



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 2E37 / pdb_00002e37
Title : Structure of TT0471 protein from *Thermus thermophilus*
Authors : Lokanath, N.K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-11-21
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

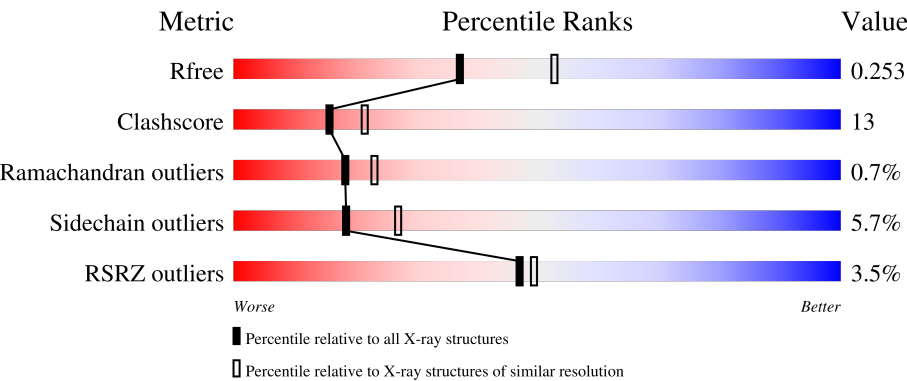
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	310	3% 74%24%..
1	B	310	4% 66%27%. .
1	C	310	75%22%. .
1	D	310	8% 63%31%. . .
1	E	310	3% 70%27%. .

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Mol	Chain	Length	Quality of chain
1	F	310	7% 66% 29%
1	G	310	% 75% 22%
1	H	310	3% 72% 25%

2 Entry composition

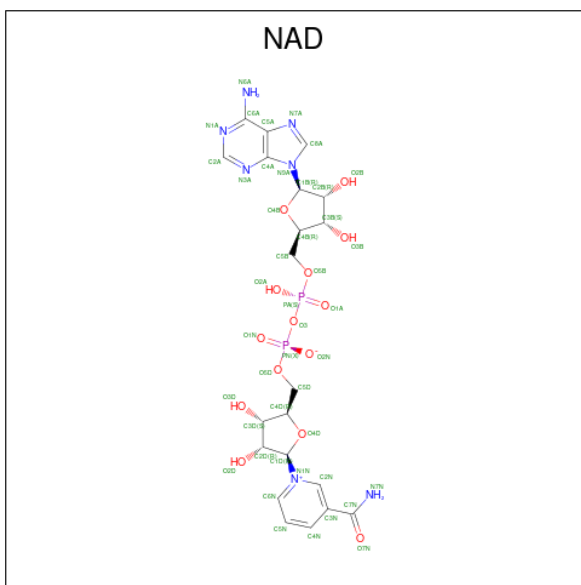
There are 4 unique types of molecules in this entry. The entry contains 19337 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-lactate dehydrogenase.

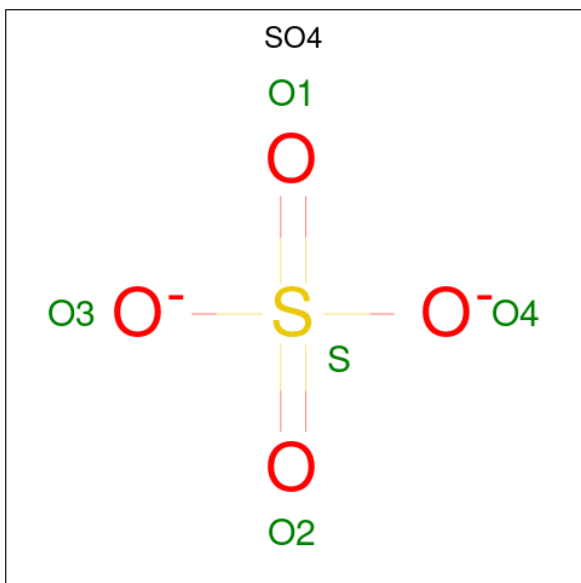
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	Se	0	0	0
			2300	1460	410	427	3			
1	B	304	Total	C	N	O	Se	0	0	0
			2268	1441	405	419	3			
1	C	310	Total	C	N	O	Se	0	0	0
			2315	1468	415	429	3			
1	D	302	Total	C	N	O	Se	0	0	0
			2253	1433	400	417	3			
1	E	304	Total	C	N	O	Se	0	0	0
			2271	1442	403	423	3			
1	F	308	Total	C	N	O	Se	0	0	0
			2300	1460	410	427	3			
1	G	310	Total	C	N	O	Se	0	0	0
			2315	1468	415	429	3			
1	H	308	Total	C	N	O	Se	0	0	0
			2300	1460	410	427	3			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

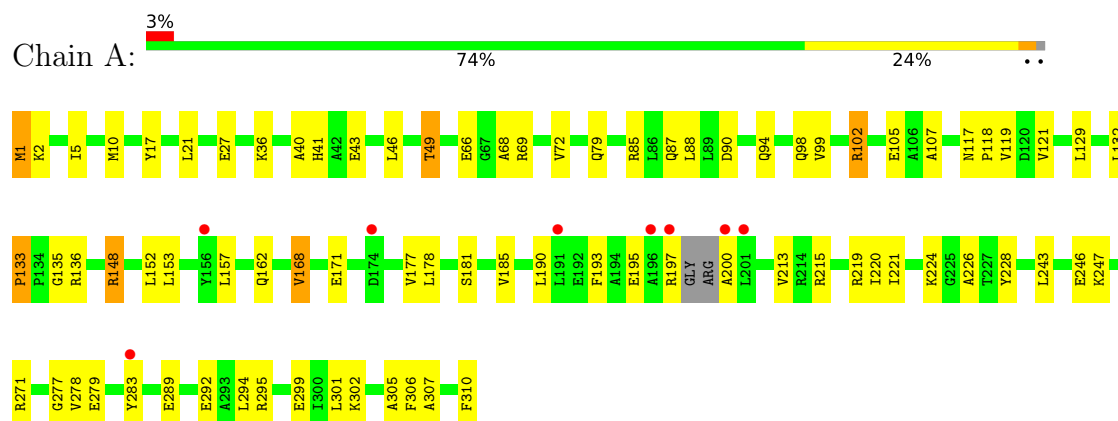
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	76	Total	O	0	0
			76	76		
4	C	140	Total	O	0	0
			140	140		
4	D	60	Total	O	0	0
			60	60		
4	E	84	Total	O	0	0
			84	84		
4	F	100	Total	O	0	0
			100	100		
4	G	129	Total	O	0	0
			129	129		
4	H	117	Total	O	0	0
			117	117		

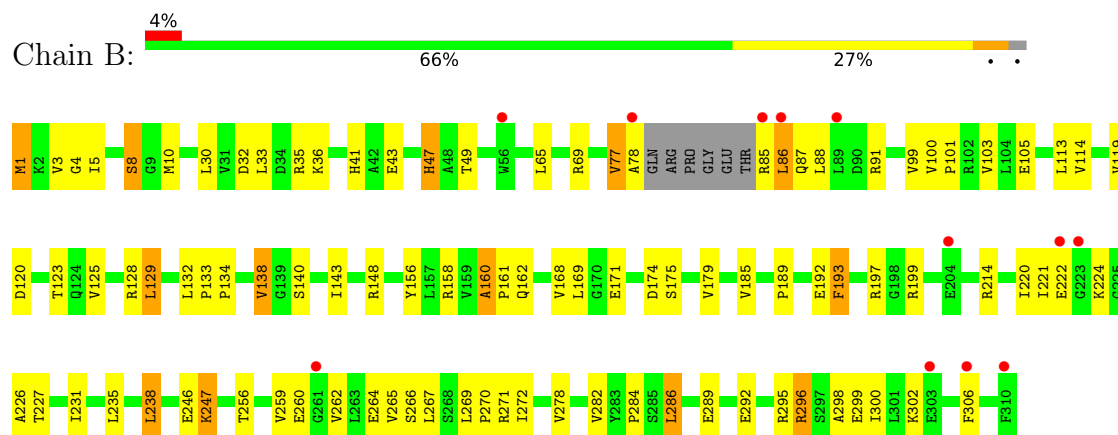
3 Residue-property plots

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.

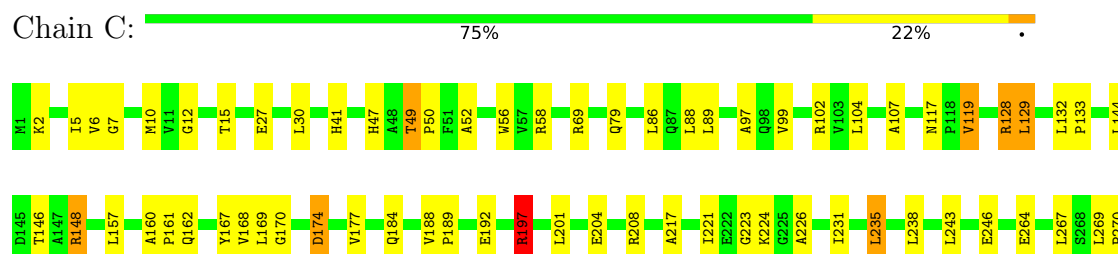
• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase

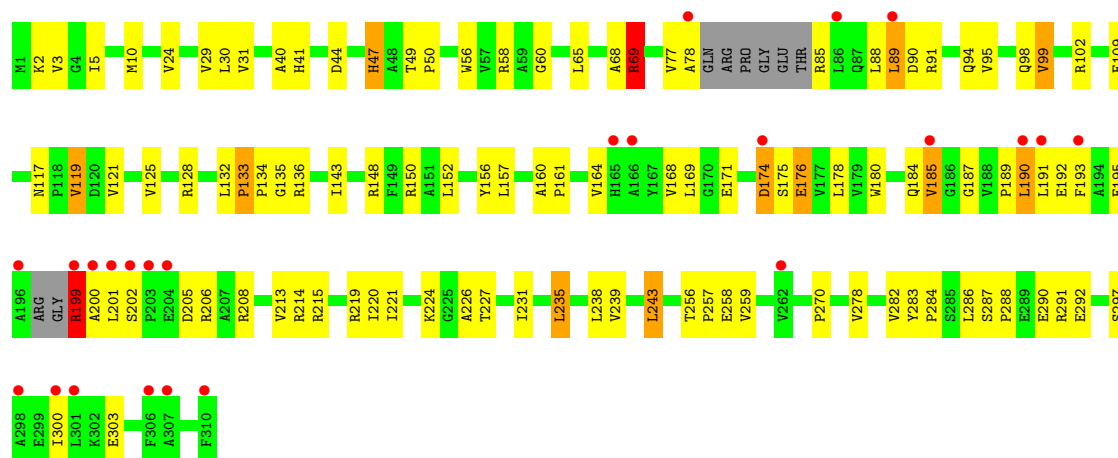


• Molecule 1: L-lactate dehydrogenase

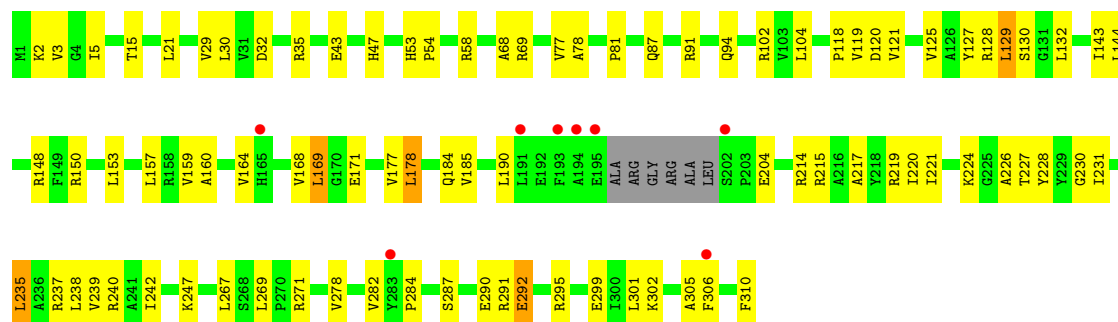




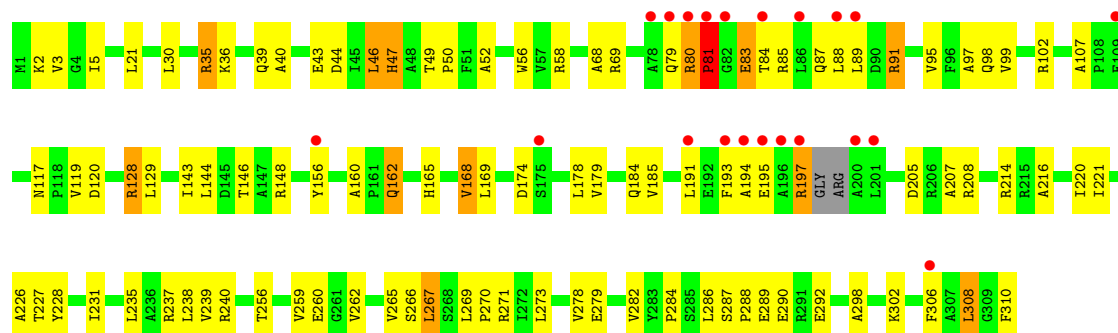
• Molecule 1: L-lactate dehydrogenase



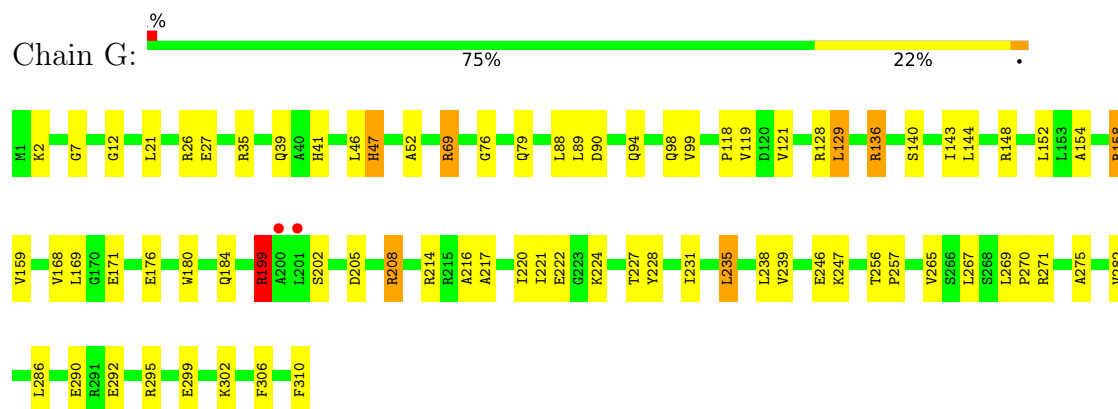
• Molecule 1: L-lactate dehydrogenase



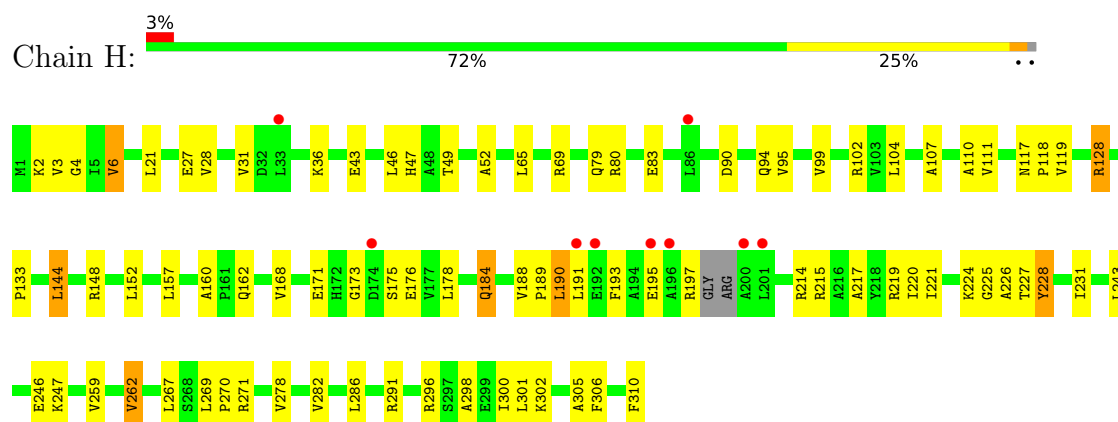
• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.74Å 135.64Å 162.06Å 90.00° 113.79° 90.00°	Depositor
Resolution (Å)	44.01 – 2.30 44.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.01-2.30) 95.2 (44.01-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.255 0.214 , 0.253	Depositor DCC
R_{free} test set	6900 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19337	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: SO4, 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	0.51	2/2337 (0.1%)	1.02	8/3175 (0.3%)
1	B	0.51	0/2304	1.05	13/3129 (0.4%)
1	C	0.52	0/2353	1.02	16/3197 (0.5%)
1	D	0.48	0/2288	1.02	9/3107 (0.3%)
1	E	0.46	0/2308	0.95	2/3136 (0.1%)
1	F	0.54	0/2337	1.06	12/3175 (0.4%)
1	G	0.58	1/2353 (0.0%)	1.05	8/3197 (0.3%)
1	H	0.54	0/2337	1.04	15/3175 (0.5%)
All	All	0.52	3/18617 (0.0%)	1.03	83/25291 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	180	TRP	NE1-CE2	10.38	1.48	1.37
1	A	1	MSE	SE-CE	-5.18	1.79	1.95
1	A	1	MSE	CG-SE	-5.04	1.80	1.95

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	119	VAL	N-CA-C	8.54	119.32	110.36
1	G	99	VAL	N-CA-C	7.83	118.41	110.82
1	A	133	PRO	N-CA-CB	7.57	107.43	103.19
1	H	214	ARG	N-CA-C	7.39	119.34	111.28
1	B	99	VAL	N-CA-C	7.21	117.30	110.74
1	C	99	VAL	N-CA-C	7.06	117.15	110.30
1	H	107	ALA	CA-C-N	6.89	126.59	119.56
1	H	107	ALA	C-N-CA	6.89	126.59	119.56
1	D	99	VAL	N-CA-C	6.84	116.96	110.53
1	A	107	ALA	CA-C-N	6.77	127.32	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ALA	C-N-CA	6.77	127.32	119.47
1	F	99	VAL	N-CA-C	6.73	116.86	110.53
1	C	119	VAL	N-CA-C	6.63	118.18	110.62
1	F	214	ARG	N-CA-C	6.59	118.47	111.28
1	B	168	VAL	N-CA-C	-6.51	98.24	107.75
1	A	99	VAL	N-CA-C	6.48	117.11	110.82
1	F	179	VAL	N-CA-C	6.46	113.12	106.21
1	A	168	VAL	N-CA-C	-6.35	98.48	107.75
1	A	181	SER	N-CA-C	6.25	117.76	111.07
1	A	119	VAL	N-CA-C	6.18	116.93	110.62
1	B	160	ALA	CA-C-N	6.14	126.60	119.47
1	B	160	ALA	C-N-CA	6.14	126.60	119.47
1	H	99	VAL	N-CA-C	6.11	116.16	110.42
1	G	168	VAL	N-CA-C	-6.10	99.57	108.11
1	H	6	VAL	N-CA-CB	-6.05	103.03	111.25
1	D	119	VAL	N-CA-C	5.98	116.64	110.36
1	B	179	VAL	N-CA-C	5.93	112.56	106.21
1	E	119	VAL	N-CA-C	5.91	116.57	110.36
1	B	193	PHE	N-CA-C	-5.90	104.76	111.14
1	D	133	PRO	CA-C-N	5.90	127.21	119.84
1	D	133	PRO	C-N-CA	5.90	127.21	119.84
1	F	168	VAL	N-CA-C	-5.87	99.17	107.75
1	H	111	VAL	N-CA-C	-5.85	99.98	108.87
1	C	170	GLY	O-C-N	5.76	130.19	122.70
1	C	133	PRO	CA-C-N	5.61	126.86	119.84
1	C	133	PRO	C-N-CA	5.61	126.86	119.84
1	H	190	LEU	N-CA-C	5.61	117.84	111.11
1	C	246	GLU	N-CA-C	5.55	118.05	111.33
1	G	214	ARG	N-CA-C	5.51	117.29	111.28
1	C	177	VAL	N-CA-C	5.49	115.76	107.80
1	B	256	THR	CA-C-N	5.43	124.89	119.24
1	B	256	THR	C-N-CA	5.43	124.89	119.24
1	H	95	VAL	N-CA-C	-5.43	105.20	110.42
1	D	214	ARG	N-CA-C	5.42	117.26	111.36
1	F	107	ALA	CA-C-N	5.41	125.23	119.28
1	F	107	ALA	C-N-CA	5.41	125.23	119.28
1	C	107	ALA	CA-C-N	5.37	125.03	119.56
1	C	107	ALA	C-N-CA	5.37	125.03	119.56
1	F	207	ALA	N-CA-C	-5.37	105.51	111.36
1	H	133	PRO	N-CA-CB	5.34	106.00	103.22
1	A	177	VAL	N-CA-C	5.34	115.55	107.80
1	B	214	ARG	N-CA-C	5.33	117.17	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	TYR	N-CA-C	5.33	117.78	109.52
1	C	69	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	F	69	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	D	24	VAL	N-CA-C	5.31	115.52	110.53
1	H	160	ALA	CA-C-N	5.28	125.33	119.32
1	H	160	ALA	C-N-CA	5.28	125.33	119.32
1	H	69	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	E	214	ARG	N-CA-C	5.23	117.73	111.71
1	F	91	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	D	190	LEU	N-CA-C	5.19	116.63	110.97
1	B	138	VAL	N-CA-C	5.17	115.36	108.11
1	B	86	LEU	N-CA-C	5.15	116.58	111.07
1	G	136	ARG	CD-NE-CZ	-5.10	117.25	124.40
1	G	69	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	C	167	TYR	CA-C-N	5.10	129.96	123.13
1	C	167	TYR	C-N-CA	5.10	129.96	123.13
1	C	197	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	D	69	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	D	199	ARG	CD-NE-CZ	-5.08	117.28	124.40
1	G	158	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	F	237	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	F	240	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	F	197	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	B	148	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	G	199	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	C	148	ARG	CD-NE-CZ	-5.04	117.35	124.40
1	H	184	GLN	N-CA-C	5.03	117.02	109.23
1	H	197	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	H	110	ALA	N-CA-C	5.01	117.57	110.50
1	C	174	ASP	N-CA-C	5.00	118.16	111.75
1	B	197	ARG	CD-NE-CZ	-5.00	117.40	124.40

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	2300	0	2350	64	0
1	B	2268	0	2322	73	0
1	C	2315	0	2367	47	0
1	D	2253	0	2305	94	0
1	E	2271	0	2316	72	0
1	F	2300	0	2350	85	0
1	G	2315	0	2367	50	0
1	H	2300	0	2350	50	0
2	A	44	0	26	0	0
2	C	44	0	26	0	0
2	E	44	0	26	0	0
2	G	44	0	26	1	0
3	B	5	0	0	1	0
3	H	5	0	0	0	0
4	A	123	0	0	4	0
4	B	76	0	0	2	0
4	C	140	0	0	4	0
4	D	60	0	0	0	0
4	E	84	0	0	3	0
4	F	100	0	0	5	0
4	G	129	0	0	2	0
4	H	117	0	0	2	0
All	All	19337	0	18831	496	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 (496) 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:F:79:GLN:HE22	1:F:84:THR:HA	1.14	1.09
1:D:156:TYR:CE2	1:D:201:LEU:HD23	1.96	1.01
1:D:69:ARG:HH11	1:D:69:ARG:HB3	1.24	0.99
1:D:192:GLU:HG3	1:D:193:PHE:H	1.32	0.93
1:D:192:GLU:HG3	1:D:193:PHE:N	1.85	0.92
1:F:79:GLN:NE2	1:F:84:THR:HA	1.88	0.88
1:D:189:PRO:HB2	1:D:192:GLU:HG2	1.56	0.87
1:F:262:VAL:HG21	1:F:298:ALA:HB1	1.56	0.87
1:F:79:GLN:HE22	1:F:84:THR:CA	1.88	0.86
1:D:69:ARG:HH11	1:D:69:ARG:CB	1.88	0.86
1:F:85:ARG:HB2	1:F:88:LEU:HB3	1.58	0.86
1:D:185:VAL:HG11	1:D:193:PHE:CD2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLN:O	1:D:102:ARG:HD3	1.79	0.82
1:D:88:LEU:HD13	1:D:91:ARG:NH2	1.94	0.82
1:B:220:ILE:HG21	1:B:227:THR:HG22	1.62	0.82
1:C:204:GLU:HG3	4:C:1515:HOH:O	1.81	0.81
1:D:220:ILE:HG21	1:D:227:THR:HG22	1.63	0.80
1:H:171:GLU:HG3	1:H:301:LEU:HD21	1.64	0.80
1:F:80:ARG:HB2	1:F:81:PRO:HD3	1.65	0.79
1:E:2:LYS:HG3	1:E:68:ALA:HA	1.64	0.79
1:H:220:ILE:HG21	1:H:227:THR:HG22	1.65	0.78
1:G:231:ILE:HG13	1:G:235:LEU:HD22	1.63	0.78
1:H:171:GLU:OE1	1:H:175:SER:HB3	1.85	0.77
1:D:156:TYR:HE2	1:D:201:LEU:HD23	1.45	0.76
1:D:2:LYS:HG3	1:D:68:ALA:HA	1.68	0.76
1:D:202:SER:HB2	1:D:205:ASP:OD2	1.86	0.76
1:A:148:ARG:HH12	1:B:47:HIS:CD2	2.05	0.75
1:D:69:ARG:HB3	1:D:69:ARG:NH1	2.01	0.75
1:A:49:THR:HG21	4:A:1513:HOH:O	1.86	0.74
1:F:56:TRP:CZ2	1:F:58:ARG:HD3	2.21	0.74
1:G:158:ARG:NH1	1:G:199:ARG:HH22	1.86	0.74
1:B:220:ILE:CG2	1:B:227:THR:HG22	2.18	0.73
1:F:80:ARG:HB2	1:F:81:PRO:CD	2.18	0.73
1:F:35:ARG:O	1:F:39:GLN:HG3	1.88	0.73
1:E:21:LEU:HD12	1:F:21:LEU:HD12	1.71	0.73
1:G:158:ARG:HD2	1:G:199:ARG:HH12	1.53	0.72
1:H:262:VAL:HG11	1:H:298:ALA:CB	2.18	0.72
1:C:157:LEU:O	1:C:197:ARG:HG2	1.90	0.72
1:B:86:LEU:HD22	1:B:86:LEU:H	1.52	0.72
1:C:41:HIS:CD2	1:D:224:LYS:HD2	2.25	0.72
1:E:169:LEU:N	1:E:169:LEU:HD12	2.05	0.71
1:E:269:LEU:HB2	1:E:271:ARG:NH1	2.05	0.71
1:A:197:ARG:NH2	4:A:1459:HOH:O	2.24	0.71
1:E:215:ARG:HB2	1:E:219:ARG:NH1	2.04	0.71
1:B:162:GLN:CD	1:B:162:GLN:H	1.99	0.70
1:D:56:TRP:CZ2	1:D:58:ARG:HD3	2.27	0.69
1:H:90:ASP:O	1:H:94:GLN:HG3	1.93	0.69
1:H:168:VAL:HG22	1:H:178:LEU:HD22	1.72	0.69
1:E:171:GLU:HG3	1:E:301:LEU:HD21	1.74	0.69
1:H:262:VAL:HG11	1:H:298:ALA:HB1	1.75	0.69
1:G:2:LYS:HD3	1:G:27:GLU:OE2	1.94	0.68
1:F:162:GLN:CD	1:F:162:GLN:H	2.01	0.68
1:A:289:GLU:CD	1:A:289:GLU:H	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:VAL:HG22	1:H:31:VAL:HB	1.76	0.67
1:A:2:LYS:HG3	1:A:68:ALA:HA	1.75	0.67
1:B:162:GLN:CD	1:B:162:GLN:N	2.53	0.67
1:A:157:LEU:HD11	1:A:190:LEU:CD1	2.25	0.67
1:G:220:ILE:HG21	1:G:227:THR:HG22	1.76	0.66
1:B:1:MSE:HE3	1:B:1:MSE:N	2.10	0.66
1:G:79:GLN:HB2	1:G:88:LEU:HD22	1.76	0.66
1:G:302:LYS:HE3	1:G:306:PHE:CZ	2.31	0.66
1:F:128:ARG:HD2	1:F:310:PHE:O	1.95	0.66
1:F:117:ASN:OD1	1:F:119:VAL:HG23	1.95	0.65
1:H:220:ILE:CG2	1:H:227:THR:HG22	2.26	0.65
1:C:49:THR:HG21	4:C:1441:HOH:O	1.95	0.65
1:F:220:ILE:HG21	1:F:227:THR:HG22	1.79	0.64
1:A:292:GLU:OE2	1:A:295:ARG:NH2	2.29	0.64
1:A:221:ILE:HD13	1:A:226:ALA:HA	1.78	0.64
1:A:195:GLU:HA	1:A:200:ALA:HB2	1.80	0.64
1:H:128:ARG:HD2	1:H:310:PHE:O	1.98	0.64
1:A:168:VAL:HG22	1:A:178:LEU:HD22	1.79	0.64
1:E:295:ARG:O	1:E:299:GLU:HG3	1.96	0.64
1:B:185:VAL:HG11	1:B:193:PHE:CE2	2.34	0.63
1:C:231:ILE:HG13	1:C:235:LEU:HD22	1.78	0.63
1:E:190:LEU:C	1:E:190:LEU:HD23	2.23	0.63
1:E:291:ARG:HG3	1:E:291:ARG:HH11	1.63	0.63
1:F:2:LYS:HG3	1:F:68:ALA:HA	1.80	0.63
1:B:85:ARG:NH1	4:B:1574:HOH:O	2.30	0.63
1:F:184:GLN:NE2	4:F:367:HOH:O	2.23	0.63
1:A:148:ARG:HH11	1:A:148:ARG:HB2	1.63	0.62
1:D:169:LEU:HD22	1:D:270:PRO:HD3	1.80	0.62
1:E:305:ALA:HB1	1:E:310:PHE:OXT	1.99	0.62
1:A:136:ARG:NH1	4:A:1492:HOH:O	2.23	0.62
1:G:217:ALA:O	1:G:221:ILE:HG12	2.00	0.61
1:C:197:ARG:NH2	1:F:279:GLU:HG2	2.15	0.61
1:F:220:ILE:CG2	1:F:227:THR:HG22	2.31	0.61
1:F:269:LEU:H	1:F:271:ARG:NH1	1.98	0.61
1:D:184:GLN:NE2	1:D:187:GLY:O	2.34	0.61
1:E:77:VAL:HG21	1:E:91:ARG:NH1	2.15	0.61
1:B:220:ILE:O	1:B:224:LYS:HB3	2.01	0.61
1:A:271:ARG:HB3	1:A:278:VAL:HG13	1.83	0.61
1:D:89:LEU:N	1:D:89:LEU:HD23	2.15	0.61
1:F:259:VAL:HG11	1:F:267:LEU:HD21	1.82	0.60
1:F:5:ILE:HB	1:F:30:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD22	1:B:86:LEU:N	2.17	0.60
1:D:221:ILE:CD1	1:D:226:ALA:HA	2.32	0.60
1:E:148:ARG:HH22	1:F:43:GLU:HG2	1.65	0.60
1:D:143:ILE:HD13	1:D:238:LEU:HD11	1.82	0.60
1:G:220:ILE:CG2	1:G:227:THR:HG22	2.32	0.60
1:D:221:ILE:HD13	1:D:226:ALA:HA	1.84	0.60
1:E:153:LEU:HD22	1:E:190:LEU:HD11	1.83	0.60
1:F:102:ARG:NH1	4:F:381:HOH:O	2.31	0.60
1:B:158:ARG:HD2	1:B:199:ARG:NH2	2.17	0.60
1:F:162:GLN:NE2	4:F:369:HOH:O	2.27	0.60
1:G:69:ARG:NH2	1:G:275:ALA:O	2.34	0.59
1:H:270:PRO:HB2	1:H:282:VAL:HB	1.84	0.59
1:C:128:ARG:HD2	1:C:310:PHE:O	2.02	0.59
1:A:148:ARG:NH1	1:B:47:HIS:CD2	2.70	0.59
1:B:120:ASP:OD2	1:B:171:GLU:HA	2.02	0.59
1:D:69:ARG:HH11	1:D:69:ARG:CG	2.15	0.59
1:B:231:ILE:O	1:B:235:LEU:HB2	2.01	0.59
1:B:69:ARG:HG2	1:B:69:ARG:HH11	1.66	0.59
1:F:89:LEU:HG	1:F:308:LEU:HD21	1.84	0.59
1:A:41:HIS:CD2	1:B:224:LYS:HE3	2.38	0.58
1:A:220:ILE:HD11	1:B:43:GLU:HG2	1.85	0.58
1:B:302:LYS:HE3	1:B:306:PHE:CE2	2.38	0.58
1:F:302:LYS:HE3	1:F:306:PHE:CE2	2.39	0.58
1:E:271:ARG:HD3	1:E:278:VAL:HG11	1.85	0.58
1:D:135:GLY:HA2	1:D:278:VAL:CG2	2.34	0.58
1:E:120:ASP:OD2	1:E:171:GLU:HA	2.03	0.58
1:H:117:ASN:HA	1:H:119:VAL:N	2.19	0.58
1:H:286:LEU:HB2	1:H:291:ARG:HG2	1.86	0.58
1:C:5:ILE:HB	1:C:30:LEU:HD23	1.86	0.58
1:F:98:GLN:O	1:F:102:ARG:HG2	2.04	0.58
1:H:305:ALA:HB1	1:H:310:PHE:OXT	2.04	0.58
1:B:87:GLN:HG3	1:B:91:ARG:HH21	1.69	0.57
1:B:113:LEU:HD21	1:B:238:LEU:HD23	1.86	0.57
1:G:292:GLU:OE1	1:G:295:ARG:NH2	2.36	0.57
1:A:295:ARG:NH1	1:A:299:GLU:OE2	2.38	0.57
1:B:1:MSE:HE3	1:B:1:MSE:H3	1.68	0.57
1:C:184:GLN:NE2	1:F:184:GLN:HE22	2.03	0.57
1:D:287:SER:OG	1:D:290:GLU:HG3	2.05	0.57
1:F:80:ARG:CB	1:F:81:PRO:HD3	2.34	0.57
1:B:5:ILE:HB	1:B:30:LEU:HD23	1.85	0.57
1:C:291:ARG:NE	4:C:1540:HOH:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HD13	1:B:226:ALA:HA	1.88	0.56
1:D:171:GLU:HB3	1:D:175:SER:HB2	1.85	0.56
1:H:262:VAL:HG11	1:H:298:ALA:HB3	1.87	0.56
1:B:169:LEU:HD22	1:B:269:LEU:HA	1.88	0.56
1:D:287:SER:O	1:D:291:ARG:HG2	2.05	0.56
1:E:302:LYS:HE3	1:E:306:PHE:CZ	2.41	0.56
1:C:117:ASN:ND2	4:C:1487:HOH:O	2.20	0.56
1:F:117:ASN:HA	1:F:119:VAL:N	2.22	0.56
1:F:282:VAL:O	1:F:284:PRO:HD3	2.06	0.55
1:G:292:GLU:CD	1:G:295:ARG:HH21	2.14	0.55
1:C:169:LEU:HD22	1:C:270:PRO:HD3	1.88	0.55
1:G:202:SER:HG	1:G:205:ASP:CG	2.15	0.55
1:C:146:THR:HA	1:C:168:VAL:HG23	1.89	0.55
1:F:289:GLU:CD	1:F:289:GLU:H	2.15	0.55
1:G:202:SER:OG	1:G:205:ASP:OD2	2.21	0.55
1:A:118:PRO:HG2	1:A:121:VAL:HB	1.88	0.54
1:B:189:PRO:HB2	1:B:192:GLU:HG2	1.88	0.54
1:D:174:ASP:C	1:D:176:GLU:H	2.14	0.54
1:E:159:VAL:HG22	1:E:160:ALA:H	1.73	0.54
1:F:169:LEU:HD22	1:F:270:PRO:HD3	1.89	0.54
1:B:158:ARG:HG2	1:B:158:ARG:HH11	1.73	0.54
1:D:156:TYR:CE2	1:D:201:LEU:CD2	2.83	0.54
1:E:224:LYS:HG3	1:F:40:ALA:CB	2.38	0.54
1:F:79:GLN:HG2	1:F:88:LEU:CD2	2.38	0.54
1:E:238:LEU:O	1:E:242:ILE:HG13	2.08	0.53
1:F:238:LEU:HD22	1:F:273:LEU:CD2	2.38	0.53
1:A:302:LYS:HE3	1:A:306:PHE:CZ	2.42	0.53
1:F:88:LEU:HB2	1:F:91:ARG:NH2	2.23	0.53
1:G:265:VAL:CG1	1:G:302:LYS:HD3	2.38	0.53
1:E:150:ARG:HD3	1:E:164:VAL:O	2.09	0.53
1:E:215:ARG:HB2	1:E:219:ARG:HH12	1.71	0.53
1:D:69:ARG:NH1	1:D:69:ARG:CG	2.70	0.53
1:D:168:VAL:HG22	1:D:178:LEU:HD22	1.90	0.53
1:A:171:GLU:HG3	1:A:301:LEU:HD21	1.91	0.53
1:F:191:LEU:O	1:F:194:ALA:HB3	2.09	0.53
1:C:2:LYS:HD3	1:C:27:GLU:OE2	2.09	0.52
1:E:224:LYS:HG3	1:F:40:ALA:HB3	1.90	0.52
1:G:129:LEU:HD13	1:G:310:PHE:HE1	1.73	0.52
1:B:296:ARG:HG2	1:B:296:ARG:HH11	1.74	0.52
1:E:291:ARG:HG3	1:E:291:ARG:NH1	2.23	0.52
1:E:118:PRO:HG2	1:E:121:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HE2	1:A:228:TYR:CE2	2.45	0.52
1:D:152:LEU:HD12	1:D:213:VAL:HG23	1.92	0.52
1:D:191:LEU:HD23	1:D:201:LEU:HD12	1.92	0.52
1:E:217:ALA:O	1:E:221:ILE:HG12	2.10	0.52
1:A:40:ALA:HB3	1:B:224:LYS:HB2	1.92	0.52
1:B:140:SER:O	1:B:143:ILE:HG12	2.08	0.52
1:G:35:ARG:O	1:G:39:GLN:HG3	2.10	0.52
1:A:40:ALA:CB	1:B:224:LYS:HB2	2.40	0.52
1:A:271:ARG:HD3	1:A:278:VAL:HG21	1.92	0.52
1:C:15:THR:OG1	1:C:235:LEU:HD23	2.09	0.52
1:C:47:HIS:HE1	1:D:148:ARG:NH1	2.06	0.52
1:C:302:LYS:HE3	1:C:306:PHE:CZ	2.44	0.52
1:E:47:HIS:CE1	1:F:148:ARG:HD2	2.44	0.52
1:F:287:SER:OG	1:F:290:GLU:HG3	2.10	0.52
1:A:307:ALA:O	1:D:91:ARG:NH1	2.43	0.51
1:E:287:SER:OG	1:E:290:GLU:HG3	2.10	0.51
1:E:302:LYS:HE3	1:E:306:PHE:CE2	2.45	0.51
1:G:158:ARG:HH11	1:G:199:ARG:HH22	1.58	0.51
1:A:305:ALA:HB1	1:A:310:PHE:OXT	2.09	0.51
1:H:246:GLU:O	1:H:247:LYS:HB2	2.10	0.51
1:B:86:LEU:H	1:B:86:LEU:CD2	2.21	0.51
1:B:100:VAL:HB	1:B:101:PRO:HD3	1.93	0.51
1:E:69:ARG:HH11	1:E:69:ARG:HG2	1.76	0.51
1:C:2:LYS:HD3	1:C:27:GLU:CD	2.35	0.51
1:E:32:ASP:O	1:E:35:ARG:HD3	2.11	0.51
1:E:169:LEU:HD23	1:E:269:LEU:HD23	1.93	0.51
1:A:41:HIS:NE2	1:B:224:LYS:HE3	2.26	0.51
1:C:47:HIS:CE1	1:D:148:ARG:NH1	2.79	0.51
1:F:216:ALA:O	1:F:220:ILE:HG13	2.11	0.51
1:D:185:VAL:CG1	1:D:193:PHE:CD2	2.91	0.51
1:F:80:ARG:CB	1:F:81:PRO:CD	2.87	0.51
1:F:165:HIS:ND1	4:F:366:HOH:O	2.32	0.50
1:B:125:VAL:HG12	1:B:129:LEU:HD22	1.93	0.50
1:A:132:LEU:HB3	1:A:133:PRO:HD2	1.93	0.50
1:A:153:LEU:HD22	1:A:190:LEU:HD21	1.93	0.50
1:B:33:LEU:HG	3:B:1501:SO4:O1	2.11	0.50
1:G:46:LEU:O	1:G:46:LEU:HG	2.11	0.50
1:G:295:ARG:HD2	1:G:299:GLU:OE2	2.12	0.50
1:A:271:ARG:HD3	1:A:278:VAL:HG11	1.92	0.50
1:D:291:ARG:HG3	1:D:291:ARG:HH11	1.77	0.50
1:A:193:PHE:HD1	1:A:197:ARG:HH21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:O	1:A:102:ARG:HD3	2.12	0.50
1:F:169:LEU:CD2	1:F:270:PRO:HD3	2.42	0.50
1:D:5:ILE:HB	1:D:30:LEU:HD23	1.94	0.50
1:C:47:HIS:CE1	1:D:148:ARG:HH11	2.30	0.49
1:E:235:LEU:O	1:E:239:VAL:HG23	2.12	0.49
1:G:47:HIS:CE1	1:H:148:ARG:NH1	2.80	0.49
1:H:188:VAL:HG13	1:H:189:PRO:HD2	1.94	0.49
1:G:47:HIS:CE1	1:H:148:ARG:HH11	2.29	0.49
1:F:221:ILE:CD1	1:F:226:ALA:HA	2.42	0.49
1:B:262:VAL:HG21	1:B:298:ALA:HB1	1.94	0.49
1:B:262:VAL:CG1	1:B:299:GLU:HG3	2.43	0.49
1:G:216:ALA:O	1:G:220:ILE:HG13	2.12	0.49
1:D:224:LYS:HE3	1:D:226:ALA:O	2.12	0.49
1:G:270:PRO:HB2	1:G:282:VAL:HB	1.94	0.49
1:A:193:PHE:HD1	1:A:197:ARG:NH2	2.10	0.49
1:B:282:VAL:O	1:B:284:PRO:HD3	2.12	0.49
1:F:156:TYR:CE1	1:F:208:ARG:NH2	2.81	0.49
1:E:5:ILE:HB	1:E:30:LEU:HD23	1.93	0.49
1:H:162:GLN:H	1:H:162:GLN:CD	2.20	0.49
1:E:269:LEU:HB2	1:E:271:ARG:HH12	1.73	0.49
1:B:289:GLU:O	1:B:292:GLU:HB2	2.13	0.49
1:D:220:ILE:CG2	1:D:227:THR:HG22	2.38	0.49
1:F:97:ALA:HA	1:F:129:LEU:HD13	1.94	0.48
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.78	0.48
1:A:10:MSE:HE1	1:B:10:MSE:CE	2.44	0.48
1:C:217:ALA:O	1:C:221:ILE:HG12	2.13	0.48
1:G:76:GLY:HA3	2:G:1404:NAD:O3D	2.14	0.48
1:H:2:LYS:HD3	1:H:27:GLU:OE2	2.12	0.48
1:E:77:VAL:HG21	1:E:91:ARG:HH12	1.77	0.48
1:D:297:SER:HA	1:D:300:ILE:HD12	1.94	0.48
1:F:49:THR:OG1	1:F:50:PRO:HD3	2.13	0.48
1:B:296:ARG:O	1:B:300:ILE:HG13	2.14	0.48
1:B:284:PRO:O	1:B:286:LEU:HD22	2.13	0.48
1:E:143:ILE:HG13	1:E:144:LEU:N	2.29	0.48
1:A:36:LYS:HD2	1:A:36:LYS:N	2.29	0.48
1:D:157:LEU:HD11	1:D:190:LEU:CD1	2.44	0.48
1:A:85:ARG:HG3	1:A:85:ARG:HH11	1.79	0.48
1:G:158:ARG:CD	1:G:199:ARG:HH12	2.23	0.48
1:A:2:LYS:HD2	1:A:66:GLU:O	2.14	0.47
1:D:56:TRP:CE2	1:D:58:ARG:HD3	2.49	0.47
1:A:102:ARG:O	1:A:105:GLU:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:GLY:HA3	1:D:40:ALA:HB2	1.96	0.47
1:D:202:SER:O	1:D:206:ARG:HG3	2.14	0.47
1:G:94:GLN:O	1:G:98:GLN:HG2	2.14	0.47
1:C:79:GLN:HA	1:C:88:LEU:HD13	1.97	0.47
1:C:97:ALA:HA	1:C:129:LEU:HD21	1.97	0.47
1:D:288:PRO:O	1:D:292:GLU:HG2	2.14	0.47
1:E:215:ARG:O	1:E:219:ARG:HG3	2.15	0.47
1:F:238:LEU:HD22	1:F:273:LEU:HD22	1.96	0.47
1:B:33:LEU:HA	1:B:35:ARG:HH12	1.79	0.47
1:C:162:GLN:H	1:C:162:GLN:CD	2.22	0.47
1:H:117:ASN:CG	1:H:118:PRO:HA	2.40	0.47
1:D:185:VAL:HG13	1:D:185:VAL:O	2.15	0.47
1:E:102:ARG:HG3	1:E:102:ARG:HH11	1.80	0.47
1:E:221:ILE:HD13	1:E:226:ALA:HA	1.97	0.47
1:F:156:TYR:HE2	1:F:205:ASP:CG	2.22	0.47
1:G:208:ARG:NH1	4:G:1493:HOH:O	2.28	0.47
1:H:271:ARG:HB3	1:H:278:VAL:HG13	1.96	0.47
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.79	0.47
1:E:94:GLN:HB3	4:E:1460:HOH:O	2.13	0.47
1:A:195:GLU:O	1:A:195:GLU:HG2	2.14	0.47
1:D:88:LEU:CD1	1:D:91:ARG:NH2	2.73	0.47
1:G:169:LEU:HD22	1:G:269:LEU:HA	1.97	0.47
1:B:260:GLU:O	1:B:295:ARG:HG3	2.15	0.47
1:E:3:VAL:HG21	1:E:239:VAL:HG11	1.97	0.47
1:E:125:VAL:O	1:E:129:LEU:HB2	2.15	0.46
1:C:295:ARG:O	1:C:299:GLU:HG3	2.14	0.46
1:D:29:VAL:HG11	1:D:65:LEU:HD23	1.97	0.46
1:F:308:LEU:HB3	1:F:310:PHE:HD2	1.78	0.46
1:G:148:ARG:HH22	1:H:43:GLU:HG3	1.79	0.46
1:A:247:LYS:HE2	1:A:279:GLU:OE1	2.15	0.46
1:C:197:ARG:HH22	1:F:279:GLU:HG2	1.79	0.46
1:B:259:VAL:HG13	1:B:262:VAL:HG22	1.97	0.46
1:C:117:ASN:HA	1:C:119:VAL:N	2.31	0.46
1:E:169:LEU:N	1:E:169:LEU:CD1	2.77	0.46
1:E:269:LEU:N	1:E:271:ARG:HH12	2.13	0.46
1:H:228:TYR:HA	1:H:231:ILE:HG22	1.98	0.46
1:A:2:LYS:HE2	1:A:27:GLU:OE2	2.16	0.46
1:E:168:VAL:C	1:E:169:LEU:HD12	2.40	0.46
1:G:246:GLU:O	1:G:247:LYS:HB2	2.16	0.46
1:G:265:VAL:HG13	1:G:302:LYS:HD3	1.97	0.46
1:C:49:THR:N	1:C:50:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:THR:OG1	1:D:50:PRO:HD3	2.16	0.46
1:D:132:LEU:HB3	1:D:133:PRO:HD2	1.98	0.46
1:F:91:ARG:O	1:F:95:VAL:HG23	2.16	0.46
1:D:90:ASP:O	1:D:94:GLN:HG3	2.15	0.46
1:D:231:ILE:O	1:D:235:LEU:HB2	2.15	0.46
1:E:35:ARG:NH2	4:E:1472:HOH:O	2.23	0.46
1:A:43:GLU:HG2	1:B:220:ILE:HD11	1.98	0.45
1:B:8:SER:HB2	1:B:32:ASP:HB2	1.98	0.45
1:D:291:ARG:HG3	1:D:291:ARG:NH1	2.31	0.45
1:A:152:LEU:HD12	1:A:213:VAL:HG23	1.99	0.45
1:H:193:PHE:CD1	1:H:193:PHE:C	2.93	0.45
1:B:246:GLU:O	1:B:247:LYS:HB2	2.16	0.45
1:D:69:ARG:CB	1:D:69:ARG:NH1	2.69	0.45
1:F:120:ASP:OD1	1:F:267:LEU:HA	2.16	0.45
1:H:157:LEU:HD11	1:H:190:LEU:CD1	2.46	0.45
1:B:271:ARG:HD3	1:B:278:VAL:HG11	1.99	0.45
1:D:88:LEU:HD13	1:D:91:ARG:HH22	1.80	0.45
1:H:215:ARG:HB2	1:H:219:ARG:NH1	2.32	0.45
1:D:117:ASN:HA	1:D:119:VAL:N	2.31	0.45
1:E:269:LEU:O	1:E:271:ARG:HG3	2.15	0.45
1:F:265:VAL:HG22	1:F:266:SER:N	2.30	0.45
1:C:269:LEU:O	1:C:271:ARG:HG3	2.17	0.45
1:E:104:LEU:HD11	1:E:130:SER:HB2	1.98	0.45
1:E:157:LEU:CD1	1:E:185:VAL:HG21	2.47	0.45
1:F:235:LEU:O	1:F:239:VAL:HG23	2.17	0.45
1:B:158:ARG:HG2	1:B:158:ARG:NH1	2.31	0.45
1:C:148:ARG:HH11	1:C:148:ARG:HD2	1.60	0.45
1:E:87:GLN:O	1:E:91:ARG:HG3	2.17	0.45
1:F:56:TRP:CE2	1:F:58:ARG:HD3	2.52	0.45
1:G:140:SER:HB2	1:G:231:ILE:HD11	1.99	0.45
1:B:77:VAL:HG12	1:B:78:ALA:N	2.31	0.45
1:D:199:ARG:HG3	1:D:200:ALA:H	1.81	0.45
1:D:231:ILE:HG13	1:D:235:LEU:HD22	1.98	0.45
1:H:225:GLY:O	1:H:226:ALA:HB2	2.17	0.45
1:E:292:GLU:OE1	1:E:295:ARG:NH2	2.49	0.45
1:A:221:ILE:CD1	1:A:226:ALA:HA	2.46	0.44
1:C:56:TRP:CZ2	1:C:58:ARG:HD3	2.53	0.44
1:D:180:TRP:CH2	1:D:206:ARG:HA	2.51	0.44
1:D:202:SER:HB2	1:D:205:ASP:CG	2.40	0.44
1:H:3:VAL:CG1	1:H:28:VAL:HG22	2.47	0.44
1:D:171:GLU:CD	1:D:175:SER:HB2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:ALA:O	1:H:221:ILE:HG12	2.17	0.44
1:A:215:ARG:HB2	1:A:219:ARG:NH1	2.31	0.44
1:D:235:LEU:O	1:D:239:VAL:HG23	2.17	0.44
1:H:117:ASN:HA	1:H:119:VAL:H	1.83	0.44
1:D:95:VAL:O	1:D:99:VAL:HG23	2.18	0.44
1:F:288:PRO:O	1:F:292:GLU:HG2	2.18	0.44
1:B:1:MSE:HE3	1:B:1:MSE:H1	1.82	0.44
1:D:31:VAL:HG22	1:D:60:GLY:O	2.17	0.44
1:D:109:GLU:HA	1:D:136:ARG:HH22	1.83	0.44
1:E:15:THR:OG1	1:E:235:LEU:HD23	2.18	0.44
1:G:118:PRO:HG2	1:G:121:VAL:HB	1.99	0.44
1:D:283:TYR:CD1	1:D:283:TYR:N	2.86	0.44
1:E:190:LEU:C	1:E:190:LEU:CD2	2.89	0.44
1:G:235:LEU:O	1:G:239:VAL:HG23	2.18	0.44
1:A:90:ASP:O	1:A:94:GLN:HG3	2.18	0.44
1:A:283:TYR:CD1	1:A:283:TYR:N	2.86	0.44
1:C:188:VAL:HG13	1:C:189:PRO:HD2	1.99	0.44
1:C:286:LEU:HB3	1:C:291:ARG:HG3	2.00	0.44
1:D:109:GLU:C	1:D:136:ARG:NH2	2.76	0.44
1:E:104:LEU:CD2	1:E:132:LEU:HD11	2.48	0.44
1:E:168:VAL:HA	1:E:177:VAL:O	2.18	0.44
1:D:160:ALA:HA	1:D:161:PRO:HD3	1.91	0.43
1:B:247:LYS:O	1:B:272:ILE:HG23	2.18	0.43
1:F:256:THR:OG1	1:F:271:ARG:NH2	2.51	0.43
1:H:302:LYS:HE3	1:H:306:PHE:CZ	2.53	0.43
1:B:265:VAL:HG22	1:B:266:SER:N	2.34	0.43
1:D:157:LEU:HD11	1:D:190:LEU:HD11	2.00	0.43
1:E:43:GLU:HG2	1:F:220:ILE:HD11	2.00	0.43
1:D:148:ARG:HH11	1:D:148:ARG:HG2	1.83	0.43
1:D:169:LEU:CD2	1:D:270:PRO:HD3	2.47	0.43
1:A:10:MSE:HE1	1:B:10:MSE:HE2	2.00	0.43
1:E:190:LEU:HD23	1:E:190:LEU:O	2.17	0.43
1:F:83:GLU:O	1:F:84:THR:HB	2.18	0.43
1:F:185:VAL:HG11	1:F:193:PHE:CE2	2.52	0.43
1:F:271:ARG:HD3	1:F:278:VAL:HG21	2.01	0.43
1:G:41:HIS:CE1	1:H:224:LYS:HE3	2.54	0.43
1:H:215:ARG:HB2	1:H:219:ARG:HH12	1.83	0.43
1:B:4:GLY:HA3	1:B:65:LEU:HD22	2.01	0.43
1:C:270:PRO:HB2	1:C:282:VAL:HB	2.01	0.43
1:D:174:ASP:C	1:D:176:GLU:N	2.77	0.43
1:A:117:ASN:ND2	4:A:1460:HOH:O	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:CG2	1:E:227:THR:HG22	2.49	0.43
1:C:208:ARG:HG2	1:C:208:ARG:HH11	1.84	0.43
1:F:270:PRO:HB2	1:F:282:VAL:HB	2.01	0.43
1:G:148:ARG:HD3	4:H:1587:HOH:O	2.18	0.43
1:H:224:LYS:HE2	1:H:228:TYR:CE1	2.54	0.43
1:B:132:LEU:HB3	1:B:133:PRO:HD2	2.00	0.42
1:D:286:LEU:HB3	1:D:290:GLU:HB2	2.00	0.42
1:F:79:GLN:HG2	1:F:88:LEU:HD23	2.01	0.42
1:A:152:LEU:HD12	1:A:213:VAL:CG2	2.49	0.42
1:A:157:LEU:HD11	1:A:190:LEU:HD12	2.01	0.42
1:B:169:LEU:HD21	1:B:270:PRO:HD3	2.01	0.42
1:B:292:GLU:OE1	1:B:295:ARG:NH2	2.52	0.42
1:D:282:VAL:O	1:D:284:PRO:HD3	2.19	0.42
1:F:79:GLN:HE22	1:F:84:THR:N	2.17	0.42
1:F:160:ALA:HB1	1:F:162:GLN:HE22	1.83	0.42
1:F:168:VAL:HG22	1:F:178:LEU:HD22	2.01	0.42
1:G:21:LEU:HD12	1:H:21:LEU:HD12	2.00	0.42
1:F:79:GLN:CD	1:F:84:THR:HA	2.42	0.42
1:F:165:HIS:CE1	4:F:366:HOH:O	2.69	0.42
1:G:256:THR:OG1	1:G:271:ARG:NH2	2.52	0.42
1:B:133:PRO:HA	1:B:134:PRO:HD3	1.95	0.42
1:D:29:VAL:CG1	1:D:65:LEU:HD23	2.49	0.42
1:E:21:LEU:HD12	1:F:21:LEU:CD1	2.46	0.42
1:G:158:ARG:HD2	1:G:199:ARG:NH1	2.27	0.42
1:B:156:TYR:HE1	1:B:199:ARG:O	2.03	0.42
1:D:195:GLU:OE1	1:D:195:GLU:HA	2.20	0.42
1:H:191:LEU:O	1:H:195:GLU:HG3	2.19	0.42
1:E:168:VAL:HG22	1:E:178:LEU:HD22	2.01	0.42
1:E:230:GLY:HA3	1:F:47:HIS:HB3	2.01	0.42
1:B:222:GLU:OE1	1:B:222:GLU:HA	2.20	0.42
1:A:17:TYR:CZ	1:A:21:LEU:HD11	2.55	0.42
1:D:184:GLN:NE2	1:E:184:GLN:OE1	2.53	0.42
1:E:237:ARG:CZ	1:E:240:ARG:NH2	2.82	0.42
1:H:117:ASN:OD1	1:H:118:PRO:HA	2.20	0.42
1:B:160:ALA:HA	1:B:161:PRO:HD3	1.85	0.42
1:D:121:VAL:O	1:D:125:VAL:HG23	2.20	0.42
1:D:243:LEU:HD12	1:D:243:LEU:HA	1.90	0.42
1:G:90:ASP:O	1:G:94:GLN:HG2	2.19	0.42
1:H:269:LEU:O	1:H:271:ARG:HG3	2.20	0.42
1:D:150:ARG:HD3	1:D:164:VAL:O	2.19	0.41
1:G:171:GLU:O	1:G:176:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:LEU:HB3	1:G:290:GLU:HB2	2.02	0.41
1:A:246:GLU:O	1:A:247:LYS:HB2	2.21	0.41
1:B:292:GLU:CD	1:B:295:ARG:HH22	2.27	0.41
1:C:104:LEU:HD21	1:C:132:LEU:HD11	2.01	0.41
1:E:29:VAL:HA	1:E:58:ARG:O	2.20	0.41
1:F:259:VAL:HG13	1:F:262:VAL:HG22	2.02	0.41
1:A:1:MSE:SE	1:A:69:ARG:NH1	3.04	0.41
1:C:10:MSE:HE1	1:D:10:MSE:CE	2.51	0.41
1:C:221:ILE:HD13	1:C:226:ALA:HA	2.02	0.41
1:E:69:ARG:NH2	1:E:242:ILE:O	2.54	0.41
1:E:295:ARG:HH11	1:E:299:GLU:CD	2.29	0.41
1:F:143:ILE:HG13	1:F:144:LEU:N	2.36	0.41
1:A:5:ILE:HG12	1:A:72:VAL:HB	2.03	0.41
1:A:292:GLU:OE2	1:A:295:ARG:CZ	2.68	0.41
1:C:86:LEU:HD12	1:C:308:LEU:HD13	2.03	0.41
1:D:156:TYR:OH	1:D:200:ALA:O	2.37	0.41
1:E:231:ILE:HG13	1:E:235:LEU:HD22	2.02	0.41
1:F:262:VAL:CG2	1:F:298:ALA:HB1	2.39	0.41
1:H:4:GLY:HA3	1:H:65:LEU:HD22	2.03	0.41
1:F:228:TYR:HA	1:F:231:ILE:HG22	2.03	0.41
1:G:154:ALA:HB1	1:G:159:VAL:O	2.21	0.41
1:C:231:ILE:O	1:C:235:LEU:HB2	2.21	0.41
1:C:279:GLU:OE2	1:F:197:ARG:NH2	2.53	0.41
1:F:302:LYS:HE3	1:F:306:PHE:CZ	2.55	0.41
1:H:79:GLN:NE2	1:H:83:GLU:O	2.54	0.41
1:H:220:ILE:O	1:H:224:LYS:HB3	2.21	0.41
1:A:79:GLN:HA	1:A:88:LEU:HD13	2.03	0.41
1:C:224:LYS:HE3	1:D:41:HIS:CE1	2.56	0.41
1:D:199:ARG:HH11	1:D:199:ARG:HD3	1.63	0.41
1:F:146:THR:HA	1:F:168:VAL:HG23	2.03	0.41
1:G:136:ARG:NH1	4:G:1419:HOH:O	2.53	0.41
1:G:148:ARG:HH11	1:H:47:HIS:CD2	2.38	0.41
1:H:296:ARG:O	1:H:300:ILE:HG13	2.20	0.41
1:B:246:GLU:O	1:B:247:LYS:CB	2.67	0.41
1:C:7:GLY:O	1:C:12:GLY:HA3	2.21	0.41
1:D:215:ARG:HB2	1:D:219:ARG:NH1	2.34	0.41
1:D:256:THR:HA	1:D:257:PRO:HD3	1.95	0.41
1:E:53:HIS:HA	1:E:54:PRO:HD3	1.90	0.41
1:H:286:LEU:CB	1:H:291:ARG:HG2	2.50	0.41
1:B:103:VAL:C	1:B:105:GLU:N	2.77	0.41
1:B:113:LEU:HA	1:B:138:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:HA	1:C:161:PRO:HD3	1.97	0.41
1:G:231:ILE:HD12	1:G:231:ILE:HA	1.93	0.41
1:H:80:ARG:HB2	1:H:83:GLU:CD	2.46	0.41
1:H:90:ASP:OD2	1:H:94:GLN:NE2	2.54	0.41
1:A:148:ARG:HH11	1:A:148:ARG:CB	2.32	0.40
1:E:77:VAL:HG22	1:E:78:ALA:N	2.36	0.40
1:F:44:ASP:O	1:F:47:HIS:HB2	2.20	0.40
1:F:128:ARG:CD	1:F:310:PHE:O	2.65	0.40
1:F:269:LEU:H	1:F:271:ARG:HH12	1.67	0.40
1:D:44:ASP:O	1:D:47:HIS:HB2	2.21	0.40
1:E:81:PRO:HA	1:G:224:LYS:O	2.21	0.40
1:G:7:GLY:O	1:G:12:GLY:HA3	2.22	0.40
1:A:90:ASP:CG	1:D:77:VAL:HG11	2.46	0.40
1:A:162:GLN:H	1:A:162:GLN:CD	2.29	0.40
1:A:289:GLU:CD	1:A:289:GLU:N	2.75	0.40
1:B:171:GLU:HB3	1:B:175:SER:HB2	2.03	0.40
1:D:77:VAL:HG12	1:D:78:ALA:N	2.36	0.40
1:E:247:LYS:NZ	4:E:1434:HOH:O	2.53	0.40
1:H:173:GLY:O	1:H:176:GLU:HG2	2.21	0.40
1:A:79:GLN:HB2	1:A:88:LEU:HD22	2.03	0.40
1:B:35:ARG:NH2	4:B:1519:HOH:O	2.54	0.40
1:B:88:LEU:HA	1:B:91:ARG:CZ	2.52	0.40
1:B:114:VAL:HG21	1:B:123:THR:HA	2.04	0.40
1:C:102:ARG:HG3	1:C:102:ARG:NH1	2.37	0.40
1:E:282:VAL:O	1:E:284:PRO:HD3	2.21	0.40
1:F:269:LEU:O	1:F:271:ARG:HG3	2.21	0.40
1:G:143:ILE:HG13	1:G:144:LEU:N	2.36	0.40
1:A:135:GLY:O	1:A:277:GLY:HA3	2.21	0.40
1:A:157:LEU:CD1	1:A:185:VAL:HG21	2.51	0.40
1:B:69:ARG:HG2	1:B:69:ARG:NH1	2.33	0.40
1:D:201:LEU:HD23	1:D:201:LEU:HA	1.80	0.40
1:F:46:LEU:HD23	1:F:46:LEU:HA	1.92	0.40
1:H:144:LEU:HB2	4:H:1537:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/310 (98%)	290 (95%)	14 (5%)	0	100	100
1	B	300/310 (97%)	279 (93%)	19 (6%)	2 (1%)	18	23
1	C	308/310 (99%)	295 (96%)	10 (3%)	3 (1%)	12	15
1	D	296/310 (96%)	282 (95%)	13 (4%)	1 (0%)	36	46
1	E	300/310 (97%)	282 (94%)	16 (5%)	2 (1%)	18	23
1	F	304/310 (98%)	288 (95%)	12 (4%)	4 (1%)	9	10
1	G	308/310 (99%)	296 (96%)	10 (3%)	2 (1%)	21	27
1	H	304/310 (98%)	294 (97%)	8 (3%)	2 (1%)	18	23
All	All	2424/2480 (98%)	2306 (95%)	102 (4%)	16 (1%)	18	23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	GLU
1	F	80	ARG
1	F	81	PRO
1	H	228	TYR
1	C	52	ALA
1	C	201	LEU
1	E	127	TYR
1	F	83	GLU
1	G	52	ALA
1	G	228	TYR
1	H	52	ALA
1	B	264	GLU
1	E	228	TYR
1	F	52	ALA
1	D	134	PRO
1	B	77	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/229 (101%)	223 (96%)	8 (4%)	32	48
1	B	227/229 (99%)	211 (93%)	16 (7%)	14	19
1	C	232/229 (101%)	217 (94%)	15 (6%)	15	22
1	D	226/229 (99%)	211 (93%)	15 (7%)	15	21
1	E	229/229 (100%)	221 (96%)	8 (4%)	32	48
1	F	231/229 (101%)	216 (94%)	15 (6%)	15	22
1	G	232/229 (101%)	218 (94%)	14 (6%)	17	25
1	H	231/229 (101%)	218 (94%)	13 (6%)	19	28
All	All	1839/1832 (100%)	1735 (94%)	104 (6%)	18	27

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	49	THR
1	A	87	GLN
1	A	102	ARG
1	A	129	LEU
1	A	148	ARG
1	A	243	LEU
1	A	294	LEU
1	B	1	MSE
1	B	3	VAL
1	B	8	SER
1	B	36	LYS
1	B	41	HIS
1	B	47	HIS
1	B	49	THR
1	B	119	VAL
1	B	128	ARG
1	B	129	LEU
1	B	174	ASP

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Mol	Chain	Res	Type
1	B	238	LEU
1	B	247	LYS
1	B	267	LEU
1	B	286	LEU
1	B	296	ARG
1	C	6	VAL
1	C	49	THR
1	C	89	LEU
1	C	128	ARG
1	C	129	LEU
1	C	144	LEU
1	C	174	ASP
1	C	192	GLU
1	C	197	ARG
1	C	235	LEU
1	C	238	LEU
1	C	243	LEU
1	C	267	LEU
1	C	286	LEU
1	C	308	LEU
1	D	3	VAL
1	D	47	HIS
1	D	69	ARG
1	D	85	ARG
1	D	89	LEU
1	D	128	ARG
1	D	174	ASP
1	D	176	GLU
1	D	185	VAL
1	D	199	ARG
1	D	235	LEU
1	D	243	LEU
1	D	258	GLU
1	D	259	VAL
1	D	303	GLU
1	E	128	ARG
1	E	129	LEU
1	E	169	LEU
1	E	178	LEU
1	E	204	GLU
1	E	235	LEU
1	E	267	LEU

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Mol	Chain	Res	Type
1	E	292	GLU
1	F	3	VAL
1	F	35	ARG
1	F	36	LYS
1	F	46	LEU
1	F	47	HIS
1	F	81	PRO
1	F	87	GLN
1	F	128	ARG
1	F	162	GLN
1	F	174	ASP
1	F	195	GLU
1	F	260	GLU
1	F	267	LEU
1	F	286	LEU
1	F	308	LEU
1	G	26	ARG
1	G	47	HIS
1	G	89	LEU
1	G	128	ARG
1	G	129	LEU
1	G	152	LEU
1	G	184	GLN
1	G	199	ARG
1	G	208	ARG
1	G	222	GLU
1	G	235	LEU
1	G	238	LEU
1	G	257	PRO
1	G	267	LEU
1	H	36	LYS
1	H	46	LEU
1	H	49	THR
1	H	102	ARG
1	H	104	LEU
1	H	128	ARG
1	H	144	LEU
1	H	152	LEU
1	H	184	GLN
1	H	243	LEU
1	H	259	VAL
1	H	262	VAL

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Mol	Chain	Res	Type
1	H	267	LEU

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

Mol	Chain	Res	Type
1	A	41	HIS
1	A	53	HIS
1	A	184	GLN
1	B	87	GLN
1	B	98	GLN
1	C	41	HIS
1	C	184	GLN
1	D	53	HIS
1	D	165	HIS
1	D	172	HIS
1	E	41	HIS
1	E	47	HIS
1	E	94	GLN
1	E	117	ASN
1	F	79	GLN
1	F	184	GLN
1	G	41	HIS
1	G	117	ASN
1	H	39	GLN
1	H	47	HIS
1	H	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	1401	-	46,48,48	2.93	18 (39%)	64,73,73	2.08	20 (31%)
2	NAD	C	1402	-	46,48,48	2.87	19 (41%)	64,73,73	2.06	20 (31%)
3	SO4	H	1502	-	4,4,4	0.40	0	6,6,6	0.08	0
3	SO4	B	1501	-	4,4,4	0.55	0	6,6,6	0.80	0
2	NAD	E	1403	-	46,48,48	2.93	19 (41%)	64,73,73	2.05	20 (31%)
2	NAD	G	1404	-	46,48,48	2.94	19 (41%)	64,73,73	2.08	19 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1401	-	-	1/30/62/62	0/5/5/5
2	NAD	E	1403	-	-	1/30/62/62	0/5/5/5
2	NAD	G	1404	-	-	1/30/62/62	0/5/5/5
2	NAD	C	1402	-	-	0/30/62/62	0/5/5/5

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1403	NAD	C2N-N1N	9.70	1.45	1.35
2	G	1404	NAD	C2N-N1N	9.54	1.45	1.35
2	A	1401	NAD	C2N-N1N	9.42	1.45	1.35
2	C	1402	NAD	C2N-N1N	9.12	1.45	1.35
2	A	1401	NAD	C4N-C3N	6.63	1.49	1.39
2	G	1404	NAD	C4N-C3N	6.61	1.49	1.39
2	C	1402	NAD	C4N-C3N	6.53	1.49	1.39
2	E	1403	NAD	C4N-C3N	6.45	1.49	1.39
2	G	1404	NAD	O7N-C7N	6.29	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	NAD	O7N-C7N	6.27	1.35	1.24
2	C	1402	NAD	O7N-C7N	5.92	1.35	1.24
2	E	1403	NAD	O7N-C7N	5.75	1.34	1.24
2	E	1403	NAD	C2A-N1A	5.57	1.43	1.33
2	C	1402	NAD	C2A-N1A	5.51	1.43	1.33
2	G	1404	NAD	C2A-N1A	5.51	1.43	1.33
2	A	1401	NAD	C2A-N1A	5.50	1.43	1.33
2	A	1401	NAD	C6N-N1N	4.56	1.45	1.35
2	G	1404	NAD	C2A-N3A	4.56	1.42	1.33
2	C	1402	NAD	C2A-N3A	4.54	1.42	1.33
2	A	1401	NAD	C2A-N3A	4.52	1.42	1.33
2	E	1403	NAD	C2A-N3A	4.51	1.41	1.33
2	G	1404	NAD	C6N-N1N	4.49	1.45	1.35
2	E	1403	NAD	C6N-N1N	4.45	1.45	1.35
2	E	1403	NAD	C4A-N3A	4.42	1.42	1.34
2	C	1402	NAD	C6N-N1N	4.39	1.45	1.35
2	C	1402	NAD	C4A-N3A	4.38	1.42	1.34
2	G	1404	NAD	C4A-N3A	4.36	1.42	1.34
2	A	1401	NAD	C4A-N3A	4.33	1.42	1.34
2	E	1403	NAD	C5B-C4B	4.21	1.64	1.51
2	A	1401	NAD	C5B-C4B	4.19	1.64	1.51
2	G	1404	NAD	C5B-C4B	4.18	1.64	1.51
2	C	1402	NAD	C5B-C4B	4.14	1.64	1.51
2	G	1404	NAD	C5N-C4N	4.13	1.46	1.38
2	E	1403	NAD	C5N-C4N	4.12	1.46	1.38
2	C	1402	NAD	C5N-C4N	4.12	1.45	1.38
2	A	1401	NAD	C5N-C4N	4.11	1.45	1.38
2	E	1403	NAD	C2N-C3N	3.37	1.44	1.39
2	G	1404	NAD	C2N-C3N	3.35	1.44	1.39
2	E	1403	NAD	C6A-N1A	3.33	1.45	1.35
2	C	1402	NAD	C6A-N1A	3.32	1.45	1.35
2	E	1403	NAD	O4D-C1D	3.31	1.45	1.40
2	A	1401	NAD	C6A-N1A	3.29	1.45	1.35
2	G	1404	NAD	C6A-N1A	3.29	1.45	1.35
2	G	1404	NAD	O4D-C1D	3.26	1.45	1.40
2	A	1401	NAD	C2N-C3N	3.25	1.44	1.39
2	A	1401	NAD	O4D-C1D	3.23	1.45	1.40
2	C	1402	NAD	O4D-C1D	3.01	1.44	1.40
2	C	1402	NAD	C2N-C3N	2.99	1.43	1.39
2	A	1401	NAD	C5A-C4A	2.84	1.44	1.39
2	G	1404	NAD	C5A-C4A	2.81	1.44	1.39
2	E	1403	NAD	C5A-C4A	2.79	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1402	NAD	C5A-C4A	2.74	1.44	1.39
2	C	1402	NAD	C2D-C3D	-2.70	1.46	1.53
2	E	1403	NAD	C2D-C3D	-2.68	1.46	1.53
2	G	1404	NAD	C2D-C3D	-2.59	1.46	1.53
2	G	1404	NAD	O3D-C3D	2.57	1.49	1.43
2	A	1401	NAD	C2D-C3D	-2.55	1.46	1.53
2	E	1403	NAD	O3D-C3D	2.55	1.49	1.43
2	A	1401	NAD	O3D-C3D	2.52	1.49	1.43
2	C	1402	NAD	O3D-C3D	2.51	1.49	1.43
2	A	1401	NAD	C6N-C5N	2.41	1.43	1.38
2	G	1404	NAD	C6N-C5N	2.39	1.43	1.38
2	C	1402	NAD	C6N-C5N	2.35	1.43	1.38
2	E	1403	NAD	C6N-C5N	2.35	1.43	1.38
2	C	1402	NAD	O4D-C4D	-2.27	1.39	1.45
2	A	1401	NAD	C5A-N7A	-2.20	1.35	1.39
2	E	1403	NAD	O4D-C4D	-2.19	1.40	1.45
2	G	1404	NAD	C5A-N7A	-2.18	1.35	1.39
2	C	1402	NAD	C5A-N7A	-2.15	1.35	1.39
2	E	1403	NAD	C5A-N7A	-2.13	1.35	1.39
2	A	1401	NAD	O4D-C4D	-2.12	1.40	1.45
2	G	1404	NAD	O4D-C4D	-2.09	1.40	1.45
2	C	1402	NAD	O4B-C1B	2.04	1.46	1.42
2	G	1404	NAD	PN-O3	2.01	1.61	1.59
2	E	1403	NAD	O4B-C1B	2.00	1.46	1.42

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1402	NAD	N3A-C2A-N1A	-6.64	118.54	128.58
2	A	1401	NAD	N3A-C2A-N1A	-6.62	118.56	128.58
2	G	1404	NAD	N3A-C2A-N1A	-6.61	118.57	128.58
2	E	1403	NAD	N3A-C2A-N1A	-6.61	118.57	128.58
2	G	1404	NAD	C3N-C7N-N7N	5.45	124.46	117.74
2	A	1401	NAD	C3N-C7N-N7N	5.43	124.42	117.74
2	E	1403	NAD	C3N-C7N-N7N	5.37	124.35	117.74
2	C	1402	NAD	C3N-C7N-N7N	5.33	124.31	117.74
2	C	1402	NAD	O3D-C3D-C2D	-4.74	96.63	111.82
2	A	1401	NAD	O3D-C3D-C2D	-4.72	96.70	111.82
2	G	1404	NAD	O3D-C3D-C2D	-4.68	96.81	111.82
2	E	1403	NAD	O3D-C3D-C2D	-4.68	96.82	111.82
2	A	1401	NAD	C4B-O4B-C1B	-4.59	99.32	109.47
2	G	1404	NAD	C4B-O4B-C1B	-4.59	99.34	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1403	NAD	C4B-O4B-C1B	-4.58	99.36	109.47
2	C	1402	NAD	C4B-O4B-C1B	-4.53	99.47	109.47
2	A	1401	NAD	C2D-C3D-C4D	3.60	109.57	102.61
2	G	1404	NAD	C2D-C3D-C4D	3.41	109.20	102.61
2	A	1401	NAD	O4B-C4B-C3B	3.41	111.91	105.15
2	E	1403	NAD	O4B-C4B-C3B	3.40	111.91	105.15
2	G	1404	NAD	O4B-C4B-C3B	3.39	111.88	105.15
2	C	1402	NAD	O4B-C1B-C2B	3.33	113.74	106.62
2	A	1401	NAD	C2A-N3A-C4A	3.33	119.96	111.83
2	E	1403	NAD	C2A-N3A-C4A	3.32	119.94	111.83
2	C	1402	NAD	O4B-C4B-C3B	3.32	111.74	105.15
2	G	1404	NAD	C2A-N3A-C4A	3.31	119.92	111.83
2	C	1402	NAD	C2A-N3A-C4A	3.31	119.91	111.83
2	G	1404	NAD	O4B-C1B-C2B	3.28	113.63	106.62
2	A	1401	NAD	O4B-C1B-C2B	3.26	113.60	106.62
2	E	1403	NAD	O4B-C1B-C2B	3.23	113.52	106.62
2	G	1404	NAD	C5A-N7A-C8A	3.07	108.27	103.45
2	A	1401	NAD	C5A-N7A-C8A	3.05	108.24	103.45
2	C	1402	NAD	C5A-N7A-C8A	3.03	108.21	103.45
2	E	1403	NAD	C5A-N7A-C8A	3.01	108.19	103.45
2	G	1404	NAD	N9A-C8A-N7A	-3.01	109.67	113.94
2	A	1401	NAD	N9A-C8A-N7A	-2.97	109.72	113.94
2	C	1402	NAD	N9A-C8A-N7A	-2.95	109.75	113.94
2	E	1403	NAD	N9A-C8A-N7A	-2.92	109.79	113.94
2	G	1404	NAD	O7N-C7N-N7N	-2.80	118.58	122.62
2	E	1403	NAD	O7N-C7N-N7N	-2.73	118.67	122.62
2	A	1401	NAD	O7N-C7N-N7N	-2.68	118.74	122.62
2	C	1402	NAD	C2D-C3D-C4D	2.63	107.70	102.61
2	E	1403	NAD	C5A-C4A-N3A	-2.62	123.11	126.72
2	G	1404	NAD	C5A-C4A-N3A	-2.57	123.17	126.72
2	A	1401	NAD	C5A-C4A-N3A	-2.56	123.18	126.72
2	C	1402	NAD	C5A-C4A-N3A	-2.55	123.21	126.72
2	C	1402	NAD	O7N-C7N-C3N	-2.51	116.53	119.60
2	E	1403	NAD	C2D-C3D-C4D	2.45	107.35	102.61
2	G	1404	NAD	C3B-C2B-C1B	-2.40	96.92	101.46
2	C	1402	NAD	O7N-C7N-N7N	-2.39	119.16	122.62
2	C	1402	NAD	C3B-C2B-C1B	-2.39	96.93	101.46
2	C	1402	NAD	C5N-C4N-C3N	2.33	122.66	120.36
2	A	1401	NAD	C3B-C2B-C1B	-2.31	97.08	101.46
2	A	1401	NAD	O7N-C7N-C3N	-2.26	116.84	119.60
2	E	1403	NAD	C3B-C2B-C1B	-2.26	97.19	101.46
2	A	1401	NAD	C5N-C4N-C3N	2.24	122.57	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1404	NAD	O2B-C2B-C1B	2.23	117.80	110.10
2	A	1401	NAD	O2B-C2B-C1B	2.23	117.79	110.10
2	C	1402	NAD	O2B-C2B-C1B	2.22	117.74	110.10
2	E	1403	NAD	C4A-C5A-N7A	-2.22	108.05	110.58
2	E	1403	NAD	O2B-C2B-C1B	2.21	117.70	110.10
2	E	1403	NAD	C5N-C4N-C3N	2.21	122.53	120.36
2	G	1404	NAD	C4A-C5A-N7A	-2.20	108.06	110.58
2	G	1404	NAD	C5N-C4N-C3N	2.20	122.53	120.36
2	A	1401	NAD	O5D-PN-O1N	2.19	117.61	108.94
2	C	1402	NAD	C4A-C5A-N7A	-2.18	108.09	110.58
2	A	1401	NAD	C4A-C5A-N7A	-2.17	108.11	110.58
2	E	1403	NAD	O7N-C7N-C3N	-2.17	116.95	119.60
2	G	1404	NAD	O7N-C7N-C3N	-2.15	116.97	119.60
2	E	1403	NAD	O2B-C2B-C3B	2.12	118.62	111.82
2	C	1402	NAD	O2B-C2B-C3B	2.12	118.61	111.82
2	G	1404	NAD	O2B-C2B-C3B	2.11	118.59	111.82
2	A	1401	NAD	O2B-C2B-C3B	2.11	118.58	111.82
2	E	1403	NAD	O5D-PN-O1N	2.11	117.29	108.94
2	C	1402	NAD	O5D-PN-O1N	2.11	117.28	108.94
2	G	1404	NAD	C4A-N9A-C1B	-2.09	121.75	126.63
2	A	1401	NAD	C4A-N9A-C1B	-2.08	121.76	126.63
2	E	1403	NAD	C4A-N9A-C1B	-2.06	121.82	126.63
2	C	1402	NAD	C4A-N9A-C1B	-2.03	121.88	126.63

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1403	NAD	O4D-C1D-N1N-C6N
2	A	1401	NAD	O4B-C4B-C5B-O5B
2	G	1404	NAD	O4B-C4B-C5B-O5B

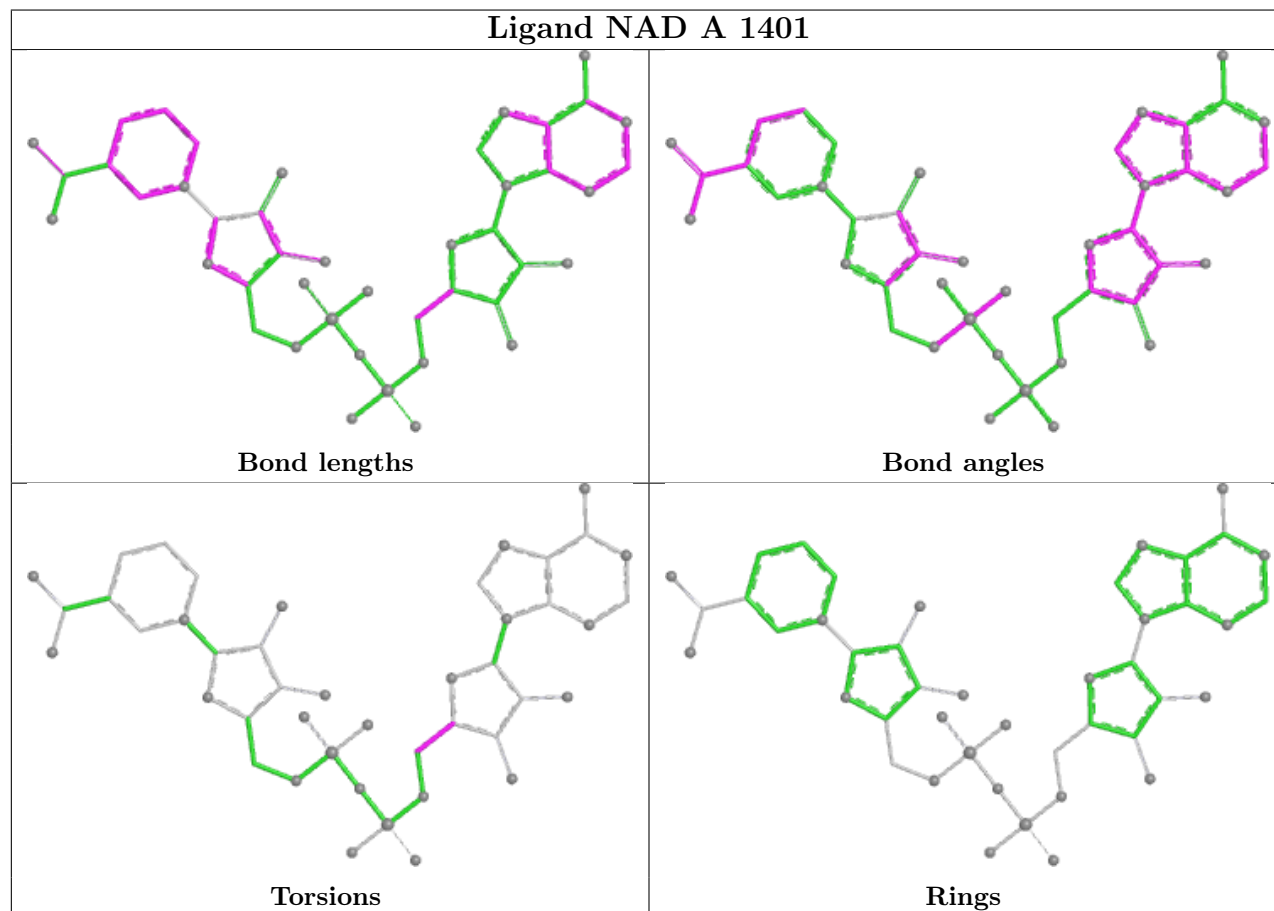
There are no ring outliers.

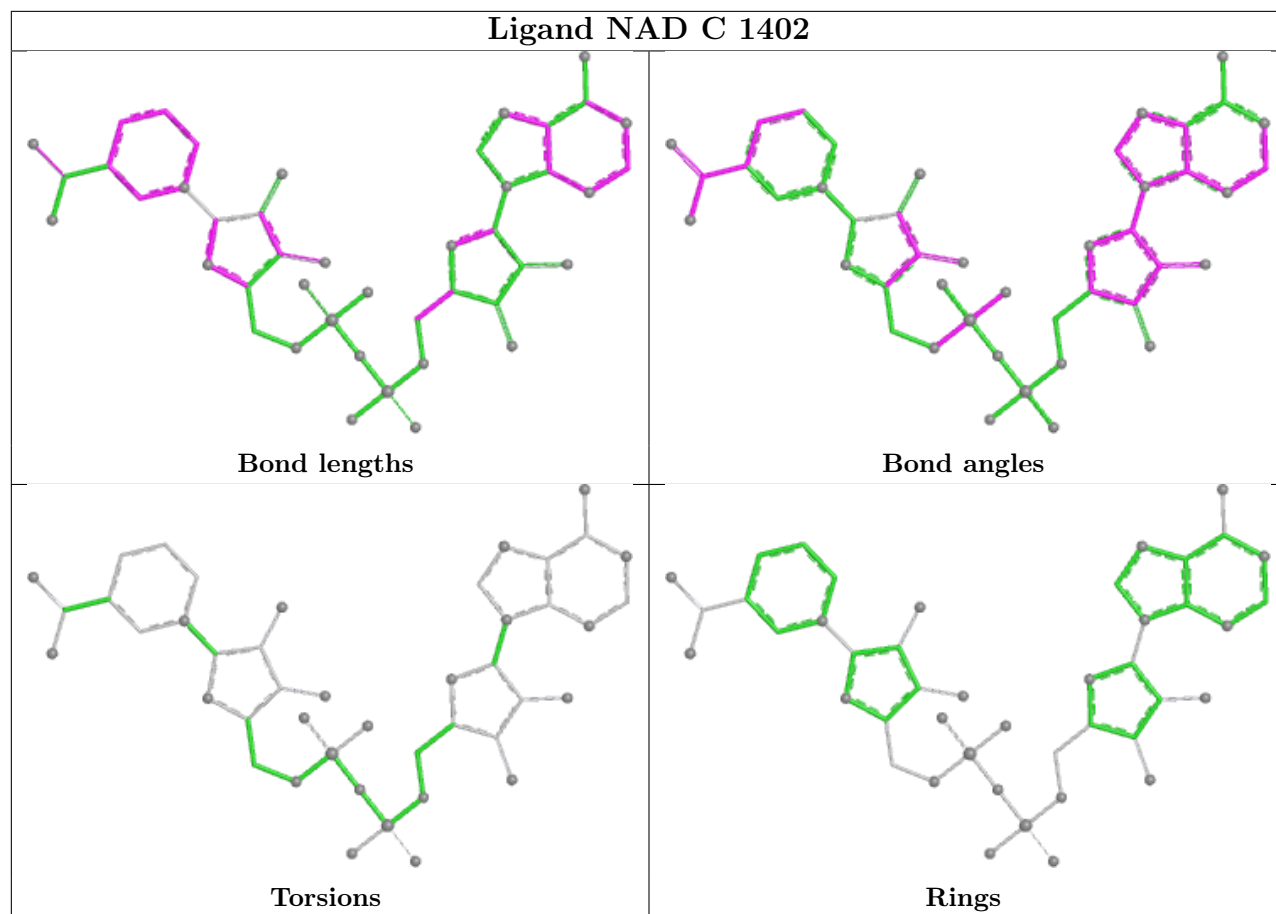
2 monomers are involved in 2 short contacts:

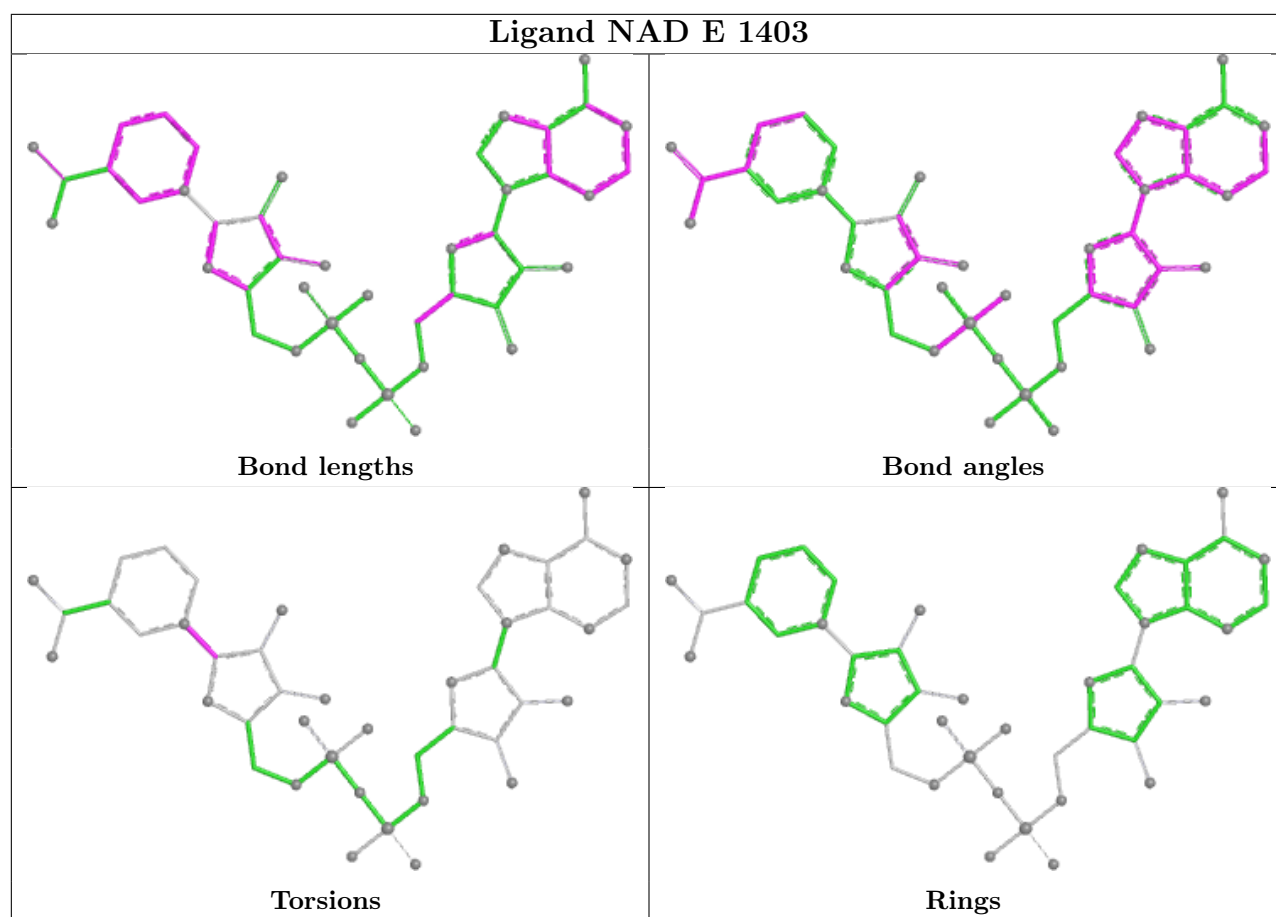
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	SO4	1	0
2	G	1404	NAD	1	0

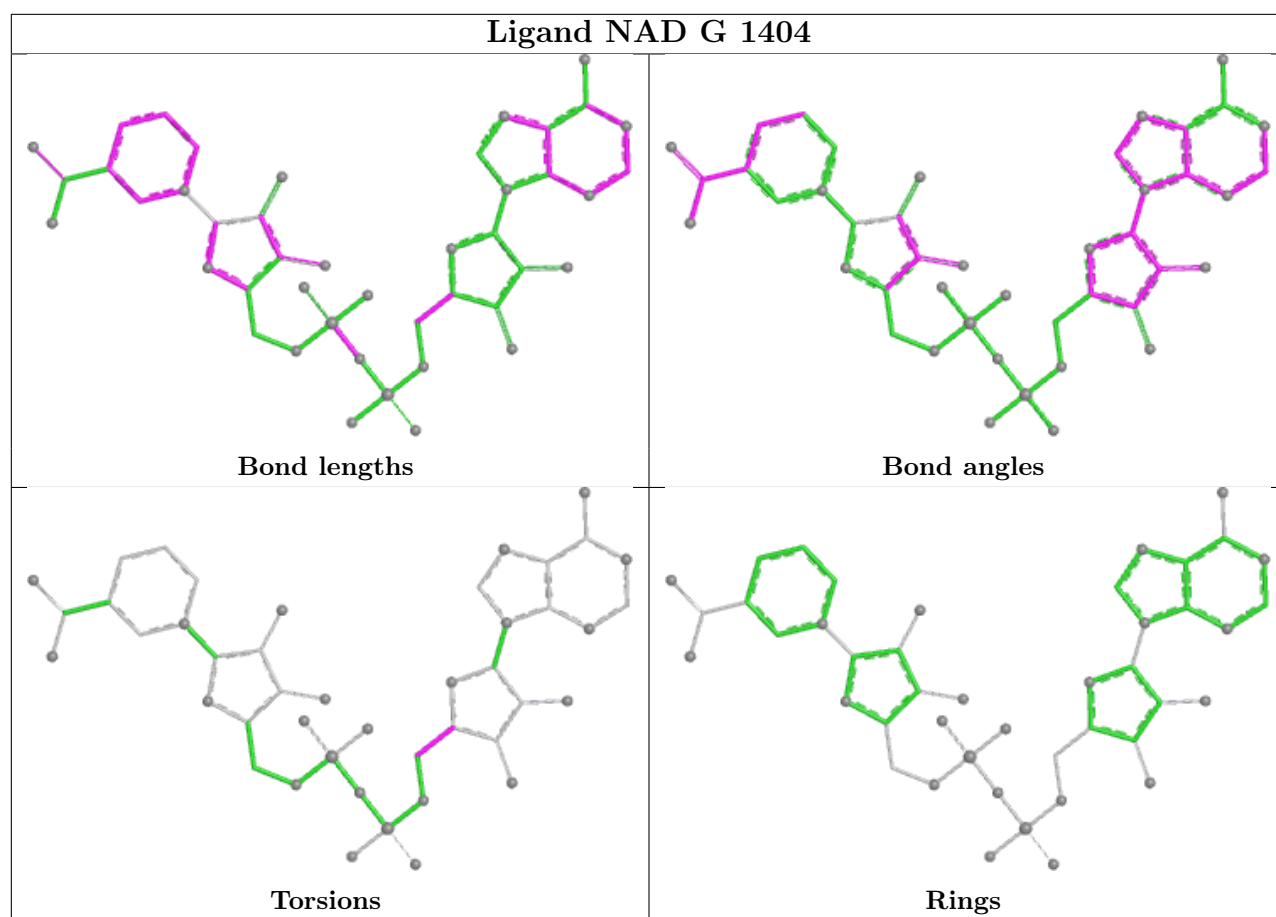
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/310 (98%)	0.15	8 (2%) 57 59	31, 43, 60, 91	0
1	B	301/310 (97%)	0.45	12 (3%) 42 44	28, 47, 72, 98	0
1	C	307/310 (99%)	-0.02	1 (0%) 90 90	26, 40, 52, 61	0
1	D	299/310 (96%)	0.66	24 (8%) 18 20	32, 55, 83, 99	0
1	E	301/310 (97%)	0.35	8 (2%) 56 58	32, 46, 67, 93	0
1	F	305/310 (98%)	0.32	21 (6%) 23 25	31, 43, 73, 103	0
1	G	307/310 (99%)	-0.01	2 (0%) 84 85	27, 39, 55, 68	0
1	H	305/310 (98%)	0.03	9 (2%) 52 54	24, 38, 63, 80	0
All	All	2430/2480 (97%)	0.24	85 (3%) 47 49	24, 43, 70, 103	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	ALA	5.7
1	F	200	ALA	5.0
1	H	200	ALA	4.9
1	A	200	ALA	4.4
1	D	78	ALA	4.3
1	A	196	ALA	4.2
1	F	156	TYR	4.2
1	F	81	PRO	4.2
1	B	306	PHE	4.2
1	F	196	ALA	4.1
1	B	86	LEU	3.9
1	E	195	GLU	3.7
1	E	194	ALA	3.7
1	E	193	PHE	3.6
1	D	306	PHE	3.6
1	H	196	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	191	LEU	3.5
1	B	78	ALA	3.4
1	F	306	PHE	3.2
1	B	261	GLY	3.2
1	H	201	LEU	3.2
1	D	300	ILE	3.2
1	A	201	LEU	3.2
1	F	88	LEU	3.1
1	D	86	LEU	3.1
1	F	201	LEU	3.1
1	H	33	LEU	3.0
1	H	174	ASP	2.9
1	D	200	ALA	2.9
1	D	193	PHE	2.8
1	A	197	ARG	2.8
1	D	174	ASP	2.8
1	F	86	LEU	2.8
1	A	283	TYR	2.7
1	D	191	LEU	2.7
1	D	165	HIS	2.6
1	D	201	LEU	2.6
1	F	79	GLN	2.6
1	F	89	LEU	2.6
1	D	190	LEU	2.5
1	B	85	ARG	2.5
1	F	82	GLY	2.5
1	H	86	LEU	2.5
1	D	262	VAL	2.5
1	A	191	LEU	2.5
1	D	89	LEU	2.5
1	H	191	LEU	2.5
1	F	197	ARG	2.4
1	B	310	PHE	2.4
1	E	202	SER	2.4
1	F	78	ALA	2.4
1	A	156	TYR	2.4
1	D	203	PRO	2.4
1	F	194	ALA	2.4
1	G	200	ALA	2.4
1	D	199	ARG	2.3
1	F	175	SER	2.3
1	G	201	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	165	HIS	2.3
1	F	195	GLU	2.3
1	F	191	LEU	2.3
1	B	89	LEU	2.2
1	D	301	LEU	2.2
1	B	303	GLU	2.2
1	F	84	THR	2.2
1	H	195	GLU	2.2
1	F	193	PHE	2.2
1	B	222	GLU	2.2
1	C	292	GLU	2.2
1	H	192	GLU	2.2
1	A	174	ASP	2.2
1	D	185	VAL	2.2
1	B	204	GLU	2.2
1	D	202	SER	2.2
1	D	204	GLU	2.1
1	D	307	ALA	2.1
1	E	283	TYR	2.1
1	F	109	GLU	2.1
1	D	310	PHE	2.1
1	D	166	ALA	2.1
1	E	306	PHE	2.1
1	B	223	GLY	2.1
1	F	80	ARG	2.1
1	D	298	ALA	2.0
1	B	56	TRP	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,

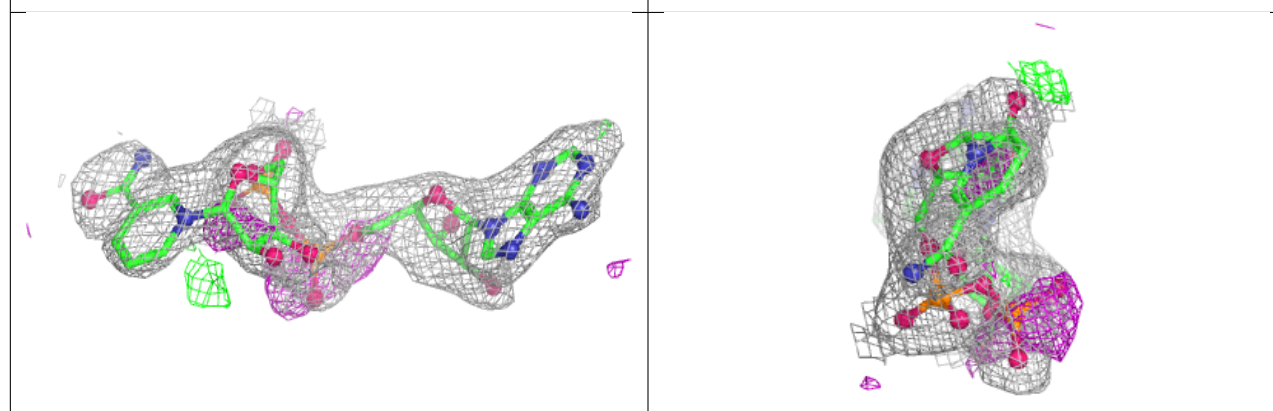
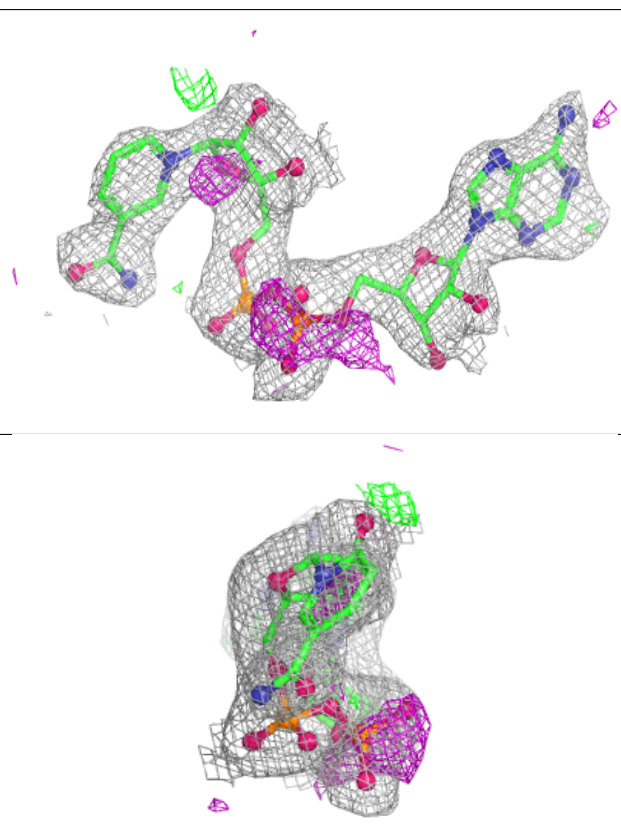
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	1501	5/5	0.77	0.16	112,112,112,113	0
2	NAD	C	1402	44/44	0.88	0.13	59,64,71,72	0
2	NAD	G	1404	44/44	0.89	0.13	50,56,67,68	0
2	NAD	E	1403	44/44	0.89	0.13	50,63,80,81	0
3	SO4	H	1502	5/5	0.90	0.13	100,101,102,102	0
2	NAD	A	1401	44/44	0.92	0.12	48,56,69,70	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.

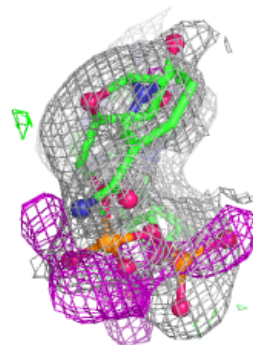
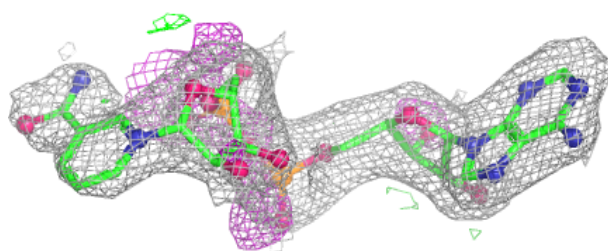
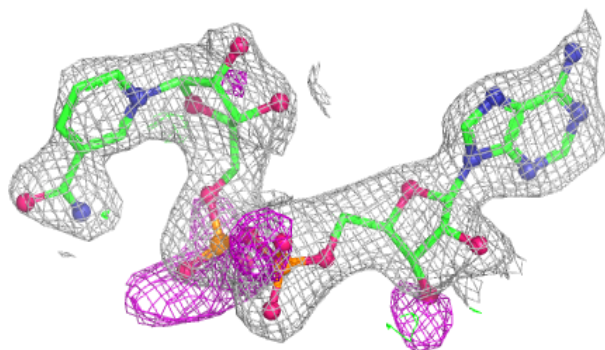
Electron density around NAD C 1402:

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

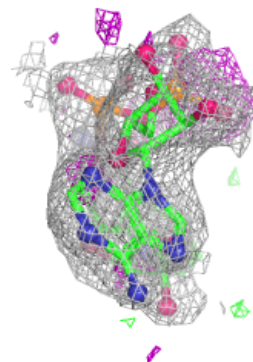
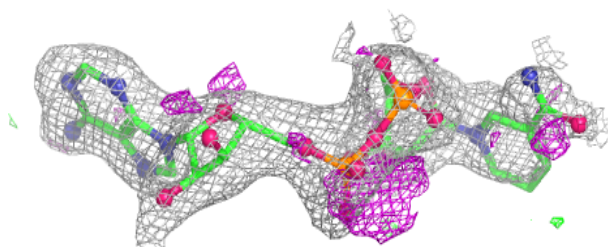
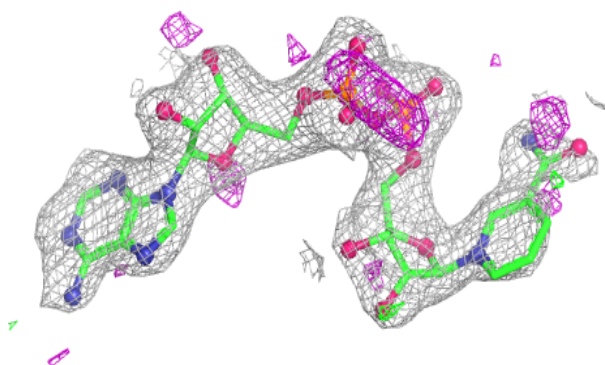


Electron density around NAD G 1404:

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

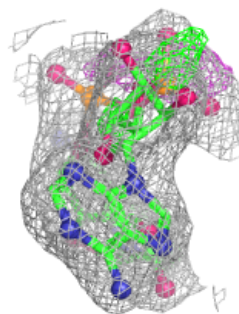
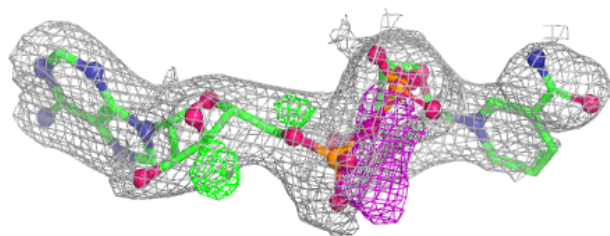
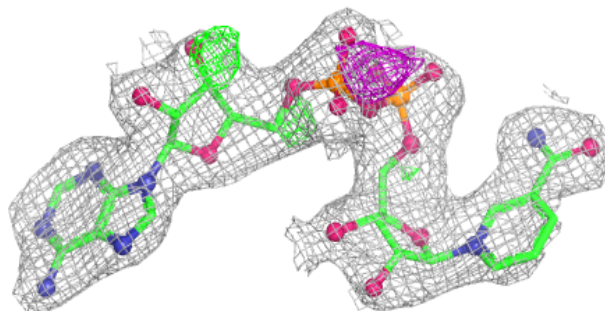
**Electron density around NAD E 1403:**

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



Electron density around NAD A 1401:

$2mF_o-DF_c$ (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.