Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:02 PM GMT

PDB ID	:	1DO8
Title	:	CRYSTAL STRUCTURE OF A CLOSED FORM OF HUMAN MITOCHONDRIAL NAD(P)+-DEPENDENT MALIC ENZYME
Authors	:	Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on	:	1999-12-19
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

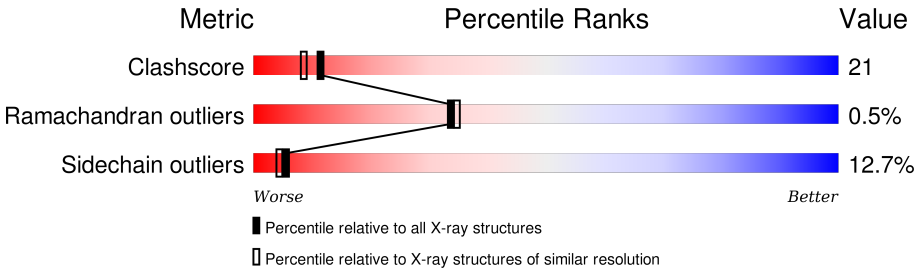
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	564	59% 31% 8% •
1	B	564	57% 35% 5% •
1	C	564	63% 30% 5% •
1	D	564	63% 28% 7% •

2 Entry composition (i)

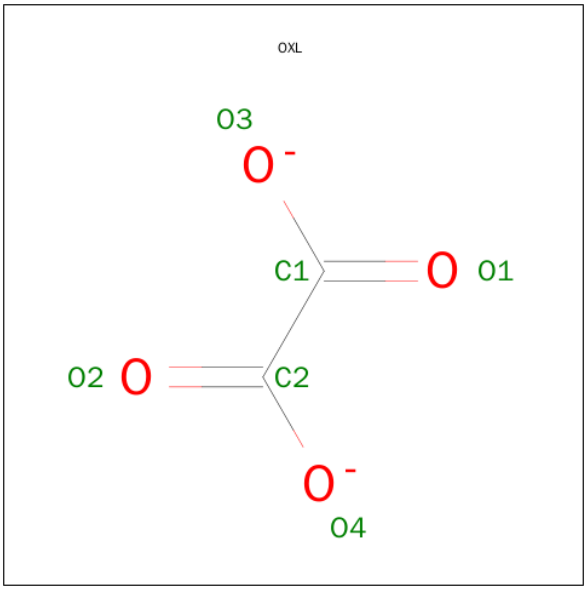
There are 5 unique types of molecules in this entry. The entry contains 18807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		

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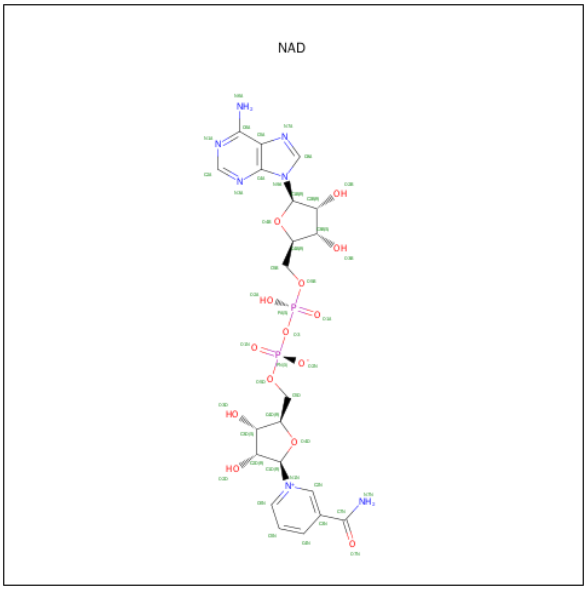
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 2 4	0	0
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 44 21 7 14 2	0	0
4	A	1	Total C N O P 44 21 7 14 2	9	0
4	B	1	Total C N O P 44 21 7 14 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	9	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	9	0
			44	21	7	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	199	Total	O	0	0
			199	199		
5	C	275	Total	O	0	0
			275	275		
5	D	246	Total	O	0	0
			246	246		

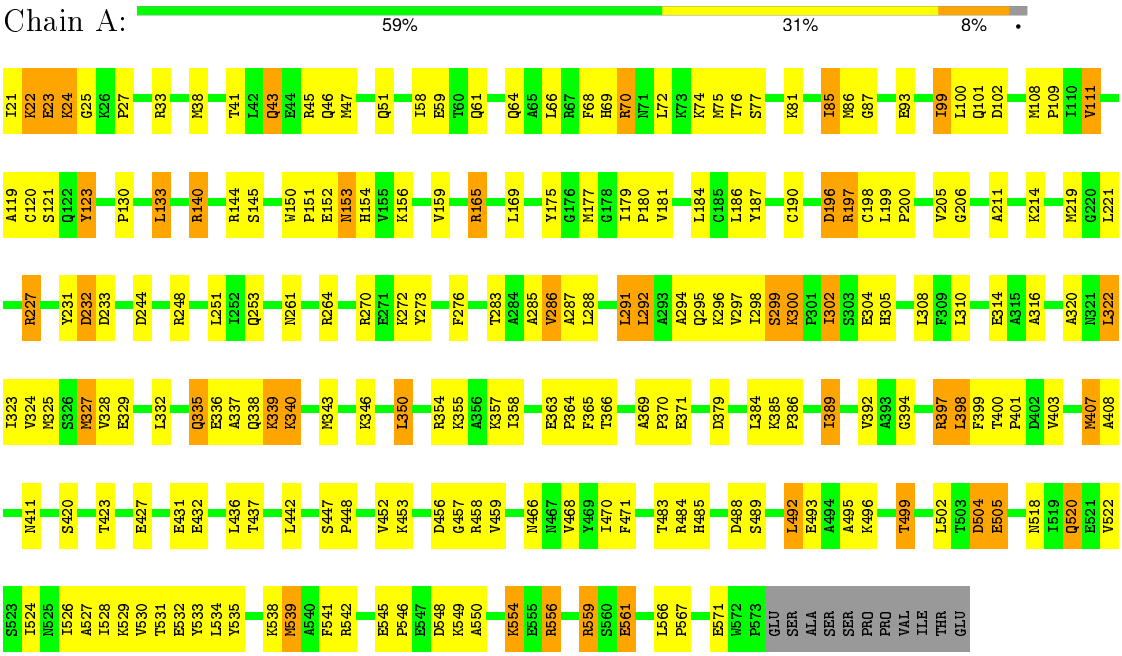
3 Residue-property plots (i)

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.

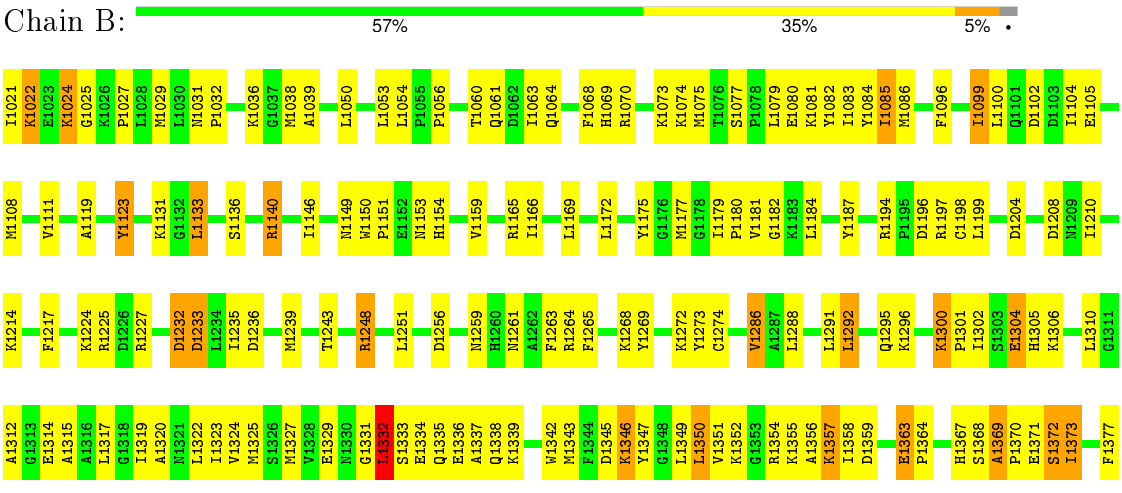
- Molecule 1: MALIC ENZYME

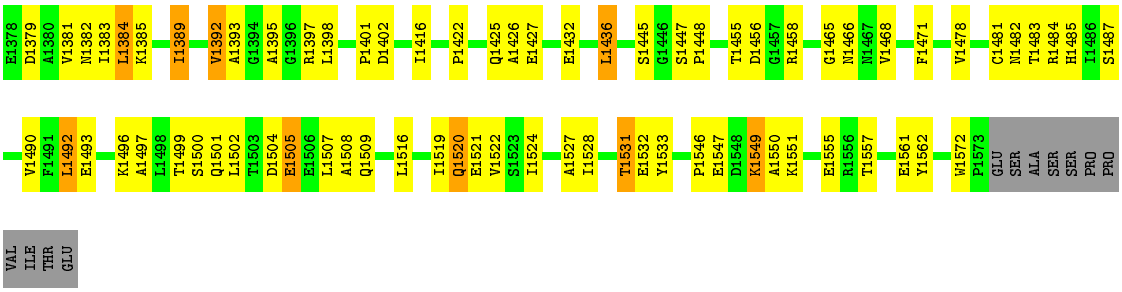
Chain A:



- Molecule 1: MALIC ENZYME

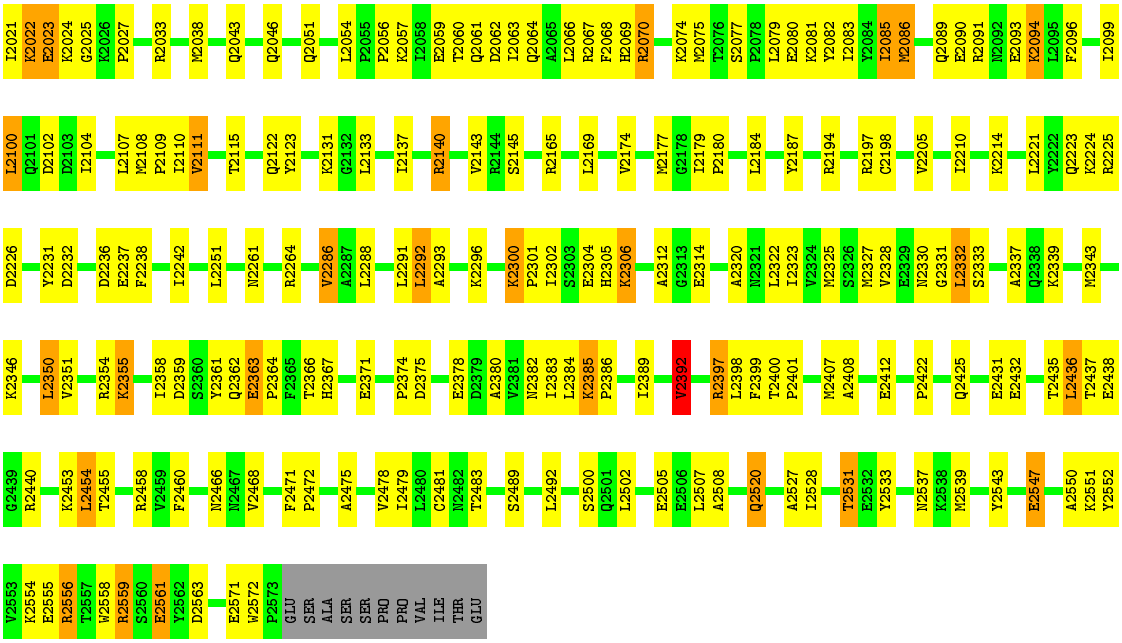
Chain B:





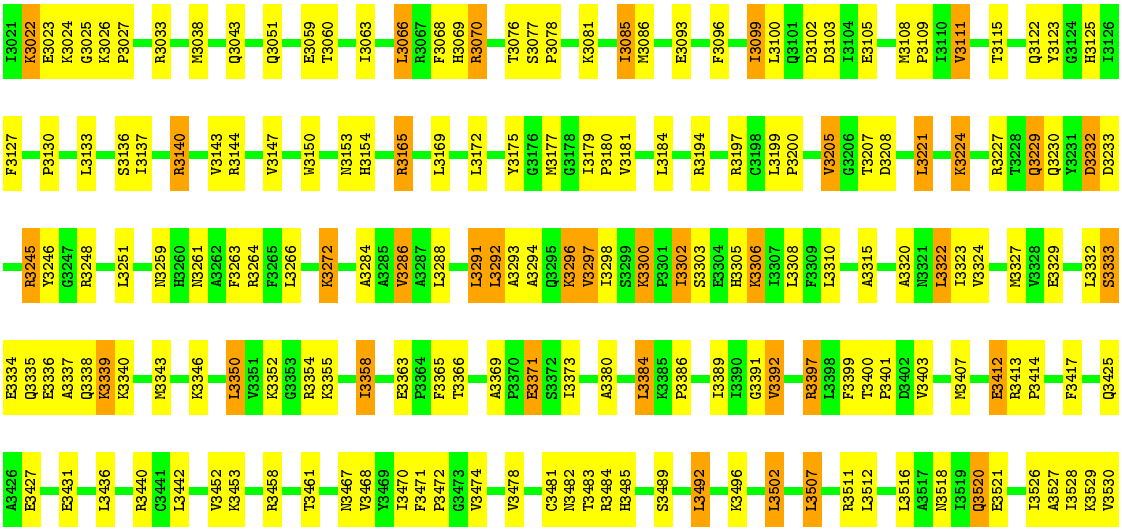
• Molecule 1: MALIC ENZYME

Chain C:



• Molecule 1: MALIC ENZYME

Chain D:




T3531
E3532
N3537
K3538
M3539
A3540
E3545
P3546
E3547
D3548
K3549
A3550
K3551
E3555
R3556
T3557
W3558
R3559
E3571
W3572
P3573
GLU
SER
ALA
SER
SER
PRO
PRO
VAL
ILE
THR
GLU

4 Data and refinement statistics (i)

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	229.00Å 118.70Å 113.00Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18807	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: OXL, MN, 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	0.37	0/4447	0.61	0/5998
1	B	0.37	0/4447	0.61	0/5998
1	C	0.38	0/4447	0.61	0/5998
1	D	0.38	0/4447	0.60	0/5998
All	All	0.37	0/17788	0.61	0/23992

There are no bond length outliers.

There are no bond angle outliers.

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	4367	0	4407	203	0
1	B	4367	0	4407	229	0
1	C	4367	0	4407	141	0
1	D	4367	0	4407	179	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	52	2	0
4	B	88	0	52	3	0
4	C	88	0	52	2	0
4	D	88	0	52	1	0
5	A	239	0	0	14	0
5	B	199	0	0	30	0
5	C	275	0	0	18	0
5	D	246	0	0	12	0
All	All	18807	0	17836	731	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 21.

All (731) 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:A:177:MSE:HE2	1:A:181:VAL:HG23	1.29	1.14
1:D:3177:MSE:HE2	1:D:3181:VAL:HG23	1.35	1.08
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.18	1.06
1:B:1358:ILE:HG22	5:B:4650:HOH:O	1.54	1.06
1:A:140:ARG:HH22	1:A:233:ASP:HB3	1.14	1.05
1:D:3389:ILE:HG21	5:D:4639:HOH:O	1.58	1.03
1:B:1302:ILE:HG12	1:B:1332:LEU:HD11	1.41	0.99
1:B:1332:LEU:HD12	1:B:1332:LEU:H	1.28	0.96
1:D:3140:ARG:HH22	1:D:3233:ASP:HB3	1.26	0.96
1:C:2422:PRO:HD2	1:C:2425:GLN:HE21	1.31	0.95
1:D:3327:MSE:HE3	1:D:3337:ALA:HB1	1.44	0.95
1:A:300:LYS:HZ3	1:A:304:GLU:HB2	1.33	0.92
1:B:1371:GLU:H	1:B:1371:GLU:CD	1.71	0.91
1:B:1342:TRP:HE3	1:B:1349:LEU:HD11	1.32	0.91
1:D:3520:GLN:H	1:D:3520:GLN:HE21	1.19	0.91
1:D:3086:MSE:HE1	1:D:3111:VAL:HG22	1.53	0.90
1:D:3261:ASN:HD22	1:D:3264:ARG:HE	1.16	0.90
1:C:2210:ILE:HG22	1:C:2214:LYS:HE2	1.53	0.89
1:B:1022:LYS:HE2	1:D:3025:GLY:HA3	1.52	0.89
1:B:1422:PRO:HD2	1:B:1425:GLN:HE21	1.37	0.89
1:C:2300:LYS:HB3	1:C:2300:LYS:HZ2	1.34	0.89
1:B:1024:LYS:HZ2	1:D:3022:LYS:HD2	1.34	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MSE:HE1	1:A:180:PRO:HB2	1.54	0.89
1:A:261:ASN:HD22	1:A:264:ARG:HE	1.19	0.88
1:B:1315:ALA:HB3	1:B:1392:VAL:HG21	1.55	0.87
1:D:3343:MSE:HE2	1:D:3365:PHE:HB2	1.56	0.87
1:B:1261:ASN:HD22	1:B:1264:ARG:HD3	1.40	0.87
1:C:2302:ILE:HD13	1:C:2332:LEU:HD13	1.56	0.87
1:D:3527:ALA:O	1:D:3531:THR:HG22	1.75	0.86
1:B:1029:MSE:HE2	1:B:1050:LEU:HD22	1.57	0.86
1:D:3369:ALA:HB1	1:D:3373:ILE:HD11	1.58	0.85
1:A:66:LEU:HD21	1:A:70:ARG:NH1	1.91	0.85
1:A:154:HIS:HB2	5:A:4947:HOH:O	1.76	0.84
1:B:1327:MSE:HE3	1:B:1337:ALA:HB1	1.59	0.84
1:A:140:ARG:NH2	1:A:233:ASP:HB3	1.92	0.83
1:C:2527:ALA:O	1:C:2531:THR:HG23	1.78	0.83
1:A:371:GLU:H	1:A:371:GLU:CD	1.82	0.83
1:C:2520:GLN:HE21	1:C:2520:GLN:H	1.22	0.83
1:C:2300:LYS:HB3	1:C:2300:LYS:NZ	1.92	0.83
1:B:1377:PHE:O	1:B:1381:VAL:HG23	1.79	0.82
1:B:1389:ILE:HG21	5:B:4275:HOH:O	1.80	0.82
1:D:3177:MSE:HE1	1:D:3180:PRO:HB2	1.62	0.81
1:A:294:ALA:O	1:A:297:VAL:HG22	1.79	0.81
1:B:1060:THR:H	1:B:1063:ILE:HD12	1.46	0.81
1:D:3332:LEU:HD21	1:D:3340:LYS:HE2	1.63	0.81
1:A:123:TYR:CD2	1:A:219:MSE:HE1	2.11	0.81
1:D:3085:ILE:HD11	1:D:3111:VAL:CG2	2.10	0.80
1:A:66:LEU:HD22	1:B:1217:PHE:HZ	1.47	0.80
1:B:1363:GLU:HB3	1:B:1364:PRO:HD3	1.64	0.80
1:B:1081:LYS:O	1:B:1085:ILE:HG23	1.82	0.80
1:A:343:MSE:HE2	1:A:365:PHE:HB2	1.63	0.80
1:B:1335:GLN:HB2	5:B:4934:HOH:O	1.82	0.80
1:C:2090:GLU:OE1	1:C:2131:LYS:HE3	1.82	0.80
1:C:2081:LYS:O	1:C:2085:ILE:HG23	1.82	0.80
1:B:1029:MSE:CE	1:B:1050:LEU:HD22	2.12	0.79
1:B:1395:ALA:HB3	5:B:4720:HOH:O	1.80	0.79
1:D:3261:ASN:ND2	1:D:3264:ARG:HE	1.80	0.79
1:B:1021:ILE:HD11	5:B:4943:HOH:O	1.82	0.78
1:A:407:MSE:CE	1:A:407:MSE:HA	2.14	0.78
1:A:33:ARG:HD3	1:A:93:GLU:OE2	1.82	0.78
1:A:527:ALA:O	1:A:531:THR:HG23	1.83	0.77
1:C:2327:MSE:HE3	1:C:2337:ALA:HB1	1.66	0.77
1:A:300:LYS:HZ2	1:A:300:LYS:HB3	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1343:MSE:HE1	5:B:4327:HOH:O	1.84	0.77
1:C:2085:ILE:HG13	1:C:2086:MSE:N	2.00	0.77
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.67	0.76
1:B:1261:ASN:ND2	1:B:1264:ARG:HH11	1.84	0.76
1:C:2454:LEU:HD11	1:C:2460:PHE:HE2	1.50	0.76
1:C:2392:VAL:HG13	1:C:2392:VAL:O	1.86	0.76
1:A:177:MSE:HE3	1:A:180:PRO:HD2	1.68	0.75
1:A:534:LEU:HA	1:A:539:MSE:HG3	1.69	0.75
1:A:550:ALA:O	1:A:554:LYS:HG2	1.86	0.75
1:C:2293:ALA:HA	1:C:2296:LYS:HE2	1.68	0.75
1:C:2389:ILE:HG21	5:C:4314:HOH:O	1.86	0.75
1:D:3177:MSE:HE3	1:D:3177:MSE:O	1.86	0.75
1:B:1370:PRO:HD2	1:B:1373:ILE:HD12	1.69	0.74
1:A:156:LYS:HG2	1:A:197:ARG:HG2	1.69	0.74
1:B:1263:PHE:HE1	5:B:4936:HOH:O	1.69	0.74
1:D:3081:LYS:O	1:D:3085:ILE:HG23	1.87	0.74
1:B:1478:VAL:HG13	1:B:1483:THR:HB	1.67	0.74
1:D:3286:VAL:HG21	1:D:3467:ASN:HA	1.70	0.74
1:C:2371:GLU:CD	1:C:2371:GLU:H	1.91	0.74
1:A:261:ASN:ND2	1:A:264:ARG:HE	1.86	0.74
1:B:1393:ALA:HB3	5:B:4720:HOH:O	1.88	0.74
1:A:219:MSE:HG2	1:B:1038:MSE:HE1	1.70	0.73
1:D:3338:GLN:HB2	1:D:3339:LYS:NZ	2.03	0.73
1:C:2323:ILE:HG22	1:C:2327:MSE:HE2	1.69	0.73
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.54	0.73
1:B:1397:ARG:HH21	1:B:1426:ALA:HB3	1.54	0.72
1:A:22:LYS:HE2	1:C:2024:LYS:O	1.89	0.72
1:B:1024:LYS:NZ	1:D:3022:LYS:HA	2.04	0.72
1:C:2086:MSE:HE1	1:C:2111:VAL:HG22	1.70	0.72
1:A:495:ALA:O	1:A:499:THR:HG22	1.90	0.72
1:A:407:MSE:HE2	1:A:411:ASN:HD22	1.56	0.71
1:D:3323:ILE:HG22	1:D:3327:MSE:HE2	1.71	0.71
1:D:3571:GLU:HG3	5:D:4551:HOH:O	1.90	0.71
1:A:493:GLU:HG3	1:A:533:TYR:CD1	2.26	0.71
1:C:2301:PRO:HB2	1:C:2304:GLU:HG3	1.70	0.71
1:D:3300:LYS:HB3	1:D:3300:LYS:NZ	2.04	0.71
1:D:3520:GLN:NE2	1:D:3520:GLN:H	1.88	0.70
1:B:1085:ILE:HD12	1:B:1096:PHE:HE1	1.56	0.70
1:D:3137:ILE:HB	1:D:3205:VAL:HG12	1.73	0.70
1:C:2094:LYS:HE2	1:C:2558:TRP:CZ2	2.27	0.70
1:C:2306:LYS:HG2	1:C:2386:PRO:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:GLU:N	5:B:4650:HOH:O	2.24	0.70
1:B:1546:PRO:HG2	1:B:1549:LYS:HD2	1.73	0.69
1:A:493:GLU:HG2	5:A:4484:HOH:O	1.92	0.69
1:B:1069:HIS:HE1	1:B:1102:ASP:OD2	1.74	0.69
1:A:392:VAL:CG1	1:A:392:VAL:O	2.40	0.69
1:D:3272:LYS:NZ	1:D:3272:LYS:HB3	2.08	0.69
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.75	0.69
1:C:2520:GLN:HG2	5:C:4086:HOH:O	1.92	0.69
1:C:2551:LYS:O	1:C:2555:GLU:HB2	1.91	0.69
1:D:3400:THR:OG1	1:D:3403:VAL:HG23	1.93	0.69
1:A:177:MSE:HE3	1:A:177:MSE:O	1.92	0.69
1:B:1029:MSE:HE1	1:B:1053:LEU:HD12	1.73	0.69
1:A:320:ALA:HB2	5:A:4862:HOH:O	1.93	0.69
1:B:1397:ARG:NH2	1:B:1426:ALA:HB3	2.08	0.68
1:B:1342:TRP:CE3	1:B:1349:LEU:HD11	2.23	0.68
1:B:1333:SER:OG	1:B:1336:GLU:HG2	1.93	0.68
1:C:2422:PRO:HD2	1:C:2425:GLN:NE2	2.06	0.68
1:A:302:ILE:HD11	1:A:327:MSE:HG2	1.74	0.68
1:B:1393:ALA:CB	5:B:4720:HOH:O	2.41	0.67
1:B:1370:PRO:HG2	1:B:1372:SER:O	1.95	0.67
1:B:1501:GLN:NE2	1:B:1522:VAL:HG13	2.08	0.67
1:D:3548:ASP:OD2	1:D:3551:LYS:HG3	1.95	0.67
1:B:1268:LYS:HD3	1:B:1269:TYR:CZ	2.30	0.67
1:A:130:PRO:HG3	1:B:1054:LEU:HD23	1.76	0.67
1:B:1233:ASP:HB2	5:B:4649:HOH:O	1.95	0.67
1:D:3086:MSE:HE1	1:D:3111:VAL:CG2	2.25	0.66
1:A:300:LYS:NZ	1:A:304:GLU:HB2	2.07	0.66
1:A:324:VAL:HA	1:A:327:MSE:CE	2.25	0.66
1:B:1524:ILE:O	1:B:1528:ILE:HG13	1.96	0.66
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.59	0.66
1:C:2061:GLN:HA	1:C:2064:GLN:HE21	1.61	0.66
1:A:175:TYR:HD2	1:A:219:MSE:HE2	1.61	0.66
1:B:1177:MSE:O	1:B:1180:PRO:HD2	1.95	0.66
1:B:1261:ASN:HA	1:B:1264:ARG:HG2	1.75	0.66
1:B:1302:ILE:HA	1:B:1305:HIS:ND1	2.11	0.66
1:B:1369:ALA:HB1	1:B:1373:ILE:HD11	1.77	0.66
1:C:2468:VAL:HA	1:C:2471:PHE:CE2	2.31	0.66
1:A:77:SER:C	5:A:4952:HOH:O	2.34	0.66
1:B:1354:ARG:HD3	1:B:1358:ILE:HD11	1.78	0.65
1:D:3177:MSE:O	1:D:3180:PRO:HD2	1.97	0.65
1:D:3551:LYS:NZ	1:D:3551:LYS:HB3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:MSE:HG2	1:B:1080:GLU:CD	2.17	0.65
1:B:1332:LEU:CD1	1:B:1332:LEU:H	2.08	0.65
1:D:3261:ASN:HD22	1:D:3264:ARG:NE	1.91	0.65
1:D:3551:LYS:HZ2	1:D:3551:LYS:HB3	1.60	0.65
1:A:559:ARG:HG3	1:A:561:GLU:OE1	1.97	0.65
1:A:184:LEU:HD22	1:A:198:CYS:HB3	1.77	0.65
1:C:2261:ASN:ND2	1:C:2264:ARG:HH21	1.95	0.65
1:B:1342:TRP:CZ3	1:B:1349:LEU:HD21	2.32	0.64
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.79	0.64
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.80	0.64
1:D:3334:GLU:O	1:D:3338:GLN:HG3	1.97	0.64
1:D:3184:LEU:HD12	1:D:3200:PRO:HG3	1.80	0.64
1:A:350:LEU:HD22	1:A:354:ARG:NH1	2.13	0.63
1:B:1181:VAL:HG11	5:B:4503:HOH:O	1.97	0.63
1:D:3431:GLU:OE1	1:D:3452:VAL:HG13	1.97	0.63
1:A:24:LYS:O	1:C:2022:LYS:HE2	1.98	0.63
1:B:1528:ILE:HD13	1:B:1550:ALA:HA	1.80	0.63
1:D:3528:ILE:O	1:D:3531:THR:HG23	1.99	0.63
1:D:3286:VAL:HG22	1:D:3470:ILE:HG13	1.81	0.63
1:A:177:MSE:O	1:A:180:PRO:HD2	1.99	0.62
1:A:85:ILE:HD11	1:A:111:VAL:CG2	2.29	0.62
1:B:1389:ILE:HG12	5:B:4275:HOH:O	1.99	0.62
1:B:1075:MSE:HG2	1:B:1080:GLU:OE1	1.98	0.62
1:A:211:ALA:HA	1:A:214:LYS:HE2	1.81	0.62
1:D:3327:MSE:CE	1:D:3337:ALA:HB1	2.25	0.62
1:B:1371:GLU:CD	1:B:1371:GLU:N	2.50	0.62
1:A:153:ASN:H	1:A:153:ASN:HD22	1.45	0.62
1:A:23:GLU:HG3	1:A:27:PRO:HB2	1.81	0.62
1:A:177:MSE:CE	1:A:180:PRO:HB2	2.28	0.62
1:B:1312:ALA:CB	1:B:1343:MSE:HE3	2.29	0.62
1:C:2425:GLN:HG3	5:C:4790:HOH:O	1.99	0.62
1:B:1368:SER:HA	5:B:4846:HOH:O	1.99	0.62
1:B:1323:ILE:HG22	1:B:1327:MSE:HE2	1.82	0.61
1:D:3338:GLN:HB2	1:D:3339:LYS:HZ2	1.63	0.61
1:D:3284:ALA:HB1	1:D:3322:LEU:HD13	1.81	0.61
1:A:456:ASP:OD1	1:A:458:ARG:HD3	2.00	0.61
1:D:3125:HIS:CE1	5:D:4912:HOH:O	2.52	0.61
1:A:175:TYR:CD2	1:A:219:MSE:HE2	2.35	0.61
1:A:363:GLU:HB3	1:A:364:PRO:HD3	1.82	0.61
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.35	0.61
1:B:1367:HIS:CB	5:B:4824:HOH:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:ND2	1:A:153:ASN:H	1.97	0.61
1:B:1505:GLU:CD	1:B:1505:GLU:H	2.04	0.61
1:A:407:MSE:HE3	1:A:407:MSE:HA	1.81	0.61
1:A:153:ASN:ND2	1:A:153:ASN:N	2.49	0.61
1:B:1133:LEU:HB2	1:B:1199:LEU:HD11	1.83	0.61
1:C:2520:GLN:NE2	1:C:2520:GLN:H	1.96	0.60
1:A:144:ARG:HH12	1:A:244:ASP:HB3	1.64	0.60
1:C:2179:ILE:HB	1:C:2180:PRO:HD3	1.83	0.60
1:D:3272:LYS:HZ3	1:D:3272:LYS:HB3	1.64	0.60
1:B:1352:LYS:HB2	5:B:4846:HOH:O	1.99	0.60
1:B:1079:LEU:O	1:B:1083:ILE:HG13	2.02	0.60
1:A:505:GLU:N	1:A:505:GLU:CD	2.54	0.60
1:D:3335:GLN:HG2	1:D:3339:LYS:HE2	1.82	0.60
1:C:2552:TYR:O	1:C:2556:ARG:HG3	2.01	0.60
1:B:1261:ASN:HA	1:B:1264:ARG:HD3	1.83	0.60
1:B:1085:ILE:HD12	1:B:1096:PHE:CE1	2.37	0.60
1:A:25:GLY:HA3	1:C:2022:LYS:HE2	1.83	0.60
1:B:1140:ARG:HB2	1:B:1140:ARG:CZ	2.32	0.60
1:A:38:MSE:HE3	1:A:59:GLU:CD	2.22	0.60
1:B:1312:ALA:HB1	1:B:1343:MSE:CE	2.31	0.60
1:D:3085:ILE:HG13	1:D:3086:MSE:HE2	1.84	0.60
1:A:305:HIS:O	1:A:340:LYS:HG2	2.01	0.60
5:B:4632:HOH:O	4:C:2602:NAD:H51N	2.01	0.60
1:B:1085:ILE:HG13	1:B:1086:MSE:N	2.15	0.60
1:C:2361:TYR:O	1:C:2364:PRO:HD2	2.02	0.59
1:A:407:MSE:CE	1:A:411:ASN:ND2	2.64	0.59
1:C:2075:MSE:HE2	5:C:4558:HOH:O	2.03	0.59
1:D:3528:ILE:O	1:D:3532:GLU:HG3	2.01	0.59
1:D:3315:ALA:HB3	1:D:3392:VAL:HG21	1.84	0.59
1:D:3179:ILE:HB	1:D:3180:PRO:HD3	1.85	0.59
1:B:1357:LYS:O	1:B:1358:ILE:HD13	2.03	0.59
1:D:3154:HIS:HB2	5:D:4342:HOH:O	2.02	0.59
1:D:3298:ILE:HD11	1:D:3442:LEU:HD12	1.85	0.59
1:B:1370:PRO:HD2	1:B:1373:ILE:CD1	2.32	0.59
1:D:3060:THR:H	1:D:3063:ILE:HD12	1.68	0.59
1:C:2300:LYS:NZ	1:C:2304:GLU:HB2	2.17	0.59
1:C:2184:LEU:HD22	1:C:2198:CYS:HB3	1.85	0.58
1:B:1140:ARG:HH22	1:B:1233:ASP:HB3	1.66	0.58
1:B:1261:ASN:HB3	1:B:1265:PHE:CE1	2.38	0.58
1:A:324:VAL:HA	1:A:327:MSE:HE3	1.85	0.58
1:C:2094:LYS:HE2	1:C:2558:TRP:HZ2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:MSE:HE2	1:A:411:ASN:ND2	2.17	0.58
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.67	0.58
1:D:3177:MSE:CE	1:D:3180:PRO:HB2	2.32	0.58
1:D:3140:ARG:NH2	1:D:3233:ASP:HB3	2.09	0.58
1:A:505:GLU:H	1:A:505:GLU:CD	2.06	0.58
1:D:3293:ALA:HA	1:D:3296:LYS:HE2	1.86	0.58
1:C:2323:ILE:O	1:C:2327:MSE:HG3	2.03	0.58
1:B:1392:VAL:HG22	1:B:1392:VAL:O	2.02	0.58
1:D:3144:ARG:NH2	1:D:3245:ARG:HB2	2.18	0.58
1:D:3177:MSE:HE3	1:D:3180:PRO:HD2	1.86	0.58
1:A:286:VAL:HG11	1:A:466:ASN:O	2.04	0.57
1:B:1505:GLU:OE2	1:B:1505:GLU:N	2.37	0.57
1:B:1350:LEU:HD23	1:B:1354:ARG:NH1	2.20	0.57
1:D:3302:ILE:HG12	1:D:3332:LEU:HD11	1.84	0.57
1:D:3324:VAL:HA	1:D:3327:MSE:CE	2.35	0.57
1:B:1159:VAL:HG23	1:B:1184:LEU:HD21	1.87	0.57
1:C:2312:ALA:HB1	1:C:2343:MSE:HE3	1.86	0.57
1:A:332:LEU:HD21	1:A:340:LYS:HE2	1.86	0.57
1:C:2382:ASN:O	1:C:2385:LYS:HD2	2.03	0.57
1:A:520:GLN:HE21	1:A:520:GLN:H	1.52	0.57
1:B:1527:ALA:O	1:B:1531:THR:CG2	2.53	0.57
1:D:3492:LEU:HD22	1:D:3496:LYS:HE3	1.87	0.57
1:C:2210:ILE:O	1:C:2214:LYS:HG3	2.04	0.57
1:B:1024:LYS:NZ	1:D:3022:LYS:HD2	2.16	0.57
1:C:2293:ALA:O	1:C:2296:LYS:HB2	2.05	0.57
1:C:2061:GLN:HA	1:C:2064:GLN:NE2	2.19	0.57
1:C:2320:ALA:CB	5:C:4058:HOH:O	2.52	0.57
1:C:2392:VAL:CG1	1:C:2392:VAL:O	2.52	0.56
1:C:2359:ASP:OD2	1:C:2362:GLN:HG3	2.05	0.56
1:B:1261:ASN:HA	1:B:1264:ARG:CG	2.35	0.56
1:A:47:MSE:HG2	5:C:4312:HOH:O	2.04	0.56
1:B:1334:GLU:O	1:B:1338:GLN:HG3	2.03	0.56
1:B:1354:ARG:NE	1:B:1358:ILE:HD11	2.20	0.56
1:B:1343:MSE:SE	5:B:4104:HOH:O	2.73	0.56
1:D:3085:ILE:HD11	1:D:3111:VAL:HG23	1.87	0.56
1:B:1354:ARG:CD	1:B:1358:ILE:HD11	2.35	0.56
1:C:2397:ARG:NH1	5:C:4346:HOH:O	2.38	0.56
1:A:358:ILE:HD12	1:A:366:THR:OG1	2.06	0.56
1:D:3358:ILE:HD13	1:D:3366:THR:HG21	1.88	0.56
1:D:3085:ILE:HD11	1:D:3111:VAL:HG21	1.86	0.56
1:A:38:MSE:HE3	1:A:59:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3093:GLU:O	1:D:3096:PHE:HB3	2.05	0.55
1:C:2547:GLU:HB2	5:C:4930:HOH:O	2.06	0.55
1:A:68:PHE:CD2	1:A:99:ILE:HG13	2.41	0.55
1:D:3392:VAL:O	1:D:3392:VAL:HG13	2.06	0.55
1:D:3060:THR:OG1	1:D:3063:ILE:HG13	2.06	0.55
1:A:408:ALA:HB2	1:A:437:THR:HG22	1.88	0.55
1:B:1301:PRO:HD2	1:B:1304:GLU:HG3	1.88	0.55
1:C:2060:THR:H	1:C:2063:ILE:HD12	1.72	0.55
1:C:2184:LEU:O	1:C:2187:TYR:HB2	2.07	0.55
1:B:1302:ILE:CG1	1:B:1332:LEU:HD11	2.26	0.55
1:B:1261:ASN:HA	1:B:1264:ARG:CD	2.37	0.55
1:C:2343:MSE:SE	5:C:4058:HOH:O	2.74	0.55
1:C:2478:VAL:HG13	1:C:2483:THR:HB	1.87	0.55
1:D:3412:GLU:O	1:D:3440:ARG:HD2	2.06	0.55
1:D:3066:LEU:HD22	1:D:3070:ARG:HE	1.70	0.55
1:D:3538:LYS:N	1:D:3538:LYS:HD2	2.21	0.55
1:B:1025:GLY:C	1:B:1027:PRO:HD2	2.26	0.55
1:A:285:ALA:HB1	1:A:470:ILE:HD12	1.89	0.55
1:D:3023:GLU:HG3	1:D:3027:PRO:HB2	1.89	0.55
1:A:392:VAL:O	1:A:392:VAL:HG13	2.06	0.55
1:C:2054:LEU:HD23	1:D:3130:PRO:HG3	1.89	0.55
1:C:2293:ALA:HA	1:C:2296:LYS:CE	2.37	0.55
1:C:2137:ILE:O	1:C:2140:ARG:HG2	2.07	0.55
1:D:3371:GLU:CD	1:D:3371:GLU:H	2.07	0.54
1:B:1077:SER:O	1:B:1081:LYS:HG3	2.07	0.54
1:A:85:ILE:HD11	1:A:111:VAL:HG21	1.89	0.54
1:C:2177:MSE:O	1:C:2180:PRO:HD2	2.07	0.54
1:A:302:ILE:HG12	1:A:332:LEU:CD1	2.38	0.54
1:A:144:ARG:NH1	1:A:244:ASP:HB3	2.21	0.54
1:B:1300:LYS:HZ3	1:B:1304:GLU:C	2.11	0.54
1:B:1432:GLU:O	1:B:1436:LEU:HB2	2.07	0.54
1:A:33:ARG:NH1	1:A:93:GLU:OE1	2.40	0.54
1:A:407:MSE:HE2	1:A:407:MSE:HA	1.87	0.54
1:D:3315:ALA:CB	1:D:3392:VAL:HG21	2.38	0.54
1:A:549:LYS:HG2	5:A:4766:HOH:O	2.07	0.54
1:B:1379:ASP:O	1:B:1383:ILE:HD12	2.07	0.54
1:B:1493:GLU:HG3	1:B:1533:TYR:CD1	2.43	0.54
1:B:1349:LEU:HG	1:B:1351:VAL:HG13	1.90	0.54
1:B:1024:LYS:HZ2	1:D:3022:LYS:HA	1.69	0.54
1:A:298:ILE:HD11	1:A:442:LEU:HD12	1.90	0.54
1:B:1154:HIS:O	1:B:1197:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:HZ1	1:A:457:GLY:HA2	1.73	0.54
1:B:1496:LYS:O	1:B:1500:SER:HB3	2.08	0.54
1:A:298:ILE:HD11	1:A:442:LEU:CD1	2.38	0.54
1:B:1346:LYS:HD2	1:B:1346:LYS:H	1.73	0.54
1:D:3284:ALA:CB	1:D:3322:LEU:HD13	2.38	0.53
1:A:45:ARG:NH2	1:A:58:ILE:HD13	2.23	0.53
1:B:1315:ALA:HB3	1:B:1392:VAL:CG2	2.35	0.53
1:B:1358:ILE:CG2	5:B:4650:HOH:O	2.31	0.53
1:C:2559:ARG:HB3	1:C:2561:GLU:HG2	1.91	0.53
1:C:2355:LYS:HE2	1:C:2355:LYS:HA	1.90	0.53
1:B:1024:LYS:HZ1	1:D:3022:LYS:HA	1.73	0.53
1:A:546:PRO:O	1:A:549:LYS:NZ	2.40	0.53
1:C:2358:ILE:HD13	1:C:2366:THR:HG21	1.90	0.53
1:B:1312:ALA:HB1	1:B:1343:MSE:HE3	1.90	0.53
1:C:2559:ARG:HG3	1:C:2561:GLU:OE1	2.07	0.53
1:D:3177:MSE:O	1:D:3177:MSE:CE	2.56	0.53
1:B:1320:ALA:O	1:B:1324:VAL:HG23	2.09	0.53
1:C:2131:LYS:O	1:C:2177:MSE:HE3	2.07	0.53
1:C:2325:MSE:HE1	1:C:2489:SER:HA	1.91	0.53
1:C:2328:VAL:HA	1:C:2332:LEU:O	2.08	0.53
1:C:2086:MSE:CE	1:C:2111:VAL:HG22	2.37	0.53
1:A:483:THR:OG1	1:A:534:LEU:HD13	2.08	0.53
1:A:453:LYS:NZ	1:A:457:GLY:HA2	2.24	0.53
1:D:3208:ASP:OD2	1:D:3227:ARG:NH2	2.40	0.53
1:D:3380:ALA:O	1:D:3384:LEU:HB2	2.08	0.53
1:D:3229:GLN:O	1:D:3229:GLN:HG2	2.09	0.53
1:A:81:LYS:O	1:A:85:ILE:HG23	2.09	0.52
1:D:3343:MSE:CE	1:D:3365:PHE:HB2	2.34	0.52
1:C:2302:ILE:HA	1:C:2305:HIS:ND1	2.25	0.52
1:C:2069:HIS:HE1	1:C:2102:ASP:OD2	1.93	0.52
1:A:302:ILE:HG12	1:A:332:LEU:HD11	1.92	0.52
1:B:1029:MSE:HE1	1:B:1053:LEU:CD1	2.39	0.52
1:B:1325:MSE:HE2	1:B:1492:LEU:CD1	2.39	0.52
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.90	0.52
1:A:397:ARG:HA	1:A:427:GLU:O	2.10	0.52
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.24	0.52
1:C:2355:LYS:CE	1:C:2355:LYS:HA	2.40	0.52
1:B:1286:VAL:HG11	1:B:1466:ASN:O	2.10	0.51
1:B:1300:LYS:NZ	1:B:1304:GLU:HG3	2.25	0.51
1:B:1068:PHE:CD2	1:B:1099:ILE:HG13	2.46	0.51
1:D:3389:ILE:HG12	5:D:4639:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3324:VAL:HA	1:D:3327:MSE:HE3	1.93	0.51
1:A:386:PRO:O	1:A:407:MSE:HE1	2.10	0.51
1:D:3068:PHE:CD2	1:D:3099:ILE:HG13	2.45	0.51
1:B:1505:GLU:O	1:B:1508:ALA:HB3	2.10	0.51
1:B:1314:GLU:HG3	4:B:1601:NAD:O2A	2.11	0.51
1:B:1196:ASP:N	1:B:1196:ASP:OD1	2.44	0.51
1:D:3338:GLN:HB2	1:D:3339:LYS:HZ3	1.76	0.51
1:A:273:TYR:O	1:A:485:HIS:HD2	1.93	0.51
1:A:288:LEU:HG	1:A:292:LEU:HD22	1.92	0.51
1:D:3333:SER:HB3	1:D:3336:GLU:HB3	1.92	0.51
1:B:1177:MSE:C	1:B:1180:PRO:HD2	2.31	0.51
1:A:85:ILE:HD11	1:A:111:VAL:HG23	1.92	0.51
1:B:1345:ASP:HB2	4:B:1601:NAD:O2B	2.10	0.51
1:B:1325:MSE:HE2	1:B:1492:LEU:HD12	1.92	0.51
1:D:3350:LEU:HD22	1:D:3354:ARG:NH1	2.26	0.51
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.24	0.51
1:A:177:MSE:HE3	1:A:180:PRO:CD	2.39	0.51
1:C:2481:CYS:SG	1:C:2531:THR:HB	2.50	0.51
1:D:3412:GLU:HG3	1:D:3413:ARG:HG2	1.93	0.51
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.93	0.51
1:D:3389:ILE:HG23	1:D:3399:PHE:CE1	2.46	0.50
1:B:1342:TRP:HZ3	1:B:1349:LEU:HD21	1.74	0.50
1:B:1528:ILE:O	1:B:1532:GLU:HG3	2.10	0.50
1:D:3502:LEU:CD1	1:D:3507:LEU:HG	2.41	0.50
1:C:2505:GLU:O	1:C:2508:ALA:HB3	2.10	0.50
1:D:3320:ALA:HB2	5:D:4695:HOH:O	2.11	0.50
1:A:350:LEU:HD13	1:A:358:ILE:CD1	2.41	0.50
1:A:119:ALA:O	1:A:123:TYR:N	2.45	0.50
1:B:1022:LYS:HD2	1:B:1022:LYS:O	2.12	0.50
1:A:397:ARG:NH2	1:A:423:THR:O	2.44	0.50
1:A:177:MSE:SE	5:A:4018:HOH:O	2.79	0.50
1:C:2350:LEU:HD22	1:C:2354:ARG:NH1	2.27	0.50
1:D:3085:ILE:HG13	1:D:3086:MSE:N	2.24	0.50
1:C:2300:LYS:HE2	5:C:4931:HOH:O	2.10	0.50
1:C:2301:PRO:HD2	1:C:2304:GLU:OE1	2.11	0.50
1:B:1261:ASN:HD22	1:B:1264:ARG:HH11	1.57	0.50
1:C:2454:LEU:HD11	1:C:2460:PHE:CE2	2.39	0.50
1:D:3023:GLU:CG	1:D:3027:PRO:HB2	2.42	0.50
1:B:1445:SER:O	1:B:1465:GLY:N	2.44	0.50
1:B:1343:MSE:HE2	1:B:1350:LEU:HD12	1.92	0.50
1:C:2312:ALA:HB1	1:C:2343:MSE:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2412:GLU:O	1:C:2440:ARG:HD2	2.12	0.50
1:B:1346:LYS:HD2	4:B:1601:NAD:O2B	2.11	0.50
1:B:1481:CYS:SG	1:B:1531:THR:HB	2.52	0.50
1:C:2079:LEU:O	1:C:2083:ILE:HG13	2.11	0.50
1:A:484:ARG:HG3	1:A:541:PHE:CE1	2.47	0.50
1:B:1136:SER:HA	1:B:1204:ASP:O	2.12	0.50
1:B:1338:GLN:OE1	1:B:1364:PRO:HB3	2.11	0.49
1:B:1350:LEU:CD2	1:B:1354:ARG:NH1	2.75	0.49
1:B:1383:ILE:HG22	1:B:1384:LEU:HD13	1.94	0.49
1:D:3150:TRP:CE2	1:D:3199:LEU:HD13	2.47	0.49
1:B:1312:ALA:HB1	1:B:1343:MSE:HE1	1.94	0.49
1:D:3343:MSE:HE2	1:D:3365:PHE:CB	2.36	0.49
1:D:3122:GLN:HE22	1:D:3125:HIS:CD2	2.30	0.49
1:C:2556:ARG:HH11	1:C:2556:ARG:CG	2.25	0.49
1:B:1081:LYS:HE3	5:B:4336:HOH:O	2.11	0.49
1:A:407:MSE:HE1	1:A:411:ASN:HD21	1.76	0.49
1:B:1036:LYS:HG2	1:B:1562:TYR:CD2	2.47	0.49
1:C:2238:PHE:CE1	1:C:2242:ILE:HG13	2.47	0.49
1:B:1315:ALA:CB	1:B:1392:VAL:HG21	2.36	0.49
1:D:3300:LYS:HB3	1:D:3300:LYS:HZ2	1.78	0.49
1:A:400:THR:OG1	1:A:403:VAL:HG23	2.13	0.49
1:A:310:LEU:HD21	1:A:398:LEU:HB2	1.93	0.49
1:B:1227:ARG:HG2	1:B:1227:ARG:NH1	2.26	0.49
1:D:3315:ALA:HB3	1:D:3392:VAL:CG2	2.43	0.49
1:B:1301:PRO:HG2	1:B:1304:GLU:OE2	2.13	0.49
1:A:72:LEU:HA	1:A:75:MSE:HG3	1.94	0.49
1:B:1505:GLU:CD	1:B:1505:GLU:N	2.65	0.49
1:C:2075:MSE:HG2	1:C:2080:GLU:CD	2.33	0.49
1:D:3302:ILE:CD1	1:D:3332:LEU:HD13	2.42	0.49
1:C:2527:ALA:O	1:C:2531:THR:CG2	2.58	0.49
1:B:1527:ALA:O	1:B:1531:THR:HG22	2.13	0.49
1:C:2091:ARG:HB3	5:C:4893:HOH:O	2.12	0.49
1:A:299:SER:HB3	5:A:4513:HOH:O	2.12	0.49
1:A:219:MSE:HG2	1:B:1038:MSE:CE	2.41	0.48
1:A:535:TYR:OH	1:A:542:ARG:HB3	2.12	0.48
1:A:308:LEU:HD23	1:A:389:ILE:HD11	1.94	0.48
1:C:2067:ARG:HD2	5:C:4187:HOH:O	2.13	0.48
1:D:3520:GLN:N	1:D:3520:GLN:HE21	1.99	0.48
1:A:85:ILE:HG13	1:A:86:MSE:N	2.28	0.48
1:D:3537:ASN:C	1:D:3538:LYS:HD2	2.33	0.48
1:A:526:ILE:O	1:A:530:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MSE:HE1	1:A:488:ASP:CB	2.43	0.48
1:D:3401:PRO:HA	1:D:3436:LEU:CD1	2.44	0.48
1:C:2363:GLU:HB3	1:C:2364:PRO:HD3	1.96	0.48
1:A:184:LEU:O	1:A:187:TYR:HB2	2.13	0.48
1:D:3288:LEU:HG	1:D:3292:LEU:HD22	1.95	0.48
1:D:3306:LYS:HG2	1:D:3386:PRO:HA	1.95	0.48
1:D:3521:GLU:HG2	5:D:4042:HOH:O	2.13	0.48
1:C:2068:PHE:CD2	1:C:2099:ILE:HG13	2.47	0.48
1:D:3302:ILE:HG23	1:D:3303:SER:N	2.28	0.48
1:D:3551:LYS:O	1:D:3555:GLU:HB2	2.13	0.48
1:A:46:GLN:HG2	1:A:51:GLN:HG3	1.96	0.48
1:B:1029:MSE:HE2	1:B:1050:LEU:HB3	1.95	0.48
1:B:1343:MSE:HE2	1:B:1350:LEU:CD1	2.44	0.48
1:B:1350:LEU:HD22	1:B:1358:ILE:HD11	1.94	0.48
1:B:1302:ILE:HA	1:B:1305:HIS:CE1	2.49	0.48
1:B:1336:GLU:HA	1:B:1339:LYS:HG3	1.96	0.48
1:B:1140:ARG:NH1	1:B:1140:ARG:HB2	2.29	0.47
1:A:186:LEU:O	1:A:190:CYS:HB2	2.13	0.47
1:D:3051:GLN:HE21	1:D:3051:GLN:HA	1.79	0.47
1:D:3528:ILE:HG12	1:D:3550:ALA:HA	1.96	0.47
1:A:350:LEU:HB3	1:A:358:ILE:HD11	1.96	0.47
1:D:3291:LEU:HD13	1:D:3417:PHE:CE2	2.49	0.47
1:C:2226:ASP:OD1	1:C:2226:ASP:C	2.53	0.47
1:D:3143:VAL:O	1:D:3147:VAL:HG23	2.14	0.47
1:B:1169:LEU:HD13	1:B:1422:PRO:HD3	1.96	0.47
1:A:66:LEU:HD23	1:A:66:LEU:O	2.14	0.47
1:D:3300:LYS:C	1:D:3300:LYS:HZ2	2.18	0.47
1:D:3033:ARG:NH1	1:D:3093:GLU:OE2	2.39	0.47
1:B:1520:GLN:NE2	1:B:1520:GLN:H	2.12	0.47
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.96	0.47
1:D:3302:ILE:HG12	1:D:3332:LEU:CD1	2.43	0.47
1:D:3144:ARG:HD2	1:D:3144:ARG:HA	1.72	0.47
1:A:407:MSE:HE1	1:A:411:ASN:ND2	2.29	0.47
1:B:1194:ARG:HB2	1:B:1197:ARG:HG3	1.96	0.47
1:B:1288:LEU:HG	1:B:1292:LEU:HD22	1.96	0.47
1:A:165:ARG:NE	1:A:165:ARG:O	2.47	0.47
1:B:1295:GLN:HA	1:B:1295:GLN:OE1	2.13	0.47
1:D:3245:ARG:HG2	1:D:3246:TYR:CD1	2.50	0.47
1:A:492:LEU:O	1:A:496:LYS:HG3	2.15	0.47
1:A:120:CYS:O	1:A:175:TYR:HB3	2.14	0.47
1:B:1022:LYS:HE2	1:D:3024:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:O	1:A:74:LYS:HE3	2.14	0.47
1:D:3286:VAL:CG2	1:D:3467:ASN:HA	2.43	0.47
1:D:3038:MSE:HE3	1:D:3059:GLU:CD	2.35	0.47
1:A:518:ASN:O	1:A:522:VAL:HG23	2.14	0.47
1:B:1274:CYS:HB2	1:B:1484:ARG:O	2.14	0.47
1:C:2528:ILE:HG12	1:C:2550:ALA:HA	1.95	0.47
1:D:3154:HIS:O	1:D:3197:ARG:HD3	2.15	0.47
1:A:548:ASP:C	1:A:548:ASP:OD1	2.52	0.47
1:D:3232:ASP:CG	1:D:3264:ARG:HH22	2.19	0.47
1:A:401:PRO:HA	1:A:436:LEU:CD2	2.45	0.47
1:D:3310:LEU:HB3	1:D:3391:GLY:HA2	1.96	0.47
1:A:206:GLY:HA2	5:A:4098:HOH:O	2.14	0.47
1:A:177:MSE:O	1:A:177:MSE:CE	2.62	0.47
1:A:314:GLU:HB2	4:A:601:NAD:O1N	2.15	0.47
1:D:3512:LEU:HG	5:D:4471:HOH:O	2.16	0.46
1:A:253:GLN:HB2	1:A:276:PHE:CE2	2.49	0.46
1:A:504:ASP:N	1:A:504:ASP:OD2	2.48	0.46
1:C:2085:ILE:HD12	1:C:2096:PHE:HE1	1.80	0.46
1:D:3400:THR:HB	1:D:3401:PRO:HD2	1.98	0.46
1:D:3481:CYS:HB3	1:D:3540:ALA:CB	2.44	0.46
1:D:3300:LYS:HZ1	1:D:3305:HIS:CE1	2.33	0.46
1:D:3140:ARG:NH2	1:D:3230:GLN:O	2.49	0.46
1:A:43:GLN:OE1	1:A:47:MSE:HE1	2.16	0.46
1:B:1146:ILE:O	1:B:1149:ASN:HB2	2.16	0.46
1:B:1166:ILE:HA	1:B:1256:ASP:OD2	2.16	0.46
1:D:3144:ARG:HH21	1:D:3245:ARG:HB2	1.80	0.46
1:B:1248:ARG:HH22	1:B:1272:LYS:HG2	1.81	0.46
1:D:3468:VAL:HA	1:D:3471:PHE:CE2	2.50	0.46
1:C:2571:GLU:HG3	1:C:2572:TRP:N	2.30	0.46
1:A:177:MSE:HE1	1:A:200:PRO:HB2	1.98	0.46
1:C:2331:GLY:O	1:C:2332:LEU:O	2.33	0.46
1:D:3272:LYS:NZ	1:D:3272:LYS:CB	2.77	0.46
1:B:1325:MSE:O	1:B:1329:GLU:HB2	2.16	0.46
1:D:3397:ARG:HA	1:D:3427:GLU:O	2.16	0.46
1:C:2288:LEU:HG	1:C:2292:LEU:HD22	1.98	0.46
1:B:1367:HIS:HB2	5:B:4824:HOH:O	2.14	0.46
1:A:392:VAL:O	1:A:392:VAL:HG12	2.14	0.46
1:A:23:GLU:OE1	1:A:23:GLU:HA	2.14	0.46
1:B:1527:ALA:O	1:B:1531:THR:HG23	2.16	0.46
1:D:3099:ILE:HA	1:D:3099:ILE:HD12	1.68	0.46
1:A:150:TRP:CE2	1:A:199:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1532:GLU:HG2	1:B:1549:LYS:HG2	1.98	0.46
1:B:1235:ILE:O	1:B:1239:MSE:HG2	2.16	0.45
1:A:21:ILE:N	1:A:21:ILE:HD12	2.31	0.45
1:D:3526:ILE:O	1:D:3530:VAL:HG23	2.16	0.45
1:A:156:LYS:CG	1:A:197:ARG:HG2	2.44	0.45
1:A:332:LEU:HA	1:A:336:GLU:OE2	2.16	0.45
1:D:3066:LEU:HD22	1:D:3070:ARG:NE	2.32	0.45
1:C:2145:SER:HB3	5:C:4036:HOH:O	2.15	0.45
1:C:2022:LYS:HD2	1:C:2022:LYS:O	2.16	0.45
1:C:2471:PHE:CG	1:C:2472:PRO:HD3	2.52	0.45
5:C:4932:HOH:O	1:D:3063:ILE:HD13	2.15	0.45
1:C:2374:PRO:HB3	1:C:2383:ILE:HD12	1.98	0.45
1:C:2194:ARG:NH1	1:C:2197:ARG:NH2	2.65	0.45
1:A:177:MSE:CE	1:A:200:PRO:HB2	2.47	0.45
1:B:1367:HIS:HB3	5:B:4824:HOH:O	2.16	0.45
1:D:3339:LYS:N	1:D:3339:LYS:HD3	2.29	0.45
1:C:2069:HIS:HD2	5:C:4306:HOH:O	1.99	0.45
1:B:1172:LEU:O	1:B:1175:TYR:HB2	2.16	0.45
1:C:2408:ALA:HB2	1:C:2437:THR:HG22	1.98	0.45
1:B:1232:ASP:OD1	1:B:1264:ARG:NH2	2.49	0.45
1:A:528:ILE:O	1:A:532:GLU:HG3	2.16	0.45
1:A:538:LYS:HA	5:A:4882:HOH:O	2.16	0.45
1:A:287:ALA:O	1:A:291:LEU:HD22	2.17	0.45
1:B:1315:ALA:O	1:B:1319:ILE:HG13	2.17	0.45
1:B:1335:GLN:O	1:B:1339:LYS:HG3	2.16	0.45
1:B:1401:PRO:HA	1:B:1436:LEU:HD23	1.97	0.45
1:A:453:LYS:HD2	1:A:459:VAL:HG22	1.98	0.45
1:A:338:GLN:HB2	1:A:339:LYS:NZ	2.31	0.45
1:B:1350:LEU:HD22	1:B:1358:ILE:CD1	2.47	0.45
1:A:66:LEU:HD21	1:A:70:ARG:HH11	1.75	0.45
1:B:1259:ASN:ND2	5:B:4936:HOH:O	2.49	0.45
1:B:1268:LYS:NZ	5:B:4587:HOH:O	2.49	0.45
1:A:108:MSE:N	1:A:109:PRO:CD	2.79	0.45
1:C:2286:VAL:HG11	1:C:2466:ASN:O	2.17	0.45
1:D:3343:MSE:SE	5:D:4695:HOH:O	2.84	0.45
1:B:1075:MSE:HE1	1:B:1084:TYR:CD2	2.51	0.45
1:B:1481:CYS:O	1:B:1482:ASN:HB2	2.17	0.45
1:B:1456:ASP:OD1	1:B:1458:ARG:HD3	2.16	0.45
1:B:1104:ILE:HG23	1:B:1105:GLU:N	2.32	0.45
1:B:1312:ALA:HB2	1:B:1343:MSE:HE3	1.98	0.44
1:B:1024:LYS:HZ2	1:D:3022:LYS:CD	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3184:LEU:HD12	1:D:3200:PRO:CG	2.46	0.44
1:D:3026:LYS:N	1:D:3027:PRO:CD	2.80	0.44
1:D:3481:CYS:HB3	1:D:3540:ALA:HB1	1.99	0.44
1:A:133:LEU:HB2	1:A:199:LEU:HD11	1.99	0.44
1:C:2454:LEU:HD12	1:C:2458:ARG:HB2	1.99	0.44
1:D:3555:GLU:HB3	1:D:3556:ARG:NH1	2.31	0.44
1:C:2412:GLU:HG2	5:C:4719:HOH:O	2.17	0.44
1:C:2432:GLU:O	1:C:2436:LEU:HB2	2.17	0.44
1:A:554:LYS:H	1:A:554:LYS:HG2	1.38	0.44
1:C:2205:VAL:HG11	1:C:2231:TYR:HD1	1.82	0.44
1:D:3286:VAL:HG22	1:D:3470:ILE:CG1	2.47	0.44
1:D:3484:ARG:O	1:D:3485:HIS:CD2	2.70	0.44
1:A:66:LEU:HD22	1:B:1217:PHE:CZ	2.38	0.44
1:D:3496:LYS:NZ	5:D:4699:HOH:O	2.50	0.44
1:C:2033:ARG:HD3	1:C:2093:GLU:OE2	2.16	0.44
1:B:1208:ASP:OD1	1:B:1224:LYS:HB3	2.17	0.44
1:A:545:GLU:OE2	1:A:549:LYS:NZ	2.47	0.44
1:B:1484:ARG:HG2	1:C:2543:TYR:CZ	2.52	0.44
1:D:3259:ASN:O	1:D:3263:PHE:HD1	2.01	0.44
1:B:1351:VAL:HA	1:B:1367:HIS:O	2.18	0.44
1:A:297:VAL:HG23	1:A:298:ILE:HG13	1.98	0.44
1:D:3078:PRO:HD2	5:D:4900:HOH:O	2.17	0.44
1:C:2300:LYS:HZ3	1:C:2304:GLU:HB2	1.82	0.43
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.80	0.43
1:A:339:LYS:NZ	1:A:339:LYS:N	2.65	0.43
1:C:2314:GLU:HB2	4:C:2601:NAD:O1N	2.18	0.43
1:D:3399:PHE:CG	1:D:3427:GLU:HB3	2.53	0.43
1:C:2089:GLN:OE1	1:C:2131:LYS:HE2	2.17	0.43
1:B:1248:ARG:NH2	1:B:1272:LYS:HG2	2.33	0.43
1:B:1456:ASP:C	1:B:1456:ASP:OD1	2.56	0.43
1:B:1108:MSE:HE3	1:B:1516:LEU:HD11	2.00	0.43
1:B:1060:THR:N	1:B:1063:ILE:HD12	2.25	0.43
1:A:432:GLU:O	1:A:436:LEU:HB2	2.18	0.43
1:D:3194:ARG:HG2	1:D:3558:TRP:CD1	2.53	0.43
1:D:3172:LEU:O	1:D:3175:TYR:HB2	2.19	0.43
1:D:3108:MSE:N	1:D:3109:PRO:CD	2.81	0.43
1:C:2300:LYS:CB	1:C:2300:LYS:NZ	2.62	0.43
1:A:24:LYS:HD3	1:C:2024:LYS:HB3	2.01	0.43
1:A:154:HIS:O	1:A:197:ARG:HG3	2.18	0.43
1:C:2082:TYR:O	1:C:2086:MSE:HB2	2.19	0.43
1:B:1036:LYS:HE2	1:B:1562:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:HG23	1:A:399:PHE:CZ	2.54	0.43
1:D:3478:VAL:HG13	1:D:3483:THR:HB	2.01	0.43
1:D:3177:MSE:SE	5:D:4067:HOH:O	2.86	0.43
1:C:2431:GLU:O	1:C:2435:THR:HG23	2.18	0.43
1:C:2038:MSE:HE2	1:D:3127:PHE:CE2	2.53	0.43
1:D:3022:LYS:O	1:D:3022:LYS:HD2	2.19	0.43
1:B:1300:LYS:NZ	1:B:1301:PRO:O	2.52	0.43
1:D:3115:THR:HG22	1:D:3115:THR:O	2.19	0.43
1:B:1335:GLN:HG3	1:B:1339:LYS:HE2	2.00	0.43
1:C:2100:LEU:HA	1:C:2107:LEU:HD12	1.99	0.43
1:C:2556:ARG:NH1	1:C:2556:ARG:CG	2.80	0.43
1:C:2070:ARG:O	1:C:2074:LYS:HD3	2.18	0.43
1:B:1521:GLU:HG2	5:B:4059:HOH:O	2.18	0.43
1:D:3105:GLU:OE2	1:D:3516:LEU:HB3	2.19	0.43
1:A:152:GLU:HG2	1:A:196:ASP:O	2.19	0.43
1:B:1351:VAL:CG1	1:B:1369:ALA:HA	2.49	0.43
1:A:350:LEU:HD23	1:A:350:LEU:N	2.34	0.43
1:B:1401:PRO:HA	1:B:1436:LEU:CD2	2.48	0.43
1:A:66:LEU:HD21	1:A:70:ARG:CZ	2.46	0.42
1:C:2539:MSE:HE2	1:C:2539:MSE:HB3	1.91	0.42
1:A:431:GLU:CD	1:A:452:VAL:HG13	2.40	0.42
1:B:1273:TYR:O	1:B:1485:HIS:HD2	2.02	0.42
1:B:1317:LEU:CG	5:B:4327:HOH:O	2.67	0.42
1:B:1320:ALA:CB	5:B:4104:HOH:O	2.66	0.42
1:A:33:ARG:HH11	1:A:93:GLU:CD	2.23	0.42
1:A:350:LEU:HD13	1:A:358:ILE:HD13	2.00	0.42
1:B:1505:GLU:O	1:B:1509:GLN:HG3	2.18	0.42
1:A:87:GLY:HA3	5:A:4428:HOH:O	2.18	0.42
1:A:392:VAL:CG1	5:A:4007:HOH:O	2.67	0.42
1:A:466:ASN:HA	4:A:601:NAD:O7N	2.19	0.42
1:B:1031:ASN:HA	1:B:1032:PRO:HD2	1.87	0.42
1:D:3207:THR:O	1:D:3224:LYS:HA	2.18	0.42
1:A:232:ASP:CG	1:A:264:ARG:HH22	2.23	0.42
1:B:1140:ARG:CZ	1:B:1140:ARG:CB	2.97	0.42
1:A:447:SER:HB3	1:A:448:PRO:HD2	2.00	0.42
1:A:549:LYS:HG2	1:A:549:LYS:H	1.62	0.42
1:A:41:THR:O	1:A:45:ARG:HG3	2.19	0.42
1:A:159:VAL:O	1:A:180:PRO:HB3	2.19	0.42
1:D:3194:ARG:HE	1:D:3197:ARG:HG3	1.84	0.42
1:A:283:THR:HA	1:A:286:VAL:HG23	2.00	0.42
1:B:1182:GLY:HA3	5:B:4647:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2389:ILE:HG23	1:C:2399:PHE:CZ	2.54	0.42
1:C:2475:ALA:O	1:C:2479:ILE:HG13	2.19	0.42
1:A:297:VAL:HG21	1:A:442:LEU:CD2	2.50	0.42
1:C:2077:SER:O	1:C:2081:LYS:HG3	2.18	0.42
1:B:1355:LYS:HA	1:B:1355:LYS:HD2	1.89	0.42
1:D:3407:MSE:HG3	1:D:3414:PRO:HB3	2.02	0.42
1:B:1332:LEU:HD12	1:B:1332:LEU:N	2.13	0.42
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.34	0.42
1:A:205:VAL:HG11	1:A:231:TYR:HD1	1.85	0.42
1:C:2110:ILE:O	1:C:2115:THR:HB	2.19	0.42
1:A:322:LEU:HA	1:A:322:LEU:HD22	1.79	0.42
1:B:1322:LEU:HD12	1:B:1322:LEU:HA	1.91	0.42
1:A:159:VAL:HG23	1:A:184:LEU:HD21	2.02	0.42
1:C:2300:LYS:HZ1	1:C:2304:GLU:HB2	1.85	0.42
1:A:150:TRP:CD2	1:A:151:PRO:HD2	2.55	0.42
1:C:2351:VAL:HA	1:C:2367:HIS:O	2.20	0.42
1:B:1347:TYR:HB2	1:B:1354:ARG:HH22	1.85	0.41
1:A:24:LYS:HZ2	1:C:2022:LYS:HD2	1.84	0.41
1:B:1497:ALA:O	1:B:1501:GLN:HG3	2.20	0.41
1:B:1184:LEU:O	1:B:1187:TYR:HB2	2.20	0.41
1:B:1487:SER:OG	1:B:1490:VAL:HG23	2.20	0.41
1:C:2177:MSE:C	1:C:2180:PRO:HD2	2.40	0.41
1:A:520:GLN:O	1:A:524:ILE:HG12	2.20	0.41
1:D:3545:GLU:HA	1:D:3546:PRO:HD3	1.92	0.41
1:C:2400:THR:HB	1:C:2401:PRO:HD2	2.02	0.41
1:B:1317:LEU:HD11	5:B:4327:HOH:O	2.21	0.41
1:B:1261:ASN:CA	1:B:1264:ARG:HG2	2.49	0.41
1:B:1310:LEU:HD13	1:B:1377:PHE:CD1	2.56	0.41
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.94	0.41
1:B:1036:LYS:HB3	1:B:1039:ALA:HB3	2.02	0.41
1:C:2539:MSE:CE	5:C:4084:HOH:O	2.67	0.41
1:C:2533:TYR:O	1:C:2537:ASN:ND2	2.47	0.41
1:C:2025:GLY:C	1:C:2027:PRO:HD2	2.41	0.41
1:A:69:HIS:HE1	1:A:102:ASP:OD2	2.03	0.41
1:B:1119:ALA:O	1:B:1123:TYR:N	2.53	0.41
1:A:371:GLU:N	1:A:371:GLU:CD	2.62	0.41
1:B:1310:LEU:HD21	1:B:1398:LEU:HD23	2.02	0.41
1:C:2407:MSE:HG3	5:C:4314:HOH:O	2.20	0.41
1:A:335:GLN:O	1:A:339:LYS:HD2	2.19	0.41
1:D:3474:VAL:O	1:D:3478:VAL:HG23	2.20	0.41
1:C:2322:LEU:HA	1:C:2322:LEU:HD12	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2046:GLN:HG2	1:C:2051:GLN:HG3	2.00	0.41
1:C:2385:LYS:N	1:C:2386:PRO:CD	2.83	0.41
1:B:1184:LEU:HD22	1:B:1198:CYS:HB3	2.02	0.41
1:A:379:ASP:HA	5:A:4486:HOH:O	2.19	0.41
1:B:1210:ILE:CD1	5:B:4445:HOH:O	2.69	0.41
1:D:3069:HIS:HE1	1:D:3102:ASP:OD2	2.04	0.41
1:B:1331:GLY:O	1:B:1332:LEU:O	2.38	0.41
1:D:3335:GLN:O	1:D:3339:LYS:HE2	2.20	0.41
1:B:1069:HIS:CE1	1:B:1102:ASP:OD2	2.65	0.41
1:D:3136:SER:HB2	1:D:3221:LEU:HD22	2.03	0.41
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.84	0.41
1:C:2174:VAL:O	1:C:2174:VAL:HG12	2.20	0.41
1:D:3077:SER:O	1:D:3081:LYS:HG3	2.21	0.41
1:B:1397:ARG:HA	1:B:1427:GLU:O	2.20	0.41
1:D:3482:ASN:HD21	4:D:3602:NAD:H4B	1.86	0.41
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.92	0.41
1:D:3308:LEU:HD23	1:D:3389:ILE:HD11	2.03	0.41
1:B:1261:ASN:HD21	1:B:1264:ARG:HH11	1.62	0.41
1:B:1082:TYR:CZ	1:B:1086:MSE:HG3	2.56	0.41
1:A:400:THR:HB	1:A:401:PRO:HD2	2.02	0.41
1:B:1273:TYR:O	1:B:1485:HIS:CD2	2.74	0.41
1:D:3453:LYS:HA	1:D:3458:ARG:O	2.21	0.41
1:B:1166:ILE:HD12	1:B:1179:ILE:HG13	2.01	0.41
1:B:1354:ARG:HH21	1:B:1356:ALA:HB3	1.86	0.40
1:C:2300:LYS:HZ2	1:C:2300:LYS:CB	2.16	0.40
1:D:3492:LEU:O	1:D:3496:LYS:HG3	2.21	0.40
1:D:3294:ALA:O	1:D:3297:VAL:HG22	2.21	0.40
1:C:2380:ALA:O	1:C:2384:LEU:HB2	2.20	0.40
1:B:1382:ASN:O	1:B:1385:LYS:HG3	2.22	0.40
1:A:33:ARG:NH2	5:A:4407:HOH:O	2.54	0.40
1:A:324:VAL:O	1:A:328:VAL:HG23	2.21	0.40
1:D:3051:GLN:NE2	1:D:3051:GLN:HA	2.35	0.40
1:A:369:ALA:HA	1:A:370:PRO:HD3	1.92	0.40
1:B:1551:LYS:O	1:B:1555:GLU:HB2	2.21	0.40
1:B:1468:VAL:HA	1:B:1471:PHE:CE2	2.56	0.40
1:C:2023:GLU:OE1	1:C:2023:GLU:HA	2.22	0.40
1:D:3165:ARG:NH2	2:D:3603:OXL:O1	2.45	0.40
1:A:66:LEU:CD2	1:A:70:ARG:HD3	2.51	0.40
1:A:343:MSE:SE	5:A:4862:HOH:O	2.89	0.40
1:A:316:ALA:N	1:A:392:VAL:HG11	2.36	0.40
1:D:3350:LEU:HD23	1:D:3350:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3471:PHE:N	1:D:3472:PRO:CD	2.84	0.40
1:D:3165:ARG:NE	1:D:3165:ARG:O	2.54	0.40
1:B:1447:SER:HB3	1:B:1448:PRO:HD2	2.03	0.40
1:C:2143:VAL:HB	1:C:2237:GLU:HG2	2.04	0.40
1:C:2057:LYS:HE2	1:C:2059:GLU:HG2	2.03	0.40
1:A:219:MSE:O	1:B:1056:PRO:HD2	2.22	0.40
1:B:1140:ARG:NH2	1:B:1233:ASP:OD2	2.55	0.40
1:D:3296:LYS:HE2	1:D:3296:LYS:HB2	1.89	0.40
1:B:1150:TRP:HA	1:B:1151:PRO:HD3	1.89	0.40
1:C:2108:MSE:N	1:C:2109:PRO:CD	2.85	0.40
1:A:295:GLN:OE1	1:A:295:GLN:HA	2.22	0.40
1:D:3461:THR:HG21	1:D:3511:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	39	42
1	B	551/564 (98%)	522 (95%)	26 (5%)	3 (0%)	34	35
1	C	551/564 (98%)	530 (96%)	17 (3%)	4 (1%)	26	25
1	D	551/564 (98%)	528 (96%)	20 (4%)	3 (0%)	34	35
All	All	2204/2256 (98%)	2110 (96%)	82 (4%)	12 (0%)	34	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1332	LEU
1	C	2332	LEU
1	A	397	ARG

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Mol	Chain	Res	Type
1	C	2392	VAL
1	D	3302	ILE
1	C	2397	ARG
1	B	1392	VAL
1	D	3103	ASP
1	A	270	ARG
1	D	3392	VAL
1	C	2056	PRO
1	B	1369	ALA

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	469/465 (101%)	406 (87%)	63 (13%)	5 4
1	B	469/465 (101%)	412 (88%)	57 (12%)	6 5
1	C	469/465 (101%)	409 (87%)	60 (13%)	5 4
1	D	469/465 (101%)	410 (87%)	59 (13%)	5 4
All	All	1876/1860 (101%)	1637 (87%)	239 (13%)	5 4

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

Mol	Chain	Res	Type
1	A	22	LYS
1	A	23	GLU
1	A	24	LYS
1	A	43	GLN
1	A	70	ARG
1	A	76	THR
1	A	85	ILE
1	A	99	ILE
1	A	100	LEU
1	A	101	GLN
1	A	111	VAL
1	A	121	SER

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Mol	Chain	Res	Type
1	A	123	TYR
1	A	133	LEU
1	A	140	ARG
1	A	145	SER
1	A	153	ASN
1	A	165	ARG
1	A	169	LEU
1	A	196	ASP
1	A	197	ARG
1	A	221	LEU
1	A	227	ARG
1	A	232	ASP
1	A	248	ARG
1	A	251	LEU
1	A	272	LYS
1	A	286	VAL
1	A	291	LEU
1	A	292	LEU
1	A	296	LYS
1	A	299	SER
1	A	300	LYS
1	A	302	ILE
1	A	322	LEU
1	A	327	MSE
1	A	329	GLU
1	A	335	GLN
1	A	339	LYS
1	A	340	LYS
1	A	346	LYS
1	A	350	LEU
1	A	355	LYS
1	A	357	LYS
1	A	384	LEU
1	A	385	LYS
1	A	389	ILE
1	A	398	LEU
1	A	407	MSE
1	A	489	SER
1	A	492	LEU
1	A	499	THR
1	A	502	LEU
1	A	504	ASP

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Mol	Chain	Res	Type
1	A	505	GLU
1	A	520	GLN
1	A	529	LYS
1	A	539	MSE
1	A	554	LYS
1	A	556	ARG
1	A	559	ARG
1	A	561	GLU
1	A	571	GLU
1	B	1022	LYS
1	B	1024	LYS
1	B	1070	ARG
1	B	1073	LYS
1	B	1074	LYS
1	B	1085	ILE
1	B	1099	ILE
1	B	1100	LEU
1	B	1111	VAL
1	B	1123	TYR
1	B	1131	LYS
1	B	1133	LEU
1	B	1140	ARG
1	B	1153	ASN
1	B	1165	ARG
1	B	1214	LYS
1	B	1225	ARG
1	B	1232	ASP
1	B	1233	ASP
1	B	1236	ASP
1	B	1243	THR
1	B	1248	ARG
1	B	1251	LEU
1	B	1286	VAL
1	B	1291	LEU
1	B	1292	LEU
1	B	1296	LYS
1	B	1300	LYS
1	B	1304	GLU
1	B	1306	LYS
1	B	1332	LEU
1	B	1346	LYS
1	B	1350	LEU

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Mol	Chain	Res	Type
1	B	1357	LYS
1	B	1359	ASP
1	B	1363	GLU
1	B	1372	SER
1	B	1373	ILE
1	B	1384	LEU
1	B	1389	ILE
1	B	1402	ASP
1	B	1436	LEU
1	B	1455	THR
1	B	1492	LEU
1	B	1499	THR
1	B	1502	LEU
1	B	1504	ASP
1	B	1505	GLU
1	B	1507	LEU
1	B	1519	ILE
1	B	1520	GLN
1	B	1531	THR
1	B	1547	GLU
1	B	1549	LYS
1	B	1557	THR
1	B	1561	GLU
1	B	1572	TRP
1	C	2021	ILE
1	C	2022	LYS
1	C	2023	GLU
1	C	2043	GLN
1	C	2062	ASP
1	C	2066	LEU
1	C	2070	ARG
1	C	2085	ILE
1	C	2086	MSE
1	C	2094	LYS
1	C	2100	LEU
1	C	2104	ILE
1	C	2111	VAL
1	C	2122	GLN
1	C	2123	TYR
1	C	2133	LEU
1	C	2140	ARG
1	C	2165	ARG

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Mol	Chain	Res	Type
1	C	2169	LEU
1	C	2221	LEU
1	C	2223	GLN
1	C	2224	LYS
1	C	2225	ARG
1	C	2232	ASP
1	C	2236	ASP
1	C	2251	LEU
1	C	2286	VAL
1	C	2291	LEU
1	C	2292	LEU
1	C	2300	LYS
1	C	2306	LYS
1	C	2330	ASN
1	C	2333	SER
1	C	2339	LYS
1	C	2346	LYS
1	C	2350	LEU
1	C	2355	LYS
1	C	2363	GLU
1	C	2375	ASP
1	C	2378	GLU
1	C	2385	LYS
1	C	2392	VAL
1	C	2398	LEU
1	C	2436	LEU
1	C	2438	GLU
1	C	2453	LYS
1	C	2454	LEU
1	C	2455	THR
1	C	2492	LEU
1	C	2500	SER
1	C	2502	LEU
1	C	2507	LEU
1	C	2520	GLN
1	C	2531	THR
1	C	2547	GLU
1	C	2554	LYS
1	C	2556	ARG
1	C	2559	ARG
1	C	2561	GLU
1	C	2563	ASP

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Mol	Chain	Res	Type
1	D	3022	LYS
1	D	3043	GLN
1	D	3066	LEU
1	D	3070	ARG
1	D	3076	THR
1	D	3085	ILE
1	D	3099	ILE
1	D	3100	LEU
1	D	3111	VAL
1	D	3123	TYR
1	D	3133	LEU
1	D	3140	ARG
1	D	3153	ASN
1	D	3165	ARG
1	D	3169	LEU
1	D	3205	VAL
1	D	3221	LEU
1	D	3224	LYS
1	D	3229	GLN
1	D	3232	ASP
1	D	3245	ARG
1	D	3248	ARG
1	D	3251	LEU
1	D	3266	LEU
1	D	3272	LYS
1	D	3286	VAL
1	D	3291	LEU
1	D	3292	LEU
1	D	3296	LYS
1	D	3297	VAL
1	D	3300	LYS
1	D	3306	LYS
1	D	3322	LEU
1	D	3329	GLU
1	D	3333	SER
1	D	3339	LYS
1	D	3346	LYS
1	D	3350	LEU
1	D	3352	LYS
1	D	3355	LYS
1	D	3358	ILE
1	D	3363	GLU

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Mol	Chain	Res	Type
1	D	3371	GLU
1	D	3384	LEU
1	D	3397	ARG
1	D	3412	GLU
1	D	3425	GLN
1	D	3489	SER
1	D	3492	LEU
1	D	3502	LEU
1	D	3507	LEU
1	D	3518	ASN
1	D	3520	GLN
1	D	3529	LYS
1	D	3531	THR
1	D	3538	LYS
1	D	3547	GLU
1	D	3559	ARG
1	D	3571	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	69	HIS
1	A	125	HIS
1	A	153	ASN
1	A	261	ASN
1	A	305	HIS
1	A	330	ASN
1	A	411	ASN
1	A	482	ASN
1	A	485	HIS
1	A	520	GLN
1	B	1043	GLN
1	B	1051	GLN
1	B	1064	GLN
1	B	1069	HIS
1	B	1154	HIS
1	B	1229	GLN
1	B	1261	ASN
1	B	1425	GLN
1	B	1518	ASN
1	B	1520	GLN

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Mol	Chain	Res	Type
1	C	2051	GLN
1	C	2064	GLN
1	C	2069	HIS
1	C	2154	HIS
1	C	2229	GLN
1	C	2261	ASN
1	C	2425	GLN
1	C	2520	GLN
1	D	3051	GLN
1	D	3064	GLN
1	D	3069	HIS
1	D	3125	HIS
1	D	3153	ASN
1	D	3230	GLN
1	D	3261	ASN
1	D	3482	ASN
1	D	3485	HIS
1	D	3518	ASN
1	D	3520	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
4	NAD	A	601	-	38,48,48	1.77	9 (23%)	47,73,73	1.96	5 (10%)
4	NAD	A	602	-	38,48,48	1.89	11 (28%)	47,73,73	1.92	4 (8%)
2	OXL	A	603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	B	1601	-	38,48,48	1.70	10 (26%)	47,73,73	2.00	6 (12%)
4	NAD	B	1602	-	38,48,48	2.02	10 (26%)	47,73,73	1.98	5 (10%)
2	OXL	B	1603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	C	2601	-	38,48,48	1.56	6 (15%)	47,73,73	1.97	6 (12%)
4	NAD	C	2602	-	38,48,48	2.26	10 (26%)	47,73,73	2.04	6 (12%)
2	OXL	C	2603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	D	3601	-	38,48,48	1.83	9 (23%)	47,73,73	1.99	6 (12%)
4	NAD	D	3602	-	38,48,48	1.92	8 (21%)	47,73,73	1.97	5 (10%)
2	OXL	D	3603	3	0,5,5	0.00	-	0,6,6	0.00	-

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
4	NAD	A	601	-	-	0/22/62/62	0/5/5/5
4	NAD	A	602	-	-	0/22/62/62	0/5/5/5
2	OXL	A	603	3	-	0/0/4/4	0/0/0/0
4	NAD	B	1601	-	-	0/22/62/62	0/5/5/5
4	NAD	B	1602	-	-	0/22/62/62	0/5/5/5
2	OXL	B	1603	3	-	0/0/4/4	0/0/0/0
4	NAD	C	2601	-	-	0/22/62/62	0/5/5/5
4	NAD	C	2602	-	-	0/22/62/62	0/5/5/5
2	OXL	C	2603	3	-	0/0/4/4	0/0/0/0
4	NAD	D	3601	-	-	0/22/62/62	0/5/5/5
4	NAD	D	3602	-	-	0/22/62/62	0/5/5/5
2	OXL	D	3603	3	-	0/0/4/4	0/0/0/0

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAD	C5A-C4A	-3.30	1.33	1.40
4	D	3601	NAD	C5A-C4A	-3.17	1.33	1.40
4	A	601	NAD	C5A-C4A	-3.16	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3602	NAD	C5A-C4A	-2.97	1.33	1.40
4	B	1601	NAD	C5A-C4A	-2.90	1.33	1.40
4	A	602	NAD	C5A-C4A	-2.89	1.34	1.40
4	C	2602	NAD	C5A-C4A	-2.87	1.34	1.40
4	B	1602	NAD	C5A-C4A	-2.76	1.34	1.40
4	B	1601	NAD	C5A-N7A	-2.53	1.30	1.39
4	A	602	NAD	C5A-N7A	-2.43	1.31	1.39
4	D	3602	NAD	C5A-N7A	-2.38	1.31	1.39
4	A	601	NAD	C5A-N7A	-2.34	1.31	1.39
4	D	3601	NAD	C5A-N7A	-2.31	1.31	1.39
4	C	2602	NAD	C5A-N7A	-2.27	1.31	1.39
4	C	2601	NAD	C5A-N7A	-2.21	1.31	1.39
4	B	1602	NAD	C5A-N7A	-2.12	1.32	1.39
4	B	1601	NAD	C2A-N1A	2.01	1.37	1.33
4	A	602	NAD	C2A-N1A	2.02	1.37	1.33
4	D	3601	NAD	C2A-N1A	2.03	1.37	1.33
4	B	1601	NAD	C4N-C3N	2.07	1.42	1.39
4	C	2602	NAD	O3B-C3B	2.09	1.48	1.43
4	B	1601	NAD	O4D-C4D	2.09	1.49	1.45
4	B	1602	NAD	O4D-C4D	2.11	1.49	1.45
4	A	602	NAD	C4N-C3N	2.12	1.42	1.39
4	A	602	NAD	C2N-C3N	2.14	1.42	1.39
4	B	1602	NAD	C2A-N1A	2.15	1.38	1.33
4	A	601	NAD	C2A-N1A	2.16	1.38	1.33
4	C	2602	NAD	C2N-C3N	2.20	1.42	1.39
4	C	2602	NAD	C5N-C4N	2.21	1.43	1.38
4	C	2601	NAD	C3N-C7N	2.22	1.54	1.50
4	A	602	NAD	O4D-C4D	2.33	1.50	1.45
4	D	3601	NAD	C4N-C3N	2.35	1.43	1.39
4	B	1601	NAD	C3N-C7N	2.39	1.54	1.50
4	B	1602	NAD	C3N-C7N	2.42	1.54	1.50
4	B	1602	NAD	C4N-C3N	2.70	1.43	1.39
4	A	601	NAD	C4N-C3N	2.74	1.44	1.39
4	D	3602	NAD	O4D-C4D	2.83	1.51	1.45
4	D	3602	NAD	C2A-N3A	2.86	1.37	1.32
4	D	3602	NAD	C4N-C3N	2.86	1.44	1.39
4	B	1601	NAD	C2A-N3A	2.89	1.37	1.32
4	A	601	NAD	C3N-C7N	2.95	1.55	1.50
4	B	1602	NAD	C6N-N1N	3.01	1.43	1.35
4	A	602	NAD	C2A-N3A	3.11	1.37	1.32
4	B	1601	NAD	O4D-C1D	3.11	1.45	1.41
4	B	1602	NAD	C2A-N3A	3.16	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2601	NAD	C2A-N3A	3.23	1.37	1.32
4	A	601	NAD	O4D-C1D	3.28	1.45	1.41
4	A	602	NAD	C3N-C7N	3.29	1.55	1.50
4	D	3602	NAD	O4B-C1B	3.32	1.45	1.41
4	D	3601	NAD	C2A-N3A	3.37	1.38	1.32
4	A	601	NAD	C2A-N3A	3.40	1.38	1.32
4	C	2602	NAD	C2A-N3A	3.44	1.38	1.32
4	A	601	NAD	C6N-N1N	3.45	1.44	1.35
4	D	3601	NAD	C6N-N1N	3.45	1.44	1.35
4	D	3602	NAD	C6N-N1N	3.47	1.44	1.35
4	C	2601	NAD	C6N-N1N	3.47	1.44	1.35
4	D	3601	NAD	C3N-C7N	3.50	1.56	1.50
4	A	602	NAD	C6N-N1N	3.53	1.44	1.35
4	C	2601	NAD	O4B-C1B	3.67	1.45	1.41
4	B	1601	NAD	C6N-N1N	3.68	1.45	1.35
4	D	3601	NAD	O4D-C1D	3.90	1.46	1.41
4	C	2602	NAD	C4N-C3N	4.08	1.46	1.39
4	A	602	NAD	O4B-C1B	4.11	1.46	1.41
4	B	1601	NAD	O4B-C1B	4.15	1.46	1.41
4	B	1602	NAD	O4B-C1B	4.31	1.46	1.41
4	A	601	NAD	O4B-C1B	4.76	1.47	1.41
4	D	3601	NAD	O4B-C1B	5.02	1.47	1.41
4	C	2602	NAD	C6N-N1N	5.57	1.50	1.35
4	C	2602	NAD	O4B-C1B	5.65	1.48	1.41
4	A	602	NAD	O4D-C1D	5.81	1.48	1.41
4	D	3602	NAD	O4D-C1D	6.83	1.49	1.41
4	C	2602	NAD	O4D-C1D	7.11	1.50	1.41
4	B	1602	NAD	O4D-C1D	7.80	1.51	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3602	NAD	N3A-C2A-N1A	-10.70	120.70	128.89
4	A	601	NAD	N3A-C2A-N1A	-10.62	120.76	128.89
4	B	1601	NAD	N3A-C2A-N1A	-10.61	120.77	128.89
4	C	2601	NAD	N3A-C2A-N1A	-10.59	120.79	128.89
4	B	1602	NAD	N3A-C2A-N1A	-10.53	120.83	128.89
4	D	3601	NAD	N3A-C2A-N1A	-10.47	120.88	128.89
4	A	602	NAD	N3A-C2A-N1A	-10.26	121.04	128.89
4	C	2602	NAD	N3A-C2A-N1A	-10.18	121.10	128.89
4	D	3601	NAD	C4B-O4B-C1B	-2.94	106.49	109.72
4	C	2601	NAD	C4B-O4B-C1B	-2.92	106.50	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2602	NAD	C3N-C7N-N7N	-2.81	114.74	117.82
4	D	3601	NAD	C4D-O4D-C1D	-2.39	107.10	109.72
4	B	1601	NAD	C3N-C7N-N7N	-2.38	115.21	117.82
4	B	1601	NAD	C4D-O4D-C1D	-2.26	107.23	109.72
4	A	601	NAD	C4D-O4D-C1D	-2.22	107.28	109.72
4	D	3602	NAD	C3N-C7N-N7N	-2.18	115.43	117.82
4	C	2601	NAD	C3N-C7N-N7N	-2.16	115.45	117.82
4	B	1602	NAD	C3N-C7N-N7N	-2.10	115.51	117.82
4	C	2602	NAD	C3N-C2N-N1N	-2.07	117.98	120.36
4	A	601	NAD	O4B-C1B-N9A	2.05	112.39	108.10
4	D	3602	NAD	C2D-C3D-C4D	2.13	107.00	102.61
4	A	602	NAD	C2D-C3D-C4D	2.16	107.05	102.61
4	C	2601	NAD	O4B-C1B-N9A	2.28	112.88	108.10
4	D	3601	NAD	O4B-C1B-N9A	2.31	112.94	108.10
4	B	1602	NAD	C2D-C3D-C4D	2.34	107.41	102.61
4	B	1601	NAD	O4B-C1B-N9A	2.34	113.00	108.10
4	C	2602	NAD	C2D-C3D-C4D	2.40	107.54	102.61
4	C	2601	NAD	O4D-C1D-N1N	2.95	111.37	108.13
4	D	3602	NAD	O4D-C1D-N1N	3.33	111.79	108.13
4	B	1601	NAD	O4D-C1D-N1N	3.37	111.83	108.13
4	A	601	NAD	O4D-C1D-N1N	3.42	111.89	108.13
4	A	602	NAD	O4D-C1D-N1N	3.44	111.91	108.13
4	D	3601	NAD	O4D-C1D-N1N	3.66	112.15	108.13
4	C	2602	NAD	C4A-C5A-N7A	4.24	113.38	109.48
4	D	3601	NAD	C4A-C5A-N7A	4.24	113.38	109.48
4	A	601	NAD	C4A-C5A-N7A	4.40	113.53	109.48
4	C	2601	NAD	C4A-C5A-N7A	4.41	113.53	109.48
4	B	1602	NAD	O4D-C1D-N1N	4.42	112.99	108.13
4	B	1602	NAD	C4A-C5A-N7A	4.46	113.59	109.48
4	D	3602	NAD	C4A-C5A-N7A	4.55	113.67	109.48
4	A	602	NAD	C4A-C5A-N7A	4.61	113.72	109.48
4	B	1601	NAD	C4A-C5A-N7A	4.78	113.88	109.48
4	C	2602	NAD	O4D-C1D-N1N	5.14	113.78	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1601	NAD	3	0
4	C	2601	NAD	1	0
4	C	2602	NAD	1	0
4	D	3602	NAD	1	0
2	D	3603	OXL	1	0

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.