



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:21 PM GMT

PDB ID : 3TDK
Title : Crystal Structure of Human UDP-Glucose Dehydrogenase
Authors : Rajakannan, V.; Han, C.; Robinson, R.
Deposited on : 2011-08-11
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

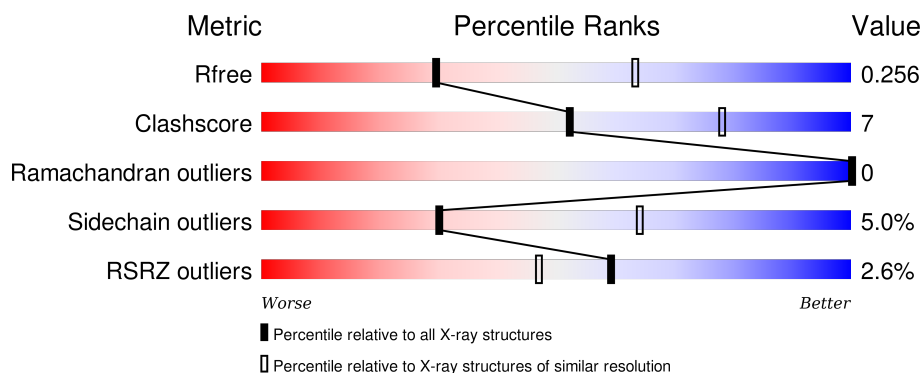
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	487	
1	B	487	
1	C	487	
1	D	487	
1	E	487	

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Mol	Chain	Length	Quality of chain
1	F	487	 3% 79% 14% • 6%
1	G	487	 % 80% 13% • 6%
1	H	487	 78% 15% • 6%
1	I	487	 5% 80% 13% • 6%
1	J	487	 2% 83% 11% 6%
1	K	487	 5% 78% 16% • 6%
1	L	487	 2% 76% 16% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	E	500	-	-	-	X
2	NAD	J	500	-	-	-	X

2 Entry composition

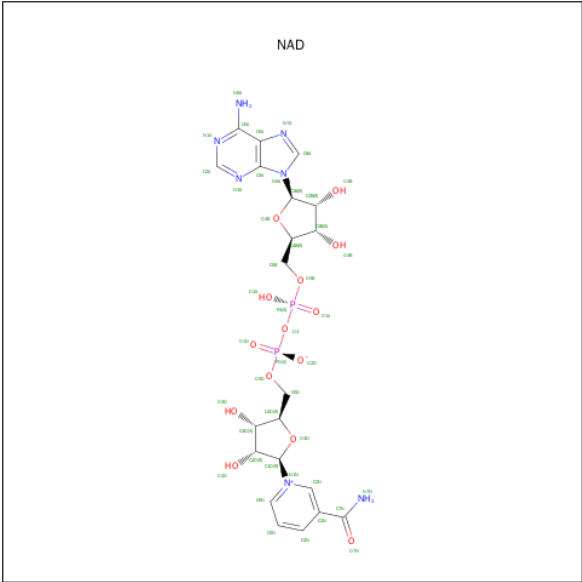
There are 4 unique types of molecules in this entry. The entry contains 44667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glucose 6-dehydrogenase.

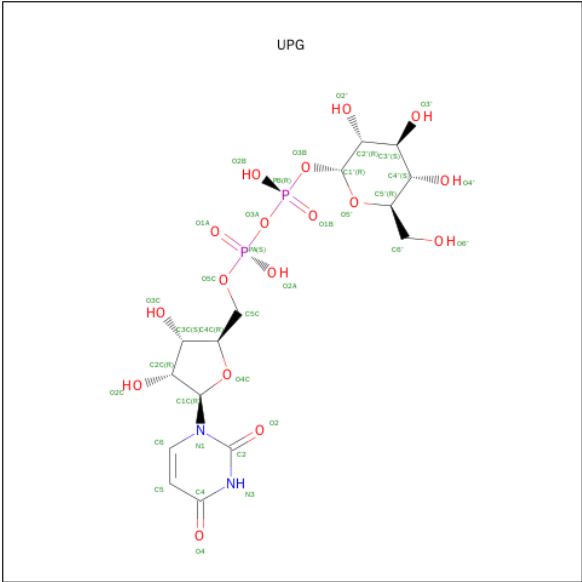
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	B	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	G	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	H	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	L	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	K	458	Total	C	N	O	S	0	0	0
			3588	2272	619	677	20			
1	F	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	E	458	Total	C	N	O	S	0	0	0
			3588	2272	619	677	20			
1	D	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	C	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	J	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			
1	I	460	Total	C	N	O	S	0	0	0
			3606	2282	623	681	20			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	G	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	H	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	L	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	K	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	F	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	E	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	D	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	J	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	I	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂).

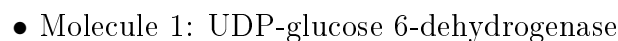
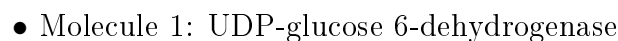


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	G	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	H	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	L	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	K	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	F	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	E	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	J	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	I	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total 77	O 77	0	0
4	B	75	Total 75	O 75	0	0
4	G	69	Total 69	O 69	0	0
4	H	85	Total 85	O 85	0	0
4	L	26	Total 26	O 26	0	0
4	K	18	Total 18	O 18	0	0
4	F	33	Total 33	O 33	0	0
4	E	29	Total 29	O 29	0	0
4	D	40	Total 40	O 40	0	0
4	C	38	Total 38	O 38	0	0
4	J	44	Total 44	O 44	0	0
4	I	45	Total 45	O 45	0	0

- Molecule 1: UDP-glucose 6-dehydrogenase



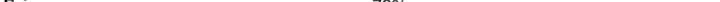
Chain H: 

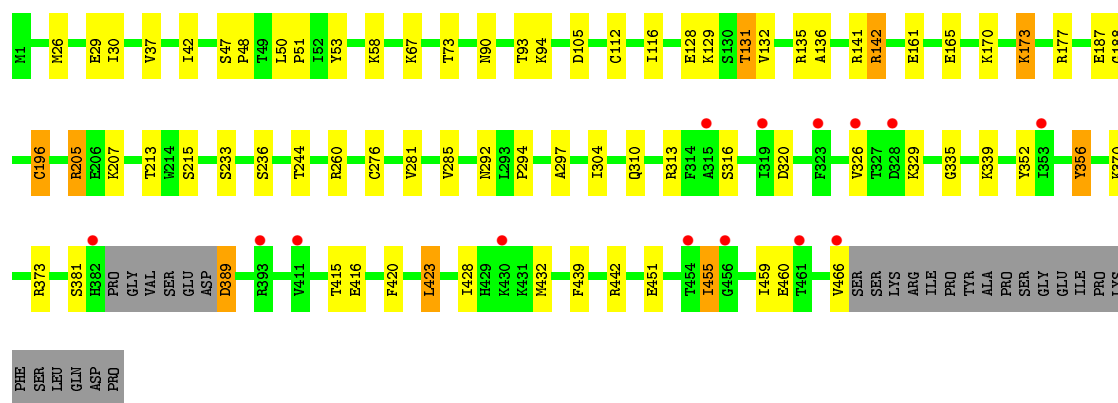
Chain L:

Amino Acid	Count
M1	1
F2	2
E3	3
I7	7
G13	13
A24	24
C27	27
F28	28
E29	29
I30	30
R31	31
V32	32
D36	36
V37	37
N38	38
E39	39
L50	50
P51	51
K58	58
N68	68
T73	73
E81	81
L84	84
T93	93
D105	105
C112	112
I116	116
V117	117
T127	127
E128	128
K129	129
I130	130
T131	131
V132	132
A136	136
R141	141
R142	142
N147	147
M159	159
E165	165
N174	174
R177	177
E187	187
G188	188
C196	196
R205	205
T213	213
W214	214
S215	215
K220	220
L221	221
A222	222
F226	226
S238	238
E242	242
R260	260
F265	265
L266	266
K267	267
S275	275
V296	296
S316	316
I319	319
D320	320
N324	324
T325	325
V326	326
K329	329
K339	339
R346	346
Y352	352
I353	353
Y356	356
E360	360
P360	360

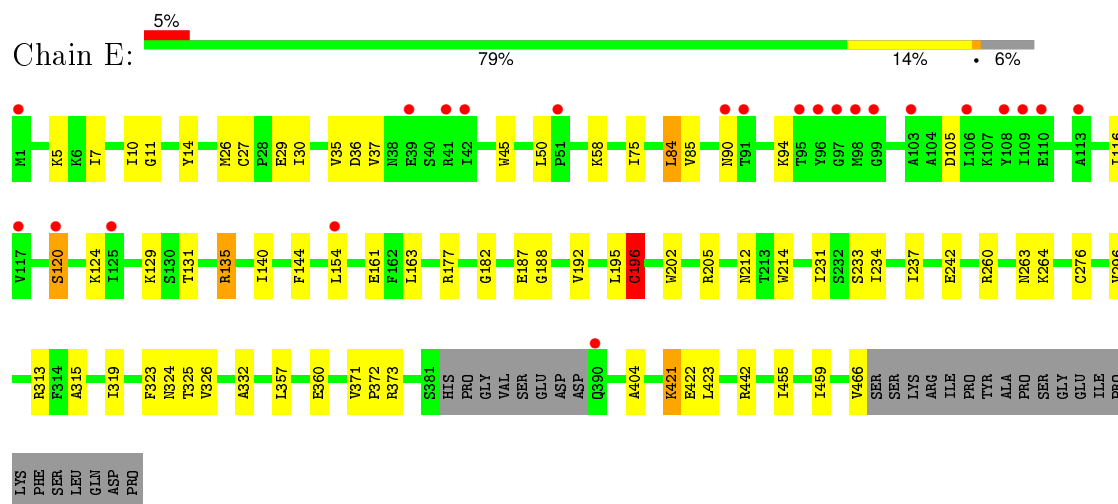
Chain K:

5% 78% 16% 6%

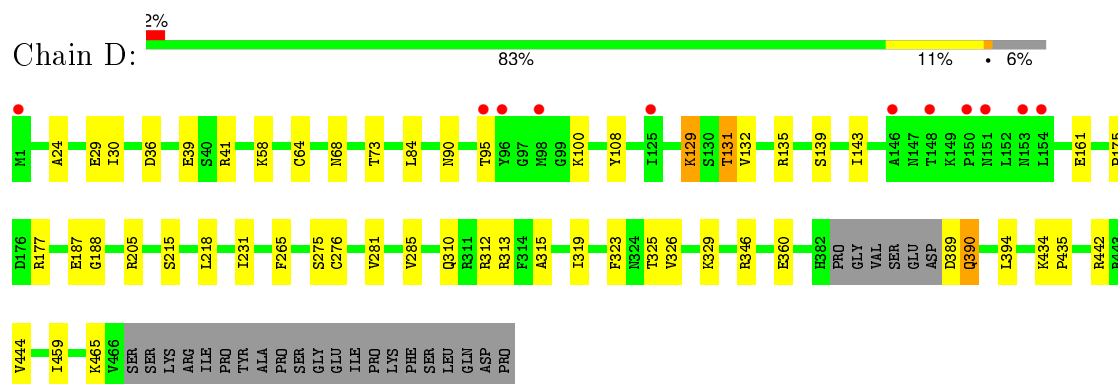
Chain F:  3% 79% 14% 6%



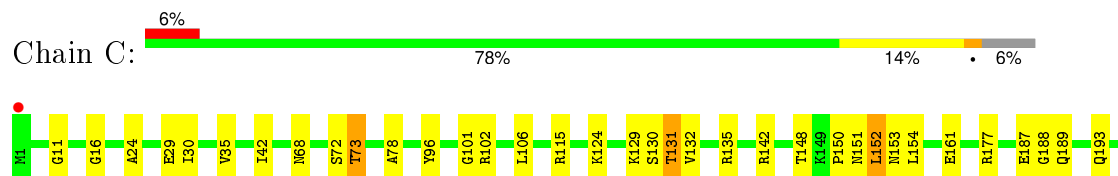
• Molecule 1: UDP-glucose 6-dehydrogenase

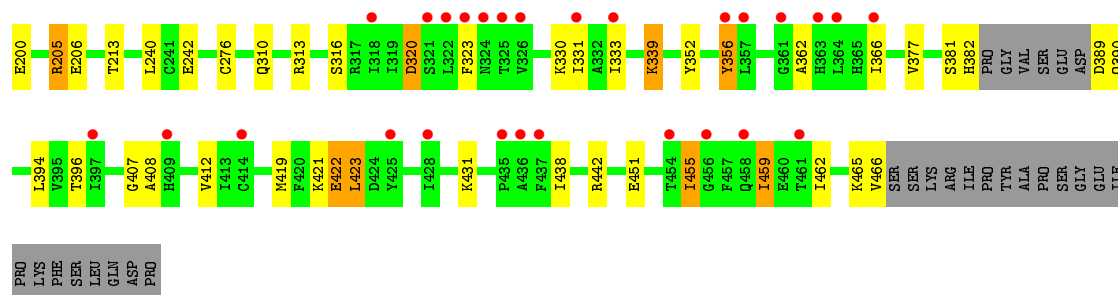


• Molecule 1: UDP-glucose 6-dehydrogenase

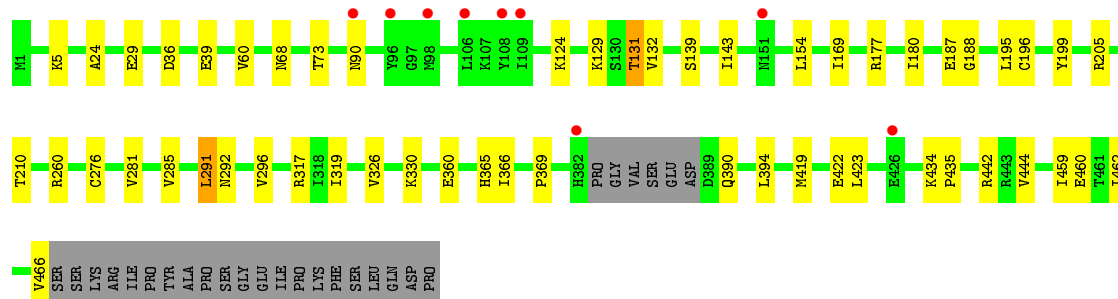
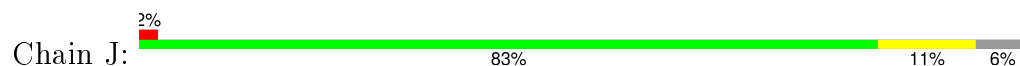


• Molecule 1: UDP-glucose 6-dehydrogenase

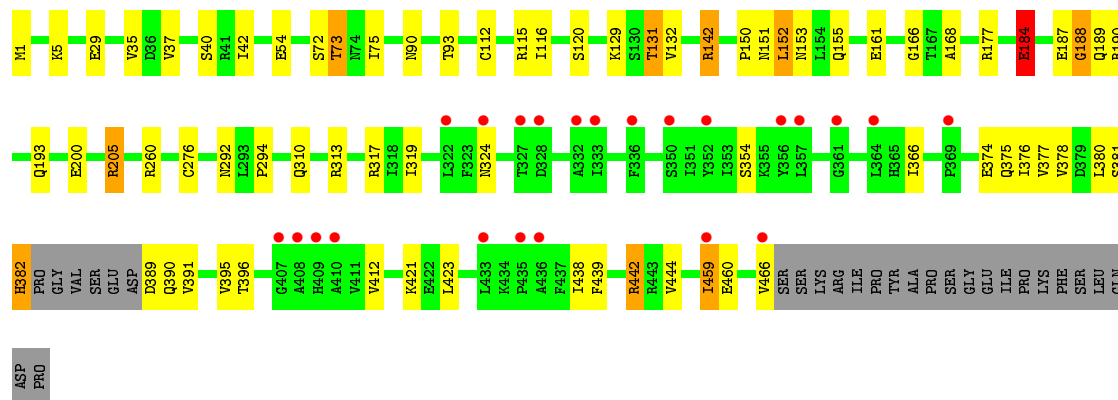
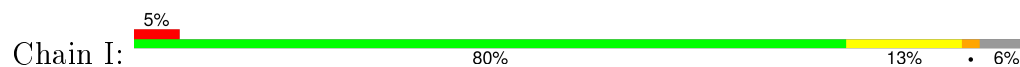




- Molecule 1: UDP-glucose 6-dehydrogenase



- Molecule 1: UDP-glucose 6-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.13Å 191.18Å 225.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.91 – 2.80 49.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.8 (145.91-2.80) 95.8 (49.40-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.261 0.229 , 0.256	Depositor DCC
R_{free} test set	8844 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 176230 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	44667	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 48.42 % 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 8.6196e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UPG, 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	0.76	2/3671 (0.1%)	0.74	0/4966
1	B	0.76	1/3671 (0.0%)	0.72	0/4966
1	C	0.69	0/3671	0.69	0/4966
1	D	0.73	1/3671 (0.0%)	0.71	0/4966
1	E	0.63	1/3652 (0.0%)	0.63	0/4940
1	F	0.67	0/3671	0.68	0/4966
1	G	0.73	0/3671	0.70	2/4966 (0.0%)
1	H	0.80	2/3671 (0.1%)	0.74	1/4966 (0.0%)
1	I	0.67	1/3671 (0.0%)	0.69	1/4966 (0.0%)
1	J	0.73	0/3671	0.69	0/4966
1	K	0.58	0/3652	0.62	0/4940
1	L	0.66	0/3671	0.66	0/4966
All	All	0.70	8/44014 (0.0%)	0.69	4/59540 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	389	ASP	CB-CG	5.98	1.64	1.51
1	D	64	CYS	CB-SG	-5.62	1.72	1.81
1	H	403	GLU	CG-CD	5.49	1.60	1.51
1	I	184	GLU	CG-CD	5.48	1.60	1.51
1	B	161	GLU	CG-CD	5.37	1.60	1.51
1	E	196	CYS	CB-SG	-5.31	1.73	1.81
1	A	29	GLU	CG-CD	5.23	1.59	1.51
1	A	374	GLU	CG-CD	5.18	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	240	LEU	CB-CG-CD2	-5.79	101.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	188	GLY	N-CA-C	-5.78	98.65	113.10
1	G	183	ASP	CB-CG-OD1	5.44	123.19	118.30
1	H	188	GLY	N-CA-C	-5.18	100.15	113.10

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	3606	0	3627	59	0
1	B	3606	0	3627	32	0
1	C	3606	0	3627	52	0
1	D	3606	0	3627	37	0
1	E	3588	0	3616	58	0
1	F	3606	0	3627	50	0
1	G	3606	0	3627	45	0
1	H	3606	0	3627	63	0
1	I	3606	0	3627	54	0
1	J	3606	0	3627	27	0
1	K	3588	0	3616	61	0
1	L	3606	0	3627	60	0
2	A	35	0	19	4	0
2	B	35	0	19	0	0
2	C	35	0	19	2	0
2	D	35	0	19	7	0
2	E	35	0	19	7	0
2	F	35	0	19	3	0
2	G	35	0	19	4	0
2	H	35	0	19	1	0
2	I	35	0	19	1	0
2	J	35	0	19	3	0
2	K	35	0	19	4	0
2	L	35	0	19	5	0
3	A	36	0	21	9	0
3	B	36	0	21	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	36	0	21	7	0
3	D	36	0	22	4	0
3	E	36	0	22	6	0
3	F	36	0	22	5	0
3	G	36	0	21	7	0
3	H	36	0	21	9	0
3	I	36	0	21	3	0
3	J	36	0	22	4	0
3	K	36	0	21	13	0
3	L	36	0	22	4	0
4	A	77	0	0	0	0
4	B	75	0	0	2	0
4	C	38	0	0	0	0
4	D	40	0	0	1	0
4	E	29	0	0	0	0
4	F	33	0	0	1	0
4	G	69	0	0	1	0
4	H	85	0	0	0	0
4	I	45	0	0	2	0
4	J	44	0	0	1	0
4	K	18	0	0	0	0
4	L	26	0	0	1	0
All	All	44667	0	43987	588	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 7.

All (588) 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:C:152:LEU:HD12	1:C:153:ASN:N	1.57	1.18
1:B:319:ILE:HD12	1:B:360:GLU:HG3	1.28	1.15
1:I:42:ILE:HG21	1:I:73:THR:HG22	1.30	1.08
1:I:42:ILE:HG21	1:I:73:THR:CG2	1.87	1.05
1:H:135:ARG:HG2	1:H:135:ARG:HH11	1.17	1.04
1:I:381:SER:HB3	1:I:391:VAL:HG21	1.39	1.03
1:C:152:LEU:HD12	1:C:153:ASN:H	1.17	0.99
1:H:325:THR:CG2	1:L:105:ASP:OD1	2.10	0.99
1:I:152:LEU:HD12	1:I:153:ASN:N	1.77	0.99
1:I:152:LEU:HD12	1:I:153:ASN:H	1.27	0.99
1:H:276:CYS:SG	3:H:501:UPG:O6'	2.21	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HG2	1:B:135:ARG:HH11	1.25	0.98
1:B:326:VAL:HG22	1:B:360:GLU:HB3	1.46	0.95
1:I:54:GLU:OE2	1:I:166:GLY:N	2.00	0.93
1:I:381:SER:CB	1:I:391:VAL:HG21	2.00	0.92
1:I:382:HIS:CD2	1:I:382:HIS:C	2.43	0.92
1:K:165:GLU:O	1:K:339:LYS:HE3	1.71	0.91
1:A:131:THR:N	2:A:500:NAD:O3D	2.03	0.91
1:G:276:CYS:SG	3:G:501:UPG:O6'	2.29	0.91
1:K:462:ILE:HD12	1:K:462:ILE:C	1.92	0.90
1:A:276:CYS:SG	3:A:501:UPG:O6'	2.29	0.90
1:K:462:ILE:O	1:K:462:ILE:HD12	1.72	0.90
1:H:323:PHE:HE1	1:L:142:ARG:HD3	1.35	0.90
1:H:110:GLU:HG3	1:H:143:ILE:HD11	1.52	0.89
1:H:142:ARG:HD3	1:H:142:ARG:O	1.70	0.88
1:H:325:THR:HG21	1:L:105:ASP:OD1	1.71	0.88
1:K:276:CYS:SG	3:K:501:UPG:O6'	2.31	0.87
1:H:319:ILE:HD12	1:H:360:GLU:HG3	1.54	0.87
1:B:319:ILE:CD1	1:B:360:GLU:HG3	2.05	0.85
1:C:276:CYS:SG	3:C:501:UPG:O6'	2.35	0.84
1:F:42:ILE:HG13	1:F:73:THR:HG22	1.59	0.84
1:F:131:THR:HG22	1:F:132:VAL:HG23	1.59	0.84
1:A:165:GLU:O	1:A:339:LYS:HE3	1.79	0.82
1:A:323:PHE:HE1	1:C:142:ARG:HD3	1.45	0.82
1:E:276:CYS:SG	3:E:501:UPG:H6'1	2.20	0.81
3:F:501:UPG:O1A	3:F:501:UPG:H1'	1.82	0.80
1:G:276:CYS:HG	3:G:501:UPG:C6'	1.94	0.80
1:G:319:ILE:HD12	1:G:360:GLU:HG3	1.64	0.79
1:H:135:ARG:HG2	1:H:135:ARG:NH1	1.89	0.79
1:G:260:ARG:NH1	3:H:501:UPG:O2'	2.15	0.78
1:C:390:GLN:HG2	1:C:394:LEU:HD12	1.64	0.78
1:L:1:MET:N	1:L:1:MET:SD	2.56	0.77
1:H:165:GLU:O	1:H:339:LYS:HE3	1.85	0.77
1:H:142:ARG:HH11	1:H:146:ALA:HB2	1.48	0.77
1:D:319:ILE:HD12	1:D:360:GLU:HG3	1.67	0.77
1:E:36:ASP:OD2	2:E:500:NAD:O2B	2.02	0.76
1:H:310:GLN:OE1	1:H:313:ARG:NH2	2.19	0.76
1:A:165:GLU:O	1:A:339:LYS:CE	2.33	0.76
1:L:131:THR:HG22	1:L:132:VAL:HG23	1.67	0.76
1:H:325:THR:HG22	1:L:105:ASP:OD1	1.86	0.75
1:D:187:GLU:N	1:D:188:GLY:HA3	2.00	0.75
1:E:326:VAL:HG22	1:E:360:GLU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:CYS:HG	3:A:501:UPG:C6'	1.99	0.75
1:D:326:VAL:HG22	1:D:360:GLU:HB3	1.68	0.74
1:E:187:GLU:N	1:E:188:GLY:HA3	2.01	0.74
1:F:187:GLU:H	1:F:188:GLY:HA3	1.53	0.74
1:E:187:GLU:H	1:E:188:GLY:HA3	1.53	0.74
1:E:85:VAL:HG11	1:E:116:ILE:HD11	1.69	0.74
1:L:352:TYR:CD1	1:L:352:TYR:C	2.60	0.73
1:F:187:GLU:N	1:F:188:GLY:HA3	2.03	0.73
1:E:276:CYS:HB2	3:E:501:UPG:O6'	1.88	0.73
1:B:187:GLU:N	1:B:188:GLY:HA3	2.04	0.73
1:L:356:TYR:O	1:L:356:TYR:HD1	1.72	0.73
1:B:135:ARG:NH1	1:B:135:ARG:HG2	1.98	0.73
1:K:421:LYS:O	1:K:422:GLU:HB2	1.89	0.73
1:K:102:ARG:NH2	1:K:289:GLU:OE2	2.21	0.73
1:E:84:LEU:HD11	1:E:195:LEU:HD13	1.71	0.73
1:G:187:GLU:N	1:G:188:GLY:HA3	2.03	0.73
1:H:39:GLU:HG2	1:H:73:THR:HG21	1.71	0.73
1:H:187:GLU:N	1:H:188:GLY:HA3	2.04	0.72
1:H:421:LYS:O	1:H:422:GLU:HB2	1.90	0.72
1:E:421:LYS:O	1:E:422:GLU:HB2	1.89	0.72
1:B:276:CYS:SG	3:B:501:UPG:O6'	2.46	0.71
1:C:200:GLU:OE1	1:C:205:ARG:NH1	2.23	0.71
3:H:501:UPG:H1'	3:H:501:UPG:O1A	1.89	0.71
1:E:36:ASP:CG	2:E:500:NAD:O2B	2.29	0.71
1:C:150:PRO:O	1:C:151:ASN:HB2	1.90	0.71
1:I:310:GLN:OE1	1:I:313:ARG:NH2	2.24	0.71
1:I:150:PRO:O	1:I:151:ASN:HB2	1.90	0.70
1:G:130:SER:HB2	2:G:500:NAD:O3D	1.91	0.70
1:K:276:CYS:CB	3:K:501:UPG:O6'	2.38	0.70
1:J:187:GLU:N	1:J:188:GLY:HA3	2.04	0.70
1:A:187:GLU:N	1:A:188:GLY:HA3	2.05	0.70
1:G:276:CYS:SG	3:G:501:UPG:C6'	2.79	0.70
1:L:356:TYR:O	1:L:356:TYR:CD1	2.44	0.70
1:K:102:ARG:HH22	1:K:289:GLU:CD	1.95	0.70
1:A:326:VAL:HG22	1:A:360:GLU:HB3	1.74	0.70
1:H:142:ARG:CD	1:H:142:ARG:O	2.39	0.70
1:K:187:GLU:N	1:K:188:GLY:HA3	2.07	0.70
1:G:112:CYS:O	1:G:116:ILE:HG12	1.92	0.69
1:C:152:LEU:HD12	1:C:152:LEU:C	2.09	0.69
3:K:501:UPG:H1'	3:K:501:UPG:O1A	1.92	0.69
1:E:35:VAL:HB	1:E:75:ILE:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:389:ASP:O	1:I:390:GLN:HB2	1.92	0.69
1:G:39:GLU:HG2	1:G:73:THR:HG21	1.75	0.69
1:K:263:ASN:OD1	1:K:264:LYS:HE3	1.93	0.69
1:D:310:GLN:OE1	1:D:313:ARG:NH2	2.25	0.68
3:E:501:UPG:H1'	3:E:501:UPG:O1A	1.92	0.68
3:J:501:UPG:H1'	3:J:501:UPG:O1A	1.93	0.68
1:J:326:VAL:HG22	1:J:360:GLU:HB3	1.74	0.68
1:I:184:GLU:CD	1:I:184:GLU:H	1.96	0.68
1:A:319:ILE:HD12	1:A:360:GLU:HG3	1.74	0.68
1:I:72:SER:O	1:I:73:THR:HG23	1.93	0.67
1:H:326:VAL:O	1:H:326:VAL:HG23	1.94	0.67
1:D:187:GLU:H	1:D:188:GLY:HA3	1.60	0.67
1:C:42:ILE:HG13	1:C:73:THR:HG22	1.75	0.67
1:E:319:ILE:HD12	1:E:360:GLU:HG3	1.76	0.67
1:I:381:SER:HB3	1:I:391:VAL:CG2	2.22	0.67
1:I:190:ARG:NH1	4:I:497:HOH:O	2.27	0.67
1:H:276:CYS:HB2	3:H:501:UPG:H6'2	1.77	0.67
1:H:323:PHE:CE1	1:L:142:ARG:HD3	2.26	0.66
1:D:326:VAL:HG22	1:D:360:GLU:CB	2.25	0.66
1:A:7:ILE:CD1	1:A:30:ILE:HD11	2.26	0.66
1:H:141:ARG:HH22	1:H:213:THR:HG21	1.61	0.66
1:B:390:GLN:HG2	1:B:394:LEU:HD12	1.77	0.65
1:L:131:THR:H	2:L:500:NAD:HO3N	1.45	0.65
3:B:501:UPG:O1A	3:B:501:UPG:H1'	1.97	0.65
1:C:72:SER:O	1:C:73:THR:HG23	1.96	0.65
1:L:416:GLU:HG2	1:L:416:GLU:O	1.95	0.65
1:L:356:TYR:C	1:L:356:TYR:CD1	2.70	0.64
3:A:501:UPG:O2'	1:B:260:ARG:NH1	2.29	0.64
1:H:276:CYS:HG	3:H:501:UPG:C6'	2.04	0.64
1:I:382:HIS:C	1:I:382:HIS:HD2	2.01	0.64
1:A:260:ARG:NH1	3:B:501:UPG:O2'	2.28	0.64
1:H:110:GLU:HG3	1:H:143:ILE:CD1	2.25	0.64
1:L:326:VAL:HA	1:L:329:LYS:HD2	1.78	0.64
1:L:356:TYR:C	1:L:356:TYR:HD1	2.00	0.64
1:G:429:HIS:CE1	1:G:434:LYS:HE3	2.33	0.64
1:B:131:THR:HG22	1:B:132:VAL:HG23	1.79	0.64
1:F:416:GLU:O	1:F:416:GLU:HG2	1.98	0.64
1:E:116:ILE:O	1:E:120:SER:HB2	1.98	0.64
1:H:141:ARG:NH2	1:H:213:THR:HG21	2.13	0.64
1:F:420:PHE:HA	1:F:423:LEU:HD22	1.80	0.63
1:H:189:GLN:O	1:H:193:GLN:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:131:THR:HG22	2:K:500:NAD:O3D	1.99	0.63
1:H:421:LYS:O	1:H:422:GLU:CB	2.46	0.63
1:D:276:CYS:HB2	3:D:501:UPG:O6'	1.99	0.63
1:I:42:ILE:CG2	1:I:73:THR:HG22	2.18	0.62
1:I:131:THR:HG22	1:I:132:VAL:HG23	1.81	0.62
1:B:323:PHE:HE1	1:F:142:ARG:HD3	1.66	0.61
1:L:165:GLU:O	1:L:339:LYS:CE	2.48	0.61
1:B:102:ARG:HD3	4:B:561:HOH:O	2.00	0.61
1:I:90:ASN:HA	2:I:500:NAD:H3D	1.81	0.61
1:I:35:VAL:HB	1:I:75:ILE:HG13	1.82	0.61
1:G:389:ASP:HA	1:G:392:SER:HB2	1.82	0.61
1:A:129:LYS:HE2	1:A:161:GLU:OE1	2.01	0.61
1:B:462:ILE:HG13	1:B:462:ILE:O	2.00	0.61
1:B:47:SER:HB2	1:B:48:PRO:HD2	1.82	0.61
1:E:90:ASN:HB3	2:E:500:NAD:H52A	1.82	0.61
1:L:390:GLN:O	1:L:390:GLN:HG2	2.01	0.61
1:I:374:GLU:O	1:I:377:VAL:HG22	2.01	0.61
1:G:276:CYS:CB	3:G:501:UPG:H6'2	2.31	0.61
1:C:377:VAL:O	1:C:381:SER:OG	2.15	0.61
1:B:326:VAL:HA	1:B:329:LYS:HD2	1.83	0.61
1:D:312:ARG:NH1	4:D:497:HOH:O	2.33	0.60
1:H:319:ILE:CD1	1:H:360:GLU:HG3	2.30	0.60
1:F:260:ARG:NH1	3:E:501:UPG:O2'	2.24	0.60
1:A:205:ARG:CG	1:A:205:ARG:HH11	2.14	0.60
1:I:382:HIS:O	1:I:382:HIS:CD2	2.54	0.60
1:A:276:CYS:CB	3:A:501:UPG:H6'2	2.32	0.60
1:H:419:MET:O	1:H:423:LEU:HD13	2.00	0.60
1:H:276:CYS:CB	3:H:501:UPG:H6'2	2.31	0.60
1:L:165:GLU:O	1:L:339:LYS:HE2	2.01	0.60
1:H:328:ASP:HA	1:H:363:HIS:CE1	2.37	0.60
1:C:130:SER:HB2	2:C:500:NAD:O3D	2.01	0.59
1:H:135:ARG:HH11	1:H:135:ARG:CG	2.05	0.59
1:G:276:CYS:SG	3:G:501:UPG:H6'2	2.42	0.59
1:E:182:GLY:O	1:E:212:ASN:HA	2.01	0.59
1:A:323:PHE:CE1	1:C:142:ARG:HD3	2.34	0.59
1:H:165:GLU:O	1:H:339:LYS:CE	2.49	0.58
1:A:187:GLU:H	1:A:188:GLY:HA3	1.66	0.58
1:G:326:VAL:HG22	1:G:360:GLU:HB3	1.84	0.58
1:K:326:VAL:CG2	1:K:360:GLU:HB3	2.32	0.58
1:H:131:THR:HG22	1:H:132:VAL:HG23	1.84	0.58
1:E:11:GLY:HA2	2:E:500:NAD:H1B	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:GLU:N	1:L:188:GLY:HA3	2.19	0.58
1:C:276:CYS:HG	3:C:501:UPG:C6'	2.11	0.57
1:I:54:GLU:HG2	1:I:168:ALA:HB3	1.86	0.57
1:H:112:CYS:O	1:H:116:ILE:HG12	2.04	0.57
1:E:135:ARG:HB3	1:E:135:ARG:HH11	1.68	0.57
1:D:131:THR:HG22	2:D:500:NAD:O2D	2.05	0.57
1:F:316:SER:O	1:F:320:ASP:HB2	2.02	0.57
1:K:98:MET:HG3	1:K:98:MET:O	2.04	0.57
1:A:325:THR:HG21	1:C:106:LEU:H	1.69	0.57
1:F:141:ARG:HH22	1:F:213:THR:HG21	1.69	0.56
1:A:130:SER:HB2	2:A:500:NAD:O3D	2.04	0.56
1:E:276:CYS:SG	3:E:501:UPG:C6'	2.93	0.56
1:F:352:TYR:CD1	1:F:352:TYR:C	2.78	0.56
1:A:131:THR:HB	2:A:500:NAD:H4D	1.86	0.56
1:K:165:GLU:O	1:K:339:LYS:CE	2.50	0.56
1:C:131:THR:H	2:C:500:NAD:H4D	1.69	0.56
1:F:276:CYS:HB2	3:F:501:UPG:O6'	2.05	0.56
3:L:501:UPG:O2'	3:L:501:UPG:O1A	2.24	0.56
1:F:335:GLY:HA3	1:F:415:THR:HB	1.88	0.56
1:E:233:SER:O	1:E:237:ILE:HG12	2.04	0.56
1:F:129:LYS:HE3	1:F:161:GLU:HB2	1.88	0.55
1:K:426:GLU:OE2	1:K:455:ILE:HG13	2.06	0.55
1:G:323:PHE:HE1	1:I:142:ARG:HD3	1.69	0.55
1:F:53:TYR:CD2	1:F:370:LYS:HG2	2.42	0.55
1:A:276:CYS:HB2	3:A:501:UPG:H6'2	1.88	0.55
1:D:218:LEU:HD11	1:C:240:LEU:HD23	1.88	0.55
1:I:187:GLU:N	1:I:188:GLY:HA3	2.21	0.55
1:G:98:MET:HG2	1:K:360:GLU:OE2	2.06	0.55
1:H:326:VAL:HG23	1:H:362:ALA:HB2	1.89	0.55
1:I:189:GLN:O	1:I:193:GLN:HG2	2.06	0.55
1:C:339:LYS:HE3	3:C:501:UPG:O2A	2.06	0.55
1:C:131:THR:HG22	1:C:132:VAL:HG23	1.88	0.55
1:F:141:ARG:NH2	1:F:213:THR:HG21	2.21	0.55
1:F:326:VAL:HA	1:F:329:LYS:HD2	1.87	0.55
1:H:381:SER:O	1:H:382:HIS:HB2	2.05	0.55
1:K:451:GLU:O	1:K:455:ILE:HD13	2.07	0.55
1:L:417:TRP:HB2	1:L:420:PHE:CE2	2.42	0.55
1:B:315:ALA:O	1:B:319:ILE:HG12	2.07	0.55
3:D:501:UPG:H1'	3:D:501:UPG:O1A	2.07	0.55
3:A:501:UPG:H1'	3:A:501:UPG:O1A	2.07	0.54
1:G:362:ALA:O	1:G:394:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:CYS:O	1:A:116:ILE:HG12	2.07	0.54
1:I:389:ASP:OD1	1:I:391:VAL:HG23	2.07	0.54
1:E:319:ILE:HD11	1:E:357:LEU:HD23	1.89	0.54
1:L:296:VAL:HG13	1:K:236:SER:HB2	1.89	0.54
1:K:50:LEU:HB3	1:K:51:PRO:HD2	1.88	0.54
1:I:412:VAL:HG22	1:I:439:PHE:HB2	1.89	0.54
1:J:390:GLN:HG2	1:J:394:LEU:HD12	1.88	0.54
1:A:276:CYS:SG	3:A:501:UPG:C6'	2.93	0.54
1:I:112:CYS:O	1:I:116:ILE:HG12	2.07	0.54
1:B:326:VAL:HG22	1:B:360:GLU:CB	2.28	0.54
1:H:319:ILE:HG22	1:H:324:ASN:HA	1.90	0.54
1:E:124:LYS:HB2	1:E:154:LEU:HD23	1.89	0.54
1:C:276:CYS:HB2	3:C:501:UPG:H6'2	1.90	0.54
1:F:451:GLU:O	1:F:455:ILE:HD12	2.07	0.54
1:J:24:ALA:O	1:J:68:ASN:ND2	2.41	0.54
1:H:326:VAL:CG2	1:H:362:ALA:HB2	2.38	0.53
1:K:326:VAL:CG2	1:K:360:GLU:CB	2.86	0.53
1:E:263:ASN:OD1	1:E:264:LYS:HE3	2.08	0.53
1:G:187:GLU:H	1:G:188:GLY:HA3	1.71	0.53
1:I:319:ILE:HG22	1:I:324:ASN:HA	1.90	0.53
1:C:310:GLN:OE1	1:C:313:ARG:NH2	2.41	0.53
1:B:319:ILE:HG22	1:B:324:ASN:HA	1.91	0.53
1:A:7:ILE:HD11	1:A:30:ILE:HD11	1.90	0.53
1:E:94:LYS:HG2	1:E:105:ASP:HB2	1.90	0.53
1:F:42:ILE:HG21	1:F:73:THR:HG23	1.90	0.53
1:A:340:LYS:HB3	1:A:416:GLU:HG2	1.90	0.53
1:H:276:CYS:SG	3:H:501:UPG:C6'	2.93	0.53
1:K:462:ILE:CD1	1:K:462:ILE:C	2.68	0.53
1:I:129:LYS:HE3	1:I:161:GLU:HB2	1.89	0.53
1:B:451:GLU:O	1:B:455:ILE:HG13	2.09	0.53
1:K:417:TRP:HB2	1:K:420:PHE:CD2	2.44	0.53
1:A:165:GLU:O	1:A:339:LYS:HE2	2.07	0.52
1:C:419:MET:O	1:C:423:LEU:HD13	2.09	0.52
1:C:187:GLU:N	1:C:188:GLY:HA3	2.24	0.52
1:F:131:THR:H	2:F:500:NAD:HO3N	1.55	0.52
1:E:10:ILE:HA	1:E:35:VAL:HG23	1.92	0.52
1:A:242:GLU:HB3	1:A:465:LYS:HE3	1.91	0.52
1:D:390:GLN:HG2	1:D:390:GLN:O	2.09	0.52
1:L:112:CYS:O	1:L:116:ILE:HG12	2.10	0.52
1:A:39:GLU:HG2	1:A:73:THR:HG21	1.92	0.52
1:L:267:LYS:HG2	4:L:506:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:GLN:OE1	1:G:313:ARG:NH2	2.42	0.52
1:F:310:GLN:OE1	1:F:313:ARG:NH2	2.41	0.52
1:A:200:GLU:OE2	1:A:205:ARG:CD	2.58	0.52
1:K:333:ILE:HD13	1:K:412:VAL:HB	1.92	0.52
1:J:317:ARG:NH2	1:J:460:GLU:HB3	2.25	0.52
1:D:41:ARG:NE	2:D:500:NAD:O3B	2.43	0.52
1:B:142:ARG:HD3	1:D:323:PHE:HE1	1.73	0.52
1:D:39:GLU:HG2	1:D:73:THR:HG21	1.91	0.52
1:E:276:CYS:CB	3:E:501:UPG:O6'	2.55	0.51
1:L:39:GLU:HG2	1:L:73:THR:HG21	1.91	0.51
1:B:129:LYS:HE2	1:B:161:GLU:OE1	2.09	0.51
1:K:405:CYS:HB3	1:K:428:ILE:HG23	1.92	0.51
1:G:281:VAL:HB	1:G:304:ILE:HD11	1.91	0.51
1:K:90:ASN:OD1	2:K:500:NAD:H8A	2.11	0.51
1:K:276:CYS:HB2	3:K:501:UPG:O6'	2.11	0.51
1:C:276:CYS:CB	3:C:501:UPG:H6'2	2.41	0.51
1:G:58:LYS:HE3	1:G:62:GLU:OE1	2.11	0.51
1:C:451:GLU:O	1:C:455:ILE:HD12	2.10	0.51
1:L:265:PHE:HZ	3:L:501:UPG:O1A	1.94	0.51
1:F:233:SER:O	1:F:236:SER:OG	2.26	0.51
1:F:47:SER:HB2	1:F:48:PRO:HD2	1.93	0.51
3:J:501:UPG:O2'	1:I:260:ARG:NH1	2.42	0.50
1:C:152:LEU:HD11	1:C:154:LEU:HG	1.93	0.50
3:G:501:UPG:O1A	3:G:501:UPG:H1'	2.11	0.50
1:G:131:THR:HG22	2:G:500:NAD:O2D	2.11	0.50
1:I:276:CYS:SG	3:I:501:UPG:O6'	2.59	0.50
1:C:352:TYR:HH	1:C:356:TYR:HD2	1.59	0.50
1:F:281:VAL:HB	1:F:304:ILE:HD11	1.94	0.50
1:L:141:ARG:NH2	1:L:213:THR:HG21	2.26	0.50
1:L:319:ILE:HG22	1:L:324:ASN:HA	1.93	0.50
1:K:14:TYR:HB2	2:K:500:NAD:O1N	2.12	0.50
1:I:374:GLU:O	1:I:377:VAL:CG2	2.60	0.50
1:H:131:THR:H	2:H:500:NAD:H4D	1.77	0.50
1:A:380:LEU:O	1:A:391:VAL:HG22	2.12	0.50
1:A:401:PRO:O	1:A:404:ALA:HB3	2.12	0.50
3:K:501:UPG:C1'	3:K:501:UPG:O1A	2.60	0.50
1:K:328:ASP:HA	1:K:363:HIS:ND1	2.27	0.49
3:C:501:UPG:O1A	3:C:501:UPG:H1'	2.12	0.49
1:F:90:ASN:OD1	2:F:500:NAD:H8A	2.11	0.49
1:A:315:ALA:O	1:A:319:ILE:HG12	2.13	0.49
1:J:276:CYS:SG	3:J:501:UPG:H6'1	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:GLN:HG2	1:D:394:LEU:HD12	1.93	0.49
1:K:124:LYS:HB2	1:K:154:LEU:HD23	1.94	0.49
1:I:116:ILE:O	1:I:120:SER:HB2	2.12	0.49
1:G:318:ILE:HA	1:G:439:PHE:CZ	2.47	0.49
1:E:242:GLU:OE1	1:E:313:ARG:NH1	2.46	0.49
1:G:236:SER:HB2	1:H:296:VAL:HG13	1.94	0.49
1:I:42:ILE:HG21	1:I:73:THR:HG21	1.87	0.49
1:C:200:GLU:OE1	1:C:205:ARG:CZ	2.61	0.49
1:H:213:THR:O	1:H:216:SER:HB3	2.12	0.49
1:D:231:ILE:HD11	1:D:265:PHE:CD2	2.48	0.49
1:B:276:CYS:HB2	3:B:501:UPG:H6'2	1.95	0.49
1:J:90:ASN:OD1	2:J:500:NAD:H8A	2.13	0.49
1:G:389:ASP:O	1:G:390:GLN:C	2.52	0.48
1:D:326:VAL:CG2	1:D:360:GLU:HB2	2.42	0.48
1:A:205:ARG:NH1	1:A:205:ARG:CG	2.71	0.48
1:K:93:THR:HA	1:K:104:ALA:HA	1.95	0.48
1:I:376:ILE:O	1:I:376:ILE:HG22	2.13	0.48
1:E:7:ILE:HG13	1:E:30:ILE:HD11	1.95	0.48
1:H:315:ALA:O	1:H:319:ILE:HG12	2.13	0.48
1:E:85:VAL:HG11	1:E:116:ILE:CD1	2.40	0.48
1:L:130:SER:HB2	2:L:500:NAD:O3D	2.13	0.48
1:J:319:ILE:HD12	1:J:360:GLU:HG3	1.95	0.48
1:A:205:ARG:HG3	1:A:205:ARG:HH11	1.76	0.48
1:C:189:GLN:O	1:C:193:GLN:HG2	2.12	0.48
1:C:242:GLU:HB3	1:C:465:LYS:HE2	1.95	0.48
1:K:182:GLY:O	1:K:212:ASN:HA	2.13	0.48
1:K:276:CYS:HB2	3:K:501:UPG:C6'	2.44	0.48
1:F:131:THR:HB	2:F:500:NAD:O3D	2.14	0.48
1:L:131:THR:HG23	3:L:501:UPG:H6'2	1.95	0.48
1:G:45:TRP:O	1:G:65:ARG:NH1	2.44	0.48
1:B:104:ALA:HB3	1:B:134:VAL:HG21	1.94	0.48
1:F:356:TYR:CD1	1:F:356:TYR:C	2.86	0.48
1:H:405:CYS:HB3	1:H:428:ILE:HG23	1.96	0.48
1:K:131:THR:HG21	1:K:276:CYS:HB2	1.96	0.47
1:L:27:CYS:HB2	1:L:30:ILE:HG12	1.95	0.47
1:K:242:GLU:OE1	1:K:313:ARG:NH1	2.47	0.47
1:G:56:GLY:HA2	1:G:59:GLU:OE2	2.13	0.47
1:E:326:VAL:CG2	1:E:360:GLU:CB	2.92	0.47
1:K:102:ARG:NH2	1:K:289:GLU:CD	2.63	0.47
1:L:7:ILE:HB	1:L:32:VAL:HG22	1.95	0.47
1:F:244:THR:HB	1:E:214:TRP:NE1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:ALA:O	1:L:226:PHE:HD1	1.97	0.47
1:D:276:CYS:CB	3:D:501:UPG:O6'	2.62	0.47
1:I:153:ASN:OD1	1:I:155:GLN:NE2	2.48	0.47
1:K:417:TRP:HB2	1:K:420:PHE:CE2	2.49	0.47
1:L:260:ARG:HH12	3:K:501:UPG:HO2'	1.61	0.47
1:G:27:CYS:HB3	1:G:30:ILE:CG2	2.44	0.47
1:I:200:GLU:OE1	1:I:205:ARG:CZ	2.63	0.47
1:H:277:PHE:CE2	3:H:501:UPG:H5C2	2.49	0.47
1:K:131:THR:HG22	1:K:132:VAL:HG23	1.96	0.47
1:K:131:THR:HG23	3:K:501:UPG:O6'	2.15	0.47
1:E:315:ALA:O	1:E:319:ILE:HG12	2.15	0.47
1:L:128:GLU:HG3	1:L:136:ALA:HB1	1.94	0.47
1:A:135:ARG:NH1	1:A:138:GLU:OE1	2.48	0.47
1:K:131:THR:CG2	3:K:501:UPG:H6'1	2.44	0.47
1:L:36:ASP:OD2	2:L:500:NAD:H1B	2.14	0.47
1:H:326:VAL:CG2	1:H:326:VAL:O	2.61	0.47
1:I:378:VAL:O	1:I:378:VAL:HG12	2.15	0.47
1:G:165:GLU:O	1:G:339:LYS:HE2	2.15	0.47
1:A:24:ALA:O	1:A:68:ASN:ND2	2.48	0.47
1:L:275:SER:HB3	1:L:346:ARG:HD2	1.96	0.47
1:A:429:HIS:HB2	1:A:457:PHE:CE2	2.49	0.47
1:K:220:LYS:NZ	1:K:224:ASN:HD21	2.13	0.47
1:L:369:PRO:O	1:L:370:LYS:HD2	2.15	0.47
1:I:442:ARG:HB3	1:I:444:VAL:HG13	1.96	0.47
1:E:332:ALA:HB2	1:E:404:ALA:O	2.15	0.47
1:A:130:SER:HB2	2:A:500:NAD:HO3N	1.78	0.46
1:J:131:THR:HG22	1:J:132:VAL:HG23	1.96	0.46
1:J:39:GLU:HG2	1:J:73:THR:HG21	1.96	0.46
1:K:98:MET:HA	1:K:99:GLY:HA2	1.64	0.46
1:D:24:ALA:O	1:D:68:ASN:ND2	2.49	0.46
1:I:381:SER:HB2	1:I:391:VAL:HG21	1.91	0.46
1:C:72:SER:C	1:C:73:THR:HG23	2.36	0.46
1:D:131:THR:HB	2:D:500:NAD:O3D	2.15	0.46
1:B:329:LYS:HG2	1:B:409:HIS:CD2	2.51	0.46
1:A:434:LYS:HA	1:A:435:PRO:C	2.35	0.46
1:F:285:VAL:HG13	1:F:297:ALA:HB1	1.98	0.46
1:E:140:ILE:HG22	1:E:144:PHE:CE2	2.51	0.46
1:E:326:VAL:CG2	1:E:360:GLU:HB3	2.42	0.46
1:D:131:THR:HG22	1:D:132:VAL:HG23	1.96	0.46
1:L:417:TRP:HB2	1:L:420:PHE:CD2	2.51	0.46
1:D:95:THR:O	1:D:100:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LYS:HA	1:D:435:PRO:C	2.36	0.46
1:H:6:LYS:HD3	1:H:81:GLU:HG2	1.97	0.46
1:D:36:ASP:OD2	2:D:500:NAD:H1B	2.16	0.46
1:C:330:LYS:HB3	1:C:408:ALA:HA	1.97	0.46
1:A:192:VAL:O	1:A:196:CYS:HB2	2.16	0.46
1:C:242:GLU:OE1	1:C:313:ARG:NH1	2.49	0.46
1:L:24:ALA:O	1:L:68:ASN:ND2	2.49	0.46
1:C:407:GLY:N	1:C:431:LYS:O	2.43	0.46
1:A:242:GLU:CD	1:A:313:ARG:HH12	2.18	0.46
1:D:108:TYR:HB3	2:D:500:NAD:H61A	1.81	0.45
1:L:238:SER:O	1:L:242:GLU:HG3	2.17	0.45
1:D:139:SER:O	1:D:143:ILE:HG12	2.15	0.45
1:L:13:GLY:HA3	2:L:500:NAD:O2A	2.16	0.45
1:G:312:ARG:HG2	4:G:531:HOH:O	2.16	0.45
1:I:421:LYS:HB3	1:I:421:LYS:HE2	1.82	0.45
1:I:382:HIS:O	1:I:382:HIS:CG	2.68	0.45
1:B:105:ASP:OD1	1:D:325:THR:HG21	2.16	0.45
1:A:189:GLN:O	1:A:193:GLN:HG2	2.17	0.45
1:F:389:ASP:C	1:F:389:ASP:OD2	2.55	0.45
1:C:30:ILE:O	1:C:68:ASN:OD1	2.34	0.45
1:D:326:VAL:HA	1:D:329:LYS:HD2	1.98	0.45
1:F:207:LYS:HE2	4:F:499:HOH:O	2.17	0.45
1:C:438:ILE:HB	1:C:459:ILE:HD12	1.99	0.45
1:A:382:HIS:O	1:A:382:HIS:CG	2.69	0.45
3:J:501:UPG:O1A	3:J:501:UPG:C1'	2.63	0.45
1:E:161:GLU:HG3	1:E:163:LEU:HG	1.97	0.45
1:C:11:GLY:O	1:C:16:GLY:HA3	2.17	0.45
1:K:13:GLY:HA3	2:K:500:NAD:O5B	2.17	0.45
1:J:291:LEU:O	1:J:292:ASN:HB2	2.17	0.45
1:K:276:CYS:CB	3:K:501:UPG:C6'	2.94	0.45
1:G:315:ALA:O	1:G:319:ILE:HG12	2.17	0.45
1:G:226:PHE:CZ	1:H:233:SER:HB3	2.51	0.45
1:K:56:GLY:O	1:K:60:VAL:HG23	2.16	0.45
1:H:26:MET:HG3	1:H:202:TRP:CD2	2.52	0.45
1:L:352:TYR:HD1	1:L:353:ILE:N	2.15	0.44
1:G:389:ASP:OD2	1:G:390:GLN:N	2.48	0.44
1:F:26:MET:CE	1:F:173:LYS:HG2	2.47	0.44
1:E:326:VAL:HG22	1:E:360:GLU:CB	2.42	0.44
1:F:244:THR:CB	1:E:214:TRP:HE1	2.31	0.44
1:G:38:ASN:ND2	1:G:41:ARG:HB2	2.33	0.44
1:J:124:LYS:HB2	1:J:154:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:LEU:HD11	1:L:127:THR:OG1	2.16	0.44
1:L:424:ASP:OD2	1:L:427:ARG:HB2	2.17	0.44
1:B:101:GLY:C	1:B:102:ARG:HG3	2.37	0.44
1:J:36:ASP:OD2	2:J:500:NAD:H1B	2.18	0.44
1:J:281:VAL:O	1:J:285:VAL:HG23	2.16	0.44
1:K:39:GLU:HG2	1:K:73:THR:HG21	1.99	0.44
1:C:276:CYS:SG	3:C:501:UPG:C6'	3.04	0.44
1:D:90:ASN:HA	2:D:500:NAD:H51N	1.99	0.44
1:C:129:LYS:HE3	1:C:161:GLU:HB2	1.99	0.44
1:G:106:LEU:H	1:K:325:THR:HG21	1.82	0.44
1:J:210:THR:HB	4:J:515:HOH:O	2.16	0.44
1:H:27:CYS:HB2	1:H:30:ILE:HG23	2.00	0.44
1:A:106:LEU:HD21	1:A:134:VAL:O	2.16	0.44
1:A:429:HIS:HB2	1:A:457:PHE:CZ	2.53	0.44
1:C:333:ILE:HD13	1:C:412:VAL:HB	2.00	0.44
1:E:27:CYS:HB2	1:E:30:ILE:CG2	2.48	0.44
1:G:135:ARG:NH1	1:G:138:GLU:OE1	2.45	0.44
1:E:135:ARG:HB3	1:E:135:ARG:NH1	2.33	0.44
1:H:368:ASP:OD2	1:H:371:VAL:HG23	2.18	0.44
1:J:129:LYS:NZ	1:J:199:TYR:OH	2.51	0.44
1:K:131:THR:CG2	1:K:276:CYS:HB2	2.48	0.44
1:K:221:LEU:HD23	1:K:280:ASP:OD1	2.17	0.44
1:C:331:ILE:HD12	1:C:362:ALA:HB1	2.00	0.44
1:D:129:LYS:HE2	1:D:161:GLU:HB2	2.00	0.43
1:A:142:ARG:HD3	1:E:323:PHE:HE1	1.83	0.43
1:L:316:SER:O	1:L:320:ASP:HB2	2.18	0.43
1:L:129:LYS:NZ	1:L:159:ASN:OD1	2.50	0.43
1:B:276:CYS:CB	3:B:501:UPG:H6'2	2.48	0.43
1:D:276:CYS:SG	3:D:501:UPG:H6'1	2.58	0.43
1:I:276:CYS:HB2	3:I:501:UPG:H6'2	1.99	0.43
1:C:316:SER:O	1:C:320:ASP:HB2	2.17	0.43
1:C:421:LYS:HE3	1:C:422:GLU:OE1	2.18	0.43
1:H:462:ILE:HG13	1:H:462:ILE:O	2.18	0.43
1:I:380:LEU:HD13	1:I:395:VAL:HG21	2.01	0.43
1:K:27:CYS:HB2	1:K:30:ILE:CG2	2.48	0.43
1:K:131:THR:CG2	3:K:501:UPG:C6'	2.96	0.43
1:E:90:ASN:OD1	2:E:500:NAD:H8A	2.18	0.43
1:E:35:VAL:HG11	1:E:75:ILE:HA	2.00	0.43
1:F:236:SER:HB2	1:E:296:VAL:HG13	1.99	0.43
1:F:356:TYR:HD1	1:F:356:TYR:C	2.20	0.43
1:D:90:ASN:OD1	2:D:500:NAD:H8A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:LYS:HG2	1:F:105:ASP:HB2	2.00	0.43
1:E:26:MET:HG3	1:E:202:TRP:CD2	2.54	0.43
1:F:276:CYS:CB	3:F:501:UPG:O6'	2.67	0.43
1:L:131:THR:N	2:L:500:NAD:O3D	2.50	0.43
1:A:27:CYS:HB3	1:A:30:ILE:HG23	2.00	0.43
1:J:139:SER:O	1:J:143:ILE:HG12	2.19	0.43
1:F:128:GLU:HG3	1:F:136:ALA:HB1	2.00	0.43
1:J:434:LYS:HA	1:J:435:PRO:C	2.39	0.43
1:E:319:ILE:CD1	1:E:360:GLU:HG3	2.45	0.43
1:J:131:THR:HG22	2:J:500:NAD:O2D	2.19	0.43
1:D:129:LYS:HE2	1:D:161:GLU:OE1	2.19	0.43
1:J:60:VAL:HG21	1:J:169:ILE:HD12	2.00	0.43
1:D:281:VAL:O	1:D:285:VAL:HG23	2.18	0.43
1:A:276:CYS:SG	3:A:501:UPG:H6'2	2.59	0.43
1:G:90:ASN:OD1	2:G:500:NAD:H8A	2.19	0.43
1:L:374:GLU:O	1:L:377:VAL:HG22	2.18	0.43
1:B:279:LYS:NZ	4:B:553:HOH:O	2.50	0.43
1:J:462:ILE:O	1:J:462:ILE:HG13	2.18	0.43
1:K:421:LYS:HB2	1:K:421:LYS:HE2	1.63	0.43
1:A:277:PHE:O	1:A:281:VAL:HG23	2.19	0.42
1:E:192:VAL:O	1:E:196:CYS:HB2	2.19	0.42
1:G:107:LYS:HE3	1:G:108:TYR:CZ	2.54	0.42
1:F:165:GLU:O	1:F:339:LYS:NZ	2.32	0.42
1:B:268:ALA:HB1	1:B:462:ILE:HD11	2.00	0.42
1:A:20:CYS:HB3	1:A:32:VAL:HG11	2.01	0.42
1:C:124:LYS:HB2	1:C:154:LEU:HD23	2.01	0.42
1:A:277:PHE:CE2	3:A:501:UPG:H5C2	2.54	0.42
1:A:416:GLU:HG2	1:A:416:GLU:O	2.19	0.42
1:E:163:LEU:HD12	1:E:163:LEU:O	2.19	0.42
1:I:317:ARG:NH2	1:I:460:GLU:HB3	2.34	0.42
1:C:101:GLY:C	1:C:102:ARG:HG3	2.39	0.42
1:F:428:ILE:O	1:F:432:MET:HG3	2.18	0.42
1:I:72:SER:C	1:I:73:THR:HG23	2.40	0.42
1:E:319:ILE:CD1	1:E:357:LEU:HD23	2.50	0.42
1:H:327:THR:O	1:H:328:ASP:HB2	2.19	0.42
1:B:434:LYS:HA	1:B:435:PRO:C	2.40	0.42
1:E:14:TYR:HB2	2:E:500:NAD:O1N	2.20	0.42
1:L:326:VAL:O	1:L:329:LYS:HB2	2.19	0.42
1:L:451:GLU:O	1:L:455:ILE:HD12	2.19	0.42
1:G:163:LEU:C	1:G:163:LEU:HD12	2.40	0.42
1:G:382:HIS:ND1	1:G:382:HIS:C	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:CE1	1:A:434:LYS:HE3	2.55	0.42
1:C:24:ALA:O	1:C:68:ASN:ND2	2.53	0.42
1:E:129:LYS:HE2	1:E:161:GLU:OE1	2.20	0.42
1:H:317:ARG:NH2	1:H:460:GLU:OE1	2.47	0.42
1:E:231:ILE:O	1:E:234:ILE:HG22	2.20	0.42
1:J:326:VAL:HG22	1:J:360:GLU:CB	2.45	0.42
1:L:450:ASN:O	1:L:454:THR:HG23	2.20	0.42
1:L:174:ASN:CG	1:L:174:ASN:O	2.58	0.42
1:D:315:ALA:O	1:D:319:ILE:HG12	2.20	0.42
1:L:416:GLU:N	1:L:442:ARG:HG2	2.35	0.42
1:I:377:VAL:HG23	1:I:378:VAL:N	2.35	0.42
1:H:374:GLU:O	1:H:378:VAL:HG23	2.20	0.42
1:H:54:GLU:OE2	1:H:166:GLY:N	2.50	0.42
1:A:369:PRO:HG3	1:A:419:MET:SD	2.59	0.42
1:E:14:TYR:N	2:E:500:NAD:O1N	2.53	0.42
1:A:131:THR:HG22	1:A:132:VAL:HG23	2.02	0.41
1:A:129:LYS:HE3	1:A:161:GLU:HB2	2.02	0.41
1:L:406:ASP:OD1	1:L:431:LYS:HD3	2.20	0.41
1:L:220:LYS:HZ3	3:L:501:UPG:C6'	2.33	0.41
1:C:42:ILE:HG21	1:C:73:THR:CG2	2.50	0.41
1:C:423:LEU:HD12	1:C:423:LEU:HA	1.68	0.41
1:F:53:TYR:CG	1:F:370:LYS:HG2	2.55	0.41
1:J:260:ARG:NH1	3:I:501:UPG:O2'	2.52	0.41
1:H:403:GLU:OE1	1:H:403:GLU:O	2.39	0.41
1:F:439:PHE:HA	1:F:460:GLU:O	2.19	0.41
3:H:501:UPG:C1'	3:H:501:UPG:O1A	2.64	0.41
1:D:326:VAL:CG2	1:D:360:GLU:CB	2.95	0.41
1:E:319:ILE:HG22	1:E:324:ASN:HA	2.01	0.41
1:A:124:LYS:HB2	1:A:154:LEU:HD23	2.03	0.41
1:E:371:VAL:HA	1:E:372:PRO:HD3	1.96	0.41
1:C:150:PRO:C	1:C:152:LEU:H	2.24	0.41
1:H:389:ASP:HB2	1:H:390:GLN:H	1.69	0.41
1:G:128:GLU:HG3	1:G:136:ALA:HB1	2.02	0.41
1:J:369:PRO:HG3	1:J:419:MET:SD	2.60	0.41
1:A:236:SER:HB2	1:B:296:VAL:HG13	2.02	0.41
1:F:276:CYS:SG	3:F:501:UPG:H6'1	2.60	0.41
3:F:501:UPG:O2'	1:E:260:ARG:NH1	2.32	0.41
1:J:317:ARG:HH21	1:J:460:GLU:HB3	1.85	0.41
1:I:354:SER:HB2	1:I:380:LEU:HD21	2.02	0.41
1:H:56:GLY:O	1:H:60:VAL:HG23	2.21	0.41
1:F:112:CYS:O	1:F:116:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:OD1	1:A:107:LYS:HG2	2.21	0.41
1:K:369:PRO:C	1:K:370:LYS:HD2	2.41	0.41
1:F:356:TYR:CD1	1:F:356:TYR:O	2.74	0.41
1:L:50:LEU:HB3	1:L:51:PRO:HD2	2.03	0.41
1:F:292:ASN:C	1:F:294:PRO:HD3	2.40	0.41
1:I:72:SER:C	1:I:73:THR:CG2	2.89	0.41
1:G:276:CYS:HB2	3:G:501:UPG:H6'2	2.01	0.41
1:G:131:THR:H	2:G:500:NAD:HO3N	1.64	0.41
1:L:420:PHE:HA	1:L:423:LEU:HD22	2.03	0.41
1:E:45:TRP:CE3	1:E:50:LEU:HD22	2.56	0.41
1:H:183:ASP:C	1:H:185:THR:H	2.24	0.41
1:I:438:ILE:HB	1:I:459:ILE:HD12	2.03	0.41
1:I:1:MET:N	4:I:498:HOH:O	2.52	0.41
1:F:50:LEU:HB3	1:F:51:PRO:HD2	2.03	0.41
1:L:369:PRO:HD2	1:L:417:TRP:CE2	2.56	0.41
1:L:369:PRO:HG3	1:L:419:MET:SD	2.60	0.41
1:F:244:THR:HB	1:E:214:TRP:HE1	1.84	0.41
1:K:24:ALA:O	1:K:68:ASN:ND2	2.54	0.41
1:G:35:VAL:HA	1:G:72:SER:O	2.22	0.41
1:L:117:VAL:HG11	1:L:147:ASN:HB3	2.02	0.41
1:K:326:VAL:CG2	1:K:360:GLU:HB2	2.51	0.40
1:K:281:VAL:O	1:K:285:VAL:HG23	2.21	0.40
1:C:35:VAL:HG11	1:C:78:ALA:CB	2.51	0.40
1:J:330:LYS:HE3	1:J:365:HIS:CD2	2.56	0.40
1:A:424:ASP:OD1	1:A:426:GLU:HB2	2.21	0.40
1:H:213:THR:HG22	1:H:214:TRP:N	2.37	0.40
1:F:47:SER:HB2	1:F:48:PRO:CD	2.51	0.40
1:K:15:VAL:O	1:K:16:GLY:C	2.60	0.40
1:I:292:ASN:C	1:I:294:PRO:HD3	2.42	0.40
1:J:180:ILE:HG12	1:J:195:LEU:HD23	2.02	0.40
1:H:251:VAL:O	1:H:255:ILE:HG13	2.21	0.40
1:E:94:LYS:HG2	1:E:105:ASP:CB	2.51	0.40
1:K:328:ASP:HA	1:K:363:HIS:CE1	2.57	0.40
1:K:84:LEU:HD12	1:K:125:ILE:HB	2.03	0.40
1:K:319:ILE:HG22	1:K:324:ASN:HA	2.04	0.40
1:C:462:ILE:HD13	1:C:462:ILE:HG21	1.72	0.40
1:H:443:ARG:HD3	1:H:443:ARG:HH11	1.70	0.40
1:K:265:PHE:HA	3:K:501:UPG:O4	2.22	0.40
1:K:131:THR:HG21	3:K:501:UPG:C6'	2.52	0.40
1:B:277:PHE:CE2	3:B:501:UPG:H5C2	2.57	0.40
1:C:200:GLU:OE1	1:C:205:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:CYS:SG	1:F:205:ARG:NH2	2.94	0.40
1:D:275:SER:HB3	1:D:346:ARG:HD2	2.03	0.40
1:G:336:PHE:CD1	1:G:366:ILE:HG21	2.57	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	456/487 (94%)	438 (96%)	18 (4%)	0	100	100
1	B	456/487 (94%)	439 (96%)	17 (4%)	0	100	100
1	C	456/487 (94%)	441 (97%)	15 (3%)	0	100	100
1	D	456/487 (94%)	440 (96%)	16 (4%)	0	100	100
1	E	454/487 (93%)	438 (96%)	16 (4%)	0	100	100
1	F	456/487 (94%)	433 (95%)	23 (5%)	0	100	100
1	G	456/487 (94%)	441 (97%)	15 (3%)	0	100	100
1	H	456/487 (94%)	442 (97%)	14 (3%)	0	100	100
1	I	456/487 (94%)	436 (96%)	20 (4%)	0	100	100
1	J	456/487 (94%)	436 (96%)	20 (4%)	0	100	100
1	K	454/487 (93%)	436 (96%)	18 (4%)	0	100	100
1	L	456/487 (94%)	434 (95%)	22 (5%)	0	100	100
All	All	5468/5844 (94%)	5254 (96%)	214 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	395/419 (94%)	377 (95%)	18 (5%)	33	67
1	B	395/419 (94%)	372 (94%)	23 (6%)	25	57
1	C	395/419 (94%)	369 (93%)	26 (7%)	21	51
1	D	395/419 (94%)	378 (96%)	17 (4%)	35	70
1	E	393/419 (94%)	374 (95%)	19 (5%)	31	66
1	F	395/419 (94%)	371 (94%)	24 (6%)	23	55
1	G	395/419 (94%)	377 (95%)	18 (5%)	33	67
1	H	395/419 (94%)	375 (95%)	20 (5%)	29	63
1	I	395/419 (94%)	374 (95%)	21 (5%)	28	61
1	J	395/419 (94%)	380 (96%)	15 (4%)	40	74
1	K	393/419 (94%)	377 (96%)	16 (4%)	37	72
1	L	395/419 (94%)	373 (94%)	22 (6%)	26	59
All	All	4736/5028 (94%)	4497 (95%)	239 (5%)	30	64

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	29	GLU
1	A	30	ILE
1	A	37	VAL
1	A	129	LYS
1	A	131	THR
1	A	177	ARG
1	A	205	ARG
1	A	320	ASP
1	A	373	ARG
1	A	377	VAL
1	A	382	HIS
1	A	389	ASP

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Mol	Chain	Res	Type
1	A	422	GLU
1	A	423	LEU
1	A	442	ARG
1	A	459	ILE
1	B	5	LYS
1	B	29	GLU
1	B	30	ILE
1	B	39	GLU
1	B	49	THR
1	B	98	MET
1	B	129	LYS
1	B	131	THR
1	B	134	VAL
1	B	135	ARG
1	B	177	ARG
1	B	205	ARG
1	B	325	THR
1	B	326	VAL
1	B	373	ARG
1	B	377	VAL
1	B	380	LEU
1	B	422	GLU
1	B	423	LEU
1	B	442	ARG
1	B	459	ILE
1	B	462	ILE
1	B	465	LYS
1	G	5	LYS
1	G	29	GLU
1	G	30	ILE
1	G	129	LYS
1	G	131	THR
1	G	177	ARG
1	G	196	CYS
1	G	215	SER
1	G	319	ILE
1	G	339	LYS
1	G	366	ILE
1	G	373	ARG
1	G	382	HIS
1	G	389	ASP
1	G	422	GLU

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Mol	Chain	Res	Type
1	G	423	LEU
1	G	442	ARG
1	G	459	ILE
1	H	5	LYS
1	H	29	GLU
1	H	30	ILE
1	H	129	LYS
1	H	131	THR
1	H	135	ARG
1	H	142	ARG
1	H	177	ARG
1	H	205	ARG
1	H	213	THR
1	H	325	THR
1	H	366	ILE
1	H	377	VAL
1	H	389	ASP
1	H	390	GLN
1	H	396	THR
1	H	403	GLU
1	H	442	ARG
1	H	459	ILE
1	H	465	LYS
1	L	1	MET
1	L	3	GLU
1	L	29	GLU
1	L	37	VAL
1	L	58	LYS
1	L	81	GLU
1	L	93	THR
1	L	116	ILE
1	L	177	ARG
1	L	187	GLU
1	L	196	CYS
1	L	205	ARG
1	L	215	SER
1	L	356	TYR
1	L	373	ARG
1	L	382	HIS
1	L	390	GLN
1	L	400	ASP
1	L	423	LEU

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Mol	Chain	Res	Type
1	L	442	ARG
1	L	455	ILE
1	L	459	ILE
1	K	29	GLU
1	K	37	VAL
1	K	100	LYS
1	K	102	ARG
1	K	131	THR
1	K	135	ARG
1	K	177	ARG
1	K	196	CYS
1	K	205	ARG
1	K	373	ARG
1	K	396	THR
1	K	421	LYS
1	K	423	LEU
1	K	442	ARG
1	K	459	ILE
1	K	464	LYS
1	F	29	GLU
1	F	30	ILE
1	F	37	VAL
1	F	58	LYS
1	F	67	LYS
1	F	93	THR
1	F	131	THR
1	F	135	ARG
1	F	142	ARG
1	F	170	LYS
1	F	173	LYS
1	F	177	ARG
1	F	196	CYS
1	F	205	ARG
1	F	215	SER
1	F	356	TYR
1	F	373	ARG
1	F	381	SER
1	F	389	ASP
1	F	423	LEU
1	F	442	ARG
1	F	455	ILE
1	F	459	ILE

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Mol	Chain	Res	Type
1	F	466	VAL
1	E	5	LYS
1	E	29	GLU
1	E	37	VAL
1	E	58	LYS
1	E	84	LEU
1	E	120	SER
1	E	131	THR
1	E	135	ARG
1	E	177	ARG
1	E	196	CYS
1	E	205	ARG
1	E	325	THR
1	E	373	ARG
1	E	421	LYS
1	E	423	LEU
1	E	442	ARG
1	E	455	ILE
1	E	459	ILE
1	E	466	VAL
1	D	29	GLU
1	D	30	ILE
1	D	58	LYS
1	D	84	LEU
1	D	129	LYS
1	D	131	THR
1	D	135	ARG
1	D	175	PRO
1	D	177	ARG
1	D	205	ARG
1	D	215	SER
1	D	389	ASP
1	D	390	GLN
1	D	442	ARG
1	D	444	VAL
1	D	459	ILE
1	D	465	LYS
1	C	29	GLU
1	C	73	THR
1	C	96	TYR
1	C	115	ARG
1	C	131	THR

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Mol	Chain	Res	Type
1	C	135	ARG
1	C	148	THR
1	C	152	LEU
1	C	177	ARG
1	C	205	ARG
1	C	206	GLU
1	C	213	THR
1	C	320	ASP
1	C	323	PHE
1	C	339	LYS
1	C	356	TYR
1	C	366	ILE
1	C	382	HIS
1	C	389	ASP
1	C	396	THR
1	C	422	GLU
1	C	423	LEU
1	C	442	ARG
1	C	455	ILE
1	C	459	ILE
1	C	466	VAL
1	J	5	LYS
1	J	29	GLU
1	J	131	THR
1	J	177	ARG
1	J	196	CYS
1	J	205	ARG
1	J	291	LEU
1	J	296	VAL
1	J	366	ILE
1	J	422	GLU
1	J	423	LEU
1	J	442	ARG
1	J	444	VAL
1	J	459	ILE
1	J	466	VAL
1	I	5	LYS
1	I	29	GLU
1	I	37	VAL
1	I	40	SER
1	I	73	THR
1	I	93	THR

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Mol	Chain	Res	Type
1	I	115	ARG
1	I	131	THR
1	I	142	ARG
1	I	152	LEU
1	I	177	ARG
1	I	184	GLU
1	I	205	ARG
1	I	366	ILE
1	I	375	GLN
1	I	382	HIS
1	I	396	THR
1	I	423	LEU
1	I	442	ARG
1	I	459	ILE
1	I	466	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	229	GLN
1	B	68	ASN
1	B	365	HIS
1	G	68	ASN
1	G	363	HIS
1	G	429	HIS
1	G	450	ASN
1	H	68	ASN
1	H	174	ASN
1	H	259	GLN
1	H	363	HIS
1	L	68	ASN
1	L	155	GLN
1	L	292	ASN
1	L	365	HIS
1	L	449	HIS
1	K	224	ASN
1	E	229	GLN
1	D	68	ASN
1	D	363	HIS
1	C	68	ASN
1	C	155	GLN

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Mol	Chain	Res	Type
1	C	193	GLN
1	C	409	HIS
1	J	68	ASN
1	J	363	HIS
1	J	365	HIS
1	I	68	ASN
1	I	153	ASN
1	I	155	GLN
1	I	365	HIS
1	I	375	GLN
1	I	382	HIS
1	I	449	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

24 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	500	-	31,38,48	1.24	4 (12%)	39,58,73	2.39	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UPG	A	501	-	29,38,38	1.44	3 (10%)	43,58,58	2.21	9 (20%)
2	NAD	B	500	-	31,38,48	1.17	2 (6%)	39,58,73	2.16	6 (15%)
3	UPG	B	501	-	29,38,38	1.71	4 (13%)	43,58,58	2.19	10 (23%)
2	NAD	C	500	-	31,38,48	1.12	1 (3%)	39,58,73	2.37	6 (15%)
3	UPG	C	501	-	29,38,38	1.50	2 (6%)	43,58,58	1.81	8 (18%)
2	NAD	D	500	-	31,38,48	1.34	3 (9%)	39,58,73	2.61	4 (10%)
3	UPG	D	501	-	29,38,38	0.81	1 (3%)	43,58,58	2.05	8 (18%)
2	NAD	E	500	-	31,38,48	1.31	3 (9%)	39,58,73	2.37	4 (10%)
3	UPG	E	501	-	29,38,38	0.65	0	43,58,58	1.71	7 (16%)
2	NAD	F	500	-	31,38,48	1.07	2 (6%)	39,58,73	2.55	7 (17%)
3	UPG	F	501	-	29,38,38	0.87	1 (3%)	43,58,58	1.96	9 (20%)
2	NAD	G	500	-	31,38,48	1.19	3 (9%)	39,58,73	2.27	5 (12%)
3	UPG	G	501	-	29,38,38	1.55	3 (10%)	43,58,58	1.96	10 (23%)
2	NAD	H	500	-	31,38,48	1.10	2 (6%)	39,58,73	1.97	7 (17%)
3	UPG	H	501	-	29,38,38	1.58	3 (10%)	43,58,58	2.41	9 (20%)
2	NAD	I	500	-	31,38,48	1.15	2 (6%)	39,58,73	2.27	6 (15%)
3	UPG	I	501	-	29,38,38	1.50	2 (6%)	43,58,58	1.94	9 (20%)
2	NAD	J	500	-	31,38,48	1.26	2 (6%)	39,58,73	2.59	6 (15%)
3	UPG	J	501	-	29,38,38	1.11	2 (6%)	43,58,58	1.88	8 (18%)
2	NAD	K	500	-	31,38,48	1.40	4 (12%)	39,58,73	2.20	5 (12%)
3	UPG	K	501	-	29,38,38	2.28	3 (10%)	43,58,58	2.21	10 (23%)
2	NAD	L	500	-	31,38,48	1.23	2 (6%)	39,58,73	2.37	4 (10%)
3	UPG	L	501	-	29,38,38	0.75	0	43,58,58	1.59	7 (16%)

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	500	-	-	0/18/51/62	0/4/4/5
3	UPG	A	501	-	-	0/19/59/59	0/3/3/3
2	NAD	B	500	-	-	0/18/51/62	0/4/4/5
3	UPG	B	501	-	-	0/19/59/59	0/3/3/3
2	NAD	C	500	-	-	0/18/51/62	0/4/4/5
3	UPG	C	501	-	-	0/19/59/59	0/3/3/3
2	NAD	D	500	-	-	0/18/51/62	0/4/4/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UPG	D	501	-	-	0/19/59/59	0/3/3/3
2	NAD	E	500	-	-	0/18/51/62	0/4/4/5
3	UPG	E	501	-	-	0/19/59/59	0/3/3/3
2	NAD	F	500	-	-	0/18/51/62	0/4/4/5
3	UPG	F	501	-	-	0/19/59/59	0/3/3/3
2	NAD	G	500	-	-	0/18/51/62	0/4/4/5
3	UPG	G	501	-	-	0/19/59/59	0/3/3/3
2	NAD	H	500	-	-	0/18/51/62	0/4/4/5
3	UPG	H	501	-	-	0/19/59/59	0/3/3/3
2	NAD	I	500	-	-	0/18/51/62	0/4/4/5
3	UPG	I	501	-	-	0/19/59/59	0/3/3/3
2	NAD	J	500	-	-	0/18/51/62	0/4/4/5
3	UPG	J	501	-	-	0/19/59/59	0/3/3/3
2	NAD	K	500	-	-	0/18/51/62	0/4/4/5
3	UPG	K	501	-	-	0/19/59/59	0/3/3/3
2	NAD	L	500	-	-	0/18/51/62	0/4/4/5
3	UPG	L	501	-	-	0/19/59/59	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	UPG	O6'-C6'	-4.51	1.22	1.42
3	G	501	UPG	O6'-C6'	-4.50	1.22	1.42
3	K	501	UPG	O6'-C6'	-4.37	1.23	1.42
3	C	501	UPG	O6'-C6'	-4.23	1.24	1.42
3	I	501	UPG	O6'-C6'	-4.21	1.24	1.42
3	B	501	UPG	O6'-C6'	-4.21	1.24	1.42
3	A	501	UPG	O6'-C6'	-4.19	1.24	1.42
2	A	500	NAD	O4B-C4B	-2.62	1.39	1.45
3	G	501	UPG	C6-N1	-2.48	1.32	1.35
3	K	501	UPG	C6-N1	-2.32	1.32	1.35
3	A	501	UPG	PB-O2B	-2.30	1.45	1.54
2	A	500	NAD	PN-O2N	-2.18	1.45	1.54
2	G	500	NAD	PN-O2N	-2.10	1.46	1.54
2	K	500	NAD	O4B-C1B	2.06	1.43	1.41
2	E	500	NAD	C4A-N3A	2.08	1.38	1.35
2	H	500	NAD	C2A-N1A	2.10	1.37	1.33
2	K	500	NAD	C4A-N3A	2.18	1.38	1.35
3	H	501	UPG	PB-O3B	2.20	1.66	1.60
3	B	501	UPG	C4-N3	2.22	1.37	1.33
2	D	500	NAD	C4A-N3A	2.26	1.38	1.35
3	B	501	UPG	PB-O3B	2.30	1.66	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	C2A-N1A	2.33	1.38	1.33
3	J	501	UPG	O4C-C1C	2.33	1.44	1.41
2	F	500	NAD	C2A-N1A	2.35	1.38	1.33
2	G	500	NAD	C2A-N1A	2.45	1.38	1.33
2	I	500	NAD	C2A-N1A	2.50	1.38	1.33
3	D	501	UPG	O4C-C1C	2.57	1.44	1.41
2	L	500	NAD	C2A-N1A	2.69	1.39	1.33
3	F	501	UPG	O4C-C1C	2.83	1.44	1.41
2	B	500	NAD	C2A-N1A	2.88	1.39	1.33
2	J	500	NAD	C2A-N1A	3.07	1.39	1.33
2	H	500	NAD	C2A-N3A	3.10	1.37	1.32
2	D	500	NAD	C2A-N1A	3.21	1.40	1.33
2	K	500	NAD	C2A-N1A	3.31	1.40	1.33
2	C	500	NAD	C2A-N3A	3.50	1.38	1.32
2	A	500	NAD	C2A-N3A	3.52	1.38	1.32
2	F	500	NAD	C2A-N3A	3.52	1.38	1.32
2	E	500	NAD	C2A-N1A	3.55	1.40	1.33
3	J	501	UPG	O4-C4	3.60	1.33	1.24
2	B	500	NAD	C2A-N3A	3.68	1.38	1.32
2	G	500	NAD	C2A-N3A	4.02	1.39	1.32
2	I	500	NAD	C2A-N3A	4.23	1.39	1.32
2	L	500	NAD	C2A-N3A	4.38	1.39	1.32
2	E	500	NAD	C2A-N3A	4.52	1.40	1.32
2	J	500	NAD	C2A-N3A	4.53	1.40	1.32
3	A	501	UPG	O4-C4	4.80	1.36	1.24
3	G	501	UPG	O4-C4	4.84	1.36	1.24
3	C	501	UPG	O4-C4	4.95	1.36	1.24
2	D	500	NAD	C2A-N3A	4.95	1.40	1.32
3	I	501	UPG	O4-C4	5.07	1.36	1.24
3	H	501	UPG	O4-C4	5.07	1.36	1.24
2	K	500	NAD	C2A-N3A	5.15	1.41	1.32
3	B	501	UPG	O4-C4	6.08	1.39	1.24
3	K	501	UPG	O4-C4	10.53	1.49	1.24

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	NAD	N3A-C2A-N1A	-12.99	118.95	128.89
2	J	500	NAD	N3A-C2A-N1A	-12.79	119.10	128.89
2	A	500	NAD	N3A-C2A-N1A	-12.24	119.52	128.89
2	L	500	NAD	N3A-C2A-N1A	-11.91	119.78	128.89
2	F	500	NAD	N3A-C2A-N1A	-11.77	119.88	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NAD	N3A-C2A-N1A	-11.69	119.94	128.89
2	G	500	NAD	N3A-C2A-N1A	-11.43	120.14	128.89
2	E	500	NAD	N3A-C2A-N1A	-10.97	120.50	128.89
2	I	500	NAD	N3A-C2A-N1A	-10.96	120.50	128.89
2	K	500	NAD	N3A-C2A-N1A	-10.54	120.83	128.89
2	B	500	NAD	N3A-C2A-N1A	-10.27	121.03	128.89
3	A	501	UPG	O5'-C1'-O3B	-9.02	99.47	111.36
3	K	501	UPG	O5'-C1'-O3B	-8.41	100.27	111.36
2	H	500	NAD	N3A-C2A-N1A	-8.34	122.51	128.89
3	H	501	UPG	O5'-C1'-O3B	-7.42	101.58	111.36
2	D	500	NAD	PN-O3-PA	-7.17	112.60	132.73
3	B	501	UPG	O5'-C1'-O3B	-6.66	102.58	111.36
2	E	500	NAD	PN-O3-PA	-6.56	114.32	132.73
2	F	500	NAD	PN-O3-PA	-6.22	115.25	132.73
2	L	500	NAD	PN-O3-PA	-6.14	115.48	132.73
2	K	500	NAD	PN-O3-PA	-6.02	115.83	132.73
3	G	501	UPG	O5'-C1'-O3B	-5.98	103.48	111.36
3	D	501	UPG	O5'-C1'-O3B	-5.74	103.79	111.36
2	J	500	NAD	PN-O3-PA	-5.54	117.16	132.73
2	B	500	NAD	PN-O3-PA	-5.38	117.62	132.73
2	C	500	NAD	PN-O3-PA	-5.22	118.07	132.73
3	I	501	UPG	C6'-C5'-C4'	-5.17	100.26	113.02
3	G	501	UPG	C6'-C5'-C4'	-5.15	100.31	113.02
2	I	500	NAD	PN-O3-PA	-4.92	118.92	132.73
3	F	501	UPG	C1'-O5'-C5'	-4.67	104.69	113.75
3	A	501	UPG	C6'-C5'-C4'	-4.64	101.58	113.02
2	G	500	NAD	PN-O3-PA	-4.59	119.83	132.73
3	B	501	UPG	O3A-PA-O5C	-4.59	90.76	102.94
3	C	501	UPG	C6'-C5'-C4'	-4.55	101.80	113.02
2	F	500	NAD	C2B-C1B-N9A	-4.35	107.64	114.29
3	I	501	UPG	O5'-C1'-O3B	-4.34	105.64	111.36
3	J	501	UPG	O5'-C1'-O3B	-4.29	105.71	111.36
3	H	501	UPG	C3'-C4'-C5'	-4.27	102.76	110.20
3	B	501	UPG	C6'-C5'-C4'	-4.13	102.84	113.02
2	D	500	NAD	C2B-C1B-N9A	-4.07	108.07	114.29
3	E	501	UPG	C3'-C4'-C5'	-3.89	103.42	110.20
2	H	500	NAD	C4A-C5A-N7A	-3.64	106.13	109.48
2	H	500	NAD	PN-O3-PA	-3.55	122.77	132.73
3	F	501	UPG	O5'-C1'-O3B	-3.42	106.85	111.36
3	F	501	UPG	O6'-C6'-C5'	-3.42	100.02	111.33
3	F	501	UPG	C3'-C4'-C5'	-3.41	104.25	110.20
3	I	501	UPG	PB-O3A-PA	-3.39	123.20	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	NAD	N6A-C6A-N1A	-3.34	112.03	119.20
2	C	500	NAD	C4A-C5A-N7A	-3.33	106.42	109.48
3	G	501	UPG	O3'-C3'-C4'	-3.28	102.94	110.34
3	H	501	UPG	C6'-C5'-C4'	-3.26	104.97	113.02
2	G	500	NAD	C4B-O4B-C1B	-3.24	106.16	109.72
3	K	501	UPG	O3A-PA-O5C	-3.21	94.43	102.94
3	L	501	UPG	C4'-C3'-C2'	-3.17	104.87	110.79
3	J	501	UPG	C3'-C4'-C5'	-3.14	104.72	110.20
3	D	501	UPG	C1'-O5'-C5'	-3.14	107.65	113.75
3	H	501	UPG	C4C-O4C-C1C	-3.14	106.27	109.72
3	H	501	UPG	PB-O3A-PA	-3.09	124.05	132.73
2	A	500	NAD	C4B-O4B-C1B	-2.99	106.44	109.72
2	E	500	NAD	C4B-O4B-C1B	-2.95	106.47	109.72
3	G	501	UPG	C4'-C3'-C2'	-2.87	105.43	110.79
3	L	501	UPG	C6'-C5'-C4'	-2.85	105.98	113.02
3	K	501	UPG	PB-O3A-PA	-2.85	124.73	132.73
2	A	500	NAD	O3-PN-O5D	-2.81	95.49	102.94
2	H	500	NAD	C1B-N9A-C4A	-2.80	122.72	126.94
2	F	500	NAD	C4A-C5A-N7A	-2.78	106.93	109.48
3	E	501	UPG	PB-O3A-PA	-2.77	124.95	132.73
3	K	501	UPG	C6'-C5'-C4'	-2.69	106.37	113.02
3	J	501	UPG	PB-O3A-PA	-2.69	125.18	132.73
3	D	501	UPG	PB-O3A-PA	-2.67	125.22	132.73
3	A	501	UPG	O4C-C1C-N1	-2.65	102.50	108.08
3	A	501	UPG	O3'-C3'-C4'	-2.62	104.44	110.34
3	D	501	UPG	C6'-C5'-C4'	-2.59	106.62	113.02
3	E	501	UPG	O5'-C1'-O3B	-2.57	107.97	111.36
3	E	501	UPG	O6'-C6'-C5'	-2.57	102.83	111.33
3	B	501	UPG	O3'-C3'-C4'	-2.55	104.60	110.34
3	C	501	UPG	O5'-C1'-O3B	-2.54	108.01	111.36
3	J	501	UPG	C1'-O5'-C5'	-2.53	108.84	113.75
3	K	501	UPG	O3A-PB-O3B	-2.51	96.39	103.63
3	B	501	UPG	O3C-C3C-C4C	-2.51	103.52	111.05
3	D	501	UPG	C3'-C4'-C5'	-2.49	105.85	110.20
2	A	500	NAD	O3D-C3D-C4D	-2.48	103.61	111.05
3	J	501	UPG	O3'-C3'-C4'	-2.46	104.80	110.34
3	C	501	UPG	O3'-C3'-C4'	-2.43	104.87	110.34
3	A	501	UPG	C3'-C4'-C5'	-2.40	106.01	110.20
2	B	500	NAD	C1B-N9A-C4A	-2.39	123.34	126.94
2	I	500	NAD	C4A-C5A-N7A	-2.38	107.29	109.48
3	K	501	UPG	O5'-C5'-C6'	-2.38	100.35	106.36
3	F	501	UPG	PB-O3A-PA	-2.37	126.07	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	UPG	PB-O3A-PA	-2.36	126.11	132.73
3	F	501	UPG	O3'-C3'-C4'	-2.36	105.03	110.34
3	G	501	UPG	C3'-C4'-C5'	-2.33	106.13	110.20
3	G	501	UPG	O5'-C5'-C6'	-2.32	100.49	106.36
2	A	500	NAD	C2B-C1B-N9A	-2.30	110.78	114.29
3	H	501	UPG	O5'-C5'-C6'	-2.29	100.56	106.36
3	C	501	UPG	C3'-C4'-C5'	-2.29	106.20	110.20
3	L	501	UPG	O2'-C2'-C3'	-2.27	105.23	110.34
3	B	501	UPG	C4'-C3'-C2'	-2.26	106.57	110.79
2	K	500	NAD	C4A-C5A-N7A	-2.23	107.43	109.48
3	I	501	UPG	O5C-C5C-C4C	-2.20	100.99	109.12
2	C	500	NAD	O3-PA-O5B	-2.19	97.13	102.94
3	J	501	UPG	O6'-C6'-C5'	-2.15	104.23	111.33
2	G	500	NAD	C1B-N9A-C4A	-2.11	123.76	126.94
2	B	500	NAD	C2B-C1B-N9A	-2.10	111.09	114.29
2	L	500	NAD	C4A-C5A-N7A	-2.09	107.56	109.48
2	C	500	NAD	O3D-C3D-C2D	-2.07	106.77	111.68
3	K	501	UPG	C4'-C3'-C2'	-2.06	106.95	110.79
3	I	501	UPG	O3C-C3C-C4C	-2.04	104.93	111.05
2	J	500	NAD	C5D-C4D-C3D	-2.03	107.15	115.21
2	I	500	NAD	C1B-N9A-C4A	-2.00	123.92	126.94
3	A	501	UPG	O6'-C6'-C5'	2.01	117.98	111.33
3	G	501	UPG	O5'-C5'-C4'	2.03	113.49	109.68
2	D	500	NAD	O3D-C3D-C2D	2.03	116.50	111.68
3	E	501	UPG	O3A-PB-O3B	2.04	109.49	103.63
2	F	500	NAD	C1D-O4D-C4D	2.04	113.21	108.08
2	G	500	NAD	O2A-PA-O3	2.06	114.44	105.09
2	A	500	NAD	O2A-PA-O3	2.06	114.46	105.09
3	K	501	UPG	O2B-PB-O3B	2.09	114.88	106.49
2	A	500	NAD	C1D-O4D-C4D	2.11	113.38	108.08
2	I	500	NAD	O2A-PA-O3	2.12	114.73	105.09
2	I	500	NAD	O2N-PN-O1N	2.13	124.05	112.53
2	C	500	NAD	O4B-C1B-N9A	2.14	112.57	108.10
3	L	501	UPG	O3A-PA-O5C	2.14	108.62	102.94
3	I	501	UPG	C1'-C2'-C3'	2.17	114.24	109.97
2	F	500	NAD	O2A-PA-O3	2.18	114.98	105.09
2	A	500	NAD	C1D-C2D-C3D	2.24	105.25	101.64
2	K	500	NAD	O2A-PA-O3	2.26	115.35	105.09
2	H	500	NAD	O2A-PA-O3	2.30	115.52	105.09
3	B	501	UPG	C6-C5-C4	2.36	121.69	117.28
3	G	501	UPG	O3B-C1'-C2'	2.38	112.83	108.39
3	B	501	UPG	O3B-PB-O1B	2.41	118.94	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	UPG	C6-C5-C4	2.41	121.79	117.28
2	B	500	NAD	C1D-O4D-C4D	2.43	114.19	108.08
2	B	500	NAD	C1D-C2D-C3D	2.46	105.60	101.64
2	K	500	NAD	C1D-C2D-C3D	2.47	105.62	101.64
2	H	500	NAD	O2D-C2D-C3D	2.51	116.05	111.23
3	A	501	UPG	C6-C5-C4	2.53	122.02	117.28
3	D	501	UPG	O2C-C2C-C3C	2.54	120.08	111.83
3	I	501	UPG	O4'-C4'-C3'	2.55	116.09	110.34
2	J	500	NAD	O3D-C3D-C2D	2.65	117.97	111.68
3	H	501	UPG	O3'-C3'-C2'	2.70	116.41	110.34
2	E	500	NAD	C1D-C2D-C3D	2.72	106.02	101.64
3	C	501	UPG	O2B-PB-O3B	2.73	117.45	106.49
2	J	500	NAD	C4B-O4B-C1B	2.83	112.83	109.72
2	F	500	NAD	O4D-C4D-C5D	2.83	115.72	109.53
2	L	500	NAD	O4D-C4D-C5D	2.99	116.07	109.53
3	F	501	UPG	O3B-C1'-C2'	3.16	114.30	108.39
3	L	501	UPG	C1'-O5'-C5'	3.20	119.96	113.75
2	J	500	NAD	O4D-C4D-C5D	3.26	116.66	109.53
3	F	501	UPG	O4C-C1C-N1	3.46	115.38	108.08
3	L	501	UPG	O5'-C5'-C4'	3.77	116.76	109.68
3	A	501	UPG	O3B-C1'-C2'	3.83	115.54	108.39
3	I	501	UPG	O3B-C1'-C2'	4.10	116.06	108.39
3	C	501	UPG	O3B-C1'-C2'	4.16	116.16	108.39
3	E	501	UPG	O3B-C1'-C2'	4.41	116.62	108.39
3	G	501	UPG	C4-N3-C2	4.59	118.69	114.14
3	H	501	UPG	O3B-C1'-C2'	4.73	117.22	108.39
3	B	501	UPG	C4-N3-C2	4.83	118.92	114.14
3	D	501	UPG	O3B-C1'-C2'	4.94	117.62	108.39
3	K	501	UPG	O3B-C1'-C2'	4.94	117.62	108.39
3	J	501	UPG	O3B-C1'-C2'	5.15	118.00	108.39
3	A	501	UPG	C4-N3-C2	5.40	119.49	114.14
3	E	501	UPG	C4-N3-C2	5.43	119.52	114.14
3	I	501	UPG	C4-N3-C2	5.50	119.59	114.14
3	L	501	UPG	C4-N3-C2	5.56	119.65	114.14
3	B	501	UPG	O3B-C1'-C2'	6.12	119.82	108.39
3	J	501	UPG	C4-N3-C2	6.29	120.37	114.14
3	K	501	UPG	C4-N3-C2	6.71	120.79	114.14
3	C	501	UPG	C4-N3-C2	6.77	120.85	114.14
3	F	501	UPG	C4-N3-C2	6.77	120.85	114.14
3	D	501	UPG	C4-N3-C2	6.94	121.01	114.14
3	H	501	UPG	C4-N3-C2	8.59	122.64	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAD	4	0
3	A	501	UPG	9	0
3	B	501	UPG	6	0
2	C	500	NAD	2	0
3	C	501	UPG	7	0
2	D	500	NAD	7	0
3	D	501	UPG	4	0
2	E	500	NAD	7	0
3	E	501	UPG	6	0
2	F	500	NAD	3	0
3	F	501	UPG	5	0
2	G	500	NAD	4	0
3	G	501	UPG	7	0
2	H	500	NAD	1	0
3	H	501	UPG	9	0
2	I	500	NAD	1	0
3	I	501	UPG	3	0
2	J	500	NAD	3	0
3	J	501	UPG	4	0
2	K	500	NAD	4	0
3	K	501	UPG	13	0
2	L	500	NAD	5	0
3	L	501	UPG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/487 (94%)	-0.17	1 (0%) 95 94	23, 34, 55, 71	0
1	B	460/487 (94%)	-0.24	0 100 100	22, 37, 54, 70	0
1	C	460/487 (94%)	0.23	28 (6%) 25 15	29, 48, 88, 103	0
1	D	460/487 (94%)	0.05	11 (2%) 62 50	26, 45, 73, 99	0
1	E	458/487 (94%)	0.36	23 (5%) 32 21	37, 62, 99, 113	0
1	F	460/487 (94%)	0.13	14 (3%) 54 41	35, 52, 85, 110	0
1	G	460/487 (94%)	0.08	5 (1%) 82 74	23, 47, 73, 88	0
1	H	460/487 (94%)	-0.25	0 100 100	20, 33, 50, 70	0
1	I	460/487 (94%)	0.35	23 (5%) 32 21	27, 55, 95, 110	0
1	J	460/487 (94%)	0.13	9 (1%) 68 58	23, 45, 79, 105	0
1	K	458/487 (94%)	0.45	23 (5%) 32 21	42, 75, 106, 117	0
1	L	460/487 (94%)	0.10	8 (1%) 73 63	33, 54, 84, 106	0
All	All	5516/5844 (94%)	0.10	145 (2%) 59 47	20, 47, 89, 117	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	96	TYR	4.8
1	E	1	MET	4.6
1	J	151	ASN	4.6
1	E	95	THR	4.6
1	E	98	MET	4.5
1	E	96	TYR	4.4
1	I	435	PRO	4.3
1	K	90	ASN	4.2
1	K	95	THR	4.1
1	K	109	ILE	4.1
1	K	1	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	428	ILE	4.0
1	C	356	TYR	4.0
1	J	109	ILE	3.9
1	C	326	VAL	3.8
1	L	356	TYR	3.7
1	I	409	HIS	3.7
1	F	466	VAL	3.7
1	K	98	MET	3.7
1	C	435	PRO	3.6
1	E	113	ALA	3.6
1	I	328	ASP	3.6
1	I	333	ILE	3.5
1	J	108	TYR	3.5
1	F	326	VAL	3.5
1	C	1	MET	3.4
1	C	436	ALA	3.3
1	K	110	GLU	3.3
1	K	104	ALA	3.2
1	C	323	PHE	3.1
1	D	98	MET	3.1
1	I	327	THR	3.1
1	D	151	ASN	3.1
1	C	324	ASN	3.1
1	J	106	LEU	3.0
1	I	361	GLY	3.0
1	C	364	LEU	3.0
1	K	97	GLY	3.0
1	D	1	MET	2.9
1	I	336	PHE	2.9
1	C	331	ILE	2.8
1	F	328	ASP	2.8
1	I	407	GLY	2.8
1	D	153	ASN	2.8
1	L	452	LEU	2.7
1	C	322	LEU	2.7
1	C	318	ILE	2.7
1	G	436	ALA	2.7
1	C	397	ILE	2.6
1	K	378	VAL	2.6
1	L	450	ASN	2.6
1	F	315	ALA	2.6
1	D	96	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	393	ARG	2.6
1	G	438	ILE	2.6
1	K	197	ALA	2.6
1	I	356	TYR	2.6
1	J	96	TYR	2.6
1	C	437	PHE	2.6
1	D	95	THR	2.6
1	E	108	TYR	2.6
1	I	357	LEU	2.5
1	G	1	MET	2.5
1	F	454	THR	2.5
1	E	117	VAL	2.5
1	I	364	LEU	2.5
1	F	353	ILE	2.5
1	I	350	SER	2.4
1	E	97	GLY	2.4
1	I	332	ALA	2.4
1	L	466	VAL	2.4
1	J	90	ASN	2.4
1	I	466	VAL	2.4
1	C	357	LEU	2.4
1	C	366	ILE	2.4
1	I	459	ILE	2.4
1	E	99	GLY	2.4
1	I	408	ALA	2.4
1	I	324	ASN	2.4
1	C	363	HIS	2.4
1	K	71	PHE	2.3
1	G	449	HIS	2.3
1	L	324	ASN	2.3
1	D	150	PRO	2.3
1	K	62	GLU	2.3
1	I	322	LEU	2.3
1	C	409	HIS	2.3
1	C	456	GLY	2.3
1	E	41	ARG	2.3
1	E	42	ILE	2.3
1	E	154	LEU	2.3
1	C	333	ILE	2.3
1	E	110	GLU	2.3
1	C	325	THR	2.3
1	C	454	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	424	ASP	2.3
1	K	140	ILE	2.3
1	D	148	THR	2.3
1	F	411	VAL	2.2
1	D	154	LEU	2.2
1	F	319	ILE	2.2
1	E	106	LEU	2.2
1	E	109	ILE	2.2
1	A	1	MET	2.2
1	C	361	GLY	2.2
1	F	382	HIS	2.2
1	F	461	THR	2.2
1	K	106	LEU	2.2
1	C	321	SER	2.2
1	E	103	ALA	2.2
1	F	430	LYS	2.2
1	C	461	THR	2.2
1	K	451	GLU	2.2
1	E	39	GLU	2.2
1	J	382	HIS	2.2
1	C	425	TYR	2.2
1	C	458	GLN	2.2
1	I	369	PRO	2.2
1	E	120	SER	2.1
1	G	400	ASP	2.1
1	K	151	ASN	2.1
1	I	410	ALA	2.1
1	K	185	THR	2.1
1	L	360	GLU	2.1
1	E	90	ASN	2.1
1	I	352	TYR	2.1
1	E	390	GLN	2.1
1	C	414	CYS	2.1
1	L	439	PHE	2.1
1	F	456	GLY	2.1
1	K	5	LYS	2.1
1	D	125	ILE	2.1
1	J	98	MET	2.0
1	L	454	THR	2.0
1	E	51	PRO	2.0
1	K	105	ASP	2.0
1	J	426	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	125	ILE	2.0
1	K	123	TYR	2.0
1	K	377	VAL	2.0
1	E	91	THR	2.0
1	I	436	ALA	2.0
1	I	433	LEU	2.0
1	D	146	ALA	2.0
1	F	323	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	E	500	35/44	0.84	0.40	2.05	55,65,70,71	0
2	NAD	J	500	35/44	0.88	0.36	2.04	49,61,64,66	0
2	NAD	D	500	35/44	0.90	0.31	1.90	52,60,65,66	0
2	NAD	K	500	35/44	0.86	0.38	1.58	58,66,71,71	0
2	NAD	C	500	35/44	0.94	0.20	1.17	42,47,57,59	0
2	NAD	A	500	35/44	0.97	0.19	1.12	37,45,55,59	0
3	UPG	A	501	36/36	0.97	0.21	1.12	34,37,48,56	0
3	UPG	I	501	36/36	0.96	0.20	1.10	35,44,59,67	0
2	NAD	I	500	35/44	0.92	0.23	0.93	44,55,57,59	0
3	UPG	J	501	36/36	0.97	0.20	0.75	35,40,47,50	0
2	NAD	G	500	35/44	0.95	0.21	0.66	43,50,59,60	0
3	UPG	H	501	36/36	0.98	0.19	0.64	27,35,45,56	0
3	UPG	F	501	36/36	0.95	0.21	0.64	43,47,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAD	B	500	35/44	0.95	0.18	0.60	40,46,53,54	0
3	UPG	C	501	36/36	0.97	0.19	0.57	34,41,52,64	0
3	UPG	D	501	36/36	0.97	0.19	0.52	34,38,47,51	0
2	NAD	L	500	35/44	0.96	0.19	0.44	44,48,57,57	0
2	NAD	H	500	35/44	0.97	0.17	0.41	39,45,49,52	0
3	UPG	B	501	36/36	0.97	0.18	0.39	26,33,49,63	0
2	NAD	F	500	35/44	0.94	0.18	0.33	44,52,56,57	0
3	UPG	E	501	36/36	0.97	0.19	0.15	41,47,53,57	0
3	UPG	G	501	36/36	0.97	0.20	-0.01	36,41,47,57	0
3	UPG	L	501	36/36	0.96	0.18	-0.69	43,47,52,56	0
3	UPG	K	501	36/36	0.95	0.18	-0.70	40,52,62,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.