



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:18 am BST

PDB ID : 1ZCD
Title : Crystal structure of the Na⁺/H⁺ antiporter NhaA
Authors : Hunte, C.; Screpanti, E.; Venturi, M.; Rimon, A.; Padan, E.; Michel, H.
Deposited on : 2005-04-11
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

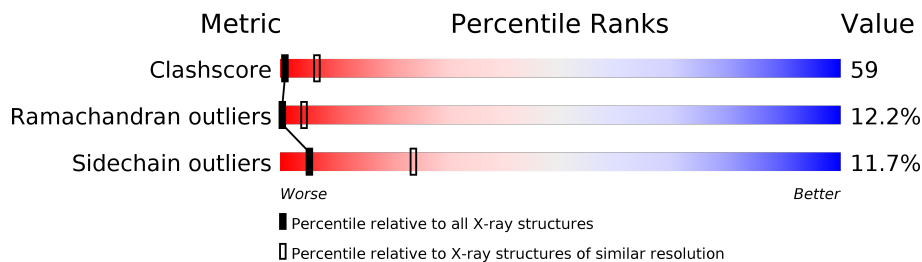
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	 27% 54% 15% ..
1	B	388	 28% 53% 15% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5616 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 Na(+)/H(+) antiporter 1.

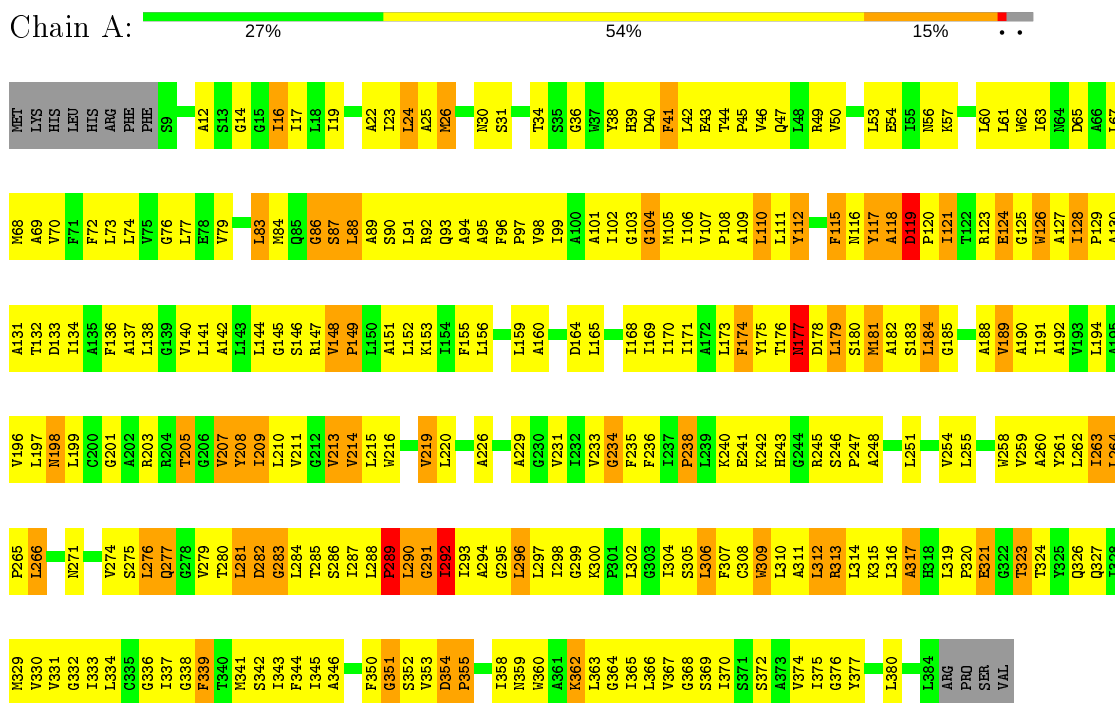
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	Total 2808	C 1865	N 457	O 473	S 13	0	0	0
1	B	376	Total 2808	C 1865	N 457	O 473	S 13	0	0	0

3 Residue-property plots

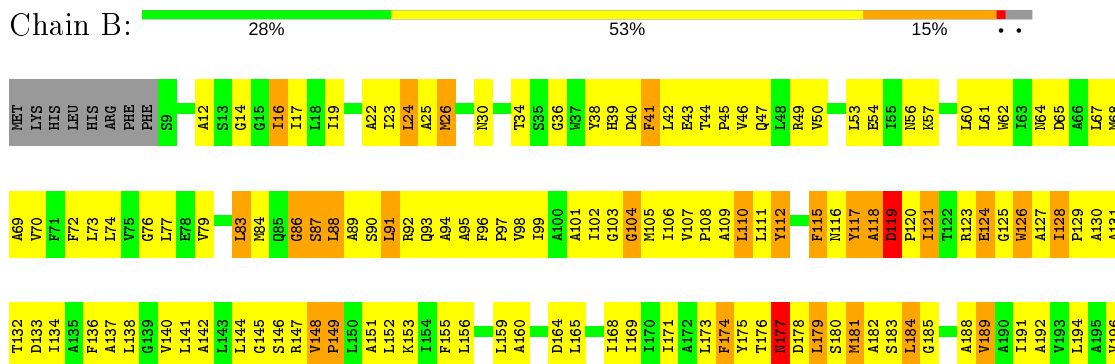
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

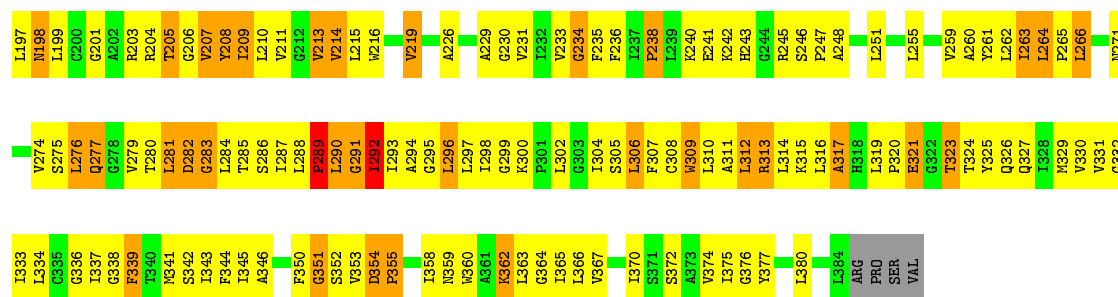
Note EDS was not executed.

- Molecule 1: Na(+)/H(+) antiporter 1



- Molecule 1: Na(+)/H(+) antiporter 1





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.87Å 121.72Å 123.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.45	Depositor
% Data completeness (in resolution range)	91.2 (15.00-3.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.316 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5616	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/2867	0.73	1/3910 (0.0%)
1	B	0.49	0/2867	0.73	1/3910 (0.0%)
All	All	0.49	0/5734	0.73	2/7820 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	119	ASP	N-CA-C	5.04	124.60	111.00
1	B	119	ASP	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	TYR	Sidechain
1	B	112	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2808	0	2993	352	0
1	B	2808	0	2993	339	0
All	All	5616	0	5986	684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (684) 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:119:ASP:HB3	1:A:120:PRO:HD3	1.19	1.13
1:B:119:ASP:HB3	1:B:120:PRO:HD3	1.20	1.10
1:A:330:VAL:HG11	1:A:380:LEU:HB2	1.32	1.09
1:B:330:VAL:HG11	1:B:380:LEU:HB2	1.32	1.06
1:B:96:PHE:HB3	1:B:97:PRO:HD3	1.47	0.97
1:A:96:PHE:HB3	1:A:97:PRO:HD3	1.48	0.95
1:A:290:LEU:HD22	1:A:291:GLY:H	1.34	0.93
1:A:119:ASP:HB3	1:A:120:PRO:CD	2.00	0.92
1:A:112:TYR:CD2	1:A:125:GLY:HA2	2.04	0.91
1:B:112:TYR:CD2	1:B:125:GLY:HA2	2.04	0.91
1:B:290:LEU:HD22	1:B:291:GLY:H	1.35	0.91
1:A:121:ILE:HB	1:A:124:GLU:OE1	1.71	0.91
1:B:304:ILE:HD13	1:B:333:ILE:HG12	1.52	0.90
1:B:119:ASP:HB3	1:B:120:PRO:CD	2.01	0.89
1:B:134:ILE:HB	1:B:160:ALA:HB1	1.53	0.89
1:A:374:VAL:HG23	1:A:375:ILE:HD12	1.55	0.88
1:A:125:GLY:O	1:A:127:ALA:N	2.06	0.88
1:B:121:ILE:HB	1:B:124:GLU:OE1	1.71	0.88
1:B:374:VAL:HG23	1:B:375:ILE:HD12	1.55	0.88
1:A:134:ILE:HB	1:A:160:ALA:HB1	1.55	0.87
1:B:107:VAL:HB	1:B:306:LEU:HD12	1.56	0.87
1:A:281:LEU:HD22	1:A:360:TRP:CH2	2.08	0.87
1:A:297:LEU:HD21	1:A:367:VAL:HG12	1.56	0.86
1:A:304:ILE:HD13	1:A:333:ILE:HG12	1.55	0.86
1:A:128:ILE:HB	1:A:129:PRO:HD3	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:HD2	1:A:175:TYR:N	1.74	0.85
1:A:107:VAL:HB	1:A:306:LEU:HD12	1.57	0.85
1:B:88:LEU:HD23	1:B:88:LEU:O	1.77	0.84
1:B:125:GLY:O	1:B:127:ALA:N	2.10	0.84
1:B:128:ILE:HB	1:B:129:PRO:HD3	1.58	0.84
1:B:281:LEU:HD22	1:B:360:TRP:CH2	2.12	0.84
1:B:174:PHE:HD2	1:B:175:TYR:N	1.74	0.83
1:A:12:ALA:HB2	1:A:142:ALA:HB3	1.60	0.83
1:A:148:VAL:HG13	1:A:324:THR:HG21	1.60	0.83
1:B:112:TYR:CE2	1:B:125:GLY:HA2	2.14	0.83
1:A:88:LEU:HD23	1:A:88:LEU:O	1.78	0.83
1:A:108:PRO:HD3	1:A:306:LEU:HD12	1.62	0.82
1:A:103:GLY:O	1:A:306:LEU:HD11	1.80	0.82
1:A:112:TYR:CE2	1:A:125:GLY:HA2	2.14	0.81
1:B:108:PRO:HD3	1:B:306:LEU:HD12	1.63	0.81
1:B:290:LEU:HD13	1:B:291:GLY:N	1.94	0.81
1:A:290:LEU:HD13	1:A:291:GLY:N	1.96	0.81
1:B:49:ARG:HD3	1:B:54:GLU:HG2	1.62	0.81
1:B:297:LEU:HD21	1:B:367:VAL:HG12	1.62	0.81
1:B:148:VAL:HG13	1:B:324:THR:HG21	1.63	0.80
1:B:12:ALA:HB2	1:B:142:ALA:HB3	1.61	0.80
1:B:103:GLY:O	1:B:306:LEU:HD11	1.81	0.80
1:A:128:ILE:HG21	1:A:296:LEU:HD12	1.64	0.79
1:A:284:LEU:O	1:A:288:LEU:HB3	1.84	0.78
1:A:49:ARG:HD3	1:A:54:GLU:HG2	1.64	0.78
1:B:124:GLU:HB2	1:B:350:PHE:CZ	2.18	0.78
1:B:99:ILE:HG21	1:B:314:LEU:HD21	1.66	0.77
1:A:124:GLU:HB2	1:A:350:PHE:CZ	2.18	0.77
1:A:119:ASP:CB	1:A:120:PRO:HD3	2.10	0.77
1:A:99:ILE:HG21	1:A:314:LEU:HD21	1.66	0.76
1:B:128:ILE:HG21	1:B:296:LEU:HD12	1.66	0.76
1:A:104:GLY:CA	1:A:306:LEU:HD11	2.17	0.75
1:A:50:VAL:HB	1:A:53:LEU:HD21	1.69	0.75
1:A:312:LEU:C	1:A:314:LEU:H	1.88	0.75
1:B:284:LEU:O	1:B:288:LEU:HB3	1.86	0.75
1:A:104:GLY:N	1:A:306:LEU:HD21	2.00	0.74
1:A:104:GLY:HA2	1:A:306:LEU:CD1	2.17	0.74
1:B:194:LEU:HB3	1:B:236:PHE:CD2	2.22	0.74
1:B:312:LEU:C	1:B:314:LEU:H	1.88	0.74
1:A:288:LEU:HB3	1:A:289:PRO:HD3	1.69	0.74
1:B:104:GLY:CA	1:B:306:LEU:HD11	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLY:HA2	1:B:306:LEU:CD1	2.18	0.74
1:A:124:GLU:HB2	1:A:350:PHE:HZ	1.51	0.74
1:B:104:GLY:N	1:B:306:LEU:HD21	2.02	0.73
1:B:131:ALA:HB1	1:B:341:MET:HB3	1.70	0.73
1:B:129:PRO:HG3	1:B:296:LEU:HB2	1.70	0.73
1:A:285:THR:O	1:A:289:PRO:HG2	1.88	0.72
1:B:14:GLY:HA2	1:B:17:ILE:HG22	1.71	0.72
1:B:288:LEU:HB3	1:B:289:PRO:HD3	1.70	0.72
1:B:124:GLU:HB2	1:B:350:PHE:HZ	1.53	0.72
1:A:286:SER:C	1:A:289:PRO:HD2	2.10	0.71
1:A:334:LEU:O	1:A:337:ILE:HG12	1.89	0.71
1:B:262:LEU:O	1:B:266:LEU:HB2	1.90	0.71
1:B:285:THR:O	1:B:289:PRO:HG2	1.89	0.71
1:B:337:ILE:HG13	1:B:337:ILE:O	1.90	0.71
1:B:39:HIS:O	1:B:43:GLU:HG2	1.90	0.71
1:A:131:ALA:HB1	1:A:341:MET:HB3	1.71	0.71
1:A:366:LEU:O	1:A:370:ILE:HG13	1.90	0.71
1:B:50:VAL:HB	1:B:53:LEU:HD21	1.71	0.71
1:B:83:LEU:O	1:B:89:ALA:HA	1.90	0.71
1:A:194:LEU:HB3	1:A:236:PHE:CD2	2.26	0.71
1:A:39:HIS:O	1:A:43:GLU:HG2	1.90	0.71
1:A:14:GLY:HA2	1:A:17:ILE:HG22	1.73	0.71
1:B:74:LEU:HD13	1:B:259:VAL:HG21	1.71	0.71
1:B:286:SER:C	1:B:289:PRO:HD2	2.11	0.71
1:B:119:ASP:CB	1:B:120:PRO:HD3	2.12	0.71
1:A:83:LEU:O	1:A:89:ALA:HA	1.91	0.70
1:B:366:LEU:O	1:B:370:ILE:HG13	1.91	0.70
1:A:104:GLY:HA2	1:A:306:LEU:HD11	1.73	0.70
1:B:334:LEU:O	1:B:337:ILE:HG12	1.92	0.70
1:B:68:MET:HG3	1:B:344:PHE:CE1	2.27	0.70
1:B:105:MET:HG3	1:B:130:ALA:HB1	1.73	0.70
1:B:91:LEU:H	1:B:91:LEU:HD12	1.57	0.70
1:B:140:VAL:HG11	1:B:334:LEU:HD22	1.73	0.70
1:B:334:LEU:C	1:B:336:GLY:H	1.95	0.70
1:A:286:SER:O	1:A:289:PRO:HD2	1.92	0.69
1:A:129:PRO:HG3	1:A:296:LEU:HB2	1.73	0.69
1:A:91:LEU:H	1:A:91:LEU:HD12	1.58	0.69
1:A:276:LEU:HD12	1:A:277:GLN:H	1.58	0.69
1:A:74:LEU:HB2	1:A:255:LEU:HD23	1.75	0.69
1:B:104:GLY:HA2	1:B:306:LEU:HD11	1.75	0.69
1:A:74:LEU:HD13	1:A:259:VAL:HG21	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PRO:HB3	1:A:153:LYS:HG3	1.74	0.68
1:A:296:LEU:HD23	1:A:297:LEU:N	2.08	0.68
1:B:111:LEU:O	1:B:115:PHE:HB2	1.93	0.68
1:B:149:PRO:HB3	1:B:153:LYS:HG3	1.75	0.68
1:B:194:LEU:HB3	1:B:236:PHE:HD2	1.58	0.68
1:B:286:SER:O	1:B:289:PRO:HD2	1.92	0.68
1:B:297:LEU:O	1:B:297:LEU:HD23	1.94	0.68
1:A:334:LEU:C	1:A:336:GLY:H	1.96	0.68
1:A:105:MET:HG3	1:A:130:ALA:HB1	1.76	0.68
1:A:292:ILE:O	1:A:292:ILE:HD13	1.94	0.68
1:A:353:VAL:HG13	1:B:36:GLY:HA2	1.74	0.68
1:A:30:ASN:HD21	1:A:276:LEU:H	1.40	0.68
1:A:360:TRP:CD1	1:B:279:VAL:HG21	2.29	0.68
1:B:292:ILE:HD13	1:B:292:ILE:O	1.94	0.68
1:A:140:VAL:HG11	1:A:334:LEU:HD22	1.77	0.67
1:A:261:TYR:O	1:A:265:PRO:HG2	1.94	0.67
1:B:96:PHE:HB3	1:B:97:PRO:CD	2.23	0.67
1:B:101:ALA:HB2	1:B:159:LEU:HD23	1.77	0.67
1:B:174:PHE:C	1:B:174:PHE:CD2	2.68	0.67
1:A:36:GLY:HA2	1:B:353:VAL:HG13	1.77	0.67
1:A:337:ILE:O	1:A:337:ILE:HG13	1.95	0.66
1:A:36:GLY:O	1:A:40:ASP:HB2	1.94	0.66
1:B:291:GLY:HA2	1:B:295:GLY:H	1.60	0.66
1:B:105:MET:O	1:B:105:MET:HG2	1.95	0.66
1:A:198:ASN:C	1:A:198:ASN:ND2	2.49	0.66
1:A:210:LEU:O	1:A:213:VAL:HG13	1.95	0.66
1:A:262:LEU:O	1:A:266:LEU:HB2	1.96	0.66
1:A:291:GLY:HA2	1:A:295:GLY:H	1.60	0.66
1:B:74:LEU:HB2	1:B:255:LEU:HD23	1.78	0.65
1:A:165:LEU:O	1:A:165:LEU:HD23	1.97	0.65
1:B:198:ASN:C	1:B:198:ASN:ND2	2.50	0.65
1:A:174:PHE:C	1:A:174:PHE:CD2	2.70	0.65
1:B:276:LEU:HD12	1:B:277:GLN:H	1.61	0.65
1:A:188:ALA:O	1:A:191:ILE:HG22	1.96	0.65
1:A:105:MET:HG2	1:A:105:MET:O	1.96	0.65
1:B:210:LEU:O	1:B:213:VAL:HG13	1.97	0.65
1:B:67:LEU:HD22	1:B:263:ILE:HG23	1.79	0.65
1:A:374:VAL:HG23	1:A:375:ILE:CD1	2.27	0.64
1:A:374:VAL:HA	1:A:377:TYR:HB3	1.79	0.64
1:B:101:ALA:HB2	1:B:159:LEU:CD2	2.27	0.64
1:B:296:LEU:HD23	1:B:297:LEU:N	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:HD21	1:A:291:GLY:HA3	1.62	0.64
1:A:297:LEU:HD23	1:A:297:LEU:O	1.98	0.64
1:B:116:ASN:HD21	1:B:291:GLY:HA3	1.63	0.64
1:B:30:ASN:HD21	1:B:276:LEU:H	1.44	0.64
1:B:374:VAL:HA	1:B:377:TYR:HB3	1.79	0.64
1:A:68:MET:HG3	1:A:344:PHE:CE1	2.33	0.64
1:A:291:GLY:O	1:A:293:ILE:N	2.31	0.64
1:B:291:GLY:O	1:B:293:ILE:N	2.30	0.64
1:B:374:VAL:HG23	1:B:375:ILE:CD1	2.28	0.64
1:A:306:LEU:O	1:A:310:LEU:N	2.31	0.64
1:A:374:VAL:C	1:A:376:GLY:H	2.01	0.64
1:A:112:TYR:HD2	1:A:125:GLY:HA2	1.63	0.63
1:A:296:LEU:C	1:A:296:LEU:HD23	2.18	0.63
1:A:304:ILE:O	1:A:306:LEU:N	2.29	0.63
1:A:96:PHE:HB3	1:A:97:PRO:CD	2.24	0.63
1:B:134:ILE:HB	1:B:160:ALA:CB	2.28	0.63
1:B:36:GLY:O	1:B:40:ASP:HB2	1.99	0.63
1:B:293:ILE:O	1:B:297:LEU:HB2	1.99	0.63
1:A:174:PHE:CD2	1:A:175:TYR:N	2.64	0.63
1:B:121:ILE:CB	1:B:124:GLU:OE1	2.47	0.63
1:A:141:LEU:HD23	1:A:153:LYS:HG2	1.81	0.63
1:A:175:TYR:CE2	1:A:177:ASN:HA	2.34	0.62
1:B:280:THR:C	1:B:281:LEU:HG	2.19	0.62
1:B:304:ILE:O	1:B:306:LEU:N	2.26	0.62
1:B:306:LEU:O	1:B:310:LEU:N	2.31	0.62
1:A:194:LEU:HB3	1:A:236:PHE:HD2	1.63	0.62
1:A:293:ILE:O	1:A:297:LEU:HB2	2.00	0.62
1:B:68:MET:HG3	1:B:344:PHE:CD1	2.35	0.62
1:A:101:ALA:HB2	1:A:159:LEU:HD23	1.81	0.62
1:B:261:TYR:O	1:B:265:PRO:HG2	1.99	0.62
1:A:127:ALA:O	1:A:129:PRO:N	2.33	0.61
1:A:111:LEU:O	1:A:115:PHE:HB2	1.99	0.61
1:A:330:VAL:CG1	1:A:380:LEU:HB2	2.22	0.61
1:B:275:SER:H	1:B:359:ASN:HD21	1.49	0.61
1:A:285:THR:O	1:A:289:PRO:CG	2.49	0.61
1:B:188:ALA:HA	1:B:191:ILE:HG22	1.81	0.61
1:B:374:VAL:C	1:B:376:GLY:H	2.02	0.61
1:B:138:LEU:HD23	1:B:156:LEU:HD23	1.83	0.61
1:A:101:ALA:HB2	1:A:159:LEU:CD2	2.30	0.60
1:B:175:TYR:CE2	1:B:177:ASN:HA	2.35	0.60
1:A:111:LEU:HD23	1:A:111:LEU:C	2.21	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLN:O	1:A:279:VAL:N	2.33	0.60
1:B:141:LEU:HD23	1:B:153:LYS:HG2	1.83	0.60
1:B:188:ALA:O	1:B:191:ILE:HG22	2.01	0.60
1:B:233:VAL:C	1:B:235:PHE:H	2.04	0.60
1:B:316:LEU:O	1:B:317:ALA:HB2	2.01	0.60
1:A:316:LEU:O	1:A:317:ALA:HB2	2.01	0.60
1:B:238:PRO:HB2	1:B:247:PRO:HG3	1.83	0.60
1:A:188:ALA:HA	1:A:191:ILE:HG22	1.83	0.60
1:B:300:LYS:HE2	1:B:336:GLY:O	2.00	0.60
1:A:324:THR:OG1	1:A:327:GLN:HB3	2.02	0.59
1:A:304:ILE:HG12	1:A:333:ILE:HA	1.84	0.59
1:B:76:GLY:O	1:B:79:VAL:HG12	2.01	0.59
1:B:174:PHE:CD2	1:B:175:TYR:N	2.63	0.59
1:A:263:ILE:O	1:A:264:LEU:C	2.40	0.59
1:A:138:LEU:HD23	1:A:156:LEU:HD23	1.84	0.59
1:A:238:PRO:HB2	1:A:247:PRO:HG3	1.83	0.59
1:A:259:VAL:HG23	1:A:260:ALA:N	2.17	0.59
1:B:296:LEU:C	1:B:296:LEU:HD23	2.23	0.59
1:A:296:LEU:HG	1:A:365:ILE:HG22	1.83	0.59
1:A:280:THR:C	1:A:281:LEU:HG	2.23	0.59
1:A:94:ALA:O	1:A:97:PRO:HD2	2.02	0.59
1:A:290:LEU:HD22	1:A:291:GLY:N	2.13	0.59
1:A:57:LYS:HA	1:B:45:PRO:HG2	1.83	0.59
1:B:127:ALA:O	1:B:129:PRO:N	2.36	0.59
1:B:285:THR:O	1:B:289:PRO:CG	2.50	0.59
1:A:275:SER:H	1:A:359:ASN:HD21	1.51	0.58
1:B:277:GLN:O	1:B:279:VAL:N	2.35	0.58
1:B:279:VAL:O	1:B:281:LEU:HG	2.02	0.58
1:B:304:ILE:HG12	1:B:333:ILE:HA	1.83	0.58
1:A:76:GLY:O	1:A:79:VAL:HG12	2.04	0.58
1:B:324:THR:OG1	1:B:327:GLN:HB3	2.04	0.58
1:B:91:LEU:N	1:B:91:LEU:HD12	2.17	0.58
1:B:111:LEU:HD23	1:B:111:LEU:C	2.23	0.58
1:B:233:VAL:O	1:B:235:PHE:N	2.36	0.58
1:A:103:GLY:C	1:A:306:LEU:HD11	2.24	0.58
1:A:290:LEU:HD13	1:A:292:ILE:H	1.69	0.58
1:B:112:TYR:HD2	1:B:125:GLY:HA2	1.64	0.58
1:A:41:PHE:HA	1:A:44:THR:CG2	2.33	0.58
1:A:91:LEU:HD12	1:A:91:LEU:N	2.17	0.58
1:A:121:ILE:CB	1:A:124:GLU:OE1	2.46	0.57
1:A:132:THR:HA	1:A:338:GLY:HA2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:HA	1:B:44:THR:CG2	2.34	0.57
1:A:117:TYR:HD1	1:A:117:TYR:H	1.52	0.57
1:B:117:TYR:H	1:B:117:TYR:HD1	1.52	0.57
1:A:233:VAL:C	1:A:235:PHE:H	2.07	0.57
1:B:296:LEU:HG	1:B:365:ILE:HG22	1.85	0.57
1:A:134:ILE:HB	1:A:160:ALA:CB	2.31	0.57
1:A:276:LEU:HD12	1:A:277:GLN:N	2.19	0.57
1:A:68:MET:HG3	1:A:344:PHE:CD1	2.39	0.57
1:B:132:THR:HA	1:B:338:GLY:HA2	1.87	0.57
1:A:312:LEU:C	1:A:314:LEU:N	2.57	0.57
1:B:296:LEU:HD21	1:B:364:GLY:HA3	1.86	0.57
1:B:330:VAL:CG1	1:B:380:LEU:HB2	2.22	0.57
1:B:86:GLY:O	1:B:88:LEU:N	2.35	0.57
1:A:108:PRO:HD3	1:A:306:LEU:CD1	2.33	0.57
1:A:300:LYS:HE2	1:A:336:GLY:O	2.05	0.57
1:A:297:LEU:HD21	1:A:367:VAL:CG1	2.31	0.57
1:A:179:LEU:HA	1:A:184:LEU:HD23	1.86	0.57
1:A:210:LEU:HA	1:A:213:VAL:CG1	2.35	0.57
1:A:306:LEU:HD23	1:A:306:LEU:C	2.25	0.57
1:A:375:ILE:O	1:A:375:ILE:HG22	2.05	0.57
1:A:353:VAL:O	1:A:354:ASP:C	2.44	0.57
1:B:165:LEU:O	1:B:165:LEU:HD23	2.05	0.57
1:B:306:LEU:HD23	1:B:306:LEU:C	2.25	0.57
1:A:279:VAL:O	1:A:281:LEU:HG	2.04	0.56
1:A:233:VAL:O	1:A:235:PHE:N	2.38	0.56
1:B:79:VAL:O	1:B:83:LEU:HB2	2.05	0.56
1:B:375:ILE:HG22	1:B:375:ILE:O	2.04	0.56
1:B:179:LEU:HA	1:B:184:LEU:HD23	1.87	0.56
1:B:290:LEU:HD13	1:B:292:ILE:H	1.71	0.56
1:B:94:ALA:O	1:B:97:PRO:HD2	2.05	0.56
1:A:86:GLY:O	1:A:88:LEU:N	2.37	0.56
1:A:103:GLY:C	1:A:306:LEU:HD21	2.25	0.56
1:A:128:ILE:CB	1:A:129:PRO:HD3	2.34	0.56
1:A:41:PHE:O	1:A:44:THR:HG23	2.05	0.56
1:B:103:GLY:C	1:B:306:LEU:HD11	2.25	0.56
1:B:304:ILE:HG12	1:B:332:GLY:O	2.06	0.56
1:B:90:SER:OG	1:B:93:GLN:HG3	2.06	0.56
1:A:351:GLY:H	1:A:358:ILE:HD12	1.71	0.56
1:A:304:ILE:HG12	1:A:332:GLY:O	2.06	0.56
1:B:103:GLY:C	1:B:306:LEU:HD21	2.25	0.56
1:B:350:PHE:O	1:B:352:SER:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD22	1:A:263:ILE:HG23	1.88	0.55
1:B:116:ASN:ND2	1:B:291:GLY:HA3	2.22	0.55
1:A:79:VAL:O	1:A:83:LEU:HB2	2.06	0.55
1:B:233:VAL:C	1:B:235:PHE:N	2.57	0.55
1:B:210:LEU:HA	1:B:213:VAL:CG1	2.36	0.55
1:B:259:VAL:HG23	1:B:260:ALA:N	2.21	0.55
1:A:90:SER:OG	1:A:93:GLN:HG3	2.06	0.55
1:A:72:PHE:HB3	1:A:231:VAL:HG23	1.89	0.55
1:B:353:VAL:O	1:B:354:ASP:C	2.44	0.55
1:B:108:PRO:HD3	1:B:306:LEU:CD1	2.33	0.55
1:B:290:LEU:HD22	1:B:291:GLY:N	2.13	0.55
1:B:291:GLY:C	1:B:293:ILE:N	2.61	0.54
1:A:174:PHE:HD2	1:A:174:PHE:C	2.09	0.54
1:A:116:ASN:ND2	1:A:291:GLY:HA3	2.22	0.54
1:B:98:VAL:O	1:B:102:ILE:HG22	2.07	0.54
1:B:41:PHE:O	1:B:44:THR:HG23	2.06	0.54
1:A:233:VAL:C	1:A:235:PHE:N	2.59	0.54
1:A:341:MET:O	1:A:345:ILE:HG12	2.07	0.54
1:B:298:ILE:O	1:B:302:LEU:HB2	2.06	0.54
1:A:350:PHE:O	1:A:352:SER:N	2.41	0.54
1:B:276:LEU:HD12	1:B:277:GLN:N	2.22	0.54
1:B:341:MET:O	1:B:345:ILE:HG12	2.07	0.54
1:A:125:GLY:C	1:A:127:ALA:H	2.11	0.54
1:A:125:GLY:C	1:A:127:ALA:N	2.61	0.54
1:A:16:ILE:O	1:A:19:ILE:HG22	2.08	0.54
1:B:72:PHE:HB3	1:B:231:VAL:HG23	1.90	0.54
1:B:263:ILE:O	1:B:264:LEU:C	2.46	0.54
1:B:304:ILE:HG23	1:B:332:GLY:C	2.29	0.53
1:A:304:ILE:HG23	1:A:332:GLY:C	2.29	0.53
1:A:307:PHE:O	1:A:311:ALA:N	2.39	0.53
1:B:264:LEU:CB	1:B:265:PRO:HD3	2.38	0.53
1:B:264:LEU:HB3	1:B:265:PRO:HD3	1.91	0.53
1:B:90:SER:C	1:B:92:ARG:H	2.11	0.53
1:A:99:ILE:HA	1:A:102:ILE:HG22	1.89	0.53
1:A:94:ALA:O	1:A:96:PHE:N	2.42	0.53
1:B:308:CYS:SG	1:B:329:MET:HB2	2.49	0.53
1:B:362:LYS:O	1:B:366:LEU:HB2	2.08	0.53
1:A:90:SER:C	1:A:92:ARG:H	2.12	0.53
1:B:16:ILE:O	1:B:19:ILE:HG22	2.09	0.53
1:B:306:LEU:O	1:B:310:LEU:HB2	2.08	0.53
1:B:320:PRO:O	1:B:321:GLU:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ILE:HA	1:B:102:ILE:HG22	1.90	0.53
1:B:147:ARG:O	1:B:149:PRO:HD3	2.09	0.52
1:A:296:LEU:HD21	1:A:364:GLY:HA3	1.90	0.52
1:B:101:ALA:C	1:B:103:GLY:N	2.63	0.52
1:B:307:PHE:O	1:B:311:ALA:N	2.40	0.52
1:A:312:LEU:O	1:A:314:LEU:N	2.42	0.52
1:A:326:GLN:O	1:A:329:MET:HG2	2.10	0.52
1:B:41:PHE:HA	1:B:44:THR:HG23	1.90	0.52
1:A:219:VAL:HG23	1:A:219:VAL:O	2.08	0.52
1:A:45:PRO:HG2	1:B:57:LYS:HA	1.90	0.52
1:B:326:GLN:O	1:B:329:MET:HG2	2.10	0.52
1:A:292:ILE:HG23	1:A:293:ILE:HG12	1.91	0.52
1:B:125:GLY:C	1:B:127:ALA:N	2.62	0.52
1:B:312:LEU:C	1:B:314:LEU:N	2.58	0.52
1:B:94:ALA:O	1:B:96:PHE:N	2.42	0.52
1:A:41:PHE:HA	1:A:44:THR:HG23	1.92	0.52
1:B:128:ILE:CB	1:B:129:PRO:HD3	2.35	0.52
1:B:274:VAL:HG21	1:B:363:LEU:HG	1.92	0.52
1:A:147:ARG:O	1:A:149:PRO:HD3	2.10	0.52
1:B:275:SER:N	1:B:359:ASN:HD21	2.08	0.52
1:A:127:ALA:O	1:A:129:PRO:CD	2.58	0.51
1:B:291:GLY:O	1:B:292:ILE:C	2.47	0.51
1:B:297:LEU:HD21	1:B:367:VAL:CG1	2.37	0.51
1:A:115:PHE:C	1:A:116:ASN:HD22	2.12	0.51
1:A:115:PHE:HD1	1:A:115:PHE:O	1.92	0.51
1:A:320:PRO:O	1:A:321:GLU:HB2	2.09	0.51
1:A:98:VAL:O	1:A:102:ILE:HG22	2.10	0.51
1:B:219:VAL:O	1:B:219:VAL:HG23	2.09	0.51
1:B:312:LEU:O	1:B:314:LEU:N	2.43	0.51
1:A:198:ASN:HD22	1:A:198:ASN:C	2.14	0.51
1:A:50:VAL:H	1:A:53:LEU:HD23	1.76	0.51
1:B:169:ILE:O	1:B:173:LEU:HD22	2.11	0.51
1:A:291:GLY:C	1:A:293:ILE:N	2.61	0.51
1:A:291:GLY:O	1:A:292:ILE:C	2.48	0.51
1:A:148:VAL:HG11	1:A:327:GLN:OE1	2.10	0.51
1:B:351:GLY:H	1:B:358:ILE:HD12	1.75	0.51
1:A:106:ILE:O	1:A:110:LEU:HB2	2.10	0.51
1:A:308:CYS:SG	1:A:329:MET:HB2	2.50	0.51
1:A:362:LYS:O	1:A:366:LEU:HB2	2.10	0.51
1:B:107:VAL:N	1:B:108:PRO:CD	2.74	0.51
1:B:131:ALA:HA	1:B:164:ASP:OD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PHE:C	1:B:174:PHE:HD2	2.08	0.51
1:B:197:LEU:HD21	1:B:207:VAL:CG1	2.41	0.51
1:B:292:ILE:HG23	1:B:293:ILE:HG12	1.91	0.51
1:B:334:LEU:C	1:B:336:GLY:N	2.64	0.51
1:B:338:GLY:O	1:B:339:PHE:C	2.48	0.51
1:B:50:VAL:H	1:B:53:LEU:HD23	1.75	0.51
1:A:264:LEU:CB	1:A:265:PRO:HD3	2.41	0.51
1:A:298:ILE:O	1:A:302:LEU:HB2	2.11	0.51
1:B:137:ALA:HB1	1:B:156:LEU:HD21	1.93	0.51
1:B:203:ARG:HD3	1:B:243:HIS:ND1	2.25	0.51
1:A:159:LEU:O	1:A:160:ALA:C	2.49	0.50
1:A:330:VAL:HB	1:A:380:LEU:HD12	1.93	0.50
1:A:333:ILE:HG21	1:A:376:GLY:HA3	1.93	0.50
1:A:91:LEU:CD1	1:A:91:LEU:H	2.24	0.50
1:B:115:PHE:O	1:B:115:PHE:HD1	1.93	0.50
1:B:159:LEU:O	1:B:160:ALA:C	2.49	0.50
1:B:198:ASN:HD22	1:B:198:ASN:C	2.13	0.50
1:A:197:LEU:HD21	1:A:207:VAL:CG1	2.41	0.50
1:A:330:VAL:CG1	1:A:380:LEU:HD12	2.41	0.50
1:B:175:TYR:OH	1:B:178:ASP:HB2	2.12	0.50
1:B:199:LEU:C	1:B:201:GLY:H	2.14	0.50
1:A:101:ALA:C	1:A:103:GLY:N	2.63	0.50
1:A:109:ALA:C	1:A:111:LEU:H	2.14	0.50
1:B:124:GLU:CG	1:B:125:GLY:N	2.74	0.50
1:B:112:TYR:CE2	1:B:124:GLU:HG2	2.46	0.50
1:B:125:GLY:C	1:B:127:ALA:H	2.13	0.50
1:A:374:VAL:C	1:A:376:GLY:N	2.64	0.50
1:B:115:PHE:C	1:B:116:ASN:HD22	2.14	0.50
1:B:214:VAL:HG12	1:B:215:LEU:N	2.26	0.50
1:A:274:VAL:HG21	1:A:363:LEU:HG	1.94	0.50
1:B:147:ARG:O	1:B:148:VAL:HB	2.12	0.50
1:B:111:LEU:HD22	1:B:299:GLY:HA2	1.94	0.50
1:B:304:ILE:CD1	1:B:333:ILE:HA	2.41	0.50
1:B:333:ILE:HG21	1:B:376:GLY:HA3	1.93	0.50
1:A:104:GLY:HA2	1:A:306:LEU:HD13	1.93	0.50
1:A:306:LEU:O	1:A:310:LEU:HB2	2.11	0.50
1:A:112:TYR:CE2	1:A:124:GLU:HG2	2.46	0.50
1:A:152:LEU:O	1:A:155:PHE:HB3	2.12	0.50
1:A:203:ARG:HD3	1:A:243:HIS:ND1	2.27	0.49
1:A:307:PHE:CD2	1:A:332:GLY:HA3	2.47	0.49
1:A:137:ALA:HB1	1:A:156:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:HB	1:A:327:GLN:NE2	2.26	0.49
1:B:127:ALA:O	1:B:129:PRO:CD	2.60	0.49
1:B:330:VAL:HB	1:B:380:LEU:HD12	1.94	0.49
1:B:65:ASP:O	1:B:69:ALA:HB2	2.12	0.49
1:B:91:LEU:H	1:B:91:LEU:CD1	2.23	0.49
1:B:374:VAL:C	1:B:376:GLY:N	2.66	0.49
1:A:131:ALA:HA	1:A:164:ASP:OD2	2.12	0.49
1:A:124:GLU:HG2	1:A:125:GLY:N	2.26	0.49
1:A:304:ILE:CD1	1:A:333:ILE:HA	2.43	0.49
1:B:101:ALA:O	1:B:104:GLY:N	2.45	0.49
1:B:216:TRP:CD1	1:B:226:ALA:HB1	2.46	0.49
1:B:307:PHE:CD2	1:B:332:GLY:HA3	2.46	0.49
1:A:275:SER:N	1:A:359:ASN:HD21	2.10	0.49
1:B:148:VAL:HG11	1:B:327:GLN:OE1	2.12	0.49
1:A:279:VAL:HG21	1:B:360:TRP:CD1	2.48	0.49
1:A:124:GLU:CG	1:A:125:GLY:N	2.74	0.49
1:A:284:LEU:O	1:A:288:LEU:CB	2.58	0.49
1:A:288:LEU:HB3	1:A:289:PRO:CD	2.40	0.49
1:B:124:GLU:HG2	1:B:125:GLY:N	2.27	0.49
1:B:330:VAL:CG1	1:B:380:LEU:HD12	2.43	0.49
1:A:103:GLY:HA3	1:A:310:LEU:HG	1.95	0.49
1:A:316:LEU:O	1:A:317:ALA:CB	2.61	0.49
1:B:324:THR:HB	1:B:327:GLN:NE2	2.28	0.49
1:B:210:LEU:O	1:B:211:VAL:C	2.51	0.48
1:B:309:TRP:O	1:B:313:ARG:HB2	2.13	0.48
1:A:107:VAL:N	1:A:108:PRO:CD	2.75	0.48
1:A:287:ILE:O	1:A:288:LEU:C	2.51	0.48
1:A:307:PHE:C	1:A:309:TRP:H	2.16	0.48
1:B:375:ILE:O	1:B:375:ILE:CG2	2.60	0.48
1:B:307:PHE:C	1:B:309:TRP:H	2.17	0.48
1:B:152:LEU:HD11	1:B:331:VAL:HG22	1.95	0.48
1:A:147:ARG:O	1:A:148:VAL:HB	2.13	0.48
1:A:309:TRP:O	1:A:313:ARG:HB2	2.14	0.48
1:A:338:GLY:O	1:A:339:PHE:C	2.52	0.48
1:B:178:ASP:O	1:B:180:SER:N	2.44	0.48
1:B:198:ASN:HD22	1:B:199:LEU:N	2.11	0.48
1:A:214:VAL:HG12	1:A:215:LEU:N	2.28	0.48
1:B:316:LEU:O	1:B:317:ALA:CB	2.61	0.48
1:B:109:ALA:C	1:B:111:LEU:H	2.17	0.48
1:B:50:VAL:HB	1:B:53:LEU:CD2	2.41	0.48
1:B:152:LEU:O	1:B:155:PHE:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:VAL:O	1:B:214:VAL:HB	2.13	0.48
1:B:104:GLY:HA2	1:B:306:LEU:HD13	1.95	0.48
1:B:288:LEU:HB3	1:B:289:PRO:CD	2.41	0.48
1:B:313:ARG:O	1:B:313:ARG:HD3	2.13	0.48
1:A:137:ALA:HA	1:A:337:ILE:HD11	1.96	0.47
1:B:112:TYR:HE2	1:B:124:GLU:HG2	1.79	0.47
1:B:284:LEU:O	1:B:288:LEU:CB	2.61	0.47
1:A:47:GLN:NE2	1:B:47:GLN:NE2	2.62	0.47
1:B:103:GLY:HA3	1:B:310:LEU:HG	1.96	0.47
1:A:178:ASP:O	1:A:180:SER:N	2.43	0.47
1:A:375:ILE:CG2	1:A:375:ILE:O	2.61	0.47
1:B:106:ILE:O	1:B:110:LEU:HB2	2.13	0.47
1:B:275:SER:H	1:B:359:ASN:ND2	2.13	0.47
1:B:287:ILE:O	1:B:288:LEU:C	2.53	0.47
1:B:126:TRP:HD1	1:B:126:TRP:O	1.98	0.47
1:A:112:TYR:HE2	1:A:124:GLU:HG2	1.79	0.47
1:A:175:TYR:OH	1:A:178:ASP:HB2	2.15	0.47
1:B:99:ILE:HA	1:B:102:ILE:CG2	2.45	0.47
1:B:23:ILE:HG22	1:B:24:LEU:N	2.28	0.47
1:A:23:ILE:HG22	1:A:24:LEU:N	2.29	0.47
1:B:148:VAL:HB	1:B:149:PRO:HD3	1.97	0.47
1:B:287:ILE:O	1:B:294:ALA:HB2	2.14	0.47
1:B:70:VAL:O	1:B:73:LEU:HB3	2.15	0.47
1:A:111:LEU:HD22	1:A:299:GLY:HA2	1.96	0.47
1:A:126:TRP:HD1	1:A:126:TRP:O	1.97	0.47
1:A:152:LEU:HD11	1:A:331:VAL:HG22	1.96	0.47
1:A:313:ARG:O	1:A:313:ARG:HD3	2.14	0.47
1:A:65:ASP:O	1:A:69:ALA:HB2	2.15	0.47
1:A:300:LYS:HE2	1:A:300:LYS:HB3	1.70	0.46
1:A:304:ILE:C	1:A:306:LEU:N	2.69	0.46
1:A:46:VAL:O	1:A:46:VAL:HG12	2.14	0.46
1:A:77:LEU:HD23	1:A:234:GLY:O	2.15	0.46
1:B:112:TYR:OH	1:B:124:GLU:HG3	2.14	0.46
1:B:180:SER:O	1:B:181:MET:C	2.53	0.46
1:B:43:GLU:HG3	1:B:43:GLU:O	2.15	0.46
1:A:101:ALA:O	1:A:104:GLY:N	2.49	0.46
1:A:169:ILE:O	1:A:173:LEU:HD22	2.15	0.46
1:A:121:ILE:O	1:A:124:GLU:CD	2.54	0.46
1:A:229:ALA:O	1:A:233:VAL:HG23	2.15	0.46
1:B:189:VAL:O	1:B:192:ALA:HB3	2.15	0.46
1:B:343:ILE:HG23	1:B:362:LYS:HD2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:VAL:HG12	1:B:46:VAL:O	2.14	0.46
1:A:99:ILE:HA	1:A:102:ILE:CG2	2.45	0.46
1:A:127:ALA:O	1:A:129:PRO:HD2	2.16	0.46
1:A:149:PRO:HA	1:A:152:LEU:HB3	1.97	0.46
1:A:199:LEU:C	1:A:201:GLY:H	2.18	0.46
1:A:198:ASN:HD22	1:A:199:LEU:N	2.13	0.46
1:B:149:PRO:HA	1:B:152:LEU:HB3	1.97	0.46
1:B:77:LEU:HD23	1:B:234:GLY:O	2.16	0.46
1:B:281:LEU:HD12	1:B:281:LEU:O	2.16	0.46
1:A:148:VAL:HB	1:A:149:PRO:HD3	1.98	0.46
1:B:97:PRO:HG3	1:B:155:PHE:CD1	2.51	0.46
1:B:229:ALA:O	1:B:233:VAL:HG23	2.16	0.46
1:B:342:SER:O	1:B:346:ALA:N	2.48	0.46
1:A:180:SER:O	1:A:181:MET:C	2.54	0.46
1:A:31:SER:HB3	1:A:34:THR:OG1	2.16	0.46
1:A:96:PHE:CD2	1:A:314:LEU:HD12	2.51	0.46
1:B:115:PHE:O	1:B:116:ASN:ND2	2.43	0.46
1:B:138:LEU:HD23	1:B:156:LEU:CD2	2.46	0.46
1:B:136:PHE:CD1	1:B:337:ILE:HD12	2.51	0.46
1:B:320:PRO:O	1:B:323:THR:HG23	2.16	0.46
1:A:34:THR:C	1:A:36:GLY:N	2.70	0.45
1:A:50:VAL:HB	1:A:53:LEU:CD2	2.40	0.45
1:B:199:LEU:C	1:B:201:GLY:N	2.70	0.45
1:B:207:VAL:O	1:B:208:TYR:C	2.54	0.45
1:B:22:ALA:O	1:B:25:ALA:HB3	2.16	0.45
1:B:319:LEU:HA	1:B:320:PRO:HD3	1.80	0.45
1:A:112:TYR:OH	1:A:124:GLU:HG3	2.17	0.45
1:A:207:VAL:O	1:A:208:TYR:C	2.55	0.45
1:A:274:VAL:HG23	1:A:359:ASN:ND2	2.32	0.45
1:A:171:ILE:O	1:A:171:ILE:HG22	2.17	0.45
1:A:216:TRP:CD1	1:A:226:ALA:HB1	2.51	0.45
1:B:14:GLY:HA2	1:B:17:ILE:CG2	2.45	0.45
1:A:320:PRO:O	1:A:323:THR:HG23	2.15	0.45
1:B:238:PRO:O	1:B:248:ALA:HB2	2.17	0.45
1:A:112:TYR:CD1	1:A:295:GLY:C	2.90	0.45
1:A:287:ILE:O	1:A:294:ALA:HB2	2.16	0.45
1:B:204:ARG:O	1:B:206:GLY:N	2.49	0.45
1:B:304:ILE:C	1:B:306:LEU:H	2.14	0.45
1:B:304:ILE:CG1	1:B:333:ILE:HA	2.46	0.45
1:A:22:ALA:O	1:A:25:ALA:HB3	2.17	0.45
1:A:264:LEU:HB3	1:A:265:PRO:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ILE:HG23	1:A:362:LYS:HD2	1.99	0.45
1:B:245:ARG:HG3	1:B:246:SER:N	2.32	0.45
1:B:290:LEU:C	1:B:290:LEU:HD13	2.36	0.45
1:B:34:THR:C	1:B:36:GLY:N	2.70	0.45
1:B:320:PRO:O	1:B:321:GLU:CB	2.66	0.44
1:A:141:LEU:CD2	1:A:153:LYS:HG2	2.45	0.44
1:A:290:LEU:HD13	1:A:290:LEU:C	2.38	0.44
1:A:209:ILE:HG22	1:A:210:LEU:N	2.33	0.44
1:B:60:LEU:HD21	1:B:271:ASN:HD21	1.83	0.44
1:B:116:ASN:C	1:B:118:ALA:H	2.20	0.44
1:B:121:ILE:O	1:B:124:GLU:CD	2.56	0.44
1:B:176:THR:O	1:B:177:ASN:C	2.56	0.44
1:A:179:LEU:O	1:A:181:MET:N	2.51	0.44
1:A:320:PRO:O	1:A:321:GLU:CB	2.65	0.44
1:A:97:PRO:HG3	1:A:155:PHE:CD1	2.52	0.44
1:A:293:ILE:HG22	1:A:294:ALA:N	2.33	0.44
1:B:127:ALA:O	1:B:129:PRO:HD2	2.17	0.44
1:A:241:GLU:HG2	1:A:241:GLU:O	2.18	0.44
1:A:286:SER:O	1:A:293:ILE:HG21	2.18	0.44
1:B:203:ARG:O	1:B:205:THR:N	2.51	0.44
1:A:144:LEU:HD13	1:A:380:LEU:HD22	2.00	0.43
1:A:26:MET:H	1:A:26:MET:HG2	1.59	0.43
1:A:77:LEU:HD11	1:A:251:LEU:HD23	2.00	0.43
1:A:138:LEU:HD23	1:A:156:LEU:CD2	2.48	0.43
1:B:209:ILE:O	1:B:213:VAL:HG12	2.18	0.43
1:B:274:VAL:HG23	1:B:359:ASN:ND2	2.33	0.43
1:A:203:ARG:HB3	1:A:243:HIS:CE1	2.53	0.43
1:B:26:MET:H	1:B:26:MET:HG2	1.58	0.43
1:B:96:PHE:CD2	1:B:314:LEU:HD12	2.53	0.43
1:A:96:PHE:CE2	1:A:314:LEU:HD12	2.54	0.43
1:B:304:ILE:C	1:B:306:LEU:N	2.68	0.43
1:B:309:TRP:HD1	1:B:310:LEU:HD22	1.82	0.43
1:B:53:LEU:O	1:B:53:LEU:HD23	2.18	0.43
1:A:298:ILE:C	1:A:300:LYS:N	2.70	0.43
1:B:103:GLY:O	1:B:306:LEU:CD1	2.61	0.43
1:B:141:LEU:CD2	1:B:153:LYS:HG2	2.47	0.43
1:B:241:GLU:O	1:B:241:GLU:HG2	2.19	0.43
1:A:109:ALA:O	1:A:111:LEU:N	2.52	0.43
1:A:168:ILE:CD1	1:A:345:ILE:HD11	2.48	0.43
1:A:211:VAL:O	1:A:214:VAL:HB	2.18	0.43
1:A:53:LEU:O	1:A:53:LEU:HD23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:NH1	1:B:126:TRP:HZ3	2.17	0.43
1:B:298:ILE:C	1:B:300:LYS:N	2.70	0.43
1:A:309:TRP:HD1	1:A:310:LEU:HD22	1.82	0.43
1:A:147:ARG:O	1:A:148:VAL:CB	2.67	0.43
1:A:176:THR:O	1:A:177:ASN:C	2.57	0.43
1:A:203:ARG:O	1:A:205:THR:N	2.52	0.43
1:A:245:ARG:HG3	1:A:246:SER:N	2.33	0.43
1:B:171:ILE:O	1:B:171:ILE:HG22	2.19	0.43
1:B:79:VAL:CG1	1:B:235:PHE:CE1	3.02	0.43
1:A:124:GLU:OE2	1:A:125:GLY:N	2.52	0.43
1:A:12:ALA:HB2	1:A:142:ALA:CB	2.42	0.43
1:A:281:LEU:O	1:A:281:LEU:HD12	2.18	0.43
1:B:147:ARG:O	1:B:148:VAL:CB	2.67	0.43
1:B:197:LEU:HD21	1:B:207:VAL:HG11	2.01	0.43
1:A:197:LEU:HD21	1:A:207:VAL:HG11	2.00	0.42
1:B:179:LEU:O	1:B:181:MET:N	2.51	0.42
1:B:182:ALA:O	1:B:185:GLY:N	2.51	0.42
1:B:229:ALA:O	1:B:230:GLY:C	2.57	0.42
1:B:22:ALA:O	1:B:26:MET:HG2	2.19	0.42
1:A:60:LEU:HD21	1:A:271:ASN:HD21	1.82	0.42
1:A:142:ALA:C	1:A:144:LEU:H	2.23	0.42
1:B:282:ASP:O	1:B:283:GLY:C	2.58	0.42
1:A:282:ASP:O	1:A:283:GLY:C	2.58	0.42
1:A:298:ILE:HG12	1:A:302:LEU:HD23	2.01	0.42
1:A:136:PHE:CD1	1:A:337:ILE:HD12	2.54	0.42
1:B:203:ARG:HB3	1:B:243:HIS:CE1	2.54	0.42
1:B:298:ILE:HG12	1:B:302:LEU:HD23	2.01	0.42
1:A:261:TYR:C	1:A:265:PRO:HG2	2.39	0.42
1:A:286:SER:O	1:A:289:PRO:CD	2.65	0.42
1:A:70:VAL:O	1:A:73:LEU:HB3	2.19	0.42
1:B:137:ALA:HA	1:B:337:ILE:HD11	2.00	0.42
1:B:144:LEU:HD13	1:B:380:LEU:HD22	2.01	0.42
1:B:50:VAL:H	1:B:53:LEU:CD2	2.33	0.42
1:A:123:ARG:NH1	1:A:126:TRP:HZ3	2.17	0.42
1:A:127:ALA:O	1:A:128:ILE:C	2.57	0.42
1:A:334:LEU:C	1:A:336:GLY:N	2.65	0.42
1:A:116:ASN:C	1:A:118:ALA:H	2.23	0.42
1:A:330:VAL:HG11	1:A:380:LEU:CB	2.24	0.42
1:B:116:ASN:HD21	1:B:291:GLY:CA	2.32	0.42
1:A:116:ASN:HD21	1:A:291:GLY:CA	2.32	0.42
1:A:62:TRP:CZ3	1:A:220:LEU:HD21	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ASN:N	1:B:64:ASN:HD22	2.16	0.42
1:A:101:ALA:C	1:A:103:GLY:H	2.23	0.42
1:A:182:ALA:O	1:A:185:GLY:N	2.50	0.42
1:A:189:VAL:CG2	1:A:190:ALA:N	2.83	0.42
1:B:101:ALA:C	1:B:103:GLY:H	2.23	0.42
1:B:183:SER:O	1:B:184:LEU:C	2.57	0.42
1:B:168:ILE:CD1	1:B:345:ILE:HD11	2.50	0.42
1:A:240:LYS:C	1:A:242:LYS:H	2.22	0.41
1:A:275:SER:H	1:A:359:ASN:ND2	2.15	0.41
1:A:304:ILE:C	1:A:306:LEU:H	2.15	0.41
1:B:284:LEU:C	1:B:286:SER:N	2.71	0.41
1:B:300:LYS:HE3	1:B:338:GLY:H	1.85	0.41
1:A:119:ASP:C	1:A:121:ILE:H	2.23	0.41
1:A:238:PRO:O	1:A:248:ALA:HB2	2.20	0.41
1:A:300:LYS:HE3	1:A:338:GLY:H	1.86	0.41
1:A:63:ILE:O	1:A:67:LEU:HG	2.20	0.41
1:B:240:LYS:C	1:B:242:LYS:H	2.22	0.41
1:B:380:LEU:O	1:B:380:LEU:CD2	2.68	0.41
1:B:96:PHE:CE2	1:B:314:LEU:HD12	2.56	0.41
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.84	0.41
1:A:304:ILE:CG1	1:A:333:ILE:HA	2.47	0.41
1:A:367:VAL:HG12	1:A:368:GLY:N	2.36	0.41
1:A:97:PRO:HG3	1:A:155:PHE:CE1	2.56	0.41
1:B:197:LEU:HD21	1:B:207:VAL:HG12	2.03	0.41
1:B:293:ILE:HG22	1:B:294:ALA:N	2.34	0.41
1:A:22:ALA:O	1:A:26:MET:HG2	2.19	0.41
1:A:307:PHE:CE2	1:A:332:GLY:CA	3.04	0.41
1:A:342:SER:O	1:A:346:ALA:N	2.50	0.41
1:A:57:LYS:HG3	1:A:62:TRP:CE2	2.56	0.41
1:A:133:ASP:OD2	1:A:339:PHE:HB3	2.21	0.41
1:A:189:VAL:O	1:A:192:ALA:HB3	2.21	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.84	0.41
1:A:333:ILE:HG21	1:A:376:GLY:CA	2.51	0.41
1:A:50:VAL:H	1:A:53:LEU:CD2	2.33	0.41
1:B:116:ASN:OD1	1:B:291:GLY:HA3	2.20	0.41
1:B:97:PRO:HG3	1:B:155:PHE:CE1	2.55	0.41
1:B:77:LEU:HD11	1:B:251:LEU:HD23	2.03	0.41
1:A:16:ILE:HG22	1:A:17:ILE:N	2.36	0.41
1:A:199:LEU:C	1:A:201:GLY:N	2.73	0.41
1:B:112:TYR:OH	1:B:124:GLU:CG	2.69	0.41
1:B:290:LEU:CD1	1:B:291:GLY:N	2.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HD23	1:A:307:PHE:N	2.36	0.41
1:A:380:LEU:HD23	1:A:380:LEU:O	2.21	0.41
1:B:101:ALA:HB2	1:B:159:LEU:HD22	2.01	0.41
1:B:103:GLY:O	1:B:106:ILE:HG22	2.21	0.41
1:B:112:TYR:CD1	1:B:295:GLY:C	2.93	0.41
1:A:319:LEU:HA	1:A:320:PRO:HD3	1.80	0.41
1:A:380:LEU:O	1:A:380:LEU:CD2	2.68	0.41
1:B:325:TYR:C	1:B:327:GLN:H	2.24	0.41
1:A:183:SER:O	1:A:184:LEU:C	2.58	0.41
1:B:142:ALA:C	1:B:144:LEU:H	2.24	0.41
1:B:209:ILE:HG22	1:B:210:LEU:N	2.36	0.41
1:B:286:SER:O	1:B:293:ILE:HG21	2.20	0.41
1:B:77:LEU:HA	1:B:77:LEU:HD23	1.86	0.41
1:A:79:VAL:CG1	1:A:235:PHE:CE1	3.04	0.41
1:B:119:ASP:C	1:B:121:ILE:H	2.24	0.41
1:B:147:ARG:C	1:B:149:PRO:HD3	2.41	0.41
1:B:57:LYS:HG3	1:B:62:TRP:CE2	2.55	0.41
1:A:188:ALA:CA	1:A:191:ILE:HG22	2.50	0.40
1:A:210:LEU:O	1:A:211:VAL:C	2.59	0.40
1:A:284:LEU:C	1:A:286:SER:N	2.72	0.40
1:A:49:ARG:HG3	1:A:53:LEU:O	2.22	0.40
1:A:103:GLY:O	1:A:106:ILE:HG22	2.21	0.40
1:A:254:VAL:O	1:A:258:TRP:HD1	2.04	0.40
1:A:290:LEU:CD1	1:A:291:GLY:N	2.77	0.40
1:A:34:THR:C	1:A:36:GLY:H	2.25	0.40
1:A:367:VAL:O	1:A:369:SER:N	2.55	0.40
1:B:290:LEU:HD13	1:B:291:GLY:CA	2.51	0.40
1:B:133:ASP:OD2	1:B:339:PHE:HB3	2.21	0.40
1:A:107:VAL:HB	1:A:108:PRO:HD3	2.03	0.40
1:A:115:PHE:O	1:A:116:ASN:ND2	2.44	0.40
1:A:188:ALA:HA	1:A:191:ILE:CG2	2.51	0.40
1:A:30:ASN:ND2	1:A:276:LEU:HD12	2.37	0.40
1:A:49:ARG:HA	1:A:53:LEU:O	2.22	0.40
1:B:49:ARG:HA	1:B:53:LEU:O	2.21	0.40
1:A:144:LEU:CD1	1:A:380:LEU:HD22	2.52	0.40
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.88	0.40
1:B:124:GLU:OE2	1:B:125:GLY:N	2.54	0.40
1:A:103:GLY:HA2	1:A:106:ILE:HG22	2.04	0.40
1:A:147:ARG:C	1:A:149:PRO:HD3	2.42	0.40
1:A:169:ILE:O	1:A:170:ILE:C	2.59	0.40
1:A:298:ILE:C	1:A:300:LYS:H	2.24	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:HA2	1:B:106:ILE:HG22	2.04	0.40
1:B:134:ILE:HG12	1:B:134:ILE:O	2.22	0.40
1:B:298:ILE:C	1:B:300:LYS:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/388 (96%)	235 (63%)	94 (25%)	45 (12%)	0	4
1	B	374/388 (96%)	234 (63%)	94 (25%)	46 (12%)	0	4
All	All	748/776 (96%)	469 (63%)	188 (25%)	91 (12%)	0	4

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLY
1	A	87	SER
1	A	95	ALA
1	A	119	ASP
1	A	126	TRP
1	A	128	ILE
1	A	148	VAL
1	A	263	ILE
1	A	277	GLN
1	A	282	ASP
1	A	283	GLY
1	A	309	TRP
1	A	317	ALA
1	A	321	GLU
1	A	339	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	351	GLY
1	A	372	SER
1	B	86	GLY
1	B	87	SER
1	B	95	ALA
1	B	119	ASP
1	B	126	TRP
1	B	128	ILE
1	B	148	VAL
1	B	263	ILE
1	B	282	ASP
1	B	283	GLY
1	B	309	TRP
1	B	317	ALA
1	B	321	GLU
1	B	339	PHE
1	B	351	GLY
1	B	372	SER
1	A	38	TYR
1	A	110	LEU
1	A	145	GLY
1	A	146	SER
1	A	149	PRO
1	A	179	LEU
1	A	290	LEU
1	A	292	ILE
1	A	305	SER
1	A	323	THR
1	B	38	TYR
1	B	110	LEU
1	B	145	GLY
1	B	146	SER
1	B	149	PRO
1	B	151	ALA
1	B	179	LEU
1	B	205	THR
1	B	277	GLN
1	B	290	LEU
1	B	292	ILE
1	B	305	SER
1	B	313	ARG
1	B	323	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	104	GLY
1	A	151	ALA
1	A	177	ASN
1	A	205	THR
1	A	208	TYR
1	A	313	ARG
1	A	355	PRO
1	B	177	ASN
1	B	181	MET
1	B	208	TYR
1	B	355	PRO
1	A	88	LEU
1	A	118	ALA
1	A	181	MET
1	A	219	VAL
1	B	88	LEU
1	B	104	GLY
1	B	118	ALA
1	B	219	VAL
1	A	207	VAL
1	B	91	LEU
1	A	42	LEU
1	A	354	ASP
1	B	42	LEU
1	B	207	VAL
1	B	291	GLY
1	B	354	ASP
1	A	289	PRO
1	A	291	GLY
1	B	234	GLY
1	B	289	PRO
1	A	234	GLY
1	B	238	PRO
1	A	238	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/303 (96%)	257 (88%)	34 (12%)	5	24
1	B	291/303 (96%)	257 (88%)	34 (12%)	5	24
All	All	582/606 (96%)	514 (88%)	68 (12%)	5	24

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	24	LEU
1	A	26	MET
1	A	41	PHE
1	A	56	ASN
1	A	61	LEU
1	A	83	LEU
1	A	84	MET
1	A	87	SER
1	A	115	PHE
1	A	117	TYR
1	A	121	ILE
1	A	124	GLU
1	A	174	PHE
1	A	177	ASN
1	A	184	LEU
1	A	189	VAL
1	A	196	VAL
1	A	198	ASN
1	A	209	ILE
1	A	213	VAL
1	A	214	VAL
1	A	264	LEU
1	A	266	LEU
1	A	276	LEU
1	A	281	LEU
1	A	289	PRO
1	A	292	ILE
1	A	296	LEU
1	A	306	LEU
1	A	312	LEU
1	A	315	LYS
1	A	355	PRO
1	A	362	LYS
1	B	16	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	24	LEU
1	B	26	MET
1	B	41	PHE
1	B	56	ASN
1	B	61	LEU
1	B	83	LEU
1	B	84	MET
1	B	87	SER
1	B	115	PHE
1	B	117	TYR
1	B	121	ILE
1	B	124	GLU
1	B	174	PHE
1	B	177	ASN
1	B	184	LEU
1	B	189	VAL
1	B	196	VAL
1	B	198	ASN
1	B	209	ILE
1	B	213	VAL
1	B	214	VAL
1	B	264	LEU
1	B	266	LEU
1	B	276	LEU
1	B	281	LEU
1	B	289	PRO
1	B	292	ILE
1	B	296	LEU
1	B	306	LEU
1	B	312	LEU
1	B	315	LYS
1	B	355	PRO
1	B	362	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	47	GLN
1	A	56	ASN
1	A	64	ASN
1	A	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	198	ASN
1	A	271	ASN
1	A	318	HIS
1	A	359	ASN
1	B	30	ASN
1	B	47	GLN
1	B	56	ASN
1	B	64	ASN
1	B	93	GLN
1	B	198	ASN
1	B	271	ASN
1	B	318	HIS
1	B	359	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.