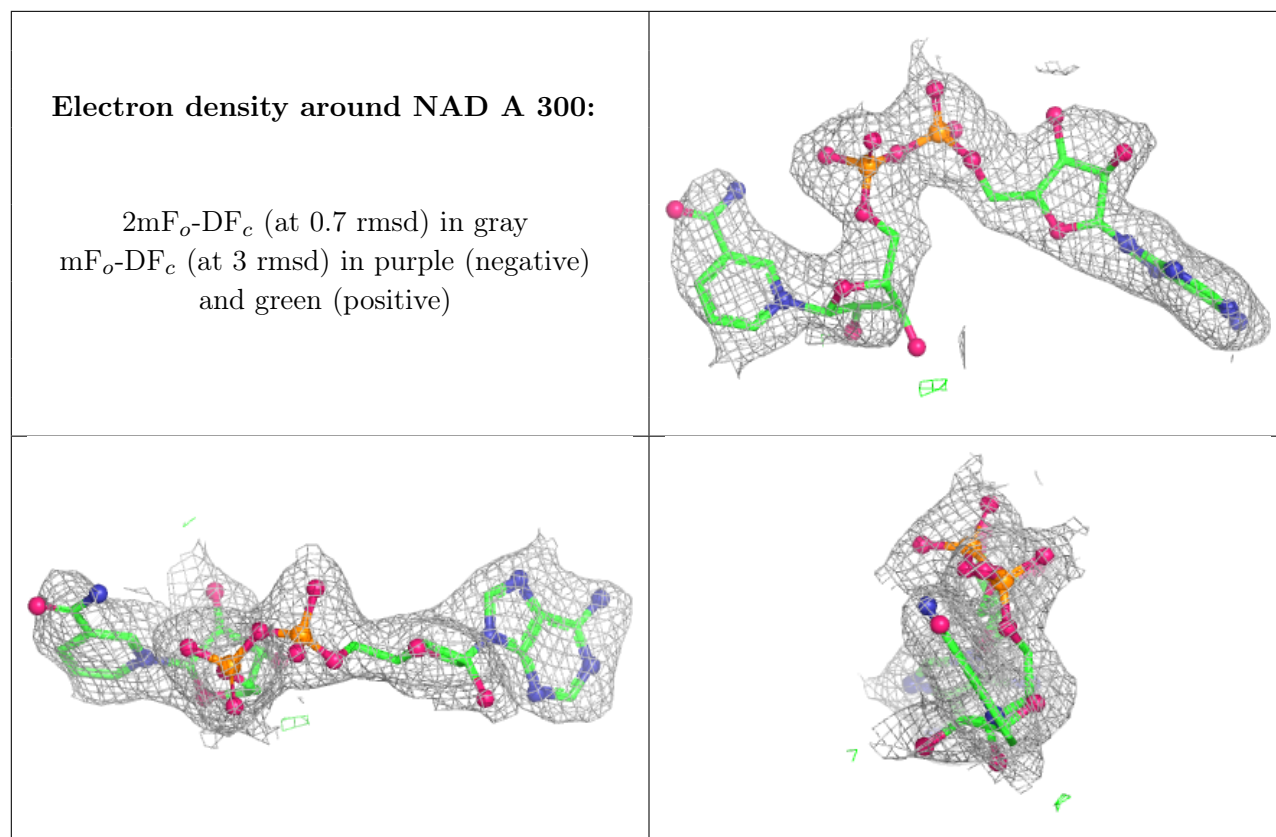
Electron density around GEQ C 550:

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

**Electron density around GEQ D 650:**

$2mF_o-DF_c$ (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.