Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID	:	6ADH
Title	:	STRUCTURE OF TRICLINIC TERNARY COMPLEX OF HORSE LIVER ALCOHOL DEHYDROGENASE AT 2.9 ANGSTROMS RESOLUTION
Authors	:	Eklund, H.
Deposited on	:	1984-01-16
Resolution	:	2.90 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:

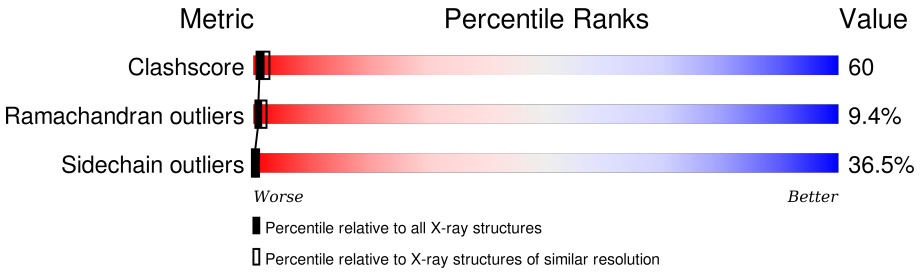
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	374	24% 44% 27% 5%
1	B	374	24% 44% 26% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5669 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.

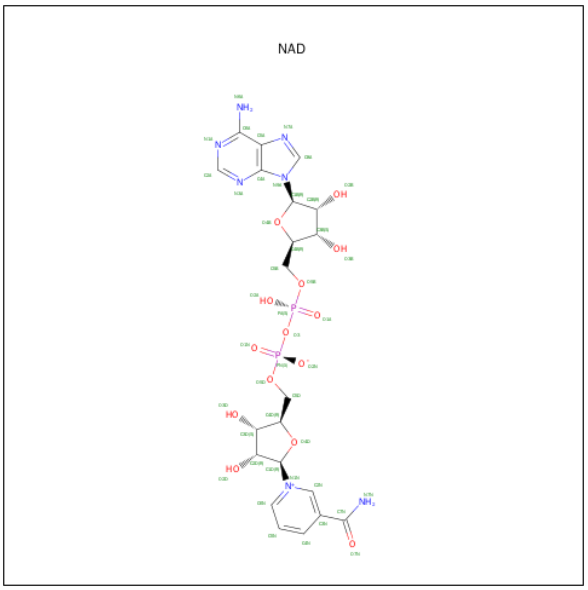
- Molecule 1 is a protein called HOLO-LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	154	0	0
			2784	1769	472	520	23			
1	B	374	Total	C	N	O	S	151	0	0
			2785	1769	472	521	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

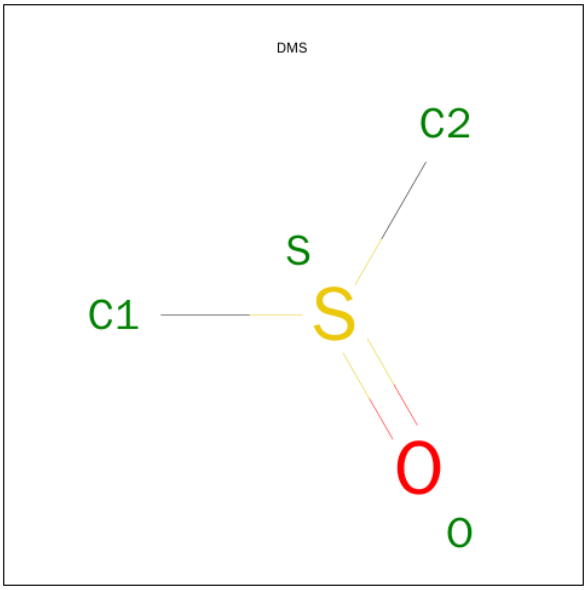
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

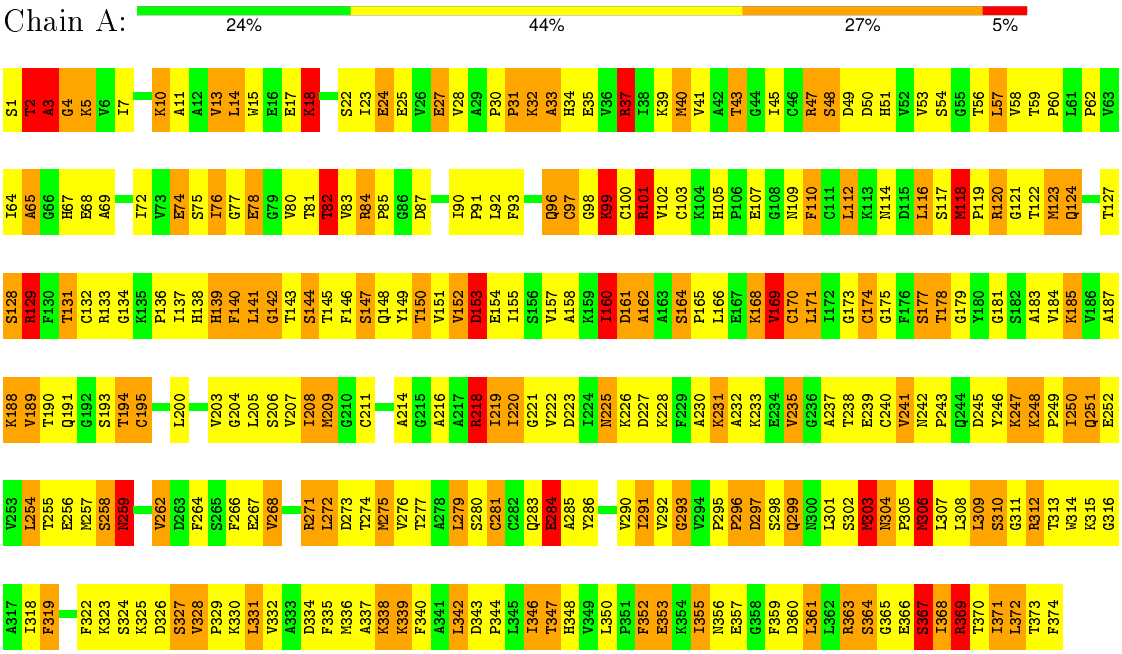
3 Residue-property plots (i)

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.

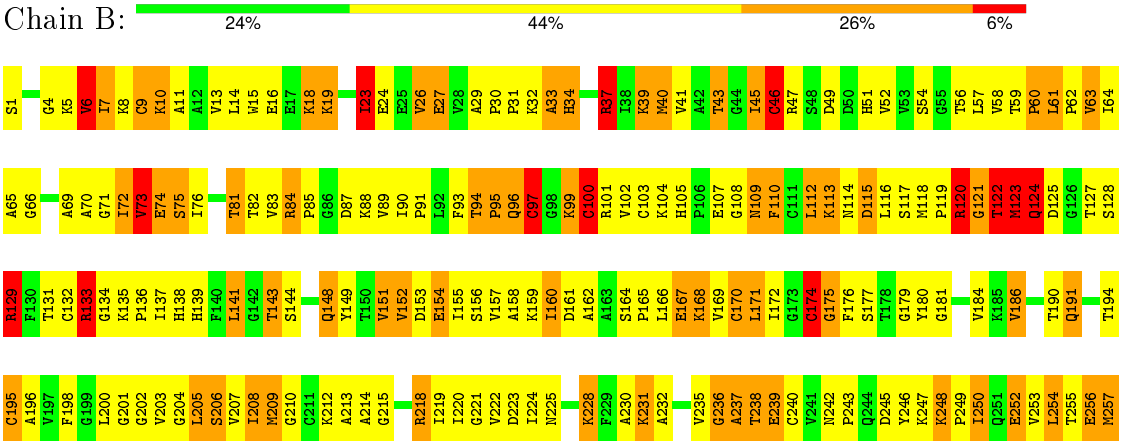
- Molecule 1: HOLO-LIVER ALCOHOL DEHYDROGENASE

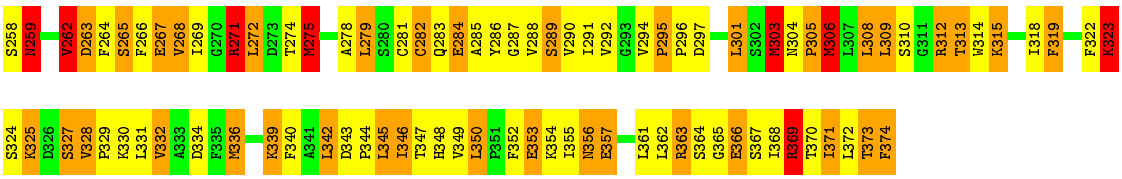
Chain A:



- Molecule 1: HOLO-LIVER ALCOHOL DEHYDROGENASE

Chain B:




S258
N259
V262
D263
F264
S265
F266
E267
V268
I269
G270
R271
L272
D273
T274
W275
A278
L279
S280
C281
C282
Q283
E284
A285
Y286
G287
V288
S289
V290
I291
V292
G293
V294
P295
P296
D297
L301
S302
W303
N304
P305
W306
L307
L308
L309
S310
G311
R312
T313
W314
K315
I318
F319
F322
K323
S324
K325
D326
S327
V328
P329
K330
L331
V332
A333
D334
F335
N336
K339
F340
A341
L342
D343
P344
L345
I346
T347
H348
V349
L350
P351
F352
E353
K354
I355
N356
E357
L361
L362
R363
S364
G365
E366
S367
I368
R369
T370
I371
L372
T373
F374

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	52.00Å 44.60Å 94.40Å 104.40° 101.90° 70.70°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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: ZN, DMS, 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	1.03	1/2836 (0.0%)	1.51	43/3834 (1.1%)
1	B	1.15	6/2837 (0.2%)	1.65	54/3834 (1.4%)
All	All	1.09	7/5673 (0.1%)	1.58	97/7668 (1.3%)

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	B	1	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	CYS	CA-CB	8.44	1.72	1.53
1	B	282	CYS	CA-CB	7.60	1.70	1.53
1	A	240	CYS	CB-SG	7.06	1.94	1.82
1	B	170	CYS	CB-SG	7.06	1.94	1.82
1	B	9	CYS	CB-SG	6.70	1.93	1.82
1	B	282	CYS	CB-SG	6.61	1.93	1.82
1	B	46	CYS	CA-C	6.30	1.69	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	46	CYS	N-CA-CB	23.70	153.26	110.60
1	B	122	THR	O-C-N	11.07	140.41	122.70
1	A	195	CYS	CA-CB-SG	9.37	130.87	114.00
1	A	1	SER	O-C-N	9.19	137.40	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	VAL	O-C-N	9.15	137.34	122.70
1	B	100	CYS	N-CA-CB	-8.79	94.78	110.60
1	A	3	ALA	O-C-N	8.55	137.74	123.20
1	B	282	CYS	CA-CB-SG	-8.49	98.72	114.00
1	B	9	CYS	CA-CB-SG	-8.26	99.13	114.00
1	B	122	THR	CA-C-N	-8.04	99.51	117.20
1	A	367	SER	O-C-N	8.03	135.55	122.70
1	A	37	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	A	133	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	B	271	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	B	292	VAL	O-C-N	7.67	136.24	123.20
1	A	363	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	A	47	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	129	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	B	218	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	369	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	120	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	218	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	312	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	B	363	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	101	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	120	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	B	47	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	369	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	282	CYS	N-CA-CB	7.36	123.85	110.60
1	A	84	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	B	84	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	B	312	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	B	58	VAL	O-C-N	7.28	134.35	122.70
1	B	129	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	A	3	ALA	CA-C-N	-7.16	101.87	116.20
1	B	127	THR	O-C-N	7.12	134.10	122.70
1	B	101	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	B	37	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	B	133	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	A	1	SER	CA-C-N	-6.80	102.23	117.20
1	A	271	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	B	73	VAL	CA-C-N	-6.60	102.68	117.20
1	A	361	LEU	O-C-N	6.58	133.23	122.70
1	B	63	VAL	CB-CA-C	-6.46	99.13	111.40
1	B	123	MET	CG-SD-CE	6.43	110.49	100.20
1	B	6	VAL	O-C-N	6.38	132.90	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	PRO	O-C-N	6.33	132.82	122.70
1	B	118	MET	CG-SD-CE	6.32	110.32	100.20
1	B	10	LYS	O-C-N	6.26	132.72	122.70
1	A	209	MET	CG-SD-CE	6.22	110.16	100.20
1	B	306	MET	CG-SD-CE	6.22	110.15	100.20
1	B	279	LEU	O-C-N	6.19	132.60	122.70
1	B	275	MET	CG-SD-CE	6.18	110.08	100.20
1	A	275	MET	CG-SD-CE	6.18	110.08	100.20
1	B	259	ASN	O-C-N	6.17	133.70	123.20
1	A	118	MET	CG-SD-CE	6.16	110.06	100.20
1	A	336	MET	CG-SD-CE	6.14	110.03	100.20
1	B	100	CYS	O-C-N	6.13	132.52	122.70
1	A	306	MET	CG-SD-CE	6.13	110.01	100.20
1	A	257	MET	CG-SD-CE	6.13	110.01	100.20
1	B	336	MET	CG-SD-CE	6.11	109.98	100.20
1	B	257	MET	CG-SD-CE	6.10	109.97	100.20
1	A	40	MET	CG-SD-CE	6.10	109.96	100.20
1	B	40	MET	CG-SD-CE	6.10	109.95	100.20
1	B	303	MET	CG-SD-CE	6.09	109.94	100.20
1	A	123	MET	CG-SD-CE	6.08	109.93	100.20
1	A	367	SER	C-N-CA	6.08	136.90	121.70
1	A	367	SER	CA-C-N	-6.03	103.94	117.20
1	A	45	ILE	O-C-N	6.02	132.33	122.70
1	B	209	MET	CG-SD-CE	5.98	109.77	100.20
1	A	303	MET	CG-SD-CE	5.97	109.75	100.20
1	A	240	CYS	CA-CB-SG	-5.95	103.29	114.00
1	B	95	PRO	O-C-N	5.93	132.19	122.70
1	A	118	MET	O-C-N	5.87	132.25	121.10
1	B	9	CYS	N-CA-CB	5.82	121.08	110.60
1	B	100	CYS	CB-CA-C	5.79	121.97	110.40
1	B	46	CYS	N-CA-C	-5.76	95.46	111.00
1	B	101	ARG	CB-CA-C	-5.66	99.07	110.40
1	B	350	LEU	CB-CA-C	-5.63	99.51	110.20
1	B	127	THR	CA-C-N	-5.56	104.96	117.20
1	B	127	THR	C-N-CA	5.51	135.48	121.70
1	B	60	PRO	O-C-N	5.47	131.45	122.70
1	B	58	VAL	CA-C-N	-5.45	105.22	117.20
1	A	194	THR	O-C-N	5.41	131.36	122.70
1	B	238	THR	O-C-N	5.40	131.34	122.70
1	B	121	GLY	O-C-N	5.39	131.32	122.70
1	B	259	ASN	CA-C-N	-5.37	105.47	116.20
1	A	296	PRO	O-C-N	5.36	131.28	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	GLU	CB-CA-C	5.32	121.04	110.40
1	A	3	ALA	C-N-CA	5.27	133.36	122.30
1	B	23	ILE	O-C-N	5.26	131.12	122.70
1	A	24	GLU	O-C-N	5.21	131.03	122.70
1	A	284	GLU	CB-CA-C	-5.21	99.99	110.40
1	B	6	VAL	CA-C-N	-5.19	105.79	117.20
1	A	361	LEU	CA-C-N	-5.17	105.83	117.20
1	A	37	ARG	CB-CA-C	5.16	120.73	110.40
1	A	3	ALA	CB-CA-C	-5.16	102.36	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	46	CYS	CA

There are no planarity outliers.

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	2784	0	2848	324	55
1	B	2785	0	2849	358	59
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	25	4	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
All	All	5669	0	5760	655	63

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 60.

All (655) 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:132:CYS:HB2	1:A:137:ILE:CD1	1.61	1.29
1:A:255:THR:O	1:A:259:ASN:HA	1.42	1.18
1:B:24:GLU:HG2	1:B:132:CYS:SG	1.86	1.15
1:A:23:ILE:CD1	1:A:353:GLU:HA	1.77	1.13
1:A:132:CYS:HB2	1:A:137:ILE:HD11	1.22	1.12
1:A:339:LYS:HE2	1:A:339:LYS:HA	1.31	1.11
1:B:59:THR:HG23	1:B:60:PRO:HD2	1.26	1.10
1:B:346:ILE:HD12	1:B:371:ILE:HG12	1.26	1.10
1:B:41:VAL:HG23	1:B:71:GLY:HA2	1.27	1.09
1:B:90:ILE:HG13	1:B:160:ILE:HD13	1.36	1.06
1:B:23:ILE:CD1	1:B:353:GLU:HA	1.86	1.04
1:A:205:LEU:HD22	1:A:235:VAL:HG21	1.41	1.02
1:A:243:PRO:HB3	1:A:250:ILE:HG13	1.42	1.01
1:A:23:ILE:HD11	1:A:353:GLU:HA	1.43	1.01
1:A:132:CYS:HB2	1:A:137:ILE:HD12	1.44	1.00
1:A:62:PRO:O	1:A:138:HIS:HB2	1.62	0.98
1:B:255:THR:O	1:B:259:ASN:HA	1.63	0.98
1:B:5:LYS:HA	1:B:30:PRO:HG3	1.46	0.98
1:B:69:ALA:O	1:B:91:PRO:HD2	1.62	0.98
1:A:82:THR:HG23	1:A:154:GLU:OE2	1.64	0.98
1:B:121:GLY:HA3	1:B:138:HIS:HD2	1.23	0.98
1:A:179:GLY:O	1:A:207:VAL:HA	1.64	0.97
1:B:328:VAL:HG22	1:B:329:PRO:HD3	1.46	0.97
1:B:15:TRP:HZ2	1:B:132:CYS:HG	1.02	0.97
1:B:74:GLU:O	1:B:85:PRO:HB3	1.62	0.96
1:B:45:ILE:HG13	1:B:370:THR:HG23	1.45	0.95
1:B:29:ALA:HB1	1:B:30:PRO:HD2	1.46	0.94
1:B:129:ARG:HB3	1:B:139:HIS:CE1	2.02	0.93
1:A:60:PRO:HG2	1:A:121:GLY:HA3	1.49	0.92
1:B:346:ILE:CD1	1:B:371:ILE:HG12	2.00	0.92
1:B:89:VAL:CG1	1:B:157:VAL:HG23	1.99	0.92
1:A:301:LEU:HD21	1:B:303:MET:CE	2.00	0.91
1:B:23:ILE:HD13	1:B:353:GLU:HA	1.52	0.91
1:B:343:ASP:HA	1:B:346:ILE:HG22	1.51	0.91
1:B:349:VAL:HG12	1:B:373:THR:CG2	2.02	0.90
1:A:165:PRO:HB2	1:A:168:LYS:HB2	1.53	0.90
1:B:88:LYS:HD3	1:B:166:LEU:HD21	1.53	0.90
1:A:124:GLN:HB2	1:A:153:ASP:OD2	1.72	0.90
1:B:232:ALA:O	1:B:237:ALA:HB3	1.70	0.89
1:A:132:CYS:CB	1:A:137:ILE:HD11	2.02	0.89
1:A:179:GLY:HA2	1:A:207:VAL:HG23	1.53	0.89
1:A:208:ILE:HD12	1:A:237:ALA:HB2	1.53	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HG2	1:B:151:VAL:HG13	1.53	0.88
1:B:59:THR:CG2	1:B:60:PRO:HD2	2.02	0.88
1:A:206:SER:HA	1:A:209:MET:HG2	1.56	0.87
1:A:140:PHE:CE1	1:A:141:LEU:HG	2.10	0.87
1:B:262:VAL:HG13	1:B:263:ASP:H	1.39	0.86
1:B:334:ASP:OD2	1:B:339:LYS:HE3	1.75	0.85
1:B:269:ILE:HD12	1:B:274:THR:HG21	1.58	0.85
1:B:327:SER:C	1:B:329:PRO:HD2	1.97	0.85
1:A:37:ARG:HB3	1:A:151:VAL:HG22	1.58	0.85
1:A:179:GLY:CA	1:A:207:VAL:HG23	2.06	0.85
1:B:352:PHE:O	1:B:353:GLU:HB2	1.76	0.85
1:A:208:ILE:CD1	1:A:237:ALA:HB2	2.06	0.85
1:B:51:HIS:HB3	1:B:57:LEU:HB2	1.59	0.85
1:A:304:ASN:ND2	1:A:306:MET:HB2	1.91	0.85
1:A:190:THR:HG23	1:A:264:PHE:CZ	2.12	0.84
1:B:206:SER:HA	1:B:209:MET:HG3	1.59	0.84
1:A:301:LEU:HD21	1:B:303:MET:HE3	1.60	0.84
1:A:165:PRO:HG2	1:A:335:PHE:HE1	1.42	0.83
1:B:121:GLY:HA3	1:B:138:HIS:CD2	2.11	0.83
1:B:349:VAL:HG12	1:B:373:THR:HG23	1.60	0.83
1:A:147:SER:HB3	1:A:149:TYR:O	1.77	0.83
1:B:262:VAL:CG1	1:B:263:ASP:H	1.92	0.82
1:B:283:GLN:HG2	1:B:286:TYR:CD2	2.15	0.81
1:A:355:ILE:O	1:A:355:ILE:HG13	1.78	0.81
1:A:5:LYS:HA	1:A:30:PRO:HG3	1.61	0.81
1:B:8:LYS:HG2	1:B:27:GLU:HB2	1.61	0.81
1:B:349:VAL:CG1	1:B:373:THR:CG2	2.59	0.80
1:B:121:GLY:CA	1:B:138:HIS:HD2	1.94	0.80
1:B:90:ILE:CG1	1:B:160:ILE:HD13	2.10	0.80
1:A:307:LEU:O	1:A:312:ARG:HD2	1.81	0.80
1:A:368:ILE:HG13	1:A:369:ARG:N	1.96	0.80
1:B:31:PRO:CG	1:B:75:SER:HB3	2.11	0.80
1:A:206:SER:HA	1:A:209:MET:CG	2.12	0.79
1:A:33:ALA:HA	1:A:78:GLU:H	1.46	0.79
1:A:140:PHE:CD1	1:A:141:LEU:HG	2.17	0.79
1:B:275:MET:HE1	1:B:295:PRO:HG3	1.63	0.79
1:B:343:ASP:HA	1:B:346:ILE:CG2	2.12	0.79
1:B:203:VAL:HG23	1:B:268:VAL:HG21	1.64	0.78
1:B:345:LEU:O	1:B:368:ILE:HG22	1.83	0.78
1:B:97:CYS:HB2	1:B:99:LYS:HB2	1.64	0.78
1:A:174:CYS:O	1:A:178:THR:HG23	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLY:HA3	1:B:206:SER:HB2	1.67	0.77
1:B:90:ILE:HG13	1:B:160:ILE:CD1	2.13	0.77
1:B:195:CYS:HB3	1:B:266:PHE:HE1	1.49	0.76
1:A:2:THR:O	1:A:3:ALA:HB2	1.83	0.76
1:A:339:LYS:CE	1:A:339:LYS:HA	2.10	0.76
1:A:304:ASN:HD22	1:A:306:MET:H	1.33	0.76
1:A:13:VAL:HG22	1:A:137:ILE:HG21	1.68	0.75
1:A:232:ALA:O	1:A:235:VAL:HG23	1.86	0.75
1:A:315:LYS:HG2	1:B:313:THR:HB	1.67	0.75
1:A:231:LYS:O	1:A:235:VAL:HG22	1.87	0.74
1:B:89:VAL:HG13	1:B:157:VAL:HG23	1.70	0.74
1:B:16:GLU:HB3	1:B:19:LYS:HG2	1.69	0.74
1:A:272:LEU:HD12	1:B:305:PRO:HG3	1.68	0.74
1:B:262:VAL:CG1	1:B:263:ASP:N	2.50	0.74
1:B:171:LEU:HD11	1:B:369:ARG:HG2	1.69	0.73
1:B:45:ILE:HG13	1:B:370:THR:CG2	2.17	0.73
1:A:32:LYS:HB2	1:A:129:ARG:NH1	2.02	0.73
1:B:225:ASN:HD22	1:B:228:LYS:HD2	1.52	0.73
1:B:59:THR:HG23	1:B:60:PRO:CD	2.13	0.73
1:B:186:VAL:CG2	1:B:290:VAL:HG11	2.18	0.73
1:B:29:ALA:HB1	1:B:30:PRO:CD	2.19	0.73
1:B:31:PRO:HG2	1:B:75:SER:HB3	1.70	0.72
1:B:89:VAL:HG11	1:B:157:VAL:HG23	1.70	0.72
1:A:4:GLY:O	1:A:30:PRO:HB3	1.89	0.72
1:B:218:ARG:HH21	1:B:220:ILE:HD11	1.54	0.72
1:A:17:GLU:O	1:A:18:LYS:HB2	1.88	0.72
1:A:96:GLN:HG3	1:A:97:CYS:H	1.53	0.72
1:B:190:THR:HG22	1:B:191:GLN:N	2.05	0.72
1:B:271:ARG:HB3	1:B:274:THR:HB	1.71	0.72
1:B:84:ARG:O	1:B:87:ASP:HB2	1.88	0.71
1:B:232:ALA:O	1:B:237:ALA:CB	2.37	0.71
1:A:183:ALA:O	1:A:189:VAL:HG23	1.89	0.71
1:B:157:VAL:HG22	1:B:158:ALA:N	2.05	0.71
1:B:268:VAL:O	1:B:268:VAL:CG2	2.37	0.71
1:B:129:ARG:HG2	1:B:151:VAL:CG1	2.21	0.71
1:A:13:VAL:HG23	1:A:64:ILE:HD13	1.71	0.70
1:B:132:CYS:H	1:B:137:ILE:HG12	1.55	0.70
1:B:256:GLU:C	1:B:259:ASN:H	1.94	0.70
1:B:8:LYS:CG	1:B:27:GLU:HB2	2.21	0.70
1:B:328:VAL:N	1:B:329:PRO:HD2	2.07	0.70
1:A:169:VAL:HG13	1:A:169:VAL:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:HB2	1:B:168:LYS:HB2	1.73	0.69
1:B:268:VAL:O	1:B:268:VAL:HG22	1.93	0.69
1:A:232:ALA:HA	1:A:235:VAL:CG2	2.22	0.69
1:B:122:THR:OG1	1:B:123:MET:N	2.18	0.69
1:A:160:ILE:HG12	1:A:161:ASP:N	2.06	0.69
1:A:251:GLN:HG3	1:A:277:THR:HG23	1.74	0.69
1:A:205:LEU:O	1:A:209:MET:HG2	1.93	0.69
1:A:190:THR:HG23	1:A:264:PHE:HZ	1.57	0.69
1:B:131:THR:O	1:B:131:THR:HG23	1.91	0.69
1:A:243:PRO:HB3	1:A:250:ILE:CG1	2.21	0.68
1:A:363:ARG:HG3	1:A:364:SER:N	2.08	0.68
1:A:13:VAL:HG21	1:A:137:ILE:HD13	1.74	0.68
1:B:169:VAL:CG1	1:B:332:VAL:HG22	2.24	0.68
1:A:37:ARG:CB	1:A:151:VAL:HG22	2.23	0.68
1:A:255:THR:CG2	1:A:281:CYS:HA	2.24	0.68
1:A:337:ALA:C	1:A:338:LYS:HG2	2.13	0.67
1:A:68:GLU:HG3	1:A:174:CYS:HB3	1.74	0.67
1:A:350:LEU:HB2	1:A:372:LEU:HD12	1.75	0.67
1:A:98:GLY:O	1:A:99:LYS:HB2	1.94	0.67
1:A:179:GLY:O	1:A:207:VAL:CA	2.42	0.67
1:B:64:ILE:HB	1:B:144:SER:HB3	1.77	0.67
1:A:187:ALA:O	1:A:188:LYS:HB2	1.93	0.67
1:B:160:ILE:HG23	1:B:332:VAL:HG11	1.75	0.67
1:A:205:LEU:CD2	1:A:235:VAL:HG21	2.22	0.67
1:B:51:HIS:HB3	1:B:57:LEU:CB	2.25	0.66
1:A:255:THR:O	1:A:259:ASN:CA	2.33	0.66
1:A:296:PRO:HB2	1:A:299:GLN:NE2	2.09	0.66
1:B:15:TRP:HZ2	1:B:132:CYS:SG	2.13	0.66
1:B:157:VAL:CG2	1:B:158:ALA:N	2.59	0.66
1:B:301:LEU:O	1:B:301:LEU:CD1	2.44	0.66
1:B:225:ASN:ND2	1:B:228:LYS:HD2	2.11	0.66
1:A:161:ASP:O	1:A:162:ALA:HB2	1.96	0.66
1:B:88:LYS:CD	1:B:166:LEU:HD21	2.25	0.65
1:B:73:VAL:HG12	1:B:75:SER:O	1.96	0.65
1:A:350:LEU:HD22	1:A:370:THR:HG21	1.78	0.65
1:A:348:HIS:HB2	1:A:370:THR:HG23	1.78	0.65
1:B:59:THR:CG2	1:B:60:PRO:CD	2.70	0.65
1:B:87:ASP:O	1:B:89:VAL:HG23	1.97	0.65
1:A:168:LYS:HG2	1:A:335:PHE:HZ	1.61	0.65
1:A:97:CYS:SG	1:A:98:GLY:N	2.70	0.65
1:A:335:PHE:CD2	1:A:342:LEU:HD22	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PRO:HA	1:B:250:ILE:HG12	1.79	0.65
1:B:169:VAL:HG13	1:B:332:VAL:HG22	1.78	0.64
1:A:206:SER:CA	1:A:209:MET:HG2	2.27	0.64
1:B:328:VAL:N	1:B:329:PRO:CD	2.60	0.64
1:A:301:LEU:HD21	1:B:303:MET:HE2	1.78	0.64
1:A:40:MET:CE	1:A:145:THR:HG22	2.27	0.64
1:A:57:LEU:HD12	1:A:58:VAL:N	2.12	0.64
1:A:161:ASP:HB3	1:A:164:SER:OG	1.97	0.64
1:B:203:VAL:HG23	1:B:268:VAL:CG2	2.27	0.64
1:A:190:THR:HG23	1:A:264:PHE:CE1	2.32	0.64
1:A:251:GLN:CG	1:A:277:THR:HG23	2.28	0.64
1:B:39:LYS:HB2	1:B:149:TYR:CE1	2.32	0.64
1:B:283:GLN:HG3	1:B:285:ALA:H	1.63	0.64
1:A:343:ASP:N	1:A:344:PRO:HD2	2.13	0.64
1:B:91:PRO:HB2	1:B:143:THR:HG22	1.80	0.63
1:B:41:VAL:HG21	1:B:166:LEU:CD1	2.28	0.63
1:A:90:ILE:HD11	1:A:328:VAL:HG13	1.80	0.63
1:A:131:THR:HA	1:A:136:PRO:HA	1.80	0.63
1:B:169:VAL:HG13	1:B:332:VAL:CG2	2.28	0.63
1:B:102:VAL:HG11	1:B:110:PHE:O	1.98	0.63
1:B:179:GLY:O	1:B:207:VAL:HG22	1.97	0.63
1:B:31:PRO:HG3	1:B:75:SER:HB3	1.80	0.63
1:A:335:PHE:HE2	1:A:342:LEU:HB2	1.62	0.63
1:A:161:ASP:O	1:A:162:ALA:CB	2.47	0.63
1:B:41:VAL:HG21	1:B:166:LEU:HD12	1.79	0.63
1:A:205:LEU:HA	1:A:208:ILE:HG23	1.81	0.63
1:A:204:GLY:O	1:A:208:ILE:CG2	2.46	0.63
1:A:146:PHE:O	1:A:352:PHE:CZ	2.51	0.63
1:A:76:ILE:HD13	1:A:85:PRO:HD3	1.81	0.63
1:B:177:SER:O	1:B:181:GLY:N	2.31	0.63
1:B:345:LEU:O	1:B:369:ARG:HB2	1.97	0.62
1:A:205:LEU:HD22	1:A:235:VAL:CG2	2.24	0.62
1:B:334:ASP:OD2	1:B:339:LYS:CE	2.48	0.62
1:B:190:THR:CG2	1:B:191:GLN:N	2.63	0.62
1:B:343:ASP:C	1:B:345:LEU:H	2.03	0.62
1:A:165:PRO:HG2	1:A:335:PHE:CE1	2.29	0.62
1:B:129:ARG:HB3	1:B:139:HIS:NE2	2.14	0.62
1:B:121:GLY:C	1:B:122:THR:HG23	2.20	0.61
1:B:131:THR:O	1:B:131:THR:CG2	2.49	0.61
1:B:122:THR:OG1	1:B:123:MET:HG2	2.00	0.61
1:A:303:MET:CG	1:A:304:ASN:N	2.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HG12	1:A:161:ASP:H	1.65	0.61
1:B:328:VAL:CG2	1:B:329:PRO:HD3	2.27	0.61
1:A:60:PRO:HB2	1:A:138:HIS:CE1	2.35	0.61
1:A:123:MET:HG3	1:A:124:GLN:H	1.64	0.61
1:A:347:THR:HB	1:A:348:HIS:ND1	2.15	0.61
1:A:255:THR:HG23	1:A:281:CYS:HA	1.83	0.61
1:B:88:LYS:HD3	1:B:166:LEU:CD2	2.29	0.61
1:B:41:VAL:CG2	1:B:71:GLY:HA2	2.18	0.61
1:A:96:GLN:HG3	1:A:97:CYS:N	2.16	0.61
1:B:213:ALA:C	1:B:215:GLY:N	2.54	0.60
1:B:70:ALA:HB1	1:B:166:LEU:HD22	1.83	0.60
1:B:46:CYS:HB3	1:B:369:ARG:NH2	2.17	0.60
1:A:335:PHE:CE2	1:A:342:LEU:HB2	2.37	0.60
1:B:249:PRO:O	1:B:252:GLU:HG3	2.01	0.60
1:B:89:VAL:HA	1:B:158:ALA:O	2.00	0.60
1:B:343:ASP:CA	1:B:346:ILE:HG22	2.30	0.60
1:B:158:ALA:O	1:B:160:ILE:HD12	2.01	0.60
1:A:200:LEU:HD12	1:A:223:ASP:HB2	1.82	0.60
1:A:48:SER:HA	1:A:51:HIS:CD2	2.36	0.60
1:B:206:SER:CA	1:B:209:MET:HG3	2.30	0.60
1:A:117:SER:O	1:A:118:MET:HB3	2.02	0.60
1:B:129:ARG:HB3	1:B:139:HIS:HE1	1.58	0.60
1:A:350:LEU:HD13	1:A:370:THR:HG23	1.84	0.60
1:B:348:HIS:O	1:B:370:THR:HA	2.02	0.60
1:B:195:CYS:HA	1:B:264:PHE:O	2.02	0.59
1:B:271:ARG:HB3	1:B:274:THR:CB	2.32	0.59
1:A:284:GLU:O	1:A:310:SER:HB2	2.01	0.59
1:A:60:PRO:HG2	1:A:121:GLY:CA	2.28	0.59
1:A:140:PHE:O	1:A:142:GLY:N	2.35	0.59
1:B:301:LEU:C	1:B:301:LEU:CD1	2.70	0.59
1:A:328:VAL:N	1:A:329:PRO:HD2	2.18	0.59
1:B:172:ILE:HG22	1:B:172:ILE:O	2.01	0.59
1:A:92:LEU:CD1	1:A:325:LYS:HG2	2.32	0.59
1:B:180:TYR:O	1:B:184:VAL:HG23	2.02	0.59
1:A:10:LYS:HD3	1:A:23:ILE:HG22	1.84	0.59
1:B:334:ASP:O	1:B:339:LYS:HB2	2.02	0.59
1:A:37:ARG:HA	1:A:150:THR:O	2.03	0.59
1:A:220:ILE:HG22	1:A:241:VAL:HG12	1.85	0.59
1:B:132:CYS:HB3	1:B:137:ILE:HG13	1.83	0.59
1:A:355:ILE:HB	1:A:372:LEU:CD2	2.32	0.59
1:A:96:GLN:CG	1:A:97:CYS:N	2.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:HD11	1:A:235:VAL:HG23	1.85	0.59
1:B:272:LEU:HG	1:B:301:LEU:HB3	1.84	0.59
1:A:39:LYS:N	1:A:72:ILE:O	2.36	0.59
1:B:355:ILE:C	1:B:357:GLU:H	2.05	0.59
1:B:91:PRO:HB2	1:B:143:THR:CG2	2.33	0.58
1:B:132:CYS:HB3	1:B:137:ILE:CG1	2.32	0.58
1:B:194:THR:HG23	1:B:218:ARG:HB3	1.86	0.58
1:A:352:PHE:CD2	1:A:374:PHE:CE2	2.91	0.58
1:B:63:VAL:HG22	1:B:64:ILE:C	2.23	0.58
1:A:13:VAL:CG2	1:A:64:ILE:HD13	2.33	0.58
1:A:230:ALA:C	1:A:232:ALA:H	2.06	0.58
1:A:154:GLU:O	1:A:157:VAL:HG12	2.03	0.58
1:A:178:THR:HG22	1:A:319:PHE:CD1	2.39	0.58
1:A:13:VAL:HG23	1:A:64:ILE:CD1	2.33	0.58
1:A:251:GLN:HG3	1:A:277:THR:CG2	2.33	0.58
1:B:96:GLN:HG3	1:B:325:LYS:H	1.69	0.58
1:A:2:THR:O	1:A:3:ALA:CB	2.51	0.58
1:B:243:PRO:HB3	1:B:250:ILE:HG13	1.85	0.58
1:B:62:PRO:O	1:B:138:HIS:HB2	2.04	0.58
1:A:77:GLY:H	1:A:80:VAL:HG21	1.69	0.58
1:A:84:ARG:O	1:A:87:ASP:HB2	2.04	0.58
1:A:32:LYS:HB2	1:A:129:ARG:HH12	1.65	0.58
1:A:146:PHE:O	1:A:352:PHE:HZ	1.87	0.58
1:A:129:ARG:HG2	1:A:151:VAL:CG2	2.33	0.57
1:A:262:VAL:HG23	1:A:264:PHE:O	2.03	0.57
1:B:301:LEU:HD13	1:B:301:LEU:O	2.05	0.57
1:A:178:THR:HG22	1:A:319:PHE:HD1	1.69	0.57
1:A:309:LEU:HD23	1:B:318:ILE:HD11	1.87	0.57
1:B:249:PRO:HG2	1:B:252:GLU:OE1	2.04	0.57
1:A:69:ALA:O	1:A:91:PRO:HD2	2.03	0.57
1:A:343:ASP:N	1:A:344:PRO:CD	2.67	0.57
1:B:151:VAL:HG22	1:B:151:VAL:O	2.03	0.57
1:B:26:VAL:CG2	1:B:132:CYS:HB2	2.34	0.57
1:B:72:ILE:HG22	1:B:87:ASP:N	2.20	0.57
1:A:57:LEU:HD12	1:A:57:LEU:C	2.25	0.57
1:A:129:ARG:HG2	1:A:151:VAL:HB	1.87	0.57
1:B:190:THR:CG2	1:B:191:GLN:H	2.16	0.57
1:A:105:HIS:O	1:A:323:LYS:NZ	2.38	0.57
1:A:279:LEU:HD22	1:A:312:ARG:HD3	1.86	0.56
1:B:256:GLU:O	1:B:259:ASN:N	2.38	0.56
1:B:91:PRO:CB	1:B:143:THR:HG22	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HB	1:B:372:LEU:HD21	1.86	0.56
1:B:54:SER:HB2	1:B:56:THR:HG23	1.85	0.56
1:B:129:ARG:CB	1:B:139:HIS:NE2	2.69	0.56
1:B:243:PRO:HA	1:B:250:ILE:CG1	2.35	0.56
1:A:116:LEU:O	1:A:116:LEU:HD22	2.05	0.56
1:B:268:VAL:HG23	3:B:377:NAD:H51N	1.86	0.56
1:B:90:ILE:CD1	1:B:160:ILE:HD13	2.36	0.56
1:A:181:GLY:O	1:A:185:LYS:HB2	2.05	0.56
1:B:166:LEU:C	1:B:167:GLU:HG3	2.26	0.56
1:B:26:VAL:HG22	1:B:132:CYS:HB2	1.87	0.56
1:B:243:PRO:CB	1:B:250:ILE:HG13	2.36	0.56
1:A:157:VAL:HG13	1:A:157:VAL:O	2.07	0.55
1:A:173:GLY:O	1:A:174:CYS:HB2	2.04	0.55
1:B:179:GLY:HA2	1:B:207:VAL:HG22	1.88	0.55
1:B:129:ARG:CB	1:B:139:HIS:CE1	2.85	0.55
1:A:279:LEU:CD2	1:A:312:ARG:HD3	2.36	0.55
1:A:252:GLU:O	1:A:256:GLU:N	2.39	0.55
1:B:282:CYS:O	1:B:312:ARG:NH1	2.39	0.55
1:B:327:SER:C	1:B:329:PRO:CD	2.72	0.55
1:B:41:VAL:O	1:B:374:PHE:HB2	2.06	0.55
1:A:35:GLU:HG2	1:A:123:MET:CE	2.36	0.55
1:A:140:PHE:HD1	1:A:141:LEU:N	2.05	0.55
1:B:218:ARG:NH2	1:B:220:ILE:HD11	2.20	0.55
1:A:293:GLY:O	1:B:309:LEU:HD11	2.07	0.55
1:B:196:ALA:HB2	1:B:262:VAL:HG21	1.89	0.55
1:A:295:PRO:CG	1:B:305:PRO:HG2	2.37	0.55
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.89	0.55
1:A:40:MET:HE1	1:A:145:THR:HG22	1.89	0.54
1:A:161:ASP:CB	1:A:164:SER:OG	2.55	0.54
1:B:301:LEU:H	1:B:301:LEU:HD12	1.73	0.54
1:B:171:LEU:HD11	1:B:369:ARG:CG	2.37	0.54
1:B:283:GLN:HG2	1:B:286:TYR:CE2	2.41	0.54
1:B:129:ARG:CG	1:B:151:VAL:CG1	2.86	0.54
1:B:89:VAL:HG13	1:B:158:ALA:H	1.73	0.54
1:A:363:ARG:CG	1:A:364:SER:N	2.70	0.54
1:B:205:LEU:HD11	1:B:231:LYS:HB2	1.90	0.54
1:B:301:LEU:HD12	1:B:301:LEU:O	2.05	0.54
1:A:40:MET:HE3	1:A:145:THR:HG22	1.90	0.54
1:B:165:PRO:C	1:B:167:GLU:H	2.11	0.54
1:B:59:THR:CG2	1:B:60:PRO:N	2.70	0.54
1:A:243:PRO:CB	1:A:250:ILE:HG13	2.28	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:CG1	1:B:370:THR:HG23	2.30	0.54
1:A:181:GLY:HA3	1:A:322:PHE:CE2	2.43	0.54
1:A:272:LEU:HD12	1:B:305:PRO:CG	2.37	0.54
1:A:177:SER:HB3	1:A:331:LEU:HD13	1.90	0.53
1:A:17:GLU:O	1:A:18:LYS:CB	2.56	0.53
1:B:265:SER:OG	1:B:278:ALA:HB1	2.08	0.53
1:B:262:VAL:HG12	1:B:263:ASP:N	2.24	0.53
1:A:179:GLY:HA2	1:A:207:VAL:CG2	2.31	0.53
1:A:129:ARG:HG2	1:A:151:VAL:CB	2.39	0.53
1:A:359:PHE:O	1:A:363:ARG:HG2	2.09	0.53
1:A:47:ARG:C	1:A:49:ASP:H	2.11	0.53
1:B:88:LYS:HD3	1:B:166:LEU:HD11	1.90	0.53
1:B:204:GLY:N	1:B:268:VAL:HG21	2.24	0.53
1:A:168:LYS:O	1:A:170:CYS:N	2.39	0.53
1:A:371:ILE:HG22	1:A:371:ILE:O	2.07	0.53
1:B:345:LEU:O	1:B:368:ILE:CG2	2.57	0.52
1:B:195:CYS:HB3	1:B:266:PHE:CE1	2.38	0.52
1:A:285:ALA:CB	1:B:102:VAL:HG13	2.39	0.52
1:A:123:MET:HB2	1:A:127:THR:O	2.09	0.52
1:A:160:ILE:CG1	1:A:161:ASP:H	2.22	0.52
1:B:59:THR:HG22	1:B:60:PRO:N	2.23	0.52
1:B:154:GLU:HG2	1:B:154:GLU:O	2.09	0.52
1:B:301:LEU:HD13	1:B:301:LEU:C	2.29	0.52
1:A:140:PHE:CE1	1:A:141:LEU:CG	2.88	0.52
1:A:10:LYS:HA	1:A:24:GLU:O	2.10	0.52
1:B:73:VAL:HG23	1:B:87:ASP:O	2.09	0.52
1:A:96:GLN:O	1:A:155:ILE:HB	2.09	0.52
1:A:334:ASP:CA	1:A:339:LYS:HG2	2.40	0.52
1:A:68:GLU:HG3	1:A:174:CYS:CB	2.38	0.52
1:A:158:ALA:HB3	1:A:328:VAL:HG11	1.91	0.52
1:B:169:VAL:CG1	1:B:332:VAL:CG2	2.86	0.52
1:A:301:LEU:HD11	1:B:303:MET:HE2	1.92	0.52
1:A:23:ILE:CD1	1:A:353:GLU:CA	2.69	0.51
1:A:295:PRO:CB	1:A:296:PRO:HD2	2.40	0.51
1:B:336:MET:HA	1:B:336:MET:HE2	1.92	0.51
1:B:343:ASP:O	1:B:345:LEU:N	2.44	0.51
1:A:188:LYS:O	1:A:189:VAL:C	2.48	0.51
1:A:114:ASN:HD22	1:A:116:LEU:H	1.57	0.51
1:A:230:ALA:C	1:A:232:ALA:N	2.64	0.51
1:B:61:LEU:CD1	1:B:63:VAL:HG12	2.41	0.51
1:A:179:GLY:O	1:A:207:VAL:CG2	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:MET:HG2	1:A:304:ASN:N	2.22	0.51
1:A:290:VAL:HG22	1:A:315:LYS:HB2	1.92	0.51
1:B:90:ILE:CG1	1:B:160:ILE:CD1	2.82	0.51
1:B:113:LYS:HE2	1:B:124:GLN:NE2	2.25	0.51
1:A:190:THR:CG2	1:A:264:PHE:HZ	2.22	0.51
1:A:346:ILE:O	1:A:346:ILE:HG22	2.09	0.51
1:B:16:GLU:HB3	1:B:19:LYS:CG	2.38	0.51
1:B:222:VAL:HG21	1:B:254:LEU:HD11	1.92	0.51
1:B:59:THR:HA	1:B:119:PRO:HB2	1.92	0.51
1:B:203:VAL:CG2	1:B:268:VAL:CG2	2.89	0.51
1:B:9:CYS:HB2	1:B:148:GLN:OE1	2.10	0.51
1:B:236:GLY:O	1:B:237:ALA:O	2.28	0.51
1:A:346:ILE:HA	1:A:369:ARG:O	2.11	0.51
1:A:328:VAL:N	1:A:329:PRO:CD	2.74	0.51
1:A:59:THR:OG1	1:A:60:PRO:HD2	2.11	0.50
1:A:129:ARG:HD2	1:A:151:VAL:HG11	1.93	0.50
1:A:350:LEU:O	1:A:372:LEU:HA	2.11	0.50
1:B:122:THR:CG2	1:B:139:HIS:HB2	2.41	0.50
1:B:148:GLN:HA	1:B:374:PHE:CE2	2.46	0.50
1:A:335:PHE:HB2	1:A:340:PHE:CE2	2.46	0.50
1:A:305:PRO:HB2	1:B:275:MET:HE1	1.93	0.50
1:A:200:LEU:CD1	1:A:223:ASP:HB2	2.41	0.50
1:B:282:CYS:HB2	1:B:287:GLY:HA3	1.93	0.50
1:A:60:PRO:HB2	1:A:138:HIS:NE2	2.27	0.50
1:B:190:THR:HG22	1:B:191:GLN:H	1.72	0.50
1:A:355:ILE:HB	1:A:372:LEU:HD21	1.92	0.50
1:B:200:LEU:HD21	1:B:221:GLY:HA3	1.93	0.50
1:B:143:THR:HA	1:B:152:VAL:HG12	1.94	0.50
1:B:322:PHE:O	1:B:323:LYS:O	2.30	0.50
1:A:310:SER:HB3	1:B:110:PHE:CD2	2.47	0.50
1:B:63:VAL:HG22	1:B:64:ILE:N	2.25	0.50
1:A:129:ARG:HG2	1:A:151:VAL:HG21	1.94	0.50
1:A:308:LEU:HD22	1:A:312:ARG:O	2.12	0.50
1:A:184:VAL:O	1:A:184:VAL:CG1	2.60	0.50
1:A:225:ASN:ND2	1:A:227:ASP:HB2	2.27	0.50
1:B:141:LEU:C	1:B:143:THR:H	2.14	0.49
1:B:122:THR:HG23	1:B:139:HIS:HB2	1.92	0.49
1:A:74:GLU:O	1:A:85:PRO:HB3	2.12	0.49
1:A:303:MET:O	1:B:301:LEU:HD12	2.11	0.49
1:B:250:ILE:O	1:B:254:LEU:HB2	2.12	0.49
1:A:268:VAL:HG13	1:A:292:VAL:CG1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ALA:O	1:A:23:ILE:HA	2.12	0.49
1:B:160:ILE:O	1:B:162:ALA:N	2.43	0.49
1:A:140:PHE:CD1	1:A:141:LEU:N	2.81	0.49
1:B:272:LEU:HD13	1:B:296:PRO:HD2	1.95	0.49
1:A:147:SER:O	1:A:374:PHE:CE2	2.65	0.49
1:A:166:LEU:HA	1:A:169:VAL:HG12	1.94	0.49
1:A:343:ASP:HB2	1:A:344:PRO:HD3	1.93	0.49
1:B:203:VAL:HG23	1:B:204:GLY:N	2.27	0.49
1:B:154:GLU:HA	1:B:157:VAL:CG1	2.43	0.49
1:B:73:VAL:CG1	1:B:75:SER:O	2.61	0.49
1:A:102:VAL:HG11	1:A:110:PHE:O	2.12	0.49
1:B:109:ASN:HD21	1:B:319:PHE:HB3	1.77	0.49
1:A:13:VAL:HG11	1:A:15:TRP:CE2	2.47	0.49
1:B:343:ASP:C	1:B:345:LEU:N	2.66	0.49
1:A:218:ARG:O	1:A:219:ILE:HG13	2.13	0.49
1:B:154:GLU:HA	1:B:157:VAL:HG11	1.95	0.49
1:B:348:HIS:CD2	1:B:361:LEU:HD21	2.48	0.49
1:A:200:LEU:HD12	1:A:223:ASP:CB	2.42	0.49
1:B:13:VAL:HG12	1:B:14:LEU:N	2.28	0.49
1:B:231:LYS:C	1:B:235:VAL:HG22	2.32	0.49
1:B:89:VAL:HG13	1:B:157:VAL:CG2	2.40	0.49
1:A:350:LEU:HD13	1:A:370:THR:CG2	2.43	0.48
1:B:115:ASP:OD1	1:B:120:ARG:N	2.39	0.48
1:B:176:PHE:CE1	1:B:340:PHE:CZ	3.01	0.48
1:A:339:LYS:CA	1:A:339:LYS:CE	2.88	0.48
1:A:93:PHE:CE1	1:A:174:CYS:SG	3.06	0.48
1:A:194:THR:HG21	1:A:258:SER:OG	2.14	0.48
1:A:232:ALA:O	1:A:235:VAL:CG2	2.57	0.48
1:A:195:CYS:SG	1:A:211:CYS:HB3	2.53	0.48
1:B:31:PRO:HG3	1:B:37:ARG:HB2	1.96	0.48
1:A:7:ILE:HG13	1:A:37:ARG:CZ	2.44	0.48
1:A:352:PHE:CE2	1:A:374:PHE:CE2	3.02	0.48
1:B:93:PHE:HB2	1:B:141:LEU:HD23	1.96	0.48
1:A:309:LEU:HD12	1:B:291:ILE:HG22	1.95	0.48
1:B:327:SER:N	1:B:329:PRO:HD2	2.29	0.48
1:A:31:PRO:HD3	1:A:37:ARG:HG2	1.95	0.48
1:B:308:LEU:HD11	1:B:314:TRP:HB2	1.95	0.48
1:B:121:GLY:CA	1:B:138:HIS:CD2	2.85	0.48
1:A:23:ILE:HD12	1:A:353:GLU:HA	1.83	0.48
1:A:35:GLU:OE1	1:A:129:ARG:NH1	2.47	0.48
1:B:19:LYS:CD	1:B:19:LYS:N	2.76	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:O	1:A:169:VAL:CG1	2.61	0.48
1:B:71:GLY:O	1:B:88:LYS:HA	2.13	0.47
1:A:310:SER:HA	1:B:318:ILE:HD12	1.95	0.47
1:A:327:SER:O	1:A:331:LEU:HB2	2.14	0.47
1:A:5:LYS:CA	1:A:30:PRO:HG3	2.39	0.47
1:B:6:VAL:CG1	1:B:7:ILE:N	2.76	0.47
1:B:200:LEU:HD12	1:B:223:ASP:HB2	1.96	0.47
1:B:6:VAL:HG12	1:B:7:ILE:N	2.29	0.47
1:A:316:GLY:HA3	1:B:308:LEU:O	2.14	0.47
1:B:258:SER:O	1:B:259:ASN:C	2.53	0.47
1:A:200:LEU:HD21	1:A:221:GLY:HA3	1.96	0.47
1:B:133:ARG:HB3	1:B:134:GLY:H	1.55	0.47
1:B:243:PRO:HB3	1:B:250:ILE:CG1	2.45	0.47
1:B:210:GLY:O	1:B:214:ALA:N	2.30	0.47
1:B:169:VAL:O	1:B:169:VAL:CG1	2.62	0.47
1:B:15:TRP:HA	1:B:62:PRO:HB3	1.96	0.47
1:B:198:PHE:HB2	1:B:267:GLU:HA	1.97	0.47
1:B:295:PRO:CB	1:B:296:PRO:HD2	2.44	0.47
1:B:265:SER:O	1:B:289:SER:HA	2.15	0.47
1:A:275:MET:SD	1:B:305:PRO:HB3	2.55	0.47
1:A:13:VAL:CG2	1:A:137:ILE:HG21	2.40	0.47
1:A:363:ARG:C	1:A:365:GLY:H	2.16	0.47
1:A:363:ARG:C	1:A:365:GLY:N	2.68	0.46
1:B:284:GLU:HA	1:B:312:ARG:CZ	2.46	0.46
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.86	0.46
1:B:331:LEU:O	1:B:334:ASP:HB2	2.15	0.46
1:A:303:MET:CE	1:A:308:LEU:HG	2.46	0.46
1:B:88:LYS:HG2	1:B:166:LEU:HD11	1.97	0.46
1:A:168:LYS:HG2	1:A:335:PHE:CZ	2.46	0.46
1:B:39:LYS:CB	1:B:149:TYR:CE1	2.97	0.46
1:B:9:CYS:O	1:B:26:VAL:N	2.41	0.46
1:A:47:ARG:O	1:A:50:ASP:N	2.45	0.46
1:A:47:ARG:C	1:A:49:ASP:N	2.68	0.46
1:B:231:LYS:HG2	1:B:231:LYS:H	1.54	0.46
1:B:269:ILE:CD1	1:B:274:THR:HG21	2.36	0.46
1:B:172:ILE:O	1:B:172:ILE:CG2	2.64	0.46
1:A:268:VAL:HG13	1:A:292:VAL:HG11	1.97	0.46
1:B:304:ASN:O	1:B:306:MET:N	2.49	0.46
1:A:205:LEU:CA	1:A:208:ILE:HG23	2.46	0.46
1:B:348:HIS:HE1	1:B:366:GLU:O	1.99	0.46
1:A:285:ALA:CB	1:B:102:VAL:CG1	2.94	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:CYS:O	1:A:219:ILE:HA	2.16	0.46
1:B:201:GLY:O	1:B:205:LEU:HB2	2.17	0.45
1:B:256:GLU:HA	1:B:259:ASN:HA	1.97	0.45
1:B:69:ALA:HA	1:B:170:CYS:HB2	1.98	0.45
1:A:305:PRO:HG2	1:B:272:LEU:HD11	1.98	0.45
1:B:63:VAL:CG2	1:B:64:ILE:N	2.79	0.45
1:A:40:MET:HE1	1:A:145:THR:CG2	2.45	0.45
1:B:13:VAL:CG1	1:B:14:LEU:N	2.79	0.45
1:B:195:CYS:CB	1:B:266:PHE:HE1	2.26	0.45
1:A:232:ALA:HA	1:A:235:VAL:HG22	1.96	0.45
1:A:152:VAL:HG23	1:A:153:ASP:O	2.16	0.45
1:A:249:PRO:HG2	1:A:252:GLU:OE1	2.16	0.45
1:A:295:PRO:CB	1:A:296:PRO:CD	2.95	0.45
1:B:238:THR:OG1	1:B:239:GLU:N	2.49	0.45
1:B:322:PHE:O	1:B:323:LYS:C	2.55	0.45
1:A:335:PHE:CE2	1:A:342:LEU:HD22	2.51	0.45
1:A:118:MET:HA	1:A:119:PRO:HD2	1.71	0.45
1:B:231:LYS:HE2	1:B:344:PRO:O	2.17	0.45
1:A:295:PRO:HG3	1:B:305:PRO:HG2	1.98	0.45
1:B:198:PHE:CD1	1:B:274:THR:HG23	2.51	0.45
1:A:305:PRO:HB2	1:B:275:MET:CE	2.46	0.45
1:B:362:LEU:C	1:B:364:SER:H	2.20	0.45
1:B:361:LEU:HB3	1:B:367:SER:HB2	1.98	0.45
1:A:218:ARG:O	1:A:219:ILE:CG1	2.65	0.45
1:B:90:ILE:CD1	1:B:160:ILE:CD1	2.95	0.45
1:B:23:ILE:HD12	1:B:353:GLU:HA	1.88	0.45
1:B:169:VAL:HG11	1:B:332:VAL:HG22	1.96	0.44
1:B:94:THR:HG21	1:B:319:PHE:HB2	1.99	0.44
1:B:174:CYS:HB3	1:B:175:GLY:H	1.53	0.44
1:B:248:LYS:HD3	1:B:253:VAL:HG23	1.99	0.44
1:B:323:LYS:O	1:B:327:SER:OG	2.36	0.44
1:A:267:GLU:HG2	1:A:274:THR:HG22	1.99	0.44
1:A:43:THR:HG23	1:A:69:ALA:HB2	1.98	0.44
1:B:347:THR:CG2	1:B:368:ILE:HB	2.48	0.44
1:A:62:PRO:O	1:A:138:HIS:CB	2.50	0.44
1:A:64:ILE:O	1:A:65:ALA:O	2.35	0.44
1:B:223:ASP:OD2	3:B:377:NAD:H1B	2.17	0.44
1:A:250:ILE:O	1:A:254:LEU:HB2	2.18	0.44
1:B:322:PHE:C	1:B:323:LYS:O	2.54	0.44
1:A:301:LEU:CD2	1:B:303:MET:HE3	2.40	0.44
1:A:35:GLU:HG2	1:A:123:MET:HE2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:HG21	1:A:368:ILE:HG23	1.99	0.44
1:A:189:VAL:HB	1:A:214:ALA:CB	2.47	0.44
1:B:200:LEU:O	1:B:228:LYS:HG2	2.17	0.44
1:B:52:VAL:HA	1:B:57:LEU:O	2.18	0.44
1:A:14:LEU:HD11	1:A:53:VAL:HA	1.99	0.44
1:B:343:ASP:N	1:B:344:PRO:CD	2.81	0.43
1:B:347:THR:HG23	1:B:368:ILE:HB	2.00	0.43
1:A:262:VAL:CG2	1:A:264:PHE:O	2.65	0.43
1:A:147:SER:CB	1:A:149:TYR:O	2.59	0.43
1:B:248:LYS:HD3	1:B:253:VAL:CG2	2.47	0.43
1:B:223:ASP:CG	3:B:377:NAD:H1B	2.39	0.43
1:A:254:LEU:HA	1:A:254:LEU:HD22	1.74	0.43
1:A:304:ASN:HD21	1:A:306:MET:HB2	1.74	0.43
1:A:222:VAL:HG22	1:A:241:VAL:HG13	2.00	0.43
1:A:100:CYS:O	1:A:102:VAL:N	2.51	0.43
1:B:349:VAL:CG1	1:B:373:THR:HG22	2.46	0.43
1:B:61:LEU:HD11	1:B:63:VAL:HG12	2.01	0.43
1:B:306:MET:HA	1:B:309:LEU:HB2	2.00	0.43
1:A:353:GLU:CD	1:A:353:GLU:H	2.22	0.43
1:A:334:ASP:HA	1:A:339:LYS:HG2	2.00	0.43
1:B:204:GLY:CA	1:B:268:VAL:HG21	2.48	0.43
1:A:352:PHE:C	1:A:355:ILE:HG22	2.38	0.43
1:B:294:VAL:HG23	3:B:377:NAD:H2N	2.00	0.43
1:B:361:LEU:CG	1:B:367:SER:HB2	2.49	0.43
1:A:23:ILE:HD13	1:A:353:GLU:HA	1.88	0.43
1:A:105:HIS:CE1	1:B:286:TYR:CD1	3.05	0.43
1:B:74:GLU:HB3	1:B:75:SER:H	1.18	0.43
1:A:35:GLU:CG	1:A:153:ASP:HA	2.48	0.43
1:B:131:THR:HA	1:B:136:PRO:HA	2.01	0.43
1:A:128:SER:HA	1:A:139:HIS:NE2	2.33	0.43
1:B:334:ASP:O	1:B:339:LYS:CB	2.67	0.43
1:A:338:LYS:HB3	1:A:338:LYS:HE3	1.49	0.43
1:A:84:ARG:O	1:A:87:ASP:CG	2.57	0.43
1:B:304:ASN:C	1:B:306:MET:H	2.22	0.43
1:A:81:THR:OG1	1:A:82:THR:N	2.52	0.42
1:A:355:ILE:HA	1:A:372:LEU:HD21	2.00	0.42
1:B:195:CYS:CA	1:B:264:PHE:O	2.67	0.42
1:B:186:VAL:HG21	1:B:290:VAL:HG11	1.98	0.42
1:B:11:ALA:HB1	1:B:64:ILE:HD12	2.01	0.42
1:B:63:VAL:HG22	1:B:64:ILE:O	2.18	0.42
1:B:284:GLU:O	1:B:310:SER:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LYS:HG2	1:B:315:LYS:H	1.73	0.42
1:A:339:LYS:HD2	1:A:339:LYS:N	2.33	0.42
1:A:168:LYS:C	1:A:170:CYS:H	2.19	0.42
1:B:318:ILE:CG2	1:B:319:PHE:N	2.83	0.42
1:B:32:LYS:HB3	1:B:33:ALA:H	1.44	0.42
1:B:6:VAL:CG1	1:B:27:GLU:HG3	2.50	0.42
1:A:272:LEU:CD1	1:B:305:PRO:CG	2.97	0.42
1:A:271:ARG:HB3	1:A:273:ASP:OD1	2.19	0.42
1:B:362:LEU:C	1:B:364:SER:N	2.72	0.42
1:A:143:THR:O	1:A:144:SER:C	2.57	0.42
1:A:319:PHE:HD1	1:A:319:PHE:HA	1.60	0.42
1:B:179:GLY:HA2	1:B:207:VAL:CG2	2.49	0.42
1:B:179:GLY:CA	1:B:207:VAL:HG22	2.48	0.42
1:A:10:LYS:HB2	1:A:10:LYS:HE2	1.54	0.42
1:B:349:VAL:HG12	1:B:373:THR:HG21	1.95	0.42
1:B:361:LEU:HG	1:B:367:SER:HB2	2.01	0.42
1:A:93:PHE:HB2	1:A:141:LEU:HD13	2.01	0.42
1:A:84:ARG:O	1:A:87:ASP:CB	2.67	0.42
1:B:97:CYS:SG	1:B:100:CYS:SG	3.18	0.42
1:B:39:LYS:HB2	1:B:149:TYR:CZ	2.54	0.42
1:A:220:ILE:HG23	1:A:239:GLU:HB3	2.02	0.42
1:A:334:ASP:CB	1:A:339:LYS:HG2	2.50	0.42
1:A:122:THR:HB	1:A:123:MET:H	1.65	0.42
1:A:187:ALA:HB2	1:A:266:PHE:CE2	2.55	0.42
1:B:54:SER:CB	1:B:56:THR:HG23	2.48	0.42
1:A:100:CYS:O	1:A:103:CYS:N	2.51	0.42
1:B:116:LEU:O	1:B:116:LEU:HD12	2.19	0.42
1:A:355:ILE:HB	1:A:372:LEU:HD23	2.00	0.41
1:A:43:THR:OG1	1:A:374:PHE:CE1	2.73	0.41
1:A:241:VAL:HG23	1:A:246:TYR:HE1	1.84	0.41
1:A:100:CYS:HB2	1:A:112:LEU:HD22	2.01	0.41
1:B:231:LYS:HE2	1:B:231:LYS:HB3	1.73	0.41
1:B:171:LEU:CD1	1:B:371:ILE:HD11	2.50	0.41
1:A:90:ILE:HG21	1:A:90:ILE:HD13	1.81	0.41
1:B:43:THR:HG23	1:B:69:ALA:HB2	2.02	0.41
1:A:275:MET:SD	1:B:305:PRO:CB	3.08	0.41
1:A:286:TYR:CD1	1:B:105:HIS:CE1	3.08	0.41
1:B:169:VAL:O	1:B:169:VAL:HG12	2.19	0.41
1:A:306:MET:HE2	1:A:309:LEU:HD22	2.01	0.41
1:A:347:THR:CG2	1:A:368:ILE:HG23	2.51	0.41
1:B:213:ALA:C	1:B:215:GLY:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASP:OD2	1:B:66:GLY:HA2	2.21	0.41
1:B:203:VAL:C	1:B:205:LEU:H	2.23	0.41
1:B:352:PHE:O	1:B:353:GLU:CB	2.55	0.41
1:B:152:VAL:HB	1:B:153:ASP:H	1.72	0.41
1:B:288:VAL:CG1	1:B:315:LYS:HD3	2.50	0.41
1:B:72:ILE:CG2	1:B:87:ASP:N	2.83	0.41
1:B:328:VAL:HG22	1:B:329:PRO:CD	2.34	0.41
1:A:306:MET:CE	1:A:309:LEU:HD22	2.50	0.41
1:B:129:ARG:CG	1:B:151:VAL:HG11	2.51	0.41
1:A:295:PRO:HB3	1:A:296:PRO:HD2	2.02	0.41
1:A:357:GLU:O	1:A:361:LEU:HG	2.20	0.41
1:A:64:ILE:HB	1:A:144:SER:HB3	2.02	0.41
1:A:34:HIS:O	1:A:154:GLU:HB2	2.21	0.41
1:A:275:MET:SD	1:A:291:ILE:HD12	2.61	0.41
1:A:187:ALA:CB	1:A:266:PHE:CE2	3.04	0.41
1:A:203:VAL:HG12	1:A:268:VAL:HG11	2.02	0.41
1:A:100:CYS:O	1:A:100:CYS:SG	2.79	0.41
1:B:115:ASP:OD1	1:B:120:ARG:HB3	2.21	0.41
1:B:129:ARG:HG3	1:B:151:VAL:HG11	2.02	0.41
1:B:256:GLU:HA	1:B:259:ASN:CA	2.51	0.41
1:B:254:LEU:HD22	1:B:281:CYS:SG	2.61	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.89	0.41
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.88	0.41
1:B:10:LYS:HB2	1:B:148:GLN:OE1	2.21	0.41
1:B:230:ALA:O	1:B:231:LYS:C	2.59	0.41
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.85	0.41
1:A:332:VAL:C	1:A:334:ASP:H	2.25	0.40
1:A:123:MET:HE2	1:A:151:VAL:HG12	2.02	0.40
1:A:347:THR:HB	1:A:348:HIS:CE1	2.56	0.40
1:B:105:HIS:HD2	1:B:108:GLY:N	2.18	0.40
1:A:171:LEU:HD11	1:A:369:ARG:HG2	2.02	0.40
1:B:88:LYS:HD3	1:B:166:LEU:CG	2.52	0.40
1:A:208:ILE:HD11	1:A:237:ALA:HB2	1.97	0.40
1:A:181:GLY:O	1:A:185:LYS:CB	2.70	0.40
1:B:208:ILE:O	1:B:208:ILE:CG2	2.69	0.40
1:A:41:VAL:CG2	1:A:72:ILE:HD12	2.52	0.40
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.79	0.40
1:B:205:LEU:HD13	1:B:235:VAL:HG21	2.02	0.40
1:A:161:ASP:HB3	1:A:162:ALA:H	1.64	0.40

All (63) 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:248:LYS:NZ	1:B:245:ASP:OD1[1_655]	0.31	1.89
1:B:16:GLU:OE2	1:B:81:THR:CG2[1_545]	0.68	1.52
1:A:245:ASP:O	1:B:248:LYS:CB[1_655]	0.71	1.49
1:A:247:LYS:N	1:B:247:LYS:N[1_655]	0.72	1.48
1:A:248:LYS:CD	1:B:245:ASP:CB[1_655]	0.75	1.45
1:A:245:ASP:C	1:B:248:LYS:CG[1_655]	0.81	1.39
1:A:245:ASP:O	1:B:248:LYS:CG[1_655]	0.95	1.25
1:A:248:LYS:NZ	1:B:245:ASP:CG[1_655]	1.05	1.15
1:A:248:LYS:CG	1:B:245:ASP:C[1_655]	1.06	1.14
1:B:19:LYS:CE	1:B:81:THR:O[1_545]	1.07	1.13
1:B:19:LYS:NZ	1:B:81:THR:O[1_545]	1.14	1.06
1:A:248:LYS:CE	1:B:245:ASP:CG[1_655]	1.18	1.02
1:A:248:LYS:CG	1:B:245:ASP:O[1_655]	1.18	1.02
1:A:246:TYR:O	1:B:247:LYS:CG[1_655]	1.19	1.01
1:A:247:LYS:CB	1:B:246:TYR:O[1_655]	1.26	0.94
1:B:16:GLU:CD	1:B:81:THR:CG2[1_545]	1.33	0.87
1:A:247:LYS:CA	1:B:247:LYS:N[1_655]	1.41	0.79
1:A:247:LYS:CB	1:B:246:TYR:C[1_655]	1.45	0.75
1:A:245:ASP:CB	1:B:248:LYS:CE[1_655]	1.47	0.73
1:A:218:ARG:NH2	1:B:239:GLU:OE2[1_655]	1.48	0.72
1:A:248:LYS:CG	1:B:245:ASP:CA[1_655]	1.50	0.70
1:A:248:LYS:CE	1:B:245:ASP:OD1[1_655]	1.52	0.68
1:A:17:GLU:OE2	1:A:337:ALA:O[1_545]	1.52	0.68
1:A:248:LYS:CE	1:B:245:ASP:CB[1_655]	1.55	0.65
1:A:248:LYS:CB	1:B:245:ASP:O[1_655]	1.56	0.64
1:B:16:GLU:OE2	1:B:81:THR:CB[1_545]	1.58	0.62
1:A:246:TYR:N	1:B:248:LYS:CG[1_655]	1.61	0.59
1:A:247:LYS:N	1:B:246:TYR:C[1_655]	1.63	0.57
1:A:17:GLU:OE2	1:A:337:ALA:C[1_545]	1.64	0.56
1:A:245:ASP:O	1:B:248:LYS:CA[1_655]	1.67	0.53
1:A:245:ASP:C	1:B:248:LYS:CB[1_655]	1.69	0.51
1:A:248:LYS:CG	1:B:245:ASP:CB[1_655]	1.69	0.51
1:A:246:TYR:O	1:B:247:LYS:CB[1_655]	1.71	0.49
1:A:233:LYS:NZ	1:B:259:ASN:OD1[1_655]	1.73	0.47
1:A:246:TYR:C	1:B:247:LYS:N[1_655]	1.75	0.45
1:A:248:LYS:CA	1:B:245:ASP:O[1_655]	1.78	0.42
1:A:247:LYS:CA	1:B:246:TYR:C[1_655]	1.79	0.41
1:B:19:LYS:NZ	1:B:81:THR:C[1_545]	1.79	0.41
1:A:248:LYS:CB	1:B:245:ASP:C[1_655]	1.81	0.39
1:A:246:TYR:CD2	1:B:246:TYR:CD2[1_655]	1.87	0.33
1:A:248:LYS:CB	1:B:245:ASP:CA[1_655]	1.90	0.30
1:A:248:LYS:N	1:B:245:ASP:O[1_655]	1.90	0.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:NZ	1:B:245:ASP:OD2[1_655]	1.93	0.27
1:A:248:LYS:CD	1:B:245:ASP:CG[1_655]	1.94	0.26
1:B:16:GLU:OE1	1:B:81:THR:CG2[1_545]	1.95	0.25
1:A:247:LYS:CG	1:B:246:TYR:O[1_655]	1.95	0.25
1:A:17:GLU:O	1:A:338:LYS:CD[1_545]	1.96	0.24
1:A:25:GLU:OE1	1:B:72:ILE:CD1[1_544]	1.97	0.23
1:B:16:GLU:OE2	1:B:81:THR:OG1[1_545]	1.98	0.22
1:A:246:TYR:C	1:B:247:LYS:CG[1_655]	1.98	0.22
1:A:247:LYS:N	1:B:247:LYS:CA[1_655]	2.00	0.20
1:A:239:GLU:OE2	1:B:257:MET:CG[1_655]	2.00	0.20
1:A:248:LYS:CD	1:B:245:ASP:CA[1_655]	2.02	0.18
1:A:247:LYS:CA	1:B:247:LYS:CA[1_655]	2.06	0.14
1:A:17:GLU:OE2	1:A:337:ALA:CA[1_545]	2.06	0.14
1:A:248:LYS:N	1:B:245:ASP:C[1_655]	2.09	0.11
1:A:247:LYS:CB	1:B:247:LYS:N[1_655]	2.11	0.09
1:A:247:LYS:CD	1:B:246:TYR:O[1_655]	2.11	0.09
1:A:245:ASP:C	1:B:248:LYS:CD[1_655]	2.12	0.08
1:A:245:ASP:CA	1:B:248:LYS:CG[1_655]	2.14	0.06
1:A:247:LYS:N	1:B:246:TYR:CA[1_655]	2.15	0.05
1:A:246:TYR:CE2	1:B:253:VAL:CG2[1_655]	2.16	0.04
1:A:245:ASP:O	1:B:248:LYS:N[1_655]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	372/374 (100%)	281 (76%)	53 (14%)	38 (10%)	1 2
1	B	372/374 (100%)	282 (76%)	58 (16%)	32 (9%)	1 2
All	All	744/748 (100%)	563 (76%)	111 (15%)	70 (9%)	1 2

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	33	ALA
1	A	65	ALA
1	A	99	LYS
1	A	109	ASN
1	A	162	ALA
1	A	169	VAL
1	A	174	CYS
1	A	189	VAL
1	A	216	ALA
1	A	259	ASN
1	A	297	ASP
1	A	298	SER
1	A	353	GLU
1	A	367	SER
1	B	6	VAL
1	B	112	LEU
1	B	128	SER
1	B	133	ARG
1	B	161	ASP
1	B	175	GLY
1	B	237	ALA
1	B	297	ASP
1	A	18	LYS
1	A	97	CYS
1	A	101	ARG
1	A	110	PHE
1	A	141	LEU
1	A	144	SER
1	A	161	ASP
1	A	175	GLY
1	A	293	GLY
1	A	352	PHE
1	B	18	LYS
1	B	34	HIS
1	B	174	CYS
1	B	202	GLY
1	B	259	ASN
1	B	323	LYS
1	B	353	GLU
1	A	2	THR
1	A	4	GLY
1	A	67	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4	GLY
1	B	33	ALA
1	B	97	CYS
1	B	154	GLU
1	B	284	GLU
1	B	363	ARG
1	A	82	THR
1	A	134	GLY
1	A	153	ASP
1	A	188	LYS
1	A	284	GLU
1	B	65	ALA
1	B	81	THR
1	B	123	MET
1	B	124	GLN
1	A	160	ILE
1	A	177	SER
1	B	95	PRO
1	B	262	VAL
1	B	365	GLY
1	A	142	GLY
1	A	219	ILE
1	B	305	PRO
1	B	356	ASN
1	A	311	GLY
1	B	152	VAL
1	B	236	GLY

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	308/308 (100%)	196 (64%)	112 (36%)	0 0
1	B	308/308 (100%)	195 (63%)	113 (37%)	0 0
All	All	616/616 (100%)	391 (64%)	225 (36%)	0 0

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	5	LYS
1	A	10	LYS
1	A	13	VAL
1	A	14	LEU
1	A	18	LYS
1	A	22	SER
1	A	27	GLU
1	A	28	VAL
1	A	32	LYS
1	A	37	ARG
1	A	43	THR
1	A	48	SER
1	A	54	SER
1	A	56	THR
1	A	57	LEU
1	A	74	GLU
1	A	75	SER
1	A	76	ILE
1	A	78	GLU
1	A	82	THR
1	A	83	VAL
1	A	96	GLN
1	A	99	LYS
1	A	101	ARG
1	A	107	GLU
1	A	112	LEU
1	A	116	LEU
1	A	118	MET
1	A	120	ARG
1	A	124	GLN
1	A	128	SER
1	A	129	ARG
1	A	131	THR
1	A	139	HIS
1	A	140	PHE
1	A	147	SER
1	A	148	GLN
1	A	150	THR
1	A	152	VAL
1	A	153	ASP
1	A	160	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	SER
1	A	168	LYS
1	A	169	VAL
1	A	170	CYS
1	A	171	LEU
1	A	178	THR
1	A	185	LYS
1	A	191	GLN
1	A	193	SER
1	A	208	ILE
1	A	218	ARG
1	A	220	ILE
1	A	225	ASN
1	A	226	LYS
1	A	228	LYS
1	A	231	LYS
1	A	235	VAL
1	A	238	THR
1	A	241	VAL
1	A	242	ASN
1	A	247	LYS
1	A	248	LYS
1	A	250	ILE
1	A	251	GLN
1	A	254	LEU
1	A	258	SER
1	A	259	ASN
1	A	262	VAL
1	A	268	VAL
1	A	272	LEU
1	A	276	VAL
1	A	279	LEU
1	A	280	SER
1	A	281	CYS
1	A	283	GLN
1	A	291	ILE
1	A	297	ASP
1	A	299	GLN
1	A	302	SER
1	A	303	MET
1	A	304	ASN
1	A	306	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	309	LEU
1	A	310	SER
1	A	313	THR
1	A	314	TRP
1	A	318	ILE
1	A	319	PHE
1	A	324	SER
1	A	326	ASP
1	A	327	SER
1	A	328	VAL
1	A	330	LYS
1	A	331	LEU
1	A	338	LYS
1	A	339	LYS
1	A	342	LEU
1	A	346	ILE
1	A	347	THR
1	A	355	ILE
1	A	356	ASN
1	A	360	ASP
1	A	364	SER
1	A	366	GLU
1	A	367	SER
1	A	368	ILE
1	A	369	ARG
1	A	371	ILE
1	A	372	LEU
1	A	373	THR
1	B	1	SER
1	B	7	ILE
1	B	18	LYS
1	B	19	LYS
1	B	23	ILE
1	B	26	VAL
1	B	27	GLU
1	B	34	HIS
1	B	37	ARG
1	B	39	LYS
1	B	40	MET
1	B	43	THR
1	B	45	ILE
1	B	46	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	61	LEU
1	B	72	ILE
1	B	73	VAL
1	B	74	GLU
1	B	75	SER
1	B	76	ILE
1	B	82	THR
1	B	94	THR
1	B	96	GLN
1	B	97	CYS
1	B	99	LYS
1	B	100	CYS
1	B	103	CYS
1	B	104	LYS
1	B	107	GLU
1	B	109	ASN
1	B	110	PHE
1	B	112	LEU
1	B	113	LYS
1	B	114	ASN
1	B	115	ASP
1	B	117	SER
1	B	120	ARG
1	B	122	THR
1	B	124	GLN
1	B	125	ASP
1	B	129	ARG
1	B	133	ARG
1	B	135	LYS
1	B	141	LEU
1	B	143	THR
1	B	148	GLN
1	B	151	VAL
1	B	155	ILE
1	B	156	SER
1	B	160	ILE
1	B	164	SER
1	B	167	GLU
1	B	168	LYS
1	B	171	LEU
1	B	174	CYS
1	B	186	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	191	GLN
1	B	195	CYS
1	B	205	LEU
1	B	206	SER
1	B	208	ILE
1	B	212	LYS
1	B	219	ILE
1	B	224	ILE
1	B	228	LYS
1	B	231	LYS
1	B	239	GLU
1	B	240	CYS
1	B	242	ASN
1	B	248	LYS
1	B	250	ILE
1	B	252	GLU
1	B	254	LEU
1	B	256	GLU
1	B	262	VAL
1	B	263	ASP
1	B	265	SER
1	B	267	GLU
1	B	268	VAL
1	B	271	ARG
1	B	272	LEU
1	B	275	MET
1	B	279	LEU
1	B	289	SER
1	B	295	PRO
1	B	301	LEU
1	B	303	MET
1	B	306	MET
1	B	308	LEU
1	B	309	LEU
1	B	313	THR
1	B	315	LYS
1	B	319	PHE
1	B	323	LYS
1	B	324	SER
1	B	325	LYS
1	B	327	SER
1	B	328	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	330	LYS
1	B	332	VAL
1	B	339	LYS
1	B	342	LEU
1	B	345	LEU
1	B	346	ILE
1	B	350	LEU
1	B	354	LYS
1	B	356	ASN
1	B	357	GLU
1	B	366	GLU
1	B	369	ARG
1	B	371	ILE
1	B	373	THR
1	B	374	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	114	ASN
1	A	242	ASN
1	A	299	GLN
1	A	300	ASN
1	A	304	ASN
1	B	105	HIS
1	B	109	ASN
1	B	124	GLN
1	B	138	HIS
1	B	225	ASN
1	B	242	ASN
1	B	300	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	NAD	A	377	-	38,48,48	1.06	1 (2%)	47,73,73	1.68	6 (12%)
4	DMS	A	378	2	3,3,3	0.55	0	3,3,3	0.12	0
3	NAD	B	377	-	38,48,48	1.64	3 (7%)	47,73,73	1.96	9 (19%)
4	DMS	B	378	2	3,3,3	0.59	0	3,3,3	0.16	0

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
3	NAD	A	377	-	-	0/22/62/62	0/5/5/5
4	DMS	A	378	2	-	0/0/0/0	0/0/0/0
3	NAD	B	377	-	-	0/22/62/62	0/5/5/5
4	DMS	B	378	2	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	377	NAD	C5B-C4B	-7.45	1.27	1.51
3	B	377	NAD	C6N-N1N	2.06	1.41	1.35
3	B	377	NAD	C3N-C7N	3.72	1.56	1.50
3	A	377	NAD	C3N-C7N	4.32	1.57	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	377	NAD	C5N-C4N-C3N	-6.22	112.52	120.33
3	A	377	NAD	C5N-C4N-C3N	-5.81	113.03	120.33
3	B	377	NAD	C2B-C1B-N9A	-4.34	107.66	114.29
3	B	377	NAD	C5N-C6N-N1N	-3.61	114.23	120.47
3	A	377	NAD	C5N-C6N-N1N	-3.26	114.83	120.47
3	A	377	NAD	C1B-N9A-C4A	-2.51	123.16	126.94
3	A	377	NAD	C4N-C3N-C7N	-2.27	115.09	121.09
3	B	377	NAD	C3N-C7N-N7N	-2.24	115.37	117.82
3	B	377	NAD	O2A-PA-O3	2.06	114.44	105.09
3	B	377	NAD	C4A-C5A-N7A	2.36	111.65	109.48
3	A	377	NAD	C2N-C3N-C4N	3.89	122.63	118.29
3	B	377	NAD	C2N-C3N-C4N	3.92	122.66	118.29
3	B	377	NAD	O4B-C4B-C5B	4.65	125.96	109.32
3	A	377	NAD	C6N-C5N-C4N	5.49	127.74	119.44
3	B	377	NAD	C6N-C5N-C4N	5.61	127.92	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	377	NAD	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.