



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:00 AM UTC

PDB ID : 1QR6 / pdb_00001qr6
Title : HUMAN MITOCHONDRIAL NAD(P)-DEPENDENT MALIC ENZYME
Authors : Xu, Y.; Bhargava, G.; Wu, H.; Loeber, G.; Tong, L.
Deposited on : 1999-06-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

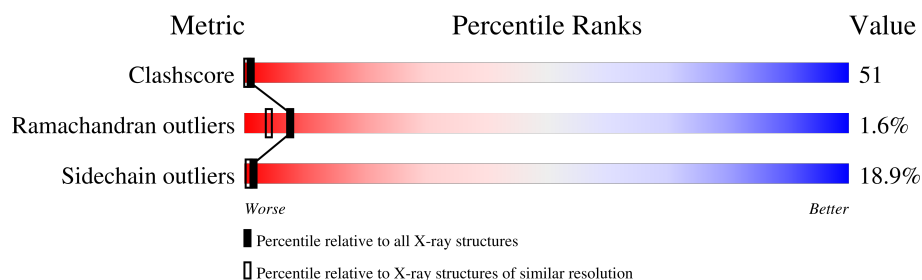
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9620 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 MALIC ENZYME 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	10	0	0
			4342	2779	739	801	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4342	2779	739	801	9	14			

There are 28 discrepancies between the modelled and reference sequences:

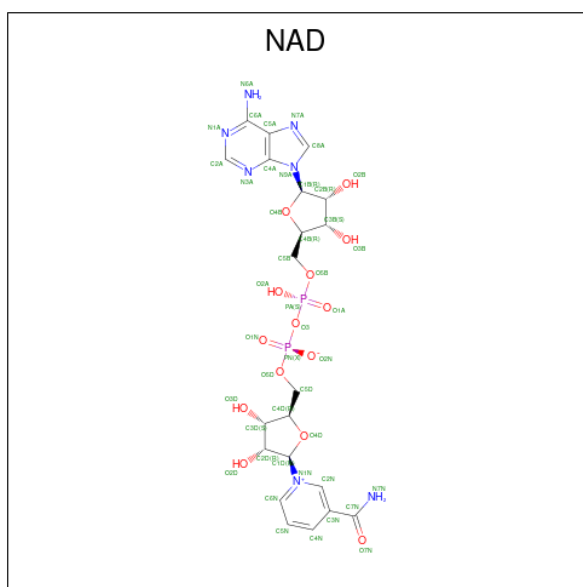
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	1029	MSE	MET	modified residue	UNP P23368
B	1038	MSE	MET	modified residue	UNP P23368
B	1047	MSE	MET	modified residue	UNP P23368
B	1075	MSE	MET	modified residue	UNP P23368
B	1086	MSE	MET	modified residue	UNP P23368
B	1108	MSE	MET	modified residue	UNP P23368
B	1177	MSE	MET	modified residue	UNP P23368
B	1219	MSE	MET	modified residue	UNP P23368
B	1239	MSE	MET	modified residue	UNP P23368
B	1325	MSE	MET	modified residue	UNP P23368
B	1327	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1343	MSE	MET	modified residue	UNP P23368
B	1407	MSE	MET	modified residue	UNP P23368
B	1539	MSE	MET	modified residue	UNP P23368

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



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

- Molecule 3 is water.

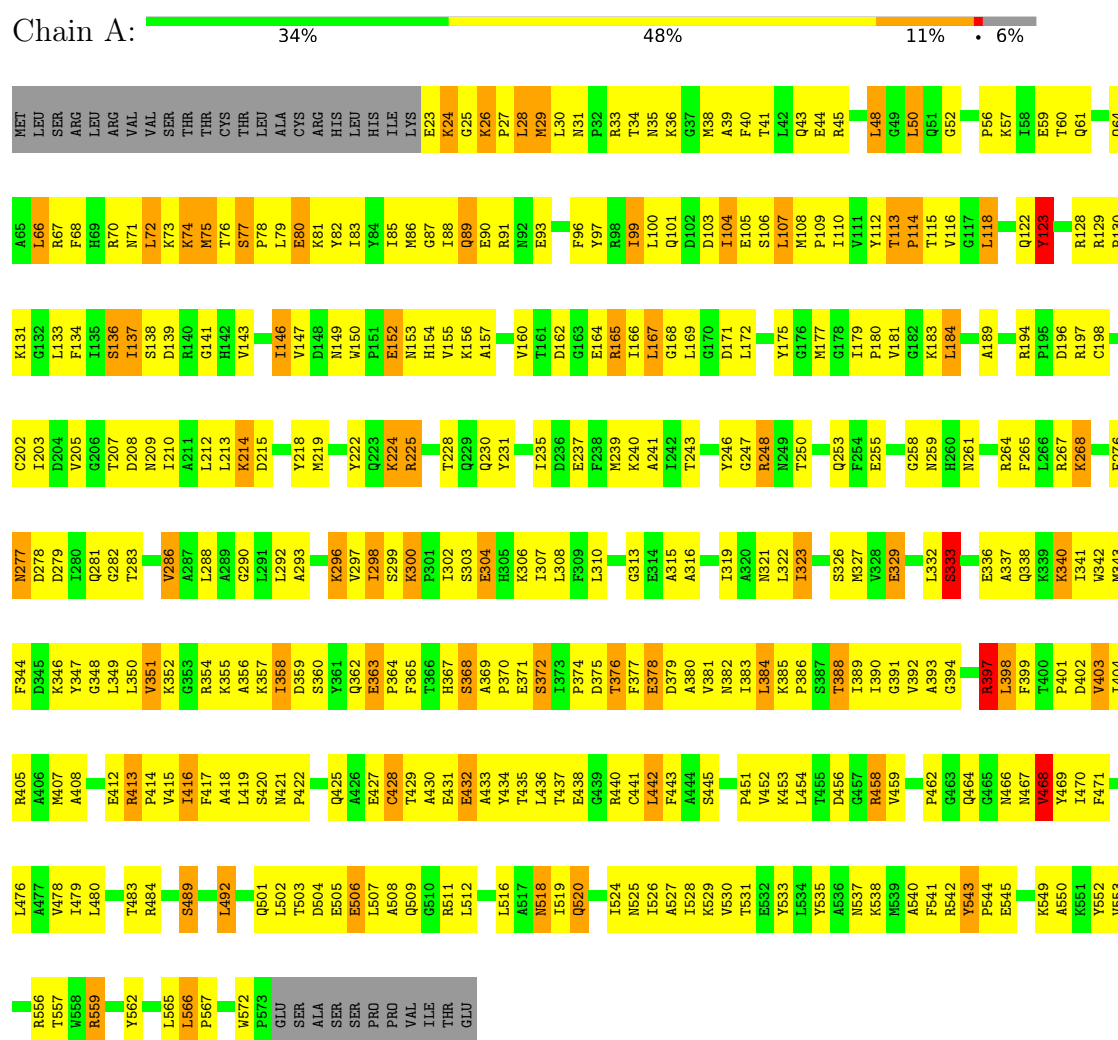
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	374	Total O 374 374	0	0
3	B	386	Total O 386 386	0	0

3 Residue-property plots

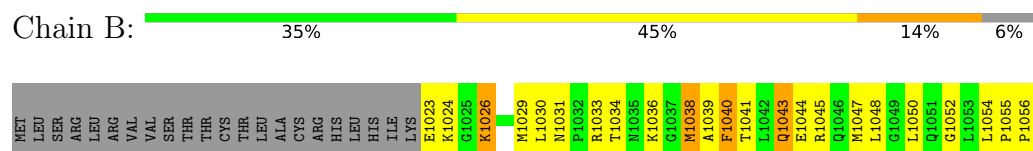
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: MALIC ENZYME 2



• Molecule 1: MALIC ENZYME 2





4 Data and refinement statistics

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	204.40 Å 107.00 Å 59.20 Å 90.00° 90.00° 101.90°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	87.0 (20.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.228 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9620	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	0.47	0/4422	0.99	20/5967 (0.3%)
1	B	0.47	0/4422	0.99	18/5967 (0.3%)
All	All	0.47	0/8844	0.99	38/11934 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1543	TYR	CA-C-N	-9.70	107.72	119.84
1	B	1543	TYR	C-N-CA	-9.70	107.72	119.84
1	B	1543	TYR	N-CA-C	9.38	130.53	109.81
1	A	543	TYR	N-CA-C	8.10	127.71	109.81
1	A	333	SER	N-CA-C	-7.82	100.79	110.41
1	A	542	ARG	N-CA-C	-7.67	95.03	108.23
1	A	281	GLN	N-CA-C	7.28	119.30	111.36
1	B	1542	ARG	N-CA-C	-7.22	95.81	108.23
1	A	543	TYR	CA-C-N	-7.22	110.82	119.84
1	A	543	TYR	C-N-CA	-7.22	110.82	119.84
1	A	375	ASP	N-CA-C	-6.93	104.01	113.30
1	A	80	GLU	N-CA-C	-6.69	103.67	110.97
1	A	104	ILE	N-CA-C	6.28	116.45	110.42
1	B	1055	PRO	CA-C-N	6.28	127.69	119.84
1	B	1055	PRO	C-N-CA	6.28	127.69	119.84
1	B	1492	LEU	N-CA-C	-6.24	104.40	111.07
1	B	1539	MSE	N-CA-C	-6.23	105.35	114.39
1	B	1125	HIS	N-CA-C	-5.87	105.78	113.12
1	A	442	LEU	N-CA-C	-5.86	98.97	108.52
1	A	73	LYS	N-CA-C	-5.78	104.90	111.14
1	B	1187	TYR	N-CA-C	-5.71	104.26	111.11
1	A	162	ASP	N-CA-C	-5.66	105.58	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1150	TRP	CA-C-N	5.57	125.93	119.47
1	B	1150	TRP	C-N-CA	5.57	125.93	119.47
1	B	1544	PRO	N-CA-C	-5.56	101.02	112.47
1	A	141	GLY	N-CA-C	-5.55	108.09	114.69
1	A	268	LYS	N-CA-C	5.45	117.98	111.71
1	A	296	LYS	N-CA-C	-5.42	106.50	113.01
1	A	507	LEU	N-CA-C	-5.41	105.41	112.23
1	B	1407	MSE	N-CA-C	-5.35	106.81	113.55
1	B	1334	GLU	N-CA-C	-5.32	105.39	111.14
1	A	323	ILE	N-CA-C	-5.29	105.56	110.53
1	B	1162	ASP	N-CA-C	-5.27	106.08	112.88
1	B	1040	PHE	N-CA-C	-5.22	102.13	109.96
1	A	492	LEU	N-CA-C	-5.16	105.65	111.28
1	B	1470	ILE	N-CA-C	5.04	119.83	109.34
1	A	544	PRO	N-CA-C	-5.02	102.12	112.47
1	A	298	ILE	CB-CA-C	-5.01	106.97	112.68

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	4342	0	4366	461	0
1	B	4342	0	4366	450	0
2	A	88	0	52	2	0
2	B	88	0	52	4	0
3	A	374	0	0	147	0
3	B	386	0	0	159	0
All	All	9620	0	8836	899	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 51.

All (899) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:LEU:HD12	3:B:2496:HOH:O	1.42	1.19
1:A:218:TYR:HB2	3:A:2698:HOH:O	1.44	1.18
1:B:1472:PRO:HB2	3:B:2252:HOH:O	1.48	1.11
1:A:215:ASP:HB3	3:A:2698:HOH:O	1.51	1.10
1:B:1243:THR:HB	1:B:1248:ARG:HE	1.20	1.06
1:B:1513:TYR:HB3	3:B:2740:HOH:O	1.55	1.05
1:A:85:ILE:HG23	1:A:86:MSE:HE3	1.39	1.05
1:B:1113:THR:HB	1:B:1114:PRO:HD3	1.39	1.05
1:A:454:LEU:HD12	3:A:2700:HOH:O	1.58	1.03
1:B:1410:ILE:HG21	3:B:2585:HOH:O	1.60	1.01
1:B:1298:ILE:HG13	3:B:2614:HOH:O	1.61	1.00
1:B:1177:MSE:HG2	1:B:1202:CYS:HB2	1.46	0.97
1:B:1287:ALA:HA	3:B:2167:HOH:O	1.62	0.97
1:A:433:ALA:HB3	3:A:2670:HOH:O	1.62	0.97
1:B:1297:VAL:HG12	1:B:1298:ILE:HD13	1.48	0.96
1:B:1454:LEU:HD11	1:B:1460:PHE:HE2	1.31	0.95
1:B:1385:LYS:HB2	3:B:2680:HOH:O	1.65	0.94
1:A:72:LEU:HA	1:A:75:MSE:HE3	1.48	0.94
1:A:104:ILE:HG13	1:A:108:MSE:HE2	1.49	0.94
1:B:1310:LEU:HD12	3:B:2076:HOH:O	1.66	0.94
1:B:1492:LEU:HB2	3:B:2514:HOH:O	1.65	0.94
1:B:1543:TYR:O	1:B:1545:GLU:N	2.01	0.93
1:A:453:LYS:HE2	3:A:2688:HOH:O	1.67	0.93
1:A:86:MSE:HE2	1:A:86:MSE:HA	1.50	0.93
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.31	0.92
1:B:1261:ASN:HD22	1:B:1264:ARG:HE	1.01	0.92
1:A:113:THR:HB	1:A:114:PRO:HD3	1.48	0.92
1:A:376:THR:HG22	1:A:379:ASP:H	1.36	0.91
1:A:543:TYR:O	1:A:545:GLU:N	2.05	0.90
1:A:393:ALA:HB3	3:A:2677:HOH:O	1.72	0.90
1:B:1526:ILE:HG23	3:B:2727:HOH:O	1.72	0.89
1:A:307:ILE:HG23	1:A:388:THR:HG22	1.53	0.88
1:B:1177:MSE:HG2	1:B:1202:CYS:CB	2.02	0.88
1:A:349:LEU:HD23	3:A:2556:HOH:O	1.74	0.88
1:A:527:ALA:O	1:A:531:THR:HG23	1.74	0.87
1:B:1057:LYS:HB3	3:B:2238:HOH:O	1.75	0.86
1:B:1086:MSE:HE2	1:B:1086:MSE:HA	1.57	0.86
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.76	0.86
1:A:44:GLU:O	1:A:48:LEU:HB2	1.75	0.85
1:A:277:ASN:HD21	1:A:279:ASP:HB2	1.39	0.85
1:A:431:GLU:HG2	1:A:452:VAL:HG22	1.58	0.85
1:B:1429:THR:HG23	1:B:1432:GLU:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:HB3	3:A:2661:HOH:O	1.75	0.85
1:A:91:ARG:HD2	3:B:2639:HOH:O	1.76	0.84
1:B:1308:LEU:HB3	1:B:1389:ILE:HD12	1.59	0.84
1:A:437:THR:HG23	3:A:2220:HOH:O	1.77	0.84
1:B:1547:GLU:HG2	3:B:2652:HOH:O	1.76	0.84
1:A:557:THR:HG22	3:A:2386:HOH:O	1.77	0.84
1:B:1515:PRO:HG2	1:B:1518:ASN:HD21	1.43	0.84
1:A:476:LEU:HD21	3:A:2386:HOH:O	1.77	0.84
1:B:1354:ARG:HD3	1:B:1358:ILE:HD11	1.58	0.84
1:A:167:LEU:HD11	3:A:2550:HOH:O	1.77	0.84
1:B:1058:ILE:HG13	3:B:2147:HOH:O	1.77	0.83
1:B:1194:ARG:HA	3:B:2518:HOH:O	1.79	0.83
1:A:374:PRO:HG3	1:A:380:ALA:HA	1.58	0.83
1:A:392:VAL:HG12	1:A:392:VAL:O	1.76	0.83
1:A:389:ILE:HG21	3:A:2333:HOH:O	1.77	0.83
1:B:1261:ASN:ND2	1:B:1264:ARG:HE	1.76	0.83
1:B:1319:ILE:HG23	3:B:2547:HOH:O	1.77	0.83
1:B:1558:TRP:HB3	3:B:2518:HOH:O	1.78	0.83
1:A:454:LEU:HA	3:A:2627:HOH:O	1.80	0.82
1:A:531:THR:HB	3:A:2234:HOH:O	1.78	0.82
1:B:1454:LEU:HD11	1:B:1460:PHE:CE2	2.13	0.82
1:A:429:THR:HG23	1:A:432:GLU:H	1.43	0.82
1:A:376:THR:HG23	1:A:378:GLU:H	1.44	0.82
1:B:1442:LEU:HD12	3:B:2614:HOH:O	1.79	0.82
1:A:109:PRO:O	1:A:114:PRO:HD2	1.79	0.82
1:A:24:LYS:HA	1:A:28:LEU:HD22	1.60	0.82
1:A:388:THR:HG23	3:A:2287:HOH:O	1.79	0.81
1:A:86:MSE:HE1	1:A:96:PHE:CE1	2.15	0.81
1:A:154:HIS:O	1:A:197:ARG:HG2	1.81	0.81
1:B:1405:ARG:HD2	3:B:2359:HOH:O	1.81	0.81
1:A:99:ILE:HG21	3:A:2715:HOH:O	1.80	0.80
1:A:378:GLU:OE1	1:A:402:ASP:HB3	1.80	0.80
1:A:338:GLN:HB3	3:A:2569:HOH:O	1.80	0.80
1:B:1406:ALA:C	3:B:2312:HOH:O	2.25	0.80
1:B:1109:PRO:O	1:B:1114:PRO:HD2	1.82	0.80
1:B:1104:ILE:HG13	1:B:1108:MSE:HG3	1.63	0.80
1:B:1039:ALA:HA	1:B:1059:GLU:O	1.82	0.79
1:A:78:PRO:HG3	3:A:2628:HOH:O	1.81	0.79
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.65	0.79
1:A:372:SER:HB2	1:A:383:ILE:HG12	1.64	0.79
1:A:390:ILE:HG12	3:A:2571:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1392:VAL:HG12	1:B:1392:VAL:O	1.82	0.79
1:A:128:ARG:HH22	1:B:1128:ARG:NH1	1.80	0.79
1:A:288:LEU:HG	3:A:2469:HOH:O	1.81	0.79
1:A:436:LEU:HB3	3:A:2512:HOH:O	1.83	0.79
1:B:1514:PRO:O	3:B:2740:HOH:O	2.01	0.78
1:A:471:PHE:CD1	3:A:2711:HOH:O	2.36	0.78
1:A:296:LYS:HE3	3:A:2737:HOH:O	1.83	0.78
1:B:1428:CYS:SG	3:B:2311:HOH:O	2.42	0.77
1:B:1351:VAL:HG11	1:B:1369:ALA:HB2	1.66	0.77
1:A:435:THR:HA	3:A:2229:HOH:O	1.83	0.77
1:B:1411:ASN:HB2	3:B:2146:HOH:O	1.84	0.77
1:A:437:THR:HG22	3:A:2063:HOH:O	1.83	0.77
1:A:310:LEU:HD23	1:A:427:GLU:HG2	1.68	0.76
1:B:1113:THR:CB	1:B:1114:PRO:HD3	2.15	0.76
1:A:386:PRO:HG2	3:A:2256:HOH:O	1.85	0.76
1:B:1085:ILE:HG23	1:B:1086:MSE:HE3	1.66	0.76
1:A:113:THR:CB	1:A:114:PRO:HD3	2.16	0.76
1:A:416:ILE:HD11	1:A:441:CYS:CB	2.16	0.75
1:A:437:THR:HG21	1:A:441:CYS:HB3	1.68	0.75
1:B:1240:LYS:HE2	3:B:2724:HOH:O	1.87	0.75
1:B:1294:ALA:HB1	1:B:1442:LEU:HD13	1.67	0.75
1:A:315:ALA:HA	3:A:2644:HOH:O	1.87	0.74
1:A:85:ILE:HG13	3:A:2715:HOH:O	1.87	0.74
1:B:1526:ILE:CG2	3:B:2727:HOH:O	2.32	0.74
1:B:1078:PRO:HB3	3:B:2741:HOH:O	1.87	0.74
1:A:212:LEU:O	3:A:2698:HOH:O	2.05	0.74
1:B:1207:THR:HG21	3:B:2716:HOH:O	1.85	0.74
1:A:183:LYS:NZ	3:A:2692:HOH:O	2.20	0.74
1:A:308:LEU:HB3	1:A:389:ILE:HD12	1.67	0.74
1:A:250:THR:HB	3:A:2279:HOH:O	1.87	0.74
1:B:1399:PHE:HD1	3:B:2311:HOH:O	1.70	0.74
1:B:1078:PRO:HD2	3:B:2507:HOH:O	1.87	0.73
1:B:1307:ILE:HG23	1:B:1388:THR:HG22	1.68	0.73
1:B:1411:ASN:ND2	3:B:2146:HOH:O	2.22	0.73
1:B:1320:ALA:HB2	3:B:2102:HOH:O	1.87	0.73
1:B:1340:LYS:HE3	3:B:2280:HOH:O	1.88	0.73
1:A:104:ILE:CG1	1:A:108:MSE:HE2	2.18	0.73
1:B:1513:TYR:OH	3:B:2167:HOH:O	2.05	0.73
1:A:440:ARG:HG2	3:A:2237:HOH:O	1.87	0.73
1:B:1308:LEU:HB2	1:B:1386:PRO:HG3	1.71	0.73
1:B:1414:PRO:HA	3:B:2146:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1043:GLN:HB3	3:B:2742:HOH:O	1.87	0.73
1:B:1526:ILE:O	1:B:1530:VAL:HG23	1.87	0.73
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.71	0.72
1:A:376:THR:CG2	1:A:379:ASP:H	2.02	0.72
1:B:1308:LEU:HB3	1:B:1389:ILE:CD1	2.19	0.72
1:A:128:ARG:HH12	1:B:1128:ARG:HH12	1.34	0.72
1:B:1261:ASN:HD22	1:B:1264:ARG:NE	1.84	0.72
1:B:1386:PRO:HG2	3:B:2265:HOH:O	1.90	0.72
1:A:292:LEU:HD11	3:A:2469:HOH:O	1.89	0.72
1:B:1165:ARG:HD3	1:B:1258:GLY:HA2	1.71	0.72
1:B:1372:SER:O	1:B:1383:ILE:HD13	1.89	0.72
1:A:23:GLU:HG2	1:A:24:LYS:N	2.04	0.72
1:A:80:GLU:C	3:A:2308:HOH:O	2.32	0.72
1:A:86:MSE:HE1	1:A:96:PHE:CZ	2.24	0.72
1:A:265:PHE:HD1	3:A:2457:HOH:O	1.72	0.72
1:A:416:ILE:HD11	1:A:441:CYS:HB2	1.70	0.72
1:A:433:ALA:O	1:A:437:THR:HG23	1.90	0.72
1:A:454:LEU:HD11	3:A:2178:HOH:O	1.89	0.72
1:B:1217:PHE:HB3	3:B:2107:HOH:O	1.90	0.71
1:B:1113:THR:HB	1:B:1114:PRO:CD	2.19	0.71
1:A:456:ASP:OD1	1:A:458:ARG:HB2	1.90	0.71
1:A:367:HIS:HE1	3:A:2569:HOH:O	1.71	0.71
1:B:1163:GLY:HA2	1:B:1166:ILE:HD11	1.72	0.71
1:A:82:TYR:HD2	1:A:83:ILE:HD13	1.54	0.71
1:A:454:LEU:HD22	3:A:2229:HOH:O	1.89	0.71
1:B:1183:LYS:HE2	1:B:1255:GLU:OE2	1.91	0.70
1:A:506:GLU:O	1:A:511:ARG:HB2	1.91	0.70
1:A:64:GLN:O	1:A:68:PHE:HD1	1.73	0.70
1:A:385:LYS:HG3	3:A:2226:HOH:O	1.91	0.70
1:A:553:VAL:HG13	3:A:2141:HOH:O	1.91	0.70
1:B:1302:ILE:HA	1:B:1305:HIS:CD2	2.27	0.70
1:B:1277:ASN:C	1:B:1277:ASN:HD22	1.99	0.70
1:A:466:ASN:CB	3:A:2681:HOH:O	2.40	0.69
1:B:1378:GLU:OE1	1:B:1402:ASP:HB3	1.92	0.69
1:B:1523:SER:HB3	3:B:2252:HOH:O	1.91	0.69
1:A:26:LYS:HE3	3:B:2492:HOH:O	1.93	0.69
1:A:152:GLU:HG2	1:A:196:ASP:O	1.92	0.69
1:A:183:LYS:HG3	3:A:2534:HOH:O	1.92	0.69
1:A:243:THR:HG22	3:A:2279:HOH:O	1.92	0.69
1:B:1086:MSE:HE1	1:B:1096:PHE:CE1	2.27	0.69
1:A:374:PRO:HD3	1:A:383:ILE:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CE2	3:A:2692:HOH:O	2.45	0.69
1:B:1152:GLU:HG2	1:B:1196:ASP:O	1.93	0.69
1:B:1090:GLU:HB3	3:B:2094:HOH:O	1.91	0.69
2:A:601:NAD:H4N	3:A:2275:HOH:O	1.93	0.69
1:B:1454:LEU:HD12	1:B:1458:ARG:HB2	1.75	0.69
1:A:79:LEU:O	1:A:83:ILE:HG12	1.93	0.68
1:A:404:ILE:CG2	3:A:2220:HOH:O	2.41	0.68
1:B:1060:THR:H	1:B:1063:ILE:HD12	1.58	0.68
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.75	0.68
1:A:381:VAL:HG22	3:A:2256:HOH:O	1.91	0.68
1:B:1061:GLN:NE2	3:B:2583:HOH:O	2.25	0.68
1:A:307:ILE:HG23	1:A:388:THR:CG2	2.24	0.68
1:B:1558:TRP:CB	3:B:2518:HOH:O	2.40	0.68
1:A:464:GLN:HA	3:A:2143:HOH:O	1.91	0.68
1:B:1511:ARG:HG2	1:B:1511:ARG:HH11	1.58	0.68
1:A:303:SER:O	1:A:340:LYS:HE2	1.94	0.68
1:B:1409:SER:N	3:B:2312:HOH:O	2.13	0.68
1:A:48:LEU:HD22	3:A:2081:HOH:O	1.94	0.68
1:B:1059:GLU:CD	1:B:1067:ARG:HH12	2.02	0.68
1:B:1325:MSE:HE2	3:B:2514:HOH:O	1.94	0.68
1:B:1325:MSE:CE	3:B:2514:HOH:O	2.41	0.67
1:B:1381:VAL:HG22	3:B:2265:HOH:O	1.93	0.67
1:A:459:VAL:HA	3:A:2189:HOH:O	1.94	0.67
1:A:376:THR:HG23	1:A:378:GLU:N	2.09	0.67
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.76	0.67
1:B:1058:ILE:HG22	3:B:2329:HOH:O	1.95	0.67
1:B:1103:ASP:HB3	1:B:1107:LEU:HD22	1.77	0.67
1:B:1392:VAL:O	1:B:1392:VAL:CG1	2.42	0.67
1:B:1484:ARG:HB2	3:B:2087:HOH:O	1.95	0.66
1:A:85:ILE:HG23	1:A:86:MSE:CE	2.20	0.66
1:B:1110:ILE:HB	3:B:2496:HOH:O	1.95	0.66
1:B:1294:ALA:CB	1:B:1442:LEU:HD13	2.26	0.66
1:B:1519:ILE:HG23	3:B:2565:HOH:O	1.93	0.66
1:A:235:ILE:O	1:A:239:MSE:HG2	1.95	0.66
1:A:327:MSE:HE1	1:A:337:ALA:O	1.94	0.66
1:B:1075:MSE:HG2	1:B:1080:GLU:CD	2.21	0.66
1:A:225:ARG:HB2	3:A:2531:HOH:O	1.95	0.65
1:B:1043:GLN:HE21	1:B:1566:LEU:HD11	1.61	0.65
1:A:415:VAL:N	3:A:2752:HOH:O	2.25	0.65
1:B:1153:ASN:HD22	1:B:1245:ARG:HH21	1.44	0.65
1:A:405:ARG:HA	3:A:2512:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLU:H	1:A:505:GLU:CD	2.04	0.65
1:B:1086:MSE:HE1	1:B:1096:PHE:CZ	2.32	0.65
1:B:1551:LYS:O	1:B:1555:GLU:HG3	1.95	0.65
1:A:128:ARG:HH12	1:B:1128:ARG:NH1	1.94	0.65
1:B:1202:CYS:SG	3:B:2416:HOH:O	2.54	0.65
1:B:1104:ILE:HD13	3:B:2565:HOH:O	1.97	0.65
1:B:1207:THR:CB	3:B:2716:HOH:O	2.44	0.65
1:A:128:ARG:NH1	1:B:1128:ARG:HH12	1.95	0.65
1:B:1038:MSE:SE	3:B:2238:HOH:O	2.64	0.65
1:B:1294:ALA:HB1	1:B:1442:LEU:CD1	2.27	0.65
1:A:471:PHE:CG	3:A:2711:HOH:O	2.49	0.64
1:A:321:ASN:HB3	3:A:2678:HOH:O	1.96	0.64
1:A:467:ASN:OD1	3:A:2275:HOH:O	2.14	0.64
1:A:129:ARG:HG3	1:A:130:PRO:HD2	1.77	0.64
1:A:377:PHE:CZ	1:A:389:ILE:HD11	2.32	0.64
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.32	0.64
1:B:1169:LEU:N	1:B:1169:LEU:HD12	2.13	0.64
1:A:347:TYR:CD1	1:A:356:ALA:HB1	2.32	0.64
1:B:1188:THR:CG2	3:B:2409:HOH:O	2.46	0.64
1:B:1137:ILE:O	1:B:1140:ARG:HG2	1.98	0.63
1:B:1250:THR:HB	3:B:2746:HOH:O	1.97	0.63
1:B:1308:LEU:HD23	1:B:1389:ILE:HD11	1.79	0.63
1:A:40:PHE:HE2	1:A:565:LEU:HD12	1.62	0.63
1:B:1538:LYS:HA	3:B:2213:HOH:O	1.97	0.63
1:B:1038:MSE:HG2	1:B:1057:LYS:O	1.99	0.63
1:B:1513:TYR:C	3:B:2740:HOH:O	2.40	0.63
1:A:413:ARG:HD2	3:A:2134:HOH:O	1.98	0.63
1:B:1376:THR:HG22	1:B:1379:ASP:H	1.63	0.63
1:B:1349:LEU:HD21	1:B:1384:LEU:HD21	1.79	0.63
1:A:524:ILE:HD12	3:A:2386:HOH:O	1.97	0.63
1:A:184:LEU:HG	1:A:198:CYS:HB3	1.81	0.63
1:A:208:ASP:N	3:A:2531:HOH:O	2.31	0.63
1:A:108:MSE:CE	1:A:519:ILE:HG21	2.29	0.62
1:A:308:LEU:HB3	1:A:389:ILE:CD1	2.28	0.62
1:B:1103:ASP:O	1:B:1107:LEU:HB2	2.00	0.62
1:B:1243:THR:HB	1:B:1248:ARG:NE	2.04	0.62
1:B:1404:ILE:HD12	1:B:1436:LEU:HD12	1.80	0.62
1:B:1414:PRO:HB3	3:B:2146:HOH:O	1.99	0.62
1:B:1214:LYS:HD3	3:B:2156:HOH:O	2.00	0.62
1:A:136:SER:OG	1:A:138:SER:HB2	2.00	0.62
1:A:85:ILE:HA	1:A:88:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:HB3	3:A:2178:HOH:O	2.00	0.62
1:A:113:THR:HB	1:A:114:PRO:CD	2.27	0.62
1:B:1177:MSE:SE	3:B:2597:HOH:O	2.68	0.61
1:B:1024:LYS:HB2	3:B:2310:HOH:O	1.99	0.61
1:B:1188:THR:HG21	3:B:2409:HOH:O	1.99	0.61
1:A:277:ASN:ND2	1:A:279:ASP:HB2	2.14	0.61
1:B:1082:TYR:HD2	1:B:1083:ILE:HD13	1.65	0.61
1:B:1207:THR:CG2	3:B:2716:HOH:O	2.44	0.61
1:B:1357:LYS:NZ	1:B:1357:LYS:HB3	2.16	0.61
1:A:189:ALA:O	1:A:520:GLN:NE2	2.34	0.61
1:B:1024:LYS:HE3	3:B:2310:HOH:O	2.00	0.61
1:A:228:THR:HG23	3:A:2560:HOH:O	2.00	0.61
1:A:86:MSE:HE2	1:A:86:MSE:CA	2.28	0.61
1:A:297:VAL:HG12	1:A:298:ILE:HD13	1.83	0.61
1:B:1494:ALA:HB1	3:B:2727:HOH:O	2.00	0.61
1:A:183:LYS:HE3	3:A:2711:HOH:O	2.00	0.61
1:A:374:PRO:CD	1:A:383:ILE:HD13	2.31	0.61
1:A:543:TYR:C	1:A:545:GLU:N	2.58	0.60
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.47	0.60
1:B:1110:ILE:CB	3:B:2496:HOH:O	2.48	0.60
1:A:177:MSE:HE1	1:A:181:VAL:HG23	1.83	0.60
1:A:454:LEU:CD2	3:A:2229:HOH:O	2.47	0.60
1:B:1389:ILE:HG21	3:B:2538:HOH:O	1.99	0.60
1:B:1112:TYR:CG	1:B:1113:THR:N	2.66	0.60
1:B:1152:GLU:HG3	3:B:2660:HOH:O	2.02	0.60
1:B:1184:LEU:HG	1:B:1198:CYS:HB3	1.83	0.60
1:B:1392:VAL:HG12	3:B:2035:HOH:O	2.01	0.60
1:B:1394:GLY:HA2	1:B:1420:SER:HB3	1.84	0.60
1:A:218:TYR:O	1:B:1057:LYS:HE2	2.01	0.60
1:A:469:TYR:CE1	3:A:2681:HOH:O	2.52	0.60
1:B:1089:GLN:HG3	1:B:1090:GLU:N	2.16	0.60
1:A:112:TYR:O	1:A:116:VAL:HG12	2.01	0.60
1:A:177:MSE:CE	1:A:181:VAL:HG23	2.31	0.60
1:B:1399:PHE:CD1	3:B:2311:HOH:O	2.51	0.60
1:A:489:SER:HB2	1:A:533:TYR:OH	2.02	0.59
1:A:518:ASN:HA	3:A:2214:HOH:O	2.03	0.59
1:A:139:ASP:CG	1:A:146:ILE:HD11	2.26	0.59
1:B:1091:ARG:HD2	3:B:2640:HOH:O	2.02	0.59
1:B:1282:GLY:O	1:B:1286:VAL:HG22	2.03	0.59
1:A:177:MSE:HG2	1:A:202:CYS:CB	2.33	0.59
1:A:342:TRP:HA	3:A:2437:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:PRO:O	1:A:405:ARG:HG2	2.03	0.59
1:B:1150:TRP:CE2	1:B:1199:LEU:HD13	2.38	0.59
1:B:1288:LEU:N	3:B:2547:HOH:O	2.34	0.59
1:A:116:VAL:HG13	3:A:2550:HOH:O	2.03	0.59
1:B:1428:CYS:HB3	3:B:2311:HOH:O	2.02	0.59
1:B:1469:TYR:CZ	1:B:1516:LEU:HD13	2.37	0.59
1:A:407:MSE:HE1	3:A:2256:HOH:O	2.03	0.59
1:B:1079:LEU:HD21	1:B:1122:GLN:HG3	1.85	0.59
1:B:1433:ALA:O	1:B:1437:THR:HG23	2.03	0.59
1:B:1515:PRO:HG2	1:B:1518:ASN:ND2	2.15	0.59
1:B:1413:ARG:HA	1:B:1440:ARG:O	2.02	0.59
1:B:1086:MSE:CE	1:B:1096:PHE:CE1	2.86	0.58
1:B:1429:THR:HG22	1:B:1432:GLU:CG	2.33	0.58
1:B:1429:THR:HG22	1:B:1432:GLU:OE1	2.03	0.58
1:A:462:PRO:HG3	3:A:2582:HOH:O	2.02	0.58
1:A:108:MSE:N	1:A:109:PRO:HD2	2.18	0.58
1:A:505:GLU:HG2	3:A:2714:HOH:O	2.03	0.58
1:B:1277:ASN:ND2	1:B:1279:ASP:H	2.01	0.58
1:A:75:MSE:SE	3:A:2308:HOH:O	2.71	0.58
1:A:103:ASP:HB3	1:A:107:LEU:HD22	1.84	0.58
1:B:1286:VAL:HG11	1:B:1466:ASN:O	2.03	0.58
1:A:72:LEU:HA	1:A:75:MSE:CE	2.28	0.58
1:A:404:ILE:HG22	3:A:2220:HOH:O	2.02	0.58
1:B:1077:SER:O	1:B:1081:LYS:HG3	2.04	0.58
1:B:1207:THR:HB	3:B:2716:HOH:O	2.03	0.58
1:A:137:ILE:HG13	1:A:137:ILE:O	2.03	0.58
1:A:379:ASP:O	1:A:383:ILE:HD12	2.03	0.58
1:A:438:GLU:HA	3:A:2555:HOH:O	2.03	0.58
1:B:1153:ASN:ND2	1:B:1245:ARG:HH21	2.02	0.58
1:B:1298:ILE:HD11	1:B:1442:LEU:HD11	1.85	0.58
1:A:416:ILE:HD11	1:A:441:CYS:SG	2.44	0.58
1:B:1298:ILE:O	1:B:1300:LYS:N	2.36	0.58
1:A:60:THR:O	1:A:64:GLN:HG3	2.03	0.58
1:B:1302:ILE:CD1	3:B:2722:HOH:O	2.52	0.58
1:B:1454:LEU:CD1	1:B:1458:ARG:HB2	2.34	0.58
1:B:1559:ARG:HG2	3:B:2338:HOH:O	2.04	0.58
1:A:277:ASN:C	1:A:277:ASN:HD22	2.11	0.58
1:A:286:VAL:HG13	1:A:470:ILE:HG12	1.84	0.58
1:A:458:ARG:NH2	3:A:2700:HOH:O	2.37	0.57
1:B:1525:ASN:O	1:B:1529:LYS:HG2	2.04	0.57
1:A:293:ALA:O	1:A:296:LYS:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:VAL:CG2	1:A:407:MSE:HE1	2.34	0.57
1:B:1573:PRO:HA	3:B:2734:HOH:O	2.03	0.57
1:A:86:MSE:CE	1:A:96:PHE:CE1	2.88	0.57
1:A:129:ARG:HB3	3:A:2434:HOH:O	2.03	0.57
1:B:1117:GLY:O	1:B:1169:LEU:HD21	2.04	0.57
1:B:1231:TYR:O	1:B:1235:ILE:HG12	2.04	0.57
1:A:405:ARG:CA	3:A:2512:HOH:O	2.52	0.57
1:B:1401:PRO:HA	1:B:1436:LEU:CD1	2.34	0.57
1:A:109:PRO:HA	1:A:113:THR:HB	1.86	0.57
1:A:505:GLU:O	1:A:509:GLN:HG3	2.04	0.57
1:B:1300:LYS:HD3	1:B:1304:GLU:HB3	1.86	0.57
1:B:1315:ALA:HB3	1:B:1392:VAL:CG1	2.34	0.57
1:A:36:LYS:O	1:A:39:ALA:HB3	2.05	0.57
1:A:166:ILE:N	1:A:166:ILE:HD12	2.20	0.57
1:A:207:THR:C	3:A:2531:HOH:O	2.47	0.57
1:A:277:ASN:ND2	1:A:279:ASP:H	2.03	0.57
1:B:1043:GLN:NE2	1:B:1566:LEU:HD11	2.20	0.57
1:B:1123:TYR:HB3	1:B:1175:TYR:CD2	2.39	0.57
1:B:1399:PHE:CG	1:B:1427:GLU:HB3	2.40	0.57
1:A:315:ALA:HB3	1:A:392:VAL:HG11	1.85	0.57
1:A:437:THR:CG2	3:A:2220:HOH:O	2.45	0.57
1:B:1073:LYS:HE2	1:B:1074:LYS:NZ	2.20	0.57
1:A:430:ALA:HB2	3:A:2582:HOH:O	2.05	0.56
1:B:1033:ARG:NH1	1:B:1093:GLU:OE1	2.38	0.56
1:A:41:THR:OG1	1:A:44:GLU:HG3	2.05	0.56
1:A:440:ARG:HB3	3:A:2134:HOH:O	2.05	0.56
1:B:1193:ILE:C	3:B:2518:HOH:O	2.46	0.56
1:B:1195:PRO:HG3	3:B:2409:HOH:O	2.06	0.56
1:B:1543:TYR:C	1:B:1545:GLU:N	2.63	0.56
1:A:248:ARG:HB3	1:A:484:ARG:NH2	2.21	0.56
1:A:397:ARG:NE	3:A:2162:HOH:O	2.37	0.56
1:A:52:GLY:HA3	1:B:1146:ILE:HG23	1.87	0.56
1:A:139:ASP:OD2	1:A:146:ILE:HD11	2.06	0.56
1:A:349:LEU:HD21	1:A:384:LEU:HD21	1.86	0.56
1:B:1218:TYR:CZ	3:B:2716:HOH:O	2.53	0.56
1:B:1177:MSE:HG2	1:B:1202:CYS:HB3	1.88	0.56
1:A:526:ILE:O	1:A:530:VAL:HG23	2.05	0.55
1:B:1177:MSE:N	3:B:2416:HOH:O	2.39	0.55
1:B:1489:SER:HA	3:B:2514:HOH:O	2.06	0.55
1:A:431:GLU:HB3	3:A:2735:HOH:O	2.05	0.55
1:B:1319:ILE:HG22	1:B:1323:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:TYR:CG	1:A:113:THR:N	2.71	0.55
1:B:1194:ARG:HB2	1:B:1197:ARG:HG3	1.88	0.55
1:A:70:ARG:O	1:A:74:LYS:HG3	2.07	0.55
1:A:282:GLY:O	1:A:286:VAL:HG22	2.06	0.55
1:B:1385:LYS:HA	3:B:2585:HOH:O	2.06	0.55
1:A:381:VAL:HG13	3:A:2256:HOH:O	2.07	0.55
1:A:382:ASN:O	1:A:385:LYS:HG3	2.07	0.55
1:B:1057:LYS:CB	3:B:2238:HOH:O	2.44	0.55
1:A:381:VAL:HG22	1:A:407:MSE:HE1	1.87	0.55
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.89	0.55
1:B:1378:GLU:CD	1:B:1402:ASP:HB3	2.31	0.55
1:A:177:MSE:HG2	1:A:202:CYS:HB2	1.88	0.55
1:B:1023:GLU:HA	3:B:2347:HOH:O	2.07	0.55
1:B:1294:ALA:O	1:B:1297:VAL:HB	2.07	0.55
1:A:342:TRP:CH2	1:A:367:HIS:HB2	2.42	0.55
1:B:1094:LYS:C	3:B:2583:HOH:O	2.50	0.55
1:A:57:LYS:HD2	1:B:1218:TYR:O	2.07	0.54
1:A:71:ASN:O	1:A:75:MSE:CE	2.55	0.54
1:B:1068:PHE:CZ	1:B:1072:LEU:HD13	2.42	0.54
1:B:1143:VAL:O	1:B:1147:VAL:HG23	2.07	0.54
1:A:219:MSE:HE3	3:A:2095:HOH:O	2.06	0.54
1:A:283:THR:HA	3:A:2275:HOH:O	2.07	0.54
1:A:315:ALA:O	1:A:319:ILE:HD12	2.06	0.54
1:A:346:LYS:HE3	1:A:347:TYR:CZ	2.41	0.54
1:A:370:PRO:HD2	3:A:2556:HOH:O	2.06	0.54
1:A:79:LEU:HD13	1:A:118:LEU:HD13	1.88	0.54
1:A:81:LYS:HE3	3:A:2451:HOH:O	2.07	0.54
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.71	0.54
1:B:1064:GLN:OE1	3:B:2704:HOH:O	2.18	0.54
1:B:1131:LYS:HE3	3:B:2094:HOH:O	2.07	0.54
1:B:1243:THR:HG22	3:B:2746:HOH:O	2.06	0.54
1:B:1253:GLN:HG3	1:B:1276:PHE:CZ	2.43	0.54
1:B:1401:PRO:HA	1:B:1436:LEU:HD13	1.89	0.54
1:A:23:GLU:HG2	1:A:24:LYS:H	1.70	0.54
1:A:520:GLN:HG3	3:A:2214:HOH:O	2.06	0.54
1:A:412:GLU:HG3	1:A:413:ARG:HG2	1.88	0.54
1:A:476:LEU:CD2	3:A:2386:HOH:O	2.45	0.54
1:A:484:ARG:HG3	1:A:541:PHE:CE1	2.42	0.54
1:B:1502:LEU:HD11	1:B:1512:LEU:C	2.32	0.54
1:B:1332:LEU:N	1:B:1332:LEU:HD12	2.22	0.54
1:A:283:THR:OG1	3:A:2275:HOH:O	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.07	0.54
1:B:1296:LYS:NZ	3:B:2480:HOH:O	2.39	0.54
1:A:416:ILE:HG22	3:A:2333:HOH:O	2.08	0.54
1:B:1344:PHE:CZ	1:B:1348:GLY:HA2	2.43	0.54
1:B:1104:ILE:HG12	1:B:1108:MSE:HE2	1.90	0.54
1:B:1047:MSE:HE3	3:B:2742:HOH:O	2.07	0.53
1:B:1144:ARG:NH1	1:B:1245:ARG:HB2	2.23	0.53
1:B:1248:ARG:HD2	1:B:1248:ARG:N	2.23	0.53
1:B:1414:PRO:CA	3:B:2146:HOH:O	2.49	0.53
1:A:225:ARG:CB	3:A:2531:HOH:O	2.54	0.53
1:A:261:ASN:ND2	1:A:264:ARG:HE	2.05	0.53
1:A:165:ARG:HD3	1:A:258:GLY:HA2	1.89	0.53
1:A:183:LYS:NZ	1:A:255:GLU:OE1	2.41	0.53
1:B:1036:LYS:NZ	3:B:2244:HOH:O	2.40	0.53
1:B:1346:LYS:HE2	1:B:1347:TYR:CZ	2.44	0.53
1:B:1043:GLN:CB	3:B:2742:HOH:O	2.53	0.53
1:B:1385:LYS:HD2	3:B:2680:HOH:O	2.07	0.53
1:B:1388:THR:OG1	1:B:1415:VAL:HB	2.08	0.53
1:A:372:SER:O	1:A:383:ILE:HG21	2.09	0.53
1:B:1261:ASN:ND2	1:B:1264:ARG:NE	2.52	0.53
1:B:1389:ILE:HG12	3:B:2538:HOH:O	2.09	0.53
1:A:343:MSE:HE2	1:A:365:PHE:HB2	1.91	0.53
1:A:344:PHE:CD1	1:A:349:LEU:N	2.76	0.53
1:B:1108:MSE:N	1:B:1109:PRO:HD2	2.23	0.53
1:B:1109:PRO:HA	1:B:1114:PRO:CD	2.39	0.53
1:B:1389:ILE:HG23	1:B:1399:PHE:CZ	2.44	0.53
1:A:213:LEU:HD11	1:A:224:LYS:HD3	1.89	0.53
1:A:374:PRO:HG3	1:A:380:ALA:CA	2.36	0.53
1:B:1177:MSE:CG	3:B:2597:HOH:O	2.57	0.53
1:B:1412:GLU:HG3	1:B:1413:ARG:HG2	1.90	0.53
1:A:177:MSE:HE1	1:A:181:VAL:CG2	2.38	0.52
1:A:452:VAL:HG12	1:A:452:VAL:O	2.09	0.52
3:A:2638:HOH:O	1:B:1125:HIS:HB3	2.09	0.52
1:A:129:ARG:HG3	1:A:130:PRO:CD	2.39	0.52
1:A:501:GLN:HE22	1:A:525:ASN:HD22	1.58	0.52
1:A:392:VAL:O	1:A:392:VAL:CG1	2.49	0.52
1:B:1205:VAL:HG22	3:B:2363:HOH:O	2.08	0.52
1:B:1310:LEU:HB3	1:B:1391:GLY:HA2	1.90	0.52
1:B:1407:MSE:HE3	3:B:2538:HOH:O	2.09	0.52
1:B:1514:PRO:N	3:B:2740:HOH:O	2.41	0.52
1:A:278:ASP:OD1	1:A:282:GLY:HA3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG12	1:A:454:LEU:HD21	1.92	0.52
1:B:1289:ALA:HA	3:B:2674:HOH:O	2.09	0.52
1:A:143:VAL:O	1:A:147:VAL:HG23	2.09	0.52
1:B:1406:ALA:O	1:B:1410:ILE:HD12	2.09	0.52
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.92	0.52
1:A:552:TYR:O	1:A:556:ARG:HD2	2.10	0.52
1:B:1523:SER:CB	3:B:2252:HOH:O	2.52	0.52
1:A:437:THR:O	1:A:438:GLU:HB2	2.09	0.52
1:A:80:GLU:HG2	3:A:2308:HOH:O	2.09	0.52
1:B:1297:VAL:HG12	1:B:1298:ILE:CD1	2.32	0.52
1:A:128:ARG:NH2	1:B:1128:ARG:NH1	2.55	0.52
1:A:377:PHE:CE2	1:A:389:ILE:HD11	2.45	0.52
1:A:386:PRO:CG	3:A:2256:HOH:O	2.53	0.52
1:B:1086:MSE:HE2	1:B:1086:MSE:CA	2.34	0.52
1:B:1373:ILE:O	1:B:1373:ILE:HG22	2.08	0.52
1:A:103:ASP:HB3	1:A:107:LEU:CD2	2.39	0.51
1:A:347:TYR:HD1	1:A:356:ALA:HB1	1.76	0.51
1:A:435:THR:HG22	3:A:2229:HOH:O	2.10	0.51
1:B:1095:LEU:HG	1:B:1099:ILE:HD12	1.91	0.51
1:B:1099:ILE:HG22	1:B:1100:LEU:N	2.23	0.51
1:B:1286:VAL:HG12	3:B:2570:HOH:O	2.10	0.51
1:A:104:ILE:O	1:A:108:MSE:HG3	2.10	0.51
1:A:378:GLU:HG3	1:A:403:VAL:HG23	1.93	0.51
1:B:1110:ILE:HG13	3:B:2496:HOH:O	2.09	0.51
1:B:1165:ARG:CZ	3:B:2673:HOH:O	2.58	0.51
1:A:265:PHE:CD1	3:A:2457:HOH:O	2.53	0.51
1:B:1079:LEU:O	1:B:1083:ILE:HG12	2.10	0.51
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.75	0.51
1:B:1287:ALA:HB3	3:B:2547:HOH:O	2.10	0.51
1:B:1453:LYS:HB2	1:B:1459:VAL:HG13	1.92	0.51
1:B:1467:ASN:ND2	2:B:1601:NAD:H71N	2.09	0.51
1:A:277:ASN:HD22	1:A:279:ASP:N	2.09	0.51
1:A:310:LEU:CD2	1:A:427:GLU:HG2	2.40	0.51
1:B:1086:MSE:CE	1:B:1096:PHE:HE1	2.23	0.51
1:B:1292:LEU:CD1	3:B:2674:HOH:O	2.59	0.51
1:B:1295:GLN:C	1:B:1297:VAL:H	2.18	0.51
1:B:1429:THR:HG22	1:B:1432:GLU:CD	2.35	0.51
1:A:91:ARG:HH12	1:B:1090:GLU:CD	2.19	0.51
1:B:1109:PRO:HA	1:B:1114:PRO:HD2	1.93	0.51
1:B:1292:LEU:HD12	3:B:2674:HOH:O	2.09	0.51
1:A:104:ILE:HG13	1:A:108:MSE:CE	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HE3	1:A:347:TYR:CE2	2.46	0.51
1:B:1068:PHE:C	1:B:1068:PHE:CD2	2.88	0.51
1:B:1315:ALA:HB3	1:B:1392:VAL:HG11	1.91	0.51
1:A:329:GLU:O	1:A:329:GLU:HG3	2.11	0.51
1:A:333:SER:HB3	1:A:336:GLU:OE2	2.11	0.51
1:B:1047:MSE:HG3	3:B:2742:HOH:O	2.11	0.51
1:A:86:MSE:HA	1:A:86:MSE:CE	2.28	0.50
1:A:108:MSE:HE1	1:A:519:ILE:HG21	1.92	0.50
1:A:459:VAL:HG13	3:A:2189:HOH:O	2.11	0.50
1:B:1301:PRO:O	1:B:1304:GLU:HB2	2.11	0.50
1:A:24:LYS:HB2	1:A:48:LEU:O	2.12	0.50
1:A:404:ILE:HG22	3:A:2063:HOH:O	2.12	0.50
1:A:458:ARG:CZ	3:A:2700:HOH:O	2.58	0.50
1:B:1086:MSE:HA	1:B:1086:MSE:CE	2.38	0.50
1:A:39:ALA:HA	1:A:59:GLU:O	2.11	0.50
1:A:122:GLN:O	1:A:123:TYR:C	2.53	0.50
1:B:1039:ALA:N	3:B:2704:HOH:O	2.44	0.50
1:B:1494:ALA:CB	3:B:2727:HOH:O	2.57	0.50
1:A:261:ASN:HD22	1:A:264:ARG:NE	2.09	0.50
1:A:352:LYS:HB2	1:A:368:SER:HA	1.93	0.50
1:B:1031:ASN:HB3	1:B:1034:THR:OG1	2.12	0.50
1:B:1068:PHE:HB2	3:B:2449:HOH:O	2.11	0.50
1:B:1354:ARG:HD3	1:B:1358:ILE:CD1	2.38	0.50
1:B:1428:CYS:CB	3:B:2311:HOH:O	2.58	0.50
1:A:171:ASP:C	1:A:171:ASP:OD1	2.53	0.50
1:A:175:TYR:HE2	1:A:219:MSE:HG3	1.77	0.50
1:A:408:ALA:HB2	3:A:2063:HOH:O	2.11	0.50
1:A:415:VAL:CG1	3:A:2287:HOH:O	2.59	0.50
1:A:78:PRO:HA	1:A:81:LYS:HG3	1.94	0.50
1:A:113:THR:CB	1:A:114:PRO:CD	2.88	0.50
1:B:1453:LYS:HA	1:B:1459:VAL:HA	1.93	0.50
1:A:45:ARG:HA	1:A:50:LEU:HD12	1.93	0.50
1:A:372:SER:O	1:A:383:ILE:HG12	2.12	0.50
1:B:1195:PRO:CG	3:B:2409:HOH:O	2.60	0.50
1:A:478:VAL:HG13	1:A:483:THR:HB	1.93	0.49
1:B:1154:HIS:O	1:B:1197:ARG:HD3	2.11	0.49
1:B:1469:TYR:HB3	1:B:1498:LEU:HD22	1.94	0.49
1:B:1381:VAL:CG2	1:B:1407:MSE:HE1	2.43	0.49
1:A:183:LYS:NZ	1:A:255:GLU:OE2	2.44	0.49
1:A:418:ALA:O	1:A:445:SER:HA	2.12	0.49
1:A:462:PRO:CB	3:A:2582:HOH:O	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1538:LYS:NZ	1:B:1543:TYR:OH	2.42	0.49
1:A:183:LYS:O	3:A:2534:HOH:O	2.20	0.49
1:B:1060:THR:O	1:B:1064:GLN:HG3	2.11	0.49
1:B:1106:SER:C	1:B:1109:PRO:HD2	2.38	0.49
1:B:1277:ASN:C	1:B:1277:ASN:ND2	2.67	0.49
1:B:1277:ASN:HD21	1:B:1279:ASP:HB2	1.77	0.49
1:B:1310:LEU:HG	1:B:1393:ALA:HB2	1.95	0.49
1:A:23:GLU:CG	1:A:24:LYS:H	2.26	0.49
1:A:452:VAL:C	3:A:2189:HOH:O	2.55	0.49
1:A:467:ASN:C	1:A:469:TYR:H	2.18	0.49
1:B:1043:GLN:CD	3:B:2742:HOH:O	2.56	0.49
1:B:1109:PRO:C	1:B:1114:PRO:HD2	2.37	0.49
1:B:1489:SER:HB2	1:B:1533:TYR:OH	2.13	0.49
1:A:128:ARG:HG3	3:A:2271:HOH:O	2.12	0.49
1:A:183:LYS:NZ	1:A:255:GLU:CD	2.71	0.49
1:A:467:ASN:ND2	3:A:2275:HOH:O	2.46	0.49
1:B:1140:ARG:HG2	1:B:1140:ARG:HH11	1.78	0.49
1:B:1357:LYS:NZ	1:B:1357:LYS:CB	2.75	0.49
1:B:1414:PRO:HD2	1:B:1440:ARG:O	2.13	0.49
1:B:1511:ARG:HH11	1:B:1511:ARG:CG	2.25	0.49
1:A:99:ILE:CG2	3:A:2715:HOH:O	2.50	0.49
1:A:112:TYR:O	1:A:113:THR:C	2.56	0.49
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.94	0.49
1:B:1513:TYR:CB	3:B:2740:HOH:O	2.33	0.49
1:A:26:LYS:HA	1:A:29:MSE:HG3	1.95	0.48
1:A:327:MSE:HE3	1:A:337:ALA:CB	2.41	0.48
1:A:378:GLU:CD	1:A:402:ASP:HB3	2.38	0.48
1:B:1061:GLN:NE2	3:B:2349:HOH:O	2.46	0.48
1:B:1294:ALA:CA	1:B:1442:LEU:HD13	2.43	0.48
1:A:35:ASN:ND2	1:A:91:ARG:O	2.44	0.48
1:A:399:PHE:HB2	1:A:428:CYS:HB3	1.94	0.48
1:A:408:ALA:HA	1:A:414:PRO:HG3	1.95	0.48
1:A:376:THR:HG22	1:A:379:ASP:N	2.18	0.48
1:A:100:LEU:HD12	1:A:100:LEU:O	2.13	0.48
1:A:443:PHE:CD2	3:A:2582:HOH:O	2.65	0.48
1:A:535:TYR:CD2	1:A:540:ALA:HB3	2.49	0.48
1:B:1169:LEU:N	1:B:1169:LEU:CD1	2.77	0.48
1:B:1069:HIS:O	1:B:1073:LYS:HB3	2.13	0.48
1:B:1144:ARG:NH1	1:B:1148:ASP:OD1	2.47	0.48
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.47	0.48
1:A:82:TYR:CD2	1:A:83:ILE:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HD2	1:A:156:LYS:HA	1.70	0.48
1:A:157:ALA:HB2	1:A:479:ILE:HD11	1.95	0.48
1:A:415:VAL:HG12	3:A:2287:HOH:O	2.13	0.48
1:A:528:ILE:HD13	1:A:550:ALA:HA	1.95	0.48
1:B:1131:LYS:NZ	3:B:2137:HOH:O	2.46	0.48
1:B:1351:VAL:CG1	1:B:1369:ALA:HB2	2.40	0.48
1:B:1415:VAL:HG22	1:B:1442:LEU:HB2	1.96	0.48
1:B:1442:LEU:CD1	3:B:2614:HOH:O	2.48	0.48
1:A:377:PHE:O	1:A:381:VAL:HG23	2.13	0.48
1:A:31:ASN:HB3	1:A:34:THR:OG1	2.12	0.48
1:A:109:PRO:HA	1:A:114:PRO:CD	2.44	0.48
1:B:1363:GLU:N	1:B:1364:PRO:HD2	2.29	0.48
1:A:203:ILE:HG22	1:A:205:VAL:HG13	1.95	0.48
1:A:214:LYS:NZ	3:A:2463:HOH:O	2.46	0.48
1:A:383:ILE:C	3:A:2226:HOH:O	2.57	0.48
1:A:467:ASN:C	1:A:469:TYR:N	2.71	0.48
1:B:1213:LEU:HB2	3:B:2156:HOH:O	2.14	0.48
1:B:1345:ASP:HB2	2:B:1601:NAD:O2B	2.14	0.48
1:A:101:GLN:NE2	3:A:2709:HOH:O	2.28	0.47
1:B:1182:GLY:O	1:B:1185:CYS:HB2	2.14	0.47
1:A:118:LEU:O	1:A:122:GLN:HG2	2.13	0.47
1:B:1073:LYS:HE2	1:B:1074:LYS:CE	2.45	0.47
1:B:1202:CYS:HB2	3:B:2416:HOH:O	2.14	0.47
1:A:231:TYR:O	1:A:235:ILE:HG12	2.14	0.47
1:A:357:LYS:O	1:A:358:ILE:HD12	2.15	0.47
1:A:421:ASN:HB3	1:A:422:PRO:HA	1.97	0.47
1:B:1177:MSE:HA	3:B:2416:HOH:O	2.14	0.47
1:B:1372:SER:O	1:B:1374:PRO:HD3	2.15	0.47
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.45	0.47
1:A:414:PRO:CA	3:A:2752:HOH:O	2.63	0.47
1:B:1105:GLU:HB3	3:B:2228:HOH:O	2.14	0.47
1:B:1165:ARG:NH2	3:B:2673:HOH:O	2.46	0.47
1:B:1301:PRO:HG3	3:B:2524:HOH:O	2.15	0.47
1:A:28:LEU:CD2	1:A:48:LEU:HG	2.45	0.47
1:A:177:MSE:CE	1:A:181:VAL:CG2	2.93	0.47
1:B:1109:PRO:CA	1:B:1114:PRO:HD2	2.44	0.47
1:B:1166:ILE:HG13	1:B:1172:LEU:HD12	1.95	0.47
1:B:1414:PRO:CB	3:B:2146:HOH:O	2.59	0.47
1:A:286:VAL:HG11	1:A:466:ASN:O	2.15	0.47
1:B:1558:TRP:CE3	3:B:2409:HOH:O	2.68	0.47
1:A:359:ASP:OD2	1:A:359:ASP:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:ILE:O	1:B:1140:ARG:NH1	2.46	0.47
1:B:1179:ILE:HG21	3:B:2405:HOH:O	2.15	0.47
1:B:1267:ARG:CZ	1:B:1267:ARG:HB3	2.45	0.47
1:A:241:ALA:HA	3:A:2305:HOH:O	2.15	0.47
1:A:310:LEU:HD23	1:A:427:GLU:CG	2.42	0.47
1:A:435:THR:CA	3:A:2229:HOH:O	2.55	0.47
1:A:109:PRO:C	1:A:114:PRO:HD2	2.40	0.46
1:A:194:ARG:NH2	1:A:196:ASP:OD2	2.48	0.46
1:B:1122:GLN:HB2	1:B:1126:ILE:HG12	1.97	0.46
1:A:133:LEU:HD13	1:A:150:TRP:HE3	1.81	0.46
1:B:1215:ASP:OD1	1:B:1216:PRO:HD2	2.15	0.46
1:B:1308:LEU:CB	1:B:1386:PRO:HG3	2.44	0.46
1:B:1328:VAL:HA	1:B:1332:LEU:O	2.16	0.46
1:A:110:ILE:O	1:A:115:THR:HB	2.15	0.46
1:A:553:VAL:HG22	3:A:2141:HOH:O	2.15	0.46
1:B:1321:ASN:HB3	3:B:2288:HOH:O	2.15	0.46
1:A:436:LEU:C	3:A:2220:HOH:O	2.58	0.46
1:B:1156:LYS:HA	1:B:1156:LYS:HD2	1.74	0.46
1:A:225:ARG:HH11	1:A:225:ARG:HG2	1.80	0.46
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.50	0.46
1:A:417:PHE:HD2	3:A:2571:HOH:O	1.98	0.46
1:A:208:ASP:HA	1:A:224:LYS:HD2	1.97	0.46
1:A:323:ILE:O	1:A:327:MSE:HG3	2.15	0.46
1:A:524:ILE:O	1:A:527:ALA:HB3	2.16	0.46
2:A:602:NAD:H52N	3:A:2302:HOH:O	2.15	0.46
1:B:1277:ASN:HD22	1:B:1279:ASP:H	1.63	0.46
1:B:1288:LEU:HD21	1:B:1492:LEU:CD1	2.45	0.46
1:A:429:THR:HG22	1:A:432:GLU:OE1	2.15	0.46
1:B:1354:ARG:HG2	1:B:1356:ALA:O	2.16	0.46
1:A:483:THR:HG23	3:A:2032:HOH:O	2.15	0.46
1:B:1267:ARG:HG2	1:B:1267:ARG:HH11	1.81	0.46
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.97	0.46
1:B:1393:ALA:HA	2:B:1601:NAD:O4B	2.16	0.46
1:A:129:ARG:HD3	3:B:2650:HOH:O	2.16	0.46
1:A:288:LEU:CG	3:A:2469:HOH:O	2.51	0.46
1:B:1325:MSE:HE1	3:B:2514:HOH:O	2.12	0.46
1:B:1502:LEU:HD23	1:B:1506:GLU:OE1	2.15	0.46
1:A:383:ILE:HG22	1:A:384:LEU:HD13	1.98	0.45
1:A:407:MSE:HE2	1:A:407:MSE:HB2	1.84	0.45
1:B:1315:ALA:HB3	1:B:1392:VAL:HG13	1.98	0.45
1:A:103:ASP:O	1:A:107:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PHE:CE2	1:A:177:MSE:HG3	2.51	0.45
1:A:384:LEU:C	3:A:2226:HOH:O	2.58	0.45
1:A:442:LEU:HA	3:A:2371:HOH:O	2.16	0.45
1:B:1167:LEU:N	1:B:1167:LEU:HD23	2.30	0.45
1:B:1243:THR:HG22	1:B:1247:GLY:O	2.16	0.45
1:A:136:SER:C	1:A:138:SER:N	2.72	0.45
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.98	0.45
1:A:462:PRO:CG	3:A:2582:HOH:O	2.62	0.45
1:A:108:MSE:N	1:A:109:PRO:CD	2.79	0.45
1:A:136:SER:C	1:A:138:SER:H	2.23	0.45
1:A:172:LEU:O	1:A:175:TYR:HB2	2.16	0.45
1:A:288:LEU:HD22	1:A:322:LEU:HG	1.99	0.45
1:A:374:PRO:HB3	1:A:379:ASP:CB	2.47	0.45
1:A:407:MSE:SE	3:A:2256:HOH:O	2.85	0.45
1:B:1376:THR:HG22	1:B:1378:GLU:N	2.31	0.45
1:A:33:ARG:NH2	1:A:196:ASP:HA	2.32	0.45
1:B:1166:ILE:HG22	1:B:1167:LEU:HG	1.99	0.45
1:B:1250:THR:N	3:B:2746:HOH:O	2.49	0.45
1:B:1416:ILE:C	1:B:1417:PHE:HD1	2.25	0.45
1:A:71:ASN:O	1:A:75:MSE:HE3	2.16	0.45
1:A:212:LEU:HD22	1:A:218:TYR:CD2	2.50	0.45
1:A:466:ASN:HB3	3:A:2681:HOH:O	2.08	0.45
1:A:538:LYS:HA	3:A:2201:HOH:O	2.17	0.45
1:B:1076:THR:N	1:B:1080:GLU:OE2	2.49	0.45
1:B:1194:ARG:CA	3:B:2518:HOH:O	2.53	0.45
1:A:25:GLY:C	1:A:27:PRO:HD2	2.41	0.45
1:A:326:SER:HB2	1:A:492:LEU:HD11	1.99	0.45
1:A:97:TYR:O	1:A:101:GLN:HG3	2.17	0.45
1:A:208:ASP:OD1	1:A:224:LYS:HD2	2.17	0.45
1:A:253:GLN:HG3	1:A:276:PHE:CZ	2.52	0.45
1:B:1120:CYS:O	1:B:1175:TYR:HB3	2.16	0.45
1:B:1238:PHE:CE1	1:B:1242:ILE:HG13	2.52	0.45
1:A:300:LYS:HE3	1:A:304:GLU:HB3	1.99	0.45
3:A:2541:HOH:O	1:B:1026:LYS:HE3	2.17	0.45
1:B:1286:VAL:HG21	1:B:1467:ASN:ND2	2.32	0.45
1:A:164:GLU:O	1:A:164:GLU:HG3	2.16	0.45
1:A:315:ALA:HB3	1:A:392:VAL:CG1	2.45	0.45
1:A:431:GLU:O	1:A:432:GLU:C	2.60	0.45
1:B:1343:MSE:SE	3:B:2102:HOH:O	2.85	0.45
1:B:1466:ASN:OD1	1:B:1468:VAL:HG13	2.16	0.45
1:A:183:LYS:CE	3:A:2711:HOH:O	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:HG3	1:A:276:PHE:CE2	2.52	0.44
1:B:1041:THR:OG1	1:B:1044:GLU:HG3	2.18	0.44
1:B:1087:GLY:HA2	1:B:1090:GLU:HG2	1.99	0.44
1:A:87:GLY:O	1:A:91:ARG:HG3	2.17	0.44
1:B:1029:MSE:SE	1:B:1050:LEU:HD22	2.67	0.44
1:B:1407:MSE:N	3:B:2312:HOH:O	2.45	0.44
1:B:1073:LYS:HG2	1:B:1074:LYS:N	2.33	0.44
1:B:1108:MSE:CE	1:B:1519:ILE:HG21	2.48	0.44
1:B:1118:LEU:HD22	1:B:1122:GLN:HE21	1.82	0.44
1:A:113:THR:CG2	1:A:114:PRO:HD3	2.47	0.44
1:A:277:ASN:ND2	1:A:279:ASP:N	2.63	0.44
1:A:381:VAL:O	1:A:385:LYS:HA	2.16	0.44
1:A:557:THR:CG2	3:A:2386:HOH:O	2.47	0.44
1:B:1381:VAL:HG22	1:B:1407:MSE:HE1	1.99	0.44
1:A:66:LEU:O	1:A:70:ARG:HG3	2.17	0.44
1:A:363:GLU:HG2	1:A:364:PRO:HD3	2.00	0.44
1:B:1376:THR:O	1:B:1379:ASP:HB2	2.17	0.44
1:A:277:ASN:HD22	1:A:279:ASP:H	1.63	0.44
1:B:1383:ILE:HG22	1:B:1384:LEU:HD13	2.00	0.44
1:A:261:ASN:ND2	1:A:264:ARG:NE	2.65	0.44
1:B:1194:ARG:N	3:B:2518:HOH:O	2.50	0.44
1:B:1333:SER:HB3	1:B:1336:GLU:CD	2.42	0.44
1:B:1407:MSE:C	3:B:2312:HOH:O	2.61	0.44
1:A:225:ARG:HH11	1:A:225:ARG:CG	2.30	0.44
1:A:430:ALA:CB	3:A:2582:HOH:O	2.65	0.44
1:A:436:LEU:HB2	3:A:2220:HOH:O	2.16	0.44
1:B:1153:ASN:HB2	3:B:2730:HOH:O	2.18	0.44
1:B:1187:TYR:O	1:B:1191:ALA:HB3	2.18	0.44
1:A:89:GLN:HG3	1:A:90:GLU:N	2.33	0.44
1:A:209:ASN:HB3	1:A:212:LEU:HD12	2.00	0.44
1:A:397:ARG:HA	1:A:427:GLU:C	2.43	0.44
1:B:1294:ALA:HA	1:B:1442:LEU:HD13	2.00	0.44
1:A:67:ARG:CZ	3:A:2659:HOH:O	2.65	0.43
1:B:1038:MSE:HE3	1:B:1038:MSE:HB2	1.95	0.43
1:B:1089:GLN:OE1	1:B:1131:LYS:HE2	2.18	0.43
1:A:430:ALA:O	1:A:434:TYR:HD1	2.02	0.43
1:A:518:ASN:CB	3:A:2661:HOH:O	2.51	0.43
1:B:1385:LYS:CA	3:B:2585:HOH:O	2.64	0.43
1:B:1469:TYR:OH	3:B:2740:HOH:O	2.21	0.43
1:A:167:LEU:HB2	1:A:168:GLY:H	1.58	0.43
1:A:397:ARG:HA	1:A:427:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:MSE:CA	3:B:2416:HOH:O	2.66	0.43
1:B:1306:LYS:HB3	1:B:1386:PRO:HA	2.00	0.43
1:B:1408:ALA:HB2	1:B:1437:THR:HG22	2.01	0.43
1:A:64:GLN:HE22	1:A:562:TYR:HE1	1.65	0.43
1:A:109:PRO:CA	1:A:114:PRO:HD2	2.48	0.43
1:A:243:THR:HG22	1:A:247:GLY:O	2.19	0.43
1:A:327:MSE:HB3	1:A:332:LEU:HD22	2.00	0.43
1:B:1040:PHE:HE2	1:B:1565:LEU:HD11	1.84	0.43
1:B:1036:LYS:O	1:B:1039:ALA:HB3	2.19	0.43
1:B:1418:ALA:O	1:B:1445:SER:HA	2.19	0.43
1:A:128:ARG:HH22	1:B:1128:ARG:HH12	1.62	0.43
1:A:277:ASN:ND2	1:A:277:ASN:C	2.73	0.43
1:A:351:VAL:HG11	1:A:369:ALA:HB2	2.00	0.43
1:A:355:LYS:HA	1:A:355:LYS:HD3	1.87	0.43
1:A:429:THR:HG22	1:A:432:GLU:HB2	1.99	0.43
1:A:344:PHE:CE1	1:A:348:GLY:HA2	2.54	0.43
1:A:434:TYR:C	3:A:2178:HOH:O	2.62	0.43
1:A:298:ILE:HD11	1:A:413:ARG:HB2	2.01	0.43
1:B:1110:ILE:CG1	3:B:2496:HOH:O	2.67	0.43
1:B:1482:ASN:HD22	1:B:1542:ARG:HA	1.82	0.43
1:A:218:TYR:HB3	1:A:222:TYR:OH	2.19	0.43
1:B:1043:GLN:NE2	3:B:2742:HOH:O	2.52	0.43
1:B:1095:LEU:N	3:B:2583:HOH:O	2.51	0.43
1:B:1385:LYS:C	3:B:2585:HOH:O	2.61	0.43
1:A:537:ASN:C	1:A:538:LYS:HG2	2.43	0.42
1:B:1073:LYS:HG2	1:B:1074:LYS:HE2	2.01	0.42
1:B:1092:ASN:HD21	1:B:1562:TYR:HH	1.62	0.42
1:B:1300:LYS:O	1:B:1301:PRO:C	2.62	0.42
1:A:310:LEU:HB3	1:A:391:GLY:HA2	2.01	0.42
1:B:1108:MSE:N	1:B:1109:PRO:CD	2.82	0.42
1:B:1277:ASN:HD22	1:B:1279:ASP:N	2.18	0.42
1:A:405:ARG:N	3:A:2512:HOH:O	2.51	0.42
1:B:1113:THR:CB	1:B:1114:PRO:CD	2.84	0.42
1:B:1453:LYS:HG2	1:B:1459:VAL:HG22	2.00	0.42
1:B:1512:LEU:HD12	1:B:1512:LEU:HA	1.87	0.42
1:A:166:ILE:HD12	1:A:166:ILE:H	1.83	0.42
1:B:1091:ARG:NH2	3:B:2646:HOH:O	2.41	0.42
1:B:1295:GLN:C	1:B:1297:VAL:N	2.71	0.42
1:B:1301:PRO:C	1:B:1303:SER:N	2.76	0.42
1:B:1467:ASN:HD21	2:B:1601:NAD:H71N	1.67	0.42
1:A:467:ASN:O	1:A:469:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:ASN:HD21	1:B:1033:ARG:HB2	1.83	0.42
1:B:1177:MSE:O	1:B:1181:VAL:HG23	2.20	0.42
1:B:1538:LYS:HE3	1:B:1543:TYR:OH	2.18	0.42
1:A:404:ILE:HG22	3:A:2512:HOH:O	2.19	0.42
1:A:503:THR:O	1:A:506:GLU:HG3	2.20	0.42
1:B:1133:LEU:HB2	1:B:1199:LEU:HD11	2.01	0.42
1:B:1161:THR:CG2	3:B:2416:HOH:O	2.67	0.42
1:A:104:ILE:HG23	1:A:105:GLU:N	2.35	0.42
1:A:146:ILE:HG23	1:B:1052:GLY:HA3	2.02	0.42
1:A:308:LEU:HB2	1:A:386:PRO:HG3	2.02	0.42
1:A:535:TYR:CD1	1:A:549:LYS:HE3	2.55	0.42
1:A:566:LEU:HD22	1:A:567:PRO:HD2	2.02	0.42
3:A:2408:HOH:O	1:B:1067:ARG:HD3	2.18	0.42
1:B:1038:MSE:HE3	3:B:2026:HOH:O	2.19	0.42
1:B:1118:LEU:O	1:B:1122:GLN:HG2	2.20	0.42
1:B:1401:PRO:O	1:B:1405:ARG:HG2	2.20	0.42
1:B:1446:GLY:O	1:B:1464:GLN:NE2	2.43	0.42
1:A:64:GLN:O	1:A:68:PHE:CD1	2.62	0.42
1:A:77:SER:HA	1:A:78:PRO:HD3	1.90	0.42
1:A:203:ILE:N	1:A:203:ILE:HD12	2.35	0.42
1:B:1167:LEU:HB2	1:B:1169:LEU:HD13	2.02	0.42
1:B:1407:MSE:SE	3:B:2265:HOH:O	2.87	0.42
1:B:1505:GLU:H	1:B:1505:GLU:HG2	1.45	0.42
1:A:86:MSE:HE1	1:A:96:PHE:HE1	1.79	0.42
1:A:466:ASN:OD1	1:A:468:VAL:HG13	2.19	0.42
1:B:1089:GLN:HE21	1:B:1089:GLN:HB2	1.57	0.42
1:B:1281:GLN:NE2	1:B:1491:PHE:CE1	2.88	0.42
1:B:1317:LEU:HD13	1:B:1361:TYR:HB3	2.02	0.42
1:B:1343:MSE:HE1	1:B:1362:GLN:HG2	2.02	0.42
1:B:1528:ILE:HD11	1:B:1554:LYS:CE	2.50	0.42
1:A:177:MSE:O	1:A:180:PRO:HD2	2.20	0.41
1:A:367:HIS:CE1	3:A:2569:HOH:O	2.58	0.41
1:B:1445:SER:O	1:B:1464:GLN:HA	2.19	0.41
1:B:1492:LEU:CB	3:B:2514:HOH:O	2.45	0.41
1:A:351:VAL:HG13	1:A:352:LYS:N	2.36	0.41
1:A:429:THR:HG22	1:A:432:GLU:CG	2.50	0.41
1:A:504:ASP:HB2	1:A:505:GLU:OE2	2.19	0.41
1:A:559:ARG:N	1:A:559:ARG:HD3	2.34	0.41
1:B:1352:LYS:HB2	1:B:1367:HIS:O	2.19	0.41
1:B:1460:PHE:O	1:B:1462:PRO:HD3	2.20	0.41
1:A:503:THR:OG1	1:A:506:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:MSE:C	3:B:2704:HOH:O	2.62	0.41
1:B:1344:PHE:CD1	1:B:1349:LEU:N	2.88	0.41
1:B:1394:GLY:N	1:B:1420:SER:OG	2.47	0.41
1:B:1520:GLN:HB2	3:B:2219:HOH:O	2.19	0.41
1:A:137:ILE:HD11	1:A:230:GLN:HB3	2.02	0.41
1:A:351:VAL:CG1	1:A:352:LYS:N	2.82	0.41
1:A:359:ASP:OD2	1:A:362:GLN:N	2.53	0.41
1:B:1310:LEU:CD2	1:B:1427:GLU:CG	2.98	0.41
1:B:1507:LEU:HD12	1:B:1507:LEU:HA	1.74	0.41
1:A:378:GLU:O	1:A:382:ASN:ND2	2.53	0.41
1:B:1112:TYR:HA	1:B:1116:VAL:HB	2.02	0.41
1:B:1227:ARG:HH11	1:B:1227:ARG:CG	2.33	0.41
1:B:1464:GLN:NE2	1:B:1466:ASN:HD22	2.19	0.41
1:A:30:LEU:HD12	3:B:2362:HOH:O	2.21	0.41
1:A:379:ASP:O	1:A:382:ASN:HB2	2.20	0.41
1:B:1066:LEU:HD12	1:B:1066:LEU:HA	1.85	0.41
1:B:1073:LYS:CG	1:B:1074:LYS:N	2.83	0.41
1:B:1317:LEU:HD13	1:B:1361:TYR:CB	2.50	0.41
1:B:1455:THR:HG23	1:B:1456:ASP:N	2.35	0.41
1:A:72:LEU:CA	1:A:75:MSE:HE3	2.35	0.41
1:B:1501:GLN:HE21	1:B:1522:VAL:HG22	1.86	0.41
1:B:1511:ARG:CG	1:B:1511:ARG:NH1	2.82	0.41
1:A:218:TYR:HB3	1:A:222:TYR:CZ	2.56	0.41
1:A:505:GLU:O	1:A:508:ALA:HB3	2.20	0.41
1:B:1100:LEU:HD21	1:B:1189:ALA:HB2	2.02	0.41
1:B:1308:LEU:HG	1:B:1377:PHE:CE1	2.56	0.41
1:A:109:PRO:HA	1:A:114:PRO:HD2	2.02	0.41
1:A:130:PRO:HG2	1:B:1054:LEU:HD23	2.03	0.41
1:A:292:LEU:HD21	3:A:2469:HOH:O	2.21	0.41
1:A:313:GLY:O	1:A:316:ALA:N	2.54	0.41
1:A:363:GLU:N	1:A:364:PRO:HD2	2.35	0.41
1:A:374:PRO:HB3	1:A:379:ASP:HB3	2.03	0.41
1:A:402:ASP:HA	1:A:405:ARG:HD2	2.03	0.41
1:A:453:LYS:N	3:A:2189:HOH:O	2.53	0.41
1:A:476:LEU:O	1:A:480:LEU:HG	2.21	0.41
1:B:1071:ASN:O	1:B:1075:MSE:HE3	2.21	0.41
1:B:1139:ASP:CG	1:B:1146:ILE:HD11	2.46	0.41
1:B:1202:CYS:CB	3:B:2416:HOH:O	2.69	0.41
1:B:1277:ASN:ND2	1:B:1279:ASP:N	2.69	0.41
1:B:1300:LYS:HD2	1:B:1305:HIS:CD2	2.56	0.41
1:B:1310:LEU:CD2	1:B:1427:GLU:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:PRO:HA	1:B:1114:PRO:HD3	2.02	0.41
1:B:1456:ASP:OD1	1:B:1458:ARG:NH1	2.53	0.41
1:B:1501:GLN:NE2	1:B:1522:VAL:HA	2.36	0.41
1:A:128:ARG:NH2	1:B:1128:ARG:HH12	2.16	0.40
1:A:155:VAL:HB	1:A:246:TYR:CD2	2.56	0.40
1:A:290:GLY:O	1:A:293:ALA:HB3	2.21	0.40
1:B:1501:GLN:HE22	1:B:1525:ASN:HD22	1.69	0.40
1:A:76:THR:HG22	1:A:77:SER:N	2.36	0.40
1:A:146:ILE:O	1:A:149:ASN:HB2	2.22	0.40
1:A:230:GLN:HE21	1:A:230:GLN:HB2	1.63	0.40
1:A:412:GLU:O	1:A:440:ARG:HB3	2.20	0.40
1:A:429:THR:CG2	1:A:432:GLU:H	2.24	0.40
1:B:1043:GLN:O	1:B:1047:MSE:HG3	2.21	0.40
1:B:1117:GLY:O	1:B:1169:LEU:CD2	2.70	0.40
1:B:1413:ARG:HE	1:B:1413:ARG:HB3	1.62	0.40
1:B:1565:LEU:HD21	3:B:2420:HOH:O	2.20	0.40
1:A:183:LYS:C	3:A:2534:HOH:O	2.64	0.40
1:A:392:VAL:HG12	3:A:2008:HOH:O	2.22	0.40
1:A:432:GLU:O	1:A:436:LEU:HD13	2.21	0.40
1:A:438:GLU:O	1:A:458:ARG:NH2	2.53	0.40
1:B:1266:LEU:O	1:B:1270:ARG:HG2	2.20	0.40
1:A:341:ILE:O	1:A:367:HIS:NE2	2.42	0.40
1:A:480:LEU:HD12	3:A:2141:HOH:O	2.20	0.40
1:B:1122:GLN:O	1:B:1123:TYR:C	2.63	0.40
1:B:1196:ASP:O	3:B:2002:HOH:O	2.22	0.40
1:B:1224:LYS:NZ	3:B:2504:HOH:O	2.54	0.40
1:B:1281:GLN:NE2	1:B:1491:PHE:HE1	2.20	0.40
1:B:1300:LYS:CD	1:B:1304:GLU:HB3	2.52	0.40
1:B:1429:THR:CG2	1:B:1432:GLU:H	2.21	0.40
1:A:91:ARG:NH1	1:B:1090:GLU:OE1	2.53	0.40
1:A:109:PRO:HA	1:A:114:PRO:HD3	2.02	0.40
1:A:118:LEU:HD22	1:A:122:GLN:HE21	1.86	0.40
1:A:177:MSE:HE3	1:A:181:VAL:HG23	2.03	0.40
1:A:343:MSE:O	1:A:350:LEU:HD23	2.21	0.40
1:A:505:GLU:HB3	3:A:2714:HOH:O	2.21	0.40
1:B:1045:ARG:HA	1:B:1050:LEU:HB2	2.04	0.40
1:B:1529:LYS:NZ	3:B:2699:HOH:O	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/584 (94%)	505 (92%)	35 (6%)	9 (2%)	7	4
1	B	549/584 (94%)	502 (91%)	38 (7%)	9 (2%)	7	4
All	All	1098/1168 (94%)	1007 (92%)	73 (7%)	18 (2%)	7	4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	B	1113	THR
1	B	1299	SER
1	B	1571	GLU
1	A	259	ASN
1	A	432	GLU
1	B	1259	ASN
1	A	114	PRO
1	A	451	PRO
1	B	1114	PRO
1	A	56	PRO
1	A	123	TYR
1	A	397	ARG
1	B	1076	THR
1	B	1354	ARG
1	A	468	VAL
1	B	1301	PRO
1	B	1056	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/484 (96%)	383 (82%)	82 (18%)	2	1
1	B	465/484 (96%)	371 (80%)	94 (20%)	1	0
All	All	930/968 (96%)	754 (81%)	176 (19%)	1	1

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	26	LYS
1	A	28	LEU
1	A	29	MSE
1	A	38	MSE
1	A	43	GLN
1	A	48	LEU
1	A	50	LEU
1	A	66	LEU
1	A	72	LEU
1	A	74	LYS
1	A	75	MSE
1	A	77	SER
1	A	89	GLN
1	A	99	ILE
1	A	106	SER
1	A	107	LEU
1	A	118	LEU
1	A	123	TYR
1	A	131	LYS
1	A	136	SER
1	A	137	ILE
1	A	146	ILE
1	A	152	GLU
1	A	153	ASN
1	A	160	VAL
1	A	165	ARG
1	A	167	LEU
1	A	169	LEU
1	A	184	LEU
1	A	210	ILE
1	A	214	LYS
1	A	224	LYS

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	237	GLU
1	A	240	LYS
1	A	248	ARG
1	A	267	ARG
1	A	268	LYS
1	A	277	ASN
1	A	286	VAL
1	A	299	SER
1	A	300	LYS
1	A	302	ILE
1	A	304	GLU
1	A	306	LYS
1	A	329	GLU
1	A	333	SER
1	A	340	LYS
1	A	351	VAL
1	A	354	ARG
1	A	358	ILE
1	A	360	SER
1	A	363	GLU
1	A	368	SER
1	A	371	GLU
1	A	372	SER
1	A	376	THR
1	A	378	GLU
1	A	384	LEU
1	A	388	THR
1	A	397	ARG
1	A	398	LEU
1	A	403	VAL
1	A	413	ARG
1	A	416	ILE
1	A	419	LEU
1	A	425	GLN
1	A	428	CYS
1	A	458	ARG
1	A	468	VAL
1	A	489	SER
1	A	502	LEU
1	A	506	GLU
1	A	512	LEU

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Mol	Chain	Res	Type
1	A	516	LEU
1	A	518	ASN
1	A	520	GLN
1	A	529	LYS
1	A	559	ARG
1	A	566	LEU
1	A	572	TRP
1	B	1026	LYS
1	B	1030	LEU
1	B	1038	MSE
1	B	1043	GLN
1	B	1048	LEU
1	B	1057	LYS
1	B	1066	LEU
1	B	1068	PHE
1	B	1070	ARG
1	B	1072	LEU
1	B	1074	LYS
1	B	1075	MSE
1	B	1088	ILE
1	B	1089	GLN
1	B	1099	ILE
1	B	1100	LEU
1	B	1104	ILE
1	B	1106	SER
1	B	1107	LEU
1	B	1118	LEU
1	B	1121	SER
1	B	1122	GLN
1	B	1123	TYR
1	B	1136	SER
1	B	1137	ILE
1	B	1144	ARG
1	B	1154	HIS
1	B	1160	VAL
1	B	1167	LEU
1	B	1174	VAL
1	B	1184	LEU
1	B	1210	ILE
1	B	1214	LYS
1	B	1224	LYS
1	B	1225	ARG

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Mol	Chain	Res	Type
1	B	1230	GLN
1	B	1240	LYS
1	B	1248	ARG
1	B	1277	ASN
1	B	1286	VAL
1	B	1295	GLN
1	B	1298	ILE
1	B	1300	LYS
1	B	1302	ILE
1	B	1306	LYS
1	B	1323	ILE
1	B	1329	GLU
1	B	1340	LYS
1	B	1346	LYS
1	B	1352	LYS
1	B	1354	ARG
1	B	1355	LYS
1	B	1357	LYS
1	B	1360	SER
1	B	1363	GLU
1	B	1368	SER
1	B	1372	SER
1	B	1373	ILE
1	B	1375	ASP
1	B	1376	THR
1	B	1384	LEU
1	B	1385	LYS
1	B	1388	THR
1	B	1389	ILE
1	B	1392	VAL
1	B	1397	ARG
1	B	1398	LEU
1	B	1409	SER
1	B	1411	ASN
1	B	1413	ARG
1	B	1419	LEU
1	B	1423	THR
1	B	1425	GLN
1	B	1428	CYS
1	B	1453	LYS
1	B	1454	LEU
1	B	1456	ASP

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Mol	Chain	Res	Type
1	B	1459	VAL
1	B	1461	THR
1	B	1489	SER
1	B	1505	GLU
1	B	1509	GLN
1	B	1511	ARG
1	B	1512	LEU
1	B	1516	LEU
1	B	1518	ASN
1	B	1520	GLN
1	B	1538	LYS
1	B	1547	GLU
1	B	1554	LYS
1	B	1559	ARG
1	B	1566	LEU
1	B	1571	GLU
1	B	1572	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	46	GLN
1	A	64	GLN
1	A	71	ASN
1	A	122	GLN
1	A	230	GLN
1	A	261	ASN
1	A	277	ASN
1	A	295	GLN
1	A	382	ASN
1	A	425	GLN
1	A	482	ASN
1	A	485	HIS
1	A	501	GLN
1	A	509	GLN
1	B	1031	ASN
1	B	1043	GLN
1	B	1046	GLN
1	B	1064	GLN
1	B	1071	ASN
1	B	1122	GLN

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Mol	Chain	Res	Type
1	B	1153	ASN
1	B	1261	ASN
1	B	1277	ASN
1	B	1330	ASN
1	B	1425	GLN
1	B	1464	GLN
1	B	1467	ASN
1	B	1482	ASN
1	B	1501	GLN
1	B	1509	GLN
1	B	1518	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	601	-	46,48,48	1.98	11 (23%)	64,73,73	1.84	10 (15%)
2	NAD	B	1601	-	46,48,48	1.82	11 (23%)	64,73,73	1.88	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	1602	-	46,48,48	2.08	11 (23%)	64,73,73	1.85	10 (15%)
2	NAD	A	602	-	46,48,48	2.27	13 (28%)	64,73,73	1.88	10 (15%)

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	601	-	-	0/30/62/62	0/5/5/5
2	NAD	B	1601	-	-	0/30/62/62	0/5/5/5
2	NAD	B	1602	-	-	14/30/62/62	0/5/5/5
2	NAD	A	602	-	-	13/30/62/62	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	NAD	C2N-N1N	9.98	1.45	1.35
2	B	1602	NAD	C2N-N1N	7.77	1.43	1.35
2	A	601	NAD	C2N-N1N	7.55	1.43	1.35
2	B	1601	NAD	C2N-N1N	6.44	1.42	1.35
2	B	1602	NAD	O4D-C1D	5.19	1.47	1.40
2	A	602	NAD	O4D-C1D	4.91	1.47	1.40
2	A	601	NAD	O4D-C1D	4.66	1.47	1.40
2	A	601	NAD	C5A-N7A	-4.33	1.31	1.39
2	B	1602	NAD	C6N-N1N	4.27	1.45	1.35
2	A	602	NAD	C3N-C7N	4.05	1.56	1.50
2	B	1601	NAD	O4D-C1D	4.03	1.46	1.40
2	B	1601	NAD	C5A-N7A	-3.93	1.31	1.39
2	B	1602	NAD	C5A-N7A	-3.83	1.32	1.39
2	B	1601	NAD	C6N-N1N	3.69	1.43	1.35
2	A	602	NAD	C6N-N1N	3.47	1.43	1.35
2	A	601	NAD	C6N-N1N	3.32	1.42	1.35
2	B	1602	NAD	C3N-C7N	3.28	1.55	1.50
2	A	602	NAD	C5A-N7A	-3.23	1.33	1.39
2	B	1602	NAD	C5A-C4A	-3.18	1.33	1.39
2	A	602	NAD	C5A-C4A	-3.07	1.33	1.39
2	A	601	NAD	C5A-C4A	-2.78	1.34	1.39
2	B	1601	NAD	C5A-C4A	-2.74	1.34	1.39
2	A	602	NAD	C2N-C3N	2.61	1.43	1.39
2	A	601	NAD	PA-O3	-2.58	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1601	NAD	C3N-C7N	2.56	1.54	1.50
2	B	1602	NAD	C8A-N7A	2.48	1.36	1.31
2	A	602	NAD	C2A-N1A	2.44	1.38	1.33
2	B	1601	NAD	C8A-N7A	2.36	1.36	1.31
2	A	601	NAD	C2A-N1A	2.35	1.38	1.33
2	A	602	NAD	O4B-C1B	2.33	1.47	1.42
2	B	1602	NAD	C4A-N9A	-2.32	1.32	1.37
2	A	601	NAD	C3N-C7N	2.32	1.54	1.50
2	A	602	NAD	PN-O3	2.28	1.62	1.59
2	A	602	NAD	C8A-N7A	2.27	1.36	1.31
2	A	601	NAD	C8A-N7A	2.21	1.35	1.31
2	B	1601	NAD	C2A-N1A	2.20	1.37	1.33
2	B	1601	NAD	C2A-N3A	2.19	1.37	1.33
2	A	602	NAD	C2A-N3A	2.19	1.37	1.33
2	B	1601	NAD	C4N-C3N	2.18	1.42	1.39
2	A	602	NAD	C4A-N3A	2.17	1.38	1.34
2	A	601	NAD	PN-O3	-2.16	1.57	1.59
2	B	1602	NAD	O4B-C1B	2.14	1.47	1.42
2	A	601	NAD	C4A-N9A	-2.14	1.33	1.37
2	B	1601	NAD	C5N-C4N	2.13	1.42	1.38
2	B	1602	NAD	C2A-N1A	2.07	1.37	1.33
2	B	1602	NAD	C2A-N3A	2.01	1.37	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1601	NAD	C5A-C4A-N3A	-6.01	118.44	126.72
2	A	602	NAD	C5A-C4A-N3A	-5.94	118.54	126.72
2	B	1602	NAD	C5A-C4A-N3A	-5.90	118.59	126.72
2	A	601	NAD	C5A-C4A-N3A	-5.86	118.64	126.72
2	A	602	NAD	N3A-C2A-N1A	-5.39	120.42	128.58
2	B	1602	NAD	N3A-C2A-N1A	-5.38	120.44	128.58
2	A	601	NAD	C6A-C5A-N7A	-5.22	122.02	132.09
2	B	1601	NAD	C6A-C5A-N7A	-5.21	122.05	132.09
2	B	1601	NAD	N3A-C4A-N9A	5.14	135.91	127.17
2	B	1601	NAD	C6A-C5A-C4A	5.12	124.17	117.18
2	A	601	NAD	N3A-C2A-N1A	-5.11	120.85	128.58
2	A	601	NAD	C6A-C5A-C4A	5.10	124.14	117.18
2	B	1601	NAD	N3A-C2A-N1A	-5.09	120.88	128.58
2	B	1602	NAD	C6A-C5A-N7A	-5.02	122.42	132.09
2	A	601	NAD	N3A-C4A-N9A	4.97	135.63	127.17
2	B	1602	NAD	C6A-C5A-C4A	4.90	123.87	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	NAD	C6A-C5A-C4A	4.86	123.82	117.18
2	A	602	NAD	N3A-C4A-N9A	4.86	135.43	127.17
2	A	602	NAD	C6A-C5A-N7A	-4.85	122.74	132.09
2	B	1602	NAD	N3A-C4A-N9A	4.72	135.19	127.17
2	A	602	NAD	C6N-N1N-C2N	-3.96	118.51	121.88
2	B	1602	NAD	N9A-C8A-N7A	-3.75	108.62	113.94
2	A	602	NAD	N9A-C8A-N7A	-3.66	108.74	113.94
2	A	601	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
2	B	1601	NAD	N9A-C8A-N7A	-3.63	108.78	113.94
2	A	602	NAD	C2A-N3A-C4A	3.30	119.90	111.83
2	B	1601	NAD	C4D-O4D-C1D	-3.25	106.95	109.92
2	B	1602	NAD	C2A-N3A-C4A	3.22	119.69	111.83
2	B	1601	NAD	C2A-N3A-C4A	3.20	119.66	111.83
2	A	601	NAD	C2A-N3A-C4A	3.14	119.49	111.83
2	B	1602	NAD	C6N-N1N-C2N	-3.03	119.30	121.88
2	A	601	NAD	C4A-C5A-N7A	2.84	113.83	110.58
2	B	1601	NAD	C4A-C5A-N7A	2.80	113.78	110.58
2	B	1602	NAD	C4A-C5A-N7A	2.73	113.71	110.58
2	A	601	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
2	A	602	NAD	C4A-C5A-N7A	2.47	113.41	110.58
2	A	602	NAD	C2D-C3D-C4D	2.28	107.01	102.61
2	A	601	NAD	C4D-O4D-C1D	-2.14	107.96	109.92
2	B	1601	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
2	B	1602	NAD	C2D-C3D-C4D	2.05	106.58	102.61

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	NAD	C5B-O5B-PA-O1A
2	A	602	NAD	C5B-O5B-PA-O2A
2	A	602	NAD	C5B-O5B-PA-O3
2	A	602	NAD	C5D-O5D-PN-O3
2	A	602	NAD	C5D-O5D-PN-O1N
2	A	602	NAD	C5D-O5D-PN-O2N
2	A	602	NAD	O4D-C4D-C5D-O5D
2	A	602	NAD	O4D-C1D-N1N-C2N
2	A	602	NAD	O4D-C1D-N1N-C6N
2	A	602	NAD	C2D-C1D-N1N-C2N
2	A	602	NAD	C2D-C1D-N1N-C6N
2	B	1602	NAD	C5B-O5B-PA-O1A
2	B	1602	NAD	C5B-O5B-PA-O3

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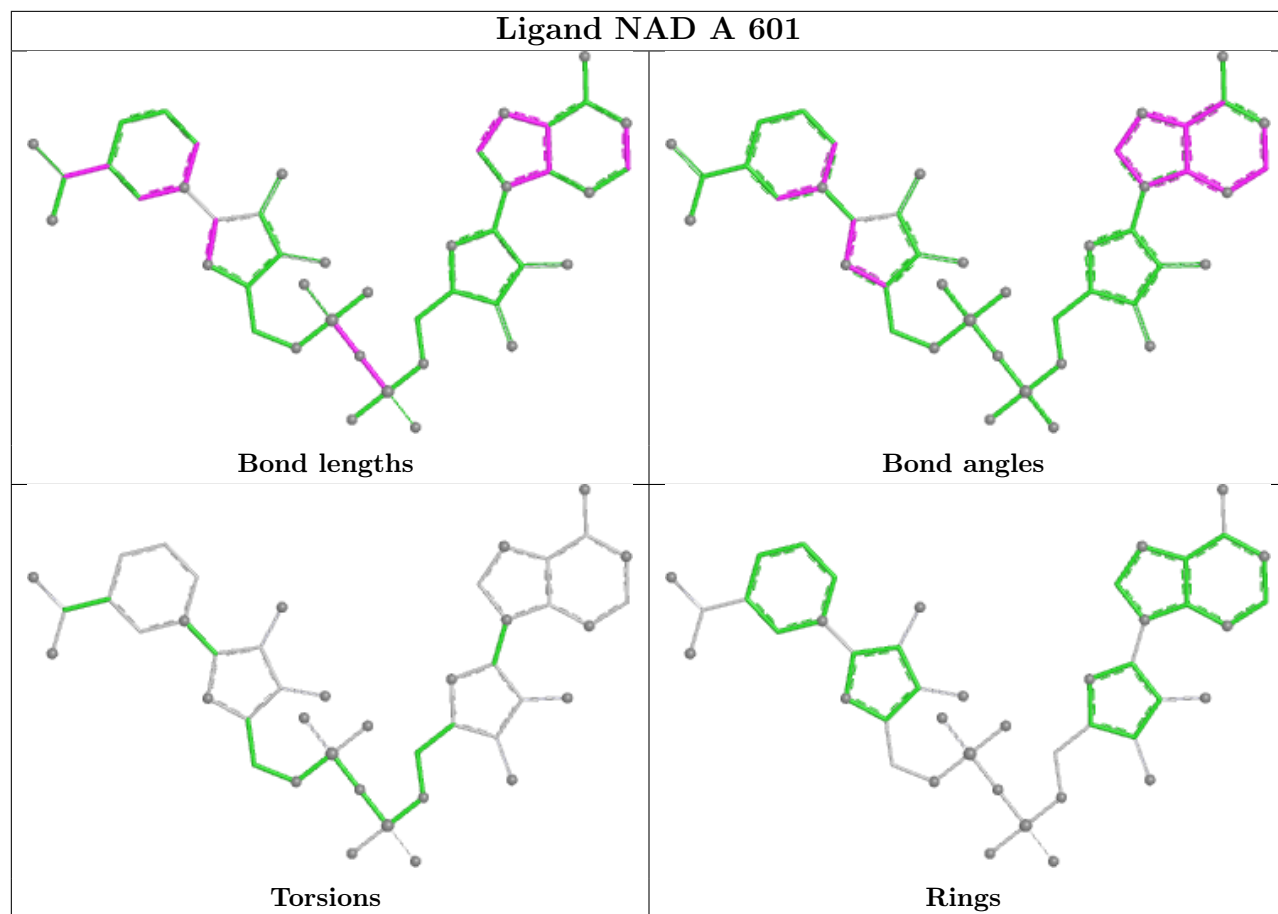
Mol	Chain	Res	Type	Atoms
2	B	1602	NAD	C5D-O5D-PN-O3
2	B	1602	NAD	C5D-O5D-PN-O1N
2	B	1602	NAD	C5D-O5D-PN-O2N
2	B	1602	NAD	O4D-C1D-N1N-C2N
2	B	1602	NAD	O4D-C1D-N1N-C6N
2	B	1602	NAD	C2D-C1D-N1N-C2N
2	B	1602	NAD	C2D-C1D-N1N-C6N
2	A	602	NAD	C3D-C4D-C5D-O5D
2	B	1602	NAD	O4D-C4D-C5D-O5D
2	B	1602	NAD	C3D-C4D-C5D-O5D
2	B	1602	NAD	C5B-O5B-PA-O2A
2	B	1602	NAD	C4D-C5D-O5D-PN
2	A	602	NAD	PA-O3-PN-O2N
2	B	1602	NAD	PN-O3-PA-O2A

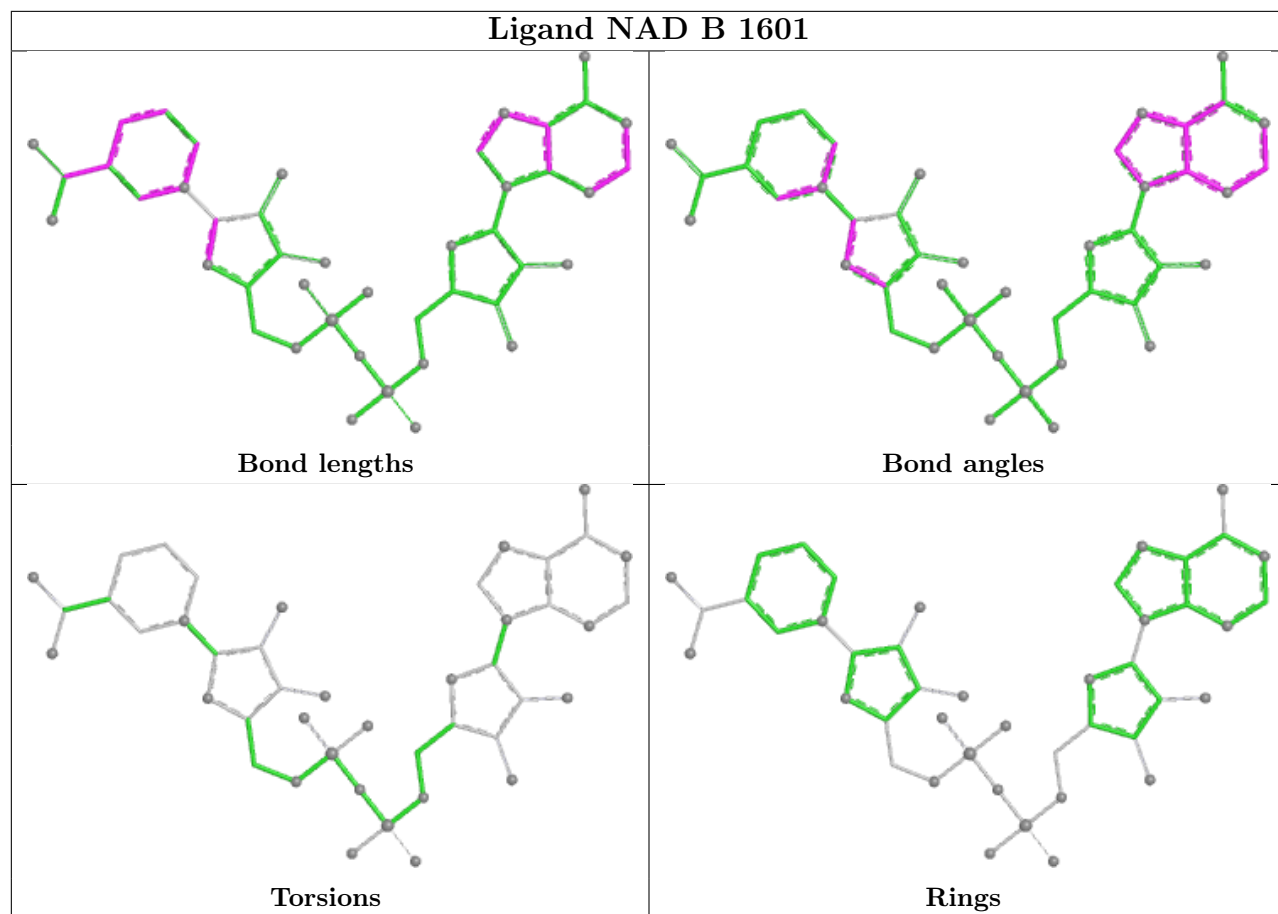
There are no ring outliers.

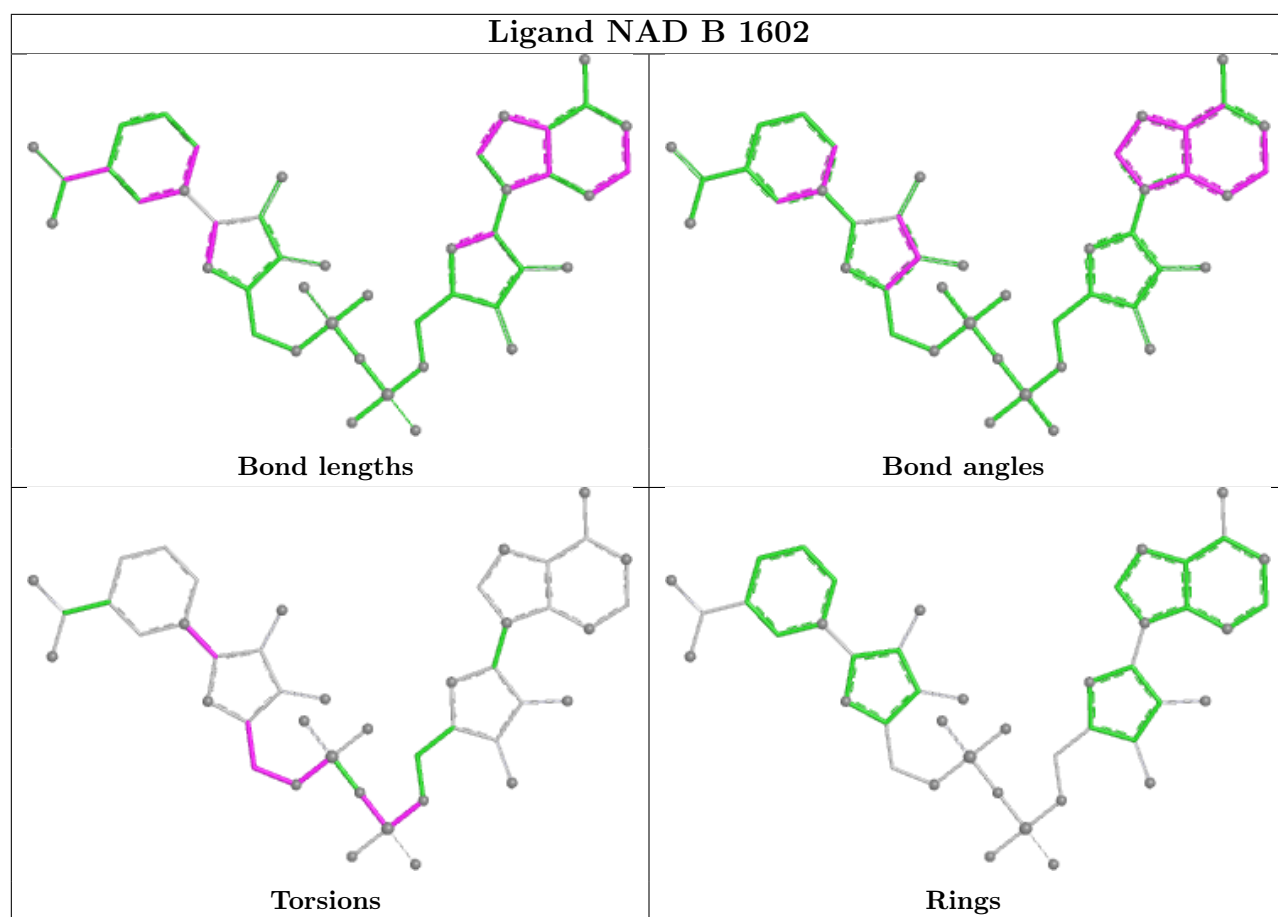
3 monomers are involved in 6 short contacts:

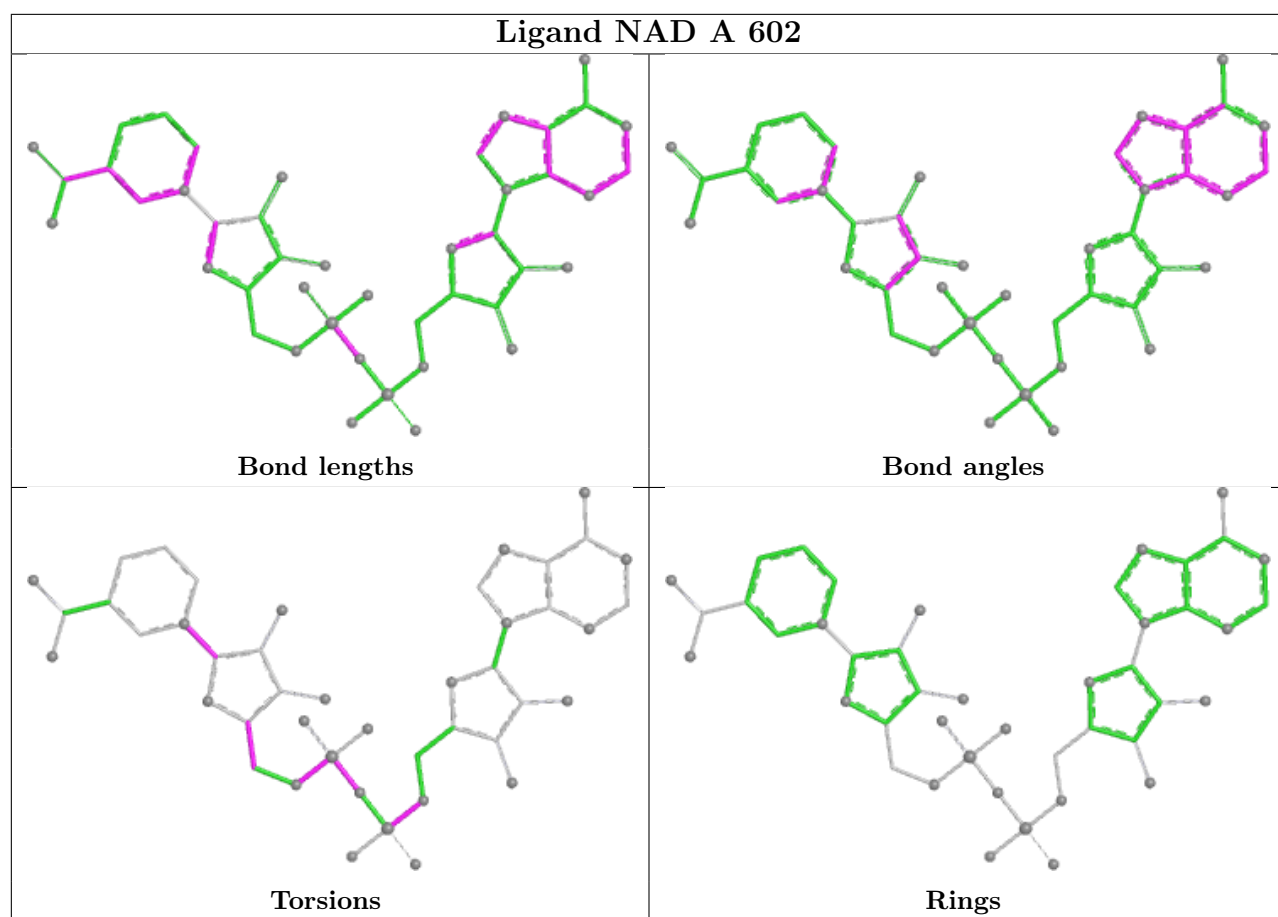
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0
2	B	1601	NAD	4	0
2	A	602	NAD	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.