Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:27 PM EDT

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

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

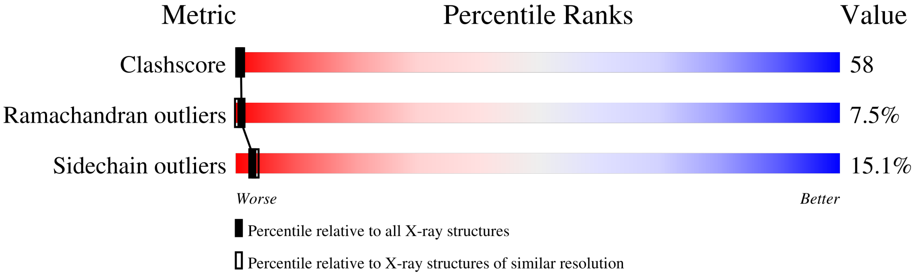
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 Å.

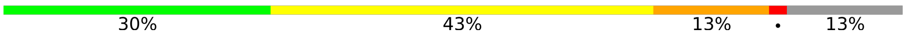
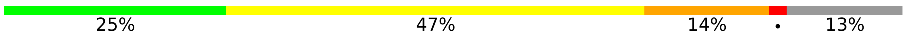
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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

Note EDS was not executed.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	610	-	-	X	-

2 Entry composition

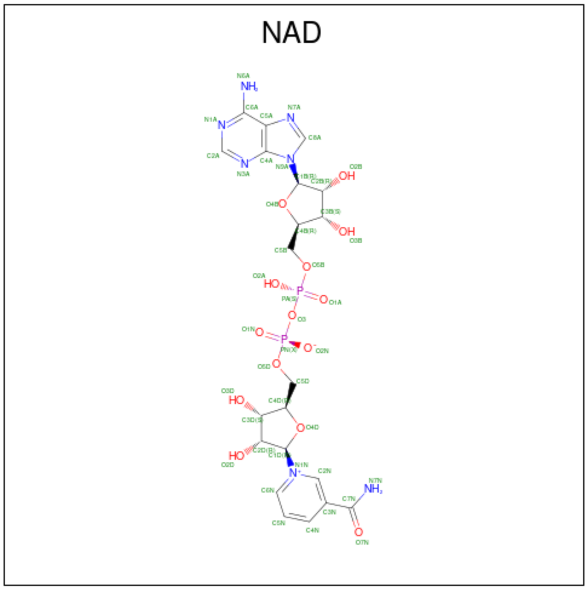
There are 3 unique types of molecules in this entry. The entry contains 7971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 myo-inositol-1-phosphate synthase.

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	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

- Molecule 3 is water.

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

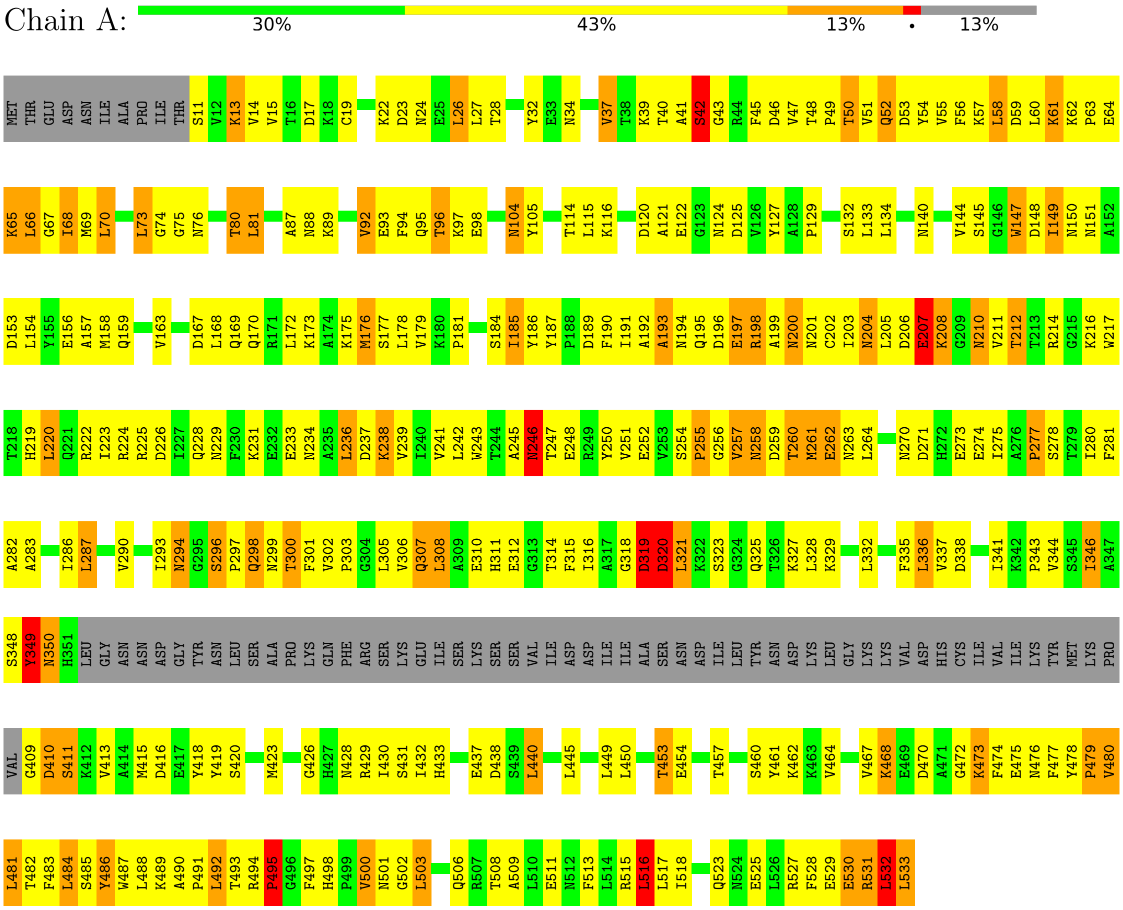
3 Residue-property plots

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.

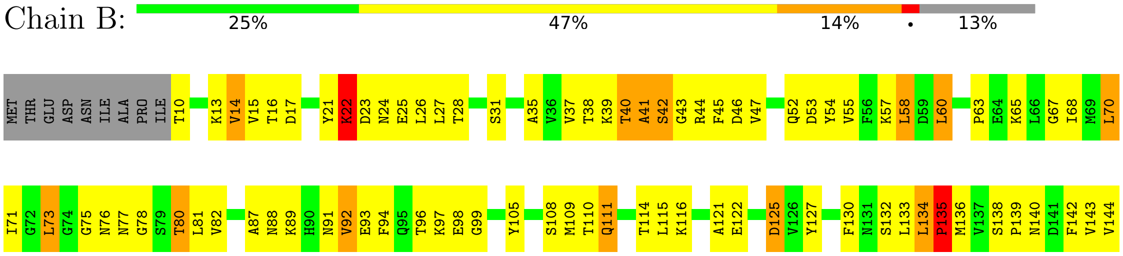
- Molecule 1: myo-inositol-1-phosphate synthase

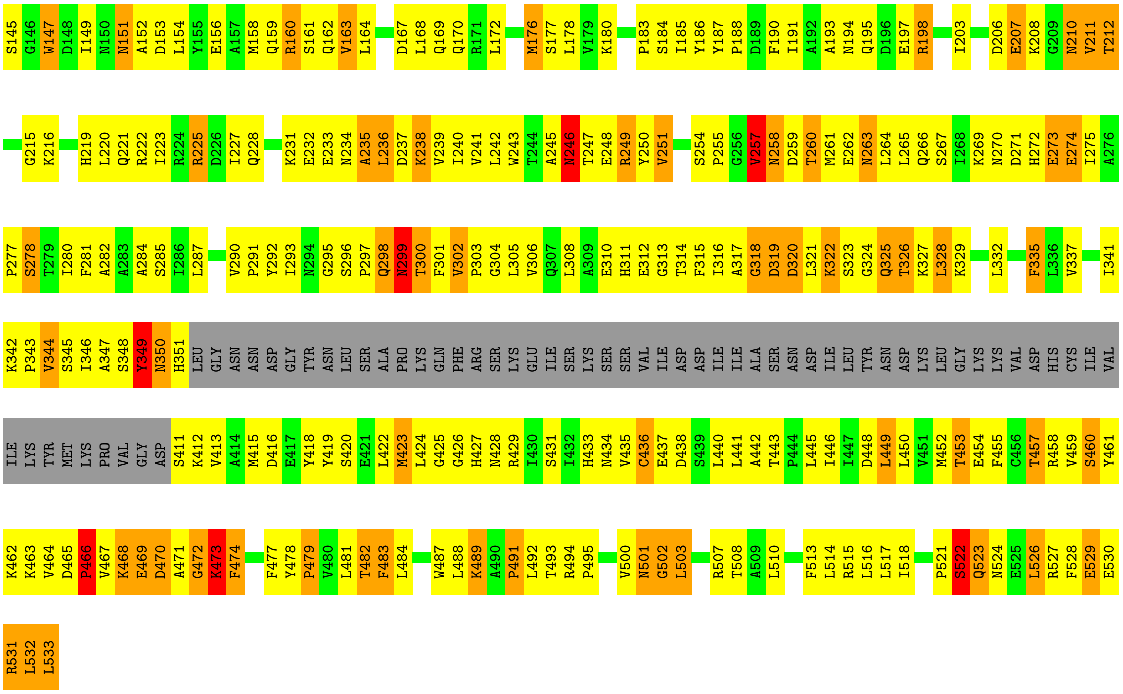
Chain A:



- Molecule 1: myo-inositol-1-phosphate synthase

Chain B:




S145
G146
W147
D148
I149
N150
N151
A152
D153
L154
Y155
E156
A157
M158
Q159
R160
S161
Q162
V163
L164
D167
L168
Q169
Q170
R171
L172
M176
S177
L178
V179
K180
P183
S184
I185
Y186
Y187
P188
D189
F190
I191
A192
A193
N194
Q195
D196
E197
R198
I203
D206
E207
K208
G209
N210
V211
T212
G215
K216
H219
L220
Q221
R222
I223
R224
R225
D226
I227
Q228
K231
E232
E233
N234
A235
L236
D237
K238
V239
I240
V241
L242
W243
T244
A245
N246
T247
E248
R249
Y250
V251
S254
P255
G256
V257
N258
D259
T260
M261
E262
N263
L264
L265
Q266
S267
I268
K269
N270
D271
H272
E273
E274
I275
A276
P277
S278
T279
I280
F281
A282
A283
A284
S285
I286
L287
V290
P291
Y292
I293
N294
G295
S296
P297
Q298
N299
T300
F301
V302
P303
G304
L305
V306
Q307
L308
A309
E310
H311
E312
G313
T314
F315
I316
A317
G318
D319
D320
L321
K322
S323
G324
Q325
T326
K327
L328
K329
L332
F335
L336
V337
I341
K342
P343
V344
S345
I346
A347
S348
Y349
N350
H351
LEU
GLY
ASN
ASN
ASP
GLY
TYR
ASN
LEU
SER
ALA
PRO
LYS
GLN
PHE
ARG
SER
LYS
GLU
ILE
SER
LYS
SER
SER
VAL
ILE
ASP
ASP
ILE
ILE
ALA
SER
ASN
ASP
ILE
LEU
TYR
ASN
ASP
LYS
LEU
GLY
LYS
LYS
VAL
ASP
HIS
CYS
ILE
VAL
ILE
LYS
TYR
MET
LYS
PRO
VAL
GLY
ASP
S411
K412
V413
A414
M415
D416
E417
Y418
Y419
S420
E421
L422
M423
L424
G425
G426
H427
N428
R429
I430
S431
I432
H433
N434
V435
C436
E437
D438
S439
L440
L441
A442
T443
P444
L445
I446
I447
D448
L449
L450
V451
M452
T453
E454
F455
C456
T457
R458
V459
S460
Y461
K462
K463
V464
D465
P466
V467
K468
E469
D470
A471
G472
K473
F474
F477
Y478
P479
V480
L481
T482
F483
L484
W487
L488
K489
A490
P491
L492
T493
R494
P495
V500
N501
G502
L503
R507
T508
A509
L510
F513
L514
R515
L516
L517
I518
P521
S522
Q523
N524
E525
L526
R527
F528
E529
E530
R531
L532
L533

4 Data and refinement statistics ⓘ

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

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

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

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

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

All (1) bond length outliers are listed below:

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

All (5) bond angle outliers are listed below:

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

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

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

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 58.

All (864) 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:149:ILE:HD11	1:B:195:GLN:HE21	1.04	1.13
1:B:293:ILE:HD11	1:B:453:THR:HG21	1.28	1.12
1:B:315:PHE:HB3	1:B:481:LEU:HD11	1.30	1.12
1:B:70:LEU:HD21	1:B:81:LEU:HD23	1.33	1.08
1:A:533:LEU:HG	1:B:494:ARG:HH22	0.92	1.08
1:A:76:ASN:O	1:A:80:THR:HG22	1.53	1.07
1:B:77:ASN:HD21	2:B:610:NAD:H6N	1.16	1.06
1:B:116:LYS:HE3	1:B:125:ASP:HB3	1.38	1.05
1:A:461:TYR:OH	1:B:533:LEU:HB2	1.53	1.04
1:B:77:ASN:ND2	2:B:610:NAD:H6N	1.70	1.04
1:A:454:GLU:O	1:A:457:THR:HG22	1.58	1.04
1:B:149:ILE:HD11	1:B:195:GLN:NE2	1.72	1.03
1:A:207:GLU:OE1	1:A:207:GLU:HA	1.57	1.02
1:A:96:THR:HG22	1:A:98:GLU:H	1.20	1.02
1:B:22:LYS:HG3	1:B:23:ASP:H	1.20	1.01
1:A:297:PRO:HB3	1:A:320:ASP:OD2	1.60	1.00

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:HE3	1:A:454:GLU:OE2	1.80	0.82
1:A:492:LEU:HD23	1:A:493:THR:N	1.94	0.81
1:B:75:GLY:HA3	2:B:610:NAD:H4B	1.62	0.81
1:B:351:HIS:HB3	1:B:413:VAL:N	1.96	0.81
1:B:76:ASN:O	1:B:80:THR:HG22	1.80	0.81
1:A:321:LEU:HD23	1:A:445:LEU:HD22	1.63	0.81
1:A:14:VAL:HG11	1:A:518:ILE:O	1.78	0.81
1:B:163:VAL:HG22	1:B:164:LEU:HD22	1.62	0.81
1:B:349:TYR:CG	1:B:415:MET:HB2	2.16	0.81
1:A:297:PRO:HD3	1:A:320:ASP:OD1	1.81	0.80
1:B:194:ASN:ND2	1:B:247:THR:HG23	1.97	0.80
1:A:258:ASN:HD22	1:A:258:ASN:H	1.30	0.80
1:B:96:THR:HA	3:B:640:HOH:O	1.81	0.80
1:B:295:GLY:O	1:B:321:LEU:HD22	1.80	0.80
1:B:427:HIS:HE1	3:B:647:HOH:O	1.63	0.80
1:A:87:ALA:HA	1:A:92:VAL:CG1	2.12	0.79
1:A:449:LEU:O	1:A:453:THR:HG23	1.80	0.79
1:A:260:THR:HG22	1:A:307:GLN:NE2	1.97	0.79
1:A:461:TYR:HH	1:B:533:LEU:HB2	1.45	0.79
1:B:134:LEU:HD21	1:B:518:ILE:HG23	1.64	0.79
1:B:322:LYS:HE2	3:B:815:HOH:O	1.81	0.78
1:B:273:GLU:O	1:B:275:ILE:N	2.16	0.78
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.19	0.78
1:B:468:LYS:NZ	3:B:828:HOH:O	2.17	0.77
1:A:415:MET:CE	1:A:431:SER:HB2	2.15	0.77
1:A:96:THR:HG22	1:A:98:GLU:N	1.99	0.76
1:A:163:VAL:HG22	1:A:410:ASP:CG	2.04	0.76
1:B:257:VAL:O	1:B:258:ASN:ND2	2.18	0.76
1:B:318:GLY:O	1:B:488:LEU:HD23	1.85	0.76
1:B:183:PRO:O	3:B:612:HOH:O	2.03	0.76
1:B:250:TYR:CE2	1:B:298:GLN:HA	2.20	0.76
1:A:64:GLU:O	1:A:65:LYS:HD2	1.86	0.76
1:A:225:ARG:HE	1:A:229:ASN:HD21	1.33	0.76
1:A:349:TYR:CG	1:A:415:MET:HB3	2.21	0.76
1:B:263:ASN:H	1:B:263:ASN:ND2	1.83	0.76
1:A:191:ILE:HD11	1:A:195:GLN:HE21	1.50	0.75
1:B:39:LYS:HB2	1:B:45:PHE:CD2	2.21	0.75
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.66	0.75
1:B:492:LEU:HD13	1:B:493:THR:N	2.01	0.75
1:A:159:GLN:HA	1:A:169:GLN:HE22	1.50	0.75
1:A:411:SER:N	1:A:437:GLU:HA	2.02	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PHE:HE2	1:B:452:MET:HE3	1.52	0.75
1:B:293:ILE:CD1	1:B:453:THR:HG21	2.15	0.75
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.69	0.75
1:A:433:HIS:HB3	1:B:431:SER:HB2	1.68	0.75
1:B:240:ILE:HG12	1:B:291:PRO:HG2	1.69	0.74
1:A:246:ASN:C	1:A:246:ASN:HD22	1.90	0.74
1:A:328:LEU:HD11	1:B:332:LEU:CD2	2.17	0.74
1:B:13:LYS:HZ3	1:B:21:TYR:HE2	1.36	0.74
1:B:310:GLU:HA	1:B:479:PRO:HG3	1.69	0.74
1:A:50:THR:HG22	3:A:611:HOH:O	1.86	0.74
1:A:62:LYS:O	1:A:62:LYS:HG2	1.87	0.74
1:B:194:ASN:HB3	1:B:246:ASN:HA	1.69	0.74
1:A:528:PHE:CD1	1:A:532:LEU:HD11	2.22	0.74
1:B:13:LYS:NZ	1:B:21:TYR:HE2	1.85	0.74
1:A:63:PRO:HG3	3:A:746:HOH:O	1.88	0.74
1:A:323:SER:HA	2:A:600:NAD:H72N	1.49	0.74
1:B:134:LEU:HB3	1:B:135:PRO:CD	2.17	0.73
1:A:200:ASN:C	1:A:200:ASN:HD22	1.91	0.73
1:B:472:GLY:O	1:B:473:LYS:HB2	1.87	0.73
1:B:297:PRO:O	1:B:298:GLN:HB3	1.88	0.73
1:A:57:LYS:O	3:A:666:HOH:O	2.06	0.73
1:B:38:THR:O	1:B:38:THR:HG23	1.88	0.72
1:B:245:ALA:O	2:B:610:NAD:O3D	2.05	0.72
1:B:321:LEU:CD2	2:B:610:NAD:C3N	2.67	0.72
1:A:486:TYR:CE2	1:A:503:LEU:HG	2.24	0.72
1:B:206:ASP:HB3	1:B:212:THR:HG21	1.72	0.72
1:B:516:LEU:HD12	1:B:517:LEU:N	2.04	0.72
1:A:440:LEU:HD23	1:B:426:GLY:HA3	1.70	0.72
3:A:649:HOH:O	1:B:500:VAL:HG11	1.89	0.72
1:B:470:ASP:O	1:B:472:GLY:N	2.23	0.72
1:B:282:ALA:CB	1:B:305:LEU:HD21	2.20	0.72
1:B:487:TRP:C	1:B:488:LEU:HD12	2.10	0.71
1:B:258:ASN:C	1:B:258:ASN:HD22	1.92	0.71
1:B:321:LEU:HD21	2:B:610:NAD:C6N	2.21	0.71
1:B:198:ARG:HD2	3:B:835:HOH:O	1.90	0.71
1:A:462:LYS:HE3	1:A:472:GLY:O	1.91	0.70
1:B:238:LYS:HG2	3:B:654:HOH:O	1.90	0.70
1:B:321:LEU:HD21	2:B:610:NAD:C3N	2.20	0.70
1:A:480:VAL:HG23	1:A:480:VAL:O	1.91	0.70
1:B:160:ARG:O	1:B:162:GLN:N	2.23	0.70
1:A:283:ALA:O	1:A:287:LEU:HD22	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLY:CA	2:B:610:NAD:O3B	2.40	0.70
1:A:70:LEU:HD21	1:A:81:LEU:HD12	1.72	0.70
1:A:298:GLN:HG3	1:A:300:THR:HG22	1.74	0.70
1:A:318:GLY:O	1:A:319:ASP:HB2	1.91	0.69
1:B:453:THR:HB	1:B:481:LEU:CD2	2.21	0.69
1:B:152:ALA:HB2	3:B:630:HOH:O	1.92	0.69
1:B:154:LEU:HB3	1:B:176:MET:HE2	1.73	0.69
1:B:243:TRP:HZ2	1:B:246:ASN:HD21	1.40	0.69
1:A:533:LEU:CB	1:B:494:ARG:HH12	2.06	0.69
1:B:260:THR:HG22	1:B:261:MET:H	1.57	0.69
1:B:320:ASP:OD2	1:B:321:LEU:N	2.25	0.69
1:B:349:TYR:HB2	1:B:415:MET:H	1.57	0.69
1:B:325:GLN:HE21	1:B:434:ASN:HD22	1.39	0.69
1:B:315:PHE:CE1	1:B:477:PHE:HB2	2.27	0.69
1:B:260:THR:CB	1:B:263:ASN:HD21	2.06	0.69
1:B:438:ASP:HB2	3:B:876:HOH:O	1.93	0.69
1:B:255:PRO:HA	1:B:259:ASP:OD1	1.93	0.68
1:A:234:ASN:CB	1:A:236:LEU:HD22	2.23	0.68
1:A:34:ASN:ND2	1:B:529:GLU:OE1	2.26	0.68
1:B:109:MET:HG3	1:B:507:ARG:HH12	1.59	0.68
1:B:163:VAL:CG2	1:B:164:LEU:HD22	2.23	0.68
1:B:299:ASN:HD22	1:B:299:ASN:N	1.91	0.68
1:B:321:LEU:HD23	2:B:610:NAD:C2N	2.21	0.68
1:A:533:LEU:HB2	1:B:494:ARG:NH1	2.07	0.68
1:A:191:ILE:HD13	1:A:195:GLN:CG	2.23	0.68
1:A:260:THR:HG22	1:A:307:GLN:HE22	1.55	0.68
1:B:500:VAL:HG13	1:B:501:ASN:N	2.07	0.68
1:B:121:ALA:HB3	1:B:122:GLU:OE1	1.94	0.68
1:B:134:LEU:HD12	1:B:517:LEU:HD23	1.75	0.68
1:B:261:MET:O	1:B:265:LEU:HD23	1.94	0.68
1:B:221:GLN:HG2	3:B:801:HOH:O	1.94	0.67
1:A:297:PRO:O	1:A:298:GLN:HB3	1.93	0.67
1:A:530:GLU:HG3	1:B:494:ARG:HE	1.59	0.67
1:A:415:MET:HE3	1:A:431:SER:HB2	1.75	0.67
1:B:75:GLY:HA2	2:B:610:NAD:O3B	1.94	0.67
1:A:185:ILE:HD13	1:A:187:TYR:CZ	2.29	0.67
1:B:273:GLU:C	1:B:275:ILE:H	1.98	0.67
1:A:55:VAL:HG23	1:A:464:VAL:CG2	2.25	0.66
1:A:219:HIS:O	1:A:223:ILE:HG12	1.94	0.66
1:A:203:ILE:HG13	1:A:204:ASN:N	2.10	0.66
1:A:461:TYR:HE1	3:A:808:HOH:O	1.79	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:C	1:A:185:ILE:HD12	2.16	0.66
1:A:257:VAL:HG21	1:A:274:GLU:OE2	1.96	0.66
1:B:282:ALA:HB1	1:B:305:LEU:HD21	1.78	0.66
1:A:214:ARG:HH11	1:A:214:ARG:HB2	1.61	0.66
1:A:239:VAL:O	1:A:290:VAL:HG23	1.95	0.66
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.77	0.66
1:A:440:LEU:CD2	1:B:426:GLY:HA3	2.26	0.66
1:A:420:SER:OG	3:A:729:HOH:O	2.13	0.66
1:B:210:ASN:HB3	3:B:857:HOH:O	1.95	0.66
1:B:193:ALA:O	1:B:194:ASN:HB2	1.96	0.66
1:B:473:LYS:HA	1:B:473:LYS:CE	2.23	0.66
1:A:428:ASN:HD22	1:B:436:CYS:HB3	1.61	0.65
1:B:87:ALA:HA	1:B:92:VAL:CG1	2.26	0.65
1:A:14:VAL:HB	1:B:47:VAL:HG13	1.77	0.65
1:B:134:LEU:CD1	1:B:517:LEU:HD23	2.27	0.65
1:B:315:PHE:CZ	1:B:477:PHE:HB2	2.31	0.65
1:A:250:TYR:CE1	1:A:298:GLN:HA	2.31	0.65
1:B:22:LYS:HG3	1:B:23:ASP:N	2.02	0.65
1:B:468:LYS:O	1:B:469:GLU:HB2	1.97	0.65
1:B:22:LYS:CG	1:B:23:ASP:N	2.56	0.65
1:B:442:ALA:CB	2:B:610:NAD:H5N	2.27	0.65
1:B:206:ASP:HB3	1:B:212:THR:CG2	2.26	0.65
1:A:61:LYS:O	1:A:61:LYS:HG2	1.96	0.65
1:A:258:ASN:HD22	1:A:258:ASN:N	1.93	0.65
1:B:429:ARG:HD3	3:B:786:HOH:O	1.97	0.65
1:A:211:VAL:O	1:A:212:THR:HG22	1.96	0.65
1:B:145:SER:HA	3:B:687:HOH:O	1.95	0.64
1:B:351:HIS:CB	1:B:413:VAL:H	2.06	0.64
1:B:515:ARG:CZ	1:B:523:GLN:HG3	2.27	0.64
1:A:206:ASP:O	1:A:208:LYS:N	2.30	0.64
1:B:65:LYS:HG3	3:B:679:HOH:O	1.97	0.64
1:B:245:ALA:O	2:B:610:NAD:C3D	2.46	0.64
1:A:64:GLU:C	1:A:65:LYS:HD2	2.17	0.64
1:B:21:TYR:CE1	1:B:26:LEU:HD13	2.33	0.64
1:B:346:ILE:HD12	1:B:346:ILE:N	2.11	0.64
1:A:70:LEU:HD21	1:A:81:LEU:CD1	2.28	0.64
1:B:149:ILE:CD1	1:B:195:GLN:HE21	1.97	0.64
1:A:190:PHE:HZ	1:A:273:GLU:O	1.81	0.63
1:A:462:LYS:CG	1:A:472:GLY:HA3	2.28	0.63
1:B:92:VAL:HG22	1:B:92:VAL:O	1.99	0.63
1:B:246:ASN:C	1:B:246:ASN:ND2	2.51	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:HG13	1:B:419:TYR:O	1.98	0.63
1:B:35:ALA:HB1	1:B:47:VAL:HG23	1.80	0.63
1:B:58:LEU:HD23	1:B:459:VAL:HG23	1.81	0.63
1:B:70:LEU:CD2	1:B:81:LEU:HD23	2.21	0.63
1:B:160:ARG:HD2	1:B:197:GLU:OE1	1.98	0.63
1:B:183:PRO:HG3	3:B:791:HOH:O	1.98	0.63
1:A:73:LEU:HD13	1:A:154:LEU:HD11	1.81	0.63
1:A:476:ASN:OD1	3:A:630:HOH:O	2.16	0.63
1:B:63:PRO:O	3:B:625:HOH:O	2.16	0.63
1:B:88:ASN:HB3	1:B:140:ASN:HD21	1.64	0.63
1:B:299:ASN:N	1:B:299:ASN:ND2	2.46	0.63
1:B:303:PRO:HG2	1:B:304:GLY:H	1.64	0.63
1:B:449:LEU:O	1:B:453:THR:CG2	2.46	0.63
1:A:462:LYS:HG3	1:A:472:GLY:HA3	1.81	0.63
1:B:297:PRO:O	1:B:298:GLN:CB	2.46	0.63
1:B:481:LEU:HB3	1:B:484:LEU:HD13	1.81	0.63
1:A:153:ASP:OD2	1:A:177:SER:HA	1.99	0.63
1:A:480:VAL:O	1:A:480:VAL:CG2	2.46	0.63
1:A:68:ILE:HG12	1:A:450:LEU:HD13	1.80	0.63
1:A:286:ILE:CG2	1:A:308:LEU:HD22	2.29	0.62
1:B:15:VAL:HG23	1:B:15:VAL:O	1.99	0.62
1:A:315:PHE:CE1	1:A:481:LEU:HD11	2.34	0.62
1:B:323:SER:OG	1:B:326:THR:HB	1.99	0.62
1:B:478:TYR:CE2	1:B:494:ARG:HB3	2.34	0.62
1:B:296:SER:OG	1:B:298:GLN:NE2	2.32	0.62
1:B:468:LYS:HE3	3:B:827:HOH:O	1.98	0.62
1:B:327:LYS:O	1:B:327:LYS:HG2	2.00	0.62
1:A:222:ARG:NH2	3:A:691:HOH:O	2.31	0.62
1:B:67:GLY:HA3	1:B:239:VAL:HG22	1.82	0.62
1:A:185:ILE:HD13	1:A:187:TYR:CE2	2.35	0.62
1:A:234:ASN:HB2	1:A:236:LEU:HD22	1.81	0.62
1:A:327:LYS:HG2	1:A:503:LEU:HD13	1.81	0.62
1:B:216:LYS:NZ	1:B:275:ILE:HB	2.15	0.62
1:A:320:ASP:O	1:A:488:LEU:HA	2.00	0.62
1:A:332:LEU:CD2	1:B:328:LEU:HD21	2.29	0.62
1:A:500:VAL:C	1:A:501:ASN:HD22	2.03	0.62
1:A:191:ILE:CD1	1:A:195:GLN:HE21	2.12	0.62
1:A:492:LEU:CD2	1:A:493:THR:N	2.63	0.61
1:A:346:ILE:HG22	1:A:346:ILE:O	2.00	0.61
1:B:130:PHE:HE2	1:B:452:MET:CE	2.12	0.61
1:B:263:ASN:H	1:B:263:ASN:HD22	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:O	1:B:306:VAL:HG23	2.00	0.61
1:B:477:PHE:HZ	1:B:513:PHE:CZ	2.18	0.61
1:B:194:ASN:HD22	1:B:247:THR:HG23	1.65	0.61
1:B:301:PHE:HE1	1:B:317:ALA:O	1.84	0.61
1:A:115:LEU:CD2	1:A:511:GLU:HG2	2.31	0.61
1:A:122:GLU:OE2	1:A:122:GLU:N	2.34	0.61
1:A:415:MET:HE1	1:A:431:SER:HB2	1.81	0.61
1:A:500:VAL:HG21	1:B:527:ARG:CZ	2.31	0.61
1:B:99:GLY:HA2	3:B:619:HOH:O	2.00	0.61
1:B:454:GLU:O	1:B:457:THR:HG22	2.01	0.61
1:A:210:ASN:N	1:A:210:ASN:ND2	2.47	0.61
1:A:212:THR:HG23	1:A:214:ARG:H	1.65	0.61
1:B:110:THR:HA	1:B:130:PHE:CD2	2.35	0.61
1:A:191:ILE:HG22	1:A:191:ILE:O	2.01	0.61
1:A:532:LEU:HB2	1:B:461:TYR:CZ	2.36	0.61
1:B:180:LYS:HB3	3:B:677:HOH:O	2.01	0.61
1:B:465:ASP:N	1:B:469:GLU:HA	2.10	0.61
1:A:286:ILE:HG21	1:A:308:LEU:HD22	1.84	0.60
1:A:328:LEU:HD11	1:B:332:LEU:HD22	1.82	0.60
1:B:93:GLU:N	3:B:620:HOH:O	2.35	0.60
1:B:349:TYR:CB	1:B:415:MET:H	2.13	0.60
1:B:527:ARG:H	1:B:531:ARG:HD2	1.66	0.60
1:A:200:ASN:HD22	1:A:201:ASN:N	2.00	0.60
1:A:205:LEU:HA	1:A:210:ASN:O	2.01	0.60
1:B:223:ILE:O	1:B:227:ILE:HG13	2.01	0.60
1:A:15:VAL:HA	3:A:773:HOH:O	2.00	0.60
1:A:17:ASP:O	3:A:713:HOH:O	2.16	0.60
1:B:52:GLN:HG3	1:B:54:TYR:CE1	2.37	0.60
1:A:92:VAL:HG22	1:A:92:VAL:O	2.01	0.60
1:B:248:GLU:OE1	1:B:278:SER:HB2	2.01	0.60
1:B:464:VAL:HG13	1:B:469:GLU:CG	2.26	0.60
1:A:214:ARG:NH1	1:A:214:ARG:CB	2.64	0.60
1:A:483:PHE:CE1	1:B:531:ARG:HD3	2.37	0.59
1:B:24:ASN:N	1:B:24:ASN:HD22	1.98	0.59
1:A:19:CYS:HB3	1:A:26:LEU:HD21	1.84	0.59
1:A:252:GLU:O	1:A:274:GLU:OE1	2.20	0.59
1:B:194:ASN:ND2	1:B:247:THR:CG2	2.64	0.59
1:B:325:GLN:NE2	1:B:434:ASN:ND2	2.51	0.59
1:B:462:LYS:HE3	1:B:472:GLY:HA2	1.84	0.59
1:B:228:GLN:O	1:B:232:GLU:HG3	2.02	0.59
1:B:481:LEU:HD12	1:B:481:LEU:H	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:HIS:O	1:B:223:ILE:HG12	2.00	0.59
1:B:321:LEU:HD23	2:B:610:NAD:C3N	2.32	0.59
1:B:449:LEU:O	1:B:453:THR:HG23	2.02	0.59
1:A:211:VAL:HG23	1:A:212:THR:N	2.14	0.59
1:A:76:ASN:O	1:A:80:THR:CG2	2.41	0.59
1:A:159:GLN:HA	1:A:169:GLN:NE2	2.17	0.59
1:B:87:ALA:HA	1:B:92:VAL:HG13	1.84	0.59
1:B:315:PHE:HE2	1:B:457:THR:HA	1.68	0.59
1:A:40:THR:O	1:A:42:SER:N	2.36	0.58
1:A:48:THR:HA	1:B:15:VAL:HG22	1.84	0.58
1:A:489:LYS:O	1:A:491:PRO:HD3	2.02	0.58
1:B:134:LEU:HB3	1:B:135:PRO:HD2	1.84	0.58
1:B:261:MET:HE2	1:B:308:LEU:HA	1.85	0.58
1:A:151:ASN:N	1:A:200:ASN:HD21	1.97	0.58
1:A:462:LYS:HD2	1:A:474:PHE:CE1	2.39	0.58
1:B:185:ILE:HG12	1:B:203:ILE:HD11	1.84	0.58
1:B:299:ASN:ND2	1:B:299:ASN:H	2.02	0.58
1:B:515:ARG:NH2	1:B:523:GLN:HG3	2.18	0.58
1:A:250:TYR:HA	1:A:299:ASN:OD1	2.03	0.58
1:A:297:PRO:O	1:A:298:GLN:CB	2.51	0.58
1:B:422:LEU:HB3	3:B:638:HOH:O	2.03	0.58
1:A:200:ASN:C	1:A:200:ASN:ND2	2.54	0.58
1:B:41:ALA:O	1:B:42:SER:HB3	2.04	0.58
1:B:423:MET:HG3	1:B:424:LEU:HG	1.84	0.58
1:A:415:MET:HA	1:A:432:ILE:O	2.04	0.57
1:A:52:GLN:OE1	1:A:53:ASP:O	2.21	0.57
1:A:234:ASN:HB3	1:A:236:LEU:HD22	1.86	0.57
1:A:172:LEU:HB3	1:A:176:MET:HE3	1.87	0.57
1:A:321:LEU:CD2	1:A:445:LEU:HD22	2.31	0.57
1:B:261:MET:O	1:B:261:MET:HG2	2.03	0.57
1:B:521:PRO:O	1:B:522:SER:CB	2.40	0.57
1:B:325:GLN:HE21	1:B:434:ASN:ND2	2.02	0.57
1:B:460:SER:HB2	1:B:474:PHE:HB3	1.85	0.57
1:A:349:TYR:CD2	1:A:415:MET:HB3	2.39	0.57
1:B:39:LYS:HD3	1:B:45:PHE:CE2	2.39	0.57
1:B:258:ASN:ND2	1:B:258:ASN:C	2.58	0.57
1:B:528:PHE:O	1:B:532:LEU:HB2	2.05	0.57
1:B:136:MET:HB3	3:B:615:HOH:O	2.04	0.57
1:B:149:ILE:CD1	1:B:195:GLN:NE2	2.59	0.57
1:B:528:PHE:CG	1:B:532:LEU:HD22	2.39	0.57
3:A:618:HOH:O	1:B:424:LEU:HA	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:311:HIS:C	1:B:313:GLY:H	2.08	0.57
1:A:14:VAL:HB	1:B:47:VAL:CG1	2.35	0.57
1:A:88:ASN:CB	1:A:140:ASN:HD21	2.18	0.57
1:A:203:ILE:CG1	1:A:204:ASN:N	2.67	0.57
1:B:130:PHE:CE2	1:B:452:MET:HE3	2.37	0.57
1:A:114:THR:O	1:A:115:LEU:HD23	2.05	0.56
1:A:430:ILE:HG12	1:B:434:ASN:OD1	2.05	0.56
1:A:293:ILE:HD11	1:A:453:THR:HG21	1.88	0.56
1:B:453:THR:HB	1:B:481:LEU:HD22	1.87	0.56
1:B:136:MET:HE1	1:B:452:MET:HE2	1.85	0.56
1:B:151:ASN:C	1:B:151:ASN:HD22	2.09	0.56
1:A:98:GLU:OE1	3:A:627:HOH:O	2.18	0.56
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.39	0.56
1:A:55:VAL:HG23	1:A:464:VAL:HG21	1.87	0.56
1:B:216:LYS:HZ2	1:B:275:ILE:HB	1.70	0.56
1:B:345:SER:C	1:B:346:ILE:HD12	2.26	0.56
1:B:266:GLN:O	1:B:270:ASN:OD1	2.23	0.56
1:A:11:SER:O	1:B:44:ARG:HA	2.05	0.56
1:B:136:MET:HE1	1:B:452:MET:CE	2.36	0.56
1:B:528:PHE:HB3	1:B:532:LEU:HD22	1.87	0.56
1:A:88:ASN:HB2	1:A:140:ASN:HD21	1.70	0.56
1:A:349:TYR:HB2	1:A:415:MET:O	2.06	0.56
1:B:136:MET:CE	1:B:452:MET:CE	2.84	0.56
1:A:121:ALA:HB3	1:A:122:GLU:OE2	2.05	0.55
1:A:214:ARG:CZ	1:A:214:ARG:HB3	2.37	0.55
1:A:341:ILE:N	1:A:341:ILE:HD12	2.21	0.55
1:B:249:ARG:HG3	1:B:249:ARG:O	2.06	0.55
1:B:257:VAL:HA	1:B:267:SER:OG	2.06	0.55
1:B:108:SER:OG	1:B:111:GLN:HB2	2.05	0.55
1:B:489:LYS:C	1:B:491:PRO:HD3	2.26	0.55
1:A:210:ASN:ND2	3:A:742:HOH:O	2.40	0.55
1:B:343:PRO:HA	1:B:420:SER:CB	2.36	0.55
1:A:40:THR:HG23	1:A:42:SER:HB3	1.88	0.55
1:A:144:VAL:HG12	1:A:145:SER:N	2.22	0.55
1:B:40:THR:O	1:B:41:ALA:C	2.44	0.55
1:B:282:ALA:HB3	1:B:305:LEU:HD21	1.89	0.55
1:B:301:PHE:CE1	1:B:317:ALA:O	2.60	0.55
1:A:298:GLN:HG3	1:A:300:THR:CG2	2.35	0.55
1:B:27:LEU:HD21	1:B:474:PHE:CZ	2.42	0.55
1:A:532:LEU:HB2	1:B:461:TYR:CE2	2.42	0.55
1:B:234:ASN:O	1:B:235:ALA:HB3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:318:GLY:C	1:B:488:LEU:HD23	2.26	0.54
1:A:56:PHE:CD2	1:A:516:LEU:HD21	2.41	0.54
1:A:134:LEU:HD21	1:A:518:ILE:HG22	1.89	0.54
1:B:160:ARG:HD3	3:B:675:HOH:O	2.06	0.54
1:B:206:ASP:C	1:B:208:LYS:H	2.10	0.54
1:B:250:TYR:CD1	1:B:299:ASN:ND2	2.74	0.54
1:B:116:LYS:HE3	1:B:125:ASP:CB	2.25	0.54
1:B:516:LEU:HD12	1:B:516:LEU:C	2.28	0.54
1:B:306:VAL:O	1:B:310:GLU:HG3	2.07	0.54
1:A:257:VAL:CG2	1:A:258:ASN:N	2.71	0.54
1:B:94:PHE:CB	1:B:168:LEU:HD23	2.35	0.54
1:B:245:ALA:O	2:B:610:NAD:H4D	2.08	0.54
1:B:464:VAL:O	1:B:466:PRO:HD3	2.07	0.54
1:A:184:SER:O	1:A:202:CYS:HA	2.07	0.54
1:B:58:LEU:HD13	1:B:60:LEU:HD12	1.89	0.54
1:A:14:VAL:CB	1:B:47:VAL:HG13	2.38	0.54
1:A:410:ASP:CG	1:A:437:GLU:HB3	2.28	0.54
1:B:311:HIS:O	1:B:312:GLU:HB2	2.08	0.54
1:B:473:LYS:HE2	1:B:473:LYS:CA	2.30	0.54
1:A:323:SER:CA	2:A:600:NAD:H72N	2.21	0.54
1:B:38:THR:O	1:B:38:THR:CG2	2.56	0.54
1:A:329:LYS:HD2	1:A:416:ASP:OD2	2.09	0.53
1:B:425:GLY:N	3:B:635:HOH:O	2.25	0.53
1:B:465:ASP:O	1:B:467:VAL:N	2.41	0.53
1:A:153:ASP:OD1	1:A:156:GLU:HG3	2.08	0.53
1:A:328:LEU:HD11	1:B:332:LEU:HD21	1.89	0.53
1:B:243:TRP:HZ2	1:B:246:ASN:ND2	2.06	0.53
1:B:274:GLU:HG2	3:B:664:HOH:O	2.08	0.53
1:B:349:TYR:HB2	1:B:415:MET:N	2.22	0.53
1:A:300:THR:HG21	3:A:602:HOH:O	2.09	0.53
1:A:516:LEU:C	1:A:516:LEU:HD23	2.28	0.53
1:B:37:VAL:HA	1:B:46:ASP:O	2.07	0.53
1:B:194:ASN:HD22	1:B:247:THR:CG2	2.22	0.53
1:B:27:LEU:HD21	1:B:474:PHE:CE2	2.44	0.53
1:B:134:LEU:HD12	1:B:455:PHE:CZ	2.29	0.53
1:B:442:ALA:HB1	2:B:610:NAD:H5N	1.91	0.53
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.90	0.53
1:A:214:ARG:HB2	1:A:214:ARG:NH1	2.22	0.53
1:A:494:ARG:CG	1:A:495:PRO:HD2	2.38	0.53
1:B:195:GLN:NE2	2:B:610:NAD:C8A	2.72	0.53
1:A:318:GLY:HA2	1:A:488:LEU:HG	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:O	1:A:343:PRO:HD3	2.08	0.53
1:B:78:GLY:O	1:B:82:VAL:HG23	2.08	0.53
1:B:474:PHE:HD1	1:B:474:PHE:H	1.57	0.53
1:B:481:LEU:C	1:B:483:PHE:H	2.12	0.53
1:A:104:ASN:HD21	1:B:423:MET:HA	1.74	0.53
1:B:293:ILE:HD11	1:B:453:THR:CG2	2.19	0.53
1:A:315:PHE:CZ	1:A:481:LEU:HD21	2.44	0.53
1:B:57:LYS:HB2	1:B:474:PHE:CE2	2.44	0.52
1:B:122:GLU:OE1	1:B:122:GLU:N	2.41	0.52
1:B:14:VAL:HG11	1:B:518:ILE:O	2.09	0.52
1:B:481:LEU:HD22	1:B:484:LEU:HD21	1.90	0.52
1:A:187:TYR:CD1	1:A:277:PRO:HD3	2.44	0.52
1:B:207:GLU:O	1:B:208:LYS:HD3	2.09	0.52
1:B:290:VAL:HG23	1:B:290:VAL:O	2.09	0.52
1:B:299:ASN:O	1:B:301:PHE:N	2.43	0.52
1:A:346:ILE:O	1:A:346:ILE:CG2	2.56	0.52
1:A:473:LYS:CD	1:A:473:LYS:C	2.77	0.52
1:A:261:MET:HE3	1:A:311:HIS:HB3	1.90	0.52
1:A:92:VAL:HG11	1:A:172:LEU:HD21	1.92	0.52
1:A:482:THR:HG21	1:B:530:GLU:OE1	2.10	0.52
1:B:39:LYS:HB2	1:B:45:PHE:CE2	2.45	0.52
1:B:42:SER:OG	1:B:43:GLY:N	2.42	0.52
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.40	0.52
1:B:311:HIS:O	1:B:313:GLY:N	2.43	0.52
1:A:28:THR:O	1:A:55:VAL:HA	2.10	0.52
1:A:55:VAL:HB	1:A:462:LYS:HB3	1.92	0.52
1:B:311:HIS:HD2	1:B:312:GLU:H	1.58	0.52
1:A:48:THR:HA	1:B:15:VAL:CG2	2.40	0.52
1:A:96:THR:HG23	1:A:97:LYS:N	2.25	0.52
1:A:332:LEU:HG	1:A:432:ILE:HD11	1.91	0.52
1:B:273:GLU:C	1:B:275:ILE:N	2.63	0.52
1:B:10:THR:HG22	1:B:132:SER:HB2	1.91	0.51
1:B:438:ASP:OD2	1:B:438:ASP:N	2.43	0.51
1:A:37:VAL:HB	1:A:47:VAL:HG22	1.92	0.51
1:A:56:PHE:CE1	1:A:461:TYR:HB3	2.45	0.51
1:A:185:ILE:HD12	1:A:186:TYR:N	2.26	0.51
1:A:225:ARG:HE	1:A:229:ASN:ND2	2.04	0.51
1:A:245:ALA:HB1	2:A:600:NAD:C4A	2.40	0.51
1:A:147:TRP:CD2	1:A:281:PHE:HE2	2.29	0.51
1:B:474:PHE:N	1:B:474:PHE:CD1	2.78	0.51
1:A:149:ILE:O	1:A:199:ALA:HA	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:OE1	1:A:207:GLU:CA	2.45	0.51
1:A:335:PHE:CE1	1:B:327:LYS:O	2.64	0.51
1:B:198:ARG:NH2	3:B:814:HOH:O	2.44	0.51
1:B:285:SER:HB3	1:B:290:VAL:HG23	1.92	0.51
1:B:351:HIS:C	1:B:412:LYS:HD2	2.30	0.51
1:B:454:GLU:OE2	3:B:654:HOH:O	2.18	0.51
1:B:526:LEU:HB3	1:B:528:PHE:CE2	2.45	0.51
1:A:335:PHE:CE2	1:B:328:LEU:HG	2.45	0.51
1:B:343:PRO:HA	1:B:420:SER:HB3	1.91	0.51
1:B:468:LYS:O	1:B:469:GLU:CB	2.59	0.51
1:A:207:GLU:HB2	3:A:791:HOH:O	2.11	0.51
1:A:231:LYS:HE2	1:A:237:ASP:O	2.11	0.51
1:A:246:ASN:CG	2:A:600:NAD:N7A	2.64	0.51
1:A:296:SER:HB2	2:A:600:NAD:O3D	2.11	0.51
1:A:52:GLN:HG3	1:A:54:TYR:CE1	2.45	0.51
1:A:238:LYS:HD3	1:A:457:THR:HG21	1.91	0.51
1:A:261:MET:HE3	1:A:308:LEU:HA	1.93	0.51
1:A:328:LEU:HD13	1:B:335:PHE:CE1	2.45	0.51
1:A:475:GLU:HA	1:A:475:GLU:OE1	2.10	0.51
1:B:260:THR:HB	1:B:263:ASN:HD21	1.75	0.51
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.45	0.51
1:B:351:HIS:ND1	1:B:412:LYS:HA	2.25	0.51
1:B:463:LYS:O	1:B:470:ASP:HB2	2.10	0.51
1:A:173:LYS:N	3:A:799:HOH:O	2.44	0.51
1:B:220:LEU:HD22	1:B:284:ALA:HB2	1.92	0.51
1:A:462:LYS:NZ	1:A:470:ASP:OD2	2.44	0.50
1:A:96:THR:CG2	1:A:97:LYS:N	2.73	0.50
1:B:321:LEU:HA	1:B:488:LEU:HA	1.92	0.50
1:B:315:PHE:HB3	1:B:481:LEU:CD1	2.22	0.50
1:A:238:LYS:HG2	3:A:796:HOH:O	2.10	0.50
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.94	0.50
1:B:73:LEU:HD22	1:B:154:LEU:HD21	1.93	0.50
1:B:242:LEU:HD23	1:B:242:LEU:C	2.31	0.50
1:B:260:THR:HB	1:B:263:ASN:ND2	2.26	0.50
1:A:37:VAL:HA	1:A:46:ASP:O	2.12	0.50
1:B:82:VAL:HG21	1:B:154:LEU:CD2	2.42	0.50
1:B:134:LEU:HD21	1:B:518:ILE:CG2	2.39	0.50
1:B:351:HIS:CB	1:B:413:VAL:O	2.60	0.50
1:A:208:LYS:C	3:A:742:HOH:O	2.49	0.50
1:B:240:ILE:HG12	1:B:291:PRO:CG	2.41	0.50
1:B:285:SER:O	1:B:290:VAL:HG22	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:OH	1:B:529:GLU:OE1	2.21	0.50
1:A:170:GLN:NE2	3:A:706:HOH:O	2.34	0.50
1:A:192:ALA:O	1:A:193:ALA:HB2	2.12	0.50
1:A:286:ILE:HG22	1:A:312:GLU:HG3	1.93	0.50
1:A:485:SER:OG	1:A:491:PRO:HB3	2.12	0.50
1:A:74:GLY:N	1:A:148:ASP:OD1	2.43	0.49
1:B:163:VAL:HB	1:B:437:GLU:HG2	1.93	0.49
1:A:54:TYR:CZ	1:B:532:LEU:HD23	2.47	0.49
1:A:95:GLN:HB2	1:A:167:ASP:OD1	2.13	0.49
1:A:493:THR:HG21	1:A:497:PHE:O	2.12	0.49
1:A:115:LEU:HD22	1:A:511:GLU:OE2	2.12	0.49
1:A:115:LEU:HD21	1:A:511:GLU:HG2	1.93	0.49
1:A:210:ASN:ND2	1:A:210:ASN:H	2.08	0.49
1:A:278:SER:HB2	3:A:602:HOH:O	2.12	0.49
1:B:24:ASN:N	1:B:24:ASN:ND2	2.60	0.49
1:B:264:LEU:HD21	1:B:305:LEU:CD1	2.42	0.49
1:A:105:TYR:OH	1:A:140:ASN:ND2	2.45	0.49
1:B:21:TYR:O	1:B:22:LYS:O	2.29	0.49
1:A:242:LEU:C	1:A:242:LEU:HD23	2.33	0.49
1:B:114:THR:O	1:B:115:LEU:HD23	2.13	0.49
1:B:510:LEU:O	1:B:514:LEU:HD23	2.12	0.49
1:B:134:LEU:HD11	1:B:517:LEU:HB3	1.95	0.49
1:B:254:SER:HB3	1:B:255:PRO:CD	2.43	0.49
1:A:50:THR:CG2	1:A:51:VAL:N	2.76	0.49
1:A:211:VAL:CG2	1:A:212:THR:H	2.19	0.49
1:B:55:VAL:HB	1:B:462:LYS:HB3	1.95	0.49
1:B:272:HIS:CE1	1:B:274:GLU:OE1	2.65	0.49
1:A:196:ASP:HB2	1:A:197:GLU:OE1	2.12	0.48
1:A:261:MET:O	1:A:263:ASN:N	2.45	0.48
1:B:462:LYS:CE	1:B:472:GLY:HA2	2.42	0.48
1:A:104:ASN:HB2	3:A:636:HOH:O	2.13	0.48
1:B:478:TYR:CE2	1:B:494:ARG:HD3	2.49	0.48
1:B:481:LEU:HD12	1:B:481:LEU:N	2.28	0.48
1:A:27:LEU:HD13	1:A:57:LYS:HG3	1.95	0.48
1:A:214:ARG:NH1	1:A:214:ARG:HB3	2.27	0.48
1:A:191:ILE:CD1	1:A:195:GLN:HG2	2.34	0.48
1:A:259:ASP:OD2	1:A:259:ASP:N	2.38	0.48
1:B:241:VAL:CG2	1:B:292:TYR:HD2	2.26	0.48
1:B:262:GLU:OE1	1:B:262:GLU:N	2.46	0.48
1:B:273:GLU:O	1:B:275:ILE:HG12	2.13	0.48
1:B:293:ILE:HG12	1:B:317:ALA:HB3	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:HD22	1:B:55:VAL:HG12	1.96	0.48
1:B:58:LEU:CD1	1:B:60:LEU:HD12	2.44	0.48
1:B:349:TYR:CD1	1:B:415:MET:CB	2.94	0.48
1:A:66:LEU:HD13	1:A:68:ILE:HD11	1.95	0.48
1:A:532:LEU:HD13	1:A:532:LEU:N	2.29	0.48
1:B:242:LEU:HD13	1:B:446:ILE:HG23	1.96	0.48
1:B:261:MET:HE2	1:B:311:HIS:HB3	1.96	0.48
1:B:14:VAL:HG11	1:B:518:ILE:HB	1.95	0.48
1:B:324:GLY:HA3	1:B:441:LEU:CD2	2.44	0.48
1:B:484:LEU:CD1	1:B:484:LEU:N	2.77	0.48
1:B:488:LEU:O	1:B:491:PRO:HD3	2.13	0.48
1:A:187:TYR:HD1	1:A:277:PRO:HD3	1.78	0.48
1:A:254:SER:H	1:A:258:ASN:HD21	1.61	0.48
1:A:532:LEU:O	1:A:532:LEU:HD22	2.13	0.48
1:B:75:GLY:HA3	2:B:610:NAD:C4B	2.40	0.48
1:B:156:GLU:O	1:B:159:GLN:HB2	2.13	0.48
1:A:196:ASP:C	1:A:197:GLU:OE2	2.52	0.48
1:A:531:ARG:HG3	1:B:482:THR:OG1	2.14	0.48
1:B:88:ASN:CB	1:B:140:ASN:HD21	2.27	0.48
1:B:245:ALA:O	2:B:610:NAD:C4D	2.61	0.48
1:A:344:VAL:HG12	1:A:419:TYR:O	2.14	0.48
1:B:10:THR:HG22	1:B:132:SER:CB	2.44	0.47
1:B:344:VAL:CG1	1:B:419:TYR:O	2.62	0.47
1:A:231:LYS:HG2	1:A:236:LEU:O	2.13	0.47
1:B:88:ASN:O	1:B:91:ASN:ND2	2.47	0.47
1:B:94:PHE:CD2	1:B:168:LEU:HD23	2.48	0.47
1:B:351:HIS:C	1:B:412:LYS:HB3	2.34	0.47
1:A:426:GLY:HA3	1:B:440:LEU:HD13	1.95	0.47
1:A:431:SER:OG	1:B:433:HIS:HB3	2.14	0.47
1:B:449:LEU:O	1:B:453:THR:HG22	2.13	0.47
1:B:457:THR:HG21	3:B:654:HOH:O	2.15	0.47
1:A:233:GLU:HG3	3:A:783:HOH:O	2.14	0.47
1:A:349:TYR:HB3	1:A:350:ASN:H	1.28	0.47
1:A:497:PHE:N	1:A:497:PHE:CD1	2.82	0.47
1:A:40:THR:HG23	1:A:43:GLY:H	1.79	0.47
1:A:308:LEU:O	1:A:312:GLU:HG2	2.14	0.47
1:B:136:MET:HE3	1:B:452:MET:HE1	1.96	0.47
1:A:104:ASN:C	1:A:104:ASN:HD22	2.17	0.47
1:A:257:VAL:HG23	1:A:258:ASN:N	2.29	0.47
1:A:529:GLU:CD	1:A:529:GLU:H	2.17	0.47
1:B:187:TYR:OH	1:B:219:HIS:HD2	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TYR:HE2	1:B:494:ARG:HB3	1.77	0.47
1:A:246:ASN:C	1:A:246:ASN:ND2	2.60	0.47
1:A:299:ASN:OD1	1:A:299:ASN:N	2.45	0.47
1:B:26:LEU:O	1:B:57:LYS:HA	2.15	0.47
1:B:139:PRO:HA	1:B:142:PHE:CD2	2.49	0.47
1:B:302:VAL:HB	1:B:303:PRO:CD	2.39	0.47
1:B:488:LEU:HD12	1:B:488:LEU:N	2.29	0.47
1:A:68:ILE:CG2	1:A:70:LEU:HD13	2.45	0.47
1:A:204:ASN:CG	1:A:204:ASN:O	2.53	0.47
1:B:341:ILE:O	1:B:343:PRO:HD3	2.14	0.47
1:A:258:ASN:N	1:A:258:ASN:ND2	2.62	0.47
1:B:235:ALA:O	1:B:236:LEU:O	2.33	0.47
1:B:515:ARG:NH1	1:B:522:SER:H	2.13	0.47
1:A:185:ILE:CD1	1:A:277:PRO:HG3	2.38	0.47
1:A:223:ILE:O	1:A:226:ASP:HB2	2.15	0.47
1:A:251:VAL:H	1:A:299:ASN:HD21	1.63	0.47
1:A:54:TYR:CE2	1:B:532:LEU:HD23	2.50	0.46
1:A:332:LEU:HD23	1:B:328:LEU:HD21	1.95	0.46
1:A:477:PHE:HZ	1:A:513:PHE:CZ	2.32	0.46
1:B:31:SER:HB2	3:B:747:HOH:O	2.15	0.46
1:B:172:LEU:HA	3:B:796:HOH:O	2.15	0.46
1:B:435:VAL:O	1:B:436:CYS:HB3	2.16	0.46
1:B:484:LEU:N	1:B:484:LEU:HD12	2.30	0.46
1:A:286:ILE:HG22	1:A:308:LEU:HD22	1.97	0.46
1:A:349:TYR:CB	1:A:415:MET:H	2.28	0.46
1:A:462:LYS:HE3	1:A:472:GLY:CA	2.46	0.46
1:A:178:LEU:HD11	3:A:797:HOH:O	2.14	0.46
1:A:238:LYS:HG3	3:A:651:HOH:O	2.15	0.46
1:B:190:PHE:HA	1:B:249:ARG:HG2	1.97	0.46
1:B:503:LEU:HD13	3:B:815:HOH:O	2.13	0.46
1:A:13:LYS:HB2	1:A:13:LYS:HE3	1.58	0.46
1:A:56:PHE:CD1	1:A:461:TYR:HB3	2.49	0.46
1:A:315:PHE:CD1	1:A:481:LEU:HD11	2.49	0.46
1:A:484:LEU:HA	1:A:487:TRP:CZ3	2.49	0.46
1:A:203:ILE:CG1	1:A:204:ASN:H	2.28	0.46
1:B:52:GLN:OE1	1:B:53:ASP:N	2.48	0.46
1:B:143:VAL:CG2	1:B:143:VAL:O	2.63	0.46
1:B:220:LEU:HD13	1:B:220:LEU:C	2.36	0.46
1:B:528:PHE:CB	1:B:532:LEU:HD22	2.46	0.46
1:A:494:ARG:HG3	1:A:495:PRO:HD2	1.97	0.46
1:A:501:ASN:HD22	1:A:501:ASN:N	2.12	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLU:OE2	1:A:527:ARG:NH2	2.47	0.46
1:A:531:ARG:C	1:A:532:LEU:HD13	2.35	0.46
1:A:243:TRP:CD1	1:A:296:SER:HB3	2.50	0.46
1:A:349:TYR:O	1:A:350:ASN:HB3	2.16	0.46
1:A:485:SER:HB3	1:A:506:GLN:NE2	2.30	0.46
1:A:502:GLY:O	1:A:503:LEU:C	2.54	0.46
1:A:508:THR:O	1:A:509:ALA:C	2.53	0.46
1:B:184:SER:OG	1:B:185:ILE:N	2.47	0.46
1:B:249:ARG:NH2	3:B:808:HOH:O	2.49	0.46
1:A:154:LEU:HD22	1:A:179:VAL:HG11	1.98	0.46
1:A:175:LYS:HA	1:A:175:LYS:HD3	1.80	0.46
1:A:286:ILE:HG23	1:A:314:THR:CG2	2.46	0.46
1:A:301:PHE:CD1	1:A:492:LEU:HD12	2.51	0.46
1:A:327:LYS:HD3	1:B:335:PHE:HE2	1.80	0.46
1:B:121:ALA:HB3	3:B:712:HOH:O	2.15	0.46
1:B:489:LYS:C	1:B:489:LYS:HD2	2.36	0.46
1:A:115:LEU:HD22	1:A:511:GLU:HG2	1.98	0.46
1:A:318:GLY:O	1:A:319:ASP:CB	2.61	0.46
1:A:480:VAL:O	1:A:482:THR:N	2.49	0.46
1:B:274:GLU:OE1	1:B:274:GLU:N	2.49	0.46
1:B:500:VAL:CG1	1:B:501:ASN:H	2.16	0.46
1:B:125:ASP:OD2	1:B:125:ASP:N	2.43	0.46
1:A:15:VAL:HG12	1:A:15:VAL:O	2.14	0.45
1:A:69:MET:HB2	1:A:241:VAL:HG22	1.97	0.45
1:A:148:ASP:C	1:A:150:ASN:H	2.20	0.45
1:A:270:ASN:O	1:A:271:ASP:HB2	2.17	0.45
1:A:229:ASN:ND2	3:A:640:HOH:O	2.49	0.45
1:A:473:LYS:C	1:A:473:LYS:HD3	2.36	0.45
1:B:28:THR:O	1:B:55:VAL:HA	2.16	0.45
1:B:301:PHE:CZ	1:B:316:ILE:HB	2.52	0.45
1:B:347:ALA:O	1:B:416:ASP:HA	2.16	0.45
1:A:69:MET:HB3	1:A:147:TRP:CZ3	2.52	0.45
1:A:275:ILE:HG22	1:A:280:ILE:HD11	1.98	0.45
1:A:311:HIS:ND1	1:A:311:HIS:C	2.69	0.45
1:B:40:THR:O	1:B:41:ALA:O	2.33	0.45
1:A:327:LYS:HE2	1:A:503:LEU:HD11	1.98	0.45
1:B:321:LEU:HD21	2:B:610:NAD:C5N	2.47	0.45
1:B:458:ARG:HA	3:B:696:HOH:O	2.15	0.45
1:B:261:MET:HE1	1:B:311:HIS:HB2	1.98	0.45
1:B:265:LEU:O	1:B:269:LYS:HG3	2.17	0.45
1:B:502:GLY:O	1:B:503:LEU:C	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASN:O	1:B:235:ALA:CB	2.64	0.45
1:A:58:LEU:HD13	1:A:60:LEU:HD23	1.98	0.45
1:B:67:GLY:HA2	1:B:143:VAL:HG22	1.99	0.45
1:B:109:MET:HE1	1:B:507:ARG:HG3	1.98	0.45
1:B:250:TYR:CZ	1:B:298:GLN:HA	2.52	0.45
1:A:241:VAL:HG12	1:A:242:LEU:N	2.32	0.45
1:A:294:ASN:C	1:A:294:ASN:ND2	2.71	0.45
1:B:258:ASN:HB2	1:B:302:VAL:HG21	1.99	0.45
1:B:25:GLU:OE1	1:B:57:LYS:HD2	2.17	0.45
1:A:24:ASN:ND2	1:A:61:LYS:HB3	2.32	0.44
1:A:87:ALA:HA	1:A:92:VAL:HG13	1.95	0.44
1:A:251:VAL:H	1:A:299:ASN:ND2	2.15	0.44
1:A:256:GLY:H	1:A:259:ASP:CG	2.19	0.44
1:A:325:GLN:HA	1:A:325:GLN:OE1	2.17	0.44
1:B:264:LEU:HD21	1:B:305:LEU:HD13	1.98	0.44
1:A:302:VAL:HB	1:A:303:PRO:HD2	2.00	0.44
1:B:89:LYS:HD3	3:B:633:HOH:O	2.16	0.44
1:B:105:TYR:OH	1:B:140:ASN:ND2	2.50	0.44
1:A:319:ASP:HB2	1:A:490:ALA:O	2.18	0.44
1:B:261:MET:HE2	1:B:311:HIS:CB	2.47	0.44
1:A:75:GLY:HA3	2:A:600:NAD:H4B	1.99	0.44
1:A:190:PHE:O	1:A:248:GLU:HA	2.16	0.44
1:A:485:SER:O	1:A:487:TRP:N	2.51	0.44
1:A:501:ASN:HA	1:A:506:GLN:NE2	2.33	0.44
1:A:531:ARG:NH2	3:A:649:HOH:O	2.51	0.44
1:A:532:LEU:O	1:A:532:LEU:CD2	2.64	0.44
1:B:121:ALA:CB	1:B:122:GLU:OE1	2.64	0.44
1:A:349:TYR:CE2	1:A:413:VAL:HG22	2.52	0.44
1:B:216:LYS:NZ	1:B:275:ILE:O	2.46	0.44
1:B:315:PHE:HD1	1:B:479:PRO:HA	1.83	0.44
1:B:348:SER:OG	1:B:416:ASP:OD1	2.32	0.44
1:A:217:TRP:O	1:A:220:LEU:HB3	2.17	0.44
1:B:68:ILE:HG22	1:B:70:LEU:HD13	2.00	0.44
1:B:136:MET:CE	1:B:452:MET:HE1	2.46	0.44
1:B:251:VAL:CG1	1:B:299:ASN:HB2	2.47	0.44
1:A:129:PRO:HB2	1:A:132:SER:HB3	2.00	0.44
1:A:158:MET:SD	1:A:169:GLN:HG3	2.57	0.44
1:A:349:TYR:HB2	1:A:415:MET:H	1.83	0.44
1:B:24:ASN:HA	1:B:60:LEU:HB2	1.99	0.44
1:B:183:PRO:HG2	3:B:612:HOH:O	2.16	0.44
1:A:22:LYS:HG2	1:A:23:ASP:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:MET:C	1:A:169:GLN:NE2	2.71	0.44
1:A:341:ILE:N	1:A:341:ILE:CD1	2.81	0.44
1:A:349:TYR:CD2	1:A:415:MET:CB	3.01	0.44
1:A:409:GLY:O	1:A:410:ASP:OD2	2.36	0.44
1:A:478:TYR:CE1	1:A:479:PRO:HG2	2.53	0.44
1:A:502:GLY:HA2	3:A:760:HOH:O	2.17	0.44
1:B:153:ASP:OD2	1:B:177:SER:HA	2.18	0.44
1:B:231:LYS:HE3	3:B:824:HOH:O	2.18	0.44
1:B:241:VAL:HG21	1:B:285:SER:OG	2.18	0.44
1:A:216:LYS:HA	1:A:219:HIS:ND1	2.32	0.44
1:B:97:LYS:HG2	1:B:98:GLU:OE1	2.17	0.43
1:B:116:LYS:HB3	1:B:523:GLN:HE22	1.83	0.43
1:B:186:TYR:CD2	1:B:188:PRO:HD3	2.53	0.43
1:B:191:ILE:O	1:B:191:ILE:HG22	2.18	0.43
1:B:467:VAL:HG21	3:B:828:HOH:O	2.01	0.43
1:A:127:TYR:CD1	1:A:127:TYR:N	2.86	0.43
1:A:210:ASN:N	1:A:210:ASN:HD22	2.16	0.43
1:A:460:SER:HB3	1:A:476:ASN:ND2	2.33	0.43
1:A:65:LYS:HB3	1:A:236:LEU:HD11	1.99	0.43
1:B:151:ASN:HD22	1:B:152:ALA:N	2.15	0.43
1:A:154:LEU:HA	1:A:157:ALA:HB3	1.99	0.43
1:B:109:MET:CE	1:B:507:ARG:HH11	2.31	0.43
1:B:231:LYS:NZ	3:B:824:HOH:O	2.52	0.43
1:A:22:LYS:HG2	1:A:23:ASP:N	2.33	0.43
1:A:122:GLU:N	1:A:122:GLU:CD	2.72	0.43
1:A:261:MET:O	1:A:262:GLU:C	2.56	0.43
1:B:225:ARG:NE	3:B:797:HOH:O	2.51	0.43
1:B:321:LEU:CD2	2:B:610:NAD:N1N	2.64	0.43
1:B:522:SER:O	1:B:522:SER:OG	2.33	0.43
1:A:58:LEU:HD22	1:A:59:ASP:O	2.18	0.43
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.54	0.43
1:A:250:TYR:CD1	1:A:298:GLN:HA	2.53	0.43
1:A:257:VAL:HG22	1:A:258:ASN:ND2	2.33	0.43
1:A:418:TYR:HA	3:A:838:HOH:O	2.18	0.43
1:A:461:TYR:O	1:A:474:PHE:HA	2.18	0.43
1:B:58:LEU:HD23	1:B:459:VAL:CG2	2.47	0.43
1:A:336:LEU:HD23	1:A:343:PRO:HG3	2.01	0.43
1:A:440:LEU:HD12	1:A:440:LEU:HA	1.88	0.43
1:B:351:HIS:O	1:B:412:LYS:HB3	2.19	0.43
1:A:68:ILE:HG22	1:A:144:VAL:HG13	2.01	0.43
1:A:429:ARG:NE	3:A:643:HOH:O	2.24	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:CD2	1:B:530:GLU:HB2	2.54	0.43
1:B:216:LYS:N	3:B:838:HOH:O	2.52	0.43
1:B:324:GLY:HA3	1:B:441:LEU:HD23	2.00	0.43
1:A:76:ASN:HD22	1:A:409:GLY:HA2	1.83	0.43
1:A:294:ASN:C	1:A:294:ASN:HD22	2.22	0.43
1:B:158:MET:HG2	1:B:169:GLN:HG2	2.01	0.43
1:A:120:ASP:OD1	1:A:124:ASN:N	2.49	0.42
1:B:517:LEU:HD12	1:B:517:LEU:HA	1.76	0.42
1:A:423:MET:HE1	1:B:443:THR:HB	2.01	0.42
1:A:501:ASN:N	1:A:501:ASN:ND2	2.66	0.42
1:A:66:LEU:HD22	1:A:67:GLY:N	2.33	0.42
1:A:423:MET:CE	1:B:443:THR:HB	2.49	0.42
1:A:531:ARG:C	1:A:532:LEU:CD1	2.87	0.42
1:A:316:ILE:HD11	1:A:480:VAL:HG12	2.00	0.42
1:A:467:VAL:HG23	1:A:467:VAL:O	2.18	0.42
1:B:245:ALA:O	1:B:246:ASN:O	2.38	0.42
1:A:264:LEU:HD22	1:A:305:LEU:CA	2.50	0.42
1:B:211:VAL:O	1:B:211:VAL:HG23	2.19	0.42
1:A:63:PRO:CG	1:A:238:LYS:HE2	2.38	0.42
1:A:468:LYS:O	1:A:468:LYS:HG2	2.19	0.42
1:B:483:PHE:O	1:B:510:LEU:HD21	2.19	0.42
1:A:257:VAL:CG2	1:A:258:ASN:ND2	2.82	0.42
1:B:344:VAL:HG12	1:B:420:SER:HA	2.02	0.42
1:A:125:ASP:HB3	1:A:127:TYR:CE1	2.55	0.42
1:A:172:LEU:HB3	1:A:176:MET:CE	2.48	0.42
1:A:245:ALA:HB1	2:A:600:NAD:C5A	2.50	0.42
1:B:337:VAL:O	1:B:337:VAL:CG1	2.66	0.42
1:B:515:ARG:HH11	1:B:522:SER:H	1.68	0.42
2:B:610:NAD:C3B	3:B:834:HOH:O	2.47	0.42
1:A:481:LEU:HB3	1:A:484:LEU:HD22	2.01	0.42
1:B:321:LEU:HD12	1:B:445:LEU:HD22	2.00	0.42
1:A:224:ARG:O	1:A:228:GLN:HG3	2.20	0.42
1:A:282:ALA:CB	1:A:305:LEU:HD21	2.50	0.42
1:A:302:VAL:O	1:A:306:VAL:HG23	2.19	0.42
1:A:410:ASP:OD1	1:A:437:GLU:OE1	2.38	0.42
1:B:170:GLN:NE2	3:B:623:HOH:O	2.53	0.42
1:A:22:LYS:CG	1:A:23:ASP:H	2.32	0.41
1:A:214:ARG:CB	1:A:214:ARG:CZ	2.97	0.41
1:A:251:VAL:O	1:A:299:ASN:ND2	2.51	0.41
1:B:215:GLY:H	1:B:271:ASP:CG	2.23	0.41
1:A:73:LEU:HD12	1:A:181:PRO:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:HE2	1:A:191:ILE:HD12	1.85	0.41
1:B:16:THR:OG1	1:B:17:ASP:N	2.53	0.41
1:B:225:ARG:NH2	3:B:797:HOH:O	2.53	0.41
1:B:242:LEU:CD1	1:B:446:ILE:HG23	2.50	0.41
1:B:311:HIS:CD2	1:B:312:GLU:H	2.37	0.41
1:B:71:ILE:HG12	1:B:147:TRP:CE3	2.55	0.41
1:B:277:PRO:O	1:B:281:PHE:HD1	2.03	0.41
1:B:321:LEU:HD21	2:B:610:NAD:C4N	2.49	0.41
1:B:411:SER:HA	1:B:437:GLU:HA	2.00	0.41
1:A:197:GLU:CD	1:A:197:GLU:N	2.73	0.41
1:A:251:VAL:N	1:A:299:ASN:HD21	2.19	0.41
1:A:261:MET:CE	1:A:308:LEU:HA	2.50	0.41
1:A:336:LEU:HA	1:A:336:LEU:HD12	1.78	0.41
1:B:58:LEU:HD13	1:B:58:LEU:O	2.20	0.41
1:B:109:MET:N	1:B:448:ASP:OD1	2.46	0.41
1:B:241:VAL:CG2	1:B:292:TYR:CD2	3.03	0.41
1:B:327:LYS:HG3	1:B:503:LEU:HD13	2.02	0.41
1:B:458:ARG:C	3:B:696:HOH:O	2.59	0.41
1:A:54:TYR:HA	1:A:462:LYS:O	2.20	0.41
1:A:194:ASN:O	1:A:246:ASN:HB3	2.21	0.41
1:B:167:ASP:OD1	1:B:167:ASP:C	2.58	0.41
1:B:195:GLN:OE1	1:B:197:GLU:N	2.43	0.41
1:B:300:THR:O	1:B:302:VAL:N	2.53	0.41
1:B:488:LEU:N	1:B:488:LEU:CD1	2.84	0.41
1:B:515:ARG:NH2	3:B:854:HOH:O	2.53	0.41
1:A:94:PHE:CD1	1:A:94:PHE:N	2.88	0.41
1:B:442:ALA:HB2	2:B:610:NAD:H5N	2.02	0.41
1:B:116:LYS:HB3	1:B:523:GLN:NE2	2.35	0.41
1:B:198:ARG:HD2	1:B:198:ARG:HA	1.59	0.41
1:B:275:ILE:HG21	1:B:280:ILE:HD11	2.02	0.41
1:A:328:LEU:HD12	1:A:328:LEU:HA	1.87	0.41
1:A:349:TYR:HB2	1:A:415:MET:N	2.36	0.41
1:B:82:VAL:HB	1:B:176:MET:HE1	2.03	0.41
1:B:303:PRO:HG2	1:B:304:GLY:N	2.32	0.41
1:B:329:LYS:HD3	3:B:837:HOH:O	2.19	0.41
1:B:346:ILE:N	1:B:346:ILE:CD1	2.81	0.41
1:B:459:VAL:O	1:B:459:VAL:HG12	2.21	0.41
1:A:76:ASN:ND2	1:A:409:GLY:HA2	2.35	0.41
1:A:198:ARG:HD2	3:A:724:HOH:O	2.21	0.41
1:A:337:VAL:HG23	1:A:338:ASP:N	2.35	0.41
1:A:461:TYR:CE1	3:A:808:HOH:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:THR:HG23	1:A:494:ARG:O	2.21	0.41
1:B:54:TYR:HA	1:B:462:LYS:O	2.21	0.41
1:B:479:PRO:O	1:B:481:LEU:HD12	2.21	0.41
1:B:492:LEU:O	1:B:493:THR:CG2	2.69	0.41
1:A:228:GLN:NE2	3:A:751:HOH:O	2.53	0.41
1:A:478:TYR:HA	1:A:479:PRO:HD2	1.62	0.41
1:A:511:GLU:O	1:A:515:ARG:HG3	2.21	0.41
1:B:272:HIS:ND1	1:B:274:GLU:OE1	2.54	0.41
1:B:464:VAL:HG12	1:B:466:PRO:HD3	2.02	0.41
1:A:89:LYS:NZ	3:A:710:HOH:O	2.23	0.40
1:B:115:LEU:O	1:B:127:TYR:HA	2.20	0.40
1:B:93:GLU:HG2	3:B:698:HOH:O	2.21	0.40
1:B:208:LYS:HD2	1:B:208:LYS:HA	1.90	0.40
1:B:351:HIS:N	1:B:413:VAL:O	2.54	0.40
1:A:94:PHE:CD1	1:A:168:LEU:HD13	2.57	0.40
1:A:247:THR:HG23	1:A:297:PRO:HG2	2.03	0.40
1:A:255:PRO:HA	1:A:259:ASP:OD1	2.22	0.40
1:A:478:TYR:HB3	1:B:531:ARG:O	2.20	0.40
1:B:342:LYS:O	1:B:343:PRO:C	2.57	0.40
1:B:446:ILE:O	1:B:450:LEU:HG	2.22	0.40
1:A:39:LYS:HG3	1:A:45:PHE:CD2	2.57	0.40
1:A:39:LYS:HG3	1:A:45:PHE:CE2	2.56	0.40
1:A:423:MET:HE1	1:B:443:THR:CG2	2.52	0.40
1:A:484:LEU:O	1:A:487:TRP:CE3	2.74	0.40
1:B:245:ALA:C	1:B:246:ASN:O	2.59	0.40
1:B:251:VAL:O	1:B:299:ASN:OD1	2.40	0.40
1:A:198:ARG:HG2	1:A:198:ARG:NH1	2.37	0.40
1:B:195:GLN:CD	1:B:197:GLU:O	2.60	0.40

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	462/533 (87%)	389 (84%)	46 (10%)	27 (6%)	1 0
1	B	461/533 (86%)	360 (78%)	59 (13%)	42 (9%)	1 0
All	All	923/1066 (87%)	749 (81%)	105 (11%)	69 (8%)	1 0

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	207	GLU
1	A	298	GLN
1	A	319	ASP
1	B	22	LYS
1	B	41	ALA
1	B	133	LEU
1	B	134	LEU
1	B	161	SER
1	B	236	LEU
1	B	246	ASN
1	B	274	GLU
1	B	298	GLN
1	B	319	ASP
1	B	349	TYR
1	B	466	PRO
1	B	469	GLU
1	B	471	ALA
1	B	473	LYS
1	B	522	SER
1	B	523	GLN
1	A	42	SER
1	A	204	ASN
1	A	246	ASN
1	A	262	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	481	LEU
1	B	135	PRO
1	B	235	ALA
1	B	273	GLU
1	B	299	ASN
1	B	472	GLY
1	A	149	ILE
1	A	193	ALA
1	A	261	MET
1	A	468	LYS
1	A	486	TYR
1	A	532	LEU
1	B	42	SER
1	B	207	GLU
1	B	287	LEU
1	B	322	LYS
1	B	495	PRO
1	B	501	ASN
1	A	41	ALA
1	A	52	GLN
1	A	208	LYS
1	A	350	ASN
1	A	503	LEU
1	B	468	LYS
1	B	479	PRO
1	B	482	THR
1	B	502	GLY
1	B	503	LEU
1	A	133	LEU
1	A	255	PRO
1	A	320	ASP
1	A	479	PRO
1	A	530	GLU
1	B	160	ARG
1	B	300	THR
1	B	350	ASN
1	B	436	CYS
1	B	257	VAL
1	B	320	ASP
1	A	495	PRO
1	B	211	VAL
1	A	49	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	491	PRO
1	B	302	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	410/471 (87%)	348 (85%)	62 (15%)	3 3
1	B	410/471 (87%)	348 (85%)	62 (15%)	3 3
All	All	820/942 (87%)	696 (85%)	124 (15%)	3 3

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

Mol	Chain	Res	Type
1	A	13	LYS
1	A	26	LEU
1	A	37	VAL
1	A	42	SER
1	A	50	THR
1	A	58	LEU
1	A	61	LYS
1	A	65	LYS
1	A	66	LEU
1	A	68	ILE
1	A	70	LEU
1	A	80	THR
1	A	81	LEU
1	A	96	THR
1	A	104	ASN
1	A	147	TRP
1	A	185	ILE
1	A	189	ASP
1	A	197	GLU
1	A	198	ARG
1	A	200	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	207	GLU
1	A	210	ASN
1	A	212	THR
1	A	220	LEU
1	A	236	LEU
1	A	238	LYS
1	A	246	ASN
1	A	257	VAL
1	A	258	ASN
1	A	260	THR
1	A	277	PRO
1	A	287	LEU
1	A	294	ASN
1	A	296	SER
1	A	300	THR
1	A	307	GLN
1	A	308	LEU
1	A	310	GLU
1	A	319	ASP
1	A	320	ASP
1	A	321	LEU
1	A	336	LEU
1	A	346	ILE
1	A	348	SER
1	A	349	TYR
1	A	410	ASP
1	A	411	SER
1	A	438	ASP
1	A	440	LEU
1	A	453	THR
1	A	473	LYS
1	A	480	VAL
1	A	484	LEU
1	A	492	LEU
1	A	495	PRO
1	A	498	HIS
1	A	500	VAL
1	A	516	LEU
1	A	531	ARG
1	A	532	LEU
1	A	533	LEU
1	B	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	22	LYS
1	B	40	THR
1	B	58	LEU
1	B	60	LEU
1	B	70	LEU
1	B	73	LEU
1	B	80	THR
1	B	92	VAL
1	B	111	GLN
1	B	125	ASP
1	B	135	PRO
1	B	138	SER
1	B	144	VAL
1	B	147	TRP
1	B	151	ASN
1	B	163	VAL
1	B	176	MET
1	B	198	ARG
1	B	210	ASN
1	B	212	THR
1	B	222	ARG
1	B	225	ARG
1	B	233	GLU
1	B	237	ASP
1	B	238	LYS
1	B	246	ASN
1	B	249	ARG
1	B	251	VAL
1	B	257	VAL
1	B	258	ASN
1	B	260	THR
1	B	263	ASN
1	B	278	SER
1	B	299	ASN
1	B	314	THR
1	B	319	ASP
1	B	325	GLN
1	B	326	THR
1	B	328	LEU
1	B	335	PHE
1	B	344	VAL
1	B	349	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	350	ASN
1	B	423	MET
1	B	428	ASN
1	B	449	LEU
1	B	453	THR
1	B	457	THR
1	B	460	SER
1	B	466	PRO
1	B	470	ASP
1	B	473	LYS
1	B	474	PHE
1	B	483	PHE
1	B	489	LYS
1	B	508	THR
1	B	522	SER
1	B	529	GLU
1	B	531	ARG
1	B	532	LEU
1	B	533	LEU

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	ASN
1	A	77	ASN
1	A	104	ASN
1	A	140	ASN
1	A	162	GLN
1	A	169	GLN
1	A	170	GLN
1	A	194	ASN
1	A	200	ASN
1	A	210	ASN
1	A	228	GLN
1	A	229	ASN
1	A	246	ASN
1	A	258	ASN
1	A	263	ASN
1	A	270	ASN
1	A	294	ASN
1	A	307	GLN

Continued on next page...

Continued from previous page...

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

5.3.3 RNA ⓘ

There are no RNA 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	B	610	-	42,48,48	2.80	16 (38%)	50,73,73	1.40	6 (12%)
2	NAD	A	600	1	42,48,48	2.68	13 (30%)	50,73,73	1.40	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	610	-	-	7/26/62/62	0/5/5/5
2	NAD	A	600	1	-	10/26/62/62	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	NAD	C4N-C3N	9.10	1.54	1.39
2	A	600	NAD	C4N-C3N	8.54	1.53	1.39
2	B	610	NAD	C2A-N1A	6.75	1.46	1.33
2	A	600	NAD	C2N-C3N	5.97	1.48	1.39
2	A	600	NAD	C6N-N1N	5.91	1.49	1.35
2	B	610	NAD	C6N-N1N	5.77	1.49	1.35
2	A	600	NAD	C2A-N1A	5.75	1.44	1.33
2	B	610	NAD	C2A-N3A	5.18	1.40	1.32
2	B	610	NAD	C3N-C7N	-5.01	1.43	1.50
2	A	600	NAD	O7N-C7N	4.58	1.32	1.24
2	B	610	NAD	C2N-C3N	4.05	1.45	1.39
2	A	600	NAD	O4B-C1B	-3.89	1.35	1.41
2	B	610	NAD	C4A-N3A	3.75	1.40	1.35
2	A	600	NAD	C3N-C7N	-3.65	1.45	1.50
2	B	610	NAD	O4D-C1D	3.55	1.46	1.41
2	A	600	NAD	C2A-N3A	3.52	1.37	1.32
2	A	600	NAD	C2B-C1B	3.23	1.58	1.53
2	A	600	NAD	C4A-N3A	3.12	1.40	1.35
2	B	610	NAD	C2B-C1B	3.06	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	NAD	C2N-N1N	2.89	1.38	1.35
2	B	610	NAD	O7N-C7N	2.87	1.29	1.24
2	A	600	NAD	C6N-C5N	2.77	1.44	1.38
2	B	610	NAD	O4B-C4B	2.48	1.50	1.45
2	A	600	NAD	C2N-N1N	2.29	1.37	1.35
2	B	610	NAD	C2D-C3D	-2.20	1.47	1.53
2	B	610	NAD	C5N-C4N	2.19	1.43	1.38
2	A	600	NAD	C5N-C4N	2.14	1.43	1.38
2	B	610	NAD	O5B-C5B	2.10	1.52	1.44
2	B	610	NAD	C5A-C4A	2.09	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	610	NAD	C3N-C7N-N7N	4.45	123.09	117.75
2	A	600	NAD	C3N-C7N-N7N	4.13	122.70	117.75
2	A	600	NAD	C3D-C2D-C1D	3.79	106.69	100.98
2	A	600	NAD	O4B-C1B-C2B	-2.96	102.60	106.93
2	A	600	NAD	N3A-C2A-N1A	-2.95	124.07	128.68
2	B	610	NAD	C5N-C4N-C3N	-2.63	117.23	120.34
2	B	610	NAD	O4D-C1D-C2D	-2.62	103.09	106.93
2	B	610	NAD	O4B-C1B-C2B	-2.56	103.19	106.93
2	B	610	NAD	N3A-C2A-N1A	-2.54	124.71	128.68
2	A	600	NAD	C5N-C4N-C3N	-2.40	117.50	120.34
2	B	610	NAD	O7N-C7N-N7N	-2.33	119.27	122.58
2	A	600	NAD	O7N-C7N-N7N	-2.15	119.52	122.58

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	NAD	C5D-O5D-PN-O3
2	A	600	NAD	C5D-O5D-PN-O2N
2	A	600	NAD	O4D-C4D-C5D-O5D
2	A	600	NAD	C3D-C4D-C5D-O5D
2	B	610	NAD	O4B-C4B-C5B-O5B
2	B	610	NAD	O4D-C4D-C5D-O5D
2	B	610	NAD	C3D-C4D-C5D-O5D
2	A	600	NAD	O4B-C4B-C5B-O5B
2	A	600	NAD	C3B-C4B-C5B-O5B
2	B	610	NAD	C3B-C4B-C5B-O5B
2	B	610	NAD	C4B-C5B-O5B-PA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	600	NAD	PA-O3-PN-O2N
2	B	610	NAD	PA-O3-PN-O2N
2	A	600	NAD	C5D-O5D-PN-O1N
2	A	600	NAD	C4B-C5B-O5B-PA
2	A	600	NAD	PA-O3-PN-O1N
2	B	610	NAD	PA-O3-PN-O1N

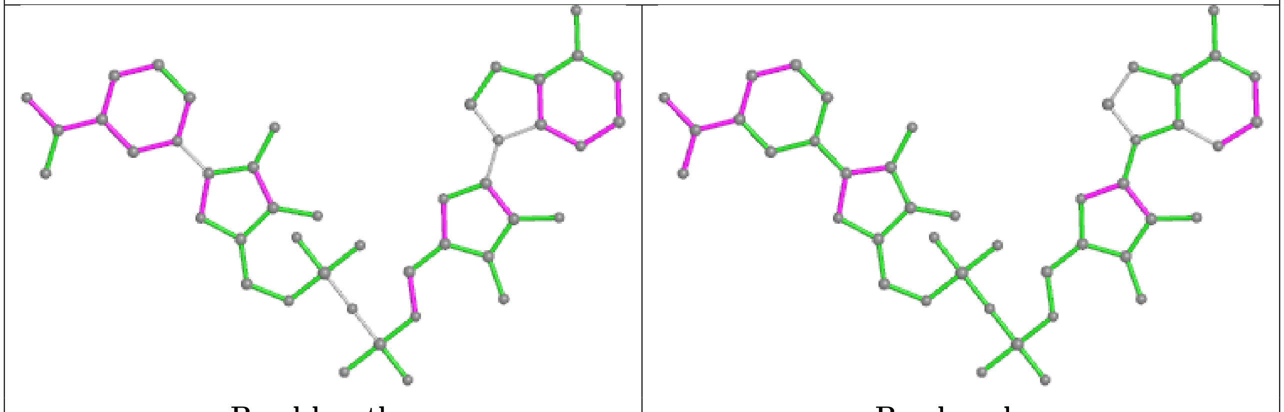
There are no ring outliers.

2 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	610	NAD	29	0
2	A	600	NAD	8	0

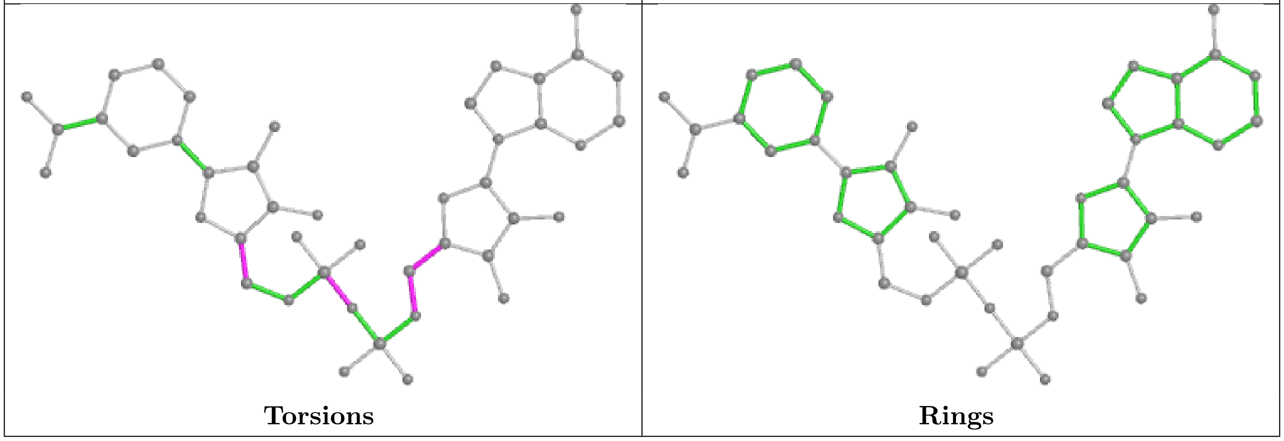
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAD B 610



Bond lengths

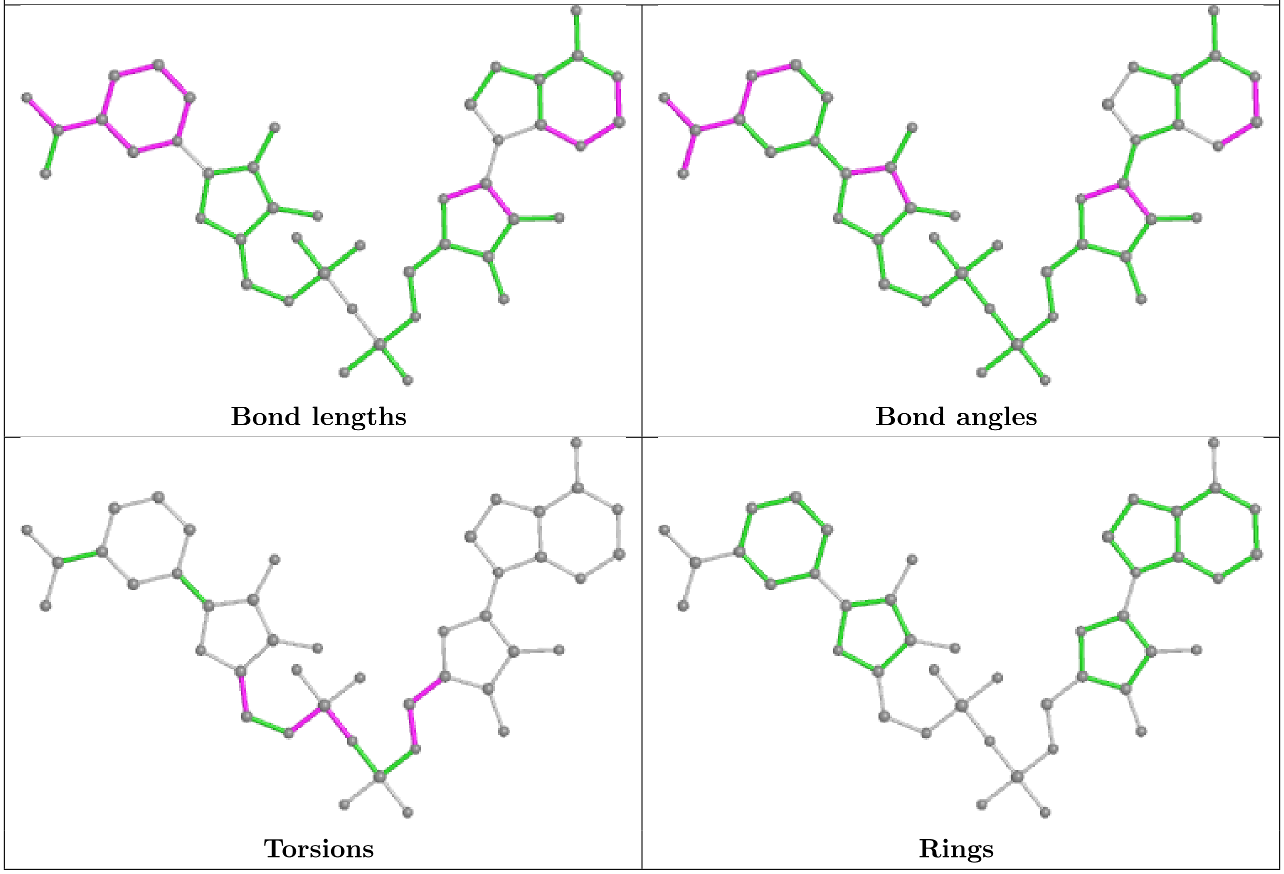
Bond angles



Torsions

Rings

Ligand NAD A 600



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.