



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:07 PM GMT

PDB ID : 1BI9  
Title : RETINAL DEHYDROGENASE TYPE TWO WITH NAD BOUND  
Authors : Newcomer, M.E.; Lamb, A.L.  
Deposited on : 1998-06-23  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

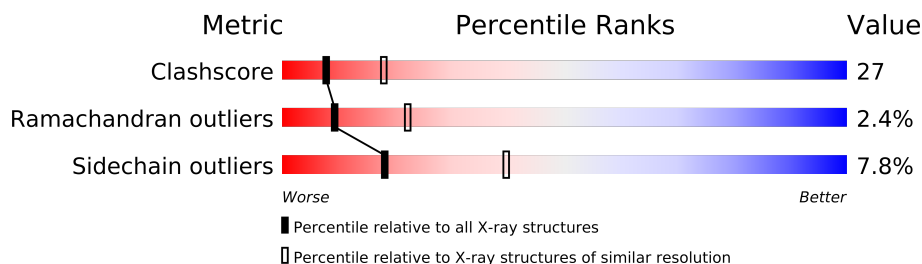
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
1	C	499	
1	D	499	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 15156 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

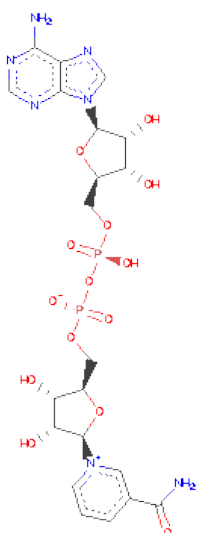
- Molecule 1 is a protein called RETINAL DEHYDROGENASE TYPE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3697	2356	628	694	19			
1	B	477	Total	C	N	O	S	0	0	0
			3689	2351	627	693	18			
1	C	480	Total	C	N	O	S	0	0	0
			3710	2363	631	697	19			
1	D	482	Total	C	N	O	S	0	0	0
			3726	2373	634	700	19			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

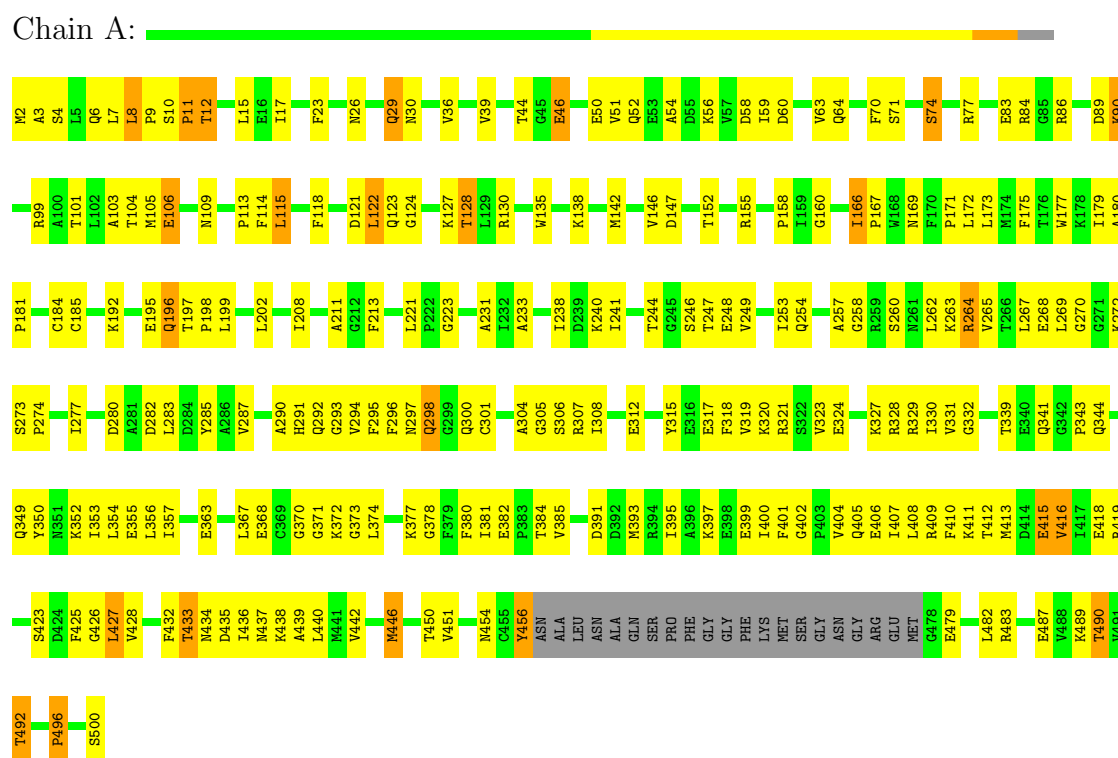
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	53	Total	O	0	0
			53	53		
4	C	68	Total	O	0	0
			68	68		
4	D	66	Total	O	0	0
			66	66		

### 3 Residue-property plots

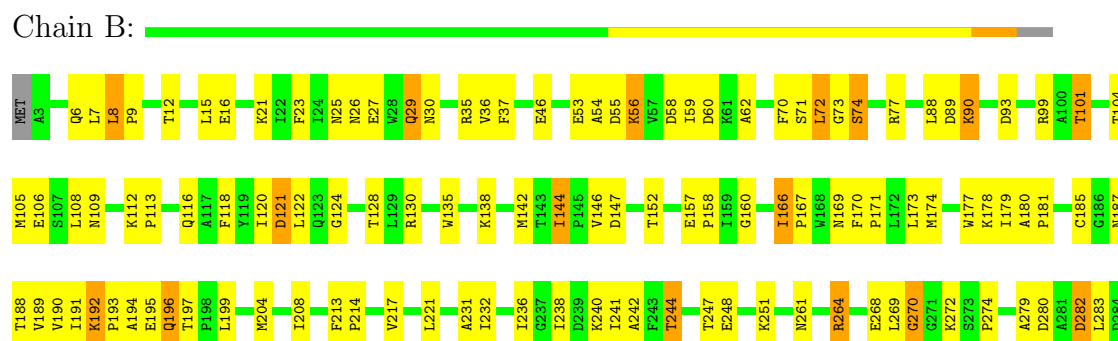
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

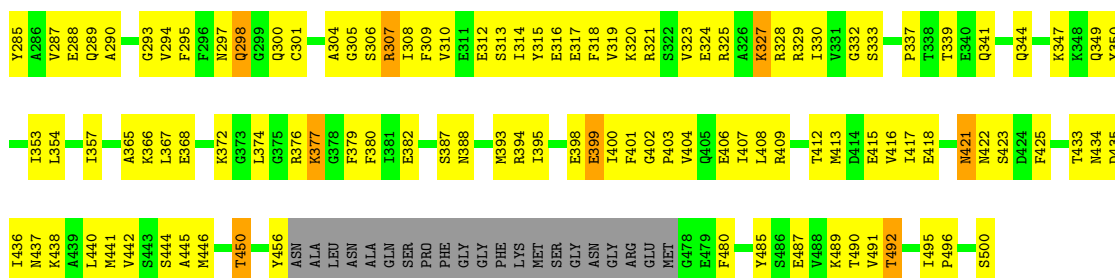
Note EDS was not executed.

#### • Molecule 1: RETINAL DEHYDROGENASE TYPE II



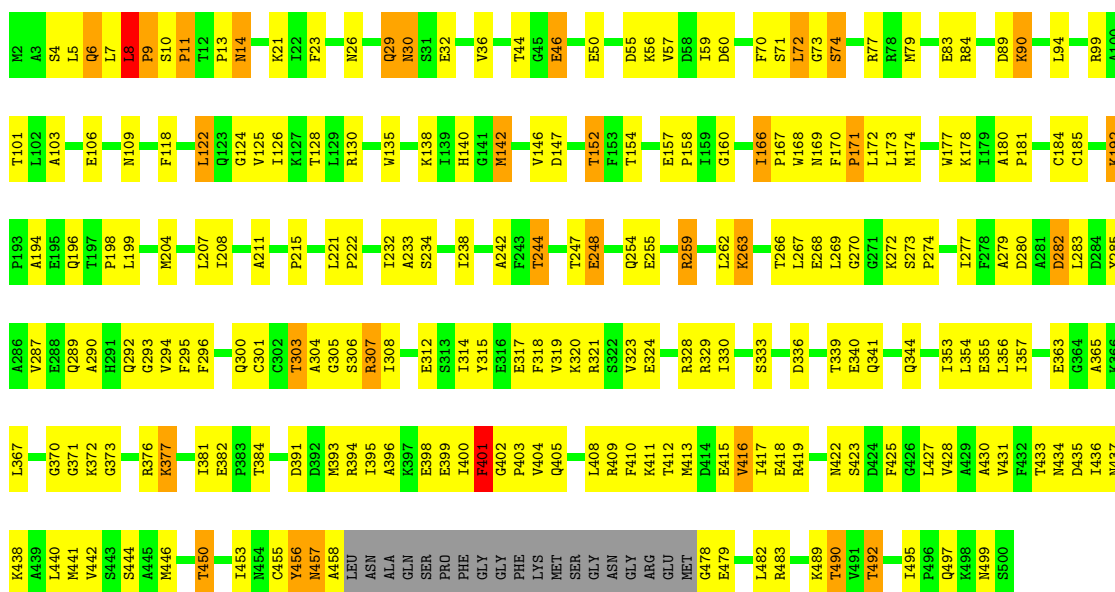
#### • Molecule 1: RETINAL DEHYDROGENASE TYPE II





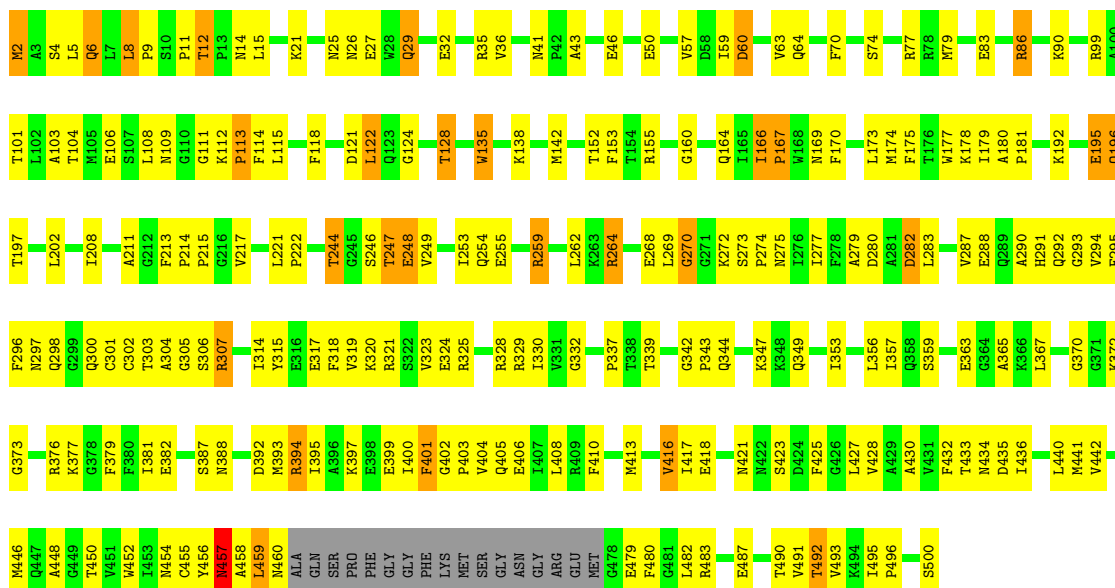
• Molecule 1: RETINAL DEHYDROGENASE TYPE II

Chain C:



• Molecule 1: RETINAL DEHYDROGENASE TYPE II

Chain D:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.80Å 167.30Å 107.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.1 (30.00-2.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.234 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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, CL

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	0.41	0/3772	0.62	0/5104
1	B	0.40	0/3764	0.61	1/5094 (0.0%)
1	C	0.43	0/3785	0.63	0/5122
1	D	0.42	0/3801	0.63	0/5144
All	All	0.42	0/15122	0.62	1/20464 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	LEU	CA-CB-CG	-5.54	102.55	115.30

There are no chirality outliers.

There are no planarity outliers.

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3697	0	3699	214	0
1	B	3689	0	3690	210	0
1	C	3710	0	3710	213	2
1	D	3726	0	3727	221	2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	2
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	37	0	0	1	0
4	B	53	0	0	3	0
4	C	68	0	0	5	0
4	D	66	0	0	2	0
All	All	15156	0	14874	811	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (811) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:152:THR:HG22	1:D:492:THR:HB	1.33	1.10
1:B:495:ILE:HG22	1:D:440:LEU:HD13	1.36	1.05
1:A:152:THR:HG22	1:A:492:THR:HB	1.38	1.04
1:C:329:ARG:NH1	1:C:341:GLN:HB2	1.74	1.01
1:C:272:LYS:HD3	1:C:423:SER:HB2	1.41	0.99
1:A:2:MET:HG2	1:A:3:ALA:H	1.28	0.98
1:B:152:THR:HG22	1:B:492:THR:HB	1.42	0.98
1:A:329:ARG:HH12	1:A:341:GLN:HB2	1.28	0.96
1:C:124:GLY:O	1:C:128:THR:HG23	1.67	0.94
1:A:329:ARG:NH1	1:A:341:GLN:HB2	1.83	0.92
1:C:329:ARG:HH12	1:C:341:GLN:HB2	1.27	0.91
1:C:433:THR:HG22	1:C:435:ASP:H	1.33	0.90
1:D:244:THR:HB	1:D:268:GLU:HB3	1.54	0.89
1:C:244:THR:HB	1:C:268:GLU:HB3	1.53	0.89
1:D:6:GLN:HE21	1:D:6:GLN:N	1.71	0.88
1:B:124:GLY:O	1:B:128:THR:HG23	1.74	0.86
1:C:4:SER:HB3	1:C:6:GLN:HE21	1.40	0.86
1:D:124:GLY:O	1:D:128:THR:HG23	1.75	0.86
1:A:433:THR:H	1:A:454:ASN:HD21	1.24	0.86
1:D:433:THR:HG22	1:D:435:ASP:H	1.40	0.84
1:D:457:ASN:HD22	1:D:458:ALA:H	1.25	0.84
1:B:329:ARG:NH1	1:B:341:GLN:HB2	1.94	0.83
1:D:372:LYS:O	1:D:382:GLU:HG2	1.79	0.83
1:C:303:THR:HB	1:C:458:ALA:HB3	1.61	0.82
1:A:440:LEU:HD13	1:C:495:ILE:HG22	1.60	0.82
1:B:29:GLN:HE21	1:B:29:GLN:HA	1.44	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:VAL:HG21	1:B:308:ILE:HD11	1.60	0.82
1:C:4:SER:HB3	1:C:6:GLN:NE2	1.95	0.81
1:B:395:ILE:O	1:B:400:ILE:HD11	1.81	0.81
1:D:109:ASN:HD21	1:D:197:THR:HA	1.46	0.80
1:A:196:GLN:HE21	1:A:196:GLN:H	1.28	0.80
1:B:433:THR:HG22	1:B:435:ASP:H	1.46	0.80
1:B:59:ILE:HD13	1:B:221:LEU:HD22	1.62	0.80
1:D:152:THR:CG2	1:D:492:THR:HB	2.11	0.80
1:D:479:GLU:HG3	1:D:483:ARG:HH21	1.46	0.80
1:A:180:ALA:HB3	1:A:181:PRO:HD3	1.64	0.80
1:D:272:LYS:HD3	1:D:423:SER:HB2	1.64	0.79
1:A:124:GLY:O	1:A:128:THR:HG23	1.83	0.78
1:A:294:VAL:HG21	1:A:308:ILE:HD11	1.64	0.78
1:A:400:ILE:HG21	1:A:404:VAL:HB	1.65	0.78
1:D:400:ILE:HG21	1:D:404:VAL:HB	1.65	0.78
1:D:6:GLN:HE21	1:D:6:GLN:CA	1.95	0.77
1:D:295:PHE:HB3	1:D:329:ARG:HH12	1.48	0.77
1:A:312:GLU:HG2	1:A:409:ARG:HD3	1.67	0.76
1:A:374:LEU:HD12	1:A:380:PHE:HB3	1.66	0.76
1:C:400:ILE:HD12	1:C:400:ILE:N	2.02	0.75
1:A:400:ILE:HD12	1:A:400:ILE:N	2.01	0.75
1:A:331:VAL:HG22	1:A:341:GLN:HB3	1.69	0.75
1:C:8:LEU:H	1:C:9:PRO:HD3	1.52	0.75
1:B:320:LYS:O	1:B:323:VAL:HG22	1.87	0.75
1:B:180:ALA:HB3	1:B:181:PRO:HD3	1.69	0.75
1:B:194:ALA:HB1	1:B:196:GLN:HE21	1.52	0.74
1:D:60:ASP:O	1:D:64:GLN:HG3	1.86	0.74
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.53	0.73
1:C:154:THR:HG22	1:C:490:THR:HB	1.70	0.73
1:A:293:GLY:HA3	1:A:456:TYR:CD2	2.23	0.73
1:C:372:LYS:O	1:C:382:GLU:HG2	1.88	0.73
1:B:329:ARG:HH12	1:B:341:GLN:HB2	1.52	0.73
1:C:293:GLY:O	1:C:304:ALA:HB1	1.88	0.73
1:B:400:ILE:N	1:B:400:ILE:HD12	2.04	0.72
1:A:90:LYS:HE2	1:A:211:ALA:O	1.89	0.72
1:B:173:LEU:HD13	1:B:177:TRP:CH2	2.24	0.72
1:D:457:ASN:HD22	1:D:458:ALA:N	1.86	0.72
1:A:283:LEU:O	1:A:287:VAL:HG23	1.90	0.72
1:D:291:HIS:HE1	1:D:329:ARG:HD3	1.54	0.72
1:D:29:GLN:HA	1:D:29:GLN:HE21	1.53	0.72
1:D:394:ARG:HB2	1:D:394:ARG:HH11	1.55	0.72
1:A:282:ASP:OD1	1:A:285:TYR:HB3	1.89	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:280:ASP:OD1	1:C:433:THR:HG23	1.89	0.71
1:D:395:ILE:HD12	1:D:406:GLU:HG2	1.70	0.71
1:C:26:ASN:ND2	1:C:215:PRO:HA	2.05	0.71
1:D:353:ILE:HD13	1:D:402:GLY:HA3	1.72	0.71
1:B:417:ILE:O	1:B:421:ASN:HB2	1.90	0.71
1:A:44:THR:OG1	1:A:46:GLU:HB3	1.91	0.71
1:A:372:LYS:O	1:A:382:GLU:HG2	1.90	0.71
1:D:413:MET:O	1:D:416:VAL:HG23	1.90	0.71
1:A:272:LYS:HD3	1:A:423:SER:HB2	1.73	0.71
1:C:272:LYS:HD3	1:C:423:SER:CB	2.19	0.70
1:C:21:LYS:HE3	1:C:30:ASN:ND2	2.06	0.70
1:B:56:LYS:HD3	1:B:231:ALA:HB2	1.73	0.70
1:C:21:LYS:HB3	1:C:29:GLN:O	1.91	0.70
1:D:103:ALA:HB2	1:D:122:LEU:HD13	1.73	0.70
1:A:2:MET:HG2	1:A:3:ALA:N	2.06	0.70
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.54	0.70
1:A:283:LEU:HD23	1:A:321:ARG:CZ	2.22	0.70
1:C:273:SER:HB3	1:C:305:GLY:N	2.07	0.70
1:B:297:ASN:HD22	1:B:301:CYS:HB3	1.58	0.69
1:D:279:ALA:HA	1:D:314:ILE:HD13	1.74	0.69
1:A:395:ILE:O	1:A:400:ILE:HD11	1.93	0.69
1:D:272:LYS:O	1:D:427:LEU:HD12	1.93	0.68
1:C:282:ASP:OD1	1:C:285:TYR:HB3	1.93	0.68
1:D:400:ILE:N	1:D:400:ILE:HD12	2.08	0.68
1:B:436:ILE:HA	1:C:436:ILE:HG12	1.76	0.68
1:C:294:VAL:HG11	1:C:405:GLN:HB3	1.75	0.68
1:C:428:VAL:HG22	1:C:450:THR:HG23	1.75	0.68
1:C:312:GLU:OE2	1:C:411:LYS:HB2	1.93	0.68
1:D:292:GLN:O	1:D:296:PHE:HB2	1.94	0.68
1:A:152:THR:CG2	1:A:492:THR:HB	2.22	0.68
1:A:306:SER:O	1:A:308:ILE:HG13	1.93	0.67
1:A:354:LEU:HD23	1:A:357:ILE:HD12	1.75	0.67
1:B:8:LEU:H	1:B:9:PRO:HD2	1.59	0.67
1:A:456:TYR:O	1:A:456:TYR:HD1	1.77	0.67
1:A:196:GLN:O	1:A:197:THR:HG23	1.95	0.67
1:B:436:ILE:HG12	1:C:436:ILE:HA	1.77	0.67
1:C:395:ILE:O	1:C:400:ILE:HD11	1.95	0.66
1:C:180:ALA:HB3	1:C:181:PRO:HD3	1.78	0.66
1:B:6:GLN:CD	1:B:6:GLN:H	1.99	0.66
1:C:194:ALA:HB1	1:C:196:GLN:HE21	1.60	0.66
1:B:365:ALA:HB2	1:B:393:MET:HE1	1.78	0.66
1:D:283:LEU:O	1:D:287:VAL:HG23	1.95	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:413:MET:CE	1:B:438:LYS:HG2	2.26	0.66
1:C:353:ILE:HD13	1:C:402:GLY:HA3	1.78	0.66
1:C:353:ILE:O	1:C:357:ILE:HG13	1.95	0.65
1:D:59:ILE:HD13	1:D:221:LEU:HD22	1.79	0.65
1:A:77:ARG:HH11	1:D:500:SER:HB2	1.61	0.65
1:A:291:HIS:HE1	1:A:329:ARG:HD2	1.60	0.65
1:A:294:VAL:HG22	1:A:305:GLY:O	1.97	0.65
1:C:317:GLU:O	1:C:321:ARG:HG2	1.97	0.65
1:C:84:ARG:NH1	1:C:184:CYS:O	2.30	0.64
1:B:353:ILE:O	1:B:357:ILE:HG13	1.97	0.64
1:C:255:GLU:HG3	1:D:255:GLU:HG3	1.79	0.64
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.31	0.64
1:D:264:ARG:HG2	1:D:264:ARG:NH1	2.11	0.64
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.60	0.64
1:A:247:THR:HA	1:A:269:LEU:HD22	1.79	0.64
1:D:328:ARG:HG2	1:D:328:ARG:HH11	1.62	0.64
1:B:56:LYS:HD3	1:B:231:ALA:CB	2.27	0.64
1:D:12:THR:HG21	1:D:101:THR:HG22	1.79	0.64
1:D:324:GLU:O	1:D:328:ARG:HG3	1.98	0.64
1:C:79:MET:HG2	1:C:83:GLU:HB3	1.80	0.64
1:B:372:LYS:HG2	1:B:382:GLU:OE2	1.98	0.64
1:B:6:GLN:CD	1:B:6:GLN:N	2.52	0.64
1:B:394:ARG:HB2	1:B:394:ARG:NH1	2.13	0.64
1:A:353:ILE:O	1:A:357:ILE:HG13	1.97	0.64
1:C:130:ARG:HH11	1:C:130:ARG:HG3	1.63	0.64
1:B:413:MET:HE2	1:B:438:LYS:HG2	1.79	0.63
1:A:247:THR:HG22	1:A:269:LEU:HB3	1.81	0.63
1:B:142:MET:HA	1:C:142:MET:HA	1.81	0.63
1:B:264:ARG:HG2	1:B:264:ARG:HH11	1.63	0.63
1:D:109:ASN:ND2	1:D:197:THR:HA	2.13	0.63
1:A:283:LEU:HD23	1:A:321:ARG:NH2	2.13	0.63
1:B:440:LEU:HD13	1:D:495:ILE:HG22	1.80	0.63
1:C:457:ASN:N	1:C:457:ASN:HD22	1.97	0.63
1:A:330:ILE:HG22	1:A:339:THR:HA	1.80	0.63
1:D:283:LEU:HD21	1:D:317:GLU:HB3	1.80	0.63
1:A:283:LEU:HD23	1:A:321:ARG:NH1	2.14	0.63
1:C:36:VAL:HG11	1:C:50:GLU:HB3	1.81	0.63
1:B:135:TRP:CE2	1:D:138:LYS:HD3	2.33	0.62
1:B:408:LEU:HD12	1:B:408:LEU:H	1.63	0.62
1:A:254:GLN:HG3	1:A:267:LEU:HD11	1.81	0.62
1:A:167:PRO:HD3	1:A:244:THR:O	1.99	0.62
1:B:7:LEU:HD23	1:B:8:LEU:N	2.15	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:344:GLN:HA	1:D:344:GLN:NE2	2.15	0.62
1:C:36:VAL:CG1	1:C:50:GLU:HB3	2.28	0.62
1:C:394:ARG:HG3	1:C:398:GLU:OE2	1.99	0.62
1:C:99:ARG:HG2	1:C:118:PHE:CE1	2.35	0.62
1:A:2:MET:CG	1:A:3:ALA:H	2.07	0.62
1:B:192:LYS:HG2	1:B:221:LEU:O	1.99	0.62
1:D:195:GLU:HG2	1:D:196:GLN:NE2	2.15	0.62
1:C:324:GLU:O	1:C:328:ARG:HG3	1.99	0.61
1:C:376:ARG:O	1:C:377:LYS:HB2	2.00	0.61
1:A:329:ARG:HH12	1:A:341:GLN:CB	2.09	0.61
1:C:319:VAL:O	1:C:323:VAL:HG13	2.00	0.61
1:A:412:THR:OG1	1:A:415:GLU:HB2	2.00	0.61
1:D:214:PRO:O	1:D:217:VAL:HG23	2.00	0.61
1:A:135:TRP:CE2	1:C:138:LYS:HD3	2.36	0.61
1:B:319:VAL:O	1:B:323:VAL:HG13	2.00	0.61
1:D:275:ASN:ND2	1:D:456:TYR:OH	2.34	0.61
1:D:479:GLU:CG	1:D:483:ARG:HH21	2.13	0.61
1:A:354:LEU:HA	1:A:357:ILE:HD12	1.82	0.61
1:C:391:ASP:OD2	1:C:419:ARG:HD2	2.01	0.61
1:C:204:MET:O	1:C:208:ILE:HG13	2.00	0.61
1:C:59:ILE:HD13	1:C:221:LEU:HD22	1.83	0.60
1:C:384:THR:HB	1:C:404:VAL:HG22	1.83	0.60
1:B:349:GLN:O	1:B:353:ILE:HG13	2.01	0.60
1:D:394:ARG:CB	1:D:394:ARG:HH11	2.13	0.60
1:C:32:GLU:HG3	1:C:57:VAL:CG1	2.30	0.60
1:C:254:GLN:HE21	1:D:254:GLN:HG2	1.66	0.60
1:B:247:THR:HG22	1:B:269:LEU:HB3	1.84	0.60
1:A:166:ILE:HB	1:A:167:PRO:HD2	1.84	0.60
1:D:2:MET:CE	1:D:4:SER:H	2.13	0.60
1:A:329:ARG:NH1	1:A:341:GLN:OE1	2.34	0.60
1:A:384:THR:HB	1:A:404:VAL:HG22	1.83	0.60
1:D:297:ASN:HD22	1:D:301:CYS:HB3	1.66	0.60
1:C:8:LEU:HD23	1:C:8:LEU:N	2.17	0.59
1:A:408:LEU:HD12	1:A:408:LEU:N	2.17	0.59
1:B:480:PHE:HB2	4:B:727:HOH:O	2.03	0.59
1:C:26:ASN:ND2	1:C:215:PRO:CA	2.65	0.59
1:A:240:LYS:HG2	1:A:241:ILE:H	1.68	0.59
1:A:290:ALA:O	1:A:294:VAL:HG23	2.03	0.59
1:D:353:ILE:O	1:D:357:ILE:HG13	2.03	0.59
1:D:344:GLN:HA	1:D:344:GLN:HE21	1.66	0.59
1:C:412:THR:OG1	1:C:415:GLU:HB2	2.03	0.59
1:A:283:LEU:HD21	1:A:317:GLU:HB3	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:ARG:NH1	1:D:500:SER:HB2	2.17	0.59
1:A:436:ILE:HA	1:D:436:ILE:HG12	1.84	0.59
1:D:291:HIS:CE1	1:D:329:ARG:HD3	2.36	0.58
1:D:295:PHE:HB3	1:D:329:ARG:NH1	2.17	0.58
1:A:433:THR:H	1:A:454:ASN:ND2	2.00	0.58
1:D:294:VAL:HG11	1:D:405:GLN:CB	2.33	0.58
1:C:370:GLY:HA2	1:C:382:GLU:OE2	2.03	0.58
1:D:294:VAL:HG11	1:D:405:GLN:HB3	1.86	0.58
1:A:109:ASN:ND2	1:A:199:LEU:HG	2.18	0.58
1:A:8:LEU:HB3	1:A:9:PRO:CD	2.33	0.58
1:A:196:GLN:NE2	1:A:196:GLN:H	1.99	0.58
1:C:26:ASN:HD22	1:C:215:PRO:CA	2.17	0.58
1:D:408:LEU:HD12	1:D:408:LEU:N	2.19	0.58
1:D:344:GLN:OE1	1:D:403:PRO:HD3	2.03	0.58
1:C:71:SER:O	1:C:74:SER:CB	2.51	0.58
1:C:10:SER:HB2	1:C:11:PRO:HD2	1.85	0.58
1:B:187:ASN:HD21	1:B:485:TYR:HB3	1.68	0.58
1:A:240:LYS:HG2	1:A:241:ILE:N	2.18	0.58
1:D:124:GLY:O	1:D:128:THR:CG2	2.51	0.58
1:D:5:LEU:C	1:D:6:GLN:HE21	2.07	0.58
1:C:8:LEU:H	1:C:9:PRO:CD	2.16	0.58
1:D:329:ARG:NH1	1:D:329:ARG:HG2	2.18	0.58
1:C:32:GLU:HG3	1:C:57:VAL:HG12	1.85	0.57
1:B:293:GLY:HA3	1:B:456:TYR:CD2	2.40	0.57
1:C:413:MET:HE1	1:C:438:LYS:HA	1.87	0.57
1:D:79:MET:HG2	1:D:83:GLU:HB3	1.84	0.57
1:D:365:ALA:HB2	1:D:393:MET:HE1	1.86	0.57
1:C:248:GLU:CD	1:C:248:GLU:H	2.06	0.57
1:A:328:ARG:O	1:A:330:ILE:HD12	2.05	0.57
1:C:320:LYS:O	1:C:324:GLU:HG3	2.03	0.57
1:D:173:LEU:HD13	1:D:177:TRP:CH2	2.38	0.57
1:A:258:GLY:HA2	1:A:262:LEU:HD23	1.86	0.57
1:C:4:SER:CB	1:C:6:GLN:HE21	2.15	0.57
1:B:264:ARG:NH1	1:B:264:ARG:HG2	2.20	0.57
1:C:446:MET:HE2	1:C:446:MET:HA	1.86	0.57
1:C:280:ASP:CG	1:C:433:THR:HG23	2.25	0.57
1:B:29:GLN:HE21	1:B:29:GLN:CA	2.14	0.57
1:C:294:VAL:HG21	1:C:308:ILE:HD11	1.86	0.57
1:D:8:LEU:HG	1:D:9:PRO:HD2	1.86	0.57
1:A:89:ASP:OD1	1:A:130:ARG:HD3	2.05	0.57
1:A:56:LYS:HD3	1:A:231:ALA:CB	2.35	0.57
1:D:315:TYR:O	1:D:319:VAL:HG23	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:109:ASN:ND2	1:C:199:LEU:HG	2.20	0.56
1:D:166:ILE:HB	1:D:167:PRO:HD2	1.87	0.56
1:B:112:LYS:HG2	1:B:113:PRO:HD2	1.86	0.56
1:C:44:THR:OG1	1:C:46:GLU:HB3	2.06	0.56
1:B:282:ASP:OD1	1:B:285:TYR:HB3	2.05	0.56
1:B:21:LYS:HE3	1:B:30:ASN:ND2	2.20	0.56
1:D:12:THR:HG23	1:D:104:THR:HG21	1.87	0.56
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.70	0.56
1:C:274:PRO:HD2	1:C:428:VAL:O	2.06	0.56
1:B:408:LEU:N	1:B:408:LEU:HD12	2.20	0.56
1:B:146:VAL:HG12	1:B:147:ASP:O	2.05	0.56
1:B:365:ALA:HB2	1:B:393:MET:CE	2.36	0.56
1:A:208:ILE:HG23	1:A:213:PHE:CD2	2.41	0.55
1:A:36:VAL:CG1	1:A:50:GLU:HB3	2.37	0.55
1:C:433:THR:HG22	1:C:434:ASN:N	2.21	0.55
1:C:400:ILE:HG21	1:C:404:VAL:HB	1.87	0.55
1:A:490:THR:O	1:B:450:THR:HA	2.06	0.55
1:D:376:ARG:O	1:D:377:LYS:HB2	2.06	0.55
1:C:166:ILE:CG2	1:C:178:LYS:HD2	2.37	0.55
1:B:365:ALA:N	1:B:393:MET:HE1	2.21	0.55
1:B:394:ARG:CB	1:B:394:ARG:HH11	2.19	0.55
1:C:89:ASP:OD1	1:C:130:ARG:HD3	2.06	0.55
1:D:320:LYS:O	1:D:323:VAL:HG22	2.06	0.55
1:A:426:GLY:O	1:A:427:LEU:HB2	2.06	0.55
1:D:400:ILE:CG2	1:D:404:VAL:HB	2.37	0.55
1:B:240:LYS:HD3	1:B:241:ILE:N	2.22	0.55
1:C:330:ILE:N	1:C:330:ILE:HD12	2.22	0.55
1:D:26:ASN:ND2	1:D:215:PRO:HA	2.21	0.55
1:A:249:VAL:O	1:A:253:ILE:HG12	2.07	0.55
1:A:301:CYS:SG	1:A:304:ALA:HB2	2.47	0.55
1:B:344:GLN:OE1	1:B:403:PRO:HD3	2.07	0.55
1:C:315:TYR:O	1:C:319:VAL:HG23	2.07	0.55
1:D:174:MET:HA	1:D:174:MET:HE3	1.89	0.55
1:A:343:PRO:HB3	1:A:380:PHE:CE1	2.42	0.54
1:A:262:LEU:HD21	1:B:251:LYS:HG2	1.88	0.54
1:D:328:ARG:O	1:D:330:ILE:HD12	2.08	0.54
1:B:70:PHE:CE2	1:B:160:GLY:HA2	2.41	0.54
1:D:264:ARG:HH11	1:D:264:ARG:CG	2.20	0.54
1:B:399:GLU:HB3	4:B:732:HOH:O	2.08	0.54
1:B:35:ARG:NH1	1:B:35:ARG:HB2	2.22	0.54
1:D:427:LEU:O	1:D:448:ALA:HB1	2.08	0.54
1:D:277:ILE:HD13	1:D:318:PHE:CE2	2.43	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:280:ASP:OD1	1:D:433:THR:HG23	2.08	0.54
1:A:400:ILE:CD1	1:A:400:ILE:N	2.71	0.54
1:D:301:CYS:SG	1:D:304:ALA:HB2	2.48	0.54
1:D:169:ASN:H	1:D:169:ASN:HD22	1.55	0.54
1:B:232:ILE:HG23	1:B:238:ILE:HD13	1.89	0.54
1:C:6:GLN:C	1:C:7:LEU:HD23	2.27	0.54
1:C:455:CYS:O	1:C:456:TYR:HB2	2.07	0.54
1:B:89:ASP:OD1	1:B:130:ARG:HD3	2.08	0.54
1:A:436:ILE:O	1:A:440:LEU:HG	2.06	0.54
1:C:400:ILE:CD1	1:C:400:ILE:N	2.71	0.54
1:D:410:PHE:CD2	1:D:416:VAL:HG22	2.43	0.54
1:C:320:LYS:O	1:C:323:VAL:HG22	2.07	0.54
1:C:71:SER:O	1:C:74:SER:HB3	2.08	0.54
1:B:187:ASN:ND2	1:B:485:TYR:HB3	2.23	0.54
1:C:247:THR:HA	1:C:269:LEU:HD22	1.89	0.54
1:A:315:TYR:O	1:A:319:VAL:HG23	2.08	0.53
1:D:399:GLU:HG2	1:D:400:ILE:N	2.22	0.53
1:D:400:ILE:HG21	1:D:404:VAL:CB	2.37	0.53
1:A:442:VAL:HG13	1:A:446:MET:HE3	1.89	0.53
1:A:297:ASN:HD22	1:A:301:CYS:HB3	1.72	0.53
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.43	0.53
1:D:480:PHE:HA	1:D:483:ARG:NE	2.24	0.53
1:A:479:GLU:HG3	1:A:483:ARG:HH21	1.74	0.53
1:B:232:ILE:HG23	1:B:238:ILE:CD1	2.39	0.53
1:A:442:VAL:HG13	1:A:446:MET:CE	2.39	0.53
1:B:109:ASN:ND2	1:B:199:LEU:HG	2.23	0.53
1:D:221:LEU:N	1:D:221:LEU:HD12	2.24	0.53
1:C:79:MET:CG	1:C:83:GLU:HB3	2.38	0.53
1:B:170:PHE:O	1:B:174:MET:HG2	2.09	0.53
1:D:247:THR:HB	1:D:269:LEU:HD13	1.90	0.53
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.44	0.53
1:A:371:GLY:H	1:A:382:GLU:HG3	1.74	0.53
1:D:288:GLU:OE1	1:D:325:ARG:CZ	2.57	0.53
1:A:90:LYS:HB2	1:A:90:LYS:NZ	2.24	0.53
1:B:194:ALA:HB1	1:B:196:GLN:NE2	2.22	0.52
1:C:353:ILE:CD1	1:C:402:GLY:HA3	2.39	0.52
1:D:290:ALA:O	1:D:294:VAL:HG23	2.09	0.52
1:C:413:MET:CE	1:C:438:LYS:HG2	2.39	0.52
1:D:273:SER:O	1:D:305:GLY:HA3	2.08	0.52
1:A:155:ARG:HH12	1:B:444:SER:HB3	1.73	0.52
1:D:394:ARG:HB2	1:D:394:ARG:NH1	2.22	0.52
1:D:12:THR:HG21	1:D:15:LEU:HD13	1.90	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:320:LYS:O	1:A:323:VAL:HG22	2.09	0.52
1:A:248:GLU:H	1:A:248:GLU:CD	2.12	0.52
1:B:90:LYS:HB2	1:B:90:LYS:NZ	2.24	0.52
1:D:6:GLN:NE2	1:D:6:GLN:CA	2.65	0.52
1:A:433:THR:HG22	1:A:434:ASN:H	1.73	0.52
1:A:405:GLN:O	1:A:405:GLN:HG3	2.10	0.52
1:D:170:PHE:HB3	1:D:173:LEU:HB2	1.91	0.52
1:B:442:VAL:HG13	1:B:446:MET:CE	2.40	0.52
1:C:168:TRP:O	1:C:171:PRO:HD3	2.09	0.52
1:A:280:ASP:OD1	1:A:433:THR:HG22	2.10	0.52
1:A:238:ILE:O	1:A:263:LYS:HE3	2.10	0.52
1:B:306:SER:HB3	1:B:406:GLU:OE1	2.09	0.52
1:D:272:LYS:HE3	1:D:307:ARG:NH1	2.25	0.52
1:D:2:MET:HE2	1:D:4:SER:H	1.73	0.52
1:B:323:VAL:O	1:B:327:LYS:HB2	2.09	0.52
1:A:244:THR:HB	1:A:268:GLU:HB2	1.91	0.52
1:A:413:MET:CE	1:A:438:LYS:HG2	2.40	0.52
1:D:367:LEU:HD11	1:D:370:GLY:O	2.10	0.51
1:D:290:ALA:HA	1:D:456:TYR:CE2	2.45	0.51
1:B:441:MET:HG3	1:D:496:PRO:HG2	1.92	0.51
1:D:272:LYS:HG3	1:D:427:LEU:HD13	1.92	0.51
1:A:264:ARG:NH2	1:A:487:GLU:HB3	2.25	0.51
1:C:169:ASN:HD22	1:C:169:ASN:H	1.58	0.51
1:C:303:THR:HB	1:C:458:ALA:CB	2.37	0.51
1:B:169:ASN:OD1	1:B:301:CYS:HA	2.10	0.51
1:B:158:PRO:HB3	1:B:185:CYS:O	2.10	0.51
1:B:433:THR:HG22	1:B:435:ASP:N	2.21	0.51
1:D:29:GLN:HE21	1:D:29:GLN:CA	2.17	0.51
1:C:328:ARG:HH11	1:C:328:ARG:HG2	1.76	0.51
1:C:336:ASP:HB3	1:C:339:THR:HG23	1.93	0.51
1:B:406:GLU:OE1	1:B:406:GLU:N	2.43	0.51
1:A:106:GLU:OE2	1:A:171:PRO:HB2	2.10	0.51
1:B:290:ALA:O	1:B:294:VAL:HG23	2.11	0.51
1:C:453:ILE:HD12	1:D:493:VAL:HG22	1.92	0.51
1:C:438:LYS:O	1:C:442:VAL:HG23	2.11	0.51
1:B:166:ILE:HB	1:B:167:PRO:HD2	1.92	0.51
1:C:106:GLU:OE1	1:C:106:GLU:HA	2.11	0.51
1:B:283:LEU:O	1:B:287:VAL:HG23	2.10	0.51
1:D:275:ASN:ND2	1:D:456:TYR:CZ	2.78	0.51
1:B:77:ARG:HH11	1:B:77:ARG:HB3	1.76	0.51
1:B:35:ARG:CB	1:B:35:ARG:HH11	2.24	0.51
1:A:12:THR:O	1:A:15:LEU:HB2	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:295:PHE:HB3	1:B:329:ARG:CZ	2.41	0.51
1:A:312:GLU:HG2	1:A:409:ARG:CD	2.39	0.51
1:B:70:PHE:CZ	1:B:160:GLY:HA2	2.46	0.51
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.51
1:A:298:GLN:C	1:A:300:GLN:H	2.14	0.51
1:D:294:VAL:HG22	1:D:305:GLY:O	2.11	0.51
1:B:248:GLU:CD	1:B:248:GLU:H	2.13	0.51
1:A:257:ALA:CB	1:A:265:VAL:HG21	2.41	0.50
1:A:233:ALA:HA	1:A:241:ILE:HD12	1.92	0.50
1:A:319:VAL:HG22	1:A:407:ILE:HG21	1.92	0.50
1:A:109:ASN:HD22	1:A:199:LEU:CG	2.23	0.50
1:A:17:ILE:HG21	1:A:199:LEU:HD22	1.93	0.50
1:B:109:ASN:HD22	1:B:199:LEU:CG	2.24	0.50
1:A:344:GLN:HA	1:A:344:GLN:NE2	2.26	0.50
1:C:174:MET:HE3	1:C:174:MET:HA	1.93	0.50
1:B:192:LYS:HD2	1:B:193:PRO:O	2.11	0.50
1:B:324:GLU:O	1:B:328:ARG:HG3	2.11	0.50
1:D:295:PHE:CB	1:D:329:ARG:HH12	2.21	0.50
1:C:178:LYS:HE3	1:C:242:ALA:HB1	1.94	0.50
1:B:214:PRO:O	1:B:217:VAL:HG23	2.12	0.50
1:D:275:ASN:ND2	1:D:430:ALA:HB3	2.26	0.50
1:B:400:ILE:H	1:B:400:ILE:HD12	1.75	0.50
1:C:430:ALA:HB2	1:C:456:TYR:CD1	2.46	0.50
1:A:36:VAL:HG13	1:A:50:GLU:HB3	1.93	0.50
1:C:482:LEU:C	1:C:482:LEU:HD12	2.32	0.50
1:B:59:ILE:HG13	1:B:231:ALA:HB3	1.93	0.50
1:C:283:LEU:O	1:C:287:VAL:HG23	2.12	0.50
1:D:294:VAL:HG13	1:D:306:SER:HA	1.94	0.49
1:B:15:LEU:HD21	1:B:105:MET:HG3	1.93	0.49
1:A:374:LEU:HD12	1:A:380:PHE:CB	2.40	0.49
1:B:433:THR:HG22	1:B:434:ASN:H	1.78	0.49
1:B:21:LYS:HB3	1:B:29:GLN:O	2.12	0.49
1:C:254:GLN:HG2	1:D:254:GLN:HE21	1.78	0.49
1:D:173:LEU:HD13	1:D:177:TRP:CZ2	2.47	0.49
1:B:330:ILE:HD12	1:B:330:ILE:N	2.28	0.49
1:C:292:GLN:HA	1:C:292:GLN:NE2	2.28	0.49
1:B:394:ARG:HG3	1:B:398:GLU:OE2	2.12	0.49
1:D:293:GLY:HA3	1:D:456:TYR:CD1	2.48	0.49
1:B:157:GLU:OE1	1:B:489:LYS:HD2	2.13	0.49
1:A:292:GLN:O	1:A:296:PHE:HB2	2.12	0.49
1:C:444:SER:HA	1:D:155:ARG:HH12	1.78	0.49
1:A:401:PHE:CD1	1:A:401:PHE:N	2.79	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:295:PHE:HE2	1:C:405:GLN:HE21	1.59	0.49
1:C:72:LEU:O	1:C:74:SER:N	2.46	0.49
1:B:274:PRO:HB3	1:B:307:ARG:NH1	2.27	0.49
1:A:195:GLU:CD	1:A:195:GLU:H	2.15	0.49
1:C:166:ILE:HG22	1:C:178:LYS:HD2	1.95	0.49
1:D:247:THR:HA	1:D:269:LEU:HD22	1.95	0.49
1:B:214:PRO:HD2	1:B:217:VAL:HG21	1.95	0.49
1:B:307:ARG:HH11	1:B:307:ARG:HG3	1.77	0.49
1:D:442:VAL:HG13	1:D:446:MET:CE	2.42	0.49
1:B:285:TYR:CZ	1:B:289:GLN:HG3	2.47	0.49
1:A:427:LEU:HD12	1:A:428:VAL:H	1.77	0.49
1:B:54:ALA:HA	1:B:58:ASP:OD2	2.13	0.49
1:C:408:LEU:N	1:C:408:LEU:HD12	2.27	0.49
1:C:329:ARG:HH12	1:C:341:GLN:CB	2.13	0.49
1:A:312:GLU:OE2	1:A:411:LYS:HB2	2.13	0.49
1:A:77:ARG:HH11	1:D:500:SER:CB	2.24	0.49
1:A:391:ASP:OD1	1:A:419:ARG:NH1	2.45	0.49
1:C:479:GLU:CG	1:C:483:ARG:HH21	2.26	0.49
1:C:7:LEU:C	1:C:8:LEU:HD23	2.33	0.49
1:D:36:VAL:CG1	1:D:50:GLU:HB3	2.43	0.48
1:B:7:LEU:HD23	1:B:8:LEU:H	1.78	0.48
1:D:365:ALA:H	1:D:393:MET:HE3	1.78	0.48
1:A:246:SER:OG	1:A:249:VAL:HG23	2.13	0.48
1:A:393:MET:O	1:A:397:LYS:HG3	2.13	0.48
1:A:410:PHE:CG	1:A:416:VAL:HG13	2.48	0.48
1:B:108:LEU:HD13	1:B:108:LEU:O	2.13	0.48
1:C:173:LEU:HD22	1:C:177:TRP:CZ2	2.49	0.48
1:C:478:GLY:N	4:C:712:HOH:O	2.46	0.48
1:C:395:ILE:HG13	1:C:396:ALA:N	2.29	0.48
1:D:433:THR:HG22	1:D:434:ASN:H	1.78	0.48
1:A:294:VAL:HG11	1:A:405:GLN:HB3	1.96	0.48
1:A:400:ILE:CG2	1:A:404:VAL:HB	2.40	0.48
1:D:29:GLN:HA	1:D:29:GLN:NE2	2.26	0.48
1:A:138:LYS:HD3	1:C:135:TRP:CD2	2.49	0.48
1:C:330:ILE:HD13	1:C:340:GLU:OE2	2.13	0.48
1:A:106:GLU:OE2	1:A:172:LEU:N	2.41	0.48
1:B:272:LYS:HD3	1:B:423:SER:HB2	1.96	0.48
1:A:29:GLN:HA	1:A:29:GLN:HE21	1.79	0.48
1:B:167:PRO:HD3	1:B:244:THR:O	2.12	0.48
1:A:30:ASN:HD22	1:A:52:GLN:CD	2.17	0.48
1:A:99:ARG:HG2	1:A:118:PHE:CE2	2.48	0.48
1:B:433:THR:HG22	1:B:434:ASN:N	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:166:ILE:CG2	1:B:178:LYS:HD2	2.43	0.48
1:C:170:PHE:HB3	1:C:173:LEU:HB2	1.96	0.48
1:A:71:SER:O	1:A:74:SER:HB3	2.14	0.48
1:C:272:LYS:HG3	1:C:427:LEU:CD1	2.44	0.48
1:A:330:ILE:HD12	1:A:330:ILE:N	2.29	0.48
1:C:394:ARG:NH1	1:C:394:ARG:HB2	2.28	0.48
1:C:330:ILE:HG22	1:C:339:THR:HA	1.96	0.48
1:C:70:PHE:CE2	1:C:160:GLY:HA2	2.48	0.48
1:B:113:PRO:HG2	1:B:116:GLN:NE2	2.29	0.48
1:D:90:LYS:HE2	1:D:211:ALA:O	2.13	0.48
1:D:32:GLU:HG3	1:D:57:VAL:CG1	2.44	0.48
1:A:173:LEU:HD22	1:A:177:TRP:CE2	2.49	0.47
1:D:395:ILE:O	1:D:400:ILE:HD11	2.14	0.47
1:D:292:GLN:HA	1:D:292:GLN:NE2	2.28	0.47
1:B:372:LYS:O	1:B:382:GLU:HG2	2.14	0.47
1:D:2:MET:HE1	1:D:4:SER:H	1.79	0.47
1:C:169:ASN:ND2	1:C:169:ASN:H	2.12	0.47
1:C:479:GLU:HG3	1:C:483:ARG:HH21	1.78	0.47
1:C:436:ILE:HG22	1:C:440:LEU:HD11	1.97	0.47
1:C:262:LEU:HD13	1:D:269:LEU:HD11	1.95	0.47
1:D:153:PHE:CZ	1:D:491:VAL:HB	2.49	0.47
1:C:435:ASP:OD1	1:C:437:ASN:HB2	2.14	0.47
1:A:158:PRO:HB3	1:A:185:CYS:O	2.14	0.47
1:B:70:PHE:CD1	1:B:77:ARG:HD3	2.49	0.47
1:D:169:ASN:H	1:D:169:ASN:ND2	2.13	0.47
1:A:315:TYR:CE1	1:A:407:ILE:HG22	2.49	0.47
1:A:352:LYS:HG2	1:A:401:PHE:HZ	1.79	0.47
1:D:246:SER:HB2	1:D:248:GLU:HG2	1.97	0.47
1:D:347:LYS:HE3	1:D:379:PHE:HE1	1.79	0.47
1:C:152:THR:HB	1:C:492:THR:HB	1.95	0.47
1:A:439:ALA:CB	1:D:436:ILE:HD11	2.45	0.47
1:B:173:LEU:HD22	1:B:177:TRP:CE2	2.49	0.47
1:D:307:ARG:HG2	1:D:307:ARG:H	1.49	0.47
1:C:412:THR:O	1:C:415:GLU:HB3	2.13	0.47
1:A:83:GLU:HG3	4:A:722:HOH:O	2.14	0.47
1:A:395:ILE:O	1:A:406:GLU:OE2	2.33	0.47
1:C:357:ILE:HG21	1:C:371:GLY:HA2	1.95	0.47
1:B:394:ARG:HB2	1:B:394:ARG:HH11	1.77	0.47
1:C:409:ARG:O	1:C:419:ARG:NH2	2.48	0.47
1:C:254:GLN:HG2	1:D:254:GLN:NE2	2.30	0.47
1:B:236:ILE:CD1	1:B:261:ASN:HB3	2.45	0.47
1:C:344:GLN:OE1	1:C:403:PRO:HD3	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:ILE:HG23	1:B:213:PHE:CD2	2.50	0.47
1:B:365:ALA:CB	1:B:393:MET:HE1	2.45	0.47
1:B:189:VAL:HG12	1:B:190:VAL:N	2.29	0.47
1:C:272:LYS:HE3	1:C:307:ARG:NH1	2.30	0.47
1:B:146:VAL:HG21	1:B:152:THR:HG21	1.95	0.47
1:D:370:GLY:HA2	1:D:382:GLU:OE2	2.14	0.47
1:C:356:LEU:HD23	1:C:400:ILE:HG13	1.96	0.47
1:D:26:ASN:ND2	1:D:215:PRO:CA	2.77	0.47
1:D:432:PHE:HA	1:D:454:ASN:OD1	2.14	0.47
1:A:500:SER:O	1:D:77:ARG:NH1	2.46	0.47
1:C:483:ARG:CZ	4:C:714:HOH:O	2.63	0.47
1:C:233:ALA:O	1:C:263:LYS:HE2	2.14	0.47
1:C:247:THR:HG22	1:C:269:LEU:HB3	1.96	0.46
1:B:204:MET:O	1:B:208:ILE:HG13	2.15	0.46
1:A:142:MET:HA	1:D:142:MET:HA	1.97	0.46
1:A:123:GLN:O	1:A:127:LYS:HG2	2.15	0.46
1:A:291:HIS:CE1	1:A:329:ARG:HD2	2.46	0.46
1:C:285:TYR:CZ	1:C:289:GLN:HG3	2.51	0.46
1:B:293:GLY:HA3	1:B:456:TYR:CE2	2.51	0.46
1:B:25:ASN:O	1:B:27:GLU:HG2	2.15	0.46
1:D:106:GLU:OE1	1:D:106:GLU:HA	2.15	0.46
1:D:86:ARG:HD3	4:D:719:HOH:O	2.16	0.46
1:D:283:LEU:HD23	1:D:321:ARG:NH2	2.31	0.46
1:C:301:CYS:SG	1:C:304:ALA:HB3	2.55	0.46
1:C:482:LEU:O	1:C:482:LEU:HD12	2.16	0.46
1:D:332:GLY:C	1:D:339:THR:HG21	2.36	0.46
1:A:59:ILE:HD13	1:A:221:LEU:HD22	1.98	0.46
1:C:167:PRO:HD3	1:C:244:THR:O	2.16	0.46
1:A:254:GLN:O	1:A:257:ALA:HB3	2.15	0.46
1:C:94:LEU:HB3	1:C:207:LEU:HD22	1.98	0.46
1:B:347:LYS:O	1:B:350:TYR:HB3	2.16	0.46
1:B:376:ARG:O	1:B:377:LYS:O	2.33	0.46
1:D:247:THR:HG22	1:D:269:LEU:HB3	1.97	0.46
1:B:166:ILE:HG22	1:B:178:LYS:HD2	1.97	0.46
1:C:152:THR:HA	1:C:492:THR:HA	1.96	0.46
1:D:356:LEU:O	1:D:359:SER:HB3	2.16	0.46
1:B:500:SER:O	1:C:77:ARG:NH1	2.47	0.46
1:A:60:ASP:O	1:A:64:GLN:HG3	2.15	0.46
1:A:451:VAL:HB	1:B:491:VAL:HG22	1.98	0.46
1:C:273:SER:HB3	1:C:305:GLY:H	1.81	0.46
1:A:323:VAL:HG12	1:A:385:VAL:HG11	1.97	0.46
1:A:39:VAL:HG21	1:A:51:VAL:HG23	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:288:GLU:OE1	1:B:325:ARG:CZ	2.64	0.46
1:B:315:TYR:O	1:B:319:VAL:HG23	2.16	0.45
1:C:354:LEU:HD23	1:C:357:ILE:HD12	1.98	0.45
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.97	0.45
1:B:62:ALA:HB2	1:B:221:LEU:HD21	1.97	0.45
1:B:301:CYS:SG	1:B:304:ALA:HB2	2.56	0.45
1:A:84:ARG:NH1	1:A:184:CYS:O	2.49	0.45
1:D:21:LYS:HB3	1:D:29:GLN:O	2.17	0.45
1:D:79:MET:CG	1:D:83:GLU:HB3	2.45	0.45
1:B:130:ARG:NH1	1:D:86:ARG:NH1	2.64	0.45
1:C:103:ALA:HB2	1:C:122:LEU:HD13	1.98	0.45
1:C:307:ARG:HG2	1:C:307:ARG:H	1.46	0.45
1:D:433:THR:HG22	1:D:434:ASN:N	2.31	0.45
1:B:221:LEU:HD12	1:B:221:LEU:N	2.31	0.45
1:D:290:ALA:HA	1:D:456:TYR:OH	2.16	0.45
1:B:12:THR:HG22	1:B:104:THR:OG1	2.17	0.45
1:C:277:ILE:HD13	1:C:318:PHE:CE2	2.52	0.45
1:B:312:GLU:HG3	1:B:409:ARG:HD3	1.99	0.45
1:D:295:PHE:CB	1:D:329:ARG:NH1	2.80	0.45
1:C:320:LYS:HA	1:C:323:VAL:HG22	1.97	0.45
1:A:11:PRO:C	1:A:12:THR:HG22	2.37	0.45
1:B:347:LYS:HB2	1:B:379:PHE:CE1	2.52	0.45
1:B:71:SER:O	1:B:72:LEU:C	2.55	0.45
1:D:373:GLY:HA2	1:D:381:ILE:HA	1.97	0.45
1:B:310:VAL:HG21	1:B:318:PHE:CD1	2.52	0.45
1:C:293:GLY:HA3	1:C:456:TYR:HD2	1.81	0.45
1:C:497:GLN:HE21	1:C:499:ASN:HD21	1.63	0.45
1:A:283:LEU:HB3	1:A:321:ARG:HH12	1.81	0.45
1:D:319:VAL:O	1:D:323:VAL:HG13	2.16	0.45
1:B:109:ASN:OD1	1:B:197:THR:HG22	2.17	0.45
1:D:164:GLN:HE22	1:D:179:ILE:HD13	1.82	0.45
1:B:88:LEU:HA	1:B:88:LEU:HD23	1.84	0.45
1:C:8:LEU:N	1:C:9:PRO:CD	2.79	0.45
1:C:293:GLY:HA3	1:C:456:TYR:CD2	2.51	0.45
1:D:202:LEU:HD21	1:D:222:PRO:HD3	1.98	0.45
1:A:295:PHE:HE2	1:A:405:GLN:HE21	1.65	0.45
1:C:391:ASP:OD2	1:C:419:ARG:CD	2.65	0.45
1:A:56:LYS:HD3	1:A:231:ALA:HB1	1.99	0.45
1:B:374:LEU:HB2	4:B:720:HOH:O	2.16	0.45
1:B:280:ASP:OD2	1:B:433:THR:HG23	2.17	0.45
1:B:408:LEU:CD1	1:B:408:LEU:H	2.30	0.45
1:A:169:ASN:OD1	1:A:301:CYS:HA	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:14:ASN:HD22	1:D:14:ASN:N	2.14	0.45
1:B:402:GLY:O	1:B:404:VAL:N	2.49	0.45
1:D:274:PRO:HB3	1:D:307:ARG:NH1	2.31	0.44
1:B:178:LYS:HE3	1:B:242:ALA:HB1	1.99	0.44
1:C:410:PHE:CG	1:C:416:VAL:HG13	2.52	0.44
1:D:459:LEU:HG	1:D:460:ASN:N	2.32	0.44
1:C:367:LEU:HD11	1:C:370:GLY:O	2.17	0.44
1:B:354:LEU:O	1:B:357:ILE:N	2.48	0.44
1:D:11:PRO:O	1:D:12:THR:C	2.56	0.44
1:A:489:LYS:NZ	1:B:444:SER:HA	2.31	0.44
1:B:283:LEU:HD13	1:B:314:ILE:HD12	1.99	0.44
1:B:247:THR:HA	1:B:269:LEU:HD13	1.99	0.44
1:C:333:SER:O	1:C:339:THR:HG21	2.16	0.44
1:A:59:ILE:O	1:A:63:VAL:HG23	2.18	0.44
1:B:146:VAL:HG21	1:B:152:THR:CG2	2.48	0.44
1:A:10:SER:O	1:A:11:PRO:O	2.36	0.44
1:A:352:LYS:CG	1:A:401:PHE:HZ	2.31	0.44
1:B:272:LYS:HE3	1:B:307:ARG:NH1	2.33	0.44
1:D:99:ARG:HG2	1:D:118:PHE:CE1	2.52	0.44
1:A:350:TYR:OH	1:A:373:GLY:HA3	2.18	0.44
1:A:370:GLY:HA2	1:A:382:GLU:OE2	2.17	0.44
1:A:367:LEU:HD21	1:A:370:GLY:O	2.18	0.44
1:A:330:ILE:CG2	1:A:339:THR:HA	2.47	0.44
1:A:109:ASN:HD22	1:A:199:LEU:HB2	1.81	0.44
1:B:293:GLY:O	1:B:456:TYR:HE2	2.00	0.44
1:D:178:LYS:NZ	1:D:244:THR:CG2	2.81	0.44
1:A:400:ILE:HG21	1:A:404:VAL:CB	2.42	0.44
1:A:306:SER:HB2	1:A:406:GLU:OE1	2.17	0.44
1:B:6:GLN:NE2	1:B:6:GLN:H	2.16	0.44
1:A:324:GLU:O	1:A:328:ARG:HG3	2.16	0.44
1:C:166:ILE:HB	1:C:167:PRO:HD2	1.99	0.44
1:C:384:THR:O	1:C:404:VAL:HA	2.17	0.44
1:D:59:ILE:O	1:D:63:VAL:HG23	2.18	0.44
1:D:365:ALA:N	1:D:393:MET:HE3	2.32	0.44
1:D:14:ASN:ND2	1:D:14:ASN:N	2.66	0.44
1:B:332:GLY:O	1:B:380:PHE:HE2	2.01	0.44
1:D:25:ASN:O	1:D:27:GLU:HG2	2.18	0.44
1:C:146:VAL:CG1	1:C:147:ASP:N	2.81	0.44
1:D:280:ASP:OD1	1:D:433:THR:CG2	2.65	0.44
1:B:294:VAL:HG22	1:B:305:GLY:O	2.18	0.44
1:A:332:GLY:O	1:A:380:PHE:HE2	2.01	0.44
1:D:208:ILE:HG23	1:D:213:PHE:CD2	2.53	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:428:VAL:HG22	1:A:450:THR:CG2	2.48	0.44
1:C:300:GLN:HB3	1:C:401:PHE:O	2.18	0.44
1:D:152:THR:HA	1:D:492:THR:HA	1.99	0.44
1:D:400:ILE:HD13	1:D:406:GLU:OE1	2.18	0.44
1:D:273:SER:HA	1:D:428:VAL:O	2.17	0.44
1:D:111:GLY:O	1:D:343:PRO:HD2	2.18	0.44
1:C:234:SER:HB2	4:C:719:HOH:O	2.17	0.44
1:B:8:LEU:H	1:B:9:PRO:CD	2.27	0.43
1:C:377:LYS:HG2	4:C:752:HOH:O	2.18	0.43
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.53	0.43
1:B:435:ASP:HA	1:C:434:ASN:O	2.18	0.43
1:A:295:PHE:HE2	1:A:405:GLN:NE2	2.16	0.43
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.26	0.43
1:A:103:ALA:HB2	1:A:122:LEU:HD13	2.00	0.43
1:C:29:GLN:HE21	1:C:29:GLN:HA	1.82	0.43
1:D:112:LYS:HG3	1:D:113:PRO:HD2	1.99	0.43
1:D:178:LYS:NZ	1:D:244:THR:HG21	2.34	0.43
1:B:436:ILE:CA	1:C:436:ILE:HG12	2.45	0.43
1:D:32:GLU:HG3	1:D:57:VAL:HG12	2.00	0.43
1:C:55:ASP:O	1:C:56:LYS:C	2.56	0.43
1:A:496:PRO:HG2	1:C:441:MET:HG3	2.01	0.43
1:D:457:ASN:ND2	1:D:458:ALA:N	2.61	0.43
1:D:274:PRO:CD	1:D:427:LEU:HD11	2.49	0.43
1:D:29:GLN:NE2	1:D:29:GLN:CA	2.81	0.43
1:A:166:ILE:HD13	1:A:166:ILE:H	1.83	0.43
1:C:32:GLU:HG3	1:C:57:VAL:HG11	2.00	0.43
1:B:247:THR:HG22	1:B:269:LEU:HD13	1.99	0.43
1:B:196:GLN:H	1:B:196:GLN:NE2	2.16	0.43
1:C:267:LEU:CD1	1:D:262:LEU:HD22	2.47	0.43
1:B:109:ASN:HD22	1:B:199:LEU:HG	1.82	0.43
1:B:236:ILE:HD12	1:B:261:ASN:HB3	2.00	0.43
1:D:454:ASN:O	1:D:455:CYS:HB3	2.19	0.43
1:B:12:THR:HG21	1:B:101:THR:HB	2.00	0.43
1:C:433:THR:HG22	1:C:434:ASN:H	1.84	0.43
1:A:273:SER:HB3	1:A:305:GLY:CA	2.49	0.43
1:B:15:LEU:HD12	1:B:16:GLU:N	2.33	0.43
1:A:70:PHE:CE2	1:A:160:GLY:HA2	2.53	0.43
1:A:356:LEU:HD23	1:A:400:ILE:HG13	2.01	0.43
1:A:109:ASN:ND2	1:A:199:LEU:CG	2.79	0.43
1:C:232:ILE:HG23	1:C:238:ILE:CD1	2.49	0.43
1:D:417:ILE:O	1:D:421:ASN:HB2	2.19	0.43
1:C:7:LEU:N	1:C:7:LEU:HD23	2.34	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:436:ILE:HG22	1:C:440:LEU:CD1	2.49	0.43
1:D:269:LEU:O	1:D:270:GLY:O	2.36	0.43
1:C:125:VAL:HG21	1:C:172:LEU:HG	2.00	0.43
1:A:114:PHE:HD2	1:A:115:LEU:HD23	1.82	0.43
1:B:280:ASP:OD1	1:B:433:THR:HA	2.19	0.43
1:A:432:PHE:HA	1:A:454:ASN:HD22	1.84	0.43
1:A:128:THR:HG21	1:A:177:TRP:NE1	2.34	0.43
1:B:421:ASN:ND2	1:B:445:ALA:O	2.42	0.43
1:D:70:PHE:CE2	1:D:160:GLY:HA2	2.54	0.43
1:A:349:GLN:O	1:A:353:ILE:HG13	2.18	0.42
1:C:365:ALA:N	1:C:393:MET:HE3	2.34	0.42
1:B:496:PRO:HG2	1:D:441:MET:HE2	2.02	0.42
1:A:436:ILE:HA	1:D:436:ILE:CG1	2.49	0.42
1:B:99:ARG:HG2	1:B:118:PHE:CE1	2.53	0.42
1:D:392:ASP:O	1:D:397:LYS:NZ	2.52	0.42
1:C:71:SER:O	1:C:74:SER:HB2	2.19	0.42
1:B:312:GLU:CG	1:B:409:ARG:HD3	2.48	0.42
1:D:6:GLN:NE2	1:D:6:GLN:HA	2.34	0.42
1:A:181:PRO:O	1:A:184:CYS:HB3	2.20	0.42
1:C:221:LEU:HD12	1:C:221:LEU:N	2.33	0.42
1:D:173:LEU:HD23	1:D:173:LEU:HA	1.89	0.42
1:A:56:LYS:HD3	1:A:231:ALA:HB2	2.00	0.42
1:C:94:LEU:HD12	1:C:211:ALA:HB2	2.01	0.42
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.54	0.42
1:A:435:ASP:OD1	1:A:437:ASN:HB2	2.19	0.42
1:A:277:ILE:HD13	1:A:318:PHE:CE2	2.55	0.42
1:A:198:PRO:O	1:A:202:LEU:HG	2.19	0.42
1:B:387:SER:O	1:B:388:ASN:C	2.56	0.42
1:C:373:GLY:HA2	1:C:381:ILE:HA	2.02	0.42
1:D:178:LYS:HZ3	1:D:244:THR:HG21	1.85	0.42
1:D:6:GLN:HE21	1:D:6:GLN:HA	1.82	0.42
1:B:329:ARG:NH1	1:B:341:GLN:OE1	2.52	0.42
1:B:400:ILE:N	1:B:400:ILE:CD1	2.76	0.42
1:D:287:VAL:O	1:D:291:HIS:HB2	2.20	0.42
1:A:169:ASN:H	1:A:169:ASN:HD22	1.67	0.42
1:C:269:LEU:HD11	1:D:262:LEU:HD13	2.01	0.42
1:B:412:THR:O	1:B:415:GLU:HB3	2.19	0.42
1:B:106:GLU:OE2	1:B:171:PRO:HB2	2.20	0.42
1:C:157:GLU:OE1	1:C:489:LYS:HD2	2.19	0.42
1:D:298:GLN:HG3	1:D:342:GLY:O	2.19	0.42
1:A:44:THR:C	1:A:46:GLU:H	2.22	0.42
1:B:264:ARG:HH22	1:B:487:GLU:HB3	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:431:VAL:HG21	1:C:442:VAL:HG11	2.02	0.42
1:B:244:THR:HB	1:B:268:GLU:HB2	2.02	0.42
1:C:363:GLU:OE2	1:C:393:MET:HA	2.19	0.42
1:B:333:SER:O	1:B:339:THR:HG21	2.19	0.42
1:D:2:MET:HE1	1:D:4:SER:N	2.35	0.42
1:B:293:GLY:HA3	1:B:456:TYR:HD2	1.83	0.42
1:D:459:LEU:HD23	4:D:731:HOH:O	2.20	0.42
1:D:292:GLN:CA	1:D:292:GLN:HE21	2.31	0.42
1:A:244:THR:HB	1:A:268:GLU:CB	2.50	0.42
1:A:39:VAL:CG2	1:A:51:VAL:HG23	2.50	0.42
1:A:373:GLY:HA2	1:A:381:ILE:HA	2.01	0.42
1:B:394:ARG:CB	1:B:394:ARG:NH1	2.78	0.42
1:B:269:LEU:O	1:B:270:GLY:O	2.38	0.42
1:C:292:GLN:O	1:C:296:PHE:HB2	2.19	0.42
1:C:56:LYS:NZ	4:C:719:HOH:O	2.53	0.42
1:B:144:ILE:HD13	1:C:140:HIS:HD2	1.85	0.42
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.85	0.42
1:C:399:GLU:C	1:C:400:ILE:HD12	2.40	0.42
1:D:11:PRO:HB3	1:D:114:PHE:CD1	2.55	0.42
1:D:11:PRO:HD3	1:D:114:PHE:CD2	2.55	0.42
1:A:8:LEU:HB3	1:A:9:PRO:HD2	2.01	0.42
1:A:479:GLU:CG	1:A:483:ARG:HH21	2.31	0.42
1:B:109:ASN:HD22	1:B:199:LEU:HD12	1.84	0.42
1:A:323:VAL:HG11	1:A:368:GLU:HB3	2.02	0.42
1:A:23:PHE:CE1	1:A:26:ASN:HA	2.55	0.42
1:B:72:LEU:O	1:B:74:SER:N	2.53	0.42
1:D:300:GLN:HB3	1:D:401:PHE:O	2.20	0.42
1:A:4:SER:C	1:A:6:GLN:H	2.23	0.42
1:D:328:ARG:CG	1:D:328:ARG:HH11	2.31	0.41
1:C:457:ASN:N	1:C:457:ASN:ND2	2.66	0.41
1:C:413:MET:C	1:C:415:GLU:N	2.73	0.41
1:B:93:ASP:OD1	1:B:130:ARG:NH2	2.47	0.41
1:D:175:PHE:O	1:D:179:ILE:HG12	2.20	0.41
1:C:306:SER:HB2	1:C:404:VAL:O	2.19	0.41
1:C:283:LEU:HD21	1:C:317:GLU:HB3	2.01	0.41
1:C:10:SER:O	1:C:11:PRO:O	2.38	0.41
1:A:402:GLY:O	1:A:404:VAL:N	2.46	0.41
1:A:312:GLU:HG2	1:A:409:ARG:CG	2.50	0.41
1:C:290:ALA:O	1:C:294:VAL:HG23	2.20	0.41
1:C:413:MET:HE1	1:C:438:LYS:HG2	2.01	0.41
1:D:8:LEU:HD21	1:D:115:LEU:HD11	2.02	0.41
1:A:427:LEU:HD12	1:A:428:VAL:N	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:77:ARG:NH1	1:B:77:ARG:HB3	2.36	0.41
1:A:292:GLN:NE2	1:A:292:GLN:HA	2.36	0.41
1:D:35:ARG:O	1:D:36:VAL:HG23	2.20	0.41
1:C:152:THR:CB	1:C:492:THR:HB	2.50	0.41
1:B:309:PHE:H	1:B:309:PHE:HD1	1.68	0.41
1:C:303:THR:CB	1:C:458:ALA:HB3	2.41	0.41
1:B:365:ALA:H	1:B:393:MET:HE1	1.83	0.41
1:B:285:TYR:CE2	1:B:289:GLN:HG3	2.55	0.41
1:B:294:VAL:O	1:B:294:VAL:HG12	2.19	0.41
1:A:15:LEU:HD21	1:A:105:MET:HG3	2.03	0.41
1:D:303:THR:CG2	1:D:459:LEU:HB3	2.50	0.41
1:A:54:ALA:HA	1:A:58:ASP:OD2	2.20	0.41
1:D:353:ILE:CD1	1:D:402:GLY:HA3	2.47	0.41
1:C:413:MET:HG2	1:C:417:ILE:CD1	2.50	0.41
1:D:41:ASN:OD1	1:D:43:ALA:HB3	2.20	0.41
1:A:15:LEU:HD22	1:A:104:THR:CG2	2.50	0.41
1:A:175:PHE:CE1	1:A:179:ILE:HG13	2.56	0.41
1:A:399:GLU:HG2	1:A:400:ILE:N	2.36	0.41
1:A:456:TYR:O	1:A:456:TYR:CD1	2.67	0.41
1:C:23:PHE:CE1	1:C:26:ASN:HA	2.55	0.41
1:A:195:GLU:HB3	1:A:223:GLY:O	2.21	0.41
1:B:366:LYS:O	1:B:368:GLU:N	2.54	0.41
1:D:108:LEU:C	1:D:108:LEU:HD13	2.41	0.41
1:D:387:SER:O	1:D:388:ASN:C	2.59	0.41
1:D:295:PHE:HD1	1:D:403:PRO:HA	1.86	0.41
1:A:282:ASP:O	1:A:282:ASP:OD1	2.39	0.41
1:B:436:ILE:HG12	1:C:436:ILE:CA	2.50	0.41
1:A:324:GLU:O	1:A:327:LYS:HB2	2.20	0.41
1:C:72:LEU:HD23	1:C:72:LEU:HA	1.79	0.41
1:B:283:LEU:HD21	1:B:317:GLU:HB3	2.01	0.41
1:A:113:PRO:HD2	1:A:298:GLN:HE22	1.86	0.41
1:B:496:PRO:HG2	1:D:441:MET:CE	2.50	0.41
1:D:298:GLN:C	1:D:300:GLN:H	2.24	0.41
1:D:349:GLN:NE2	1:D:401:PHE:CD2	2.89	0.41
1:B:309:PHE:CD1	1:B:309:PHE:N	2.88	0.41
1:C:90:LYS:NZ	1:C:90:LYS:HB2	2.36	0.41
1:C:13:PRO:O	1:C:14:ASN:C	2.58	0.41
1:B:298:GLN:C	1:B:300:GLN:H	2.25	0.41
1:B:120:ILE:O	1:B:121:ASP:C	2.58	0.41
1:A:152:THR:HG22	1:A:492:THR:CB	2.29	0.41
1:A:158:PRO:CD	1:D:500:SER:HB3	2.51	0.41
1:B:280:ASP:OD1	1:B:433:THR:HG23	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:264:ARG:HH11	1:B:264:ARG:CG	2.33	0.40
1:B:138:LYS:HE3	1:D:135:TRP:CD1	2.56	0.40
1:B:166:ILE:HD12	1:B:191:ILE:HD11	2.02	0.40
1:B:279:ALA:HA	1:B:314:ILE:HD13	2.03	0.40
1:B:317:GLU:O	1:B:321:ARG:HG2	2.21	0.40
1:B:37:PHE:HD1	1:B:53:GLU:HB2	1.85	0.40
1:A:317:GLU:OE1	1:A:321:ARG:NE	2.54	0.40
1:B:244:THR:HA	1:B:268:GLU:O	2.21	0.40
1:C:122:LEU:O	1:C:126:ILE:HG13	2.21	0.40
1:C:279:ALA:HA	1:C:314:ILE:HD13	2.04	0.40
1:A:293:GLY:HA3	1:A:456:TYR:CE2	2.54	0.40
1:D:264:ARG:NH2	1:D:487:GLU:HB3	2.37	0.40
1:D:213:PHE:HA	1:D:214:PRO:HD3	1.99	0.40
1:D:14:ASN:H	1:D:14:ASN:HD22	1.67	0.40
1:C:158:PRO:HB3	1:C:185:CYS:O	2.22	0.40
1:C:221:LEU:HA	1:C:222:PRO:HD2	1.95	0.40
1:A:274:PRO:HD2	1:A:428:VAL:O	2.21	0.40
1:D:249:VAL:O	1:D:253:ILE:HG12	2.22	0.40
1:B:435:ASP:OD1	1:B:437:ASN:HB2	2.21	0.40
1:B:319:VAL:HG22	1:B:407:ILE:HG21	2.03	0.40
1:C:192:LYS:HB3	1:C:192:LYS:HE3	1.88	0.40
1:C:192:LYS:HG2	1:C:221:LEU:O	2.20	0.40
1:A:169:ASN:N	1:A:169:ASN:HD22	2.19	0.40
1:B:283:LEU:HD21	1:B:317:GLU:CB	2.52	0.40
1:B:188:THR:HG22	1:B:217:VAL:HA	2.03	0.40
1:C:444:SER:CB	1:D:155:ARG:HH12	2.35	0.40
1:C:492:THR:HG21	1:D:452:TRP:CZ3	2.56	0.40
1:B:312:GLU:HG3	1:B:409:ARG:CG	2.51	0.40
1:A:146:VAL:HG12	1:A:147:ASP:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:503:CL:CL	2:C:503:CL:CL[2_565]	0.48	1.72
2:C:504:CL:CL	2:C:504:CL:CL[2_565]	0.48	1.72
1:C:255:GLU:OE2	1:D:259:ARG:NH2[2_565]	2.05	0.15
1:C:259:ARG:NH2	1:D:255:GLU:OE2[2_565]	2.07	0.13

## 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	474/499 (95%)	416 (88%)	48 (10%)	10 (2%)	11	27
1	B	473/499 (95%)	423 (89%)	37 (8%)	13 (3%)	8	19
1	C	476/499 (95%)	419 (88%)	42 (9%)	15 (3%)	6	14
1	D	478/499 (96%)	423 (88%)	48 (10%)	7 (2%)	15	38
All	All	1901/1996 (95%)	1681 (88%)	175 (9%)	45 (2%)	9	22

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	74	SER
1	A	260	SER
1	A	270	GLY
1	B	72	LEU
1	B	270	GLY
1	B	367	LEU
1	C	9	PRO
1	C	11	PRO
1	C	72	LEU
1	C	74	SER
1	D	74	SER
1	B	8	LEU
1	B	74	SER
1	B	316	GLU
1	B	377	LYS
1	C	8	LEU
1	C	270	GLY
1	C	425	PHE
1	D	270	GLY
1	A	425	PHE
1	B	73	GLY
1	C	73	GLY
1	C	401	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	422	ASN
1	C	456	TYR
1	D	425	PHE
1	D	457	ASN
1	A	363	GLU
1	A	377	LYS
1	B	56	LYS
1	B	313	SER
1	B	337	PRO
1	B	425	PHE
1	D	282	ASP
1	D	363	GLU
1	A	415	GLU
1	B	422	ASN
1	C	14	ASN
1	A	427	LEU
1	C	303	THR
1	C	377	LYS
1	C	171	PRO
1	A	378	GLY
1	D	337	PRO

### 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	394/409 (96%)	365 (93%)	29 (7%)	20	43
1	B	393/409 (96%)	365 (93%)	28 (7%)	21	46
1	C	395/409 (97%)	365 (92%)	30 (8%)	19	41
1	D	397/409 (97%)	361 (91%)	36 (9%)	14	30
All	All	1579/1636 (96%)	1456 (92%)	123 (8%)	18	40

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	THR
1	A	29	GLN
1	A	46	GLU
1	A	86	ARG
1	A	90	LYS
1	A	101	THR
1	A	106	GLU
1	A	115	LEU
1	A	121	ASP
1	A	122	LEU
1	A	128	THR
1	A	166	ILE
1	A	192	LYS
1	A	196	GLN
1	A	264	ARG
1	A	298	GLN
1	A	307	ARG
1	A	355	GLU
1	A	416	VAL
1	A	418	GLU
1	A	433	THR
1	A	446	MET
1	A	456	TYR
1	A	482	LEU
1	A	490	THR
1	A	492	THR
1	A	496	PRO
1	B	29	GLN
1	B	36	VAL
1	B	46	GLU
1	B	55	ASP
1	B	60	ASP
1	B	90	LYS
1	B	101	THR
1	B	121	ASP
1	B	144	ILE
1	B	166	ILE
1	B	179	ILE
1	B	192	LYS
1	B	195	GLU
1	B	196	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	244	THR
1	B	264	ARG
1	B	282	ASP
1	B	298	GLN
1	B	307	ARG
1	B	327	LYS
1	B	399	GLU
1	B	401	PHE
1	B	416	VAL
1	B	418	GLU
1	B	421	ASN
1	B	450	THR
1	B	490	THR
1	B	492	THR
1	C	5	LEU
1	C	6	GLN
1	C	8	LEU
1	C	29	GLN
1	C	30	ASN
1	C	46	GLU
1	C	60	ASP
1	C	90	LYS
1	C	101	THR
1	C	122	LEU
1	C	142	MET
1	C	152	THR
1	C	166	ILE
1	C	192	LYS
1	C	198	PRO
1	C	244	THR
1	C	248	GLU
1	C	259	ARG
1	C	263	LYS
1	C	266	THR
1	C	282	ASP
1	C	307	ARG
1	C	355	GLU
1	C	401	PHE
1	C	416	VAL
1	C	418	GLU
1	C	450	THR
1	C	457	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	490	THR
1	C	492	THR
1	D	2	MET
1	D	6	GLN
1	D	8	LEU
1	D	12	THR
1	D	29	GLN
1	D	46	GLU
1	D	60	ASP
1	D	86	ARG
1	D	113	PRO
1	D	121	ASP
1	D	122	LEU
1	D	128	THR
1	D	135	TRP
1	D	166	ILE
1	D	167	PRO
1	D	192	LYS
1	D	195	GLU
1	D	196	GLN
1	D	244	THR
1	D	247	THR
1	D	248	GLU
1	D	259	ARG
1	D	264	ARG
1	D	282	ASP
1	D	302	CYS
1	D	307	ARG
1	D	394	ARG
1	D	401	PHE
1	D	416	VAL
1	D	418	GLU
1	D	450	THR
1	D	457	ASN
1	D	459	LEU
1	D	482	LEU
1	D	490	THR
1	D	492	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	30	ASN
1	A	109	ASN
1	A	116	GLN
1	A	196	GLN
1	A	291	HIS
1	A	292	GLN
1	A	437	ASN
1	A	454	ASN
1	B	29	GLN
1	B	30	ASN
1	B	109	ASN
1	B	116	GLN
1	B	140	HIS
1	B	156	HIS
1	B	164	GLN
1	B	196	GLN
1	B	275	ASN
1	B	292	GLN
1	B	297	ASN
1	C	6	GLN
1	C	14	ASN
1	C	26	ASN
1	C	29	GLN
1	C	30	ASN
1	C	109	ASN
1	C	116	GLN
1	C	140	HIS
1	C	169	ASN
1	C	196	GLN
1	C	254	GLN
1	C	291	HIS
1	C	292	GLN
1	C	405	GLN
1	C	457	ASN
1	C	497	GLN
1	D	6	GLN
1	D	14	ASN
1	D	26	ASN
1	D	29	GLN
1	D	30	ASN
1	D	109	ASN
1	D	116	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	140	HIS
1	D	164	GLN
1	D	169	ASN
1	D	196	GLN
1	D	254	GLN
1	D	275	ASN
1	D	291	HIS
1	D	292	GLN
1	D	297	ASN
1	D	457	ASN
1	D	460	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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	701	-	29,29,48	2.29	8 (27%)	45,45,73	2.53	14 (31%)
3	NAD	B	702	-	29,29,48	2.32	8 (27%)	45,45,73	2.48	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAD	C	703	1	29,29,48	2.30	11 (37%)	45,45,73	2.44	12 (26%)
3	NAD	D	704	-	29,29,48	2.15	6 (20%)	45,45,73	2.47	11 (24%)

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	701	-	-	0/16/32/62	0/1/3/5
3	NAD	B	702	-	-	0/16/32/62	0/1/3/5
3	NAD	C	703	1	-	0/16/32/62	0/1/3/5
3	NAD	D	704	-	-	0/16/32/62	0/1/3/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAD	PN-O5D	8.04	1.65	1.51
3	A	701	NAD	PN-O5D	6.74	1.63	1.51
3	D	704	NAD	PN-O5D	6.70	1.63	1.51
3	C	703	NAD	PN-O5D	6.16	1.62	1.51
3	A	701	NAD	O4B-C1B	5.48	1.49	1.41
3	B	702	NAD	O4B-C1B	5.40	1.49	1.41
3	C	703	NAD	O4B-C1B	5.34	1.49	1.41
3	D	704	NAD	O4B-C1B	5.17	1.49	1.41
3	A	701	NAD	C4A-N3A	5.15	1.43	1.35
3	B	702	NAD	C4A-N3A	4.45	1.42	1.35
3	D	704	NAD	C4A-N3A	4.30	1.42	1.35
3	C	703	NAD	C2A-N3A	3.47	1.39	1.32
3	C	703	NAD	C4A-N3A	3.46	1.40	1.35
3	D	704	NAD	C2A-N3A	3.33	1.38	1.32
3	A	701	NAD	C2A-N3A	3.19	1.38	1.32
3	C	703	NAD	C8A-N9A	3.05	1.41	1.36
3	A	701	NAD	C2A-N1A	2.88	1.39	1.33
3	D	704	NAD	C4A-N9A	-2.80	1.33	1.37
3	B	702	NAD	C4A-N9A	-2.69	1.33	1.37
3	C	703	NAD	C4A-N9A	-2.67	1.33	1.37
3	B	702	NAD	C2A-N3A	2.66	1.37	1.32
3	A	701	NAD	C4A-N9A	-2.44	1.34	1.37
3	C	703	NAD	C5B-C4B	-2.39	1.43	1.51
3	C	703	NAD	O3B-C3B	2.34	1.48	1.43
3	C	703	NAD	C2A-N1A	2.30	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	NAD	C1B-N9A	2.24	1.55	1.48
3	A	701	NAD	C5A-N7A	-2.22	1.32	1.40
3	D	704	NAD	C5A-N7A	-2.22	1.32	1.40
3	A	701	NAD	C1B-N9A	2.15	1.55	1.48
3	B	702	NAD	C8A-N9A	2.12	1.39	1.36
3	C	703	NAD	PA-O3	-2.11	1.56	1.59
3	B	702	NAD	C1B-N9A	2.10	1.55	1.48
3	B	702	NAD	C2A-N1A	2.06	1.38	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAD	N3A-C2A-N1A	-9.72	120.58	128.71
3	D	704	NAD	N3A-C2A-N1A	-9.22	121.00	128.71
3	B	702	NAD	N3A-C2A-N1A	-9.19	121.02	128.71
3	C	703	NAD	N3A-C2A-N1A	-8.35	121.73	128.71
3	A	701	NAD	N3A-C4A-N9A	7.49	138.95	125.43
3	C	703	NAD	N3A-C4A-N9A	7.29	138.59	125.43
3	D	704	NAD	N3A-C4A-N9A	7.22	138.47	125.43
3	B	702	NAD	N3A-C4A-N9A	7.20	138.43	125.43
3	C	703	NAD	O4B-C1B-N9A	6.16	114.17	108.44
3	A	701	NAD	O4B-C1B-N9A	5.06	113.15	108.44
3	B	702	NAD	C4A-C5A-N7A	4.79	113.62	109.52
3	D	704	NAD	O4B-C1B-N9A	4.75	112.86	108.44
3	B	702	NAD	O4B-C1B-N9A	4.69	112.80	108.44
3	A	701	NAD	C4A-C5A-N7A	4.36	113.26	109.52
3	D	704	NAD	C4A-C5A-N7A	4.22	113.14	109.52
3	C	703	NAD	C4A-C5A-N7A	4.06	113.00	109.52
3	D	704	NAD	C5A-C4A-N3A	-3.85	117.31	125.70
3	C	703	NAD	C5A-C4A-N3A	-3.82	117.38	125.70
3	A	701	NAD	C5A-C4A-N3A	-3.74	117.56	125.70
3	B	702	NAD	C5A-C4A-N3A	-3.71	117.62	125.70
3	B	702	NAD	C4B-O4B-C1B	-3.47	105.98	109.75
3	D	704	NAD	O5D-PN-O1N	-3.40	104.91	112.73
3	D	704	NAD	C4B-O4B-C1B	-3.16	106.32	109.75
3	A	701	NAD	O5D-PN-O1N	-3.11	105.58	112.73
3	C	703	NAD	O5D-PN-O1N	-2.86	106.15	112.73
3	B	702	NAD	O5D-PN-O2N	-2.84	106.72	112.88
3	D	704	NAD	C2A-N3A-C4A	2.79	121.95	114.01
3	B	702	NAD	O5D-PN-O1N	-2.78	106.32	112.73
3	D	704	NAD	O2N-PN-O1N	2.74	119.04	112.73
3	D	704	NAD	O5D-PN-O2N	-2.65	107.13	112.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAD	C4B-O4B-C1B	-2.63	106.90	109.75
3	A	701	NAD	O5D-PN-O2N	-2.63	107.18	112.88
3	B	702	NAD	C2A-N3A-C4A	2.61	121.44	114.01
3	C	703	NAD	C2A-N3A-C4A	2.60	121.41	114.01
3	A	701	NAD	C5A-C4A-N9A	-2.54	103.49	107.16
3	B	702	NAD	O2N-PN-O1N	2.43	118.31	112.73
3	A	701	NAD	C2A-N3A-C4A	2.37	120.76	114.01
3	A	701	NAD	O2N-PN-O1N	2.37	118.19	112.73
3	C	703	NAD	O2N-PN-O1N	2.30	118.02	112.73
3	B	702	NAD	C5A-C4A-N9A	-2.22	103.96	107.16
3	C	703	NAD	C4B-O4B-C1B	-2.22	107.34	109.75
3	C	703	NAD	O5D-PN-O2N	-2.21	108.07	112.88
3	C	703	NAD	C5A-C4A-N9A	-2.18	104.02	107.16
3	B	702	NAD	O4B-C4B-C5B	-2.14	101.73	109.36
3	A	701	NAD	C6A-C5A-C4A	2.13	121.16	117.25
3	A	701	NAD	O2N-PN-O3	2.11	112.72	105.27
3	C	703	NAD	O4B-C4B-C5B	-2.07	101.97	109.36
3	A	701	NAD	O4B-C4B-C5B	-2.05	102.04	109.36
3	D	704	NAD	C5A-C4A-N9A	-2.05	104.21	107.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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