



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:51 PM UTC

PDB ID : 1T90 / pdb_00001t90
Title : Crystal structure of methylmalonate semialdehyde dehydrogenase from *Bacillus subtilis*
Authors : Dubourg, H.; Didierjean, C.; Stines-Chaumeil, C.; Talfournier, F.; Branlant, G.; Aubry, A.; Corbier, C.
Deposited on : 2004-05-14
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

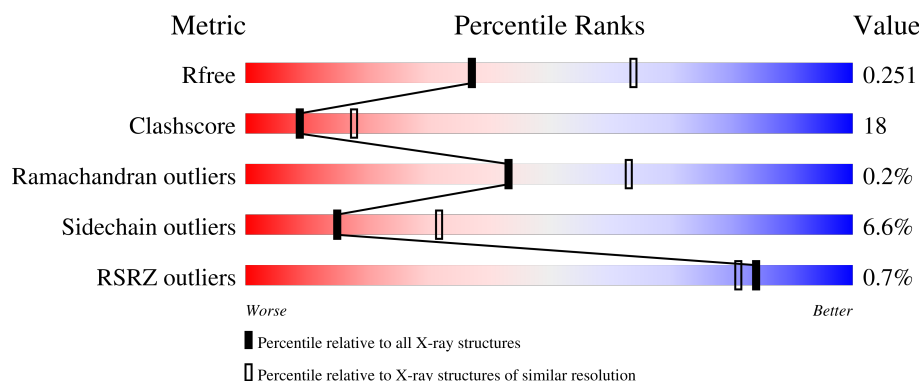
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	486	 60% 33% 6%
1	B	486	 64% 31% 5% 1%
1	C	486	 66% 29% 5%
1	D	486	 65% 31% 4% 1%

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

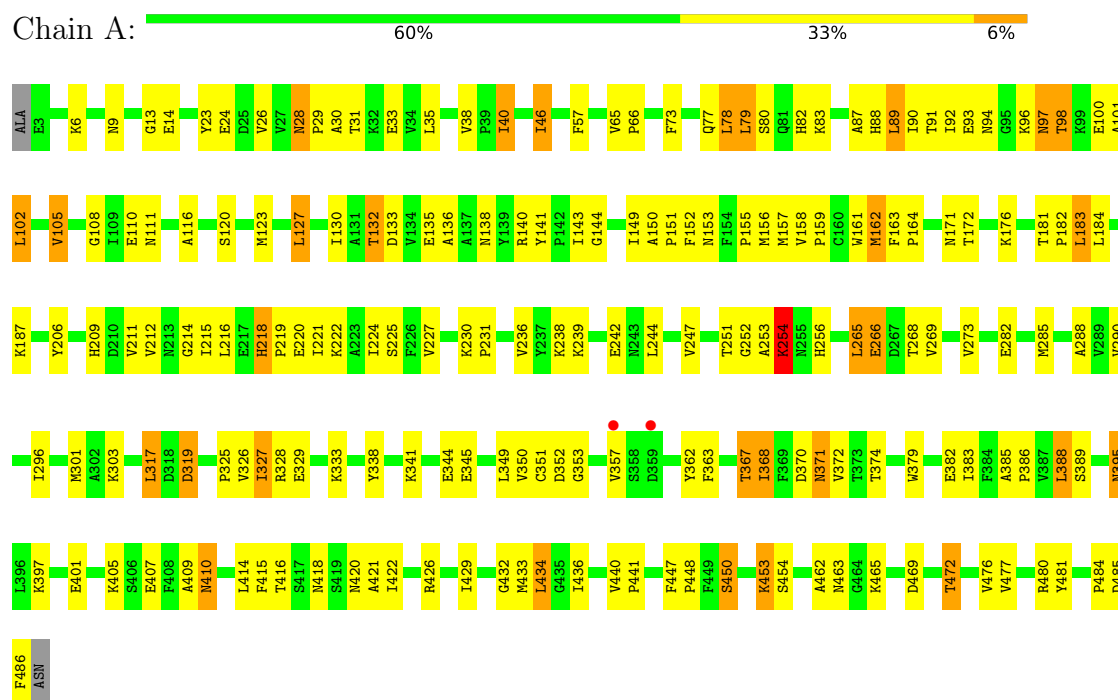
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		
3	B	229	Total	O	0	0
			229	229		
3	C	246	Total	O	0	0
			246	246		
3	D	189	Total	O	0	0
			189	189		

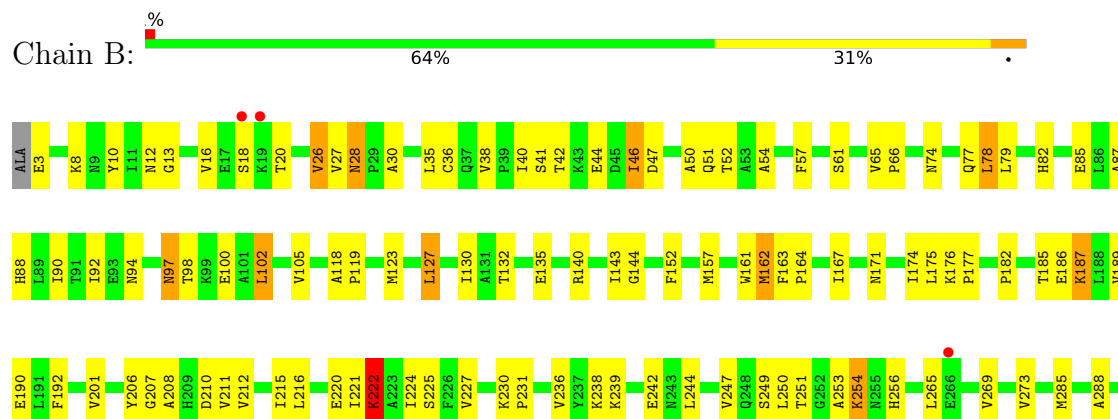
3 Residue-property plots

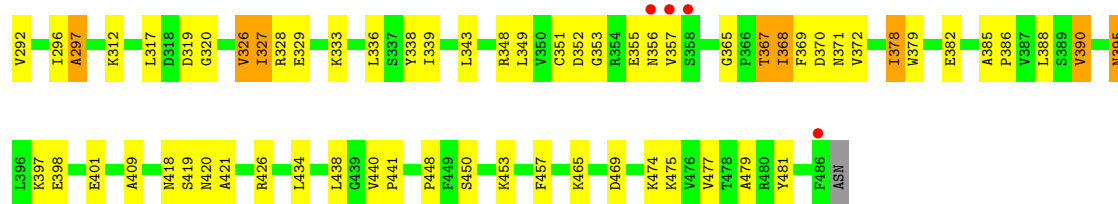
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable methylmalonate-semialdehyde dehydrogenase



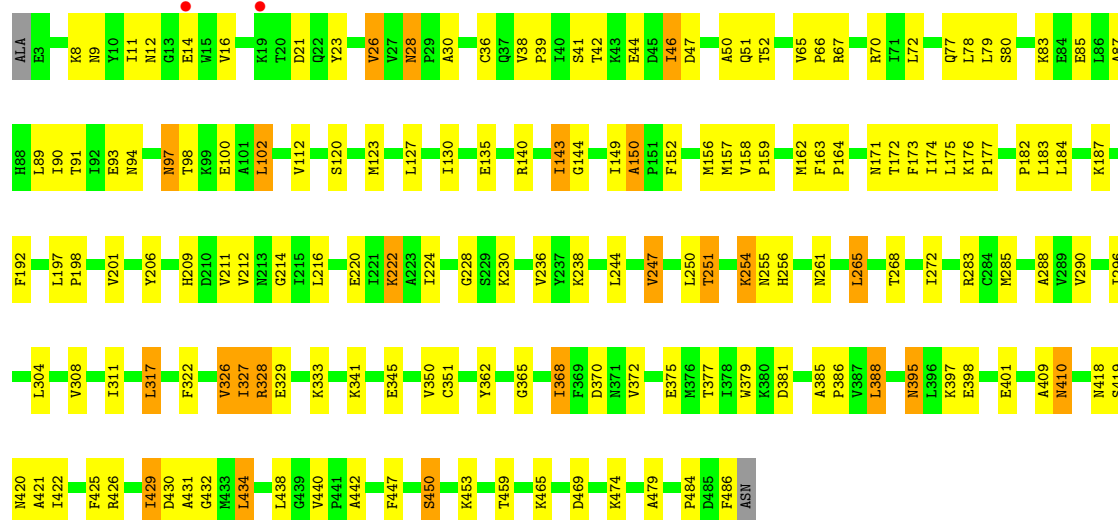
- Molecule 1: Probable methylmalonate-semialdehyde dehydrogenase





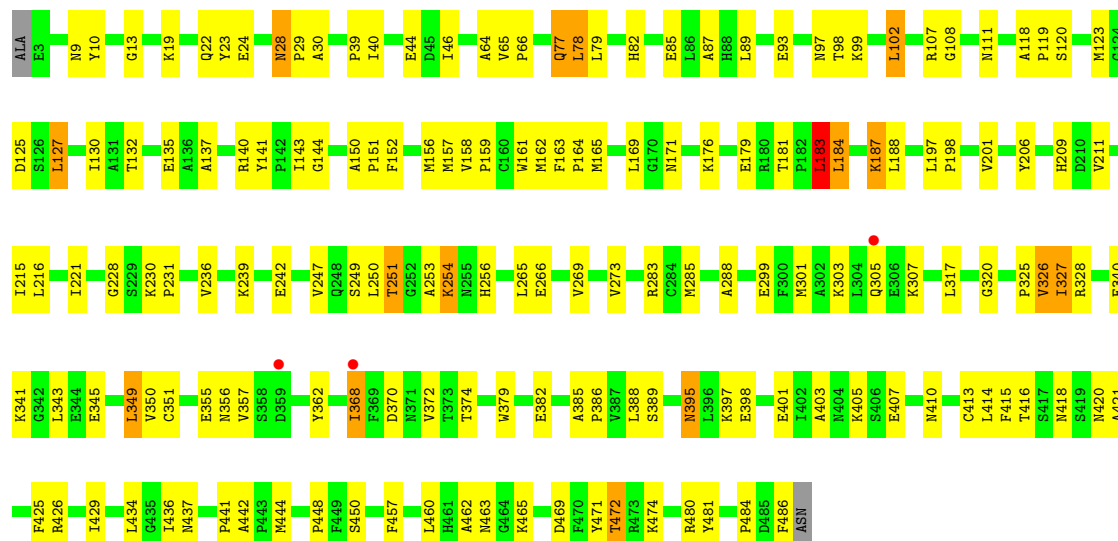
• Molecule 1: Probable methylmalonate-semialdehyde dehydrogenase

Chain C: 66% 29% 5%



• Molecule 1: Probable methylmalonate-semialdehyde dehydrogenase

Chain D: 65% 31% 4%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	195.20Å 192.50Å 83.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 99.3 (20.00-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.250 0.211 , 0.251	Depositor DCC
R_{free} test set	5418 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16006	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5701e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3818	0.96	21/5171 (0.4%)
1	B	0.42	0/3818	0.96	11/5171 (0.2%)
1	C	0.41	0/3818	0.96	17/5171 (0.3%)
1	D	0.40	0/3818	0.91	9/5171 (0.2%)
All	All	0.41	0/15272	0.95	58/20684 (0.3%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	ILE	N-CA-C	10.98	120.96	110.42
1	C	327	ILE	N-CA-C	10.01	120.03	110.42
1	A	327	ILE	N-CA-C	9.70	119.73	110.42
1	B	450	SER	N-CA-C	8.54	122.91	108.23
1	D	327	ILE	N-CA-C	8.32	118.41	110.42
1	A	450	SER	N-CA-C	8.12	121.63	108.63
1	C	450	SER	N-CA-C	7.21	121.53	107.98
1	A	251	THR	N-CA-C	7.14	120.26	109.63
1	D	450	SER	N-CA-C	7.11	121.33	108.17
1	B	326	VAL	N-CA-C	-6.88	102.55	110.05
1	C	447	PHE	CA-C-N	-6.70	113.04	120.14
1	C	447	PHE	C-N-CA	-6.70	113.04	120.14
1	A	130	ILE	N-CA-C	-6.68	106.14	113.43
1	C	209	HIS	N-CA-C	6.55	118.08	111.07
1	A	222	LYS	N-CA-C	6.55	118.50	111.36
1	C	251	THR	N-CA-C	6.44	119.22	109.63
1	D	251	THR	N-CA-C	6.37	119.12	109.63
1	D	326	VAL	N-CA-C	-6.25	103.24	110.05
1	D	320	GLY	N-CA-C	-6.10	107.82	115.08
1	A	209	HIS	N-CA-C	6.06	117.69	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	PHE	CA-C-N	-6.05	113.46	119.99
1	A	447	PHE	C-N-CA	-6.05	113.46	119.99
1	D	209	HIS	N-CA-C	5.92	117.53	111.14
1	A	162	MET	N-CA-C	5.88	121.96	110.56
1	A	181	THR	CA-C-N	5.84	127.14	119.84
1	A	181	THR	C-N-CA	5.84	127.14	119.84
1	B	157	MET	N-CA-C	5.73	117.21	110.97
1	D	130	ILE	N-CA-C	-5.67	107.25	113.43
1	C	265	LEU	N-CA-C	5.65	117.44	111.28
1	B	222	LYS	N-CA-C	5.59	119.71	113.01
1	C	173	PHE	N-CA-C	5.56	118.29	109.50
1	B	297	ALA	N-CA-C	5.54	117.75	111.11
1	C	130	ILE	N-CA-C	-5.50	107.43	113.43
1	B	161	TRP	N-CA-C	-5.48	106.09	112.89
1	A	172	THR	N-CA-C	-5.48	101.65	110.14
1	B	162	MET	N-CA-C	5.47	122.46	110.80
1	B	251	THR	N-CA-C	5.44	119.04	109.80
1	B	130	ILE	N-CA-C	-5.43	107.51	113.43
1	C	326	VAL	N-CA-C	-5.36	104.16	110.21
1	A	218	HIS	CA-C-N	5.35	125.02	119.56
1	A	218	HIS	C-N-CA	5.35	125.02	119.56
1	C	157	MET	N-CA-C	5.33	117.52	111.02
1	C	172	THR	N-CA-C	-5.32	101.89	110.14
1	C	21	ASP	N-CA-C	-5.28	106.86	113.72
1	A	254	LYS	N-CA-C	-5.20	99.73	110.80
1	D	183	LEU	N-CA-C	5.19	116.94	111.28
1	A	440	VAL	CA-C-N	5.18	126.31	119.84
1	A	440	VAL	C-N-CA	5.18	126.31	119.84
1	A	252	GLY	N-CA-C	5.17	119.18	112.25
1	C	150	ALA	CA-C-N	5.16	126.42	120.85
1	C	150	ALA	C-N-CA	5.16	126.42	120.85
1	C	222	LYS	N-CA-C	5.14	119.17	113.01
1	A	150	ALA	CA-C-N	5.08	126.42	120.98
1	A	150	ALA	C-N-CA	5.08	126.42	120.98
1	D	162	MET	N-CA-C	5.08	121.63	110.80
1	C	162	MET	N-CA-C	5.06	121.59	110.80
1	B	27	VAL	N-CA-C	5.06	116.48	109.29
1	A	40	ILE	N-CA-C	-5.05	98.84	109.34

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	3741	0	3730	173	0
1	B	3741	0	3730	144	0
1	C	3741	0	3730	145	0
1	D	3741	0	3730	141	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
3	A	202	0	0	8	0
3	B	229	0	0	7	0
3	C	246	0	0	9	0
3	D	189	0	0	8	0
All	All	16006	0	15024	557	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 18.

All (557) 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:418:ASN:HD22	1:B:421:ALA:H	1.03	1.00
1:B:77:GLN:HB2	1:D:77:GLN:HE21	1.29	0.96
1:C:143:ILE:H	1:C:171:ASN:HD21	1.14	0.93
1:A:123:MET:HE1	1:C:465:LYS:NZ	1.88	0.89
1:B:77:GLN:HG2	1:D:77:GLN:HG2	1.55	0.88
1:B:143:ILE:H	1:B:171:ASN:HD21	1.22	0.87
1:C:418:ASN:HD22	1:C:421:ALA:H	1.22	0.87
1:D:143:ILE:H	1:D:171:ASN:HD21	1.23	0.87
1:D:374:THR:HG21	1:D:405:LYS:HD3	1.55	0.87
1:B:77:GLN:HB2	1:D:77:GLN:NE2	1.88	0.86
1:A:374:THR:HG21	1:A:405:LYS:HD3	1.56	0.85
1:B:216:LEU:HD21	1:B:236:VAL:HG13	1.58	0.85
1:B:351:CYS:HB2	1:B:368:ILE:HG23	1.61	0.83
1:A:465:LYS:HZ3	1:C:123:MET:HE1	1.44	0.82
1:A:351:CYS:HB3	1:A:368:ILE:HG23	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASN:ND2	1:B:421:ALA:H	1.76	0.82
1:B:123:MET:HE1	1:D:465:LYS:NZ	1.94	0.81
1:A:77:GLN:HG3	1:C:77:GLN:CD	2.06	0.81
1:B:465:LYS:HZ3	1:D:123:MET:HE1	1.43	0.81
1:A:265:LEU:HD12	1:A:303:LYS:HD3	1.63	0.81
1:B:351:CYS:HB2	1:B:368:ILE:CG2	2.12	0.80
1:B:397:LYS:O	1:B:401:GLU:HG3	1.81	0.80
1:B:418:ASN:HD21	1:B:420:ASN:HB2	1.49	0.78
1:D:343:LEU:HD21	1:D:349:LEU:HB2	1.66	0.77
1:C:28:ASN:C	1:C:28:ASN:HD22	1.92	0.77
1:D:93:GLU:OE2	1:D:183:LEU:HB2	1.85	0.76
1:B:167:ILE:HD12	1:B:201:VAL:HG12	1.68	0.76
1:B:97:ASN:ND2	1:B:100:GLU:H	1.83	0.76
1:B:143:ILE:H	1:B:171:ASN:ND2	1.83	0.76
1:A:140:ARG:HH12	1:A:469:ASP:CG	1.94	0.76
1:A:301:MET:HE1	1:A:368:ILE:HD11	1.68	0.74
1:A:143:ILE:H	1:A:171:ASN:HD21	1.35	0.74
1:B:28:ASN:C	1:B:28:ASN:HD22	1.96	0.73
1:B:465:LYS:NZ	1:D:123:MET:HE1	2.03	0.73
1:C:143:ILE:H	1:C:171:ASN:ND2	1.86	0.73
1:B:97:ASN:C	1:B:97:ASN:HD22	1.96	0.73
1:A:265:LEU:HD23	1:A:296:ILE:HD11	1.71	0.72
1:D:46:ILE:HD11	1:D:211:VAL:HG13	1.71	0.72
1:B:162:MET:HE2	1:B:225:SER:HB3	1.70	0.72
1:A:216:LEU:HD21	1:A:236:VAL:HG13	1.71	0.72
1:D:397:LYS:O	1:D:401:GLU:HG3	1.91	0.71
1:B:216:LEU:HD13	1:B:239:LYS:HG2	1.71	0.71
1:A:353:GLY:HA3	1:A:367:THR:HG22	1.72	0.71
1:A:465:LYS:NZ	1:C:123:MET:HE1	2.07	0.70
1:B:97:ASN:HD21	1:B:100:GLU:H	1.38	0.70
1:D:87:ALA:HB2	1:D:102:LEU:HD13	1.74	0.70
1:C:97:ASN:HD21	1:C:100:GLU:HG3	1.57	0.69
1:A:123:MET:HE1	1:C:465:LYS:HZ1	1.56	0.69
1:C:350:VAL:HB	1:C:368:ILE:HG13	1.73	0.69
1:C:418:ASN:ND2	1:C:421:ALA:H	1.90	0.68
1:C:28:ASN:ND2	1:C:30:ALA:H	1.91	0.68
1:A:31:THR:OG1	1:A:33:GLU:HG2	1.94	0.67
1:A:162:MET:HE2	1:A:225:SER:HB3	1.76	0.67
1:B:26:VAL:HG11	1:B:36:CYS:SG	2.35	0.67
1:C:97:ASN:C	1:C:97:ASN:HD22	2.00	0.67
1:D:395:ASN:C	1:D:395:ASN:HD22	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3523:HOH:O	1:D:474:LYS:HE2	1.95	0.66
1:B:329:GLU:HG3	1:B:333:LYS:HE3	1.77	0.66
1:D:216:LEU:HD13	1:D:239:LYS:HD3	1.77	0.66
1:A:28:ASN:HD22	1:A:28:ASN:C	2.02	0.66
1:C:350:VAL:CG2	1:C:370:ASP:HB2	2.26	0.66
1:D:301:MET:O	1:D:305:GLN:HG2	1.95	0.66
1:A:350:VAL:HG23	1:A:370:ASP:HB2	1.76	0.66
1:D:305:GLN:HE22	1:D:368:ILE:HD11	1.60	0.66
1:A:144:GLY:H	1:A:171:ASN:HD22	1.43	0.66
1:A:101:ALA:O	1:A:105:VAL:HG12	1.95	0.66
1:D:144:GLY:H	1:D:171:ASN:HD22	1.42	0.66
1:A:97:ASN:ND2	1:A:100:GLU:H	1.94	0.66
1:A:97:ASN:HD22	1:A:97:ASN:C	2.04	0.66
1:B:353:GLY:H	1:B:367:THR:HB	1.61	0.65
1:B:87:ALA:HB2	1:B:102:LEU:HD13	1.78	0.65
1:C:418:ASN:HD21	1:C:420:ASN:HB2	1.62	0.65
1:A:77:GLN:HG3	1:C:77:GLN:CG	2.26	0.65
1:D:484:PRO:HG2	1:D:486:PHE:CZ	2.32	0.65
1:B:163:PHE:O	1:B:167:ILE:HG12	1.96	0.65
1:D:327:ILE:O	1:D:328:ARG:HD3	1.96	0.65
1:C:429:ILE:HD13	1:C:430:ASP:N	2.12	0.64
1:A:385:ALA:HB1	1:A:386:PRO:HD2	1.80	0.64
1:C:395:ASN:C	1:C:395:ASN:HD22	2.06	0.64
1:A:254:LYS:HE2	1:A:379:TRP:O	1.98	0.64
1:C:350:VAL:HG23	1:C:370:ASP:HB2	1.78	0.64
1:A:94:ASN:HD22	1:A:96:LYS:H	1.44	0.64
1:A:351:CYS:CB	1:A:368:ILE:HG23	2.29	0.63
1:A:374:THR:HG21	1:A:405:LYS:CD	2.28	0.63
1:A:157:MET:HE3	1:A:161:TRP:CZ2	2.33	0.63
1:C:26:VAL:HA	3:C:3699:HOH:O	1.99	0.63
1:D:65:VAL:CG1	1:D:66:PRO:HD3	2.29	0.62
1:B:426:ARG:HH22	1:D:135:GLU:CD	2.07	0.62
1:B:77:GLN:CB	1:D:77:GLN:HE21	2.09	0.62
1:C:255:ASN:HB2	3:C:3731:HOH:O	1.99	0.62
1:B:65:VAL:CG1	1:B:66:PRO:HD3	2.30	0.61
1:A:230:LYS:HD2	1:A:454:SER:HB3	1.82	0.61
1:A:481:TYR:HB3	1:C:420:ASN:HD22	1.65	0.61
1:D:87:ALA:CB	1:D:102:LEU:HD13	2.30	0.61
1:B:338:TYR:O	1:B:378:ILE:HD11	2.00	0.61
1:D:93:GLU:HG2	1:D:181:THR:HG22	1.80	0.61
1:A:123:MET:HE1	1:C:465:LYS:HZ2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:O	1:A:133:ASP:HB2	2.01	0.61
1:B:28:ASN:ND2	1:B:30:ALA:H	1.99	0.61
1:C:28:ASN:HD22	1:C:30:ALA:H	1.49	0.61
1:B:256:HIS:HE1	1:B:379:TRP:HE1	1.49	0.60
1:A:395:ASN:C	1:A:395:ASN:HD22	2.09	0.60
1:C:85:GLU:O	1:C:89:LEU:HD13	2.01	0.60
1:C:9:ASN:ND2	1:C:206:TYR:H	2.00	0.60
1:B:140:ARG:NH1	1:B:469:ASP:OD1	2.33	0.60
1:A:123:MET:CE	1:C:465:LYS:HZ1	2.14	0.60
1:B:47:ASP:O	1:B:51:GLN:HG3	2.01	0.60
1:A:397:LYS:O	1:A:401:GLU:HG3	2.01	0.60
1:C:65:VAL:CG1	1:C:66:PRO:HD3	2.31	0.60
1:A:87:ALA:CB	1:A:102:LEU:HD13	2.32	0.59
1:B:216:LEU:HD23	1:B:224:ILE:HD13	1.85	0.59
1:C:216:LEU:HD21	1:C:236:VAL:HG13	1.85	0.59
1:B:249:SER:HB2	1:B:457:PHE:HB2	1.85	0.59
1:B:222:LYS:HE3	3:B:2679:HOH:O	2.03	0.58
1:C:97:ASN:ND2	1:C:100:GLU:HG3	2.17	0.58
1:D:374:THR:HG21	1:D:405:LYS:CD	2.32	0.58
1:A:89:LEU:HD13	3:A:1639:HOH:O	2.03	0.58
1:A:135:GLU:CD	1:C:426:ARG:HH22	2.11	0.58
1:B:418:ASN:HD22	1:B:421:ALA:N	1.87	0.58
1:A:469:ASP:HA	1:A:472:THR:HG22	1.85	0.58
1:D:23:TYR:CE1	1:D:39:PRO:HB3	2.39	0.57
1:A:350:VAL:CG2	1:A:370:ASP:HB2	2.34	0.57
1:C:397:LYS:O	1:C:401:GLU:HG3	2.03	0.57
1:A:28:ASN:ND2	1:A:30:ALA:H	2.01	0.57
1:D:385:ALA:HB1	1:D:386:PRO:HD2	1.86	0.57
1:C:150:ALA:HB1	3:C:3513:HOH:O	2.04	0.57
1:C:426:ARG:HD2	1:D:141:TYR:OH	2.05	0.57
1:A:319:ASP:OD2	1:A:319:ASP:N	2.38	0.57
1:B:74:ASN:O	1:B:78:LEU:HD22	2.05	0.57
1:D:143:ILE:N	1:D:171:ASN:HD21	1.97	0.57
1:A:35:LEU:HD11	1:A:92:ILE:HG22	1.87	0.57
1:B:352:ASP:O	1:B:355:GLU:HG2	2.04	0.57
1:D:265:LEU:HD11	1:D:299:GLU:HG2	1.87	0.57
1:A:414:LEU:HG	1:A:416:THR:HG22	1.87	0.57
1:D:97:ASN:ND2	1:D:99:LYS:HB3	2.20	0.57
1:A:230:LYS:N	1:A:231:PRO:HD2	2.20	0.56
1:C:87:ALA:HB2	1:C:102:LEU:HD13	1.86	0.56
1:D:179:GLU:CD	1:D:179:GLU:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:LEU:HG	1:D:416:THR:HG22	1.86	0.56
1:C:28:ASN:C	1:C:28:ASN:ND2	2.64	0.56
1:C:65:VAL:HG13	1:C:66:PRO:HD3	1.86	0.56
1:A:87:ALA:HB2	1:A:102:LEU:HD13	1.88	0.56
1:A:93:GLU:OE1	1:A:183:LEU:HB2	2.06	0.56
1:A:374:THR:HG23	1:A:379:TRP:CZ3	2.40	0.56
1:B:254:LYS:HE2	1:B:379:TRP:O	2.06	0.56
1:D:9:ASN:ND2	1:D:206:TYR:H	2.03	0.56
1:C:285:MET:HB3	1:C:440:VAL:HG13	1.88	0.56
1:D:305:GLN:NE2	1:D:368:ILE:HD11	2.20	0.56
1:B:216:LEU:HD23	1:B:224:ILE:CD1	2.35	0.55
1:C:12:ASN:HB2	1:C:52:THR:HG21	1.87	0.55
1:A:220:GLU:HA	1:A:220:GLU:OE1	2.07	0.55
1:D:156:MET:HE3	1:D:188:LEU:HD21	1.89	0.55
1:A:215:ILE:HA	1:A:221:ILE:HD12	1.88	0.55
1:B:35:LEU:HD11	1:B:92:ILE:HG22	1.86	0.55
1:B:395:ASN:HD22	1:B:395:ASN:C	2.15	0.55
1:C:350:VAL:HB	1:C:368:ILE:CG1	2.35	0.55
1:A:269:VAL:O	1:A:273:VAL:HG23	2.07	0.55
1:C:143:ILE:N	1:C:171:ASN:HD21	1.94	0.55
1:D:350:VAL:CG2	1:D:370:ASP:HB2	2.36	0.55
1:C:97:ASN:ND2	1:C:100:GLU:H	2.04	0.55
1:C:317:LEU:HD22	3:C:3579:HOH:O	2.06	0.55
1:A:357:VAL:HG11	1:A:363:PHE:O	2.07	0.55
1:C:254:LYS:HD3	1:C:288:ALA:CB	2.37	0.55
1:C:197:LEU:HD12	1:C:198:PRO:HD2	1.89	0.55
1:C:385:ALA:HB1	1:C:386:PRO:HD2	1.87	0.55
1:B:395:ASN:ND2	1:B:398:GLU:H	2.05	0.54
1:B:182:PRO:HB2	1:B:206:TYR:CE2	2.42	0.54
1:C:438:LEU:HD21	1:D:480:ARG:HB2	1.89	0.54
1:B:46:ILE:HD11	1:B:211:VAL:HG13	1.90	0.54
1:C:459:THR:HB	3:D:4640:HOH:O	2.07	0.54
1:A:28:ASN:HD22	1:A:30:ALA:H	1.56	0.54
1:A:374:THR:HG23	1:A:379:TRP:CH2	2.43	0.54
1:B:208:ALA:O	1:B:212:VAL:HG23	2.07	0.54
1:C:38:VAL:CG2	1:C:182:PRO:HG3	2.38	0.54
1:D:326:VAL:HG22	1:D:362:TYR:O	2.07	0.54
1:B:370:ASP:O	1:B:371:ASN:HB2	2.07	0.54
1:A:13:GLY:O	1:A:14:GLU:HG3	2.08	0.54
1:B:28:ASN:HD22	1:B:30:ALA:H	1.55	0.54
1:B:123:MET:HE1	1:D:465:LYS:HZ1	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:HG12	1:B:171:ASN:HD21	1.73	0.54
1:C:140:ARG:NH1	1:C:469:ASP:OD1	2.41	0.54
1:A:157:MET:HE3	1:A:161:TRP:HZ2	1.70	0.54
1:A:216:LEU:HD13	1:A:239:LYS:HD3	1.89	0.54
1:C:326:VAL:HG22	1:C:362:TYR:O	2.08	0.54
1:A:254:LYS:HD3	1:A:288:ALA:CB	2.38	0.53
1:B:353:GLY:HA3	1:B:367:THR:HG22	1.90	0.53
1:C:91:THR:HG21	1:C:317:LEU:HD13	1.89	0.53
1:B:135:GLU:CD	1:D:426:ARG:HH22	2.17	0.53
1:B:144:GLY:H	1:B:171:ASN:HD22	1.56	0.53
1:D:29:PRO:HB2	1:D:325:PRO:HG2	1.91	0.53
1:A:9:ASN:ND2	1:A:206:TYR:H	2.05	0.53
1:A:35:LEU:CD1	1:A:92:ILE:HG22	2.38	0.53
1:D:85:GLU:OE1	1:D:187:LYS:HE2	2.08	0.53
1:A:242:GLU:O	1:B:238:LYS:HE2	2.08	0.53
1:C:87:ALA:CB	1:C:102:LEU:HD13	2.39	0.53
1:D:249:SER:HB2	1:D:457:PHE:HB2	1.89	0.53
1:B:285:MET:SD	1:B:441:PRO:HG2	2.48	0.53
1:A:65:VAL:CG1	1:A:66:PRO:HD3	2.39	0.53
1:A:418:ASN:ND2	1:A:421:ALA:H	2.06	0.53
1:D:269:VAL:O	1:D:273:VAL:HG23	2.09	0.53
1:A:162:MET:HE2	1:A:225:SER:CB	2.39	0.52
1:A:484:PRO:HG2	1:A:486:PHE:CZ	2.44	0.52
1:C:80:SER:O	1:C:83:LYS:HG3	2.09	0.52
1:A:65:VAL:HG12	1:A:66:PRO:HD3	1.91	0.52
1:B:269:VAL:O	1:B:273:VAL:HG23	2.09	0.52
1:C:429:ILE:HD13	1:C:430:ASP:H	1.75	0.52
1:D:253:ALA:O	1:D:382:GLU:HG3	2.09	0.52
1:A:88:HIS:O	1:A:92:ILE:HG12	2.10	0.52
1:D:24:GLU:HB2	1:D:40:ILE:HD11	1.91	0.52
1:A:46:ILE:HG21	1:A:214:GLY:HA3	1.91	0.52
1:D:107:ARG:HH12	1:D:444:MET:HA	1.73	0.52
1:A:372:VAL:HG21	1:A:389:SER:HB3	1.91	0.52
1:C:8:LYS:HB3	1:C:16:VAL:O	2.10	0.52
1:C:290:VAL:HG23	1:C:388:LEU:HD21	1.92	0.52
1:D:10:TYR:CZ	1:D:13:GLY:HA2	2.44	0.52
1:D:143:ILE:H	1:D:171:ASN:ND2	2.01	0.52
1:C:409:ALA:HB2	1:C:453:LYS:HE2	1.92	0.52
1:D:156:MET:HB2	1:D:184:LEU:CD1	2.40	0.52
1:C:395:ASN:ND2	1:C:398:GLU:H	2.08	0.52
1:A:329:GLU:OE1	1:A:333:LYS:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ASP:O	1:B:319:ASP:OD2	2.28	0.52
1:D:65:VAL:HG13	1:D:66:PRO:HD3	1.92	0.52
1:A:91:THR:HG23	1:A:96:LYS:O	2.09	0.51
1:B:65:VAL:HG13	1:B:66:PRO:HD3	1.92	0.51
1:B:26:VAL:CG1	1:B:36:CYS:SG	2.98	0.51
1:D:216:LEU:HD21	1:D:236:VAL:HG13	1.92	0.51
1:C:123:MET:HE3	3:C:3639:HOH:O	2.11	0.51
1:A:110:GLU:CG	1:C:70:ARG:HH22	2.24	0.51
1:C:47:ASP:O	1:C:51:GLN:HG3	2.09	0.51
1:B:88:HIS:O	1:B:92:ILE:HG12	2.09	0.51
1:D:28:ASN:C	1:D:28:ASN:HD22	2.18	0.51
1:B:102:LEU:O	1:B:105:VAL:HG22	2.10	0.51
1:A:98:THR:HB	3:A:1548:HOH:O	2.10	0.51
1:A:429:ILE:HG21	1:A:434:LEU:HD11	1.92	0.51
1:C:184:LEU:C	1:C:184:LEU:HD13	2.36	0.51
1:C:479:ALA:CB	1:D:436:ILE:HB	2.40	0.51
1:B:465:LYS:NZ	1:D:123:MET:CE	2.73	0.51
1:C:328:ARG:NH1	3:C:3699:HOH:O	2.43	0.51
1:B:368:ILE:HD11	1:B:390:VAL:CG1	2.41	0.51
1:D:140:ARG:NH1	1:D:469:ASP:OD2	2.44	0.51
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.11	0.50
1:C:90:ILE:O	1:C:94:ASN:HB3	2.11	0.50
1:B:418:ASN:ND2	1:B:421:ALA:N	2.54	0.50
1:C:42:THR:OG1	1:C:44:GLU:HB3	2.12	0.50
1:D:413:CYS:SG	1:D:441:PRO:HD3	2.52	0.50
1:A:152:PHE:CD1	1:A:152:PHE:C	2.89	0.50
1:B:35:LEU:CD1	1:B:92:ILE:HG22	2.42	0.50
1:B:175:LEU:HG	1:B:177:PRO:HD3	1.94	0.50
1:B:256:HIS:CE1	1:B:379:TRP:HE1	2.29	0.50
3:B:2589:HOH:O	1:D:123:MET:HE3	2.11	0.50
1:D:169:LEU:HD12	1:D:471:TYR:HB2	1.94	0.50
1:A:351:CYS:HB3	1:A:368:ILE:CG2	2.37	0.50
1:D:256:HIS:CE1	1:D:403:ALA:HA	2.46	0.50
1:A:326:VAL:HG22	1:A:362:TYR:O	2.10	0.50
3:B:2676:HOH:O	1:C:67:ARG:HD2	2.12	0.50
1:A:216:LEU:HD23	1:A:224:ILE:CD1	2.42	0.50
1:B:92:ILE:HD13	1:B:317:LEU:HD21	1.93	0.50
1:B:339:ILE:HD11	1:B:367:THR:HG21	1.94	0.50
1:A:426:ARG:HG3	1:B:477:VAL:HG21	1.93	0.50
1:C:304:LEU:O	1:C:308:VAL:HG23	2.11	0.49
1:D:120:SER:HA	1:D:123:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LYS:N	1:D:231:PRO:HD2	2.26	0.49
1:B:186:GLU:O	1:B:190:GLU:HG3	2.12	0.49
1:D:156:MET:HB2	1:D:184:LEU:HD11	1.94	0.49
1:A:349:LEU:HD21	1:A:352:ASP:HB2	1.94	0.49
1:B:38:VAL:CG2	1:B:182:PRO:HG3	2.42	0.49
1:B:385:ALA:HB1	1:B:386:PRO:HD2	1.93	0.49
1:A:353:GLY:CA	1:A:367:THR:HG22	2.40	0.49
1:D:144:GLY:H	1:D:171:ASN:ND2	2.10	0.49
1:C:216:LEU:HD23	1:C:224:ILE:CD1	2.43	0.49
1:A:254:LYS:HD3	1:A:288:ALA:HB3	1.94	0.49
1:A:268:THR:HG23	1:A:415:PHE:CG	2.48	0.49
1:A:426:ARG:HH22	1:C:135:GLU:CD	2.21	0.49
1:A:153:ASN:HB2	1:A:282:GLU:O	2.12	0.49
1:C:368:ILE:HA	1:C:388:LEU:O	2.13	0.49
1:D:107:ARG:NH1	1:D:444:MET:HA	2.28	0.49
1:C:163:PHE:CG	1:C:164:PRO:HD3	2.48	0.49
1:C:198:PRO:HG2	1:C:201:VAL:HG21	1.95	0.49
1:D:469:ASP:HA	1:D:472:THR:HG22	1.94	0.49
1:A:136:ALA:HA	1:A:477:VAL:O	2.13	0.48
1:B:123:MET:CE	1:D:465:LYS:NZ	2.74	0.48
1:C:329:GLU:OE1	1:C:333:LYS:HE3	2.12	0.48
1:D:230:LYS:HE3	1:D:407:GLU:OE2	2.13	0.48
1:A:290:VAL:HG23	1:A:388:LEU:HD21	1.94	0.48
1:B:285:MET:HB3	1:B:440:VAL:HG13	1.95	0.48
1:A:110:GLU:HG2	1:C:70:ARG:HH22	1.77	0.48
1:A:327:ILE:HG23	1:A:328:ARG:HG2	1.95	0.48
1:C:184:LEU:HD13	1:C:184:LEU:O	2.13	0.48
1:D:374:THR:HG23	1:D:379:TRP:CZ3	2.49	0.48
1:D:395:ASN:ND2	1:D:398:GLU:H	2.11	0.48
1:A:102:LEU:O	1:A:105:VAL:HG13	2.13	0.48
1:A:141:TYR:OH	1:B:426:ARG:HD2	2.13	0.48
1:A:94:ASN:ND2	1:A:96:LYS:HE3	2.29	0.48
1:A:97:ASN:HD21	1:A:100:GLU:H	1.60	0.48
1:B:92:ILE:CD1	1:B:317:LEU:HD21	2.44	0.48
1:C:26:VAL:HG11	1:C:36:CYS:SG	2.52	0.48
1:C:93:GLU:OE2	1:C:183:LEU:N	2.43	0.48
1:A:120:SER:HA	1:A:123:MET:HE2	1.96	0.48
1:D:269:VAL:HG21	1:D:303:LYS:CG	2.43	0.48
1:B:254:LYS:HD3	1:B:288:ALA:CB	2.44	0.48
1:D:65:VAL:HG12	1:D:66:PRO:HD3	1.96	0.48
1:B:163:PHE:CG	1:B:164:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ASN:C	1:C:97:ASN:ND2	2.67	0.47
1:A:374:THR:O	1:A:374:THR:HG22	2.12	0.47
3:A:1533:HOH:O	1:B:242:GLU:HG3	2.15	0.47
1:B:50:ALA:HA	1:B:174:ILE:HD11	1.96	0.47
1:B:230:LYS:N	1:B:231:PRO:HD2	2.29	0.47
1:B:254:LYS:HD3	1:B:288:ALA:HB3	1.97	0.47
1:A:90:ILE:HG23	1:A:155:PRO:CG	2.44	0.47
1:B:250:LEU:HD12	1:B:250:LEU:N	2.30	0.47
1:D:350:VAL:HG21	1:D:370:ASP:HB2	1.95	0.47
1:A:327:ILE:HG23	1:A:328:ARG:N	2.29	0.47
1:B:319:ASP:OD2	1:B:319:ASP:C	2.58	0.47
1:A:31:THR:HG1	1:A:33:GLU:HG2	1.76	0.47
1:C:429:ILE:CD1	1:C:431:ALA:H	2.27	0.47
1:D:93:GLU:HG2	1:D:181:THR:HA	1.95	0.47
1:D:228:GLY:O	2:D:4490:NAD:H1D	2.15	0.47
1:D:418:ASN:HD21	1:D:420:ASN:HB2	1.80	0.47
1:A:143:ILE:N	1:A:171:ASN:HD21	2.08	0.47
1:B:143:ILE:HG12	1:B:171:ASN:ND2	2.29	0.47
1:D:28:ASN:HD22	1:D:30:ALA:H	1.61	0.47
1:D:355:GLU:O	1:D:357:VAL:HG23	2.14	0.47
1:A:230:LYS:HE3	1:A:407:GLU:OE2	2.15	0.47
1:B:409:ALA:HB2	1:B:453:LYS:HE2	1.96	0.47
1:C:152:PHE:CE1	1:C:327:ILE:HB	2.50	0.47
1:C:228:GLY:O	1:C:251:THR:HA	2.15	0.47
1:C:365:GLY:HA3	3:C:3563:HOH:O	2.15	0.47
1:A:78:LEU:O	1:A:82:HIS:HD2	1.98	0.47
1:B:210:ASP:HB2	3:B:2499:HOH:O	2.15	0.47
1:C:143:ILE:N	1:C:171:ASN:ND2	2.57	0.47
1:B:90:ILE:O	1:B:94:ASN:HB3	2.15	0.47
1:B:87:ALA:CB	1:B:102:LEU:HD13	2.42	0.47
1:B:265:LEU:HG	1:B:296:ILE:HD11	1.97	0.47
1:D:305:GLN:HE22	1:D:350:VAL:HG12	1.80	0.47
1:A:127:LEU:HD13	1:D:123:MET:HG2	1.96	0.46
1:A:462:ALA:O	1:A:463:ASN:HB2	2.16	0.46
1:D:93:GLU:CG	1:D:181:THR:HA	2.45	0.46
1:B:351:CYS:HB2	1:B:368:ILE:HG22	1.93	0.46
1:B:357:VAL:HG11	1:B:365:GLY:H	1.80	0.46
1:D:198:PRO:HG2	1:D:201:VAL:HG21	1.97	0.46
1:C:144:GLY:H	1:C:171:ASN:HD22	1.64	0.46
1:A:329:GLU:HB2	1:A:362:TYR:CE2	2.51	0.46
1:B:152:PHE:CD1	1:B:152:PHE:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LEU:CD1	1:D:299:GLU:HG2	2.45	0.46
1:A:480:ARG:HB2	1:B:438:LEU:HD21	1.98	0.46
1:B:65:VAL:HG12	1:B:66:PRO:HD3	1.98	0.46
1:D:44:GLU:HG3	3:D:4501:HOH:O	2.15	0.46
1:A:28:ASN:C	1:A:28:ASN:ND2	2.73	0.46
1:D:163:PHE:CG	1:D:164:PRO:HD3	2.51	0.46
1:A:97:ASN:HD21	1:A:100:GLU:HG3	1.80	0.46
1:A:349:LEU:C	1:A:349:LEU:HD23	2.40	0.46
1:C:98:THR:O	1:C:102:LEU:HB2	2.16	0.46
1:C:26:VAL:CG1	1:C:36:CYS:SG	3.05	0.45
1:C:26:VAL:HG12	1:C:38:VAL:HG23	1.97	0.45
1:C:238:LYS:HE2	1:D:242:GLU:O	2.16	0.45
1:A:238:LYS:HE2	1:B:242:GLU:O	2.16	0.45
1:A:254:LYS:O	1:A:256:HIS:HD2	1.98	0.45
1:A:465:LYS:NZ	1:C:123:MET:CE	2.78	0.45
1:C:38:VAL:HG22	1:C:182:PRO:HG3	1.99	0.45
1:C:176:LYS:HG3	1:C:211:VAL:HG11	1.97	0.45
1:C:484:PRO:HG2	1:C:486:PHE:CZ	2.52	0.45
1:A:163:PHE:CG	1:A:164:PRO:HD3	2.52	0.45
1:B:368:ILE:HD12	1:B:369:PHE:N	2.31	0.45
1:A:374:THR:HG21	1:A:405:LYS:CE	2.47	0.45
1:A:410:ASN:HD22	1:A:410:ASN:HA	1.65	0.45
1:A:432:GLY:O	1:B:475:LYS:HA	2.17	0.45
1:B:10:TYR:CZ	1:B:13:GLY:HA2	2.51	0.45
1:B:38:VAL:HG22	1:B:182:PRO:HG3	1.98	0.45
1:D:46:ILE:CD1	1:D:211:VAL:HG13	2.43	0.45
1:D:151:PRO:HD2	1:D:158:VAL:HG11	1.99	0.45
1:D:462:ALA:O	1:D:463:ASN:HB2	2.16	0.45
1:A:28:ASN:HD22	1:A:29:PRO:N	2.15	0.45
1:A:91:THR:HG21	1:A:317:LEU:HD13	1.99	0.45
1:A:409:ALA:HB2	1:A:453:LYS:HG3	1.99	0.45
1:A:481:TYR:CE2	1:C:419:SER:HB3	2.51	0.45
1:C:72:LEU:HD12	1:C:112:VAL:HG13	1.98	0.45
1:B:123:MET:HE3	3:D:4570:HOH:O	2.16	0.45
1:C:285:MET:HG3	1:C:442:ALA:HB2	1.98	0.45
1:A:151:PRO:HD2	1:A:158:VAL:HG11	1.98	0.45
1:D:120:SER:CA	1:D:123:MET:HE2	2.46	0.45
1:D:197:LEU:HD12	1:D:198:PRO:HD2	1.99	0.45
1:C:254:LYS:HD3	1:C:288:ALA:HB3	1.99	0.45
1:C:425:PHE:O	1:C:429:ILE:HB	2.16	0.45
1:D:127:LEU:HD12	1:D:127:LEU:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:PHE:CD1	1:D:152:PHE:C	2.94	0.45
1:B:54:ALA:HB2	1:B:220:GLU:CG	2.47	0.45
1:B:77:GLN:CG	1:D:77:GLN:HG2	2.36	0.45
1:C:152:PHE:CD1	1:C:152:PHE:C	2.95	0.45
1:A:162:MET:HE3	1:A:227:VAL:HG23	1.99	0.44
1:B:85:GLU:OE1	1:B:187:LYS:HE2	2.17	0.44
1:C:156:MET:C	1:C:159:PRO:HD2	2.41	0.44
1:A:73:PHE:CE1	1:A:116:ALA:HB1	2.52	0.44
1:A:144:GLY:H	1:A:171:ASN:ND2	2.13	0.44
1:D:250:LEU:HD12	1:D:250:LEU:N	2.33	0.44
1:D:372:VAL:HG21	1:D:389:SER:HB3	1.99	0.44
1:A:90:ILE:O	1:A:94:ASN:HB3	2.18	0.44
1:B:215:ILE:HA	1:B:221:ILE:HD12	1.99	0.44
1:C:250:LEU:N	1:C:250:LEU:HD12	2.33	0.44
1:C:410:ASN:HD22	1:C:410:ASN:HA	1.63	0.44
1:A:285:MET:SD	1:A:441:PRO:HG2	2.58	0.44
1:A:418:ASN:HD22	1:A:421:ALA:HB2	1.83	0.44
1:C:254:LYS:NZ	1:C:381:ASP:O	2.49	0.44
1:C:311:ILE:HG23	1:C:322:PHE:HB3	1.99	0.44
1:C:459:THR:HG21	1:D:460:LEU:HD12	1.98	0.44
1:B:54:ALA:HB2	1:B:220:GLU:HG3	1.98	0.44
1:D:157:MET:HE3	1:D:161:TRP:CZ2	2.53	0.44
1:A:80:SER:O	1:A:83:LYS:HG3	2.18	0.44
1:C:97:ASN:HD21	1:C:100:GLU:H	1.65	0.44
1:A:472:THR:HG23	3:A:1510:HOH:O	2.16	0.44
1:B:152:PHE:CE1	1:B:327:ILE:HB	2.52	0.44
1:B:395:ASN:HD22	1:B:398:GLU:H	1.65	0.44
1:D:19:LYS:HE3	3:D:4556:HOH:O	2.17	0.44
1:D:28:ASN:ND2	1:D:30:ALA:H	2.15	0.44
1:D:448:PRO:HG2	3:D:4517:HOH:O	2.18	0.44
1:C:149:ILE:HG22	2:C:3490:NAD:H4B	2.00	0.44
1:A:176:LYS:HG3	1:A:211:VAL:HG11	1.99	0.43
1:B:448:PRO:HG2	3:B:2520:HOH:O	2.17	0.43
1:D:230:LYS:HA	1:D:251:THR:HB	1.99	0.43
1:D:305:GLN:HE22	1:D:350:VAL:CG1	2.32	0.43
1:A:156:MET:C	1:A:159:PRO:HD2	2.42	0.43
1:B:85:GLU:HG3	3:B:2578:HOH:O	2.17	0.43
1:D:228:GLY:O	1:D:251:THR:HA	2.18	0.43
1:C:50:ALA:HA	1:C:174:ILE:HD11	2.01	0.43
1:A:140:ARG:NH1	1:A:469:ASP:OD1	2.47	0.43
1:A:436:ILE:HB	1:B:479:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASN:ND2	1:B:97:ASN:C	2.68	0.43
1:C:156:MET:O	1:C:159:PRO:HD2	2.17	0.43
1:C:351:CYS:HB3	1:C:368:ILE:HG23	2.00	0.43
1:A:296:ILE:HG12	1:A:296:ILE:O	2.18	0.43
1:D:93:GLU:OE2	1:D:183:LEU:N	2.46	0.43
1:A:120:SER:CA	1:A:123:MET:HE2	2.49	0.43
1:A:388:LEU:HD23	1:A:389:SER:H	1.83	0.43
1:A:388:LEU:HD23	1:A:389:SER:N	2.34	0.43
1:C:224:ILE:HB	1:C:247:VAL:HB	2.00	0.43
1:B:177:PRO:HG2	1:B:206:TYR:CD2	2.54	0.43
1:B:419:SER:HB3	1:D:481:TYR:CE2	2.54	0.43
1:B:212:VAL:HG21	2:B:2490:NAD:N3A	2.34	0.43
1:B:312:LYS:HD2	1:B:320:GLY:O	2.19	0.43
1:C:38:VAL:HG21	1:C:182:PRO:HG3	2.00	0.43
1:D:64:ALA:HB1	1:D:66:PRO:HD2	2.00	0.43
1:D:108:GLY:HA2	1:D:111:ASN:HD22	1.83	0.43
1:A:132:THR:HB	3:D:4575:HOH:O	2.19	0.43
1:A:149:ILE:HD13	1:A:212:VAL:HG13	2.01	0.42
1:A:448:PRO:HG2	3:A:1530:HOH:O	2.19	0.42
1:B:57:PHE:CE2	1:B:61:SER:HB3	2.54	0.42
1:B:327:ILE:HG23	1:B:328:ARG:N	2.34	0.42
1:C:375:GLU:HG2	3:C:3714:HOH:O	2.18	0.42
1:D:317:LEU:N	1:D:317:LEU:HD22	2.34	0.42
1:D:356:ASN:N	1:D:356:ASN:HD22	2.18	0.42
1:A:253:ALA:O	1:A:382:GLU:HG3	2.19	0.42
1:A:418:ASN:HD21	1:A:420:ASN:HB2	1.85	0.42
1:B:378:ILE:HD13	1:B:378:ILE:HA	1.80	0.42
1:C:345:GLU:CD	1:C:377:THR:H	2.27	0.42
1:D:150:ALA:HB1	3:D:4659:HOH:O	2.18	0.42
1:D:350:VAL:HG23	1:D:370:ASP:HB2	2.00	0.42
1:B:8:LYS:HB3	1:B:16:VAL:O	2.18	0.42
1:C:12:ASN:HB2	1:C:52:THR:CG2	2.48	0.42
1:A:344:GLU:O	1:A:344:GLU:HG2	2.19	0.42
1:B:176:LYS:HG3	1:B:211:VAL:HG11	2.01	0.42
1:D:152:PHE:CE1	1:D:327:ILE:HB	2.55	0.42
1:D:285:MET:HG3	1:D:442:ALA:HB2	2.01	0.42
1:A:57:PHE:CE2	1:A:144:GLY:HA2	2.54	0.42
1:B:292:VAL:HG11	1:B:297:ALA:HA	2.01	0.42
1:C:261:ASN:HA	1:C:296:ILE:HB	2.02	0.42
1:B:42:THR:C	1:B:44:GLU:N	2.75	0.42
1:B:127:LEU:HD12	1:B:127:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ILE:HD13	1:C:46:ILE:HA	1.92	0.42
1:D:156:MET:HB2	1:D:184:LEU:HG	2.01	0.42
1:B:253:ALA:O	1:B:382:GLU:HG3	2.19	0.42
1:C:212:VAL:HG21	2:C:3490:NAD:N3A	2.35	0.42
1:D:143:ILE:N	1:D:171:ASN:ND2	2.65	0.42
1:D:165:MET:O	1:D:169:LEU:HG	2.20	0.42
1:C:230:LYS:HA	1:C:251:THR:HB	2.01	0.42
1:D:140:ARG:HD3	1:D:472:THR:HG21	2.02	0.42
1:D:215:ILE:HA	1:D:221:ILE:HD12	2.01	0.42
1:A:24:GLU:HB2	1:A:40:ILE:HD11	2.01	0.42
1:A:29:PRO:HB2	1:A:325:PRO:HG2	2.02	0.42
1:B:12:ASN:HB2	1:B:52:THR:HG21	2.01	0.42
1:A:26:VAL:HG21	1:A:182:PRO:HG3	2.01	0.41
1:A:370:ASP:O	1:A:371:ASN:C	2.63	0.41
1:C:120:SER:CA	1:C:123:MET:HE2	2.50	0.41
1:C:350:VAL:HB	1:C:368:ILE:CD1	2.50	0.41
1:D:183:LEU:HD12	1:D:183:LEU:HA	1.88	0.41
1:D:418:ASN:ND2	1:D:420:ASN:HB2	2.35	0.41
1:A:143:ILE:H	1:A:171:ASN:ND2	2.11	0.41
1:A:374:THR:HG21	1:A:405:LYS:NZ	2.35	0.41
1:B:419:SER:OG	1:C:422:ILE:HD12	2.20	0.41
1:C:11:ILE:O	1:C:14:GLU:OE1	2.38	0.41
1:C:158:VAL:HB	1:C:159:PRO:HD3	2.01	0.41
1:D:374:THR:HG22	1:D:374:THR:O	2.19	0.41
1:D:418:ASN:HD22	1:D:421:ALA:H	1.67	0.41
1:A:138:ASN:HA	1:A:476:VAL:HA	2.03	0.41
1:A:218:HIS:HA	1:A:219:PRO:HD2	1.93	0.41
1:B:40:ILE:HA	1:B:207:GLY:HA2	2.02	0.41
1:C:395:ASN:C	1:C:395:ASN:ND2	2.75	0.41
1:A:158:VAL:HB	1:A:159:PRO:HD3	2.02	0.41
1:A:341:LYS:O	1:A:345:GLU:HG3	2.21	0.41
1:B:185:THR:O	1:B:189:VAL:HG23	2.21	0.41
1:C:175:LEU:HG	1:C:177:PRO:HD3	2.02	0.41
1:C:368:ILE:C	1:C:368:ILE:HD12	2.46	0.41
1:D:156:MET:C	1:D:159:PRO:HD2	2.45	0.41
1:D:415:PHE:CD1	1:D:437:ASN:HA	2.56	0.41
1:A:77:GLN:HG3	1:C:77:GLN:HG2	2.01	0.41
1:A:90:ILE:HG23	1:A:155:PRO:HG3	2.02	0.41
1:A:433:MET:HG3	1:A:450:SER:O	2.20	0.41
3:A:1540:HOH:O	1:B:474:LYS:HE2	2.20	0.41
1:C:220:GLU:OE2	1:C:220:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LYS:O	1:C:256:HIS:HD2	2.04	0.41
1:D:351:CYS:HB3	1:D:368:ILE:HG23	2.03	0.41
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.93	0.41
1:B:42:THR:C	1:B:44:GLU:H	2.28	0.41
1:B:348:ARG:HB2	1:B:370:ASP:OD1	2.20	0.41
1:C:46:ILE:HG21	1:C:214:GLY:HA3	2.03	0.41
1:C:120:SER:HA	1:C:123:MET:HE2	2.03	0.41
1:C:268:THR:HG22	1:C:272:ILE:HD12	2.02	0.41
1:C:429:ILE:HG21	1:C:434:LEU:HD11	2.02	0.41
1:D:78:LEU:O	1:D:82:HIS:HD2	2.03	0.41
1:D:187:LYS:HA	1:D:187:LYS:HD3	1.84	0.41
1:D:266:GLU:OE2	1:D:307:LYS:NZ	2.47	0.41
1:D:266:GLU:CD	1:D:307:LYS:HZ1	2.27	0.41
1:D:341:LYS:O	1:D:345:GLU:HG3	2.20	0.41
1:D:341:LYS:HG3	3:D:4667:HOH:O	2.21	0.41
1:A:38:VAL:CG1	1:A:182:PRO:HG3	2.52	0.41
1:A:395:ASN:C	1:A:395:ASN:ND2	2.76	0.41
1:A:418:ASN:HD22	1:A:421:ALA:H	1.68	0.41
1:A:422:ILE:HD13	1:B:481:TYR:OH	2.21	0.41
1:B:18:SER:HB3	1:B:20:THR:HG22	2.02	0.41
1:C:26:VAL:HG13	1:C:36:CYS:O	2.21	0.41
1:B:162:MET:CE	1:B:227:VAL:HG23	2.51	0.40
1:C:14:GLU:OE1	1:C:14:GLU:N	2.53	0.40
1:C:89:LEU:O	1:C:93:GLU:HB3	2.21	0.40
1:C:140:ARG:NH1	1:C:474:LYS:NZ	2.69	0.40
1:C:265:LEU:HG	1:C:296:ILE:HD11	2.03	0.40
1:D:429:ILE:HD12	1:D:429:ILE:HA	1.95	0.40
1:A:77:GLN:HG3	1:C:77:GLN:NE2	2.36	0.40
1:A:83:LYS:HD3	3:A:1569:HOH:O	2.21	0.40
1:A:266:GLU:OE2	1:A:303:LYS:NZ	2.46	0.40
1:B:78:LEU:O	1:B:82:HIS:HD2	2.04	0.40
1:C:432:GLY:HA3	1:C:450:SER:O	2.22	0.40
1:D:125:ASP:O	1:D:137:ALA:HA	2.21	0.40
1:D:176:LYS:HG3	1:D:211:VAL:HG11	2.03	0.40
1:A:338:TYR:CG	1:A:383:ILE:HD12	2.56	0.40
1:B:98:THR:HG21	3:B:2617:HOH:O	2.20	0.40
1:D:414:LEU:HD22	1:D:425:PHE:CB	2.51	0.40
1:A:6:LYS:HE2	1:A:23:TYR:CZ	2.57	0.40
1:A:108:GLY:HA2	1:A:111:ASN:HD22	1.85	0.40
1:A:338:TYR:HA	1:A:341:LYS:HE3	2.04	0.40
1:A:385:ALA:HB1	1:A:386:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD21	1:B:349:LEU:HG	2.02	0.40
1:C:23:TYR:CE1	1:C:39:PRO:HB3	2.56	0.40
1:C:256:HIS:HE1	1:C:379:TRP:HE1	1.70	0.40
1:D:118:ALA:N	1:D:119:PRO:CD	2.85	0.40
1:A:38:VAL:HG11	1:A:182:PRO:CB	2.51	0.40
1:A:92:ILE:HD11	1:A:317:LEU:HD21	2.04	0.40
1:A:383:ILE:HB	3:A:1595:HOH:O	2.21	0.40
1:B:118:ALA:N	1:B:119:PRO:CD	2.84	0.40
1:D:254:LYS:HD3	1:D:288:ALA:HB3	2.03	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	482/486 (99%)	459 (95%)	22 (5%)	1 (0%)	43	63
1	B	482/486 (99%)	453 (94%)	27 (6%)	2 (0%)	30	49
1	C	482/486 (99%)	463 (96%)	18 (4%)	1 (0%)	43	63
1	D	482/486 (99%)	460 (95%)	22 (5%)	0	100	100
All	All	1928/1944 (99%)	1835 (95%)	89 (5%)	4 (0%)	43	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	356	ASN
1	C	41	SER
1	A	371	ASN
1	B	41	SER

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	399/400 (100%)	369 (92%)	30 (8%)	12	26
1	B	399/400 (100%)	374 (94%)	25 (6%)	16	34
1	C	399/400 (100%)	373 (94%)	26 (6%)	15	32
1	D	399/400 (100%)	375 (94%)	24 (6%)	17	36
All	All	1596/1600 (100%)	1491 (93%)	105 (7%)	15	32

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	46	ILE
1	A	78	LEU
1	A	79	LEU
1	A	89	LEU
1	A	97	ASN
1	A	98	THR
1	A	102	LEU
1	A	105	VAL
1	A	127	LEU
1	A	132	THR
1	A	183	LEU
1	A	184	LEU
1	A	187	LYS
1	A	244	LEU
1	A	247	VAL
1	A	254	LYS
1	A	265	LEU
1	A	266	GLU
1	A	317	LEU
1	A	319	ASP
1	A	367	THR
1	A	368	ILE
1	A	388	LEU

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Mol	Chain	Res	Type
1	A	395	ASN
1	A	410	ASN
1	A	434	LEU
1	A	453	LYS
1	A	472	THR
1	A	485	ASP
1	B	26	VAL
1	B	28	ASN
1	B	46	ILE
1	B	78	LEU
1	B	79	LEU
1	B	97	ASN
1	B	102	LEU
1	B	127	LEU
1	B	132	THR
1	B	187	LYS
1	B	192	PHE
1	B	222	LYS
1	B	244	LEU
1	B	247	VAL
1	B	254	LYS
1	B	326	VAL
1	B	336	LEU
1	B	367	THR
1	B	368	ILE
1	B	372	VAL
1	B	378	ILE
1	B	388	LEU
1	B	390	VAL
1	B	395	ASN
1	B	434	LEU
1	C	26	VAL
1	C	28	ASN
1	C	46	ILE
1	C	78	LEU
1	C	79	LEU
1	C	97	ASN
1	C	102	LEU
1	C	127	LEU
1	C	143	ILE
1	C	187	LYS
1	C	192	PHE

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Mol	Chain	Res	Type
1	C	222	LYS
1	C	244	LEU
1	C	247	VAL
1	C	254	LYS
1	C	283	ARG
1	C	317	LEU
1	C	328	ARG
1	C	341	LYS
1	C	368	ILE
1	C	372	VAL
1	C	388	LEU
1	C	395	ASN
1	C	410	ASN
1	C	429	ILE
1	C	434	LEU
1	D	22	GLN
1	D	28	ASN
1	D	77	GLN
1	D	78	LEU
1	D	79	LEU
1	D	89	LEU
1	D	98	THR
1	D	102	LEU
1	D	127	LEU
1	D	132	THR
1	D	183	LEU
1	D	184	LEU
1	D	187	LYS
1	D	247	VAL
1	D	254	LYS
1	D	283	ARG
1	D	340	GLU
1	D	349	LEU
1	D	368	ILE
1	D	388	LEU
1	D	395	ASN
1	D	410	ASN
1	D	434	LEU
1	D	472	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	22	GLN
1	A	28	ASN
1	A	51	GLN
1	A	74	ASN
1	A	77	GLN
1	A	81	GLN
1	A	82	HIS
1	A	94	ASN
1	A	97	ASN
1	A	111	ASN
1	A	171	ASN
1	A	248	GLN
1	A	256	HIS
1	A	356	ASN
1	A	395	ASN
1	A	410	ASN
1	A	418	ASN
1	A	420	ASN
1	A	428	ASN
1	A	463	ASN
1	B	9	ASN
1	B	28	ASN
1	B	37	GLN
1	B	51	GLN
1	B	74	ASN
1	B	77	GLN
1	B	81	GLN
1	B	82	HIS
1	B	88	HIS
1	B	97	ASN
1	B	171	ASN
1	B	256	HIS
1	B	356	ASN
1	B	395	ASN
1	B	410	ASN
1	B	418	ASN
1	B	420	ASN
1	B	428	ASN
1	B	463	ASN
1	C	9	ASN
1	C	28	ASN
1	C	37	GLN

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Mol	Chain	Res	Type
1	C	51	GLN
1	C	74	ASN
1	C	81	GLN
1	C	82	HIS
1	C	97	ASN
1	C	111	ASN
1	C	171	ASN
1	C	248	GLN
1	C	256	HIS
1	C	261	ASN
1	C	356	ASN
1	C	371	ASN
1	C	395	ASN
1	C	410	ASN
1	C	418	ASN
1	C	420	ASN
1	C	428	ASN
1	C	463	ASN
1	D	9	ASN
1	D	28	ASN
1	D	51	GLN
1	D	74	ASN
1	D	77	GLN
1	D	81	GLN
1	D	82	HIS
1	D	111	ASN
1	D	171	ASN
1	D	248	GLN
1	D	256	HIS
1	D	305	GLN
1	D	356	ASN
1	D	395	ASN
1	D	410	ASN
1	D	418	ASN
1	D	420	ASN
1	D	428	ASN
1	D	463	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](#)

4 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	1490	-	46,48,48	2.83	12 (26%)	64,73,73	1.56	12 (18%)
2	NAD	C	3490	-	46,48,48	2.80	12 (26%)	64,73,73	1.57	12 (18%)
2	NAD	D	4490	-	46,48,48	2.84	12 (26%)	64,73,73	1.57	11 (17%)
2	NAD	B	2490	-	46,48,48	2.85	11 (23%)	64,73,73	1.60	13 (20%)

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	1490	-	-	1/30/62/62	0/5/5/5
2	NAD	C	3490	-	-	1/30/62/62	0/5/5/5
2	NAD	D	4490	-	-	1/30/62/62	0/5/5/5
2	NAD	B	2490	-	-	1/30/62/62	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1490	NAD	C2N-N1N	9.68	1.45	1.35
2	B	2490	NAD	C4N-C3N	9.51	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3490	NAD	C4N-C3N	9.44	1.53	1.39
2	D	4490	NAD	C4N-C3N	9.31	1.53	1.39
2	D	4490	NAD	C2N-N1N	9.26	1.45	1.35
2	A	1490	NAD	C4N-C3N	9.09	1.53	1.39
2	B	2490	NAD	C2N-N1N	9.04	1.44	1.35
2	C	3490	NAD	C2N-N1N	8.82	1.44	1.35
2	C	3490	NAD	C5N-C4N	7.04	1.50	1.38
2	B	2490	NAD	C5N-C4N	6.95	1.50	1.38
2	A	1490	NAD	C5N-C4N	6.70	1.50	1.38
2	D	4490	NAD	C5N-C4N	6.62	1.50	1.38
2	B	2490	NAD	PN-O3	5.77	1.65	1.59
2	A	1490	NAD	PN-O3	5.56	1.65	1.59
2	D	4490	NAD	PN-O3	5.55	1.65	1.59
2	C	3490	NAD	PN-O3	4.45	1.64	1.59
2	C	3490	NAD	C6N-N1N	4.42	1.45	1.35
2	B	2490	NAD	C6N-N1N	4.19	1.44	1.35
2	D	4490	NAD	C6N-N1N	4.04	1.44	1.35
2	A	1490	NAD	C6N-N1N	3.85	1.44	1.35
2	D	4490	NAD	C2A-N3A	3.82	1.40	1.33
2	C	3490	NAD	C2A-N3A	3.79	1.40	1.33
2	B	2490	NAD	C2A-N3A	3.71	1.40	1.33
2	A	1490	NAD	C2A-N3A	3.61	1.40	1.33
2	D	4490	NAD	C4A-N3A	3.55	1.41	1.34
2	A	1490	NAD	C4A-N3A	3.54	1.41	1.34
2	B	2490	NAD	C4A-N3A	3.53	1.41	1.34
2	D	4490	NAD	O4D-C1D	3.50	1.45	1.40
2	C	3490	NAD	C4A-N3A	3.47	1.40	1.34
2	A	1490	NAD	O4D-C1D	3.37	1.45	1.40
2	C	3490	NAD	O4D-C1D	3.15	1.45	1.40
2	C	3490	NAD	C2N-C3N	-3.06	1.34	1.39
2	B	2490	NAD	C2N-C3N	-2.96	1.34	1.39
2	B	2490	NAD	O4D-C1D	2.80	1.44	1.40
2	D	4490	NAD	C2N-C3N	-2.79	1.34	1.39
2	D	4490	NAD	C5A-C6A	2.70	1.48	1.41
2	A	1490	NAD	C2N-C3N	-2.70	1.34	1.39
2	B	2490	NAD	C5A-C6A	2.53	1.48	1.41
2	B	2490	NAD	C5A-N7A	-2.41	1.34	1.39
2	C	3490	NAD	C5A-C6A	2.41	1.47	1.41
2	C	3490	NAD	C5A-N7A	-2.37	1.34	1.39
2	A	1490	NAD	C5A-C6A	2.32	1.47	1.41
2	C	3490	NAD	O4D-C4D	2.25	1.50	1.45
2	A	1490	NAD	O4D-C4D	2.19	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4490	NAD	O4D-C4D	2.16	1.49	1.45
2	D	4490	NAD	C5A-N7A	-2.09	1.35	1.39
2	A	1490	NAD	C5A-N7A	-2.01	1.35	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1490	NAD	N3A-C2A-N1A	-4.45	121.84	128.58
2	C	3490	NAD	N3A-C2A-N1A	-4.43	121.88	128.58
2	B	2490	NAD	N3A-C2A-N1A	-4.38	121.95	128.58
2	D	4490	NAD	N3A-C2A-N1A	-4.30	122.07	128.58
2	A	1490	NAD	C2A-N1A-C6A	4.27	125.74	118.73
2	B	2490	NAD	C2A-N1A-C6A	4.25	125.70	118.73
2	C	3490	NAD	C2A-N1A-C6A	4.18	125.60	118.73
2	D	4490	NAD	C2A-N1A-C6A	4.15	125.55	118.73
2	C	3490	NAD	C5N-C4N-C3N	-3.64	116.79	120.36
2	D	4490	NAD	C5N-C4N-C3N	-3.63	116.79	120.36
2	A	1490	NAD	C5N-C4N-C3N	-3.53	116.89	120.36
2	B	2490	NAD	C5N-C4N-C3N	-3.48	116.94	120.36
2	D	4490	NAD	C2N-C3N-C4N	3.04	121.80	118.26
2	C	3490	NAD	C2N-C3N-C4N	2.99	121.73	118.26
2	B	2490	NAD	C3B-C2B-C1B	2.98	107.10	101.46
2	A	1490	NAD	C3B-C2B-C1B	2.97	107.08	101.46
2	B	2490	NAD	C2N-C3N-C4N	2.91	121.65	118.26
2	D	4490	NAD	C3B-C2B-C1B	2.90	106.95	101.46
2	B	2490	NAD	C4A-N9A-C8A	-2.89	102.70	105.74
2	A	1490	NAD	C2N-C3N-C4N	2.89	121.62	118.26
2	D	4490	NAD	C1B-N9A-C8A	2.88	133.49	127.09
2	C	3490	NAD	C4A-N9A-C8A	-2.88	102.72	105.74
2	D	4490	NAD	C4A-N9A-C8A	-2.87	102.72	105.74
2	C	3490	NAD	O2A-PA-O1A	2.86	125.75	112.44
2	A	1490	NAD	C1B-N9A-C8A	2.86	133.44	127.09
2	B	2490	NAD	O2A-PA-O1A	2.85	125.71	112.44
2	D	4490	NAD	O2A-PA-O1A	2.84	125.67	112.44
2	A	1490	NAD	O2A-PA-O1A	2.78	125.38	112.44
2	C	3490	NAD	C3B-C2B-C1B	2.76	106.69	101.46
2	B	2490	NAD	C1B-N9A-C8A	2.75	133.20	127.09
2	C	3490	NAD	C1B-N9A-C8A	2.73	133.16	127.09
2	A	1490	NAD	C6N-N1N-C1D	-2.59	114.64	119.73
2	A	1490	NAD	C4A-N9A-C8A	-2.59	103.02	105.74
2	B	2490	NAD	C6N-N1N-C1D	-2.54	114.74	119.73
2	D	4490	NAD	C5A-N7A-C8A	2.51	107.40	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2490	NAD	C5A-N7A-C8A	2.48	107.35	103.45
2	C	3490	NAD	C6N-N1N-C1D	-2.45	114.92	119.73
2	C	3490	NAD	C5A-N7A-C8A	2.45	107.30	103.45
2	D	4490	NAD	C6N-N1N-C1D	-2.45	114.93	119.73
2	A	1490	NAD	C5A-N7A-C8A	2.42	107.26	103.45
2	B	2490	NAD	C6N-N1N-C2N	2.29	123.82	121.88
2	B	2490	NAD	C5A-C4A-N3A	-2.18	123.71	126.72
2	C	3490	NAD	C5A-C4A-N3A	-2.18	123.72	126.72
2	D	4490	NAD	C5A-C4A-N3A	-2.17	123.73	126.72
2	C	3490	NAD	C6N-N1N-C2N	2.07	123.64	121.88
2	B	2490	NAD	O4B-C1B-N9A	-2.04	104.17	108.09
2	A	1490	NAD	O4B-C1B-N9A	-2.03	104.20	108.09
2	A	1490	NAD	C6N-N1N-C2N	2.02	123.60	121.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1490	NAD	C4D-C5D-O5D-PN
2	D	4490	NAD	C4D-C5D-O5D-PN
2	B	2490	NAD	C4D-C5D-O5D-PN
2	C	3490	NAD	C4D-C5D-O5D-PN

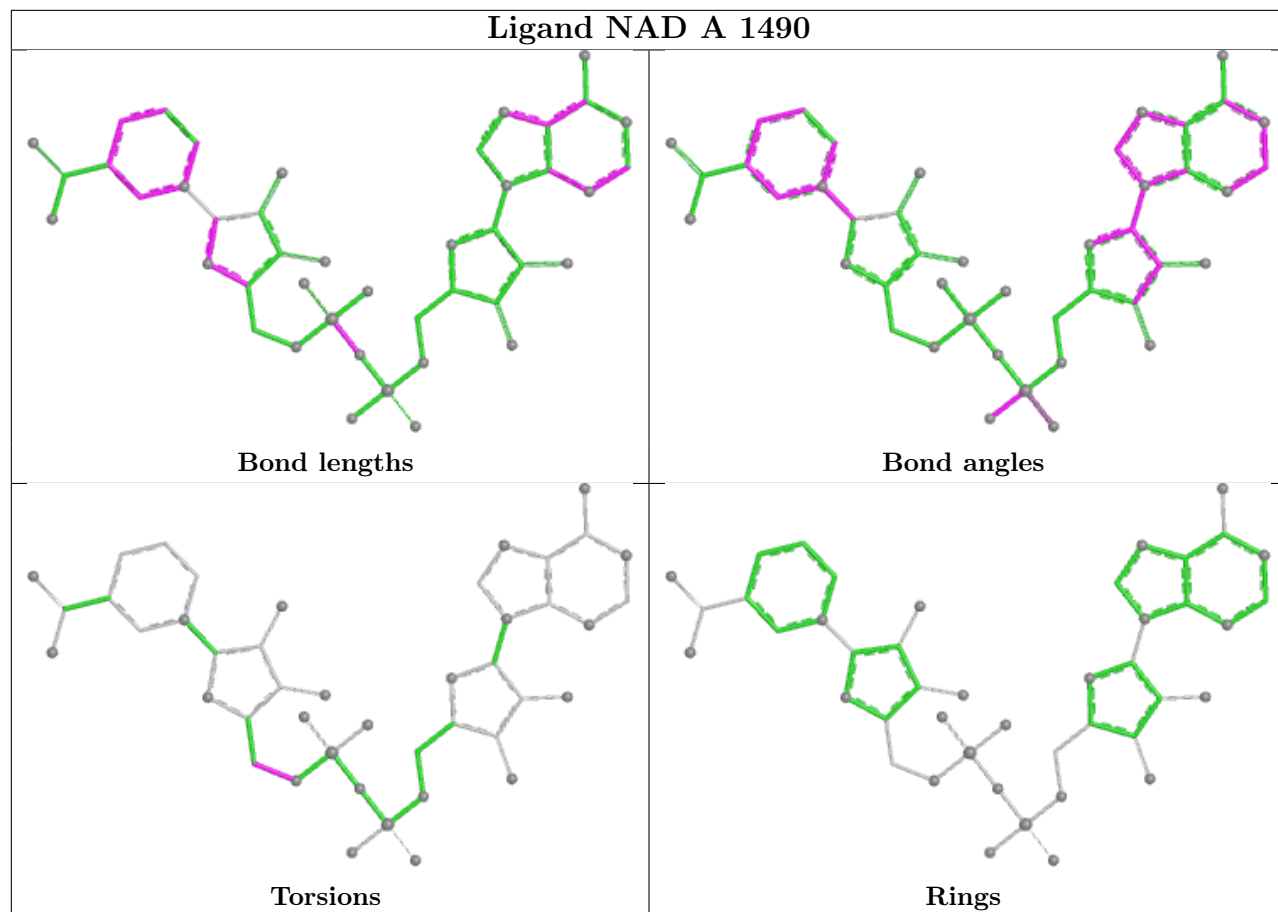
There are no ring outliers.

3 monomers are involved in 4 short contacts:

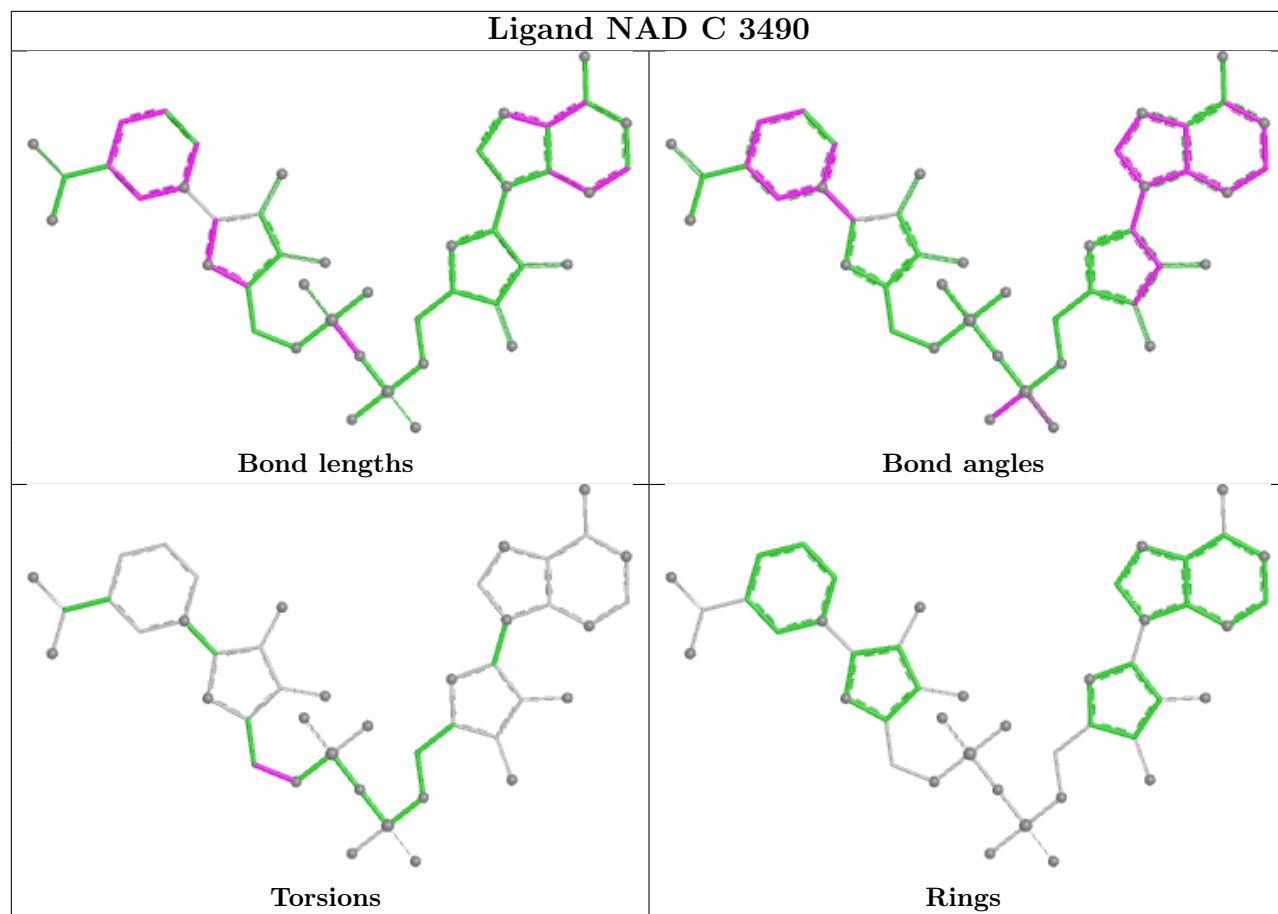
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3490	NAD	2	0
2	D	4490	NAD	1	0
2	B	2490	NAD	1	0

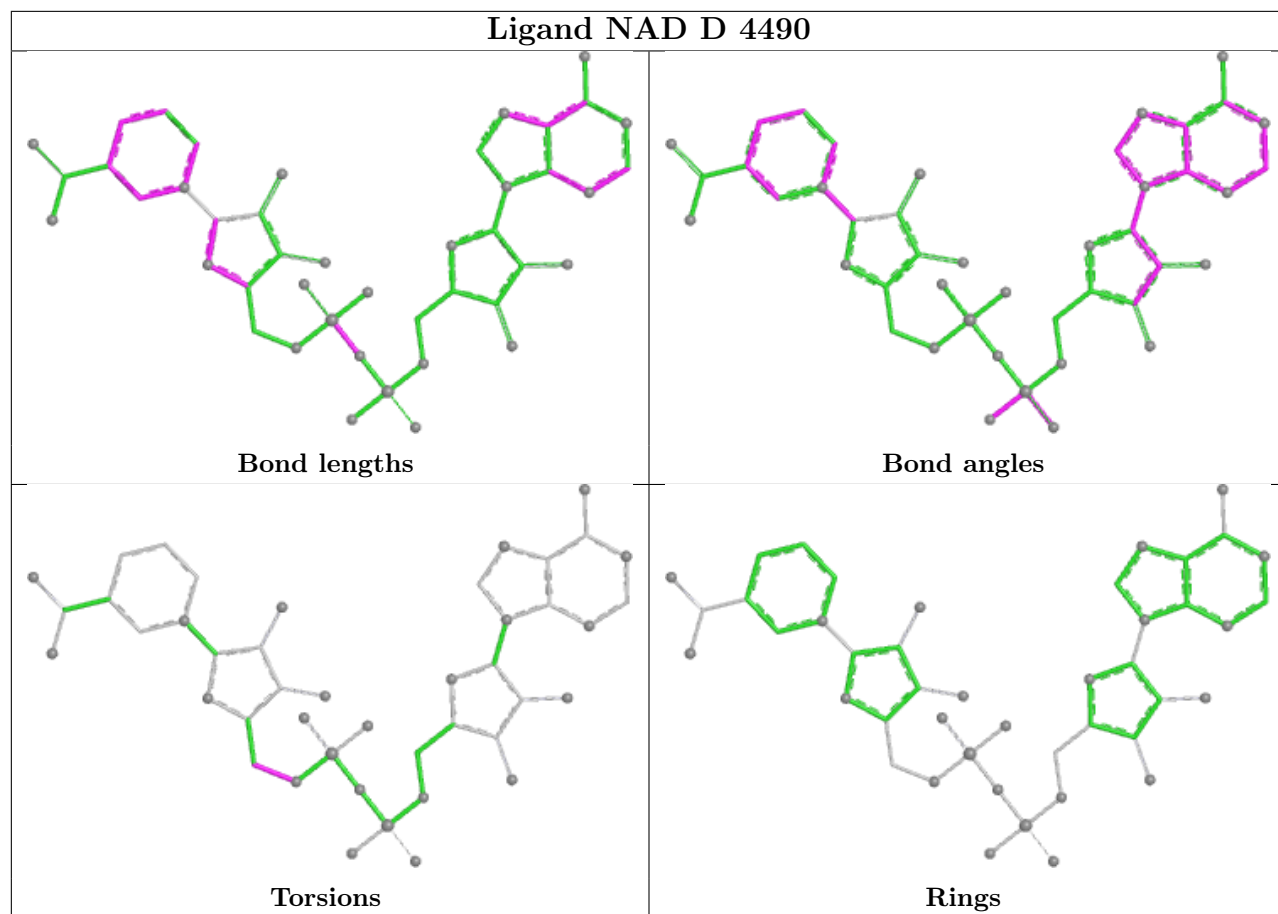
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

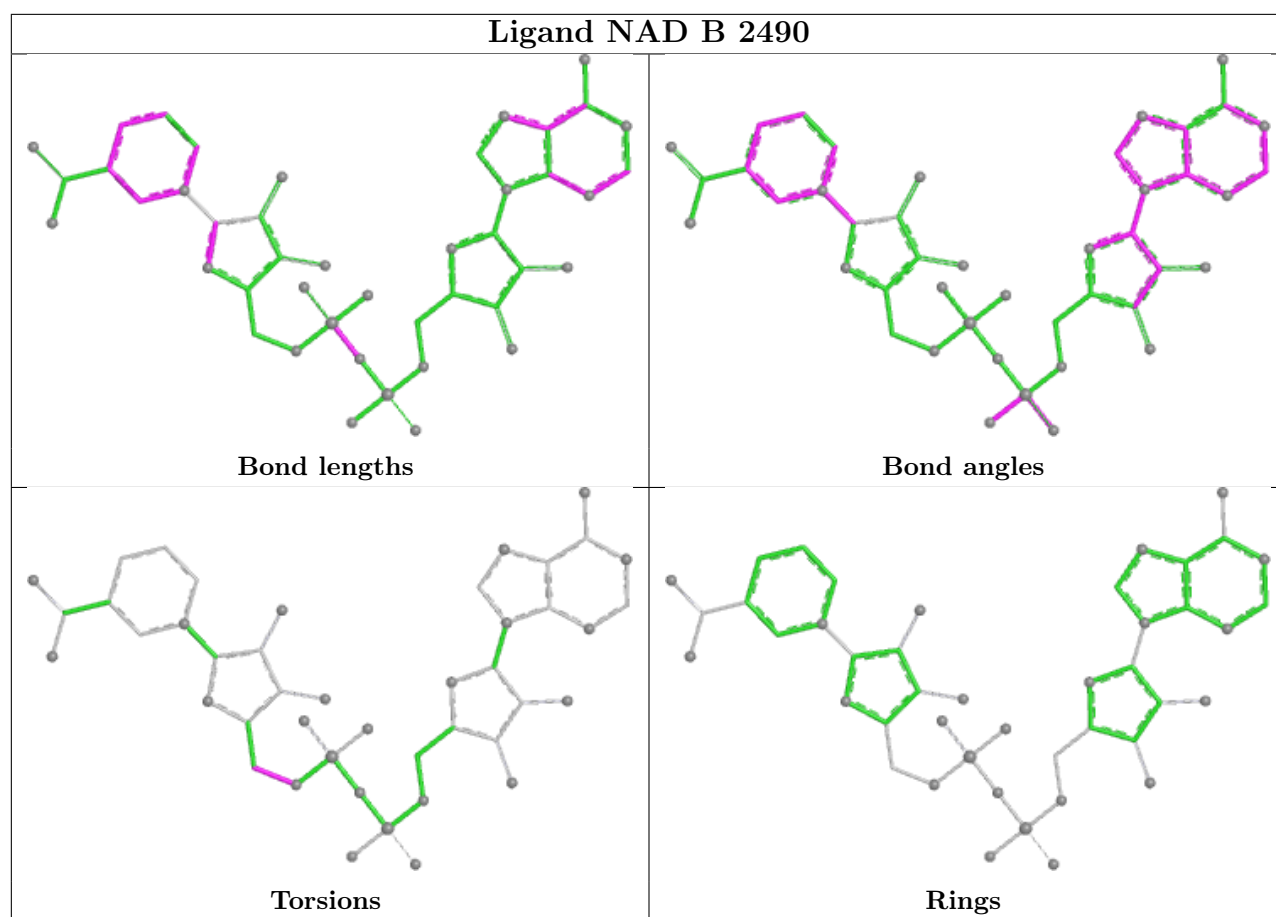
equivalents in the CSD to analyse the geometry.



Ligand NAD C 3490







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	484/486 (99%)	-0.18	2 (0%) 88 86	12, 29, 50, 67	0
1	B	484/486 (99%)	-0.26	7 (1%) 73 70	13, 26, 46, 71	0
1	C	484/486 (99%)	-0.35	2 (0%) 88 86	14, 26, 45, 64	0
1	D	484/486 (99%)	-0.21	3 (0%) 85 83	11, 30, 50, 66	0
All	All	1936/1944 (99%)	-0.25	14 (0%) 84 81	11, 27, 49, 71	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	VAL	3.3
1	B	356	ASN	3.2
1	B	266	GLU	2.6
1	A	357	VAL	2.4
1	B	358	SER	2.3
1	A	359	ASP	2.3
1	C	19	LYS	2.3
1	D	368	ILE	2.1
1	C	14	GLU	2.1
1	D	359	ASP	2.1
1	B	19	LYS	2.1
1	B	486	PHE	2.1
1	D	305	GLN	2.0
1	B	18	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

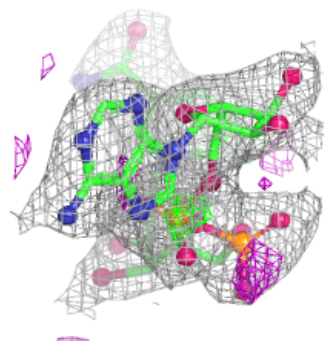
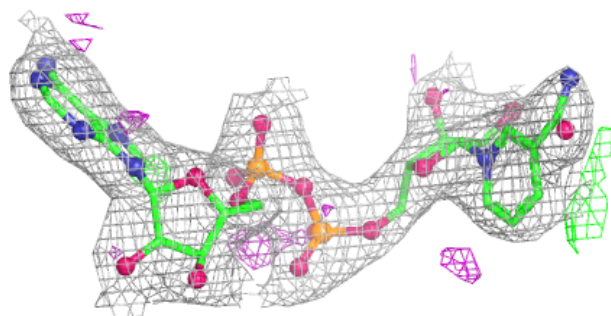
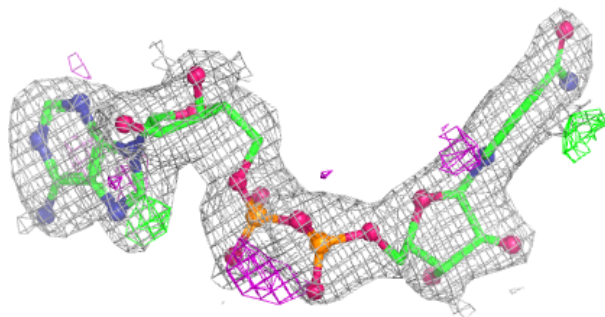
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	1490	44/44	0.95	0.08	36,40,42,44	0
2	NAD	C	3490	44/44	0.95	0.09	37,40,46,48	0
2	NAD	D	4490	44/44	0.95	0.08	37,42,44,45	0
2	NAD	B	2490	44/44	0.96	0.08	38,41,45,46	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.

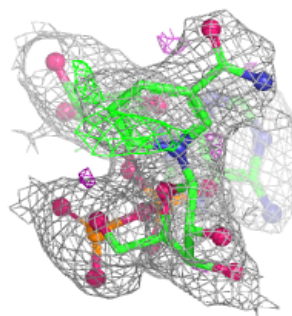
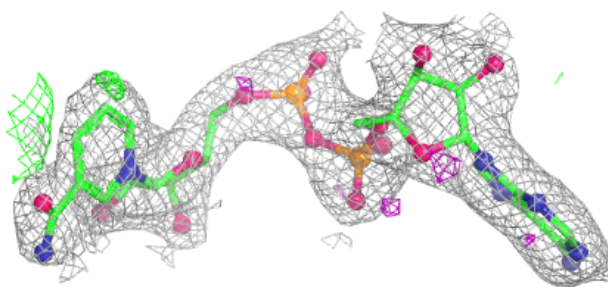
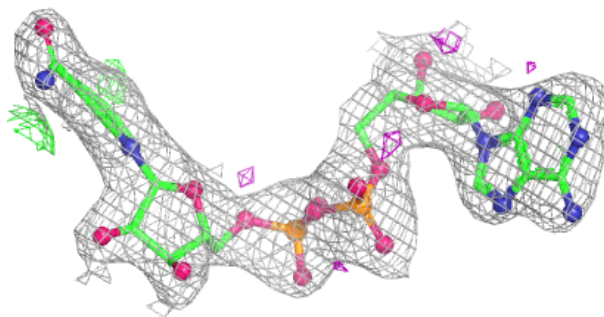
Electron density around NAD A 1490:

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

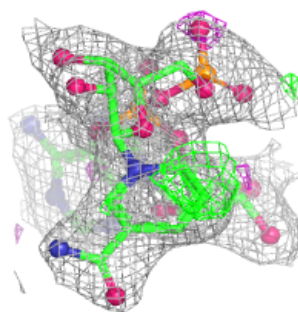
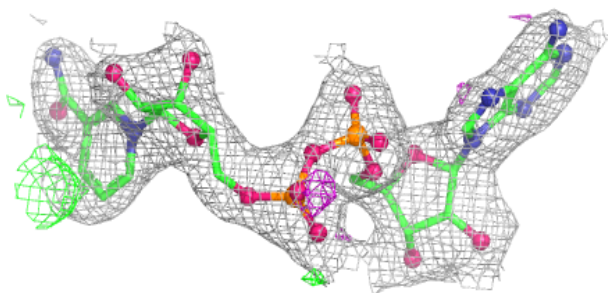
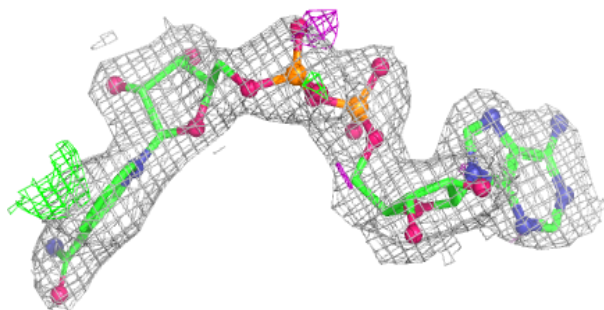


Electron density around NAD C 3490:

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

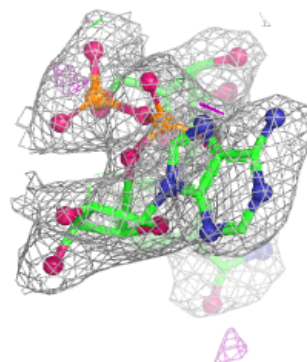
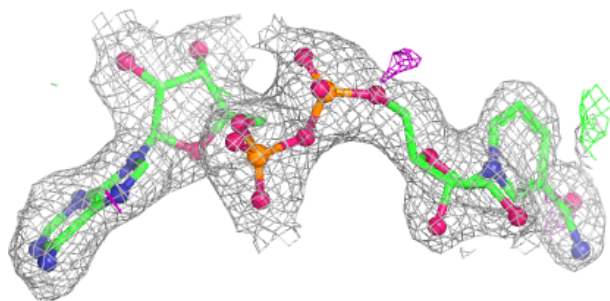
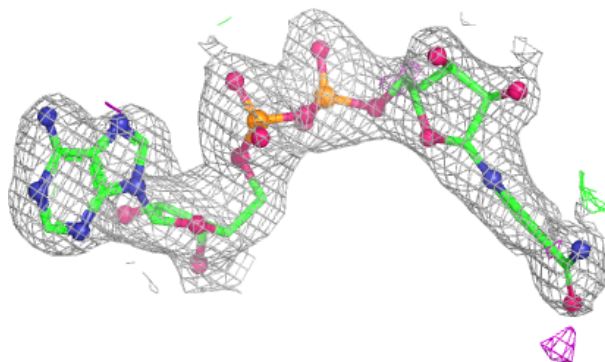
**Electron density around NAD D 4490:**

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



Electron density around NAD B 2490:

$2mF_o-DF_c$ (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.