



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:54 PM GMT

PDB ID : 1JKF
Title : Holo 1L-myo-inositol-1-phosphateSynthase
Authors : Stein, A.J.; Geiger, J.H.
Deposited on : 2001-07-12
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

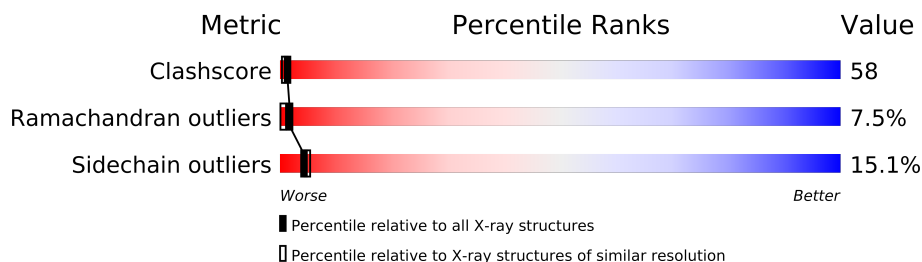
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	
1	B	533	

2 Entry composition i

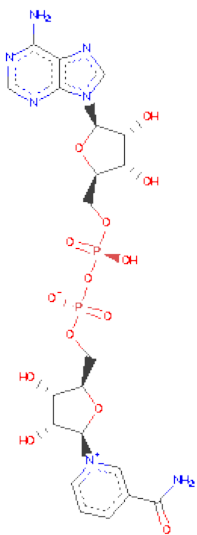
There are 3 unique types of molecules in this entry. The entry contains 7971 atoms, of which 0 are hydrogen and 0 are deuterium.

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 myo-inositol-1-phosphatesynthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3675	2338	617	706	14			
1	B	465	Total	C	N	O	S	0	0	0
			3670	2336	616	704	14			

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	256	Total 256	O 256	0	0
3	B	282	Total 282	O 282	0	0

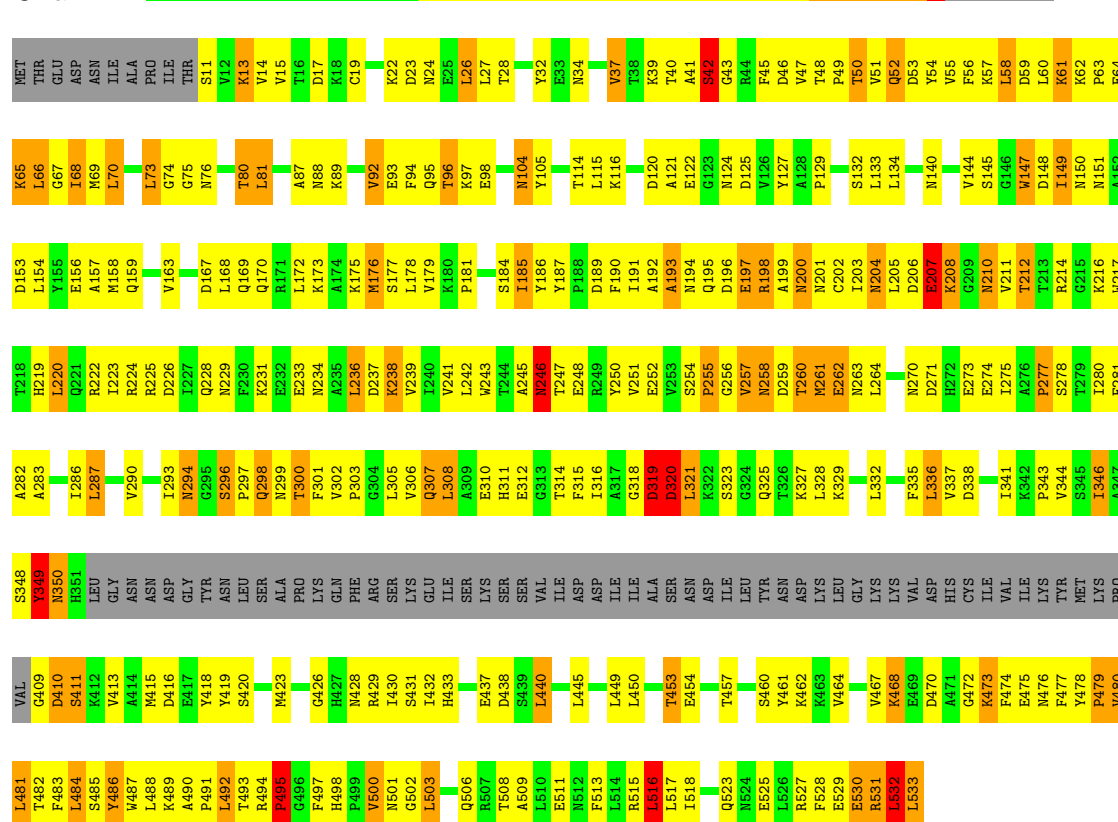
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

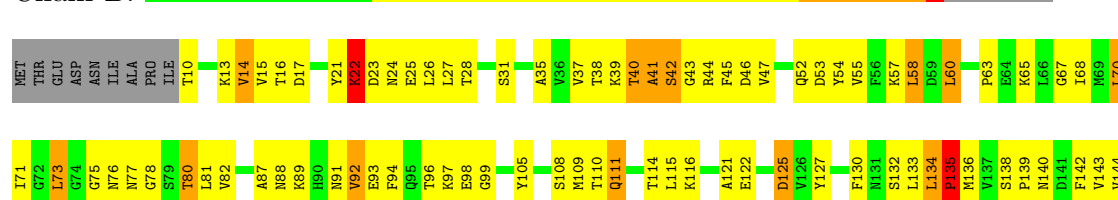
• Molecule 1: myo-inositol-1-phosphatesynthase

Chain A:



• Molecule 1: myo-inositol-1-phosphatesynthase

Chain B:





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.04Å 95.96Å 121.29Å 90.00° 126.04° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	57.3 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7971	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	1/3748 (0.0%)	0.78	2/5083 (0.0%)
1	B	0.53	0/3743	0.81	3/5077 (0.1%)
All	All	0.52	1/7491 (0.0%)	0.79	5/10160 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	MET	CG-SD	-5.11	1.67	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	GLY	N-CA-C	6.76	130.00	113.10
1	A	516	LEU	CA-CB-CG	6.10	129.34	115.30
1	A	73	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	524	ASN	N-CA-C	-5.29	96.71	111.00
1	B	526	LEU	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	TYR	Sidechain
1	B	349	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3675	0	3666	417	2
1	B	3670	0	3666	493	1
2	A	44	0	26	8	0
2	B	44	0	26	29	0
3	A	256	0	0	35	1
3	B	282	0	0	52	0
All	All	7971	0	7384	864	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 58.

All (864) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:149:ILE:HD11	1:B:195:GLN:HE21	1.04	1.13
1:B:315:PHE:HB3	1:B:481:LEU:HD11	1.30	1.12
1:B:293:ILE:HD11	1:B:453:THR:HG21	1.28	1.12
1:B:70:LEU:HD21	1:B:81:LEU:HD23	1.33	1.08
1:A:533:LEU:HG	1:B:494:ARG:HH22	0.92	1.08
1:A:76:ASN:O	1:A:80:THR:HG22	1.53	1.07
1:B:77:ASN:HD21	2:B:610:NAD:H6N	1.16	1.06
1:B:116:LYS:HE3	1:B:125:ASP:HB3	1.38	1.05
1:A:461:TYR:OH	1:B:533:LEU:HB2	1.53	1.04
1:B:77:ASN:ND2	2:B:610:NAD:H6N	1.70	1.04
1:A:454:GLU:O	1:A:457:THR:HG22	1.58	1.04
1:B:149:ILE:HD11	1:B:195:GLN:NE2	1.72	1.03
1:A:207:GLU:OE1	1:A:207:GLU:HA	1.57	1.02
1:A:96:THR:HG22	1:A:98:GLU:H	1.20	1.02
1:B:22:LYS:HG3	1:B:23:ASP:H	1.20	1.01
1:A:297:PRO:HB3	1:A:320:ASP:OD2	1.60	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:LEU:HD21	2:B:610:NAD:C2N	1.92	1.00
1:A:533:LEU:HG	1:B:494:ARG:NH2	1.75	1.00
1:B:321:LEU:CD2	2:B:610:NAD:C2N	2.40	1.00
1:B:351:HIS:HB3	1:B:413:VAL:H	1.27	1.00
1:A:411:SER:H	1:A:437:GLU:HA	1.23	0.98
1:B:464:VAL:HG13	1:B:469:GLU:HG2	1.42	0.97
1:B:521:PRO:O	1:B:522:SER:HB3	1.59	0.96
1:A:32:TYR:O	3:A:611:HOH:O	1.82	0.96
1:B:467:VAL:HG23	3:B:828:HOH:O	1.66	0.94
1:B:500:VAL:HG13	1:B:501:ASN:H	1.33	0.93
1:B:473:LYS:HA	1:B:473:LYS:HE2	1.49	0.93
1:B:465:ASP:H	1:B:469:GLU:HA	1.31	0.93
1:A:533:LEU:HB2	1:B:494:ARG:HH12	1.35	0.91
2:B:610:NAD:H3B	3:B:834:HOH:O	1.71	0.91
1:A:191:ILE:HD13	1:A:195:GLN:HG2	1.49	0.90
1:A:492:LEU:HD23	1:A:493:THR:H	1.37	0.90
1:A:151:ASN:H	1:A:200:ASN:HD21	1.19	0.89
1:B:467:VAL:CG2	3:B:828:HOH:O	2.17	0.89
1:B:160:ARG:O	1:B:162:GLN:HG3	1.72	0.89
1:A:93:GLU:HG2	3:A:727:HOH:O	1.71	0.89
1:A:211:VAL:HG23	1:A:212:THR:H	1.37	0.88
1:B:94:PHE:HB3	1:B:168:LEU:HD23	1.55	0.88
1:A:530:GLU:HA	1:B:494:ARG:HH21	1.38	0.87
1:B:134:LEU:HD12	1:B:455:PHE:HZ	1.37	0.87
1:B:76:ASN:N	2:B:610:NAD:O2A	2.06	0.87
1:B:143:VAL:HG21	1:B:236:LEU:HD11	1.55	0.87
1:B:321:LEU:HD21	2:B:610:NAD:N1N	1.87	0.87
1:A:163:VAL:HA	1:A:410:ASP:OD1	1.73	0.87
1:A:530:GLU:HA	1:B:494:ARG:NH2	1.89	0.87
1:A:185:ILE:HD11	1:A:277:PRO:HG3	1.56	0.87
1:B:246:ASN:HD22	1:B:246:ASN:C	1.77	0.87
1:B:492:LEU:HD13	1:B:493:THR:H	1.39	0.86
1:A:96:THR:CG2	1:A:98:GLU:H	1.88	0.86
1:B:77:ASN:HD21	2:B:610:NAD:C6N	1.89	0.85
1:A:409:GLY:N	2:A:600:NAD:H5N	1.92	0.85
1:A:63:PRO:HG2	1:A:238:LYS:HE2	1.60	0.84
1:B:163:VAL:HG22	3:B:790:HOH:O	1.76	0.84
1:A:116:LYS:HD3	1:A:523:GLN:HE22	1.39	0.83
1:B:22:LYS:CG	1:B:23:ASP:H	1.91	0.83
1:B:413:VAL:HG12	1:B:435:VAL:HG22	1.61	0.82
1:B:349:TYR:CD1	1:B:415:MET:HB2	2.15	0.82
1:A:238:LYS:HE3	1:A:454:GLU:OE2	1.80	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:GLY:HA3	2:B:610:NAD:H4B	1.62	0.81
1:A:492:LEU:HD23	1:A:493:THR:N	1.94	0.81
1:B:351:HIS:HB3	1:B:413:VAL:N	1.96	0.81
1:B:76:ASN:O	1:B:80:THR:HG22	1.80	0.81
1:A:321:LEU:HD23	1:A:445:LEU:HD22	1.63	0.81
1:B:163:VAL:HG22	1:B:164:LEU:HD22	1.62	0.81
1:A:14:VAL:HG11	1:A:518:ILE:O	1.78	0.81
1:B:349:TYR:CG	1:B:415:MET:HB2	2.16	0.81
1:B:194:ASN:ND2	1:B:247:THR:HG23	1.97	0.80
1:A:297:PRO:HD3	1:A:320:ASP:OD1	1.81	0.80
1:B:295:GLY:O	1:B:321:LEU:HD22	1.80	0.80
1:B:96:THR:HA	3:B:640:HOH:O	1.81	0.80
1:A:258:ASN:H	1:A:258:ASN:HD22	1.30	0.80
1:B:427:HIS:HE1	3:B:647:HOH:O	1.63	0.80
1:A:449:LEU:O	1:A:453:THR:HG23	1.80	0.79
1:A:87:ALA:HA	1:A:92:VAL:CG1	2.12	0.79
1:A:260:THR:HG22	1:A:307:GLN:NE2	1.97	0.79
1:A:461:TYR:HH	1:B:533:LEU:HB2	1.45	0.79
1:B:134:LEU:HD21	1:B:518:ILE:HG23	1.64	0.79
1:B:322:LYS:HE2	3:B:815:HOH:O	1.81	0.78
1:B:273:GLU:O	1:B:275:ILE:N	2.16	0.78
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.19	0.78
1:B:468:LYS:NZ	3:B:828:HOH:O	2.17	0.77
1:A:415:MET:CE	1:A:431:SER:HB2	2.15	0.77
1:A:96:THR:HG22	1:A:98:GLU:N	1.99	0.76
1:A:163:VAL:HG22	1:A:410:ASP:CG	2.04	0.76
1:B:318:GLY:O	1:B:488:LEU:HD23	1.85	0.76
1:B:257:VAL:O	1:B:258:ASN:ND2	2.18	0.76
1:B:250:TYR:CE2	1:B:298:GLN:HA	2.20	0.76
1:B:183:PRO:O	3:B:612:HOH:O	2.03	0.76
1:A:225:ARG:HE	1:A:229:ASN:HD21	1.33	0.76
1:A:64:GLU:O	1:A:65:LYS:HD2	1.86	0.76
1:A:349:TYR:CG	1:A:415:MET:HB3	2.21	0.76
1:B:263:ASN:ND2	1:B:263:ASN:H	1.83	0.76
1:A:191:ILE:HD11	1:A:195:GLN:HE21	1.50	0.75
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.66	0.75
1:B:39:LYS:HB2	1:B:45:PHE:CD2	2.21	0.75
1:B:492:LEU:HD13	1:B:493:THR:N	2.01	0.75
1:A:411:SER:N	1:A:437:GLU:HA	2.02	0.75
1:A:159:GLN:HA	1:A:169:GLN:HE22	1.50	0.75
1:B:293:ILE:CD1	1:B:453:THR:HG21	2.15	0.75
1:B:130:PHE:HE2	1:B:452:MET:HE3	1.52	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:433:HIS:HB3	1:B:431:SER:HB2	1.68	0.75
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.69	0.75
1:B:240:ILE:HG12	1:B:291:PRO:HG2	1.69	0.74
1:B:310:GLU:HA	1:B:479:PRO:HG3	1.69	0.74
1:A:246:ASN:C	1:A:246:ASN:HD22	1.90	0.74
1:B:13:LYS:HZ3	1:B:21:TYR:HE2	1.36	0.74
1:A:328:LEU:HD11	1:B:332:LEU:CD2	2.17	0.74
1:B:194:ASN:HB3	1:B:246:ASN:HA	1.69	0.74
1:A:50:THR:HG22	3:A:611:HOH:O	1.86	0.74
1:A:62:LYS:O	1:A:62:LYS:HG2	1.87	0.74
1:A:528:PHE:CD1	1:A:532:LEU:HD11	2.22	0.74
1:B:13:LYS:NZ	1:B:21:TYR:HE2	1.85	0.74
1:A:323:SER:HA	2:A:600:NAD:H72N	1.49	0.74
1:A:63:PRO:HG3	3:A:746:HOH:O	1.88	0.74
1:B:134:LEU:HB3	1:B:135:PRO:CD	2.17	0.73
1:A:200:ASN:HD22	1:A:200:ASN:C	1.91	0.73
1:B:472:GLY:O	1:B:473:LYS:HB2	1.87	0.73
1:B:297:PRO:O	1:B:298:GLN:HB3	1.88	0.73
1:A:57:LYS:O	3:A:666:HOH:O	2.06	0.73
1:B:38:THR:HG23	1:B:38:THR:O	1.88	0.72
1:B:245:ALA:O	2:B:610:NAD:O3D	2.05	0.72
1:B:321:LEU:CD2	2:B:610:NAD:C3N	2.67	0.72
1:B:516:LEU:HD12	1:B:517:LEU:N	2.04	0.72
1:A:486:TYR:CE2	1:A:503:LEU:HG	2.24	0.72
1:B:206:ASP:HB3	1:B:212:THR:HG21	1.72	0.72
1:B:470:ASP:O	1:B:472:GLY:N	2.23	0.72
3:A:649:HOH:O	1:B:500:VAL:HG11	1.89	0.72
1:A:440:LEU:HD23	1:B:426:GLY:HA3	1.70	0.72
1:B:282:ALA:CB	1:B:305:LEU:HD21	2.20	0.72
1:B:487:TRP:C	1:B:488:LEU:HD12	2.10	0.71
1:B:258:ASN:C	1:B:258:ASN:HD22	1.92	0.71
1:B:321:LEU:HD21	2:B:610:NAD:C6N	2.21	0.71
1:B:198:ARG:HD2	3:B:835:HOH:O	1.90	0.71
1:B:321:LEU:HD21	2:B:610:NAD:C3N	2.20	0.70
1:B:238:LYS:HG2	3:B:654:HOH:O	1.90	0.70
1:A:462:LYS:HE3	1:A:472:GLY:O	1.91	0.70
1:A:480:VAL:O	1:A:480:VAL:HG23	1.91	0.70
1:B:160:ARG:O	1:B:162:GLN:N	2.23	0.70
1:B:75:GLY:CA	2:B:610:NAD:O3B	2.40	0.70
1:A:283:ALA:O	1:A:287:LEU:HD22	1.91	0.70
1:A:298:GLN:HG3	1:A:300:THR:HG22	1.74	0.70
1:A:70:LEU:HD21	1:A:81:LEU:HD12	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:453:THR:HB	1:B:481:LEU:CD2	2.21	0.69
1:A:318:GLY:O	1:A:319:ASP:HB2	1.91	0.69
1:B:243:TRP:HZ2	1:B:246:ASN:HD21	1.40	0.69
1:B:154:LEU:HB3	1:B:176:MET:HE2	1.73	0.69
1:B:152:ALA:HB2	3:B:630:HOH:O	1.92	0.69
1:B:320:ASP:OD2	1:B:321:LEU:N	2.25	0.69
1:A:533:LEU:CB	1:B:494:ARG:HH12	2.06	0.69
1:B:349:TYR:HB2	1:B:415:MET:H	1.57	0.69
1:B:260:THR:HG22	1:B:261:MET:H	1.57	0.69
1:B:325:GLN:HE21	1:B:434:ASN:HD22	1.39	0.69
1:B:315:PHE:CE1	1:B:477:PHE:HB2	2.27	0.69
1:B:260:THR:CB	1:B:263:ASN:HD21	2.06	0.69
1:B:438:ASP:HB2	3:B:876:HOH:O	1.93	0.69
1:B:255:PRO:HA	1:B:259:ASP:OD1	1.93	0.68
1:A:234:ASN:CB	1:A:236:LEU:HD22	2.23	0.68
1:A:34:ASN:ND2	1:B:529:GLU:OE1	2.26	0.68
1:B:109:MET:HG3	1:B:507:ARG:HH12	1.59	0.68
1:B:321:LEU:HD23	2:B:610:NAD:C2N	2.21	0.68
1:B:299:ASN:HD22	1:B:299:ASN:N	1.91	0.68
1:B:163:VAL:CG2	1:B:164:LEU:HD22	2.23	0.68
1:A:533:LEU:HB2	1:B:494:ARG:NH1	2.07	0.68
1:B:500:VAL:HG13	1:B:501:ASN:N	2.07	0.68
1:A:191:ILE:HD13	1:A:195:GLN:CG	2.23	0.68
1:A:260:THR:HG22	1:A:307:GLN:HE22	1.55	0.68
1:B:134:LEU:HD12	1:B:517:LEU:HD23	1.75	0.68
1:B:261:MET:O	1:B:265:LEU:HD23	1.94	0.68
1:B:121:ALA:HB3	1:B:122:GLU:OE1	1.94	0.68
1:B:221:GLN:HG2	3:B:801:HOH:O	1.94	0.67
1:A:530:GLU:HG3	1:B:494:ARG:HE	1.59	0.67
1:A:297:PRO:O	1:A:298:GLN:HB3	1.93	0.67
1:B:75:GLY:HA2	2:B:610:NAD:O3B	1.94	0.67
1:A:415:MET:HE3	1:A:431:SER:HB2	1.75	0.67
1:A:185:ILE:HD13	1:A:187:TYR:CZ	2.29	0.67
1:B:273:GLU:C	1:B:275:ILE:H	1.98	0.67
1:A:55:VAL:HG23	1:A:464:VAL:CG2	2.25	0.66
1:A:219:HIS:O	1:A:223:ILE:HG12	1.94	0.66
1:A:461:TYR:HE1	3:A:808:HOH:O	1.79	0.66
1:A:203:ILE:HG13	1:A:204:ASN:N	2.10	0.66
1:A:185:ILE:HD12	1:A:185:ILE:C	2.16	0.66
1:A:257:VAL:HG21	1:A:274:GLU:OE2	1.96	0.66
1:B:282:ALA:HB1	1:B:305:LEU:HD21	1.78	0.66
1:A:214:ARG:HH11	1:A:214:ARG:HB2	1.61	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:VAL:O	1:A:290:VAL:HG23	1.95	0.66
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.77	0.66
1:A:440:LEU:CD2	1:B:426:GLY:HA3	2.26	0.66
1:B:210:ASN:HB3	3:B:857:HOH:O	1.95	0.66
1:A:420:SER:OG	3:A:729:HOH:O	2.13	0.66
1:B:193:ALA:O	1:B:194:ASN:HB2	1.96	0.66
1:B:473:LYS:HA	1:B:473:LYS:CE	2.23	0.66
1:A:428:ASN:HD22	1:B:436:CYS:HB3	1.61	0.65
1:B:87:ALA:HA	1:B:92:VAL:CG1	2.26	0.65
1:B:134:LEU:CD1	1:B:517:LEU:HD23	2.27	0.65
1:A:14:VAL:HB	1:B:47:VAL:HG13	1.77	0.65
1:B:315:PHE:CZ	1:B:477:PHE:HB2	2.31	0.65
1:A:250:TYR:CE1	1:A:298:GLN:HA	2.31	0.65
1:B:22:LYS:HG3	1:B:23:ASP:N	2.02	0.65
1:B:468:LYS:O	1:B:469:GLU:HB2	1.97	0.65
1:B:442:ALA:CB	2:B:610:NAD:H5N	2.27	0.65
1:B:22:LYS:CG	1:B:23:ASP:N	2.56	0.65
1:B:206:ASP:HB3	1:B:212:THR:CG2	2.26	0.65
1:A:258:ASN:HD22	1:A:258:ASN:N	1.93	0.65
1:A:61:LYS:HG2	1:A:61:LYS:O	1.96	0.65
1:B:429:ARG:HD3	3:B:786:HOH:O	1.97	0.65
1:A:211:VAL:O	1:A:212:THR:HG22	1.96	0.65
1:B:145:SER:HA	3:B:687:HOH:O	1.95	0.64
1:B:351:HIS:CB	1:B:413:VAL:H	2.06	0.64
1:B:515:ARG:CZ	1:B:523:GLN:HG3	2.27	0.64
1:B:65:LYS:HG3	3:B:679:HOH:O	1.97	0.64
1:A:206:ASP:O	1:A:208:LYS:N	2.30	0.64
1:B:245:ALA:O	2:B:610:NAD:C3D	2.46	0.64
1:B:21:TYR:CE1	1:B:26:LEU:HD13	2.33	0.64
1:A:64:GLU:C	1:A:65:LYS:HD2	2.17	0.64
1:B:346:ILE:N	1:B:346:ILE:HD12	2.11	0.64
1:B:149:ILE:CD1	1:B:195:GLN:HE21	1.97	0.64
1:A:70:LEU:HD21	1:A:81:LEU:CD1	2.28	0.64
1:B:246:ASN:ND2	1:B:246:ASN:C	2.51	0.63
1:A:462:LYS:CG	1:A:472:GLY:HA3	2.28	0.63
1:B:92:VAL:HG22	1:B:92:VAL:O	1.99	0.63
1:B:344:VAL:HG13	1:B:419:TYR:O	1.98	0.63
1:A:190:PHE:HZ	1:A:273:GLU:O	1.81	0.63
1:B:160:ARG:HD2	1:B:197:GLU:OE1	1.98	0.63
1:B:70:LEU:CD2	1:B:81:LEU:HD23	2.21	0.63
1:B:35:ALA:HB1	1:B:47:VAL:HG23	1.80	0.63
1:B:58:LEU:HD23	1:B:459:VAL:HG23	1.81	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:PRO:HG3	3:B:791:HOH:O	1.98	0.63
1:B:63:PRO:O	3:B:625:HOH:O	2.16	0.63
1:A:476:ASN:OD1	3:A:630:HOH:O	2.16	0.63
1:A:73:LEU:HD13	1:A:154:LEU:HD11	1.81	0.63
1:B:299:ASN:N	1:B:299:ASN:ND2	2.46	0.63
1:B:303:PRO:HG2	1:B:304:GLY:H	1.64	0.63
1:B:449:LEU:O	1:B:453:THR:CG2	2.46	0.63
1:B:88:ASN:HB3	1:B:140:ASN:HD21	1.64	0.63
1:B:297:PRO:O	1:B:298:GLN:CB	2.46	0.63
1:B:481:LEU:HB3	1:B:484:LEU:HD13	1.81	0.63
1:A:462:LYS:HG3	1:A:472:GLY:HA3	1.81	0.63
1:A:480:VAL:O	1:A:480:VAL:CG2	2.46	0.63
1:A:153:ASP:OD2	1:A:177:SER:HA	1.99	0.63
1:A:68:ILE:HG12	1:A:450:LEU:HD13	1.80	0.63
1:B:15:VAL:HG23	1:B:15:VAL:O	1.99	0.62
1:A:286:ILE:CG2	1:A:308:LEU:HD22	2.29	0.62
1:B:478:TYR:CE2	1:B:494:ARG:HB3	2.34	0.62
1:A:315:PHE:CE1	1:A:481:LEU:HD11	2.34	0.62
1:B:323:SER:OG	1:B:326:THR:HB	1.99	0.62
1:B:296:SER:OG	1:B:298:GLN:NE2	2.32	0.62
1:B:468:LYS:HE3	3:B:827:HOH:O	1.98	0.62
1:B:327:LYS:HG2	1:B:327:LYS:O	2.00	0.62
1:B:67:GLY:HA3	1:B:239:VAL:HG22	1.82	0.62
1:A:222:ARG:NH2	3:A:691:HOH:O	2.31	0.62
1:A:185:ILE:HD13	1:A:187:TYR:CE2	2.35	0.62
1:B:216:LYS:NZ	1:B:275:ILE:HB	2.15	0.62
1:A:234:ASN:HB2	1:A:236:LEU:HD22	1.81	0.62
1:A:327:LYS:HG2	1:A:503:LEU:HD13	1.81	0.62
1:A:320:ASP:O	1:A:488:LEU:HA	2.00	0.62
1:A:332:LEU:CD2	1:B:328:LEU:HD21	2.29	0.62
1:A:500:VAL:C	1:A:501:ASN:HD22	2.03	0.62
1:A:191:ILE:CD1	1:A:195:GLN:HE21	2.12	0.62
1:A:492:LEU:CD2	1:A:493:THR:N	2.63	0.61
1:B:130:PHE:HE2	1:B:452:MET:CE	2.12	0.61
1:A:346:ILE:HG22	1:A:346:ILE:O	2.00	0.61
1:B:302:VAL:O	1:B:306:VAL:HG23	2.00	0.61
1:B:477:PHE:HZ	1:B:513:PHE:CZ	2.18	0.61
1:B:263:ASN:HD22	1:B:263:ASN:H	1.48	0.61
1:B:194:ASN:HD22	1:B:247:THR:HG23	1.65	0.61
1:B:301:PHE:HE1	1:B:317:ALA:O	1.84	0.61
1:B:454:GLU:O	1:B:457:THR:HG22	2.01	0.61
1:A:415:MET:HE1	1:A:431:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:VAL:HG21	1:B:527:ARG:CZ	2.31	0.61
1:A:115:LEU:CD2	1:A:511:GLU:HG2	2.31	0.61
1:B:99:GLY:HA2	3:B:619:HOH:O	2.00	0.61
1:A:122:GLU:OE2	1:A:122:GLU:N	2.34	0.61
1:A:212:THR:HG23	1:A:214:ARG:H	1.65	0.61
1:B:110:THR:HA	1:B:130:PHE:CD2	2.35	0.61
1:A:210:ASN:ND2	1:A:210:ASN:N	2.47	0.61
1:A:532:LEU:HB2	1:B:461:TYR:CZ	2.36	0.61
1:A:191:ILE:O	1:A:191:ILE:HG22	2.01	0.61
1:B:180:LYS:HB3	3:B:677:HOH:O	2.01	0.61
1:B:465:ASP:N	1:B:469:GLU:HA	2.10	0.61
1:A:328:LEU:HD11	1:B:332:LEU:HD22	1.82	0.60
1:A:286:ILE:HG21	1:A:308:LEU:HD22	1.84	0.60
1:B:93:GLU:N	3:B:620:HOH:O	2.35	0.60
1:B:349:TYR:CB	1:B:415:MET:H	2.13	0.60
1:B:527:ARG:H	1:B:531:ARG:HD2	1.66	0.60
1:A:200:ASN:HD22	1:A:201:ASN:N	2.00	0.60
1:B:223:ILE:O	1:B:227:ILE:HG13	2.01	0.60
1:A:205:LEU:HA	1:A:210:ASN:O	2.01	0.60
1:B:52:GLN:HG3	1:B:54:TYR:CE1	2.37	0.60
1:A:15:VAL:HA	3:A:773:HOH:O	2.00	0.60
1:A:17:ASP:O	3:A:713:HOH:O	2.16	0.60
1:A:92:VAL:HG22	1:A:92:VAL:O	2.01	0.60
1:B:464:VAL:HG13	1:B:469:GLU:CG	2.26	0.60
1:B:248:GLU:OE1	1:B:278:SER:HB2	2.01	0.60
1:A:214:ARG:CB	1:A:214:ARG:NH1	2.64	0.60
1:A:483:PHE:CE1	1:B:531:ARG:HD3	2.37	0.59
1:B:24:ASN:N	1:B:24:ASN:HD22	1.98	0.59
1:B:194:ASN:ND2	1:B:247:THR:CG2	2.64	0.59
1:B:462:LYS:HE3	1:B:472:GLY:HA2	1.84	0.59
1:A:252:GLU:O	1:A:274:GLU:OE1	2.20	0.59
1:B:325:GLN:NE2	1:B:434:ASN:ND2	2.51	0.59
1:A:19:CYS:HB3	1:A:26:LEU:HD21	1.84	0.59
1:B:481:LEU:H	1:B:481:LEU:HD12	1.66	0.59
1:B:228:GLN:O	1:B:232:GLU:HG3	2.02	0.59
1:B:321:LEU:HD23	2:B:610:NAD:C3N	2.32	0.59
1:B:449:LEU:O	1:B:453:THR:HG23	2.02	0.59
1:B:219:HIS:O	1:B:223:ILE:HG12	2.00	0.59
1:A:211:VAL:HG23	1:A:212:THR:N	2.14	0.59
1:A:76:ASN:O	1:A:80:THR:CG2	2.41	0.59
1:A:159:GLN:HA	1:A:169:GLN:NE2	2.17	0.59
1:B:315:PHE:HE2	1:B:457:THR:HA	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:87:ALA:HA	1:B:92:VAL:HG13	1.84	0.59
1:B:134:LEU:HB3	1:B:135:PRO:HD2	1.84	0.58
1:B:261:MET:HE2	1:B:308:LEU:HA	1.85	0.58
1:A:48:THR:HA	1:B:15:VAL:HG22	1.84	0.58
1:A:489:LYS:O	1:A:491:PRO:HD3	2.02	0.58
1:A:40:THR:O	1:A:42:SER:N	2.36	0.58
1:A:462:LYS:HD2	1:A:474:PHE:CE1	2.39	0.58
1:A:151:ASN:N	1:A:200:ASN:HD21	1.97	0.58
1:B:299:ASN:H	1:B:299:ASN:ND2	2.02	0.58
1:B:515:ARG:NH2	1:B:523:GLN:HG3	2.18	0.58
1:B:185:ILE:HG12	1:B:203:ILE:HD11	1.84	0.58
1:A:250:TYR:HA	1:A:299:ASN:OD1	2.03	0.58
1:A:297:PRO:O	1:A:298:GLN:CB	2.51	0.58
1:B:422:LEU:HB3	3:B:638:HOH:O	2.03	0.58
1:A:200:ASN:ND2	1:A:200:ASN:C	2.54	0.58
1:B:41:ALA:O	1:B:42:SER:HB3	2.04	0.58
1:B:423:MET:HG3	1:B:424:LEU:HG	1.84	0.58
1:A:415:MET:HA	1:A:432:ILE:O	2.04	0.57
1:A:52:GLN:OE1	1:A:53:ASP:O	2.21	0.57
1:A:234:ASN:HB3	1:A:236:LEU:HD22	1.86	0.57
1:A:321:LEU:CD2	1:A:445:LEU:HD22	2.31	0.57
1:A:172:LEU:HB3	1:A:176:MET:HE3	1.87	0.57
1:B:521:PRO:O	1:B:522:SER:CB	2.40	0.57
1:B:261:MET:HG2	1:B:261:MET:O	2.03	0.57
1:B:460:SER:HB2	1:B:474:PHE:HB3	1.85	0.57
1:B:325:GLN:HE21	1:B:434:ASN:ND2	2.02	0.57
1:B:258:ASN:C	1:B:258:ASN:ND2	2.58	0.57
1:B:528:PHE:O	1:B:532:LEU:HB2	2.05	0.57
1:A:349:TYR:CD2	1:A:415:MET:HB3	2.39	0.57
1:B:39:LYS:HD3	1:B:45:PHE:CE2	2.39	0.57
1:B:149:ILE:CD1	1:B:195:GLN:NE2	2.59	0.57
1:B:528:PHE:CG	1:B:532:LEU:HD22	2.39	0.57
1:B:136:MET:HB3	3:B:615:HOH:O	2.04	0.57
1:B:311:HIS:C	1:B:313:GLY:H	2.08	0.57
3:A:618:HOH:O	1:B:424:LEU:HA	2.05	0.57
1:A:14:VAL:HB	1:B:47:VAL:CG1	2.35	0.57
1:B:130:PHE:CE2	1:B:452:MET:HE3	2.37	0.57
1:A:203:ILE:CG1	1:A:204:ASN:N	2.67	0.57
1:A:88:ASN:CB	1:A:140:ASN:HD21	2.18	0.57
1:A:430:ILE:HG12	1:B:434:ASN:OD1	2.05	0.56
1:A:114:THR:O	1:A:115:LEU:HD23	2.05	0.56
1:B:453:THR:HB	1:B:481:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:293:ILE:HD11	1:A:453:THR:HG21	1.88	0.56
1:B:136:MET:HE1	1:B:452:MET:HE2	1.85	0.56
1:B:151:ASN:HD22	1:B:151:ASN:C	2.09	0.56
1:A:98:GLU:OE1	3:A:627:HOH:O	2.18	0.56
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.39	0.56
1:A:55:VAL:HG23	1:A:464:VAL:HG21	1.87	0.56
1:B:216:LYS:HZ2	1:B:275:ILE:HB	1.70	0.56
1:B:345:SER:C	1:B:346:ILE:HD12	2.26	0.56
1:B:266:GLN:O	1:B:270:ASN:OD1	2.23	0.56
1:B:136:MET:HE1	1:B:452:MET:CE	2.36	0.56
1:A:11:SER:O	1:B:44:ARG:HA	2.05	0.56
1:B:528:PHE:HB3	1:B:532:LEU:HD22	1.87	0.56
1:A:349:TYR:HB2	1:A:415:MET:O	2.06	0.56
1:A:88:ASN:HB2	1:A:140:ASN:HD21	1.70	0.56
1:B:136:MET:CE	1:B:452:MET:CE	2.84	0.56
1:B:257:VAL:HA	1:B:267:SER:OG	2.06	0.55
1:A:214:ARG:HB3	1:A:214:ARG:CZ	2.37	0.55
1:A:121:ALA:HB3	1:A:122:GLU:OE2	2.05	0.55
1:B:249:ARG:O	1:B:249:ARG:HG3	2.06	0.55
1:A:341:ILE:HD12	1:A:341:ILE:N	2.21	0.55
1:B:489:LYS:C	1:B:491:PRO:HD3	2.26	0.55
1:B:108:SER:OG	1:B:111:GLN:HB2	2.05	0.55
1:A:210:ASN:ND2	3:A:742:HOH:O	2.40	0.55
1:B:343:PRO:HA	1:B:420:SER:CB	2.36	0.55
1:A:144:VAL:HG12	1:A:145:SER:N	2.22	0.55
1:A:40:THR:HG23	1:A:42:SER:HB3	1.88	0.55
1:B:40:THR:O	1:B:41:ALA:C	2.44	0.55
1:B:301:PHE:CE1	1:B:317:ALA:O	2.60	0.55
1:B:282:ALA:HB3	1:B:305:LEU:HD21	1.89	0.55
1:A:298:GLN:HG3	1:A:300:THR:CG2	2.35	0.55
1:B:27:LEU:HD21	1:B:474:PHE:CZ	2.42	0.55
1:A:532:LEU:HB2	1:B:461:TYR:CE2	2.42	0.55
1:B:234:ASN:O	1:B:235:ALA:HB3	2.05	0.55
1:B:318:GLY:C	1:B:488:LEU:HD23	2.26	0.54
1:B:160:ARG:HD3	3:B:675:HOH:O	2.06	0.54
1:A:56:PHE:CD2	1:A:516:LEU:HD21	2.41	0.54
1:A:134:LEU:HD21	1:A:518:ILE:HG22	1.89	0.54
1:B:206:ASP:C	1:B:208:LYS:H	2.10	0.54
1:B:250:TYR:CD1	1:B:299:ASN:ND2	2.74	0.54
1:B:116:LYS:HE3	1:B:125:ASP:CB	2.25	0.54
1:B:516:LEU:C	1:B:516:LEU:HD12	2.28	0.54
1:B:306:VAL:O	1:B:310:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:245:ALA:O	2:B:610:NAD:H4D	2.08	0.54
1:B:464:VAL:O	1:B:466:PRO:HD3	2.07	0.54
1:B:94:PHE:CB	1:B:168:LEU:HD23	2.35	0.54
1:A:257:VAL:CG2	1:A:258:ASN:N	2.71	0.54
1:A:184:SER:O	1:A:202:CYS:HA	2.07	0.54
1:B:58:LEU:HD13	1:B:60:LEU:HD12	1.89	0.54
1:A:410:ASP:CG	1:A:437:GLU:HB3	2.28	0.54
1:B:473:LYS:CA	1:B:473:LYS:HE2	2.30	0.54
1:A:14:VAL:CB	1:B:47:VAL:HG13	2.38	0.54
1:B:311:HIS:O	1:B:312:GLU:HB2	2.08	0.54
1:A:323:SER:CA	2:A:600:NAD:H72N	2.21	0.54
1:B:38:THR:O	1:B:38:THR:CG2	2.56	0.54
1:B:465:ASP:O	1:B:467:VAL:N	2.41	0.53
1:A:329:LYS:HD2	1:A:416:ASP:OD2	2.09	0.53
1:B:425:GLY:N	3:B:635:HOH:O	2.25	0.53
1:B:243:TRP:HZ2	1:B:246:ASN:ND2	2.06	0.53
1:A:328:LEU:HD11	1:B:332:LEU:HD21	1.89	0.53
1:A:153:ASP:OD1	1:A:156:GLU:HG3	2.08	0.53
1:B:274:GLU:HG2	3:B:664:HOH:O	2.08	0.53
1:B:349:TYR:HB2	1:B:415:MET:N	2.22	0.53
1:B:194:ASN:HD22	1:B:247:THR:CG2	2.22	0.53
1:A:516:LEU:HD23	1:A:516:LEU:C	2.28	0.53
1:A:300:THR:HG21	3:A:602:HOH:O	2.09	0.53
1:B:37:VAL:HA	1:B:46:ASP:O	2.07	0.53
1:B:442:ALA:HB1	2:B:610:NAD:H5N	1.91	0.53
1:B:27:LEU:HD21	1:B:474:PHE:CE2	2.44	0.53
1:B:134:LEU:HD12	1:B:455:PHE:CZ	2.29	0.53
1:A:214:ARG:NH1	1:A:214:ARG:HB2	2.22	0.53
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.90	0.53
1:B:195:GLN:NE2	2:B:610:NAD:C8A	2.72	0.53
1:A:494:ARG:CG	1:A:495:PRO:HD2	2.38	0.53
1:B:481:LEU:C	1:B:483:PHE:H	2.12	0.53
1:B:474:PHE:HD1	1:B:474:PHE:H	1.57	0.53
1:A:318:GLY:HA2	1:A:488:LEU:HG	1.91	0.53
1:B:78:GLY:O	1:B:82:VAL:HG23	2.08	0.53
1:A:341:ILE:O	1:A:343:PRO:HD3	2.08	0.53
1:B:293:ILE:HD11	1:B:453:THR:CG2	2.19	0.53
1:A:104:ASN:HD21	1:B:423:MET:HA	1.74	0.53
1:A:315:PHE:CZ	1:A:481:LEU:HD21	2.44	0.53
1:B:57:LYS:HB2	1:B:474:PHE:CE2	2.44	0.52
1:B:122:GLU:N	1:B:122:GLU:OE1	2.41	0.52
1:B:481:LEU:HD22	1:B:484:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:14:VAL:HG11	1:B:518:ILE:O	2.09	0.52
1:A:187:TYR:CD1	1:A:277:PRO:HD3	2.44	0.52
1:B:207:GLU:O	1:B:208:LYS:HD3	2.09	0.52
1:B:299:ASN:O	1:B:301:PHE:N	2.43	0.52
1:B:290:VAL:HG23	1:B:290:VAL:O	2.09	0.52
1:A:346:ILE:CG2	1:A:346:ILE:O	2.56	0.52
1:A:473:LYS:CD	1:A:473:LYS:C	2.77	0.52
1:A:261:MET:HE3	1:A:311:HIS:HB3	1.90	0.52
1:A:482:THR:HG21	1:B:530:GLU:OE1	2.10	0.52
1:A:92:VAL:HG11	1:A:172:LEU:HD21	1.92	0.52
1:B:39:LYS:HB2	1:B:45:PHE:CE2	2.45	0.52
1:B:42:SER:OG	1:B:43:GLY:N	2.42	0.52
1:B:311:HIS:O	1:B:313:GLY:N	2.43	0.52
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.40	0.52
1:A:28:THR:O	1:A:55:VAL:HA	2.10	0.52
1:A:55:VAL:HB	1:A:462:LYS:HB3	1.92	0.52
1:B:311:HIS:HD2	1:B:312:GLU:H	1.58	0.52
1:A:96:THR:HG23	1:A:97:LYS:N	2.25	0.52
1:A:332:LEU:HG	1:A:432:ILE:HD11	1.91	0.52
1:B:273:GLU:C	1:B:275:ILE:N	2.63	0.52
1:A:48:THR:HA	1:B:15:VAL:CG2	2.40	0.52
1:B:438:ASP:OD2	1:B:438:ASP:N	2.43	0.51
1:B:10:THR:HG22	1:B:132:SER:HB2	1.91	0.51
1:A:245:ALA:HB1	2:A:600:NAD:C4A	2.40	0.51
1:A:56:PHE:CE1	1:A:461:TYR:HB3	2.45	0.51
1:A:185:ILE:HD12	1:A:186:TYR:N	2.26	0.51
1:A:225:ARG:HE	1:A:229:ASN:ND2	2.04	0.51
1:A:37:VAL:HB	1:A:47:VAL:HG22	1.92	0.51
1:B:474:PHE:CD1	1:B:474:PHE:N	2.78	0.51
1:A:147:TRP:CD2	1:A:281:PHE:HE2	2.29	0.51
1:B:454:GLU:OE2	3:B:654:HOH:O	2.18	0.51
1:B:526:LEU:HB3	1:B:528:PHE:CE2	2.45	0.51
1:A:207:GLU:CA	1:A:207:GLU:OE1	2.45	0.51
1:B:351:HIS:C	1:B:412:LYS:HD2	2.30	0.51
1:A:335:PHE:CE1	1:B:327:LYS:O	2.64	0.51
1:B:198:ARG:NH2	3:B:814:HOH:O	2.44	0.51
1:B:285:SER:HB3	1:B:290:VAL:HG23	1.92	0.51
1:A:149:ILE:O	1:A:199:ALA:HA	2.10	0.51
1:A:335:PHE:CE2	1:B:328:LEU:HG	2.45	0.51
1:B:343:PRO:HA	1:B:420:SER:HB3	1.91	0.51
1:B:468:LYS:O	1:B:469:GLU:CB	2.59	0.51
1:A:246:ASN:CG	2:A:600:NAD:N7A	2.64	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:SER:HB2	2:A:600:NAD:O3D	2.11	0.51
1:A:207:GLU:HB2	3:A:791:HOH:O	2.11	0.51
1:A:231:LYS:HE2	1:A:237:ASP:O	2.11	0.51
1:A:52:GLN:HG3	1:A:54:TYR:CE1	2.45	0.51
1:A:238:LYS:HD3	1:A:457:THR:HG21	1.91	0.51
1:B:463:LYS:O	1:B:470:ASP:HB2	2.10	0.51
1:B:351:HIS:ND1	1:B:412:LYS:HA	2.25	0.51
1:B:260:THR:HB	1:B:263:ASN:HD21	1.75	0.51
1:A:328:LEU:HD13	1:B:335:PHE:CE1	2.45	0.51
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.45	0.51
1:A:261:MET:HE3	1:A:308:LEU:HA	1.93	0.51
1:A:475:GLU:HA	1:A:475:GLU:OE1	2.10	0.51
1:A:173:LYS:N	3:A:799:HOH:O	2.44	0.51
1:B:220:LEU:HD22	1:B:284:ALA:HB2	1.92	0.51
1:A:462:LYS:NZ	1:A:470:ASP:OD2	2.44	0.50
1:B:321:LEU:HA	1:B:488:LEU:HA	1.92	0.50
1:A:96:THR:CG2	1:A:97:LYS:N	2.73	0.50
1:B:315:PHE:HB3	1:B:481:LEU:CD1	2.22	0.50
1:A:238:LYS:HG2	3:A:796:HOH:O	2.10	0.50
1:B:260:THR:HB	1:B:263:ASN:ND2	2.26	0.50
1:B:73:LEU:HD22	1:B:154:LEU:HD21	1.93	0.50
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.94	0.50
1:B:242:LEU:C	1:B:242:LEU:HD23	2.31	0.50
1:B:351:HIS:CB	1:B:413:VAL:O	2.60	0.50
1:B:134:LEU:HD21	1:B:518:ILE:CG2	2.39	0.50
1:B:82:VAL:HG21	1:B:154:LEU:CD2	2.42	0.50
1:A:37:VAL:HA	1:A:46:ASP:O	2.12	0.50
1:B:240:ILE:HG12	1:B:291:PRO:CG	2.41	0.50
1:A:208:LYS:C	3:A:742:HOH:O	2.49	0.50
1:B:285:SER:O	1:B:290:VAL:HG22	2.12	0.50
1:A:32:TYR:OH	1:B:529:GLU:OE1	2.21	0.50
1:A:170:GLN:NE2	3:A:706:HOH:O	2.34	0.50
1:A:192:ALA:O	1:A:193:ALA:HB2	2.12	0.50
1:A:286:ILE:HG22	1:A:312:GLU:HG3	1.93	0.50
1:A:485:SER:OG	1:A:491:PRO:HB3	2.12	0.50
1:B:163:VAL:HB	1:B:437:GLU:HG2	1.93	0.49
1:A:74:GLY:N	1:A:148:ASP:OD1	2.43	0.49
1:A:54:TYR:CZ	1:B:532:LEU:HD23	2.47	0.49
1:A:493:THR:HG21	1:A:497:PHE:O	2.12	0.49
1:A:95:GLN:HB2	1:A:167:ASP:OD1	2.13	0.49
1:A:278:SER:HB2	3:A:602:HOH:O	2.12	0.49
1:B:264:LEU:HD21	1:B:305:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:ASN:ND2	1:A:210:ASN:H	2.08	0.49
1:B:24:ASN:N	1:B:24:ASN:ND2	2.60	0.49
1:A:115:LEU:HD21	1:A:511:GLU:HG2	1.93	0.49
1:A:115:LEU:HD22	1:A:511:GLU:OE2	2.12	0.49
1:B:21:TYR:O	1:B:22:LYS:O	2.29	0.49
1:A:105:TYR:OH	1:A:140:ASN:ND2	2.45	0.49
1:A:242:LEU:HD23	1:A:242:LEU:C	2.33	0.49
1:B:114:THR:O	1:B:115:LEU:HD23	2.13	0.49
1:B:510:LEU:O	1:B:514:LEU:HD23	2.12	0.49
1:B:134:LEU:HD11	1:B:517:LEU:HB3	1.95	0.49
1:B:254:SER:HB3	1:B:255:PRO:CD	2.43	0.49
1:B:55:VAL:HB	1:B:462:LYS:HB3	1.95	0.49
1:A:50:THR:CG2	1:A:51:VAL:N	2.76	0.49
1:A:211:VAL:CG2	1:A:212:THR:H	2.19	0.49
1:B:272:HIS:CE1	1:B:274:GLU:OE1	2.65	0.49
1:B:462:LYS:CE	1:B:472:GLY:HA2	2.42	0.48
1:A:261:MET:O	1:A:263:ASN:N	2.45	0.48
1:A:196:ASP:HB2	1:A:197:GLU:OE1	2.12	0.48
1:B:481:LEU:N	1:B:481:LEU:HD12	2.28	0.48
1:B:478:TYR:CE2	1:B:494:ARG:HD3	2.49	0.48
1:A:104:ASN:HB2	3:A:636:HOH:O	2.13	0.48
1:A:214:ARG:NH1	1:A:214:ARG:HB3	2.27	0.48
1:A:27:LEU:HD13	1:A:57:LYS:HG3	1.95	0.48
1:B:293:ILE:HG12	1:B:317:ALA:HB3	1.93	0.48
1:A:191:ILE:CD1	1:A:195:GLN:HG2	2.34	0.48
1:B:273:GLU:O	1:B:275:ILE:HG12	2.13	0.48
1:B:241:VAL:CG2	1:B:292:TYR:HD2	2.26	0.48
1:B:262:GLU:OE1	1:B:262:GLU:N	2.46	0.48
1:A:259:ASP:N	1:A:259:ASP:OD2	2.38	0.48
1:B:27:LEU:HD22	1:B:55:VAL:HG12	1.96	0.48
1:B:349:TYR:CD1	1:B:415:MET:CB	2.94	0.48
1:B:58:LEU:CD1	1:B:60:LEU:HD12	2.44	0.48
1:A:532:LEU:HD13	1:A:532:LEU:N	2.29	0.48
1:B:261:MET:HE2	1:B:311:HIS:HB3	1.96	0.48
1:A:66:LEU:HD13	1:A:68:ILE:HD11	1.95	0.48
1:B:242:LEU:HD13	1:B:446:ILE:HG23	1.96	0.48
1:B:488:LEU:O	1:B:491:PRO:HD3	2.13	0.48
1:B:484:LEU:CD1	1:B:484:LEU:N	2.77	0.48
1:B:14:VAL:HG11	1:B:518:ILE:HB	1.95	0.48
1:B:324:GLY:HA3	1:B:441:LEU:CD2	2.44	0.48
1:B:75:GLY:HA3	2:B:610:NAD:C4B	2.40	0.48
1:A:532:LEU:O	1:A:532:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:TYR:HD1	1:A:277:PRO:HD3	1.78	0.48
1:A:254:SER:H	1:A:258:ASN:HD21	1.61	0.48
1:B:156:GLU:O	1:B:159:GLN:HB2	2.13	0.48
1:B:245:ALA:O	2:B:610:NAD:C4D	2.61	0.48
1:A:531:ARG:HG3	1:B:482:THR:OG1	2.14	0.48
1:B:88:ASN:CB	1:B:140:ASN:HD21	2.27	0.48
1:A:196:ASP:C	1:A:197:GLU:OE2	2.52	0.48
1:A:344:VAL:HG12	1:A:419:TYR:O	2.14	0.48
1:B:344:VAL:CG1	1:B:419:TYR:O	2.62	0.47
1:B:10:THR:HG22	1:B:132:SER:CB	2.44	0.47
1:B:351:HIS:C	1:B:412:LYS:HB3	2.34	0.47
1:B:94:PHE:CD2	1:B:168:LEU:HD23	2.48	0.47
1:A:231:LYS:HG2	1:A:236:LEU:O	2.13	0.47
1:B:88:ASN:O	1:B:91:ASN:ND2	2.47	0.47
1:B:449:LEU:O	1:B:453:THR:HG22	2.13	0.47
1:B:457:THR:HG21	3:B:654:HOH:O	2.15	0.47
1:A:431:SER:OG	1:B:433:HIS:HB3	2.14	0.47
1:A:426:GLY:HA3	1:B:440:LEU:HD13	1.95	0.47
1:A:497:PHE:CD1	1:A:497:PHE:N	2.82	0.47
1:A:349:TYR:HB3	1:A:350:ASN:H	1.28	0.47
1:A:233:GLU:HG3	3:A:783:HOH:O	2.14	0.47
1:B:136:MET:HE3	1:B:452:MET:HE1	1.96	0.47
1:A:308:LEU:O	1:A:312:GLU:HG2	2.14	0.47
1:A:40:THR:HG23	1:A:43:GLY:H	1.79	0.47
1:B:478:TYR:HE2	1:B:494:ARG:HB3	1.77	0.47
1:A:257:VAL:HG23	1:A:258:ASN:N	2.29	0.47
1:B:187:TYR:OH	1:B:219:HIS:HD2	1.98	0.47
1:A:104:ASN:HD22	1:A:104:ASN:C	2.17	0.47
1:A:529:GLU:H	1:A:529:GLU:CD	2.17	0.47
1:B:488:LEU:N	1:B:488:LEU:HD12	2.29	0.47
1:B:302:VAL:HB	1:B:303:PRO:CD	2.39	0.47
1:A:246:ASN:ND2	1:A:246:ASN:C	2.60	0.47
1:B:26:LEU:O	1:B:57:LYS:HA	2.15	0.47
1:A:299:ASN:N	1:A:299:ASN:OD1	2.45	0.47
1:B:139:PRO:HA	1:B:142:PHE:CD2	2.49	0.47
1:A:68:ILE:CG2	1:A:70:LEU:HD13	2.45	0.47
1:A:204:ASN:O	1:A:204:ASN:CG	2.53	0.47
1:B:341:ILE:O	1:B:343:PRO:HD3	2.14	0.47
1:B:515:ARG:NH1	1:B:522:SER:H	2.13	0.47
1:B:235:ALA:O	1:B:236:LEU:O	2.33	0.47
1:A:258:ASN:ND2	1:A:258:ASN:N	2.62	0.47
1:A:251:VAL:H	1:A:299:ASN:HD21	1.63	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:ILE:CD1	1:A:277:PRO:HG3	2.38	0.47
1:A:223:ILE:O	1:A:226:ASP:HB2	2.15	0.47
1:B:484:LEU:N	1:B:484:LEU:HD12	2.30	0.46
1:A:54:TYR:CE2	1:B:532:LEU:HD23	2.50	0.46
1:B:435:VAL:O	1:B:436:CYS:HB3	2.16	0.46
1:A:332:LEU:HD23	1:B:328:LEU:HD21	1.95	0.46
1:B:172:LEU:HA	3:B:796:HOH:O	2.15	0.46
1:B:31:SER:HB2	3:B:747:HOH:O	2.15	0.46
1:A:477:PHE:HZ	1:A:513:PHE:CZ	2.32	0.46
1:A:462:LYS:HE3	1:A:472:GLY:CA	2.46	0.46
1:A:349:TYR:CB	1:A:415:MET:H	2.28	0.46
1:A:286:ILE:HG22	1:A:308:LEU:HD22	1.97	0.46
1:A:238:LYS:HG3	3:A:651:HOH:O	2.15	0.46
1:B:503:LEU:HD13	3:B:815:HOH:O	2.13	0.46
1:B:190:PHE:HA	1:B:249:ARG:HG2	1.97	0.46
1:A:178:LEU:HD11	3:A:797:HOH:O	2.14	0.46
1:A:56:PHE:CD1	1:A:461:TYR:HB3	2.49	0.46
1:A:315:PHE:CD1	1:A:481:LEU:HD11	2.49	0.46
1:A:484:LEU:HA	1:A:487:TRP:CZ3	2.49	0.46
1:A:13:LYS:HE3	1:A:13:LYS:HB2	1.58	0.46
1:B:528:PHE:CB	1:B:532:LEU:HD22	2.46	0.46
1:B:52:GLN:OE1	1:B:53:ASP:N	2.48	0.46
1:B:143:VAL:CG2	1:B:143:VAL:O	2.63	0.46
1:A:203:ILE:CG1	1:A:204:ASN:H	2.28	0.46
1:B:220:LEU:HD13	1:B:220:LEU:C	2.36	0.46
1:A:531:ARG:C	1:A:532:LEU:HD13	2.35	0.46
1:A:494:ARG:HG3	1:A:495:PRO:HD2	1.97	0.46
1:A:501:ASN:HD22	1:A:501:ASN:N	2.12	0.46
1:A:525:GLU:OE2	1:A:527:ARG:NH2	2.47	0.46
1:A:243:TRP:CD1	1:A:296:SER:HB3	2.50	0.46
1:A:349:TYR:O	1:A:350:ASN:HB3	2.16	0.46
1:A:502:GLY:O	1:A:503:LEU:C	2.54	0.46
1:A:485:SER:HB3	1:A:506:GLN:NE2	2.30	0.46
1:B:184:SER:OG	1:B:185:ILE:N	2.47	0.46
1:B:249:ARG:NH2	3:B:808:HOH:O	2.49	0.46
1:A:508:THR:O	1:A:509:ALA:C	2.53	0.46
1:B:489:LYS:HD2	1:B:489:LYS:C	2.36	0.46
1:A:301:PHE:CD1	1:A:492:LEU:HD12	2.51	0.46
1:A:327:LYS:HD3	1:B:335:PHE:HE2	1.80	0.46
1:B:121:ALA:HB3	3:B:712:HOH:O	2.15	0.46
1:A:154:LEU:HD22	1:A:179:VAL:HG11	1.98	0.46
1:A:286:ILE:HG23	1:A:314:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.80	0.46
1:A:318:GLY:O	1:A:319:ASP:CB	2.61	0.46
1:B:500:VAL:CG1	1:B:501:ASN:H	2.16	0.46
1:A:480:VAL:O	1:A:482:THR:N	2.49	0.46
1:A:115:LEU:HD22	1:A:511:GLU:HG2	1.98	0.46
1:B:274:GLU:OE1	1:B:274:GLU:N	2.49	0.46
1:B:125:ASP:OD2	1:B:125:ASP:N	2.43	0.46
1:A:270:ASN:O	1:A:271:ASP:HB2	2.17	0.45
1:A:15:VAL:HG12	1:A:15:VAL:O	2.14	0.45
1:A:69:MET:HB2	1:A:241:VAL:HG22	1.97	0.45
1:A:148:ASP:C	1:A:150:ASN:H	2.20	0.45
1:B:301:PHE:CZ	1:B:316:ILE:HB	2.52	0.45
1:B:28:THR:O	1:B:55:VAL:HA	2.16	0.45
1:A:229:ASN:ND2	3:A:640:HOH:O	2.49	0.45
1:A:473:LYS:C	1:A:473:LYS:HD3	2.36	0.45
1:B:347:ALA:O	1:B:416:ASP:HA	2.16	0.45
1:A:311:HIS:C	1:A:311:HIS:ND1	2.69	0.45
1:B:40:THR:O	1:B:41:ALA:O	2.33	0.45
1:A:69:MET:HB3	1:A:147:TRP:CZ3	2.52	0.45
1:A:275:ILE:HG22	1:A:280:ILE:HD11	1.98	0.45
1:B:321:LEU:HD21	2:B:610:NAD:C5N	2.47	0.45
1:A:327:LYS:HE2	1:A:503:LEU:HD11	1.98	0.45
1:B:458:ARG:HA	3:B:696:HOH:O	2.15	0.45
1:B:261:MET:HE1	1:B:311:HIS:HB2	1.98	0.45
1:B:502:GLY:O	1:B:503:LEU:C	2.54	0.45
1:B:265:LEU:O	1:B:269:LYS:HG3	2.17	0.45
1:B:234:ASN:O	1:B:235:ALA:CB	2.64	0.45
1:B:250:TYR:CZ	1:B:298:GLN:HA	2.52	0.45
1:B:67:GLY:HA2	1:B:143:VAL:HG22	1.99	0.45
1:B:109:MET:HE1	1:B:507:ARG:HG3	1.98	0.45
1:A:58:LEU:HD13	1:A:60:LEU:HD23	1.98	0.45
1:B:258:ASN:HB2	1:B:302:VAL:HG21	1.99	0.45
1:A:241:VAL:HG12	1:A:242:LEU:N	2.32	0.45
1:A:294:ASN:C	1:A:294:ASN:ND2	2.71	0.45
1:B:25:GLU:OE1	1:B:57:LYS:HD2	2.17	0.45
1:A:251:VAL:H	1:A:299:ASN:ND2	2.15	0.44
1:A:87:ALA:HA	1:A:92:VAL:HG13	1.95	0.44
1:B:264:LEU:HD21	1:B:305:LEU:HD13	1.98	0.44
1:A:24:ASN:ND2	1:A:61:LYS:HB3	2.32	0.44
1:A:256:GLY:H	1:A:259:ASP:CG	2.19	0.44
1:A:325:GLN:HA	1:A:325:GLN:OE1	2.17	0.44
1:B:105:TYR:OH	1:B:140:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:302:VAL:HB	1:A:303:PRO:HD2	2.00	0.44
1:B:89:LYS:HD3	3:B:633:HOH:O	2.16	0.44
1:A:319:ASP:HB2	1:A:490:ALA:O	2.18	0.44
1:B:261:MET:HE2	1:B:311:HIS:CB	2.47	0.44
1:A:75:GLY:HA3	2:A:600:NAD:H4B	1.99	0.44
1:A:531:ARG:NH2	3:A:649:HOH:O	2.51	0.44
1:A:532:LEU:O	1:A:532:LEU:CD2	2.64	0.44
1:B:121:ALA:CB	1:B:122:GLU:OE1	2.64	0.44
1:A:190:PHE:O	1:A:248:GLU:HA	2.16	0.44
1:A:485:SER:O	1:A:487:TRP:N	2.51	0.44
1:A:501:ASN:HA	1:A:506:GLN:NE2	2.33	0.44
1:B:315:PHE:HD1	1:B:479:PRO:HA	1.83	0.44
1:A:349:TYR:CE2	1:A:413:VAL:HG22	2.52	0.44
1:B:216:LYS:NZ	1:B:275:ILE:O	2.46	0.44
1:B:348:SER:OG	1:B:416:ASP:OD1	2.32	0.44
1:B:251:VAL:CG1	1:B:299:ASN:HB2	2.47	0.44
1:B:68:ILE:HG22	1:B:70:LEU:HD13	2.00	0.44
1:B:136:MET:CE	1:B:452:MET:HE1	2.46	0.44
1:A:217:TRP:O	1:A:220:LEU:HB3	2.17	0.44
1:A:349:TYR:HB2	1:A:415:MET:H	1.83	0.44
1:B:183:PRO:HG2	3:B:612:HOH:O	2.16	0.44
1:A:158:MET:SD	1:A:169:GLN:HG3	2.57	0.44
1:B:24:ASN:HA	1:B:60:LEU:HB2	1.99	0.44
1:A:129:PRO:HB2	1:A:132:SER:HB3	2.00	0.44
1:A:409:GLY:O	1:A:410:ASP:OD2	2.36	0.44
1:A:349:TYR:CD2	1:A:415:MET:CB	3.01	0.44
1:A:158:MET:C	1:A:169:GLN:NE2	2.71	0.44
1:A:502:GLY:HA2	3:A:760:HOH:O	2.17	0.44
1:A:478:TYR:CE1	1:A:479:PRO:HG2	2.53	0.44
1:A:341:ILE:CD1	1:A:341:ILE:N	2.81	0.44
1:B:241:VAL:HG21	1:B:285:SER:OG	2.18	0.44
1:A:22:LYS:HG2	1:A:23:ASP:H	1.83	0.44
1:B:231:LYS:HE3	3:B:824:HOH:O	2.18	0.44
1:B:153:ASP:OD2	1:B:177:SER:HA	2.18	0.44
1:A:216:LYS:HA	1:A:219:HIS:ND1	2.32	0.44
1:B:116:LYS:HB3	1:B:523:GLN:HE22	1.83	0.43
1:B:467:VAL:HG21	3:B:828:HOH:O	2.01	0.43
1:B:186:TYR:CD2	1:B:188:PRO:HD3	2.53	0.43
1:B:191:ILE:O	1:B:191:ILE:HG22	2.18	0.43
1:B:97:LYS:HG2	1:B:98:GLU:OE1	2.17	0.43
1:A:210:ASN:HD22	1:A:210:ASN:N	2.16	0.43
1:A:460:SER:HB3	1:A:476:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:TYR:CD1	1:A:127:TYR:N	2.86	0.43
1:A:65:LYS:HB3	1:A:236:LEU:HD11	1.99	0.43
1:B:151:ASN:HD22	1:B:152:ALA:N	2.15	0.43
1:B:109:MET:CE	1:B:507:ARG:HH11	2.31	0.43
1:A:154:LEU:HA	1:A:157:ALA:HB3	1.99	0.43
1:B:231:LYS:NZ	3:B:824:HOH:O	2.52	0.43
1:B:321:LEU:CD2	2:B:610:NAD:N1N	2.64	0.43
1:B:522:SER:OG	1:B:522:SER:O	2.33	0.43
1:A:261:MET:O	1:A:262:GLU:C	2.56	0.43
1:A:122:GLU:CD	1:A:122:GLU:N	2.72	0.43
1:A:22:LYS:HG2	1:A:23:ASP:N	2.33	0.43
1:B:225:ARG:NE	3:B:797:HOH:O	2.51	0.43
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.54	0.43
1:A:461:TYR:O	1:A:474:PHE:HA	2.18	0.43
1:A:250:TYR:CD1	1:A:298:GLN:HA	2.53	0.43
1:A:257:VAL:HG22	1:A:258:ASN:ND2	2.33	0.43
1:B:58:LEU:HD23	1:B:459:VAL:CG2	2.47	0.43
1:A:58:LEU:HD22	1:A:59:ASP:O	2.18	0.43
1:A:418:TYR:HA	3:A:838:HOH:O	2.18	0.43
1:B:351:HIS:O	1:B:412:LYS:HB3	2.19	0.43
1:A:440:LEU:HA	1:A:440:LEU:HD12	1.88	0.43
1:A:336:LEU:HD23	1:A:343:PRO:HG3	2.01	0.43
1:A:497:PHE:CD2	1:B:530:GLU:HB2	2.54	0.43
1:B:216:LYS:N	3:B:838:HOH:O	2.52	0.43
1:A:68:ILE:HG22	1:A:144:VAL:HG13	2.01	0.43
1:B:324:GLY:HA3	1:B:441:LEU:HD23	2.00	0.43
1:A:429:ARG:NE	3:A:643:HOH:O	2.24	0.43
1:A:76:ASN:HD22	1:A:409:GLY:HA2	1.83	0.43
1:A:294:ASN:C	1:A:294:ASN:HD22	2.22	0.43
1:B:158:MET:HG2	1:B:169:GLN:HG2	2.01	0.43
1:B:517:LEU:HA	1:B:517:LEU:HD12	1.76	0.42
1:A:120:ASP:OD1	1:A:124:ASN:N	2.49	0.42
1:A:501:ASN:ND2	1:A:501:ASN:N	2.66	0.42
1:A:423:MET:HE1	1:B:443:THR:HB	2.01	0.42
1:A:531:ARG:C	1:A:532:LEU:CD1	2.87	0.42
1:A:66:LEU:HD22	1:A:67:GLY:N	2.33	0.42
1:A:423:MET:CE	1:B:443:THR:HB	2.49	0.42
1:B:245:ALA:O	1:B:246:ASN:O	2.38	0.42
1:A:316:ILE:HD11	1:A:480:VAL:HG12	2.00	0.42
1:A:467:VAL:HG23	1:A:467:VAL:O	2.18	0.42
1:A:264:LEU:HD22	1:A:305:LEU:CA	2.50	0.42
1:B:211:VAL:O	1:B:211:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:483:PHE:O	1:B:510:LEU:HD21	2.19	0.42
1:A:63:PRO:CG	1:A:238:LYS:HE2	2.38	0.42
1:A:468:LYS:HG2	1:A:468:LYS:O	2.19	0.42
1:A:257:VAL:CG2	1:A:258:ASN:ND2	2.82	0.42
1:B:344:VAL:HG12	1:B:420:SER:HA	2.02	0.42
2:B:610:NAD:C3B	3:B:834:HOH:O	2.47	0.42
1:A:245:ALA:HB1	2:A:600:NAD:C5A	2.50	0.42
1:B:515:ARG:HH11	1:B:522:SER:H	1.68	0.42
1:A:172:LEU:HB3	1:A:176:MET:CE	2.48	0.42
1:A:125:ASP:HB3	1:A:127:TYR:CE1	2.55	0.42
1:B:337:VAL:CG1	1:B:337:VAL:O	2.66	0.42
1:B:321:LEU:HD12	1:B:445:LEU:HD22	2.00	0.42
1:A:481:LEU:HB3	1:A:484:LEU:HD22	2.01	0.42
1:A:410:ASP:OD1	1:A:437:GLU:OE1	2.38	0.42
1:A:282:ALA:CB	1:A:305:LEU:HD21	2.50	0.42
1:A:302:VAL:O	1:A:306:VAL:HG23	2.19	0.42
1:B:170:GLN:NE2	3:B:623:HOH:O	2.53	0.42
1:A:224:ARG:O	1:A:228:GLN:HG3	2.20	0.42
1:A:251:VAL:O	1:A:299:ASN:ND2	2.51	0.41
1:A:214:ARG:CB	1:A:214:ARG:CZ	2.97	0.41
1:A:22:LYS:CG	1:A:23:ASP:H	2.32	0.41
1:B:215:GLY:H	1:B:271:ASP:CG	2.23	0.41
1:A:186:TYR:HE2	1:A:191:ILE:HD12	1.85	0.41
1:B:311:HIS:CD2	1:B:312:GLU:H	2.37	0.41
1:A:73:LEU:HD12	1:A:181:PRO:HB3	2.01	0.41
1:B:242:LEU:CD1	1:B:446:ILE:HG23	2.50	0.41
1:B:225:ARG:NH2	3:B:797:HOH:O	2.53	0.41
1:B:16:THR:OG1	1:B:17:ASP:N	2.53	0.41
1:B:321:LEU:HD21	2:B:610:NAD:C4N	2.49	0.41
1:B:411:SER:HA	1:B:437:GLU:HA	2.00	0.41
1:B:277:PRO:O	1:B:281:PHE:HD1	2.03	0.41
1:B:71:ILE:HG12	1:B:147:TRP:CE3	2.55	0.41
1:A:251:VAL:N	1:A:299:ASN:HD21	2.19	0.41
1:B:327:LYS:HG3	1:B:503:LEU:HD13	2.02	0.41
1:B:109:MET:N	1:B:448:ASP:OD1	2.46	0.41
1:B:58:LEU:O	1:B:58:LEU:HD13	2.20	0.41
1:A:261:MET:CE	1:A:308:LEU:HA	2.50	0.41
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.78	0.41
1:B:241:VAL:CG2	1:B:292:TYR:CD2	3.03	0.41
1:A:197:GLU:N	1:A:197:GLU:CD	2.73	0.41
1:B:458:ARG:C	3:B:696:HOH:O	2.59	0.41
1:B:195:GLN:OE1	1:B:197:GLU:N	2.43	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:488:LEU:N	1:B:488:LEU:CD1	2.84	0.41
1:B:300:THR:O	1:B:302:VAL:N	2.53	0.41
1:A:194:ASN:O	1:A:246:ASN:HB3	2.21	0.41
1:B:515:ARG:NH2	3:B:854:HOH:O	2.53	0.41
1:A:54:TYR:HA	1:A:462:LYS:O	2.20	0.41
1:B:167:ASP:OD1	1:B:167:ASP:C	2.58	0.41
1:B:442:ALA:HB2	2:B:610:NAD:H5N	2.02	0.41
1:A:94:PHE:N	1:A:94:PHE:CD1	2.88	0.41
1:B:116:LYS:HB3	1:B:523:GLN:NE2	2.35	0.41
1:B:275:ILE:HG21	1:B:280:ILE:HD11	2.02	0.41
1:B:198:ARG:HA	1:B:198:ARG:HD2	1.59	0.41
1:B:303:PRO:HG2	1:B:304:GLY:N	2.32	0.41
1:A:349:TYR:HB2	1:A:415:MET:N	2.36	0.41
1:A:328:LEU:HA	1:A:328:LEU:HD12	1.87	0.41
1:B:82:VAL:HB	1:B:176:MET:HE1	2.03	0.41
1:B:346:ILE:CD1	1:B:346:ILE:N	2.81	0.41
1:B:459:VAL:HG12	1:B:459:VAL:O	2.21	0.41
1:B:329:LYS:HD3	3:B:837:HOH:O	2.19	0.41
1:B:479:PRO:O	1:B:481:LEU:HD12	2.21	0.41
1:A:76:ASN:ND2	1:A:409:GLY:HA2	2.35	0.41
1:A:461:TYR:CE1	3:A:808:HOH:O	2.54	0.41
1:B:54:TYR:HA	1:B:462:LYS:O	2.21	0.41
1:A:493:THR:HG23	1:A:494:ARG:O	2.21	0.41
1:B:492:LEU:O	1:B:493:THR:CG2	2.69	0.41
1:A:198:ARG:HD2	3:A:724:HOH:O	2.21	0.41
1:A:337:VAL:HG23	1:A:338:ASP:N	2.35	0.41
1:B:464:VAL:HG12	1:B:466:PRO:HD3	2.02	0.41
1:A:478:TYR:HA	1:A:479:PRO:HD2	1.62	0.41
1:A:511:GLU:O	1:A:515:ARG:HG3	2.21	0.41
1:B:272:HIS:ND1	1:B:274:GLU:OE1	2.54	0.41
1:A:228:GLN:NE2	3:A:751:HOH:O	2.53	0.41
1:B:115:LEU:O	1:B:127:TYR:HA	2.20	0.40
1:A:89:LYS:NZ	3:A:710:HOH:O	2.23	0.40
1:B:351:HIS:N	1:B:413:VAL:O	2.54	0.40
1:B:208:LYS:HA	1:B:208:LYS:HD2	1.90	0.40
1:B:93:GLU:HG2	3:B:698:HOH:O	2.21	0.40
1:A:247:THR:HG23	1:A:297:PRO:HG2	2.03	0.40
1:B:342:LYS:O	1:B:343:PRO:C	2.57	0.40
1:A:478:TYR:HB3	1:B:531:ARG:O	2.20	0.40
1:B:446:ILE:O	1:B:450:LEU:HG	2.22	0.40
1:A:255:PRO:HA	1:A:259:ASP:OD1	2.22	0.40
1:A:94:PHE:CD1	1:A:168:LEU:HD13	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:245:ALA:C	1:B:246:ASN:O	2.59	0.40
1:B:251:VAL:O	1:B:299:ASN:OD1	2.40	0.40
1:A:484:LEU:O	1:A:487:TRP:CE3	2.74	0.40
1:A:423:MET:HE1	1:B:443:THR:CG2	2.52	0.40
1:A:39:LYS:HG3	1:A:45:PHE:CD2	2.57	0.40
1:A:39:LYS:HG3	1:A:45:PHE:CE2	2.56	0.40
1:B:195:GLN:CD	1:B:197:GLU:O	2.60	0.40
1:A:198:ARG:HG2	1:A:198:ARG:NH1	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:ASN:OD1	1:B:178:LEU:O[3_455]	1.70	0.50
3:A:696:HOH:O	3:A:696:HOH:O[2_555]	2.08	0.12
1:A:23:ASP:OD2	1:A:23:ASP:OD2[2_556]	2.10	0.10

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	462/533 (87%)	389 (84%)	46 (10%)	27 (6%)	3	1
1	B	461/533 (86%)	360 (78%)	59 (13%)	42 (9%)	1	0
All	All	923/1066 (87%)	749 (81%)	105 (11%)	69 (8%)	2	0

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	207	GLU
1	A	298	GLN
1	A	319	ASP
1	B	22	LYS
1	B	41	ALA

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Mol	Chain	Res	Type
1	B	133	LEU
1	B	134	LEU
1	B	161	SER
1	B	236	LEU
1	B	246	ASN
1	B	274	GLU
1	B	298	GLN
1	B	319	ASP
1	B	349	TYR
1	B	466	PRO
1	B	469	GLU
1	B	471	ALA
1	B	473	LYS
1	B	522	SER
1	B	523	GLN
1	A	42	SER
1	A	204	ASN
1	A	246	ASN
1	A	262	GLU
1	A	481	LEU
1	B	135	PRO
1	B	235	ALA
1	B	273	GLU
1	B	299	ASN
1	B	472	GLY
1	A	149	ILE
1	A	193	ALA
1	A	261	MET
1	A	468	LYS
1	A	486	TYR
1	A	532	LEU
1	B	42	SER
1	B	207	GLU
1	B	287	LEU
1	B	322	LYS
1	B	495	PRO
1	B	501	ASN
1	A	41	ALA
1	A	52	GLN
1	A	208	LYS
1	A	350	ASN
1	A	503	LEU

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Mol	Chain	Res	Type
1	B	468	LYS
1	B	479	PRO
1	B	482	THR
1	B	502	GLY
1	B	503	LEU
1	A	133	LEU
1	A	255	PRO
1	A	320	ASP
1	A	479	PRO
1	A	530	GLU
1	B	160	ARG
1	B	300	THR
1	B	350	ASN
1	B	436	CYS
1	B	257	VAL
1	B	320	ASP
1	A	495	PRO
1	B	211	VAL
1	A	49	PRO
1	B	491	PRO
1	B	302	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/471 (87%)	348 (85%)	62 (15%)	4	5
1	B	410/471 (87%)	348 (85%)	62 (15%)	4	5
All	All	820/942 (87%)	696 (85%)	124 (15%)	4	5

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	26	LEU
1	A	37	VAL
1	A	42	SER

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Mol	Chain	Res	Type
1	A	50	THR
1	A	58	LEU
1	A	61	LYS
1	A	65	LYS
1	A	66	LEU
1	A	68	ILE
1	A	70	LEU
1	A	80	THR
1	A	81	LEU
1	A	96	THR
1	A	104	ASN
1	A	147	TRP
1	A	185	ILE
1	A	189	ASP
1	A	197	GLU
1	A	198	ARG
1	A	200	ASN
1	A	207	GLU
1	A	210	ASN
1	A	212	THR
1	A	220	LEU
1	A	236	LEU
1	A	238	LYS
1	A	246	ASN
1	A	257	VAL
1	A	258	ASN
1	A	260	THR
1	A	277	PRO
1	A	287	LEU
1	A	294	ASN
1	A	296	SER
1	A	300	THR
1	A	307	GLN
1	A	308	LEU
1	A	310	GLU
1	A	319	ASP
1	A	320	ASP
1	A	321	LEU
1	A	336	LEU
1	A	346	ILE
1	A	348	SER
1	A	349	TYR

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Mol	Chain	Res	Type
1	A	410	ASP
1	A	411	SER
1	A	438	ASP
1	A	440	LEU
1	A	453	THR
1	A	473	LYS
1	A	480	VAL
1	A	484	LEU
1	A	492	LEU
1	A	495	PRO
1	A	498	HIS
1	A	500	VAL
1	A	516	LEU
1	A	531	ARG
1	A	532	LEU
1	A	533	LEU
1	B	14	VAL
1	B	22	LYS
1	B	40	THR
1	B	58	LEU
1	B	60	LEU
1	B	70	LEU
1	B	73	LEU
1	B	80	THR
1	B	92	VAL
1	B	111	GLN
1	B	125	ASP
1	B	135	PRO
1	B	138	SER
1	B	144	VAL
1	B	147	TRP
1	B	151	ASN
1	B	163	VAL
1	B	176	MET
1	B	198	ARG
1	B	210	ASN
1	B	212	THR
1	B	222	ARG
1	B	225	ARG
1	B	233	GLU
1	B	237	ASP
1	B	238	LYS

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Mol	Chain	Res	Type
1	B	246	ASN
1	B	249	ARG
1	B	251	VAL
1	B	257	VAL
1	B	258	ASN
1	B	260	THR
1	B	263	ASN
1	B	278	SER
1	B	299	ASN
1	B	314	THR
1	B	319	ASP
1	B	325	GLN
1	B	326	THR
1	B	328	LEU
1	B	335	PHE
1	B	344	VAL
1	B	349	TYR
1	B	350	ASN
1	B	423	MET
1	B	428	ASN
1	B	449	LEU
1	B	453	THR
1	B	457	THR
1	B	460	SER
1	B	466	PRO
1	B	470	ASP
1	B	473	LYS
1	B	474	PHE
1	B	483	PHE
1	B	489	LYS
1	B	508	THR
1	B	522	SER
1	B	529	GLU
1	B	531	ARG
1	B	532	LEU
1	B	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	ASN

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Mol	Chain	Res	Type
1	A	77	ASN
1	A	104	ASN
1	A	140	ASN
1	A	162	GLN
1	A	169	GLN
1	A	170	GLN
1	A	194	ASN
1	A	200	ASN
1	A	210	ASN
1	A	228	GLN
1	A	229	ASN
1	A	246	ASN
1	A	258	ASN
1	A	263	ASN
1	A	270	ASN
1	A	294	ASN
1	A	307	GLN
1	A	476	ASN
1	A	501	ASN
1	A	504	ASN
1	A	512	ASN
1	A	523	GLN
1	B	24	ASN
1	B	77	ASN
1	B	91	ASN
1	B	95	GLN
1	B	111	GLN
1	B	140	ASN
1	B	151	ASN
1	B	159	GLN
1	B	162	GLN
1	B	194	ASN
1	B	219	HIS
1	B	228	GLN
1	B	246	ASN
1	B	258	ASN
1	B	263	ASN
1	B	307	GLN
1	B	325	GLN
1	B	427	HIS
1	B	523	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	600	1	48,48,48	2.51	13 (27%)	73,73,73	1.57	11 (15%)
2	NAD	B	610	-	48,48,48	2.65	17 (35%)	73,73,73	1.45	9 (12%)

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	600	1	-	0/30/62/62	0/3/5/5
2	NAD	B	610	-	-	0/30/62/62	0/3/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	NAD	C4N-C3N	8.98	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	NAD	C4N-C3N	8.42	1.53	1.39
2	A	600	NAD	C2N-C3N	6.63	1.48	1.38
2	B	610	NAD	C2A-N1A	6.39	1.46	1.33
2	A	600	NAD	C2A-N1A	5.44	1.44	1.33
2	A	600	NAD	C6N-N1N	5.11	1.49	1.35
2	B	610	NAD	C6N-N1N	4.98	1.49	1.35
2	B	610	NAD	C2N-C3N	4.52	1.45	1.38
2	B	610	NAD	PN-O3	4.43	1.69	1.60
2	B	610	NAD	C3N-C7N	-4.38	1.43	1.50
2	B	610	NAD	C2A-N3A	4.19	1.40	1.32
2	A	600	NAD	PN-O3	3.99	1.68	1.60
2	A	600	NAD	O7N-C7N	3.73	1.32	1.24
2	A	600	NAD	O4B-C1B	-3.69	1.35	1.41
2	A	600	NAD	C2B-C1B	3.67	1.58	1.53
2	B	610	NAD	C2B-C1B	3.49	1.58	1.53
2	B	610	NAD	C4A-N3A	3.41	1.40	1.35
2	B	610	NAD	C8A-N9A	3.35	1.41	1.36
2	A	600	NAD	C3N-C7N	-3.18	1.45	1.50
2	B	610	NAD	O4D-C1D	3.05	1.46	1.41
2	A	600	NAD	PA-O3	-2.85	1.54	1.59
2	A	600	NAD	C4A-N3A	2.84	1.40	1.35
2	A	600	NAD	C2A-N3A	2.83	1.37	1.32
2	A	600	NAD	C6N-C5N	2.65	1.44	1.38
2	B	610	NAD	C5A-C4A	2.65	1.46	1.40
2	B	610	NAD	C2N-N1N	2.52	1.38	1.35
2	B	610	NAD	O4B-C4B	2.35	1.50	1.45
2	B	610	NAD	O7N-C7N	2.34	1.29	1.24
2	B	610	NAD	PN-O1N	2.29	1.54	1.48
2	B	610	NAD	C2D-C3D	-2.18	1.47	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	NAD	N3A-C2A-N1A	-5.55	124.07	128.71
2	B	610	NAD	N3A-C2A-N1A	-4.78	124.71	128.71
2	B	610	NAD	C3N-C7N-N7N	4.67	123.09	117.77
2	A	600	NAD	C3N-C7N-N7N	4.33	122.70	117.77
2	B	610	NAD	O4D-C1D-N1N	3.72	111.76	107.95
2	A	600	NAD	O4B-C1B-N9A	-3.71	104.98	108.44
2	A	600	NAD	C3D-C2D-C1D	3.70	106.69	100.91
2	A	600	NAD	O4D-C1D-N1N	3.66	111.69	107.95
2	A	600	NAD	O4B-C1B-C2B	-2.72	102.60	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	NAD	N3A-C4A-N9A	2.69	130.29	125.43
2	A	600	NAD	C8A-N9A-C4A	2.66	108.93	106.90
2	B	610	NAD	N3A-C4A-N9A	2.59	130.11	125.43
2	B	610	NAD	C6N-N1N-C1D	-2.48	113.19	119.33
2	B	610	NAD	O4D-C1D-C2D	-2.40	103.09	106.77
2	B	610	NAD	C5N-C4N-C3N	-2.38	117.23	120.32
2	A	600	NAD	C4D-O4D-C1D	2.34	112.29	109.75
2	B	610	NAD	O4B-C1B-C2B	-2.34	103.19	106.77
2	B	610	NAD	O7N-C7N-N7N	-2.30	119.27	122.59
2	A	600	NAD	C5N-C4N-C3N	-2.17	117.50	120.32
2	A	600	NAD	O7N-C7N-N7N	-2.13	119.52	122.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.