Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 06:26 PM UTC

PDB ID	:	2GVG / pdb_00002gvg
Title	:	Crystal Structure of human NMPRTase and its complex with NMN
Authors	:	Khan, J.A.; Tao, X.; Tong, L.
Deposited on	:	2006-05-02
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

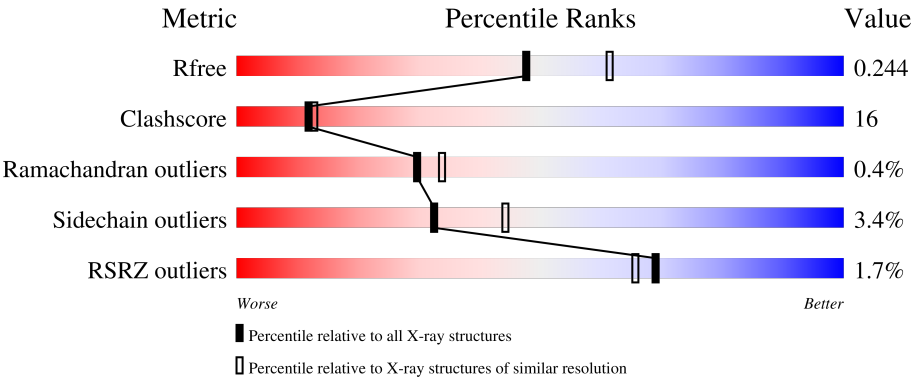
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	491	59% 32% 6%
1	B	491	67% 25% 5%
1	C	491	4% 57% 35% 6%
1	D	491	67% 25% 5%
1	E	491	69% 24% 5%

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Mol	Chain	Length	Quality of chain
1	F	491	

2 Entry composition

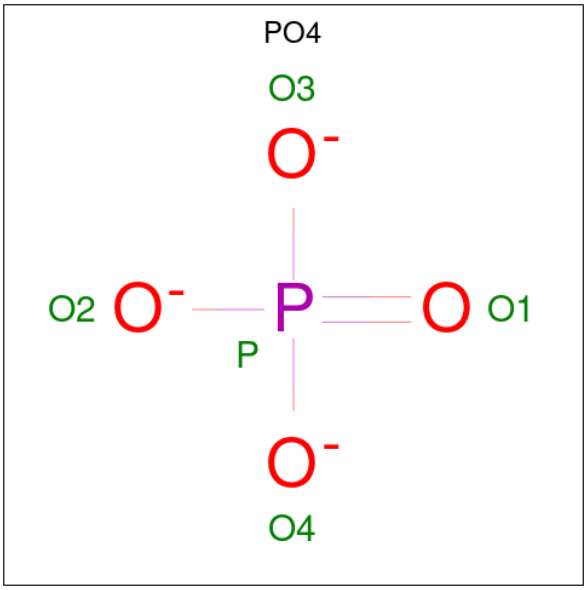
There are 4 unique types of molecules in this entry. The entry contains 23801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

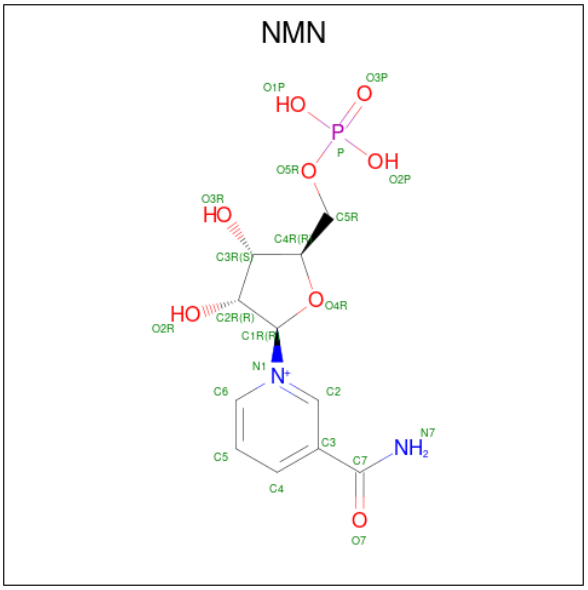
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3688	2376	609	696	7			
1	B	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	C	461	Total	C	N	O	S	0	0	0
			3688	2376	609	696	7			
1	D	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	E	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	F	463	Total	C	N	O	S	0	0	0
			3705	2385	612	701	7			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (CCD ID: NMN) (formula: $C_{11}H_{16}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	E	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	F	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 4 is water.

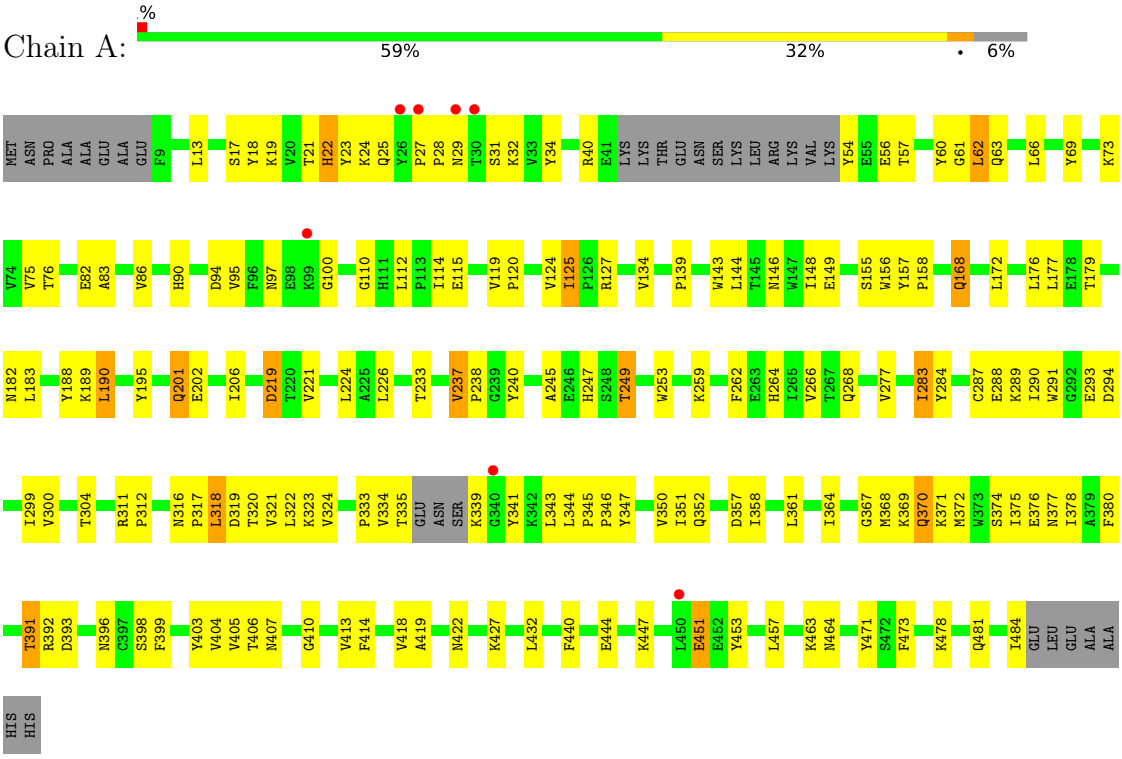
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	165	Total	O	0	0
			165	165		
4	C	125	Total	O	0	0
			125	125		
4	D	306	Total	O	0	0
			306	306		
4	E	280	Total	O	0	0
			280	280		
4	F	380	Total	O	0	0
			380	380		

3 Residue-property plots (i)

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

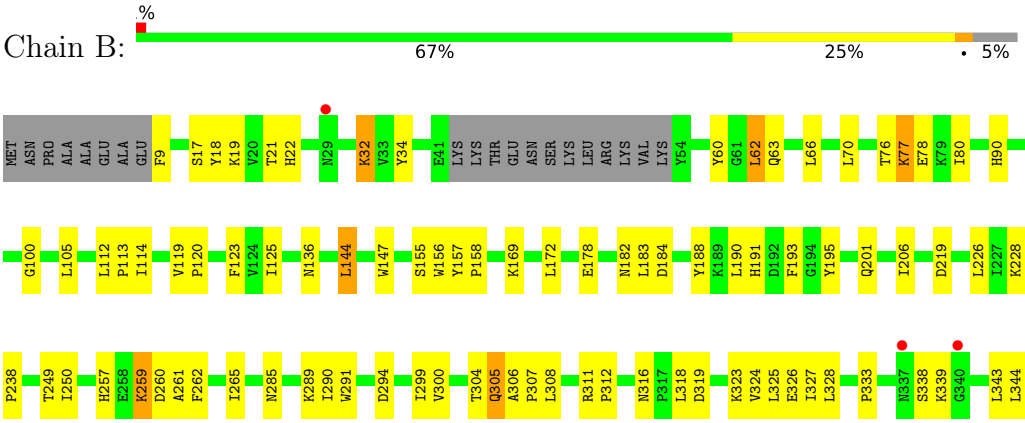
• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain A:



• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain B:

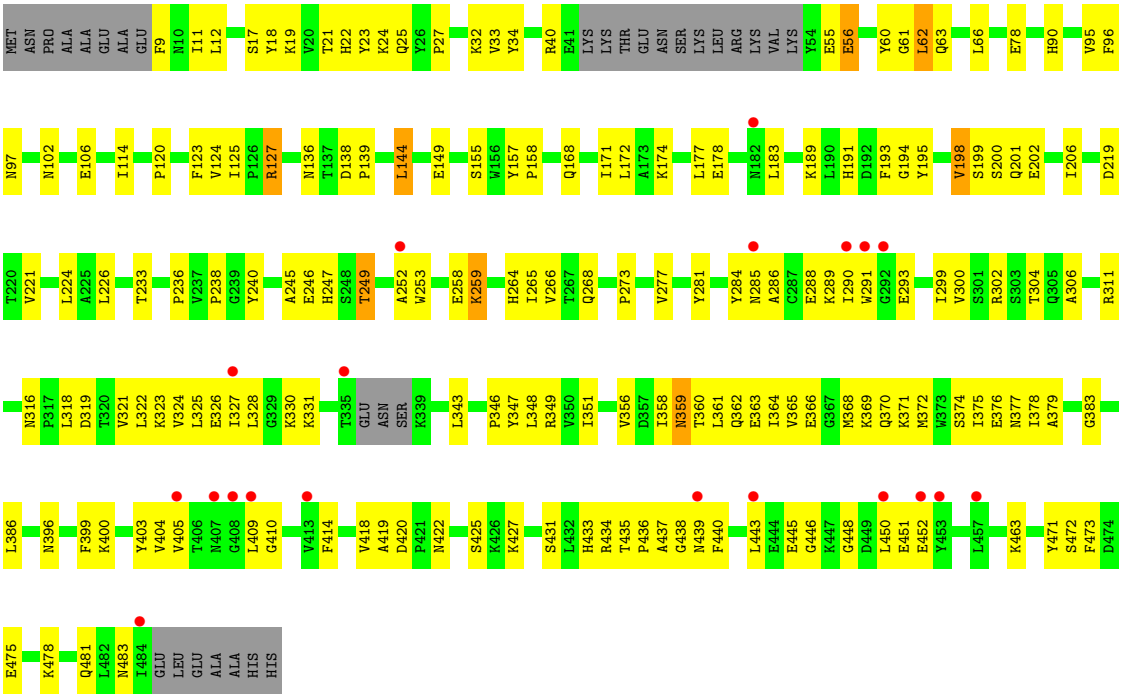




• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain C:

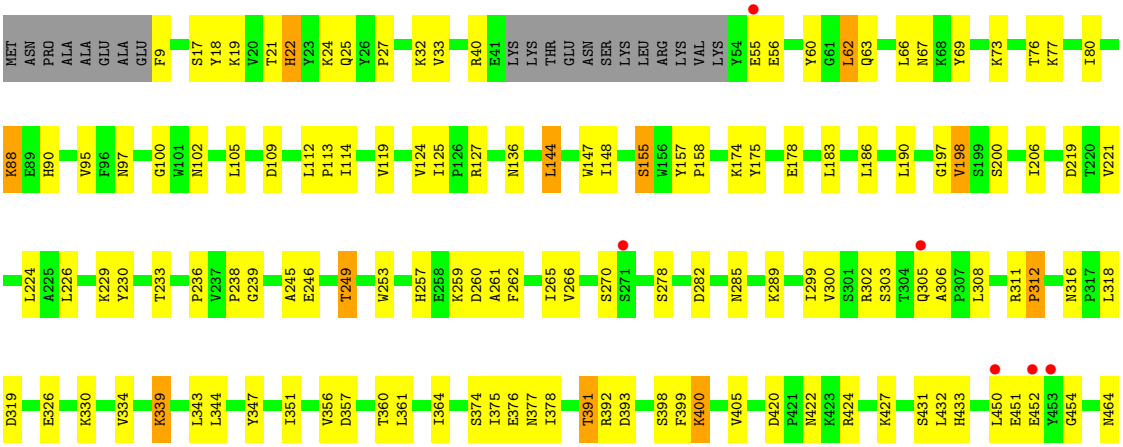


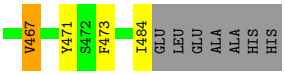


• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain D:



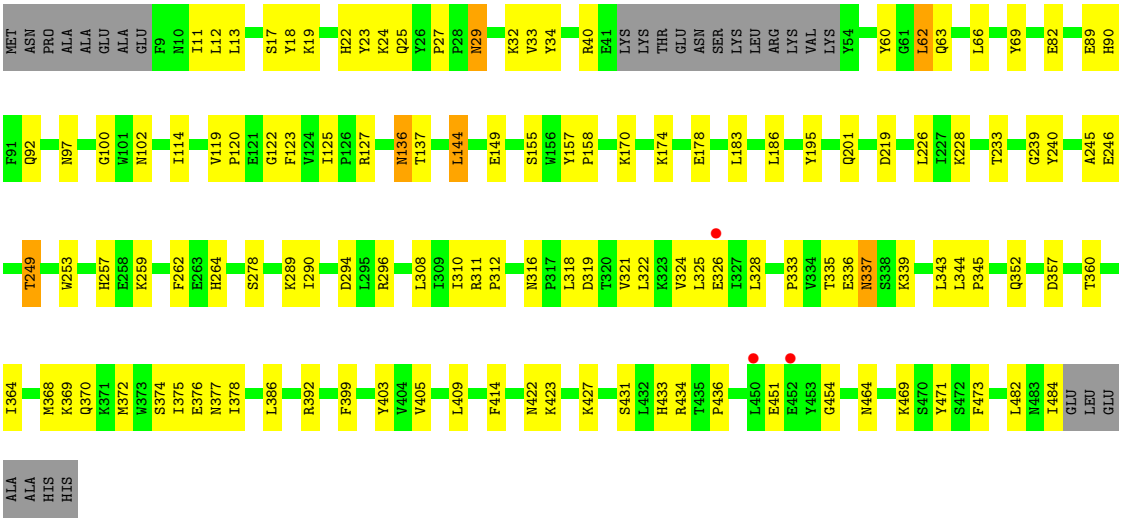




• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain E:

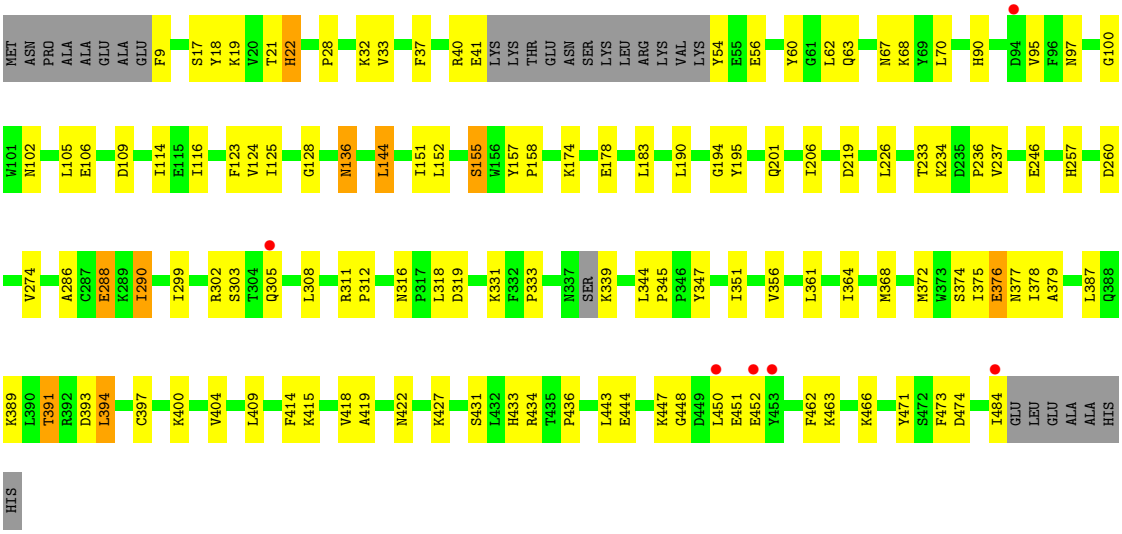




• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	253.07Å 101.37Å 148.20Å 90.00° 125.48° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 93.0 (30.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.246 0.198 , 0.244	Depositor DCC
R_{free} test set	11237 reflections (7.47%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23801	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 39.91 % 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 2.9568e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NMN

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	0.37	0/3775	0.90	7/5115 (0.1%)
1	B	0.37	0/3799	0.89	10/5149 (0.2%)
1	C	0.35	0/3775	0.87	6/5115 (0.1%)
1	D	0.42	0/3799	0.93	12/5149 (0.2%)
1	E	0.42	0/3799	0.93	9/5149 (0.2%)
1	F	0.46	0/3792	0.93	12/5138 (0.2%)
All	All	0.40	0/22739	0.91	56/30815 (0.2%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	SER	N-CA-C	-7.73	103.74	113.01
1	B	237	VAL	CA-C-N	7.10	126.59	118.85
1	B	237	VAL	C-N-CA	7.10	126.59	118.85
1	E	312	PRO	N-CA-C	-6.34	101.93	111.57
1	C	359	ASN	N-CA-C	6.08	117.71	111.14
1	F	312	PRO	N-CA-C	-5.88	101.86	111.68
1	C	127	ARG	N-CA-C	5.85	118.45	110.55
1	C	356	VAL	N-CA-C	5.84	116.52	107.99
1	D	278	SER	N-CA-C	5.83	119.70	112.59
1	B	378	ILE	N-CA-C	5.81	118.54	108.90
1	B	147	TRP	N-CA-C	-5.80	104.55	111.69
1	D	155	SER	N-CA-C	-5.80	106.04	113.01
1	C	290	ILE	N-CA-C	5.80	115.92	110.30
1	B	70	LEU	N-CA-C	5.75	120.80	113.55
1	E	69	TYR	N-CA-C	5.73	121.14	114.04
1	F	356	VAL	N-CA-C	5.68	116.92	108.23
1	F	22	HIS	N-CA-C	5.63	118.35	111.82
1	D	67	ASN	N-CA-C	5.62	117.48	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	TYR	N-CA-C	5.58	120.96	114.04
1	E	278	SER	N-CA-C	5.56	119.63	112.41
1	E	127	ARG	N-CA-C	5.55	117.86	110.53
1	E	308	LEU	N-CA-C	-5.55	100.25	109.46
1	F	288	GLU	N-CA-C	5.54	117.12	111.14
1	D	246	GLU	N-CA-C	-5.50	101.05	109.41
1	D	378	ILE	N-CA-C	5.50	118.03	108.95
1	E	378	ILE	N-CA-C	5.50	118.02	108.95
1	F	194	GLY	N-CA-C	5.48	124.59	115.66
1	A	290	ILE	N-CA-C	5.46	115.91	110.23
1	A	22	HIS	N-CA-C	5.39	118.08	111.82
1	C	125	ILE	N-CA-C	5.39	113.77	107.89
1	D	312	PRO	N-CA-C	-5.34	102.76	111.68
1	A	125	ILE	N-CA-C	5.34	113.96	107.61
1	B	312	PRO	N-CA-C	-5.31	103.49	111.57
1	D	69	TYR	N-CA-C	5.30	120.61	114.04
1	A	378	ILE	N-CA-C	5.30	117.70	108.90
1	B	290	ILE	N-CA-C	5.28	115.42	110.30
1	F	67	ASN	N-CA-C	5.26	116.82	111.14
1	D	420	ASP	CA-C-N	5.26	124.92	119.56
1	D	420	ASP	C-N-CA	5.26	124.92	119.56
1	B	308	LEU	N-CA-C	-5.23	100.78	109.46
1	D	127	ARG	N-CA-C	5.22	117.42	110.53
1	C	61	GLY	N-CA-C	5.21	120.67	114.48
1	F	70	LEU	N-CA-C	5.20	119.90	113.50
1	F	246	GLU	N-CA-C	-5.20	101.50	109.41
1	A	61	GLY	N-CA-C	5.17	120.63	114.48
1	E	92	GLN	N-CA-C	-5.17	105.62	112.24
1	D	356	VAL	N-CA-C	5.14	115.98	108.58
1	D	22	HIS	N-CA-C	5.14	117.78	111.82
1	F	237	VAL	CA-C-N	5.13	126.25	119.84
1	F	237	VAL	C-N-CA	5.13	126.25	119.84
1	B	372	MET	N-CA-C	5.10	118.77	112.24
1	E	122	GLY	N-CA-C	-5.09	108.64	114.69
1	F	155	SER	N-CA-C	-5.08	106.92	113.01
1	A	237	VAL	N-CA-C	5.06	113.34	109.19
1	E	246	GLU	N-CA-C	-5.05	101.73	109.41
1	F	387	LEU	N-CA-C	5.04	120.42	113.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3688	0	3668	156	0
1	B	3711	0	3686	114	0
1	C	3688	0	3668	162	0
1	D	3711	0	3686	116	0
1	E	3711	0	3686	102	0
1	F	3705	0	3680	97	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	22	0	12	0	0
3	B	22	0	12	0	0
3	C	22	0	12	1	0
3	D	22	0	12	1	0
3	E	22	0	12	1	0
3	F	22	0	12	1	0
4	A	139	0	0	9	0
4	B	165	0	0	8	0
4	C	125	0	0	10	0
4	D	306	0	0	14	0
4	E	280	0	0	10	0
4	F	380	0	0	14	0
All	All	23801	0	22146	704	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 16.

All (704) 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:D:391:THR:HG22	1:D:393:ASP:H	1.19	1.08
1:A:63:GLN:HE22	1:A:471:TYR:H	1.03	0.99
1:D:25:GLN:HE21	1:E:249:THR:HG21	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:LEU:H	1:E:377:ASN:HD21	1.08	0.95
1:B:391:THR:HG23	1:B:393:ASP:H	1.31	0.93
1:E:119:VAL:HG21	1:E:125:ILE:HD11	1.46	0.93
1:F:344:LEU:H	1:F:377:ASN:HD21	1.05	0.93
1:B:63:GLN:HE22	1:B:471:TYR:H	1.12	0.92
1:A:344:LEU:H	1:A:377:ASN:HD21	1.18	0.91
1:B:119:VAL:HG21	1:B:125:ILE:HD11	1.50	0.91
1:F:63:GLN:HE22	1:F:471:TYR:H	1.14	0.91
1:D:374:SER:OG	1:D:376:GLU:HG2	1.71	0.91
1:D:249:THR:HG21	1:E:25:GLN:NE2	1.86	0.91
1:C:63:GLN:HE22	1:C:471:TYR:H	1.19	0.90
1:B:344:LEU:H	1:B:377:ASN:ND2	1.70	0.89
1:D:148:ILE:HG23	4:D:1329:HOH:O	1.72	0.89
1:D:261:ALA:O	1:D:265:ILE:HG12	1.74	0.88
1:F:400:LYS:HE3	4:F:1363:HOH:O	1.74	0.88
1:D:119:VAL:HG21	1:D:125:ILE:HD11	1.56	0.88
1:F:374:SER:OG	1:F:376:GLU:HG2	1.74	0.88
1:A:316:ASN:HD22	1:A:319:ASP:H	1.19	0.87
1:E:316:ASN:HD22	1:E:319:ASP:H	1.22	0.87
1:A:224:LEU:HD12	1:A:238:PRO:HD2	1.57	0.87
1:D:316:ASN:HD22	1:D:319:ASP:H	1.14	0.86
1:D:25:GLN:NE2	1:E:249:THR:HG21	1.91	0.86
1:E:344:LEU:H	1:E:377:ASN:ND2	1.75	0.85
1:F:316:ASN:HD22	1:F:319:ASP:H	1.24	0.85
1:B:344:LEU:H	1:B:377:ASN:HD21	1.22	0.85
1:D:344:LEU:H	1:D:377:ASN:HD21	1.23	0.85
1:A:25:GLN:HE21	1:C:249:THR:HG21	1.40	0.84
1:D:249:THR:HG21	1:E:25:GLN:HE21	1.43	0.84
1:B:316:ASN:HD22	1:B:319:ASP:H	1.25	0.83
1:E:63:GLN:HE22	1:E:471:TYR:H	1.25	0.83
1:E:335:THR:HG23	1:E:343:LEU:HB3	1.59	0.83
1:D:63:GLN:HE22	1:D:471:TYR:H	1.22	0.82
1:C:343:LEU:HD12	1:C:377:ASN:HD21	1.41	0.81
1:A:391:THR:HG23	1:A:393:ASP:H	1.45	0.81
1:A:344:LEU:H	1:A:377:ASN:ND2	1.77	0.81
1:A:25:GLN:HE22	1:C:245:ALA:HA	1.44	0.81
1:A:249:THR:HG21	1:C:25:GLN:NE2	1.95	0.80
1:A:432:LEU:HG	1:A:457:LEU:HD12	1.63	0.79
1:D:344:LEU:H	1:D:377:ASN:ND2	1.80	0.79
1:F:56:GLU:HG2	1:F:124:VAL:HG12	1.64	0.79
1:C:343:LEU:HD12	1:C:377:ASN:ND2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:LYS:HD3	1:C:425:SER:HB3	1.65	0.77
1:C:316:ASN:HD22	1:C:319:ASP:H	1.30	0.76
1:A:245:ALA:HA	1:C:25:GLN:HE22	1.49	0.76
1:D:56:GLU:HG2	1:D:124:VAL:CG1	2.17	0.75
1:C:478:LYS:HD2	1:C:481:GLN:NE2	2.01	0.75
1:D:303:SER:OG	1:D:305:GLN:HG2	1.87	0.75
1:B:157:TYR:HB3	1:B:158:PRO:HD3	1.69	0.75
1:E:321:VAL:HG23	1:E:352:GLN:HE21	1.51	0.75
1:B:259:LYS:HZ2	1:B:259:LYS:HB2	1.50	0.74
1:D:316:ASN:ND2	1:D:319:ASP:H	1.84	0.74
1:A:25:GLN:NE2	1:C:249:THR:HG21	2.02	0.74
1:C:478:LYS:HA	1:C:481:GLN:HE21	1.51	0.74
1:D:147:TRP:HB3	4:D:1329:HOH:O	1.85	0.74
1:D:113:PRO:HA	1:D:464:ASN:HD22	1.52	0.74
1:F:344:LEU:H	1:F:377:ASN:ND2	1.84	0.74
1:B:77:LYS:HD2	1:B:105:LEU:HD21	1.69	0.73
1:A:63:GLN:NE2	1:A:471:TYR:H	1.83	0.73
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.70	0.73
1:C:224:LEU:HD12	1:C:238:PRO:HD2	1.70	0.73
1:B:32:LYS:O	1:B:404:VAL:HG23	1.89	0.73
1:C:322:LEU:HD22	1:C:371:LYS:HG3	1.70	0.72
1:D:25:GLN:HE22	1:E:245:ALA:HA	1.54	0.72
1:F:316:ASN:ND2	1:F:319:ASP:H	1.85	0.72
1:A:63:GLN:HE22	1:A:471:TYR:N	1.86	0.72
1:E:316:ASN:ND2	1:E:319:ASP:H	1.87	0.72
1:B:259:LYS:HB2	1:B:259:LYS:NZ	2.05	0.72
1:A:344:LEU:N	1:A:377:ASN:HD21	1.87	0.71
1:E:434:ARG:HD2	4:E:1827:HOH:O	1.90	0.71
1:D:245:ALA:HA	1:E:25:GLN:HE22	1.56	0.70
1:A:54:TYR:O	1:A:127:ARG:HD2	1.91	0.70
1:E:195:TYR:OH	1:E:201:GLN:NE2	2.23	0.70
1:F:183:LEU:HD11	1:F:484:ILE:HG22	1.73	0.70
1:F:123:PHE:HB3	1:F:125:ILE:HD11	1.73	0.70
1:E:337:ASN:C	1:E:337:ASN:HD22	2.00	0.70
1:C:277:VAL:HB	1:C:311:ARG:NH1	2.08	0.69
1:B:374:SER:OG	1:B:376:GLU:HG2	1.91	0.69
1:F:157:TYR:HB3	1:F:158:PRO:HD3	1.75	0.69
1:E:374:SER:OG	1:E:376:GLU:HG2	1.91	0.69
1:F:257:HIS:HD2	1:F:260:ASP:OD2	1.76	0.69
1:F:368:MET:HE1	1:F:378:ILE:HG21	1.75	0.69
1:E:157:TYR:HB3	1:E:158:PRO:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:ASN:HB3	1:E:319:ASP:HB3	1.76	0.67
1:D:56:GLU:HG2	1:D:124:VAL:HG12	1.74	0.67
1:F:286:ALA:HA	1:F:290:ILE:HG13	1.76	0.67
1:D:174:LYS:O	1:D:178:GLU:HG3	1.94	0.67
1:F:233:THR:HG22	1:F:473:PHE:HB3	1.75	0.67
1:A:157:TYR:HB3	1:A:158:PRO:HD3	1.77	0.67
1:D:424:ARG:HD2	4:D:1835:HOH:O	1.94	0.67
1:E:372:MET:HE3	4:E:1169:HOH:O	1.95	0.66
1:B:250:ILE:HD13	1:B:262:PHE:HE1	1.60	0.66
1:C:17:SER:OG	1:C:90:HIS:HE1	1.79	0.66
1:C:291:TRP:CE3	1:C:299:ILE:HD11	2.31	0.66
1:C:478:LYS:HD2	1:C:481:GLN:HE22	1.61	0.66
1:E:62:LEU:HD22	1:E:66:LEU:HG	1.77	0.66
1:F:56:GLU:HG2	1:F:124:VAL:CG1	2.25	0.66
1:F:174:LYS:O	1:F:178:GLU:HG3	1.96	0.66
1:B:391:THR:HG23	1:B:393:ASP:N	2.07	0.65
1:A:156:TRP:CG	1:A:392:ARG:HG3	2.32	0.65
1:A:249:THR:HG21	1:C:25:GLN:HE21	1.60	0.65
1:B:32:LYS:HA	1:B:136:ASN:HD21	1.61	0.65
1:A:21:THR:HG22	1:A:95:VAL:HG11	1.78	0.65
1:D:233:THR:HG22	1:D:473:PHE:HB3	1.79	0.65
1:E:344:LEU:N	1:E:377:ASN:HD21	1.89	0.65
1:A:195:TYR:OH	1:A:201:GLN:NE2	2.30	0.65
1:A:291:TRP:CE3	1:A:299:ILE:HD11	2.32	0.65
1:A:368:MET:HE2	1:A:375:ILE:HD13	1.77	0.65
1:D:343:LEU:HD13	1:D:376:GLU:HG3	1.79	0.64
1:A:40:ARG:HD3	1:A:422:ASN:O	1.98	0.64
1:C:195:TYR:OH	1:C:201:GLN:NE2	2.30	0.64
1:D:339:LYS:HZ1	1:D:339:LYS:HA	1.62	0.64
1:D:249:THR:CG2	1:E:25:GLN:HE21	2.09	0.64
1:C:233:THR:HG22	1:C:473:PHE:HB3	1.79	0.64
1:C:259:LYS:HB2	1:C:259:LYS:NZ	2.12	0.64
1:E:29:ASN:N	1:E:29:ASN:HD22	1.95	0.64
1:B:119:VAL:HG21	1:B:125:ILE:CD1	2.26	0.64
1:C:114:ILE:HG12	1:C:144:LEU:HD13	1.80	0.64
1:F:391:THR:CG2	1:F:393:ASP:H	2.10	0.64
1:A:27:PRO:HG3	1:C:253:TRP:CD1	2.32	0.64
1:C:221:VAL:HA	1:C:224:LEU:HD23	1.78	0.63
1:C:21:THR:HG22	1:C:95:VAL:HG11	1.80	0.63
1:F:63:GLN:HE22	1:F:471:TYR:N	1.92	0.63
1:F:339:LYS:N	4:F:1790:HOH:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD22	1:A:371:LYS:HG3	1.80	0.63
1:A:374:SER:OG	1:A:376:GLU:HG2	1.97	0.63
1:B:306:ALA:N	1:B:307:PRO:HD3	2.13	0.63
1:C:32:LYS:HA	1:C:136:ASN:HD21	1.62	0.63
1:D:25:GLN:HE21	1:E:249:THR:CG2	2.10	0.63
1:E:369:LYS:O	1:E:372:MET:HE2	1.99	0.63
1:B:447:LYS:HG2	4:B:1537:HOH:O	1.99	0.63
1:E:155:SER:O	1:E:158:PRO:HD2	1.99	0.63
1:C:19:LYS:HA	1:C:22:HIS:CD2	2.34	0.63
1:D:157:TYR:HB3	1:D:158:PRO:HD3	1.81	0.62
1:E:40:ARG:HD3	1:E:422:ASN:O	1.98	0.62
1:B:195:TYR:OH	1:B:201:GLN:NE2	2.32	0.62
1:B:305:GLN:HB3	4:B:1625:HOH:O	1.99	0.62
1:C:23:TYR:CE2	1:C:97:ASN:HB2	2.33	0.62
1:C:304:THR:HG23	1:C:346:PRO:HB2	1.81	0.62
1:F:311:ARG:NH2	3:F:506:NMN:O2R	2.32	0.62
1:E:136:ASN:H	1:E:136:ASN:HD22	1.47	0.62
1:C:157:TYR:HB3	1:C:158:PRO:HD3	1.81	0.62
1:A:316:ASN:ND2	1:A:319:ASP:H	1.95	0.62
1:F:195:TYR:OH	1:F:201:GLN:NE2	2.33	0.62
1:A:240:TYR:HA	1:C:90:HIS:CD2	2.35	0.62
1:E:32:LYS:HB3	1:E:405:VAL:HB	1.81	0.62
1:B:344:LEU:N	1:B:377:ASN:HD21	1.96	0.61
1:D:33:VAL:H	1:D:136:ASN:ND2	1.98	0.61
1:B:169:LYS:HG2	1:B:482:LEU:HD11	1.82	0.61
1:A:90:HIS:CD2	1:C:240:TYR:HA	2.35	0.61
1:A:182:ASN:C	1:A:183:LEU:HD12	2.25	0.61
1:E:114:ILE:HG12	1:E:144:LEU:HD13	1.83	0.61
1:B:93:ASP:OD1	1:B:94:ASP:N	2.34	0.61
1:A:112:LEU:O	1:A:464:ASN:HA	2.01	0.60
1:B:114:ILE:HD13	1:B:136:ASN:HA	1.83	0.60
1:C:63:GLN:HE22	1:C:471:TYR:N	1.96	0.60
1:A:119:VAL:HG21	1:A:125:ILE:HD11	1.83	0.60
1:C:127:ARG:HH21	1:C:396:ASN:HD22	1.47	0.60
1:C:400:LYS:CD	1:C:425:SER:HB3	2.30	0.60
1:D:391:THR:HG22	1:D:393:ASP:N	2.04	0.60
1:B:172:LEU:HD21	1:B:361:LEU:HD11	1.84	0.60
1:A:259:LYS:HE3	1:A:294:ASP:HB3	1.83	0.60
1:C:102:ASN:O	1:C:106:GLU:HG3	2.01	0.60
1:D:299:ILE:HD12	1:D:308:LEU:HD22	1.84	0.60
1:B:114:ILE:HG12	1:B:144:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LYS:NZ	1:C:95:VAL:HG13	2.16	0.60
1:E:63:GLN:HE22	1:E:471:TYR:N	1.97	0.60
1:A:343:LEU:HD13	1:A:376:GLU:HG3	1.84	0.60
1:D:33:VAL:H	1:D:136:ASN:HD21	1.48	0.59
1:B:261:ALA:O	1:B:265:ILE:HG12	2.02	0.59
1:C:414:PHE:CD2	1:C:427:LYS:HG2	2.38	0.59
1:A:259:LYS:CE	1:A:294:ASP:HB3	2.32	0.59
1:B:431:SER:OG	1:B:433:HIS:HE1	1.86	0.59
1:A:177:LEU:HD13	1:A:183:LEU:HD11	1.84	0.59
1:D:391:THR:HG21	4:D:1501:HOH:O	2.03	0.59
1:F:54:TYR:N	4:F:1401:HOH:O	2.34	0.59
1:A:414:PHE:CD2	1:A:427:LYS:HG2	2.38	0.59
1:B:343:LEU:HA	1:B:377:ASN:HD21	1.67	0.59
1:B:343:LEU:HD13	1:B:376:GLU:HG3	1.83	0.59
1:A:177:LEU:HD13	1:A:183:LEU:CD1	2.33	0.59
1:D:17:SER:OG	1:D:90:HIS:HE1	1.85	0.59
1:B:316:ASN:ND2	1:B:319:ASP:H	1.98	0.58
1:E:343:LEU:HD11	1:E:376:GLU:HG3	1.84	0.58
1:B:9:PHE:N	4:B:1412:HOH:O	2.35	0.58
1:B:259:LYS:HZ1	1:B:294:ASP:HB3	1.69	0.58
1:D:326:GLU:HG2	1:D:330:LYS:HE3	1.85	0.58
1:D:343:LEU:CD1	1:D:376:GLU:HG3	2.33	0.58
1:B:60:TYR:O	1:B:158:PRO:HB2	2.03	0.58
1:E:33:VAL:H	1:E:136:ASN:HD21	1.50	0.58
1:D:88:LYS:HA	1:D:88:LYS:HE2	1.85	0.58
1:A:56:GLU:HG2	1:A:124:VAL:CG1	2.34	0.58
1:F:114:ILE:HG12	1:F:144:LEU:HD13	1.85	0.58
1:C:316:ASN:ND2	1:C:319:ASP:H	2.00	0.58
1:C:60:TYR:O	1:C:158:PRO:HB2	2.03	0.58
1:E:337:ASN:ND2	1:E:339:LYS:H	2.01	0.58
1:A:168:GLN:HG3	1:A:358:ILE:HD12	1.85	0.58
1:A:361:LEU:O	1:A:361:LEU:HD23	2.03	0.58
1:A:168:GLN:HG3	1:A:358:ILE:CD1	2.33	0.58
1:C:32:LYS:HD3	4:C:1394:HOH:O	2.03	0.58
1:F:234:LYS:HG3	1:F:474:ASP:OD2	2.04	0.57
1:D:270:SER:HA	1:D:302:ARG:NH2	2.19	0.57
1:C:259:LYS:HB2	1:C:259:LYS:HZ2	1.70	0.57
1:C:321:VAL:O	1:C:325:LEU:HG	2.05	0.57
1:B:323:LYS:HA	1:B:326:GLU:HG2	1.87	0.57
1:B:392:ARG:HB3	1:B:392:ARG:NH1	2.20	0.57
1:D:155:SER:O	1:D:158:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:PRO:HG3	1:F:206:ILE:CG2	2.35	0.57
1:A:155:SER:O	1:A:158:PRO:HD2	2.04	0.56
1:E:343:LEU:CD1	1:E:376:GLU:HG3	2.35	0.56
1:F:136:ASN:H	1:F:136:ASN:HD22	1.52	0.56
1:A:155:SER:C	1:A:158:PRO:HD2	2.31	0.56
1:B:304:THR:HG22	1:B:346:PRO:HB2	1.87	0.56
1:B:418:VAL:HG13	1:B:419:ALA:N	2.20	0.56
1:D:265:ILE:CD1	1:E:25:GLN:HB3	2.36	0.56
1:F:305:GLN:HG3	4:F:1307:HOH:O	2.05	0.56
1:E:97:ASN:ND2	1:E:100:GLY:H	2.04	0.56
1:C:293:GLU:HG3	1:C:331:LYS:NZ	2.21	0.56
1:E:114:ILE:CG1	1:E:144:LEU:HD13	2.36	0.56
1:B:158:PRO:HG3	1:B:206:ILE:CG2	2.35	0.56
1:C:155:SER:O	1:C:158:PRO:HD2	2.06	0.56
1:F:299:ILE:HD12	1:F:308:LEU:HD22	1.87	0.56
1:C:446:GLY:C	1:C:448:GLY:H	2.12	0.55
1:B:478:LYS:HA	1:B:481:GLN:HE21	1.71	0.55
1:F:97:ASN:ND2	1:F:100:GLY:H	2.05	0.55
1:D:285:ASN:OD1	1:D:289:LYS:HD2	2.07	0.55
1:D:360:THR:O	1:D:364:ILE:HG13	2.06	0.55
1:A:60:TYR:O	1:A:158:PRO:HB2	2.05	0.55
1:E:149:GLU:HG3	1:E:399:PHE:CG	2.42	0.55
1:F:236:PRO:HD2	4:F:994:HOH:O	2.05	0.55
1:A:233:THR:HG22	1:A:473:PHE:HB3	1.89	0.55
1:A:404:VAL:C	4:A:1330:HOH:O	2.50	0.55
1:B:17:SER:OG	1:B:90:HIS:HE1	1.90	0.55
1:C:155:SER:C	1:C:158:PRO:HD2	2.32	0.55
1:C:249:THR:CG2	1:C:265:ILE:HD11	2.36	0.55
1:F:17:SER:OG	1:F:90:HIS:HE1	1.90	0.55
1:F:364:ILE:O	1:F:368:MET:HG3	2.07	0.55
1:C:62:LEU:HD22	1:C:66:LEU:HG	1.89	0.55
1:A:300:VAL:HG12	1:A:347:TYR:OH	2.06	0.55
1:A:25:GLN:HE21	1:C:249:THR:CG2	2.17	0.54
1:E:19:LYS:HA	1:E:22:HIS:CD2	2.42	0.54
1:F:431:SER:OG	1:F:433:HIS:HE1	1.90	0.54
1:A:90:HIS:HD2	1:C:240:TYR:HA	1.71	0.54
1:B:392:ARG:HH11	1:B:392:ARG:CB	2.20	0.54
1:E:33:VAL:H	1:E:136:ASN:ND2	2.05	0.54
1:A:168:GLN:HG2	1:A:361:LEU:HD13	1.87	0.54
1:B:233:THR:HG22	1:B:473:PHE:HB3	1.88	0.54
1:C:259:LYS:HG2	4:C:1905:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:N	1:F:377:ASN:HD21	1.88	0.54
1:D:334:VAL:HG22	4:D:1743:HOH:O	2.06	0.54
1:F:368:MET:HE3	1:F:375:ILE:HD12	1.90	0.54
1:A:56:GLU:HG2	4:A:1130:HOH:O	2.06	0.54
1:A:391:THR:CG2	1:A:393:ASP:H	2.18	0.54
1:A:57:THR:N	4:A:1130:HOH:O	2.41	0.54
1:C:149:GLU:OE2	1:C:399:PHE:HB3	2.07	0.54
1:C:359:ASN:O	1:C:363:GLU:HG3	2.07	0.54
1:D:125:ILE:HD13	1:D:432:LEU:HD21	1.90	0.54
1:F:374:SER:OG	1:F:376:GLU:CG	2.53	0.54
1:B:112:LEU:O	1:B:464:ASN:HA	2.08	0.54
1:C:56:GLU:HG2	1:C:124:VAL:CG1	2.38	0.54
1:C:330:LYS:O	1:C:331:LYS:HD2	2.08	0.54
1:D:236:PRO:HD2	4:D:1061:HOH:O	2.06	0.54
1:B:391:THR:CG2	1:B:393:ASP:HB2	2.37	0.54
1:A:23:TYR:OH	1:A:24:LYS:HE2	2.08	0.54
1:B:472:SER:OG	1:B:475:GLU:HG3	2.08	0.54
1:C:435:THR:HB	1:C:436:PRO:HD2	1.90	0.54
1:E:174:LYS:O	1:E:178:GLU:HG3	2.08	0.54
1:D:399:PHE:O	1:D:400:LYS:HE3	2.08	0.53
1:D:361:LEU:HD23	1:D:361:LEU:O	2.08	0.53
1:E:114:ILE:HD11	1:E:144:LEU:HB3	1.88	0.53
1:F:391:THR:HG23	1:F:393:ASP:H	1.73	0.53
1:C:326:GLU:HG3	1:C:327:ILE:N	2.22	0.53
1:D:90:HIS:HD2	1:E:239:GLY:O	1.91	0.53
1:D:175:TYR:HB3	1:D:375:ILE:HG13	1.90	0.53
1:A:369:LYS:O	1:A:372:MET:HE2	2.08	0.53
1:B:300:VAL:HG12	1:B:347:TYR:OH	2.08	0.53
1:B:339:LYS:HA	1:B:339:LYS:HE2	1.90	0.53
1:C:286:ALA:N	4:C:1038:HOH:O	2.41	0.53
1:E:322:LEU:O	1:E:326:GLU:HG2	2.07	0.53
1:A:283:ILE:HD13	1:A:283:ILE:O	2.08	0.53
1:C:374:SER:OG	1:C:376:GLU:HG2	2.08	0.53
1:F:41:GLU:HG3	1:F:128:GLY:HA3	1.91	0.53
1:A:312:PRO:HG2	1:A:352:GLN:NE2	2.24	0.53
1:D:32:LYS:HA	1:D:136:ASN:HD21	1.73	0.53
1:D:136:ASN:HD22	1:D:136:ASN:H	1.56	0.52
1:B:343:LEU:HD12	1:B:377:ASN:ND2	2.25	0.52
1:D:233:THR:CG2	1:D:473:PHE:HB3	2.39	0.52
1:A:168:GLN:NE2	1:A:190:LEU:HD11	2.24	0.52
1:D:21:THR:HG22	1:D:95:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ILE:HD12	1:E:25:GLN:HB3	1.91	0.52
1:C:369:LYS:O	1:C:372:MET:HE2	2.07	0.52
1:B:21:THR:HG22	1:B:95:VAL:HG11	1.91	0.52
1:C:114:ILE:HD13	1:C:136:ASN:HA	1.91	0.52
1:A:240:TYR:HA	1:C:90:HIS:HD2	1.73	0.52
1:E:29:ASN:N	1:E:29:ASN:ND2	2.58	0.52
1:D:300:VAL:HG12	1:D:347:TYR:OH	2.10	0.52
1:F:450:LEU:O	1:F:452:GLU:N	2.36	0.52
1:A:13:LEU:HD21	1:A:83:ALA:HA	1.92	0.52
1:A:32:LYS:O	1:A:404:VAL:HG23	2.09	0.52
1:A:224:LEU:H	1:A:224:LEU:HD22	1.74	0.52
1:C:446:GLY:C	1:C:448:GLY:N	2.68	0.52
1:A:27:PRO:HG3	1:C:253:TRP:CG	2.46	0.51
1:A:221:VAL:HA	1:A:224:LEU:HD23	1.92	0.51
1:A:318:LEU:HD11	1:A:367:GLY:HA3	1.93	0.51
1:D:62:LEU:HD22	1:D:66:LEU:HG	1.92	0.51
1:E:114:ILE:HD13	1:E:136:ASN:HA	1.93	0.51
1:A:418:VAL:HG13	1:A:419:ALA:N	2.26	0.51
1:E:23:TYR:CE1	1:E:24:LYS:HG3	2.46	0.51
1:E:233:THR:HG22	1:E:473:PHE:HB3	1.91	0.51
1:F:226:LEU:HD23	1:F:226:LEU:C	2.35	0.51
1:E:325:LEU:HD11	1:E:368:MET:HE3	1.91	0.51
1:F:466:LYS:HD3	4:F:848:HOH:O	2.10	0.51
1:A:317:PRO:O	1:A:321:VAL:HG23	2.11	0.51
1:F:434:ARG:HD2	4:F:1060:HOH:O	2.11	0.51
1:C:23:TYR:CE1	1:C:24:LYS:HG3	2.46	0.51
1:C:266:VAL:HG23	4:C:1561:HOH:O	2.09	0.51
1:B:392:ARG:HB3	1:B:392:ARG:HH11	1.76	0.51
1:A:168:GLN:HG2	1:A:361:LEU:CD1	2.41	0.51
1:A:253:TRP:HZ2	1:A:264:HIS:HD1	1.59	0.51
1:C:418:VAL:HG13	1:C:419:ALA:N	2.26	0.51
1:E:29:ASN:HD22	1:E:29:ASN:H	1.59	0.51
1:F:400:LYS:CE	1:F:415:LYS:HD3	2.41	0.51
1:B:63:GLN:HE22	1:B:471:TYR:N	1.94	0.50
3:D:504:NMN:H5R1	4:D:1482:HOH:O	2.11	0.50
1:F:123:PHE:HB3	1:F:125:ILE:CD1	2.40	0.50
1:D:40:ARG:HD2	1:D:422:ASN:O	2.11	0.50
1:D:113:PRO:HA	1:D:464:ASN:ND2	2.21	0.50
1:A:172:LEU:HD13	1:A:189:LYS:HB2	1.92	0.50
1:A:245:ALA:HB1	1:A:249:THR:CG2	2.42	0.50
1:F:151:ILE:HG23	1:F:152:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ARG:HB2	1:B:351:ILE:CG2	2.41	0.50
1:C:300:VAL:HG12	1:C:347:TYR:OH	2.11	0.50
1:D:344:LEU:N	1:D:377:ASN:HD21	2.03	0.50
1:E:257:HIS:HD2	4:E:781:HOH:O	1.94	0.50
1:E:333:PRO:O	1:E:345:PRO:HG3	2.12	0.50
1:F:114:ILE:CG1	1:F:144:LEU:HD13	2.41	0.50
1:A:28:PRO:O	1:A:29:ASN:HB2	2.12	0.50
1:A:249:THR:CG2	1:C:25:GLN:HE21	2.23	0.50
1:B:114:ILE:CG1	1:B:144:LEU:HD13	2.42	0.50
1:C:226:LEU:C	1:C:226:LEU:HD23	2.36	0.50
1:F:102:ASN:O	1:F:106:GLU:HG3	2.12	0.50
1:B:97:ASN:ND2	1:B:100:GLY:H	2.10	0.50
1:C:258:GLU:OE2	1:C:281:TYR:HD1	1.94	0.50
1:E:337:ASN:C	1:E:337:ASN:ND2	2.70	0.50
1:F:400:LYS:HE2	1:F:415:LYS:HD3	1.94	0.50
1:B:361:LEU:O	1:B:365:VAL:HG22	2.12	0.50
1:C:202:GLU:O	1:C:206:ILE:HG13	2.11	0.50
1:C:293:GLU:HG3	1:C:331:LYS:HZ1	1.75	0.50
1:D:224:LEU:H	1:D:224:LEU:HD22	1.77	0.50
1:C:11:ILE:HG23	1:C:12:LEU:HD12	1.94	0.49
1:E:155:SER:C	1:E:158:PRO:HD2	2.36	0.49
1:F:68:LYS:HA	4:F:2060:HOH:O	2.12	0.49
1:C:120:PRO:O	1:C:123:PHE:HB2	2.12	0.49
1:C:284:TYR:C	1:C:286:ALA:H	2.20	0.49
1:E:335:THR:OG1	1:E:336:GLU:N	2.45	0.49
1:D:257:HIS:HD2	1:D:260:ASP:OD2	1.96	0.49
1:E:23:TYR:CE2	1:E:97:ASN:HB2	2.47	0.49
1:F:37:PHE:CZ	1:F:397:CYS:HB3	2.47	0.49
1:A:226:LEU:HD23	1:A:226:LEU:C	2.38	0.49
1:A:253:TRP:CD1	1:C:27:PRO:HG3	2.47	0.49
1:C:285:ASN:C	4:C:1038:HOH:O	2.56	0.49
1:A:444:GLU:O	1:A:447:LYS:HG3	2.13	0.49
1:A:264:HIS:NE2	1:A:268:GLN:NE2	2.60	0.49
1:C:33:VAL:H	1:C:136:ASN:ND2	2.11	0.49
1:B:226:LEU:C	1:B:226:LEU:HD23	2.38	0.49
1:E:136:ASN:H	1:E:136:ASN:ND2	2.10	0.49
1:B:323:LYS:O	1:B:327:ILE:HG12	2.12	0.49
1:E:60:TYR:O	1:E:158:PRO:HB2	2.13	0.49
1:E:360:THR:O	1:E:364:ILE:HG13	2.13	0.49
1:F:19:LYS:HA	1:F:22:HIS:CD2	2.48	0.49
1:F:63:GLN:NE2	1:F:471:TYR:H	1.97	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLN:HE22	1:D:471:TYR:N	2.02	0.49
1:D:253:TRP:CD2	1:E:27:PRO:HG3	2.48	0.49
1:F:32:LYS:HA	1:F:136:ASN:HD21	1.77	0.49
1:A:318:LEU:HG	1:A:364:ILE:HA	1.95	0.48
1:A:19:LYS:HA	1:A:22:HIS:CD2	2.47	0.48
1:F:40:ARG:HD2	1:F:422:ASN:O	2.13	0.48
1:A:432:LEU:HD11	1:A:440:PHE:HB3	1.96	0.48
1:C:34:TYR:HB3	1:C:403:TYR:HB3	1.95	0.48
1:C:114:ILE:CG1	1:C:144:LEU:HD13	2.43	0.48
1:D:90:HIS:CD2	1:E:240:TYR:HA	2.47	0.48
1:E:290:ILE:HD11	4:E:1426:HOH:O	2.12	0.48
1:A:97:ASN:ND2	1:A:100:GLY:H	2.12	0.48
1:A:413:VAL:HG11	1:C:252:ALA:HA	1.94	0.48
1:B:34:TYR:HB3	1:B:403:TYR:HB3	1.95	0.48
1:E:183:LEU:HD11	1:E:484:ILE:HG21	1.94	0.48
1:F:288:GLU:HG3	1:F:331:LYS:HE3	1.96	0.48
1:A:183:LEU:HD21	1:A:484:ILE:HG21	1.95	0.48
1:C:236:PRO:HD2	4:C:1302:HOH:O	2.13	0.48
1:C:472:SER:OG	1:C:475:GLU:HG3	2.14	0.48
1:E:63:GLN:NE2	1:E:471:TYR:H	2.04	0.48
1:F:21:THR:HG22	1:F:95:VAL:HG21	1.94	0.48
1:A:361:LEU:HD23	1:A:361:LEU:C	2.39	0.48
1:B:155:SER:O	1:B:158:PRO:HD2	2.14	0.48
1:B:351:ILE:HD13	1:B:351:ILE:C	2.37	0.48
1:D:339:LYS:HA	1:D:339:LYS:NZ	2.28	0.48
1:A:114:ILE:O	1:A:463:LYS:HA	2.13	0.48
1:C:452:GLU:HG3	4:E:1169:HOH:O	2.13	0.48
1:D:427:LYS:HE3	4:D:1275:HOH:O	2.13	0.48
1:E:17:SER:OG	1:E:90:HIS:HE1	1.96	0.48
1:E:34:TYR:HB3	1:E:403:TYR:HB3	1.95	0.48
1:A:17:SER:OG	1:A:90:HIS:HE1	1.97	0.47
1:A:54:TYR:O	1:A:127:ARG:CD	2.61	0.47
1:A:62:LEU:HD22	1:A:66:LEU:HG	1.95	0.47
1:B:228:LYS:HE3	1:B:228:LYS:HB2	1.66	0.47
1:C:375:ILE:C	1:C:377:ASN:H	2.22	0.47
1:D:55:GLU:HB2	4:D:1190:HOH:O	2.13	0.47
1:C:127:ARG:NH2	1:C:396:ASN:HD22	2.11	0.47
1:C:311:ARG:HH21	3:C:503:NMN:H2RC	1.78	0.47
1:D:450:LEU:HB2	1:D:452:GLU:HG2	1.95	0.47
1:F:368:MET:HE1	1:F:378:ILE:CG2	2.42	0.47
1:C:114:ILE:O	1:C:463:LYS:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:CD1	1:C:238:PRO:HD2	2.42	0.47
1:F:136:ASN:H	1:F:136:ASN:ND2	2.12	0.47
1:C:55:GLU:O	1:C:56:GLU:HB2	2.13	0.47
1:D:80:ILE:HD13	1:D:102:ASN:ND2	2.29	0.47
1:E:311:ARG:NH1	3:E:505:NMN:O2R	2.45	0.47
1:B:351:ILE:HG23	1:B:351:ILE:O	2.13	0.47
1:D:56:GLU:CG	1:D:124:VAL:HG12	2.43	0.47
1:D:77:LYS:HA	1:D:77:LYS:HD2	1.72	0.47
1:A:312:PRO:HG2	1:A:352:GLN:HE22	1.79	0.47
1:B:478:LYS:HG3	1:B:481:GLN:NE2	2.28	0.47
1:D:60:TYR:O	1:D:158:PRO:HB2	2.15	0.47
1:A:32:LYS:HB3	1:A:405:VAL:HB	1.97	0.47
1:A:339:LYS:HB3	4:A:1129:HOH:O	2.13	0.47
1:C:224:LEU:H	1:C:224:LEU:HD22	1.79	0.47
1:C:266:VAL:O	1:C:302:ARG:NH2	2.47	0.47
1:B:120:PRO:HB2	1:B:123:PHE:CD1	2.50	0.47
1:B:250:ILE:HD13	1:B:262:PHE:CE1	2.44	0.47
1:C:78:GLU:CD	1:C:78:GLU:H	2.23	0.47
1:A:344:LEU:HG	1:A:377:ASN:ND2	2.30	0.47
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.49	0.47
1:B:392:ARG:NE	4:B:812:HOH:O	2.36	0.47
1:D:221:VAL:O	1:D:224:LEU:HD23	2.14	0.47
1:E:120:PRO:O	1:E:123:PHE:HB2	2.15	0.47
1:F:391:THR:HG22	1:F:393:ASP:H	1.77	0.47
1:A:158:PRO:HG3	1:A:206:ILE:CG2	2.45	0.46
1:C:277:VAL:HG13	1:C:277:VAL:O	2.14	0.46
1:D:158:PRO:HG3	1:D:206:ILE:CG2	2.45	0.46
1:F:155:SER:C	1:F:158:PRO:HD2	2.40	0.46
1:F:447:LYS:HE2	4:F:1479:HOH:O	2.15	0.46
1:A:291:TRP:HE3	1:A:299:ILE:HD11	1.77	0.46
1:B:62:LEU:HD22	1:B:66:LEU:HG	1.97	0.46
1:B:418:VAL:HG13	1:B:419:ALA:H	1.79	0.46
1:B:236:PRO:HD2	4:B:863:HOH:O	2.13	0.46
1:E:119:VAL:HG21	1:E:125:ILE:CD1	2.32	0.46
1:E:431:SER:OG	1:E:433:HIS:HE1	1.98	0.46
1:A:31:SER:HB2	1:A:139:PRO:HB3	1.96	0.46
1:A:146:ASN:ND2	1:C:246:GLU:OE2	2.40	0.46
1:E:316:ASN:HD22	1:E:319:ASP:N	2.02	0.46
1:F:414:PHE:CD2	1:F:427:LYS:HE2	2.51	0.46
1:A:320:THR:O	1:A:324:VAL:HG23	2.16	0.46
1:B:155:SER:C	1:B:158:PRO:HD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HD13	1:C:189:LYS:HB2	1.97	0.46
1:C:439:ASN:OD1	1:C:440:PHE:N	2.43	0.46
1:D:97:ASN:ND2	1:D:100:GLY:H	2.12	0.46
1:F:418:VAL:HG13	1:F:419:ALA:N	2.29	0.46
1:F:443:LEU:HD12	1:F:448:GLY:HA2	1.98	0.46
1:F:444:GLU:O	1:F:447:LYS:HG3	2.16	0.46
1:C:12:LEU:HD23	1:C:96:PHE:HZ	1.81	0.46
1:C:318:LEU:HD13	1:C:318:LEU:C	2.40	0.46
1:F:368:MET:HE3	1:F:375:ILE:CD1	2.45	0.46
1:A:119:VAL:HG21	1:A:125:ILE:CD1	2.44	0.46
1:A:188:TYR:HA	4:A:1001:HOH:O	2.16	0.46
1:A:351:ILE:HG23	1:A:351:ILE:O	2.15	0.46
1:B:32:LYS:HB3	1:B:405:VAL:HB	1.97	0.46
1:C:172:LEU:HD13	1:C:189:LYS:CB	2.46	0.46
1:B:76:THR:O	1:B:80:ILE:HG13	2.16	0.46
1:F:450:LEU:HB2	1:F:452:GLU:HG3	1.96	0.46
1:A:56:GLU:HG2	1:A:124:VAL:HG12	1.98	0.46
1:A:334:VAL:HG22	1:A:344:LEU:HD23	1.97	0.46
1:C:9:PHE:N	4:C:2039:HOH:O	2.48	0.46
1:D:302:ARG:HD3	1:D:306:ALA:O	2.15	0.46
1:E:262:PHE:CD2	1:E:290:ILE:HG21	2.50	0.46
1:F:375:ILE:HG22	1:F:375:ILE:O	2.16	0.46
1:C:366:GLU:HG3	1:C:370:GLN:HE21	1.81	0.45
1:C:431:SER:OG	1:C:433:HIS:HE1	1.98	0.45
1:D:239:GLY:O	1:E:90:HIS:HD2	1.99	0.45
1:E:337:ASN:HD22	1:E:339:LYS:H	1.64	0.45
1:A:119:VAL:CG2	1:A:120:PRO:HD2	2.46	0.45
1:B:291:TRP:HE3	1:B:299:ILE:HD11	1.82	0.45
1:C:318:LEU:HD23	1:C:364:ILE:HA	1.97	0.45
1:A:233:THR:CG2	1:A:473:PHE:HB3	2.46	0.45
1:C:194:GLY:N	1:C:383:GLY:HA2	2.31	0.45
1:D:9:PHE:N	4:D:1096:HOH:O	2.50	0.45
1:D:259:LYS:HB3	4:D:2028:HOH:O	2.16	0.45
1:E:13:LEU:HD11	1:E:82:GLU:OE2	2.17	0.45
1:F:155:SER:O	1:F:158:PRO:HD2	2.17	0.45
1:A:149:GLU:OE2	1:A:399:PHE:HB3	2.15	0.45
1:A:333:PRO:O	1:A:345:PRO:HG3	2.16	0.45
1:A:119:VAL:HG23	1:A:120:PRO:HD2	1.98	0.45
1:C:325:LEU:HD11	1:C:368:MET:HE3	1.98	0.45
1:B:300:VAL:HG12	1:B:347:TYR:CZ	2.52	0.45
1:C:56:GLU:HG2	1:C:124:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:HIS:CE1	1:C:277:VAL:HG21	2.51	0.45
1:F:54:TYR:CE1	1:F:394:LEU:HD11	2.52	0.45
1:A:253:TRP:CG	1:C:27:PRO:HG3	2.52	0.45
1:D:155:SER:C	1:D:158:PRO:HD2	2.41	0.45
1:D:467:VAL:HG11	4:D:1532:HOH:O	2.16	0.45
1:F:33:VAL:H	1:F:136:ASN:HD21	1.65	0.45
1:A:23:TYR:CE2	1:A:97:ASN:HB2	2.52	0.45
1:A:183:LEU:HD12	1:A:183:LEU:N	2.31	0.45
1:A:221:VAL:HG12	4:A:1786:HOH:O	2.17	0.45
1:A:288:GLU:OE2	1:E:436:PRO:HD2	2.17	0.45
1:C:33:VAL:H	1:C:136:ASN:HD21	1.64	0.45
1:C:437:ALA:HB3	1:E:336:GLU:CD	2.41	0.45
1:D:112:LEU:O	1:D:464:ASN:HA	2.17	0.45
1:F:114:ILE:HD13	1:F:136:ASN:HA	1.97	0.45
1:F:124:VAL:C	1:F:125:ILE:HD12	2.41	0.45
1:F:484:ILE:HG13	4:F:1506:HOH:O	2.17	0.45
1:A:179:THR:HG22	1:A:341:TYR:CE2	2.52	0.45
1:C:171:ILE:HG23	1:C:362:GLN:NE2	2.32	0.45
1:C:174:LYS:O	1:C:178:GLU:HG3	2.17	0.45
1:C:343:LEU:HA	1:C:377:ASN:HD21	1.82	0.45
1:C:409:LEU:C	1:C:409:LEU:HD13	2.42	0.45
1:D:24:LYS:O	1:E:264:HIS:HE1	1.98	0.45
1:D:300:VAL:HA	1:D:347:TYR:CZ	2.51	0.45
1:D:431:SER:OG	1:D:433:HIS:HE1	2.00	0.45
1:F:316:ASN:HD22	1:F:319:ASP:N	2.04	0.45
1:A:262:PHE:O	1:A:266:VAL:HG13	2.17	0.44
1:B:112:LEU:HA	1:B:113:PRO:HD3	1.82	0.44
1:C:168:GLN:HG2	1:C:358:ILE:HD12	1.99	0.44
1:D:375:ILE:HG22	1:D:375:ILE:O	2.17	0.44
1:E:228:LYS:HB2	4:E:2059:HOH:O	2.17	0.44
1:D:144:LEU:HD22	4:D:1329:HOH:O	2.16	0.44
1:D:302:ARG:HB2	1:D:347:TYR:HB2	1.99	0.44
1:C:445:GLU:HA	4:C:849:HOH:O	2.17	0.44
1:A:364:ILE:HG21	1:A:380:PHE:HE2	1.82	0.44
1:B:237:VAL:HA	1:B:238:PRO:HD3	1.81	0.44
1:E:324:VAL:O	1:E:328:LEU:HG	2.18	0.44
1:E:414:PHE:CE2	1:E:427:LYS:HE3	2.53	0.44
1:A:311:ARG:HH22	2:A:601:PO4:P	2.40	0.44
1:B:191:HIS:CD2	1:B:193:PHE:HE2	2.36	0.44
1:C:224:LEU:HD22	1:C:224:LEU:N	2.32	0.44
1:D:224:LEU:HD12	1:D:238:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:SER:OG	1:D:400:LYS:NZ	2.51	0.44
1:F:361:LEU:HD13	1:F:361:LEU:C	2.43	0.44
1:A:82:GLU:O	1:A:86:VAL:HG23	2.17	0.44
1:B:323:LYS:O	1:B:326:GLU:HG2	2.18	0.44
1:B:324:VAL:O	1:B:328:LEU:HG	2.18	0.44
1:C:291:TRP:HE3	1:C:299:ILE:HD11	1.79	0.44
1:C:404:VAL:HG12	1:C:405:VAL:N	2.33	0.44
1:E:226:LEU:C	1:E:226:LEU:HD23	2.42	0.44
1:F:378:ILE:CG1	1:F:379:ALA:N	2.81	0.44
1:A:219:ASP:CG	1:C:17:SER:HB2	2.42	0.44
1:A:357:ASP:OD1	1:A:357:ASP:C	2.61	0.44
1:A:410:GLY:HA2	4:A:1330:HOH:O	2.16	0.44
1:C:24:LYS:HZ3	1:C:95:VAL:HG13	1.83	0.44
1:C:437:ALA:HB3	1:E:336:GLU:OE2	2.17	0.44
1:E:370:GLN:CD	4:E:1418:HOH:O	2.59	0.44
1:C:172:LEU:HD21	1:C:361:LEU:HD21	1.98	0.44
1:D:32:LYS:HB3	1:D:405:VAL:HB	1.99	0.44
1:E:375:ILE:O	1:E:375:ILE:HG22	2.17	0.44
1:A:370:GLN:C	1:A:372:MET:H	2.24	0.44
1:A:376:GLU:HG2	1:A:376:GLU:H	1.62	0.44
1:A:478:LYS:HA	1:A:481:GLN:HE21	1.82	0.44
1:B:114:ILE:HD11	1:B:144:LEU:HB3	2.01	0.43
1:B:233:THR:CG2	1:B:473:PHE:HB3	2.48	0.43
1:D:229:LYS:HD3	1:D:230:TYR:CE1	2.53	0.43
1:C:177:LEU:HD13	1:C:183:LEU:CD1	2.48	0.43
1:B:378:ILE:HG12	1:B:379:ALA:N	2.33	0.43
1:B:433:HIS:HD2	1:B:454:GLY:O	2.00	0.43
1:C:420:ASP:OD1	1:C:422:ASN:HB2	2.18	0.43
1:C:443:LEU:HD12	1:C:448:GLY:HA2	2.01	0.43
1:D:136:ASN:ND2	1:D:136:ASN:H	2.17	0.43
1:D:238:PRO:HA	4:D:1452:HOH:O	2.17	0.43
1:D:326:GLU:O	1:D:330:LYS:HG3	2.17	0.43
1:F:125:ILE:HD12	1:F:125:ILE:N	2.33	0.43
1:A:283:ILE:HD13	1:A:287:CYS:SG	2.59	0.43
1:F:9:PHE:N	4:F:1116:HOH:O	2.52	0.43
1:F:40:ARG:NH2	4:F:841:HOH:O	2.49	0.43
1:F:183:LEU:HD11	1:F:484:ILE:CG2	2.46	0.43
1:B:333:PRO:O	1:B:345:PRO:HG3	2.18	0.43
1:C:127:ARG:NH2	1:C:396:ASN:ND2	2.66	0.43
1:D:105:LEU:O	1:D:109:ASP:HA	2.19	0.43
1:D:282:ASP:HB3	1:D:285:ASN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:GLU:O	1:D:452:GLU:C	2.62	0.43
1:E:357:ASP:OD1	1:E:357:ASP:C	2.61	0.43
1:A:247:HIS:CE1	1:A:277:VAL:HG21	2.54	0.43
1:A:344:LEU:HG	1:A:377:ASN:HD22	1.82	0.43
1:C:264:HIS:CE1	1:C:268:GLN:HG3	2.54	0.43
1:D:63:GLN:NE2	1:D:471:TYR:H	2.02	0.43
1:E:149:GLU:HG3	1:E:399:PHE:CD2	2.53	0.43
1:E:296:ARG:HG2	4:E:1948:HOH:O	2.18	0.43
1:F:60:TYR:O	1:F:158:PRO:HB2	2.18	0.43
1:B:182:ASN:HB2	1:B:184:ASP:OD1	2.19	0.43
1:C:191:HIS:CD2	1:C:193:PHE:HE2	2.37	0.43
1:C:246:GLU:O	1:C:249:THR:HB	2.19	0.43
1:D:351:ILE:O	1:D:351:ILE:HG23	2.19	0.43
1:D:391:THR:CG2	1:D:392:ARG:N	2.81	0.43
1:F:391:THR:HG21	4:F:1253:HOH:O	2.17	0.43
1:A:304:THR:HG23	1:A:346:PRO:HB2	2.00	0.43
1:B:391:THR:HG21	1:B:393:ASP:HB2	2.00	0.43
1:C:311:ARG:HH22	2:C:605:PO4:P	2.42	0.43
1:C:360:THR:O	1:C:364:ILE:HG13	2.19	0.43
1:D:19:LYS:HA	1:D:22:HIS:CD2	2.54	0.43
1:A:114:ILE:CG2	1:A:115:GLU:N	2.82	0.42
1:A:134:VAL:HG11	1:A:148:ILE:HD11	2.01	0.42
1:B:183:LEU:HD11	1:B:484:ILE:HD12	2.01	0.42
1:B:188:TYR:HA	4:B:1681:HOH:O	2.19	0.42
1:C:288:GLU:N	4:C:1038:HOH:O	2.51	0.42
1:C:322:LEU:CD2	1:C:371:LYS:HG3	2.44	0.42
1:F:33:VAL:H	1:F:136:ASN:ND2	2.17	0.42
1:A:73:LYS:HE3	1:A:76:THR:HG22	2.00	0.42
1:B:113:PRO:HD2	1:B:144:LEU:HD12	2.01	0.42
1:B:257:HIS:HD2	1:B:260:ASP:OD1	2.03	0.42
1:D:73:LYS:HE2	1:D:76:THR:HG22	2.02	0.42
1:D:198:VAL:HG13	1:D:200:SER:H	1.84	0.42
1:A:172:LEU:HD13	1:A:189:LYS:CB	2.48	0.42
1:B:77:LYS:CD	1:B:105:LEU:HD21	2.43	0.42
1:B:392:ARG:NH2	4:B:812:HOH:O	2.46	0.42
1:C:158:PRO:HG3	1:C:206:ILE:CG2	2.49	0.42
1:D:27:PRO:HG3	1:E:253:TRP:CG	2.54	0.42
1:D:450:LEU:C	1:D:452:GLU:H	2.28	0.42
1:A:451:GLU:N	4:A:1898:HOH:O	2.53	0.42
1:C:351:ILE:HG23	1:C:351:ILE:O	2.19	0.42
1:E:337:ASN:HB2	4:E:1717:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:ARG:HB2	1:F:347:TYR:HB2	2.01	0.42
1:B:326:GLU:HG3	1:B:327:ILE:N	2.34	0.42
1:C:358:ILE:HG23	1:C:359:ASN:N	2.35	0.42
1:C:409:LEU:HD13	1:C:410:GLY:N	2.35	0.42
1:F:226:LEU:HD23	1:F:226:LEU:O	2.20	0.42
1:F:116:ILE:HB	1:F:462:PHE:HB3	2.01	0.42
1:A:245:ALA:HB1	1:A:249:THR:HG22	2.02	0.42
1:A:406:THR:O	1:A:407:ASN:HB2	2.19	0.42
1:B:305:GLN:HB3	1:B:305:GLN:HE21	1.48	0.42
1:B:351:ILE:HD13	1:B:352:GLN:N	2.35	0.42
1:B:430:LEU:HD22	1:B:444:GLU:HG2	2.00	0.42
1:C:378:ILE:HG12	1:C:379:ALA:N	2.35	0.42
1:D:224:LEU:HD22	1:D:224:LEU:N	2.35	0.42
1:A:284:TYR:CZ	1:A:323:LYS:HD3	2.55	0.42
1:B:191:HIS:CD2	1:B:193:PHE:CE2	3.08	0.42
1:B:444:GLU:O	1:B:447:LYS:HG3	2.20	0.42
1:C:138:ASP:HA	1:C:139:PRO:HD2	1.87	0.42
1:C:450:LEU:O	1:C:452:GLU:N	2.48	0.42
1:E:170:LYS:HG2	1:E:482:LEU:HD22	2.02	0.42
1:F:274:VAL:O	1:F:274:VAL:HG13	2.18	0.42
1:F:333:PRO:O	1:F:345:PRO:HG3	2.19	0.42
1:A:283:ILE:HD12	1:A:324:VAL:CG2	2.50	0.41
1:D:226:LEU:HD23	1:D:226:LEU:C	2.45	0.41
1:F:351:ILE:O	1:F:351:ILE:HG23	2.20	0.41
1:A:202:GLU:HG2	1:C:200:SER:HB2	2.02	0.41
1:B:325:LEU:HD11	1:B:368:MET:HE3	2.02	0.41
1:C:434:ARG:HD2	1:C:438:GLY:HA2	2.02	0.41
1:A:176:LEU:HD23	1:A:183:LEU:HA	2.03	0.41
1:B:21:THR:HG22	1:B:95:VAL:CG1	2.49	0.41
1:C:375:ILE:C	1:C:377:ASN:N	2.74	0.41
1:D:316:ASN:HD22	1:D:319:ASP:N	1.98	0.41
1:E:11:ILE:HG23	1:E:12:LEU:HD12	2.01	0.41
1:B:291:TRP:CE3	1:B:299:ILE:HD11	2.55	0.41
1:C:194:GLY:HA2	4:C:977:HOH:O	2.20	0.41
1:E:469:LYS:HE3	1:E:471:TYR:CE2	2.55	0.41
1:B:369:LYS:O	1:B:372:MET:HE2	2.21	0.41
1:D:197:GLY:HA2	1:E:392:ARG:CD	2.50	0.41
1:D:311:ARG:HH22	2:D:607:PO4:P	2.43	0.41
1:E:423:LYS:HE3	4:E:1606:HOH:O	2.21	0.41
1:B:285:ASN:O	1:B:289:LYS:HB3	2.19	0.41
1:C:348:LEU:O	1:C:349:ARG:NH1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:THR:OG1	1:E:464:ASN:ND2	2.50	0.41
1:A:361:LEU:C	1:A:361:LEU:CD2	2.93	0.41
1:B:259:LYS:NZ	1:B:259:LYS:CB	2.80	0.41
1:C:288:GLU:OE2	1:F:436:PRO:HD2	2.21	0.41
1:F:105:LEU:O	1:F:109:ASP:HA	2.20	0.41
1:A:168:GLN:CD	1:A:190:LEU:HD11	2.46	0.41
1:A:224:LEU:HD22	1:A:224:LEU:N	2.35	0.41
1:A:316:ASN:HB3	1:A:319:ASP:HB2	2.02	0.41
1:A:391:THR:HG23	1:A:392:ARG:N	2.35	0.41
1:B:178:GLU:OE1	1:B:369:LYS:HE3	2.21	0.41
1:B:427:LYS:O	1:B:444:GLU:HB3	2.20	0.41
1:C:266:VAL:HB	1:C:302:ARG:HH21	1.85	0.41
1:D:262:PHE:O	1:D:266:VAL:HG22	2.20	0.41
1:D:312:PRO:HD2	1:D:351:ILE:O	2.21	0.41
1:E:259:LYS:HD2	1:E:294:ASP:HB3	2.02	0.41
1:F:303:SER:OG	1:F:305:GLN:NE2	2.54	0.41
1:A:127:ARG:NH2	1:A:396:ASN:HD22	2.19	0.41
1:B:78:GLU:CD	1:B:78:GLU:H	2.29	0.41
1:B:156:TRP:CG	1:B:392:ARG:HG3	2.56	0.41
1:F:28:PRO:HG3	4:F:1730:HOH:O	2.21	0.41
1:A:54:TYR:N	4:A:1619:HOH:O	2.54	0.40
1:A:237:VAL:HA	1:A:238:PRO:HD3	1.79	0.40
1:C:273:PRO:HG3	1:C:306:ALA:HA	2.03	0.40
1:C:284:TYR:CE2	1:C:323:LYS:HD3	2.56	0.40
1:C:362:GLN:O	1:C:365:VAL:HG22	2.21	0.40
1:C:404:VAL:O	1:C:410:GLY:HA2	2.21	0.40
1:D:357:ASP:C	1:D:357:ASP:OD1	2.64	0.40
1:F:114:ILE:O	1:F:463:LYS:HA	2.21	0.40
1:A:75:VAL:HB	1:A:110:GLY:HA2	2.03	0.40
1:A:143:TRP:CD1	1:A:143:TRP:H	2.38	0.40
1:B:262:PHE:CD2	1:B:291:TRP:CZ2	3.09	0.40
1:C:120:PRO:HB2	1:C:123:PHE:CD1	2.56	0.40
1:C:324:VAL:O	1:C:328:LEU:HG	2.21	0.40
1:A:249:THR:HG21	1:C:25:GLN:HE22	1.79	0.40
1:A:289:LYS:O	1:A:293:GLU:HB2	2.22	0.40
1:B:306:ALA:N	1:B:307:PRO:CD	2.82	0.40
1:C:198:VAL:CG1	1:C:199:SER:N	2.84	0.40
1:C:259:LYS:NZ	1:C:259:LYS:CB	2.84	0.40
1:D:236:PRO:HB3	1:E:89:GLU:HG3	2.04	0.40
1:A:62:LEU:O	1:A:66:LEU:HG	2.22	0.40
1:B:346:PRO:N	4:B:2001:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLU:HG3	1:B:370:GLN:HE21	1.86	0.40
1:A:350:VAL:HG12	1:A:351:ILE:N	2.36	0.40
1:A:453:TYR:CE2	1:F:372:MET:HE2	2.56	0.40
1:C:414:PHE:CD1	1:C:414:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/491 (93%)	424 (93%)	30 (7%)	1 (0%)	43	51
1	B	460/491 (94%)	430 (94%)	29 (6%)	1 (0%)	43	51
1	C	455/491 (93%)	425 (93%)	26 (6%)	4 (1%)	14	14
1	D	460/491 (94%)	444 (96%)	15 (3%)	1 (0%)	43	51
1	E	460/491 (94%)	442 (96%)	16 (4%)	2 (0%)	30	34
1	F	457/491 (93%)	438 (96%)	18 (4%)	1 (0%)	43	51
All	All	2747/2946 (93%)	2603 (95%)	134 (5%)	10 (0%)	30	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	483	ASN
1	D	454	GLY
1	F	451	GLU
1	C	56	GLU
1	E	451	GLU
1	B	97	ASN
1	C	451	GLU
1	E	454	GLY

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Mol	Chain	Res	Type
1	A	451	GLU
1	C	40	ARG

5.3.2 Protein sidechains (i)

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	405/430 (94%)	390 (96%)	15 (4%)	30	41
1	B	408/430 (95%)	394 (97%)	14 (3%)	32	44
1	C	405/430 (94%)	396 (98%)	9 (2%)	45	61
1	D	408/430 (95%)	391 (96%)	17 (4%)	26	36
1	E	408/430 (95%)	393 (96%)	15 (4%)	30	41
1	F	407/430 (95%)	393 (97%)	14 (3%)	32	44
All	All	2441/2580 (95%)	2357 (97%)	84 (3%)	32	44

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	62	LEU
1	A	94	ASP
1	A	144	LEU
1	A	168	GLN
1	A	190	LEU
1	A	201	GLN
1	A	219	ASP
1	A	249	THR
1	A	283	ILE
1	A	318	LEU
1	A	335	THR
1	A	370	GLN
1	A	391	THR
1	A	398	SER
1	B	18	TYR

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Mol	Chain	Res	Type
1	B	32	LYS
1	B	62	LEU
1	B	77	LYS
1	B	144	LEU
1	B	190	LEU
1	B	219	ASP
1	B	249	THR
1	B	259	LYS
1	B	305	GLN
1	B	318	LEU
1	B	351	ILE
1	B	391	THR
1	B	483	ASN
1	C	18	TYR
1	C	62	LEU
1	C	144	LEU
1	C	198	VAL
1	C	219	ASP
1	C	249	THR
1	C	259	LYS
1	C	289	LYS
1	C	386	LEU
1	D	18	TYR
1	D	62	LEU
1	D	88	LYS
1	D	114	ILE
1	D	144	LEU
1	D	183	LEU
1	D	186	LEU
1	D	190	LEU
1	D	198	VAL
1	D	219	ASP
1	D	249	THR
1	D	318	LEU
1	D	339	LYS
1	D	391	THR
1	D	400	LYS
1	D	467	VAL
1	D	484	ILE
1	E	18	TYR
1	E	29	ASN
1	E	62	LEU

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Mol	Chain	Res	Type
1	E	102	ASN
1	E	136	ASN
1	E	144	LEU
1	E	186	LEU
1	E	219	ASP
1	E	249	THR
1	E	289	LYS
1	E	310	ILE
1	E	318	LEU
1	E	337	ASN
1	E	386	LEU
1	E	409	LEU
1	F	18	TYR
1	F	62	LEU
1	F	136	ASN
1	F	144	LEU
1	F	190	LEU
1	F	219	ASP
1	F	290	ILE
1	F	318	LEU
1	F	376	GLU
1	F	389	LYS
1	F	391	THR
1	F	394	LEU
1	F	404	VAL
1	F	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	25	GLN
1	A	63	GLN
1	A	90	HIS
1	A	97	ASN
1	A	102	ASN
1	A	136	ASN
1	A	168	GLN
1	A	201	GLN
1	A	211	HIS
1	A	268	GLN
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	362	GLN
1	A	377	ASN
1	A	396	ASN
1	A	433	HIS
1	A	464	ASN
1	A	479	ASN
1	A	481	GLN
1	B	63	GLN
1	B	90	HIS
1	B	92	GLN
1	B	97	ASN
1	B	102	ASN
1	B	136	ASN
1	B	164	ASN
1	B	201	GLN
1	B	257	HIS
1	B	305	GLN
1	B	316	ASN
1	B	337	ASN
1	B	352	GLN
1	B	362	GLN
1	B	370	GLN
1	B	377	ASN
1	B	396	ASN
1	B	407	ASN
1	B	412	ASN
1	B	433	HIS
1	B	459	HIS
1	B	464	ASN
1	B	479	ASN
1	B	481	GLN
1	C	22	HIS
1	C	25	GLN
1	C	29	ASN
1	C	63	GLN
1	C	81	GLN
1	C	90	HIS
1	C	97	ASN
1	C	136	ASN
1	C	201	GLN
1	C	264	HIS

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Mol	Chain	Res	Type
1	C	285	ASN
1	C	316	ASN
1	C	362	GLN
1	C	370	GLN
1	C	377	ASN
1	C	396	ASN
1	C	407	ASN
1	C	433	HIS
1	C	464	ASN
1	C	479	ASN
1	C	481	GLN
1	C	483	ASN
1	D	25	GLN
1	D	29	ASN
1	D	63	GLN
1	D	90	HIS
1	D	97	ASN
1	D	102	ASN
1	D	136	ASN
1	D	146	ASN
1	D	257	HIS
1	D	264	HIS
1	D	268	GLN
1	D	316	ASN
1	D	377	ASN
1	D	433	HIS
1	D	455	GLN
1	D	464	ASN
1	D	479	ASN
1	E	22	HIS
1	E	25	GLN
1	E	29	ASN
1	E	63	GLN
1	E	90	HIS
1	E	97	ASN
1	E	102	ASN
1	E	111	HIS
1	E	136	ASN
1	E	146	ASN
1	E	201	GLN
1	E	264	HIS
1	E	285	ASN

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Mol	Chain	Res	Type
1	E	316	ASN
1	E	337	ASN
1	E	352	GLN
1	E	362	GLN
1	E	370	GLN
1	E	377	ASN
1	E	433	HIS
1	E	464	ASN
1	E	479	ASN
1	F	22	HIS
1	F	25	GLN
1	F	29	ASN
1	F	63	GLN
1	F	90	HIS
1	F	97	ASN
1	F	136	ASN
1	F	201	GLN
1	F	257	HIS
1	F	264	HIS
1	F	285	ASN
1	F	305	GLN
1	F	316	ASN
1	F	362	GLN
1	F	377	ASN
1	F	396	ASN
1	F	407	ASN
1	F	433	HIS
1	F	439	ASN
1	F	459	HIS
1	F	464	ASN
1	F	479	ASN
1	F	481	GLN

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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	PO4	C	602	-	4,4,4	1.81	2 (50%)	6,6,6	0.45	0
3	NMN	A	501	-	21,23,23	4.04	11 (52%)	27,34,34	3.45	12 (44%)
2	PO4	E	608	-	4,4,4	1.60	0	6,6,6	0.46	0
3	NMN	C	503	-	21,23,23	4.06	11 (52%)	27,34,34	3.32	11 (40%)
3	NMN	F	506	-	21,23,23	3.99	11 (52%)	27,34,34	3.49	12 (44%)
2	PO4	F	611	-	4,4,4	1.58	0	6,6,6	0.48	0
2	PO4	C	605	-	4,4,4	1.83	2 (50%)	6,6,6	0.45	0
2	PO4	E	609	-	4,4,4	1.73	2 (50%)	6,6,6	0.43	0
2	PO4	A	606	-	4,4,4	1.70	0	6,6,6	0.44	0
3	NMN	D	504	-	21,23,23	3.95	11 (52%)	27,34,34	3.37	10 (37%)
2	PO4	A	601	-	4,4,4	1.57	0	6,6,6	0.42	0
3	NMN	B	502	-	21,23,23	4.02	11 (52%)	27,34,34	3.37	12 (44%)
2	PO4	D	610	-	4,4,4	1.84	3 (75%)	6,6,6	0.46	0
2	PO4	B	603	-	4,4,4	1.73	1 (25%)	6,6,6	0.46	0
2	PO4	F	612	-	4,4,4	1.80	2 (50%)	6,6,6	0.47	0
3	NMN	E	505	-	21,23,23	3.97	11 (52%)	27,34,34	3.40	12 (44%)
2	PO4	D	607	-	4,4,4	1.84	2 (50%)	6,6,6	0.43	0
2	PO4	B	604	-	4,4,4	1.72	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NMN	A	501	-	-	7/14/30/30	0/2/2/2
3	NMN	C	503	-	-	7/14/30/30	0/2/2/2
3	NMN	F	506	-	-	3/14/30/30	0/2/2/2
3	NMN	D	504	-	-	6/14/30/30	0/2/2/2
3	NMN	B	502	-	-	5/14/30/30	0/2/2/2
3	NMN	E	505	-	-	3/14/30/30	0/2/2/2

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NMN	C4-C3	8.63	1.52	1.39
3	B	502	NMN	C4-C3	8.62	1.52	1.39
3	C	503	NMN	C4-C3	8.23	1.51	1.39
3	E	505	NMN	C4-C3	8.23	1.51	1.39
3	C	503	NMN	C2-N1	8.16	1.43	1.35
3	F	506	NMN	C4-C3	8.11	1.51	1.39
3	D	504	NMN	C2-N1	8.10	1.43	1.35
3	D	504	NMN	C4-C3	8.01	1.51	1.39
3	A	501	NMN	C2-N1	7.70	1.43	1.35
3	E	505	NMN	C2-N1	7.67	1.43	1.35
3	F	506	NMN	C2-N1	7.63	1.43	1.35
3	B	502	NMN	C2-N1	7.42	1.43	1.35
3	B	502	NMN	C7-N7	-6.24	1.21	1.33
3	E	505	NMN	C7-N7	-6.23	1.21	1.33
3	C	503	NMN	C7-N7	-6.18	1.21	1.33
3	F	506	NMN	C7-N7	-6.07	1.21	1.33
3	B	502	NMN	C6-N1	6.01	1.49	1.35
3	A	501	NMN	C6-N1	5.99	1.49	1.35
3	C	503	NMN	O7-C7	5.98	1.35	1.24
3	D	504	NMN	C7-N7	-5.94	1.22	1.33
3	B	502	NMN	O7-C7	5.89	1.35	1.24
3	A	501	NMN	C7-N7	-5.87	1.22	1.33
3	C	503	NMN	C6-N1	5.86	1.48	1.35
3	D	504	NMN	O7-C7	5.79	1.34	1.24
3	A	501	NMN	O7-C7	5.74	1.34	1.24
3	E	505	NMN	C6-N1	5.70	1.48	1.35
3	E	505	NMN	O7-C7	5.69	1.34	1.24
3	F	506	NMN	O7-C7	5.63	1.34	1.24
3	D	504	NMN	C6-N1	5.58	1.48	1.35
3	F	506	NMN	C6-N1	5.44	1.47	1.35
3	C	503	NMN	C3-C7	4.92	1.57	1.50
3	A	501	NMN	O4R-C4R	4.81	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	506	NMN	O4R-C4R	4.68	1.55	1.45
3	F	506	NMN	C3-C7	4.68	1.57	1.50
3	F	506	NMN	C5-C4	4.68	1.46	1.38
3	E	505	NMN	C3-C7	4.66	1.57	1.50
3	D	504	NMN	C3-C7	4.63	1.57	1.50
3	A	501	NMN	C3-C7	4.61	1.57	1.50
3	C	503	NMN	O4R-C4R	4.57	1.55	1.45
3	E	505	NMN	C5-C4	4.52	1.46	1.38
3	B	502	NMN	C3-C7	4.47	1.57	1.50
3	B	502	NMN	C5-C4	4.46	1.46	1.38
3	A	501	NMN	C5-C4	4.43	1.46	1.38
3	D	504	NMN	O4R-C4R	4.39	1.54	1.45
3	E	505	NMN	O4R-C4R	4.35	1.54	1.45
3	C	503	NMN	C5-C4	4.34	1.46	1.38
3	B	502	NMN	O4R-C4R	4.18	1.54	1.45
3	D	504	NMN	C5-C4	4.15	1.46	1.38
3	B	502	NMN	P-O3P	3.86	1.62	1.50
3	A	501	NMN	P-O3P	3.82	1.62	1.50
3	F	506	NMN	P-O3P	3.70	1.62	1.50
3	C	503	NMN	P-O3P	3.60	1.61	1.50
3	E	505	NMN	P-O3P	3.59	1.61	1.50
3	D	504	NMN	P-O3P	3.58	1.61	1.50
3	E	505	NMN	C6-C5	3.30	1.45	1.38
3	B	502	NMN	C6-C5	3.28	1.45	1.38
3	F	506	NMN	C6-C5	3.27	1.45	1.38
3	A	501	NMN	C6-C5	3.26	1.45	1.38
3	C	503	NMN	C6-C5	2.98	1.44	1.38
3	D	504	NMN	C6-C5	2.98	1.44	1.38
3	F	506	NMN	C5R-C4R	-2.40	1.44	1.51
3	E	505	NMN	C5R-C4R	-2.31	1.44	1.51
3	B	502	NMN	C5R-C4R	-2.27	1.44	1.51
3	C	503	NMN	C5R-C4R	-2.22	1.44	1.51
3	D	504	NMN	C5R-C4R	-2.19	1.45	1.51
2	C	605	PO4	P-O4	-2.17	1.48	1.54
3	A	501	NMN	C5R-C4R	-2.17	1.45	1.51
2	C	602	PO4	P-O3	-2.16	1.48	1.54
2	C	605	PO4	P-O3	-2.12	1.48	1.54
2	D	610	PO4	P-O4	-2.12	1.48	1.54
2	D	607	PO4	P-O4	-2.11	1.48	1.54
2	B	603	PO4	P-O4	-2.09	1.48	1.54
2	C	602	PO4	P-O2	-2.08	1.48	1.54
2	D	607	PO4	P-O3	-2.08	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	610	PO4	P-O2	-2.08	1.48	1.54
2	F	612	PO4	P-O3	-2.06	1.48	1.54
2	D	610	PO4	P-O3	-2.04	1.48	1.54
2	E	609	PO4	P-O4	-2.04	1.48	1.54
2	F	612	PO4	P-O4	-2.03	1.48	1.54
2	E	609	PO4	P-O2	-2.02	1.48	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	506	NMN	C3-C7-N7	9.10	128.95	117.74
3	F	506	NMN	O7-C7-C3	-8.99	108.61	119.60
3	A	501	NMN	O7-C7-C3	-8.87	108.75	119.60
3	A	501	NMN	C3-C7-N7	8.77	128.54	117.74
3	E	505	NMN	C3-C7-N7	8.76	128.53	117.74
3	B	502	NMN	O7-C7-C3	-8.65	109.02	119.60
3	B	502	NMN	C3-C7-N7	8.61	128.34	117.74
3	C	503	NMN	C3-C7-N7	8.54	128.26	117.74
3	E	505	NMN	O7-C7-C3	-8.51	109.19	119.60
3	D	504	NMN	C3-C7-N7	8.49	128.20	117.74
3	D	504	NMN	O7-C7-C3	-8.37	109.36	119.60
3	C	503	NMN	O7-C7-C3	-8.29	109.46	119.60
3	F	506	NMN	C5-C4-C3	-6.16	114.31	120.36
3	A	501	NMN	C5-C4-C3	-6.02	114.44	120.36
3	E	505	NMN	C5-C4-C3	-6.00	114.47	120.36
3	D	504	NMN	C5-C4-C3	-5.94	114.53	120.36
3	B	502	NMN	C5-C4-C3	-5.83	114.63	120.36
3	C	503	NMN	C5-C4-C3	-5.63	114.83	120.36
3	D	504	NMN	C4-C3-C7	-4.53	108.71	121.06
3	E	505	NMN	C5-C6-N1	-4.53	114.20	120.38
3	B	502	NMN	C5-C6-N1	-4.44	114.32	120.38
3	C	503	NMN	C4-C3-C7	-4.44	108.98	121.06
3	F	506	NMN	C5-C6-N1	-4.41	114.37	120.38
3	D	504	NMN	C6-C5-C4	4.40	125.79	119.45
3	E	505	NMN	C6-C5-C4	4.39	125.78	119.45
3	F	506	NMN	C6-C5-C4	4.36	125.73	119.45
3	C	503	NMN	C6-C5-C4	4.36	125.73	119.45
3	A	501	NMN	C4-C3-C7	-4.33	109.26	121.06
3	C	503	NMN	C5-C6-N1	-4.30	114.52	120.38
3	A	501	NMN	C6-C5-C4	4.27	125.60	119.45
3	E	505	NMN	C4-C3-C7	-4.24	109.50	121.06
3	B	502	NMN	C6-C5-C4	4.21	125.51	119.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	NMN	C4-C3-C7	-4.18	109.68	121.06
3	A	501	NMN	C5-C6-N1	-4.14	114.74	120.38
3	F	506	NMN	C4-C3-C7	-4.12	109.83	121.06
3	F	506	NMN	C4R-O4R-C1R	-4.11	106.16	109.92
3	A	501	NMN	C4R-O4R-C1R	-4.09	106.18	109.92
3	D	504	NMN	C5-C6-N1	-4.06	114.85	120.38
3	D	504	NMN	C4R-O4R-C1R	-4.00	106.26	109.92
3	A	501	NMN	C2-C3-C4	3.66	122.51	118.26
3	C	503	NMN	C4R-O4R-C1R	-3.63	106.60	109.92
3	D	504	NMN	C2-C3-C4	3.57	122.42	118.26
3	B	502	NMN	C2-C3-C4	3.54	122.37	118.26
3	E	505	NMN	C2-C3-C4	3.41	122.22	118.26
3	F	506	NMN	C2-C3-C4	3.40	122.22	118.26
3	B	502	NMN	C2-N1-C1R	-3.37	111.68	119.13
3	C	503	NMN	C2-C3-C4	3.37	122.18	118.26
3	D	504	NMN	C2-C3-C7	3.26	128.87	119.46
3	C	503	NMN	C2-C3-C7	3.25	128.84	119.46
3	F	506	NMN	C2-N1-C1R	-3.22	112.03	119.13
3	E	505	NMN	C2-N1-C1R	-3.16	112.16	119.13
3	B	502	NMN	C4R-O4R-C1R	-3.13	107.06	109.92
3	A	501	NMN	C2-N1-C1R	-3.10	112.28	119.13
3	E	505	NMN	C4R-O4R-C1R	-3.07	107.11	109.92
3	E	505	NMN	C2-C3-C7	3.05	128.27	119.46
3	A	501	NMN	C2-C3-C7	3.04	128.23	119.46
3	F	506	NMN	C2-C3-C7	2.94	127.96	119.46
3	B	502	NMN	C2-C3-C7	2.94	127.94	119.46
3	C	503	NMN	C2-N1-C1R	-2.78	113.00	119.13
3	D	504	NMN	C2-N1-C1R	-2.70	113.18	119.13
3	B	502	NMN	C6-N1-C2	2.59	124.08	121.88
3	C	503	NMN	C6-N1-C2	2.35	123.87	121.88
3	F	506	NMN	C6-N1-C1R	2.31	124.27	119.73
3	B	502	NMN	C6-N1-C1R	2.30	124.23	119.73
3	E	505	NMN	C6-N1-C2	2.25	123.79	121.88
3	E	505	NMN	C6-N1-C1R	2.20	124.05	119.73
3	A	501	NMN	C6-N1-C1R	2.18	124.00	119.73
3	A	501	NMN	C6-N1-C2	2.17	123.72	121.88
3	F	506	NMN	C6-N1-C2	2.14	123.70	121.88

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NMN	C5R-O5R-P-O1P
3	A	501	NMN	C5R-O5R-P-O2P
3	B	502	NMN	C5R-O5R-P-O2P
3	C	503	NMN	C5R-O5R-P-O2P
3	C	503	NMN	C2R-C1R-N1-C2
3	C	503	NMN	C2R-C1R-N1-C6
3	D	504	NMN	C2R-C1R-N1-C2
3	D	504	NMN	C2R-C1R-N1-C6
3	E	505	NMN	C2R-C1R-N1-C2
3	E	505	NMN	C2R-C1R-N1-C6
3	F	506	NMN	C2R-C1R-N1-C2
3	F	506	NMN	C2R-C1R-N1-C6
3	A	501	NMN	C3R-C4R-C5R-O5R
3	D	504	NMN	C3R-C4R-C5R-O5R
3	B	502	NMN	C3R-C4R-C5R-O5R
3	A	501	NMN	O4R-C4R-C5R-O5R
3	D	504	NMN	C4R-C5R-O5R-P
3	A	501	NMN	C5R-O5R-P-O3P
3	B	502	NMN	C5R-O5R-P-O3P
3	C	503	NMN	C5R-O5R-P-O3P
3	D	504	NMN	C5R-O5R-P-O3P
3	B	502	NMN	C5R-O5R-P-O1P
3	C	503	NMN	C5R-O5R-P-O1P
3	E	505	NMN	C4R-C5R-O5R-P
3	A	501	NMN	C4R-C5R-O5R-P
3	C	503	NMN	C4R-C5R-O5R-P
3	A	501	NMN	C2R-C1R-N1-C6
3	B	502	NMN	C2R-C1R-N1-C6
3	F	506	NMN	C4R-C5R-O5R-P
3	D	504	NMN	O4R-C4R-C5R-O5R
3	C	503	NMN	C3R-C4R-C5R-O5R

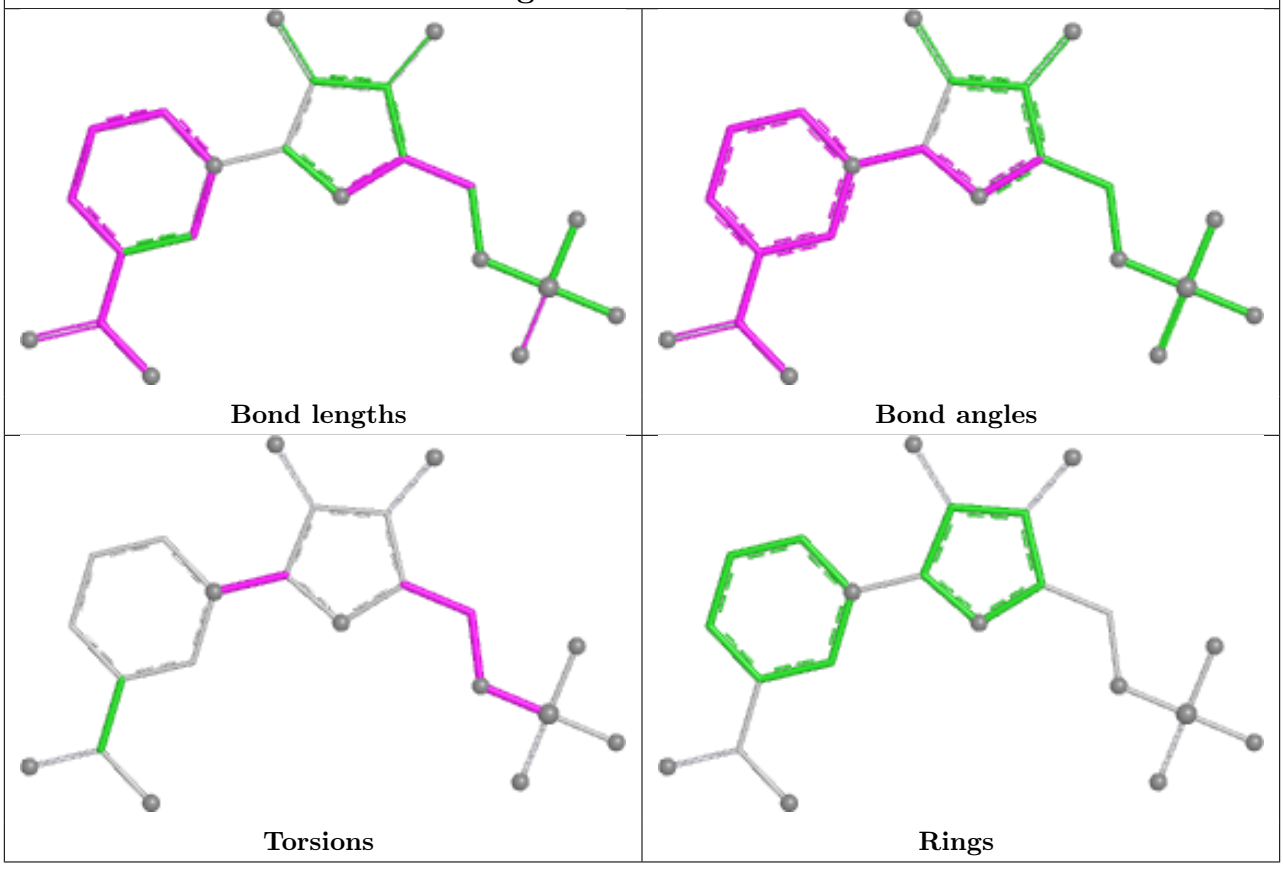
There are no ring outliers.

7 monomers are involved in 7 short contacts:

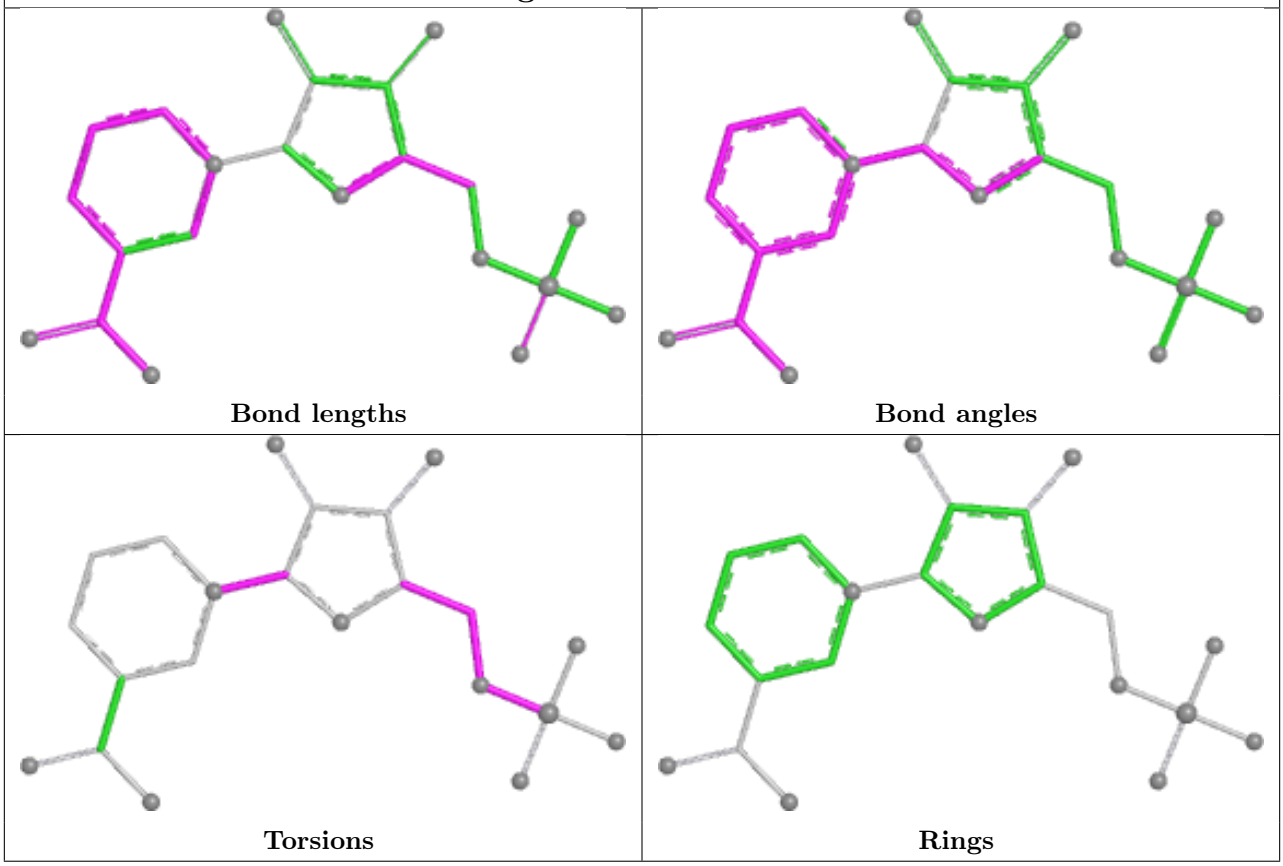
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	NMN	1	0
3	F	506	NMN	1	0
2	C	605	PO4	1	0
3	D	504	NMN	1	0
2	A	601	PO4	1	0
3	E	505	NMN	1	0
2	D	607	PO4	1	0

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 then 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.

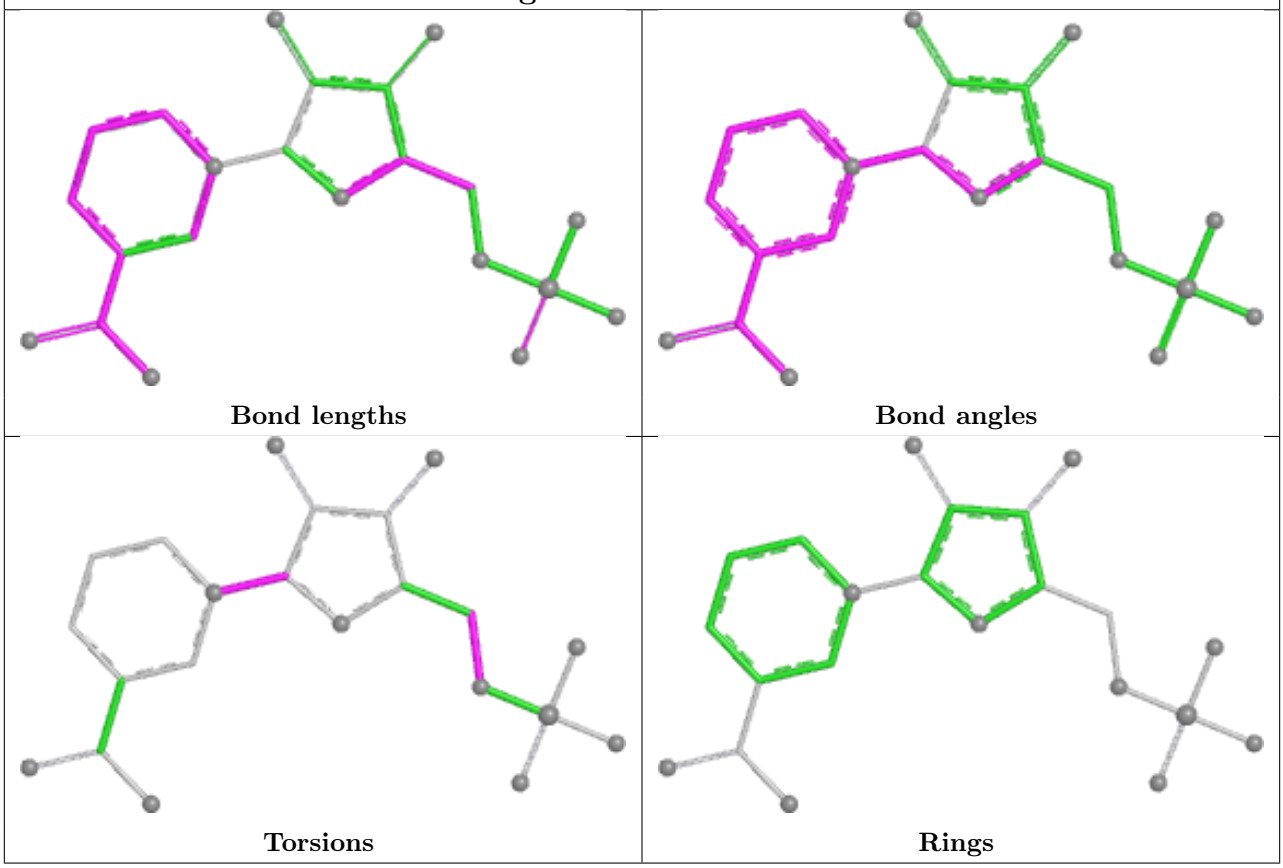
Ligand NMN A 501



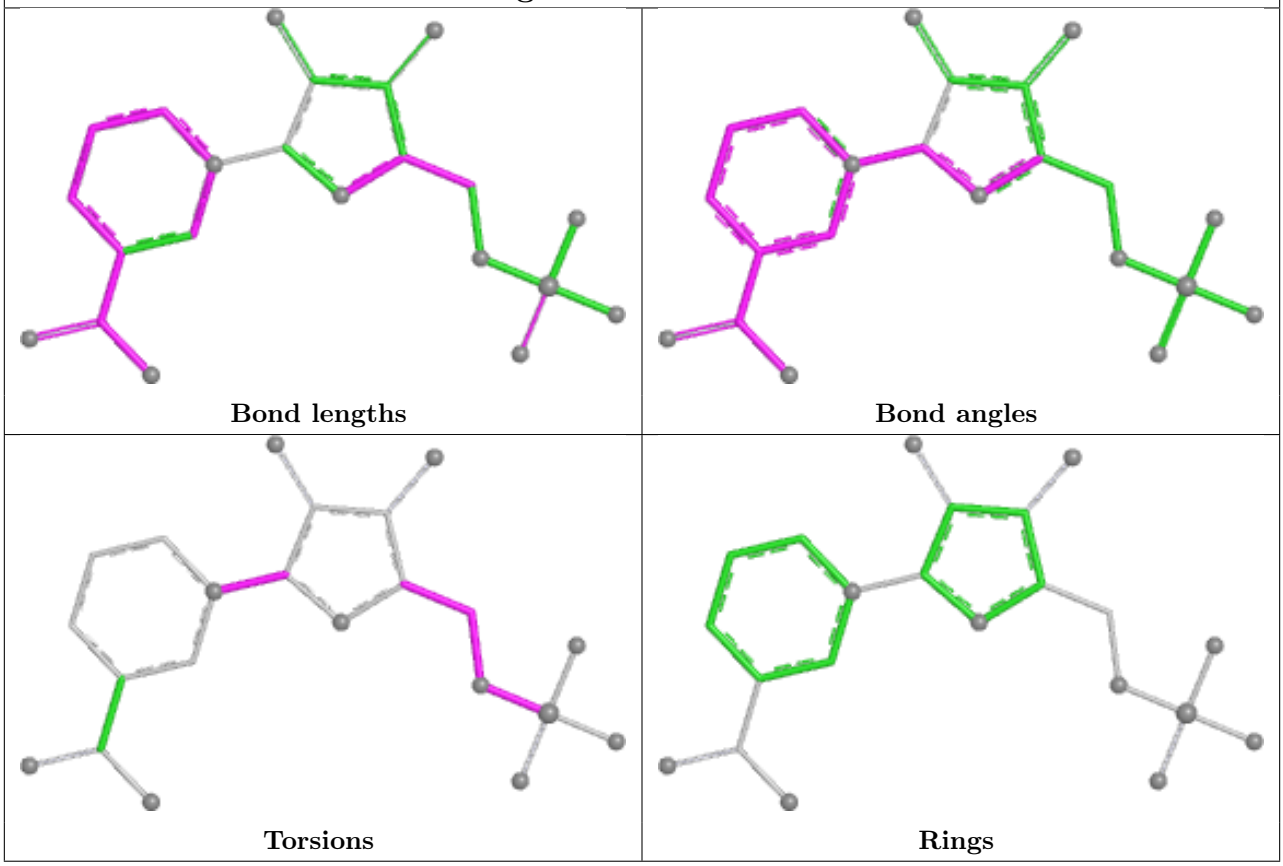
Ligand NMN C 503



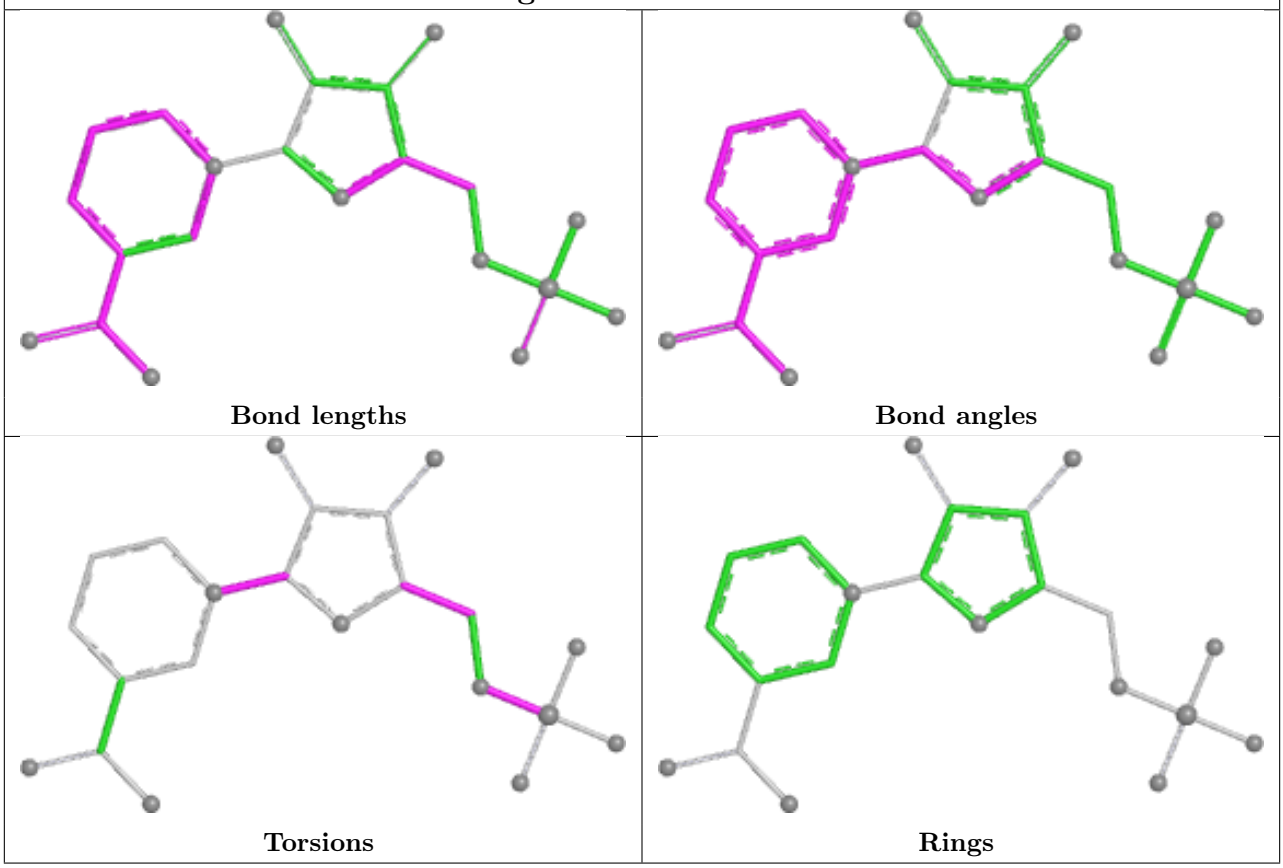
Ligand NMN F 506



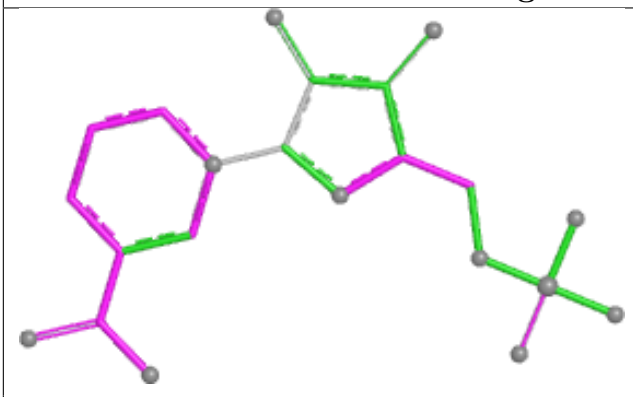
Ligand NMN D 504



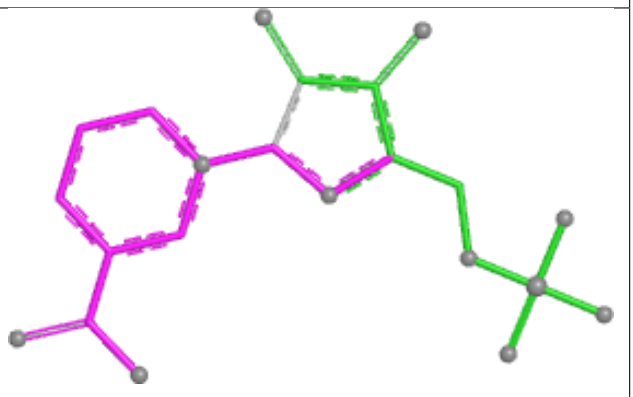
Ligand NMN B 502



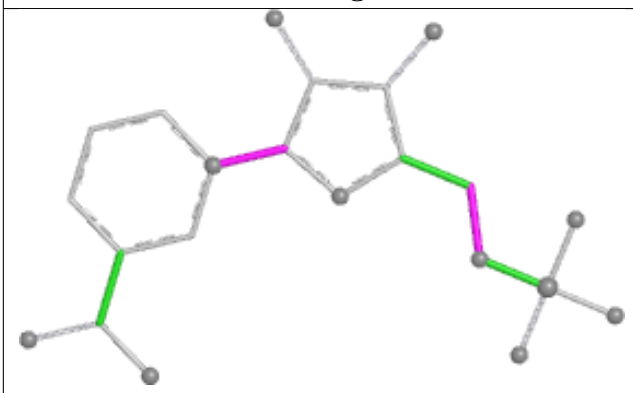
Ligand NMN E 505



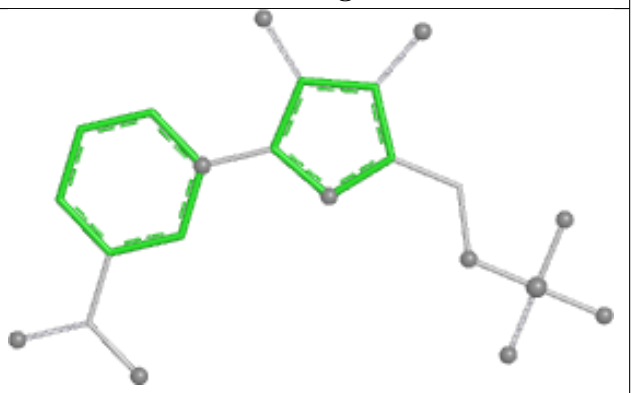
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	461/491 (93%)	0.29	7 (1%)	72	69	22, 39, 53, 67	0
1	B	464/491 (94%)	0.08	6 (1%)	75	73	19, 36, 53, 66	0
1	C	461/491 (93%)	0.49	20 (4%)	40	36	21, 42, 67, 81	0
1	D	464/491 (94%)	-0.33	6 (1%)	75	73	14, 23, 38, 69	0
1	E	464/491 (94%)	-0.32	3 (0%)	85	83	14, 24, 38, 57	0
1	F	463/491 (94%)	-0.48	6 (1%)	75	73	11, 20, 36, 64	0
All	All	2777/2946 (94%)	-0.04	48 (1%)	69	66	11, 30, 55, 81	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ASN	4.4
1	C	285	ASN	4.1
1	A	29	ASN	3.7
1	A	450	LEU	3.5
1	C	450	LEU	3.4
1	F	305	GLN	3.1
1	C	484	ILE	3.1
1	B	95	VAL	3.0
1	C	439	ASN	2.9
1	D	452	GLU	2.9
1	C	292	GLY	2.8
1	B	450	LEU	2.8
1	A	26	TYR	2.8
1	F	450	LEU	2.8
1	C	335	THR	2.7
1	F	452	GLU	2.6
1	C	405	VAL	2.4
1	B	337	ASN	2.4
1	C	452	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	484	ILE	2.3
1	D	271	SER	2.3
1	C	443	LEU	2.3
1	D	450	LEU	2.3
1	A	340	GLY	2.3
1	C	408	GLY	2.3
1	E	452	GLU	2.3
1	C	413	VAL	2.3
1	B	340	GLY	2.2
1	D	305	GLN	2.2
1	C	457	LEU	2.2
1	C	290	ILE	2.2
1	F	484	ILE	2.2
1	F	94	ASP	2.2
1	C	252	ALA	2.2
1	D	453	TYR	2.2
1	E	450	LEU	2.2
1	C	182	ASN	2.2
1	A	99	LYS	2.2
1	A	30	THR	2.2
1	C	453	TYR	2.1
1	F	453	TYR	2.1
1	C	327	ILE	2.1
1	C	407	ASN	2.1
1	C	409	LEU	2.1
1	D	55	GLU	2.1
1	E	326	GLU	2.1
1	C	291	TRP	2.1
1	A	27	PRO	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)

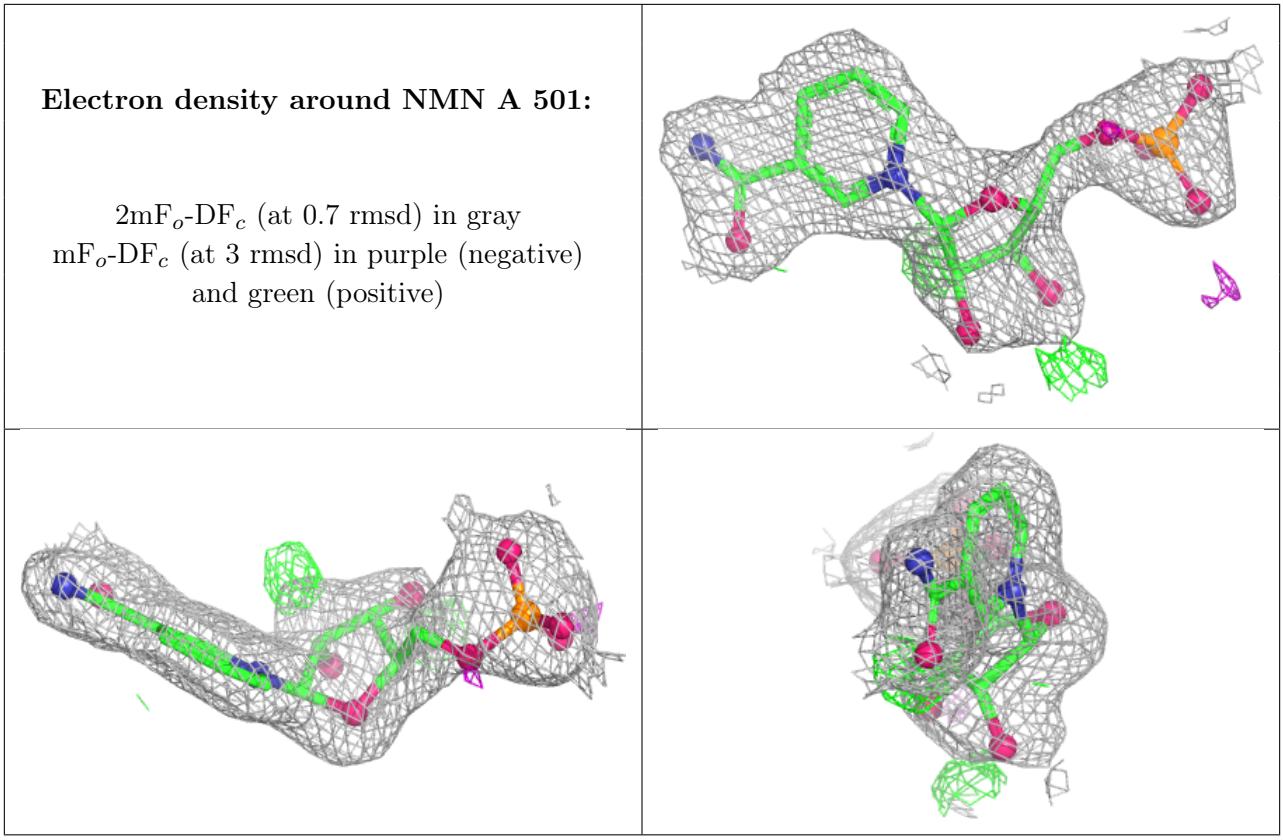
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	E	608	5/5	0.60	0.23	87,88,89,90	0
2	PO4	A	606	5/5	0.90	0.11	49,51,52,52	0
3	NMN	A	501	22/22	0.91	0.10	27,37,40,42	0
3	NMN	B	502	22/22	0.92	0.11	26,38,41,47	0
3	NMN	C	503	22/22	0.92	0.09	36,39,41,43	0
2	PO4	A	601	5/5	0.93	0.10	31,34,34,35	0
3	NMN	D	504	22/22	0.93	0.10	16,26,31,33	0
3	NMN	E	505	22/22	0.94	0.12	17,31,42,46	0
3	NMN	F	506	22/22	0.94	0.10	9,28,34,37	0
2	PO4	C	602	5/5	0.96	0.09	47,48,49,50	0
2	PO4	C	605	5/5	0.96	0.06	35,36,38,40	0
2	PO4	B	604	5/5	0.96	0.07	36,36,37,37	0
2	PO4	D	610	5/5	0.98	0.07	33,34,36,37	0
2	PO4	B	603	5/5	0.98	0.05	27,28,30,30	0
2	PO4	F	612	5/5	0.98	0.06	27,27,29,30	0
2	PO4	E	609	5/5	0.99	0.04	22,22,23,24	0
2	PO4	F	611	5/5	0.99	0.04	16,17,19,20	0
2	PO4	D	607	5/5	0.99	0.04	15,15,17,19	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.

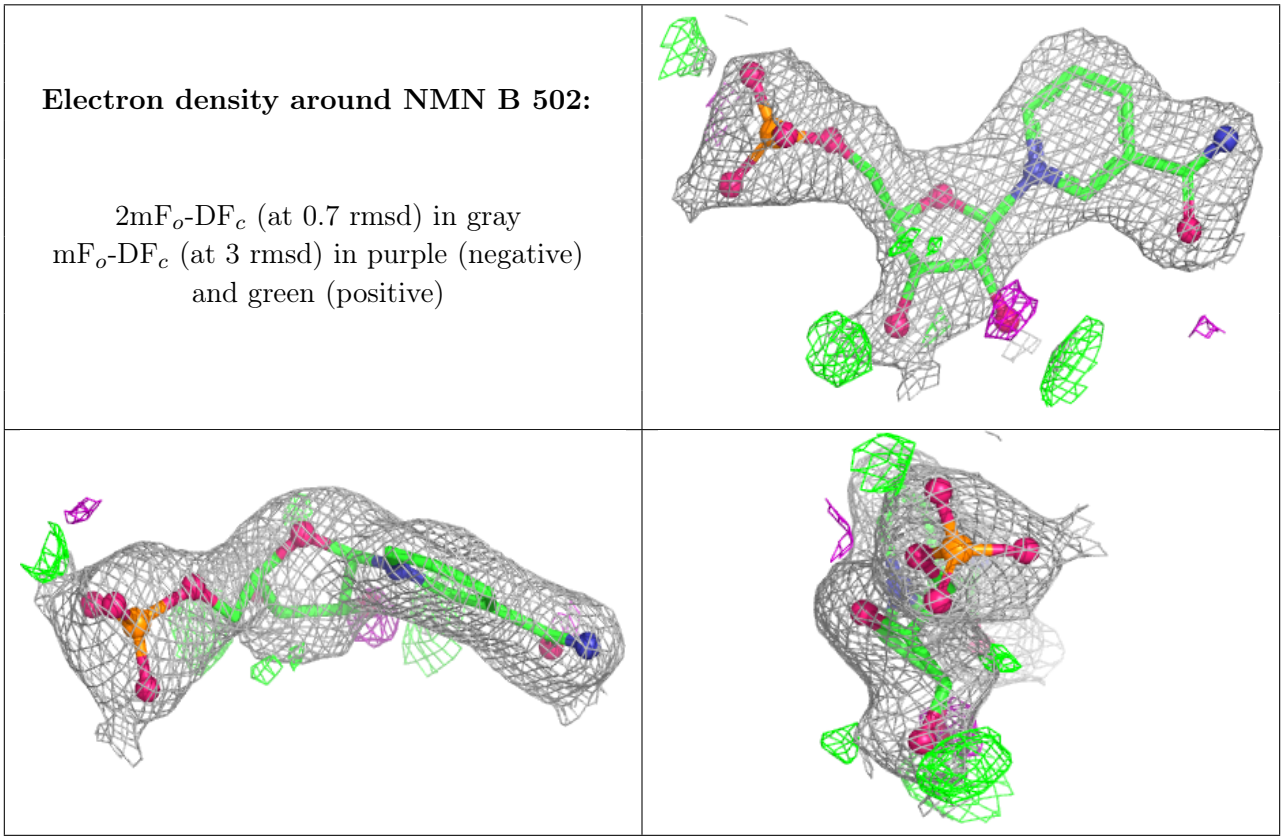
Electron density around NMN A 501:

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



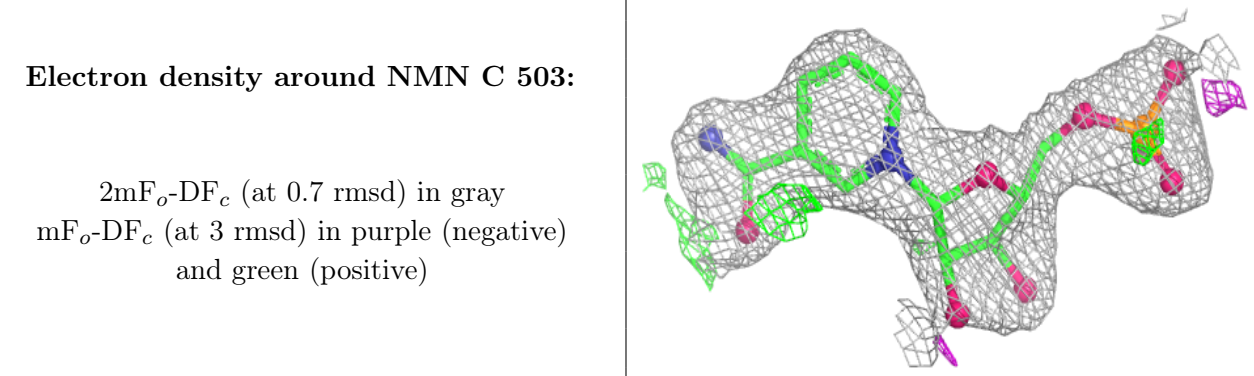
Electron density around NMN B 502:

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



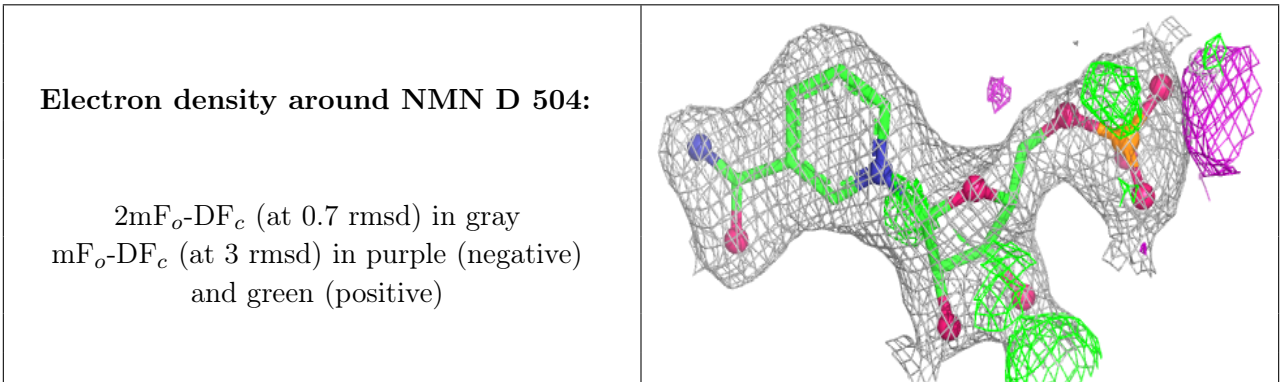
Electron density around NMN C 503:

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



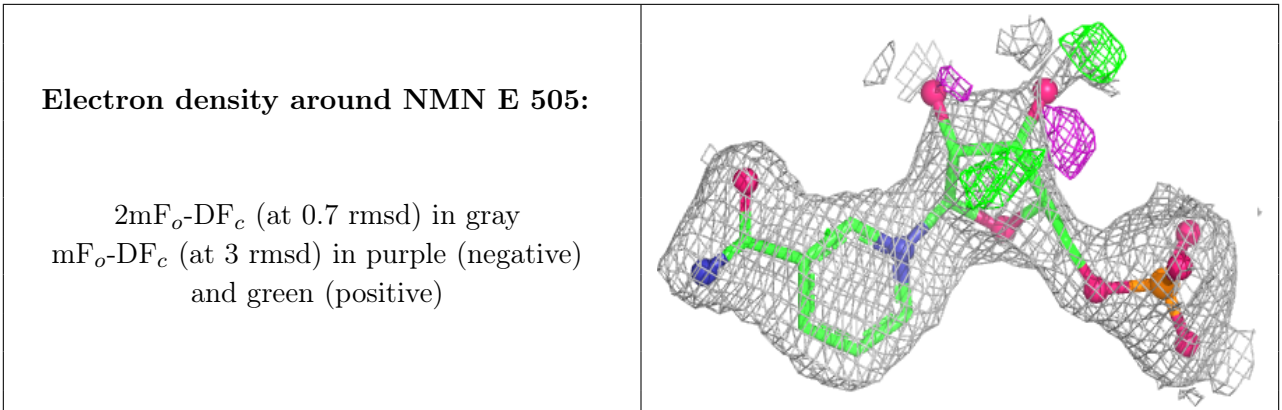
Electron density around NMN D 504:

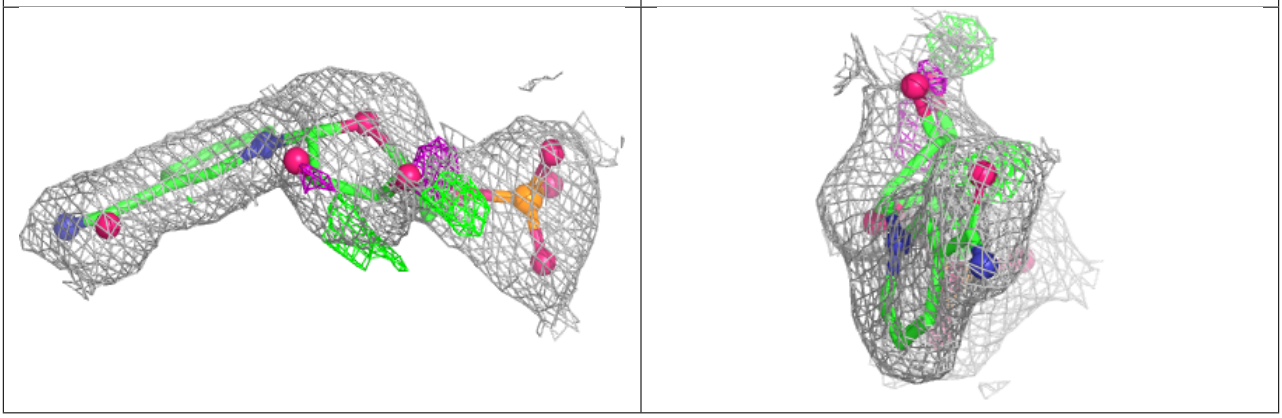
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NMN E 505:

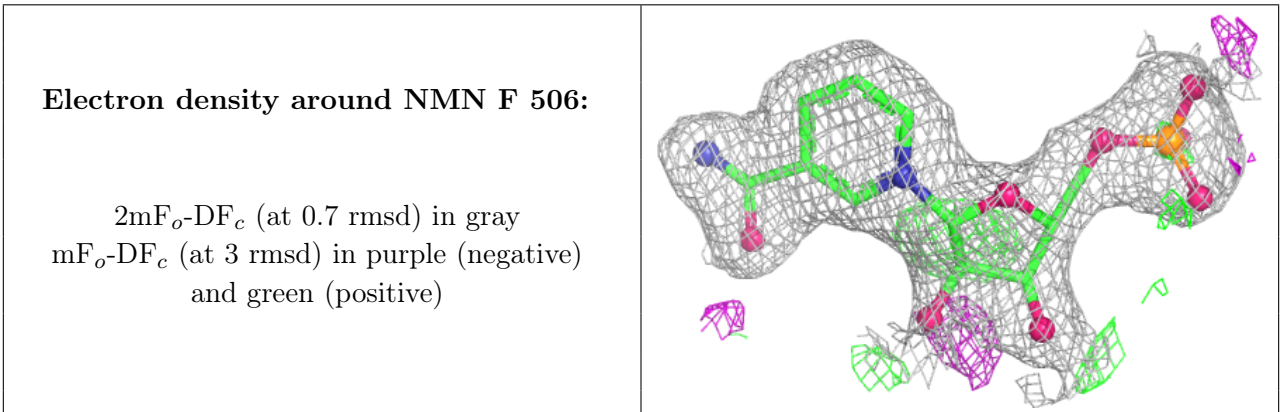
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

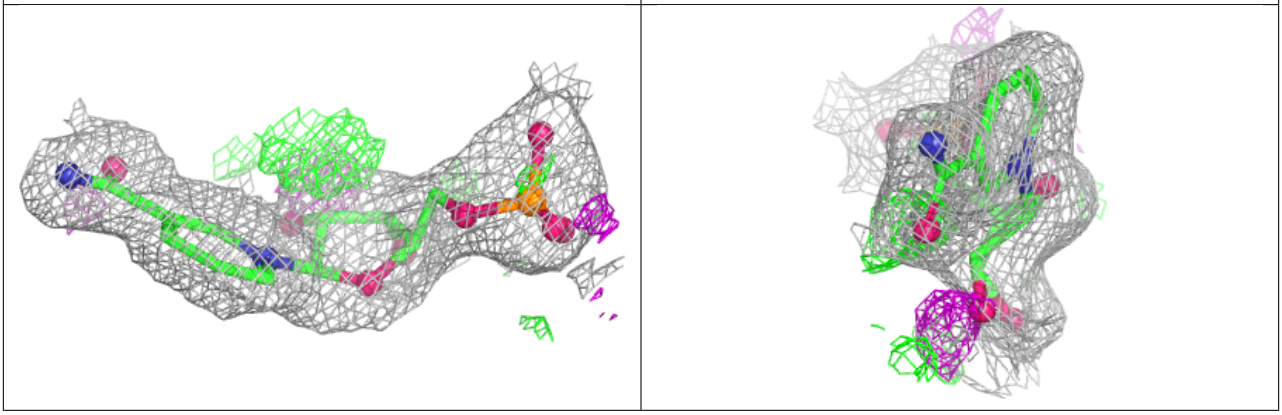




Electron density around NMN F 506:

$2mF_o$-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.