



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:59 PM GMT

PDB ID : 1ZA6
Title : The structure of an antitumor CH2-domain-deleted humanized antibody
Authors : Larson, S.B.; Day, J.S.; Glaser, S.; Braslawsky, G.; McPherson, A.
Deposited on : 2005-04-05
Resolution : 2.80 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

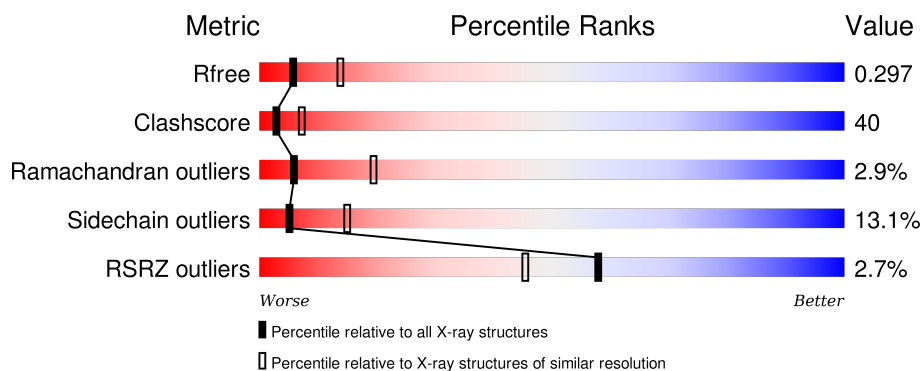
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	220	
1	C	220	
1	E	220	
1	G	220	
2	B	344	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	344	<div><div></div><div>2%</div><div>44%</div><div>42%</div><div>7%</div><div>6%</div></div>
2	F	344	<div><div></div><div>3%</div><div>38%</div><div>48%</div><div>8%</div><div>6%</div></div>
2	H	344	<div><div></div><div>6%</div><div>41%</div><div>46%</div><div>6%</div><div>6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16740 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 IGG Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1703	1069	282	346	6			
1	C	220	Total	C	N	O	S	0	0	0
			1703	1069	282	346	6			
1	E	220	Total	C	N	O	S	0	0	0
			1703	1069	282	346	6			
1	G	220	Total	C	N	O	S	0	0	0
			1703	1069	282	346	6			

- Molecule 2 is a protein called IGG Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2482	1567	416	490	9			
2	D	324	Total	C	N	O	S	0	0	0
			2482	1567	416	490	9			
2	F	324	Total	C	N	O	S	0	0	0
			2482	1567	416	490	9			
2	H	324	Total	C	N	O	S	0	0	0
			2482	1567	416	490	9			

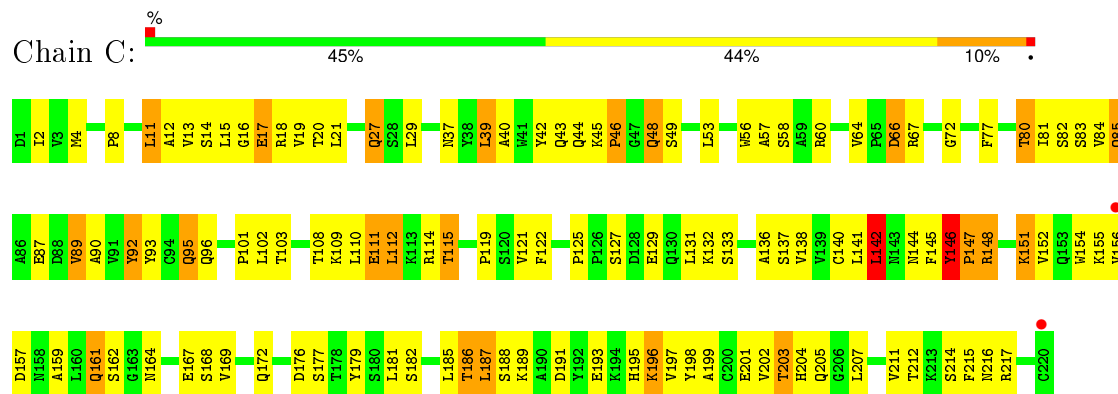
3 Residue-property plots

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.

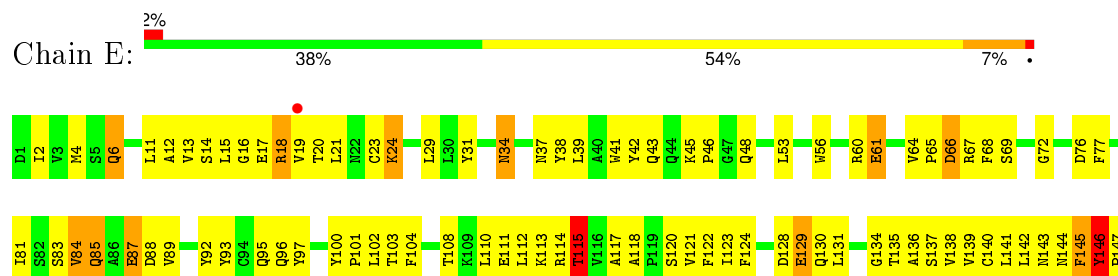
• Molecule 1: IGG Light chain

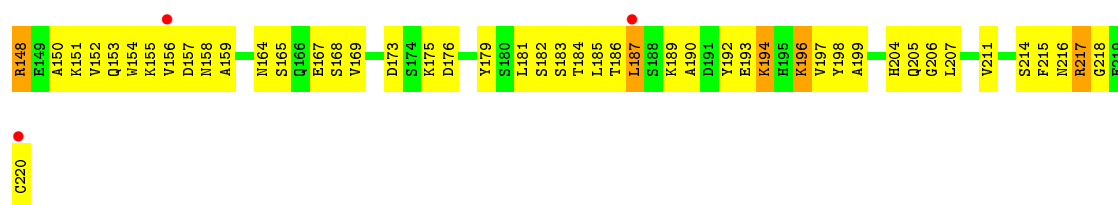


• Molecule 1: IGG Light chain

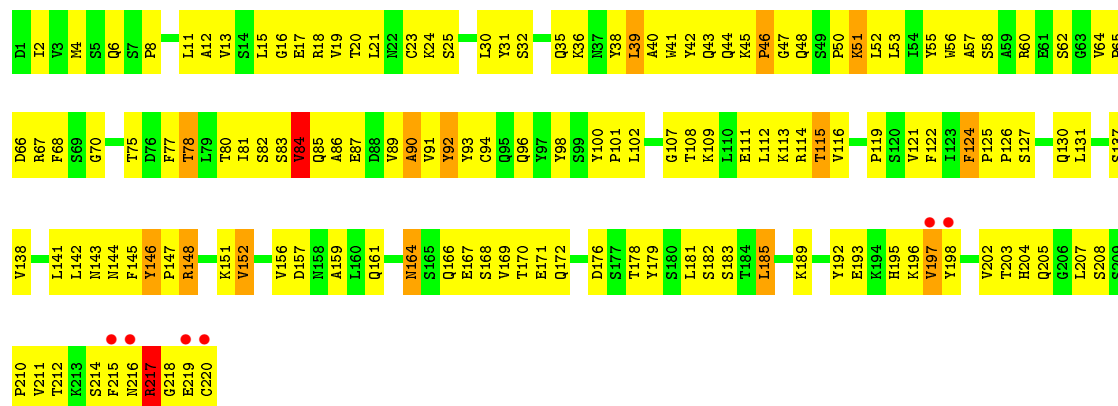


• Molecule 1: IGG Light chain

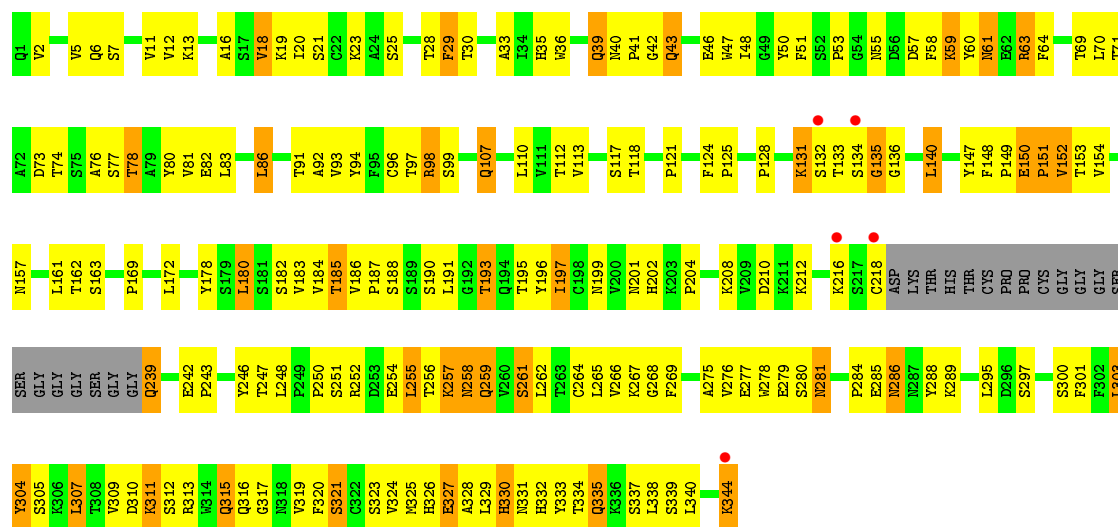




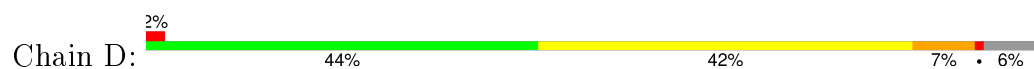
• Molecule 1: IGG Light chain

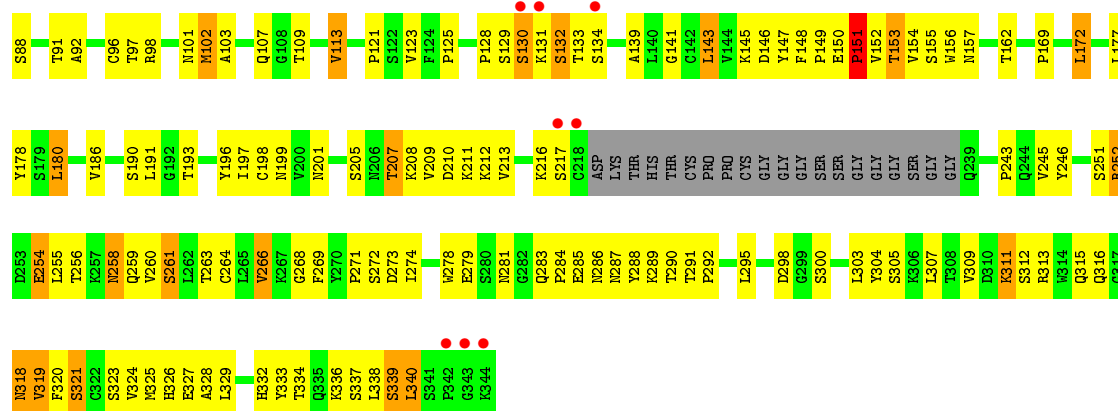


• Molecule 2: IGG Heavy chain

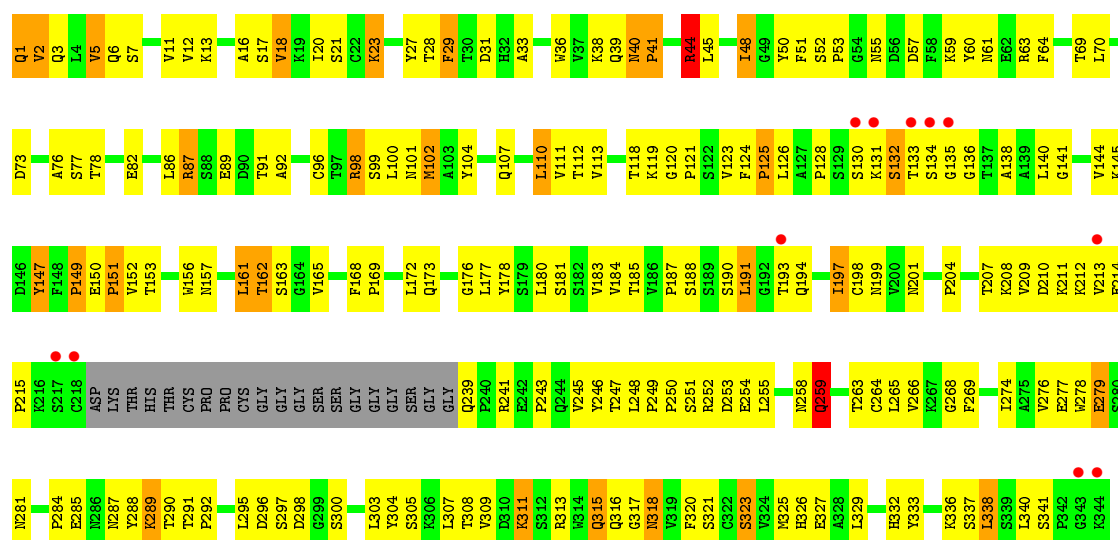


• Molecule 2: IGG Heavy chain

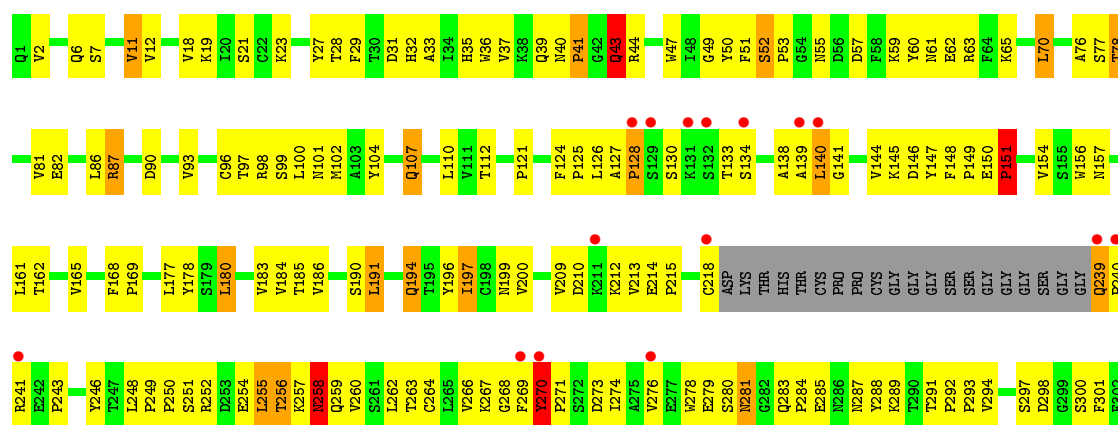
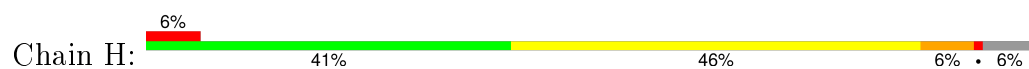


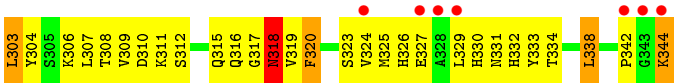


• Molecule 2: IGG Heavy chain



• Molecule 2: IGG Heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.54Å 224.20Å 166.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.13 – 2.80 45.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.13-2.80) 99.9 (45.13-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.99 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.296 0.246 , 0.297	Depositor DCC
R_{free} test set	5949 reflections (7.73%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	3 of 76929 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16740	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.71	0/1740	0.94	4/2361 (0.2%)
1	C	0.67	0/1740	0.88	1/2361 (0.0%)
1	E	0.56	0/1740	0.82	2/2361 (0.1%)
1	G	0.60	0/1740	0.81	0/2361
2	B	0.68	0/2546	0.90	4/3467 (0.1%)
2	D	0.71	0/2546	0.90	3/3467 (0.1%)
2	F	0.56	0/2546	0.80	2/3467 (0.1%)
2	H	0.57	0/2546	0.85	4/3467 (0.1%)
All	All	0.64	0/17144	0.86	20/23312 (0.1%)

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	C	0	2
1	G	0	3
2	B	0	1
2	H	0	1
All	All	0	7

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	PRO	CA-N-CD	-12.28	94.31	111.50
2	H	270	TYR	C-N-CD	9.64	148.65	128.40
1	E	146	TYR	C-N-CD	7.17	143.45	128.40
1	E	120	SER	N-CA-C	-6.47	93.53	111.00
2	B	258	ASN	N-CA-C	-6.43	93.63	111.00
1	C	142	LEU	CA-CB-CG	6.43	130.09	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	270	TYR	C-N-CA	-6.20	95.95	122.00
2	B	86	LEU	CA-CB-CG	-6.16	101.13	115.30
2	D	43	GLN	N-CA-C	5.95	127.08	111.00
2	H	258	ASN	N-CA-C	-5.77	95.42	111.00
1	A	146	TYR	C-N-CD	-5.62	108.23	120.60
2	D	258	ASN	N-CA-C	-5.61	95.86	111.00
2	H	270	TYR	N-CA-C	5.50	125.86	111.00
2	B	61	ASN	N-CA-C	-5.47	96.23	111.00
1	A	120	SER	N-CA-C	-5.37	96.50	111.00
1	A	196	LYS	N-CA-C	5.18	124.98	111.00
2	F	101	ASN	N-CA-C	-5.16	97.08	111.00
2	B	255	LEU	CA-CB-CG	-5.11	103.55	115.30
2	D	63	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	F	61	ASN	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	304	TYR	Sidechain
1	C	146	TYR	Sidechain
1	C	92	TYR	Sidechain
1	G	146	TYR	Sidechain
1	G	92	TYR	Sidechain
1	G	98	TYR	Sidechain
2	H	270	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1703	0	1648	115	0
1	C	1703	0	1648	142	0
1	E	1703	0	1648	157	0
1	G	1703	0	1648	182	0
2	B	2482	0	2414	192	0
2	D	2482	0	2414	166	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2482	0	2414	196	0
2	H	2482	0	2414	221	0
All	All	16740	0	16248	1303	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 40.

All (1303) 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:PRO:HD3	1:A:145:PHE:CB	1.60	1.31
1:A:119:PRO:CD	1:A:145:PHE:HB3	1.81	1.11
2:F:40:ASN:HB3	2:F:41:PRO:HD2	1.20	1.11
2:H:130:SER:HB2	2:H:133:THR:HB	1.36	1.07
1:A:157:ASP:HA	1:A:197:VAL:HG23	1.38	1.05
1:G:46:PRO:HG3	1:G:171:GLU:HG2	1.35	1.04
2:D:274:ILE:HG13	2:D:325:MET:O	1.60	1.01
1:A:114:ARG:O	1:A:115:THR:HB	1.56	0.98
2:F:162:THR:O	2:F:165:VAL:HG22	1.64	0.97
2:B:6:GLN:H	2:B:107:GLN:HE22	1.10	0.97
2:H:344:LYS:H	2:H:344:LYS:HD3	1.26	0.97
2:D:50:TYR:CE1	2:D:59:LYS:HB2	2.01	0.96
2:D:243:PRO:HB3	2:D:269:PHE:HB3	1.46	0.95
1:C:196:LYS:HD2	1:C:196:LYS:O	1.66	0.95
1:C:138:VAL:HG13	1:C:185:LEU:HB3	1.47	0.95
2:B:157:ASN:HD21	2:B:197:ILE:H	1.03	0.94
2:H:243:PRO:HB3	2:H:269:PHE:HB3	1.46	0.94
1:G:8:PRO:HG3	1:G:11:LEU:HD13	1.48	0.94
2:H:107:GLN:H	2:H:107:GLN:HE21	1.10	0.93
2:H:140:LEU:HD21	2:H:196:TYR:HD1	1.29	0.93
2:D:326:HIS:CD2	2:D:328:ALA:H	1.85	0.93
2:B:157:ASN:ND2	2:B:197:ILE:H	1.65	0.93
1:C:196:LYS:HZ2	1:C:216:ASN:HA	1.34	0.93
2:B:6:GLN:H	2:B:107:GLN:NE2	1.65	0.93
2:H:6:GLN:H	2:H:107:GLN:HE22	1.17	0.92
1:E:138:VAL:HG12	1:E:185:LEU:HB3	1.50	0.92
1:C:146:TYR:O	1:C:147:PRO:C	2.08	0.92
1:A:119:PRO:O	2:D:311:LYS:HE3	1.68	0.92
2:H:107:GLN:H	2:H:107:GLN:NE2	1.67	0.91
2:F:40:ASN:HB3	2:F:41:PRO:CD	1.98	0.91
1:C:15:LEU:HD23	1:C:16:GLY:N	1.87	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:PRO:HB2	2:F:213:VAL:HG23	1.54	0.90
1:A:130:GLN:HG3	2:B:124:PHE:CE2	2.07	0.89
2:B:50:TYR:CE1	2:B:59:LYS:HB3	2.06	0.89
2:H:287:ASN:HD22	2:H:308:THR:HB	1.35	0.89
1:A:199:ALA:HA	1:A:214:SER:HB2	1.55	0.89
1:E:211:VAL:HG22	2:H:256:THR:HG23	1.54	0.89
1:A:119:PRO:HD3	1:A:145:PHE:HB3	0.89	0.89
2:F:323:SER:HB3	2:F:333:TYR:CE2	2.08	0.88
1:E:29:LEU:HD12	1:E:39:LEU:HB2	1.55	0.88
1:C:138:VAL:CG1	1:C:185:LEU:HB3	2.02	0.88
2:D:121:PRO:HB3	2:D:147:TYR:HB3	1.54	0.88
1:C:39:LEU:HD13	1:C:40:ALA:N	1.89	0.88
1:C:196:LYS:NZ	1:C:216:ASN:HA	1.90	0.87
1:G:151:LYS:HG3	1:G:203:THR:HB	1.56	0.87
1:E:131:LEU:O	1:E:189:LYS:HD3	1.75	0.86
1:E:196:LYS:HD3	1:E:197:VAL:HG23	1.58	0.86
1:G:124:PHE:HB2	2:H:126:LEU:HD22	1.57	0.86
2:F:28:THR:HB	2:F:31:ASP:OD2	1.75	0.85
1:A:114:ARG:NH1	1:A:115:THR:HG22	1.91	0.85
1:E:157:ASP:HA	1:E:197:VAL:HB	1.57	0.85
2:H:157:ASN:HD21	2:H:196:TYR:HA	1.41	0.84
1:E:138:VAL:CG1	1:E:185:LEU:HB3	2.06	0.84
2:H:121:PRO:HB3	2:H:147:TYR:HB3	1.60	0.84
2:D:11:VAL:HG22	2:D:149:PRO:HG3	1.60	0.84
1:A:142:LEU:HD22	1:A:181:LEU:HD22	1.60	0.83
1:C:20:THR:HG22	1:C:80:THR:CG2	2.07	0.83
2:F:45:LEU:N	2:F:45:LEU:HD12	1.93	0.83
1:E:24:LYS:NZ	1:E:24:LYS:HB3	1.91	0.83
2:H:107:GLN:N	2:H:107:GLN:HE21	1.75	0.82
2:D:172:LEU:HD12	2:D:178:TYR:CE2	2.14	0.82
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.24	0.82
2:H:274:ILE:HG13	2:H:326:HIS:HB2	1.59	0.82
1:E:24:LYS:HZ2	1:E:24:LYS:HB3	1.45	0.81
2:D:252:ARG:HH11	2:D:252:ARG:HG2	1.45	0.81
2:F:48:ILE:HA	2:F:64:PHE:HD1	1.44	0.81
2:B:197:ILE:HG22	2:B:212:LYS:HG3	1.61	0.81
1:A:67:ARG:NH1	1:A:85:GLN:HG3	1.95	0.81
2:F:258:ASN:HA	2:F:311:LYS:HD2	1.62	0.81
1:G:114:ARG:HG2	1:G:146:TYR:CG	2.16	0.80
2:D:326:HIS:HD2	2:D:328:ALA:H	1.24	0.80
1:G:170:THR:HG22	1:G:171:GLU:H	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:ASN:HD22	2:H:258:ASN:N	1.73	0.80
2:F:145:LYS:HE2	2:F:173:GLN:HE22	1.46	0.80
1:G:170:THR:HG22	1:G:171:GLU:N	1.97	0.80
2:B:157:ASN:HD21	2:B:197:ILE:N	1.79	0.79
2:F:91:THR:HG23	2:F:112:THR:HA	1.64	0.79
2:B:239:GLN:OE1	2:B:239:GLN:N	2.15	0.79
2:B:303:LEU:HD12	2:B:303:LEU:O	1.82	0.79
2:F:12:VAL:HG21	2:F:18:VAL:HG22	1.63	0.79
1:A:114:ARG:O	1:A:115:THR:CB	2.31	0.78
1:C:13:VAL:HG21	1:C:84:VAL:HG11	1.66	0.78
1:E:147:PRO:HG2	1:E:205:GLN:NE2	1.98	0.78
1:C:42:TYR:HE1	1:C:95:GLN:HE21	1.32	0.78
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.64	0.78
2:B:257:LYS:O	2:B:311:LYS:HD2	1.83	0.78
2:H:140:LEU:HD21	2:H:196:TYR:CD1	2.17	0.77
1:C:112:LEU:HB2	1:C:172:GLN:HE22	1.49	0.77
2:B:279:GLU:HA	2:B:285:GLU:H	1.50	0.77
2:B:131:LYS:HD2	2:B:132:SER:N	2.00	0.77
2:H:125:PRO:HB3	2:H:213:VAL:HG22	1.66	0.77
1:C:11:LEU:HD11	1:C:19:VAL:HG21	1.67	0.76
2:B:128:PRO:HG3	2:B:191:LEU:HD11	1.68	0.76
2:H:327:GLU:CD	2:H:327:GLU:H	1.89	0.76
2:D:245:VAL:HG22	2:D:266:VAL:HG13	1.65	0.76
2:H:262:LEU:HD12	2:H:307:LEU:HD23	1.68	0.76
2:D:48:ILE:HG23	2:D:64:PHE:CG	2.20	0.76
2:F:125:PRO:HD3	2:F:211:LYS:HE2	1.68	0.76
2:B:172:LEU:HB2	2:B:178:TYR:HE1	1.49	0.76
2:F:323:SER:HB3	2:F:333:TYR:HE2	1.48	0.75
1:G:102:LEU:HD21	2:H:100:LEU:HD11	1.68	0.75
2:H:161:LEU:HD21	2:H:184:VAL:HG11	1.69	0.75
1:E:128:ASP:HA	1:E:131:LEU:HD12	1.69	0.74
2:D:323:SER:HB3	2:D:333:TYR:CE1	2.21	0.74
1:E:130:GLN:OE1	1:E:135:THR:HG22	1.87	0.74
2:B:243:PRO:HB3	2:B:269:PHE:HB3	1.70	0.74
2:F:327:GLU:HA	2:F:332:HIS:ND1	2.03	0.74
2:F:2:VAL:HB	2:F:104:TYR:CE1	2.23	0.74
2:F:50:TYR:CE1	2:F:59:LYS:HB3	2.22	0.74
2:H:194:GLN:HE21	2:H:194:GLN:HA	1.53	0.74
1:C:203:THR:O	1:C:203:THR:HG22	1.87	0.73
2:B:6:GLN:N	2:B:107:GLN:HE22	1.85	0.73
1:C:207:LEU:HD13	1:C:211:VAL:HG23	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:SER:HB3	2:D:333:TYR:HE1	1.53	0.73
1:A:119:PRO:CD	1:A:145:PHE:CB	2.52	0.73
1:G:217:ARG:NH1	2:H:218:CYS:HB2	2.03	0.73
2:H:312:SER:O	2:H:316:GLN:HG3	1.88	0.73
2:H:287:ASN:ND2	2:H:308:THR:HB	2.03	0.73
1:C:112:LEU:HB2	1:C:172:GLN:NE2	2.03	0.73
1:E:4:MET:HG2	1:E:103:THR:HG22	1.69	0.72
2:B:197:ILE:HD13	2:B:210:ASP:HB3	1.70	0.72
2:B:98:ARG:O	2:B:99:SER:HB3	1.88	0.72
2:D:243:PRO:HB3	2:D:269:PHE:CB	2.19	0.72
1:E:67:ARG:O	1:E:81:ILE:HA	1.89	0.72
2:F:12:VAL:HG21	2:F:18:VAL:CG2	2.19	0.72
1:A:119:PRO:HD3	1:A:145:PHE:HB2	1.70	0.72
1:G:112:LEU:N	1:G:112:LEU:HD12	2.05	0.72
1:E:137:SER:HB3	1:E:186:THR:HG22	1.72	0.72
2:D:132:SER:C	2:D:134:SER:H	1.93	0.71
2:F:274:ILE:HG13	2:F:326:HIS:HB2	1.70	0.71
1:G:157:ASP:CA	1:G:197:VAL:HG22	2.20	0.71
1:A:109:LYS:NZ	1:A:109:LYS:HB2	2.05	0.71
1:C:11:LEU:HD11	1:C:19:VAL:CG2	2.21	0.71
2:D:28:THR:HB	2:D:31:ASP:OD2	1.89	0.71
1:G:151:LYS:CG	1:G:203:THR:HB	2.20	0.71
1:A:60:ARG:CD	1:A:64:VAL:HB	2.21	0.71
1:E:15:LEU:HD23	1:E:16:GLY:N	2.06	0.71
2:F:130:SER:HB2	2:F:133:THR:HB	1.73	0.71
2:D:180:LEU:O	2:D:180:LEU:HD12	1.90	0.71
1:A:112:LEU:HD22	1:A:177:SER:OG	1.91	0.71
1:G:6:GLN:NE2	1:G:94:CYS:H	1.87	0.71
2:D:243:PRO:CB	2:D:269:PHE:HB3	2.20	0.71
1:G:13:VAL:HG21	1:G:19:VAL:CG1	2.21	0.71
2:D:121:PRO:CB	2:D:147:TYR:HB3	2.21	0.70
1:A:67:ARG:HH11	1:A:85:GLN:HG3	1.55	0.70
1:E:168:SER:OG	2:F:169:PRO:HD2	1.90	0.70
2:B:197:ILE:HD11	2:B:199:ASN:ND2	2.05	0.70
1:G:207:LEU:HD13	1:G:211:VAL:HG23	1.73	0.70
1:E:146:TYR:O	1:E:147:PRO:C	2.20	0.70
2:H:255:LEU:HD22	2:H:260:VAL:HG11	1.73	0.70
1:E:141:LEU:HD22	2:F:183:VAL:HG11	1.73	0.70
1:C:157:ASP:HA	1:C:197:VAL:HB	1.73	0.70
2:F:321:SER:HB3	2:F:337:SER:HA	1.74	0.70
1:A:60:ARG:HD3	1:A:64:VAL:HB	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG22	1:C:181:LEU:HB2	1.73	0.70
1:A:26:SER:O	1:A:27:GLN:HG3	1.90	0.70
1:A:203:THR:O	1:A:203:THR:HG22	1.91	0.70
2:D:329:LEU:HD13	2:D:334:THR:HG22	1.71	0.69
2:H:285:GLU:HB3	2:H:307:LEU:HD11	1.74	0.69
1:G:121:VAL:HG21	1:G:202:VAL:HG21	1.74	0.69
1:C:196:LYS:HD2	1:C:196:LYS:C	2.12	0.69
2:F:197:ILE:HD13	2:F:197:ILE:H	1.57	0.69
2:F:247:THR:HG23	2:F:336:LYS:HG2	1.75	0.69
2:H:191:LEU:HD21	2:H:215:PRO:HG3	1.74	0.69
1:E:123:ILE:HD12	1:E:139:VAL:O	1.93	0.69
1:C:147:PRO:HG2	1:C:204:HIS:CE1	2.26	0.69
2:D:62:GLU:HA	2:D:65:LYS:HD3	1.75	0.69
2:D:180:LEU:HD12	2:D:180:LEU:C	2.13	0.69
2:F:150:GLU:HG2	2:F:178:TYR:CE2	2.28	0.69
1:G:157:ASP:N	1:G:197:VAL:HG22	2.08	0.68
2:F:264:CYS:HB2	2:F:278:TRP:CZ2	2.27	0.68
2:H:269:PHE:CE1	2:H:301:PHE:HB2	2.28	0.68
1:E:204:HIS:CD2	1:E:206:GLY:H	2.11	0.68
2:B:258:ASN:O	2:B:259:GLN:HB2	1.91	0.68
2:D:48:ILE:HA	2:D:64:PHE:CD1	2.29	0.68
2:H:186:VAL:HG21	2:H:196:TYR:HE1	1.58	0.68
1:G:51:LYS:HE2	1:G:51:LYS:HA	1.76	0.68
2:F:145:LYS:CE	2:F:173:GLN:HE22	2.07	0.68
2:H:285:GLU:OE2	2:H:285:GLU:HA	1.92	0.68
2:F:172:LEU:HD13	2:F:178:TYR:CE1	2.28	0.68
2:D:279:GLU:HA	2:D:285:GLU:H	1.59	0.68
1:A:130:GLN:HG3	2:B:124:PHE:CD2	2.29	0.68
1:E:156:VAL:HG22	1:E:198:TYR:CE2	2.29	0.68
2:F:131:LYS:C	2:F:133:THR:H	1.96	0.68
2:B:42:GLY:O	2:B:43:GLN:O	2.12	0.68
2:D:1:GLN:HA	2:D:1:GLN:OE1	1.94	0.68
2:B:344:LYS:HE3	2:B:344:LYS:HA	1.76	0.68
2:H:130:SER:HB2	2:H:133:THR:CB	2.20	0.67
1:G:114:ARG:NH1	1:G:115:THR:O	2.27	0.67
1:E:167:GLU:HG2	1:E:181:LEU:HD21	1.75	0.67
1:G:121:VAL:CG2	1:G:202:VAL:HG21	2.23	0.67
1:E:148:ARG:HH21	1:E:169:VAL:HB	1.59	0.67
1:C:119:PRO:HD3	1:C:204:HIS:CD2	2.28	0.67
1:E:19:VAL:HG23	1:E:81:ILE:HB	1.75	0.67
1:G:44:GLN:HE22	2:H:39:GLN:HE22	1.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:ASN:ND2	1:C:132:LYS:O	2.28	0.67
1:G:68:PHE:CE2	1:G:81:ILE:HG12	2.30	0.67
2:B:195:THR:HG23	2:B:212:LYS:HE3	1.75	0.67
2:H:279:GLU:HA	2:H:285:GLU:H	1.60	0.67
1:E:129:GLU:CD	1:E:129:GLU:H	1.97	0.67
1:C:67:ARG:O	1:C:81:ILE:HA	1.95	0.67
1:E:43:GLN:HB2	1:E:53:LEU:HD11	1.75	0.67
1:E:136:ALA:O	1:E:187:LEU:HD23	1.94	0.67
2:H:40:ASN:HB3	2:H:41:PRO:HD2	1.77	0.67
2:B:35:HIS:CD2	2:B:47:TRP:HE1	2.12	0.67
2:H:86:LEU:O	2:H:87:ARG:HD2	1.95	0.66
2:H:256:THR:HG22	2:H:257:LYS:HD2	1.76	0.66
1:G:114:ARG:HG2	1:G:146:TYR:CD1	2.30	0.66
2:F:134:SER:HB2	2:F:188:SER:OG	1.96	0.66
1:G:85:GLN:OE1	1:G:87:GLU:HG2	1.96	0.66
2:F:145:LYS:HE2	2:F:173:GLN:NE2	2.10	0.66
1:E:130:GLN:HG3	2:F:124:PHE:CE2	2.31	0.66
1:E:193:GLU:HA	1:E:217:ARG:HD2	1.78	0.66
2:F:291:THR:HB	2:F:292:PRO:HD2	1.77	0.66
1:G:164:ASN:HD22	1:G:164:ASN:H	1.42	0.66
1:E:156:VAL:HG22	1:E:198:TYR:CD2	2.30	0.66
1:A:172:GLN:HB2	1:A:179:TYR:CE1	2.30	0.66
2:F:60:TYR:CZ	2:F:70:LEU:HD23	2.31	0.66
1:G:124:PHE:N	1:G:124:PHE:CD1	2.64	0.66
2:H:60:TYR:CE1	2:H:70:LEU:HD22	2.30	0.66
1:C:129:GLU:CD	1:C:129:GLU:H	2.00	0.65
1:G:19:VAL:HG21	1:G:81:ILE:HD12	1.78	0.65
1:A:4:MET:HG2	1:A:103:THR:HG22	1.78	0.65
2:B:289:LYS:HE2	2:D:295:LEU:O	1.97	0.65
2:D:121:PRO:HB3	2:D:147:TYR:CB	2.23	0.65
1:E:13:VAL:CG1	1:E:84:VAL:HG21	2.26	0.65
1:A:42:TYR:HE2	1:A:95:GLN:HE21	1.43	0.65
2:H:274:ILE:CG1	2:H:325:MET:O	2.44	0.65
1:A:67:ARG:HG3	1:A:81:ILE:HG23	1.78	0.65
2:H:303:LEU:HD12	2:H:303:LEU:O	1.96	0.65
1:G:6:GLN:HE22	1:G:93:TYR:HA	1.60	0.65
1:G:8:PRO:CG	1:G:11:LEU:HD13	2.26	0.65
1:G:17:GLU:O	1:G:84:VAL:HG22	1.97	0.65
1:C:156:VAL:HG13	1:C:198:TYR:CE1	2.32	0.65
2:F:245:VAL:O	2:F:336:LYS:HD2	1.96	0.65
1:G:168:SER:HB3	2:H:169:PRO:HG2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:HG21	2:D:340:LEU:HD13	1.78	0.65
1:E:211:VAL:CG2	2:H:256:THR:HG23	2.26	0.65
1:E:196:LYS:CD	1:E:197:VAL:HG23	2.27	0.65
1:A:86:ALA:HA	1:A:112:LEU:HD13	1.79	0.65
1:E:156:VAL:HG13	1:E:198:TYR:CE2	2.32	0.65
2:B:107:GLN:HE21	2:B:107:GLN:H	1.45	0.64
2:F:243:PRO:HB3	2:F:269:PHE:HB3	1.78	0.64
2:F:285:GLU:HG3	2:F:307:LEU:HD21	1.79	0.64
2:F:123:VAL:HB	2:F:209:VAL:HG11	1.79	0.64
2:F:197:ILE:HG22	2:F:212:LYS:HA	1.79	0.64
2:F:243:PRO:HD2	2:F:329:LEU:HD21	1.79	0.64
2:D:48:ILE:HG12	2:D:64:PHE:CZ	2.33	0.64
2:F:279:GLU:HA	2:F:285:GLU:H	1.62	0.64
2:H:291:THR:HG22	2:H:304:TYR:H	1.62	0.64
2:H:243:PRO:HB3	2:H:269:PHE:CB	2.23	0.64
1:C:42:TYR:OH	2:D:102:MET:HB2	1.98	0.64
1:C:45:LYS:HB2	1:C:48:GLN:NE2	2.13	0.64
2:H:258:ASN:N	2:H:258:ASN:ND2	2.45	0.63
2:D:205:SER:O	2:D:207:THR:HG22	1.98	0.63
1:G:101:PRO:HA	2:H:47:TRP:CZ3	2.33	0.63
1:G:67:ARG:O	1:G:81:ILE:HA	1.99	0.63
1:E:31:TYR:HB3	1:E:34:ASN:HD21	1.62	0.63
1:G:124:PHE:CB	2:H:126:LEU:HD22	2.26	0.63
2:D:252:ARG:HG2	2:D:252:ARG:NH1	2.13	0.63
2:F:249:PRO:O	2:H:248:LEU:HD21	1.97	0.63
1:A:60:ARG:HG3	1:A:60:ARG:HH11	1.63	0.63
2:H:93:VAL:HG22	2:H:110:LEU:HD23	1.80	0.63
2:D:91:THR:OG1	2:D:113:VAL:HG23	1.98	0.63
1:A:217:ARG:HG2	1:A:217:ARG:HH11	1.64	0.63
2:F:147:TYR:CE1	2:F:152:VAL:HB	2.33	0.63
1:C:15:LEU:HD23	1:C:15:LEU:C	2.18	0.63
2:B:251:SER:CB	2:D:246:TYR:HB3	2.28	0.63
2:F:16:ALA:O	2:F:86:LEU:HD12	1.99	0.63
1:G:157:ASP:HA	1:G:197:VAL:HG22	1.80	0.63
2:B:268:GLY:HA2	2:B:300:SER:OG	1.99	0.63
1:E:134:GLY:HA2	1:E:189:LYS:HE2	1.81	0.63
1:E:66:ASP:OD2	1:E:66:ASP:N	2.29	0.63
1:G:164:ASN:HD22	1:G:164:ASN:N	1.94	0.63
1:C:164:ASN:ND2	1:C:185:LEU:HD11	2.14	0.63
2:H:274:ILE:HG13	2:H:325:MET:O	1.98	0.63
2:B:63:ARG:NH1	2:B:63:ARG:HG3	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.34	0.62
2:F:197:ILE:HG22	2:F:212:LYS:CB	2.29	0.62
1:G:86:ALA:HA	1:G:112:LEU:CD2	2.30	0.62
1:G:193:GLU:HA	1:G:218:GLY:O	2.00	0.62
2:H:43:GLN:H	2:H:43:GLN:CD	2.02	0.62
2:H:320:PHE:CD1	2:H:320:PHE:N	2.67	0.62
1:G:141:LEU:HD22	2:H:183:VAL:HG21	1.81	0.62
2:F:258:ASN:O	2:F:259:GLN:HB2	1.98	0.62
1:E:19:VAL:CG2	1:E:81:ILE:HB	2.28	0.62
1:G:122:PHE:CD2	2:H:139:ALA:HB3	2.34	0.62
2:D:266:VAL:HG11	2:D:324:VAL:HG11	1.82	0.62
2:D:268:GLY:HA2	2:D:300:SER:OG	1.98	0.62
1:E:155:LYS:HA	1:E:159:ALA:O	2.00	0.62
1:A:119:PRO:O	2:D:311:LYS:CE	2.45	0.62
1:E:42:TYR:OH	2:F:102:MET:HB2	1.98	0.62
1:E:167:GLU:HA	1:E:182:SER:O	2.00	0.62
1:C:199:ALA:HA	1:C:214:SER:OG	1.99	0.62
2:B:247:THR:C	2:B:248:LEU:HD23	2.20	0.62
2:B:201:ASN:HD22	2:B:208:LYS:HG3	1.65	0.62
2:B:131:LYS:HD2	2:B:132:SER:H	1.64	0.62
2:F:48:ILE:HD13	2:F:64:PHE:CE1	2.35	0.61
1:E:187:LEU:HD23	1:E:187:LEU:H	1.65	0.61
1:G:18:ARG:HB2	1:G:82:SER:O	1.99	0.61
1:A:29:LEU:O	1:A:37:ASN:HA	1.98	0.61
1:G:148:ARG:O	1:G:148:ARG:HD3	1.99	0.61
2:D:60:TYR:HB3	2:D:65:LYS:HD2	1.82	0.61
2:F:7:SER:HB3	2:F:21:SER:OG	1.99	0.61
2:H:243:PRO:CB	2:H:269:PHE:HB3	2.24	0.61
1:E:156:VAL:HG13	1:E:198:TYR:HE2	1.65	0.61
2:F:268:GLY:HA2	2:F:300:SER:OG	2.01	0.61
2:B:330:HIS:CG	2:B:330:HIS:O	2.53	0.61
2:B:55:ASN:OD1	2:B:57:ASP:HB3	2.00	0.61
1:C:109:LYS:HD2	1:C:110:LEU:N	2.16	0.61
2:D:259:GLN:H	2:D:311:LYS:H	1.49	0.61
1:C:151:LYS:HE2	1:C:151:LYS:HA	1.81	0.61
2:D:148:PHE:CE2	2:D:149:PRO:HB3	2.36	0.61
1:C:2:ILE:HG21	1:C:96:GLN:HG2	1.82	0.61
1:G:170:THR:CG2	1:G:171:GLU:H	2.14	0.60
1:C:114:ARG:HG2	1:C:146:TYR:CG	2.36	0.60
1:C:42:TYR:HE1	1:C:95:GLN:NE2	1.99	0.60
2:B:247:THR:HB	2:B:338:LEU:HD22	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:VAL:O	2:D:3:GLN:HG2	2.01	0.60
2:B:23:LYS:HE2	2:B:78:THR:CG2	2.31	0.60
2:D:274:ILE:CG1	2:D:325:MET:O	2.45	0.60
1:C:12:ALA:HA	1:C:111:GLU:O	2.01	0.60
2:H:270:TYR:O	2:H:271:PRO:C	2.29	0.60
1:G:8:PRO:O	1:G:108:THR:HG23	2.01	0.60
1:E:141:LEU:CD2	2:F:183:VAL:HG11	2.32	0.60
1:C:18:ARG:HB2	1:C:82:SER:O	2.00	0.60
1:G:156:VAL:HG13	1:G:198:TYR:CE2	2.36	0.60
2:F:177:LEU:N	2:F:177:LEU:HD12	2.16	0.60
2:D:324:VAL:HG12	2:D:325:MET:N	2.17	0.60
1:E:187:LEU:N	1:E:187:LEU:HD23	2.17	0.60
2:H:248:LEU:HD23	2:H:249:PRO:HD2	1.82	0.60
2:H:197:ILE:C	2:H:197:ILE:HD13	2.21	0.60
2:F:48:ILE:HA	2:F:64:PHE:CD1	2.32	0.59
1:G:216:ASN:O	1:G:217:ARG:HB2	2.01	0.59
1:G:85:GLN:NE2	1:G:86:ALA:H	2.00	0.59
1:A:127:SER:OG	1:A:129:GLU:HG2	2.02	0.59
1:G:30:LEU:HD12	1:G:31:TYR:N	2.17	0.59
1:C:155:LYS:HA	1:C:159:ALA:O	2.02	0.59
2:H:243:PRO:HG2	2:H:329:LEU:HD21	1.82	0.59
1:G:51:LYS:HZ1	1:G:52:LEU:HB3	1.66	0.59
1:C:196:LYS:HZ1	1:C:197:VAL:HG22	1.67	0.59
1:G:182:SER:HB3	2:H:168:PHE:CZ	2.37	0.59
1:A:157:ASP:CA	1:A:197:VAL:HG23	2.24	0.59
1:G:124:PHE:CD2	2:H:126:LEU:HB3	2.38	0.59
2:H:276:VAL:HG22	2:H:324:VAL:HG13	1.84	0.59
2:F:76:ALA:O	2:F:77:SER:HB3	2.02	0.59
2:H:121:PRO:CB	2:H:147:TYR:HB3	2.32	0.59
1:A:67:ARG:O	1:A:81:ILE:HA	2.02	0.59
2:B:309:VAL:HG22	2:B:313:ARG:NH1	2.17	0.59
2:B:63:ARG:HH11	2:B:63:ARG:HG3	1.68	0.59
2:F:20:ILE:HG22	2:F:21:SER:N	2.18	0.59
1:E:4:MET:HE2	1:E:96:GLN:HB3	1.85	0.59
2:F:247:THR:CG2	2:F:336:LYS:HG2	2.32	0.59
2:D:6:GLN:HA	2:D:21:SER:O	2.03	0.59
2:B:321:SER:HB3	2:B:337:SER:HA	1.85	0.59
1:G:89:VAL:HB	1:G:112:LEU:HD13	1.85	0.58
1:G:170:THR:CG2	1:G:171:GLU:N	2.66	0.58
1:C:196:LYS:CD	1:C:217:ARG:H	2.16	0.58
2:H:325:MET:O	2:H:326:HIS:HB2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:CG1	1:A:81:ILE:HB	2.33	0.58
2:B:12:VAL:HG11	2:B:86:LEU:CD1	2.33	0.58
1:G:13:VAL:HG21	1:G:19:VAL:HG12	1.84	0.58
2:D:245:VAL:O	2:D:336:LYS:HG3	2.03	0.58
2:H:280:SER:HB3	2:H:285:GLU:OE1	2.03	0.58
2:F:212:LYS:HG2	2:F:214:GLU:HG2	1.84	0.58
2:F:265:LEU:HD22	2:F:304:TYR:CE2	2.38	0.58
1:A:4:MET:HE1	1:A:29:LEU:HD11	1.85	0.58
2:F:40:ASN:CB	2:F:41:PRO:HD2	2.13	0.58
1:G:148:ARG:HH21	1:G:169:VAL:HG21	1.68	0.58
2:F:87:ARG:NH1	2:F:89:GLU:OE2	2.36	0.58
2:B:48:ILE:HG23	2:B:64:PHE:CG	2.38	0.58
2:B:23:LYS:HE2	2:B:78:THR:HG21	1.86	0.58
1:A:146:TYR:CD1	1:A:146:TYR:C	2.76	0.58
2:B:12:VAL:HG11	2:B:86:LEU:HD12	1.85	0.58
1:A:168:SER:OG	2:B:169:PRO:HD2	2.04	0.58
2:B:186:VAL:HB	2:B:187:PRO:HD2	1.86	0.58
1:C:196:LYS:HD2	1:C:217:ARG:H	1.67	0.58
2:F:157:ASN:OD1	2:F:197:ILE:HD13	2.04	0.58
1:C:196:LYS:HZ3	1:C:216:ASN:CB	2.17	0.58
2:D:148:PHE:CZ	2:D:149:PRO:HB3	2.39	0.57
2:H:274:ILE:CG1	2:H:326:HIS:HB2	2.31	0.57
2:F:243:PRO:HD2	2:F:329:LEU:CD2	2.33	0.57
2:F:176:GLY:C	2:F:177:LEU:HD12	2.24	0.57
2:D:258:ASN:O	2:D:259:GLN:CB	2.51	0.57
1:C:20:THR:HG22	1:C:80:THR:HG22	1.84	0.57
1:E:187:LEU:N	1:E:187:LEU:CD2	2.67	0.57
2:D:205:SER:OG	2:D:207:THR:CG2	2.52	0.57
1:C:125:PRO:HG3	1:C:215:PHE:CD2	2.38	0.57
1:A:13:VAL:CG1	1:A:84:VAL:HG11	2.34	0.57
2:H:33:ALA:HB2	2:H:52:SER:HB2	1.86	0.57
2:H:194:GLN:NE2	2:H:194:GLN:HA	2.20	0.57
1:C:172:GLN:HE21	1:C:177:SER:HB3	1.69	0.57
2:D:180:LEU:CD1	2:D:180:LEU:C	2.73	0.57
2:B:19:LYS:HB2	2:B:82:GLU:HG3	1.87	0.57
2:H:23:LYS:HA	2:H:78:THR:HG23	1.86	0.57
1:G:116:VAL:HG21	1:G:205:GLN:HE21	1.69	0.57
1:A:89:VAL:HG13	1:A:110:LEU:O	2.04	0.57
2:H:212:LYS:NZ	2:H:214:GLU:HB3	2.19	0.57
1:G:182:SER:N	2:H:168:PHE:CE2	2.73	0.57
1:G:43:GLN:HG3	1:G:92:TYR:CE1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:PRO:HG3	1:G:11:LEU:CD1	2.31	0.57
1:G:86:ALA:HA	1:G:112:LEU:HD22	1.86	0.57
2:H:41:PRO:HG2	2:H:43:GLN:OE1	2.03	0.57
1:G:192:TYR:CE1	1:G:198:TYR:CE1	2.93	0.57
2:D:329:LEU:CD1	2:D:334:THR:HG22	2.34	0.57
2:H:194:GLN:HG3	2:H:196:TYR:CE2	2.39	0.57
2:H:324:VAL:HG12	2:H:325:MET:H	1.68	0.57
1:E:204:HIS:CG	1:E:205:GLN:H	2.23	0.56
1:E:142:LEU:HD23	1:E:142:LEU:N	2.20	0.56
2:D:152:VAL:HG23	2:D:201:ASN:O	2.05	0.56
1:C:14:SER:O	1:C:17:GLU:HG3	2.04	0.56
1:G:112:LEU:N	1:G:112:LEU:CD1	2.68	0.56
2:F:288:TYR:HB3	2:F:307:LEU:HA	1.86	0.56
2:B:276:VAL:HG22	2:B:324:VAL:HG22	1.86	0.56
2:D:59:LYS:HE3	1:E:100:TYR:CE2	2.41	0.56
1:C:146:TYR:CG	1:C:147:PRO:N	2.73	0.56
2:B:239:GLN:N	2:B:239:GLN:CD	2.57	0.56
2:B:243:PRO:HG2	2:B:329:LEU:HD21	1.86	0.56
1:G:157:ASP:H	1:G:197:VAL:HG22	1.71	0.56
2:H:320:PHE:O	2:H:338:LEU:HD13	2.05	0.56
1:C:2:ILE:O	1:C:103:THR:HG21	2.04	0.56
2:B:316:GLN:NE2	2:B:316:GLN:HA	2.21	0.56
2:D:326:HIS:O	2:D:332:HIS:HA	2.05	0.56
1:G:23:CYS:HB2	1:G:41:TRP:CH2	2.41	0.56
2:D:121:PRO:CA	2:D:147:TYR:HB3	2.35	0.56
1:A:96:GLN:HE21	1:A:103:THR:HB	1.71	0.56
2:D:152:VAL:HG22	2:D:153:THR:N	2.20	0.56
2:B:33:ALA:HA	2:B:53:PRO:HD2	1.87	0.56
2:B:19:LYS:HE2	2:B:80:TYR:CD1	2.40	0.56
2:D:209:VAL:HG12	2:D:210:ASP:N	2.19	0.56
2:B:197:ILE:HG22	2:B:212:LYS:CG	2.33	0.56
1:E:147:PRO:HG2	1:E:205:GLN:HE22	1.71	0.56
2:F:212:LYS:HD3	2:F:214:GLU:OE2	2.05	0.56
1:G:167:GLU:HA	1:G:182:SER:O	2.06	0.56
2:H:29:PHE:CD1	2:H:77:SER:HA	2.40	0.56
2:F:38:LYS:HB2	2:F:48:ILE:HD11	1.88	0.56
2:F:98:ARG:HG2	2:F:98:ARG:HH11	1.70	0.56
1:E:164:ASN:HD21	1:E:185:LEU:HD11	1.71	0.56
1:C:146:TYR:HB3	1:C:147:PRO:CD	2.36	0.56
2:D:172:LEU:HD12	2:D:178:TYR:CZ	2.41	0.56
2:H:303:LEU:HD12	2:H:303:LEU:C	2.27	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:PRO:HB3	2:F:147:TYR:HB3	1.87	0.56
1:G:146:TYR:CD2	1:G:147:PRO:N	2.74	0.56
2:B:63:ARG:HD2	2:B:64:PHE:CZ	2.40	0.56
2:H:62:GLU:HA	2:H:65:LYS:HG3	1.88	0.56
2:F:48:ILE:HD13	2:F:64:PHE:CD1	2.42	0.55
2:D:285:GLU:HA	2:D:285:GLU:OE1	2.06	0.55
1:C:144:ASN:HA	1:C:179:TYR:O	2.06	0.55
2:B:295:LEU:HA	2:B:301:PHE:CD2	2.41	0.55
2:F:258:ASN:HA	2:F:311:LYS:CD	2.34	0.55
1:A:158:ASN:O	1:A:158:ASN:OD1	2.23	0.55
1:G:217:ARG:HG3	1:G:219:GLU:CG	2.36	0.55
2:B:246:TYR:HB3	2:D:251:SER:CB	2.36	0.55
2:B:315:GLN:C	2:B:317:GLY:H	2.10	0.55
2:B:50:TYR:HE1	2:B:59:LYS:HB3	1.69	0.55
2:F:12:VAL:HG12	2:F:13:LYS:O	2.06	0.55
1:G:46:PRO:HG3	1:G:171:GLU:CG	2.23	0.55
2:B:18:VAL:HG12	2:B:86:LEU:CD1	2.33	0.55
2:B:86:LEU:HB3	2:B:113:VAL:HG21	1.88	0.55
1:C:77:PHE:CD1	1:C:77:PHE:N	2.74	0.55
1:E:114:ARG:HG3	1:E:115:THR:N	2.22	0.55
2:H:107:GLN:N	2:H:107:GLN:NE2	2.43	0.55
1:A:153:GLN:CG	1:A:160:LEU:HD21	2.37	0.55
2:B:76:ALA:CB	2:B:78:THR:HG23	2.37	0.55
2:F:156:TRP:CZ3	2:F:198:CYS:HB3	2.41	0.55
2:H:180:LEU:HD12	2:H:180:LEU:C	2.26	0.55
1:E:39:LEU:HD13	1:E:77:PHE:CD1	2.42	0.55
1:G:181:LEU:HD23	1:G:181:LEU:C	2.27	0.55
1:C:168:SER:OG	2:D:169:PRO:HG2	2.07	0.55
2:H:162:THR:O	2:H:165:VAL:HG23	2.07	0.54
2:D:287:ASN:O	2:D:307:LEU:HD12	2.07	0.54
1:E:204:HIS:CG	1:E:205:GLN:N	2.75	0.54
2:H:86:LEU:HD22	2:H:90:ASP:CB	2.37	0.54
2:D:318:ASN:ND2	2:D:318:ASN:N	2.52	0.54
2:H:209:VAL:HG12	2:H:210:ASP:N	2.22	0.54
1:C:60:ARG:HG3	1:C:64:VAL:HB	1.88	0.54
2:H:186:VAL:HG11	2:H:196:TYR:CE1	2.42	0.54
2:H:258:ASN:O	2:H:259:GLN:HB2	2.07	0.54
1:G:217:ARG:HG2	1:G:220:CYS:OXT	2.07	0.54
2:F:190:SER:O	2:F:193:THR:HG22	2.07	0.54
2:D:197:ILE:HG12	2:D:212:LYS:HB2	1.89	0.54
2:B:320:PHE:N	2:B:320:PHE:CD1	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ASN:ND2	1:E:185:LEU:CD1	2.71	0.54
1:G:20:THR:HG22	1:G:80:THR:HG23	1.89	0.54
2:D:39:GLN:OE1	2:D:45:LEU:HD21	2.06	0.54
2:F:246:TYR:HB3	2:H:251:SER:CB	2.38	0.54
2:H:186:VAL:HG21	2:H:196:TYR:CE1	2.42	0.54
2:F:123:VAL:O	2:F:211:LYS:HD3	2.07	0.54
1:C:89:VAL:HG23	1:C:112:LEU:HD23	1.90	0.54
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.56	0.54
1:E:2:ILE:HG21	1:E:96:GLN:HG2	1.89	0.54
1:C:122:PHE:N	1:C:122:PHE:CD1	2.75	0.54
1:A:161:GLN:HG3	1:A:164:ASN:HD21	1.73	0.54
2:H:150:GLU:HG3	2:H:151:PRO:HB3	1.89	0.54
2:D:326:HIS:HD2	2:D:328:ALA:N	2.01	0.54
1:A:19:VAL:HG13	1:A:81:ILE:HB	1.90	0.54
2:F:246:TYR:HB3	2:H:251:SER:HB3	1.89	0.54
1:C:196:LYS:HZ3	1:C:216:ASN:HB3	1.72	0.54
1:A:60:ARG:NH1	1:A:68:PHE:O	2.40	0.54
1:A:203:THR:O	1:A:203:THR:CG2	2.56	0.54
1:E:129:GLU:N	1:E:129:GLU:OE1	2.36	0.54
2:H:338:LEU:HD22	2:H:338:LEU:O	2.08	0.54
1:E:151:LYS:HD2	1:E:151:LYS:N	2.22	0.54
2:D:129:SER:O	2:D:130:SER:CB	2.55	0.54
2:H:266:VAL:HG12	2:H:269:PHE:HD2	1.73	0.54
1:E:196:LYS:CE	1:E:197:VAL:HG23	2.38	0.54
2:F:325:MET:HA	2:F:332:HIS:O	2.08	0.54
1:G:30:LEU:HD11	1:G:35:GLN:HA	1.88	0.54
1:A:15:LEU:HD13	1:A:16:GLY:N	2.23	0.54
1:C:187:LEU:HD23	1:C:187:LEU:H	1.72	0.54
2:H:274:ILE:HG12	2:H:325:MET:O	2.07	0.54
2:F:11:VAL:HG22	2:F:149:PRO:HG3	1.90	0.54
1:C:203:THR:O	1:C:203:THR:CG2	2.55	0.54
2:B:91:THR:O	2:B:92:ALA:HB2	2.08	0.54
2:H:320:PHE:HD1	2:H:320:PHE:N	2.05	0.53
2:D:318:ASN:ND2	2:D:318:ASN:H	2.06	0.53
2:B:59:LYS:HG3	2:B:60:TYR:N	2.24	0.53
2:H:324:VAL:HG12	2:H:325:MET:N	2.23	0.53
1:A:95:GLN:HB2	1:A:104:PHE:CD1	2.43	0.53
1:G:148:ARG:C	1:G:148:ARG:HD3	2.28	0.53
1:G:196:LYS:HA	1:G:217:ARG:O	2.08	0.53
1:E:142:LEU:HD11	1:E:152:VAL:CG2	2.37	0.53
1:C:136:ALA:O	1:C:187:LEU:HD23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:PRO:CA	2:B:147:TYR:HB3	2.38	0.53
1:A:167:GLU:HA	1:A:182:SER:O	2.08	0.53
2:D:324:VAL:CG1	2:D:325:MET:N	2.71	0.53
1:A:146:TYR:CD1	1:A:147:PRO:N	2.77	0.53
1:C:187:LEU:HD23	1:C:187:LEU:N	2.23	0.53
2:H:344:LYS:N	2:H:344:LYS:HD3	2.06	0.53
1:E:31:TYR:HB3	1:E:34:ASN:ND2	2.23	0.53
2:B:201:ASN:ND2	2:B:208:LYS:HG3	2.23	0.53
1:G:116:VAL:CG2	1:G:205:GLN:HE21	2.22	0.53
2:F:161:LEU:HD11	2:F:184:VAL:HG21	1.90	0.53
1:G:42:TYR:HB2	1:G:93:TYR:HB2	1.91	0.53
1:G:204:HIS:CD2	1:G:205:GLN:H	2.27	0.53
2:D:290:THR:CG2	2:D:303:LEU:HD13	2.38	0.53
2:D:309:VAL:HG11	2:D:320:PHE:CE2	2.44	0.53
2:F:323:SER:CB	2:F:333:TYR:HE2	2.20	0.53
2:F:12:VAL:HG11	2:F:86:LEU:HD13	1.91	0.53
1:G:217:ARG:HG3	1:G:219:GLU:HG2	1.91	0.53
2:F:288:TYR:O	2:F:289:LYS:HD3	2.08	0.53
1:E:85:GLN:HG2	1:E:87:GLU:OE2	2.08	0.53
2:F:119:LYS:HG2	2:F:120:GLY:O	2.08	0.53
2:H:319:VAL:O	2:H:319:VAL:HG23	2.09	0.53
1:E:145:PHE:N	1:E:145:PHE:CD1	2.77	0.53
1:A:114:ARG:NH2	2:D:315:GLN:O	2.42	0.53
1:E:192:TYR:CE1	1:E:198:TYR:CE1	2.97	0.53
2:D:131:LYS:O	2:D:133:THR:N	2.42	0.53
2:H:11:VAL:HA	2:H:112:THR:O	2.08	0.53
1:C:114:ARG:HG3	1:C:114:ARG:HH11	1.74	0.53
1:E:157:ASP:CA	1:E:197:VAL:HB	2.33	0.53
2:B:303:LEU:HD12	2:B:303:LEU:C	2.28	0.53
2:H:51:PHE:HB2	2:H:70:LEU:HB3	1.91	0.53
1:C:29:LEU:O	1:C:37:ASN:HA	2.09	0.53
2:B:180:LEU:HD12	2:B:180:LEU:C	2.29	0.53
2:D:41:PRO:O	2:D:43:GLN:HG2	2.08	0.53
1:C:196:LYS:NZ	1:C:216:ASN:CA	2.70	0.52
2:H:254:GLU:C	2:H:256:THR:H	2.12	0.52
2:F:70:LEU:HD22	2:F:70:LEU:N	2.24	0.52
2:D:288:TYR:C	2:D:288:TYR:CD2	2.83	0.52
2:H:191:LEU:CD2	2:H:215:PRO:HG3	2.39	0.52
1:E:134:GLY:HA2	1:E:189:LYS:CE	2.39	0.52
1:C:2:ILE:HG12	1:C:27:GLN:NE2	2.24	0.52
2:B:254:GLU:OE1	2:B:261:SER:OG	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:VAL:O	2:D:325:MET:HG3	2.09	0.52
2:F:197:ILE:HD13	2:F:197:ILE:N	2.25	0.52
1:G:182:SER:HB3	2:H:168:PHE:CE2	2.44	0.52
2:D:288:TYR:O	2:D:289:LYS:HD3	2.08	0.52
2:B:149:PRO:O	2:B:202:HIS:HE1	1.92	0.52
1:G:15:LEU:HD12	1:G:15:LEU:H	1.73	0.52
1:C:146:TYR:O	1:C:147:PRO:O	2.26	0.52
1:E:196:LYS:HD3	1:E:197:VAL:N	2.24	0.52
2:D:251:SER:O	2:D:254:GLU:N	2.41	0.52
1:G:156:VAL:HG22	1:G:198:TYR:CE2	2.45	0.52
2:B:326:HIS:O	2:B:332:HIS:HA	2.09	0.52
2:H:154:VAL:HG22	2:H:200:VAL:HG22	1.92	0.52
2:H:168:PHE:HB3	2:H:169:PRO:HD2	1.91	0.52
1:A:189:LYS:O	1:A:193:GLU:HG2	2.10	0.52
2:B:46:GLU:OE1	2:B:64:PHE:HZ	1.91	0.52
2:F:287:ASN:ND2	2:F:308:THR:HB	2.24	0.52
2:B:162:THR:HG23	2:B:163:SER:N	2.24	0.52
2:F:38:LYS:HG2	2:F:39:GLN:N	2.23	0.52
2:D:97:THR:OG1	2:D:102:MET:HG3	2.09	0.52
1:G:85:GLN:O	1:G:112:LEU:HD21	2.10	0.52
1:A:164:ASN:ND2	1:A:185:LEU:HD11	2.25	0.52
2:D:145:LYS:HG2	2:D:146:ASP:N	2.25	0.52
2:F:45:LEU:N	2:F:45:LEU:CD1	2.65	0.52
2:F:121:PRO:HD2	2:F:207:THR:OG1	2.10	0.52
2:F:6:GLN:HA	2:F:21:SER:O	2.09	0.52
2:F:110:LEU:C	2:F:110:LEU:HD12	2.30	0.52
2:B:310:ASP:O	2:B:312:SER:N	2.43	0.52
2:H:324:VAL:O	2:H:325:MET:HG3	2.10	0.52
1:E:118:ALA:HB1	1:E:207:LEU:CD2	2.40	0.52
2:B:255:LEU:O	2:B:311:LYS:NZ	2.42	0.52
1:C:39:LEU:C	1:C:39:LEU:HD13	2.30	0.52
2:H:121:PRO:HB3	2:H:147:TYR:CB	2.38	0.52
2:B:128:PRO:HD3	2:B:140:LEU:HB3	1.91	0.52
2:D:209:VAL:CG1	2:D:210:ASP:N	2.72	0.52
1:E:114:ARG:O	1:E:115:THR:HG23	2.10	0.52
1:C:21:LEU:HD22	1:C:108:THR:HB	1.92	0.52
1:C:44:GLN:NE2	1:C:93:TYR:HE1	2.08	0.51
2:H:86:LEU:C	2:H:87:ARG:HD2	2.30	0.51
2:F:152:VAL:HG22	2:F:153:THR:N	2.25	0.51
1:G:47:GLY:O	1:G:48:GLN:HG3	2.11	0.51
2:F:243:PRO:CG	2:F:329:LEU:HD21	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:317:GLY:O	2:F:318:ASN:O	2.28	0.51
1:E:199:ALA:HA	1:E:214:SER:HB2	1.91	0.51
2:B:83:LEU:HB3	2:B:86:LEU:HD21	1.93	0.51
2:F:197:ILE:HG22	2:F:212:LYS:HB2	1.92	0.51
2:F:290:THR:CG2	2:F:303:LEU:HD13	2.40	0.51
1:E:156:VAL:HA	1:E:197:VAL:O	2.10	0.51
1:A:20:THR:CG2	1:A:80:THR:HG23	2.40	0.51
2:B:107:GLN:N	2:B:107:GLN:HE21	2.08	0.51
1:C:43:GLN:HG3	1:C:92:TYR:CE1	2.46	0.51
1:C:141:LEU:HD12	1:C:142:LEU:H	1.76	0.51
2:B:344:LYS:HE3	2:B:344:LYS:CA	2.38	0.51
1:G:204:HIS:CG	1:G:205:GLN:H	2.28	0.51
2:F:162:THR:HG23	2:F:163:SER:H	1.76	0.51
2:H:250:PRO:HD3	2:H:262:LEU:HD23	1.93	0.51
1:E:164:ASN:HD21	1:E:185:LEU:CD1	2.23	0.51
1:E:141:LEU:C	1:E:142:LEU:HD23	2.31	0.51
1:G:45:LYS:O	1:G:48:GLN:HB2	2.11	0.51
2:B:286:ASN:N	2:B:286:ASN:OD1	2.44	0.51
2:F:145:LYS:NZ	2:F:173:GLN:HE22	2.08	0.51
2:F:243:PRO:CD	2:F:329:LEU:HD21	2.41	0.51
1:E:114:ARG:HG3	1:E:114:ARG:HH11	1.74	0.51
2:H:283:GLN:HG2	2:H:284:PRO:N	2.26	0.51
2:B:329:LEU:HD13	2:B:334:THR:HG22	1.92	0.51
1:G:148:ARG:C	1:G:148:ARG:CD	2.79	0.51
1:E:21:LEU:HD22	1:E:108:THR:HG21	1.92	0.51
1:E:140:CYS:HB2	1:E:154:TRP:CH2	2.46	0.50
1:E:34:ASN:ND2	1:E:34:ASN:H	2.09	0.50
2:B:48:ILE:HA	2:B:64:PHE:CD2	2.46	0.50
2:D:255:LEU:HD23	2:D:260:VAL:HG11	1.94	0.50
2:B:7:SER:HB3	2:B:21:SER:OG	2.12	0.50
1:G:130:GLN:HB2	2:H:124:PHE:CD2	2.47	0.50
1:G:102:LEU:HD12	2:H:47:TRP:CD1	2.46	0.50
2:D:91:THR:O	2:D:92:ALA:HB2	2.12	0.50
1:E:60:ARG:CG	1:E:64:VAL:HB	2.42	0.50
2:F:297:SER:N	2:H:289:LYS:NZ	2.59	0.50
2:H:266:VAL:HG12	2:H:269:PHE:CD2	2.45	0.50
1:A:109:LYS:HB2	1:A:109:LYS:HZ2	1.76	0.50
1:A:112:LEU:HD22	1:A:177:SER:CB	2.41	0.50
1:E:43:GLN:HG3	1:E:92:TYR:CE1	2.46	0.50
2:H:212:LYS:NZ	2:H:214:GLU:OE2	2.44	0.50
1:E:143:ASN:HD22	1:E:144:ASN:ND2	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:PHE:CD2	2:H:139:ALA:CB	2.94	0.50
1:G:51:LYS:NZ	1:G:52:LEU:H	2.09	0.50
2:H:76:ALA:O	2:H:77:SER:HB3	2.12	0.50
2:B:197:ILE:CD1	2:B:210:ASP:HB3	2.41	0.50
2:H:128:PRO:HG3	2:H:140:LEU:HB3	1.94	0.50
1:G:146:TYR:CD2	1:G:146:TYR:C	2.84	0.50
1:C:42:TYR:HB2	1:C:93:TYR:HB2	1.92	0.50
2:F:60:TYR:CE2	2:F:70:LEU:CD2	2.95	0.50
2:F:247:THR:OG1	2:F:338:LEU:HB2	2.12	0.50
2:F:264:CYS:HB3	2:F:305:SER:HB3	1.94	0.50
2:D:20:ILE:HD13	2:D:109:THR:HB	1.93	0.50
1:C:140:CYS:HB2	1:C:154:TRP:CH2	2.47	0.50
2:D:319:VAL:HA	2:D:339:SER:HB3	1.93	0.50
1:C:167:GLU:HA	1:C:182:SER:O	2.11	0.50
2:F:340:LEU:HD12	2:F:341:SER:H	1.76	0.50
1:G:89:VAL:HG13	1:G:89:VAL:O	2.12	0.50
2:F:33:ALA:HA	2:F:53:PRO:HD2	1.92	0.50
1:G:111:GLU:HG2	1:G:172:GLN:HE22	1.77	0.50
1:A:176:ASP:OD2	1:A:176:ASP:C	2.50	0.50
1:E:146:TYR:HB3	1:E:147:PRO:HD3	1.94	0.50
1:A:8:PRO:O	1:A:108:THR:HG23	2.12	0.50
2:H:317:GLY:O	2:H:318:ASN:O	2.30	0.50
2:H:110:LEU:C	2:H:110:LEU:HD13	2.32	0.50
2:B:55:ASN:OD1	2:B:57:ASP:CB	2.59	0.50
1:C:17:GLU:O	1:C:83:SER:HA	2.10	0.50
1:C:121:VAL:HG21	1:C:202:VAL:HG21	1.93	0.50
1:A:204:HIS:H	1:A:207:LEU:HD12	1.76	0.50
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.46	0.50
1:E:204:HIS:HB3	1:E:207:LEU:HG	1.94	0.50
2:H:279:GLU:CB	2:H:284:PRO:HA	2.42	0.50
1:A:39:LEU:HG	1:A:40:ALA:N	2.26	0.50
1:G:119:PRO:HD3	1:G:204:HIS:ND1	2.27	0.50
2:D:128:PRO:HG3	2:D:191:LEU:HD11	1.93	0.50
1:G:207:LEU:HD13	1:G:211:VAL:CG2	2.40	0.49
1:E:148:ARG:NH2	1:E:169:VAL:HB	2.26	0.49
2:B:59:LYS:HD2	2:H:59:LYS:NZ	2.27	0.49
2:F:258:ASN:O	2:F:259:GLN:CB	2.57	0.49
2:H:33:ALA:HA	2:H:53:PRO:HD2	1.94	0.49
1:A:91:VAL:HG22	1:A:109:LYS:HB3	1.94	0.49
1:A:42:TYR:HE2	1:A:95:GLN:NE2	2.08	0.49
2:H:291:THR:CG2	2:H:304:TYR:H	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:PHE:HE1	1:G:148:ARG:O	1.94	0.49
1:C:4:MET:CE	1:C:96:GLN:HB3	2.42	0.49
2:D:7:SER:HB3	2:D:21:SER:OG	2.12	0.49
1:E:115:THR:HG21	2:H:342:PRO:HA	1.94	0.49
1:G:126:PRO:HD3	1:G:138:VAL:HG22	1.93	0.49
1:A:38:TYR:N	1:A:38:TYR:CD1	2.79	0.49
2:B:51:PHE:HB2	2:B:70:LEU:HB3	1.94	0.49
2:D:315:GLN:HA	2:D:340:LEU:HD12	1.94	0.49
1:C:156:VAL:HA	1:C:197:VAL:O	2.12	0.49
2:H:128:PRO:HB2	2:H:215:PRO:HB3	1.94	0.49
2:B:35:HIS:HB2	2:B:97:THR:HG23	1.95	0.49
2:B:252:ARG:O	2:B:255:LEU:HB2	2.13	0.49
2:B:131:LYS:C	2:B:133:THR:H	2.15	0.49
2:F:197:ILE:HG22	2:F:212:LYS:CA	2.40	0.49
2:F:303:LEU:HD12	2:F:303:LEU:C	2.32	0.49
1:C:67:ARG:HD2	1:C:81:ILE:CG2	2.43	0.49
2:F:132:SER:H	2:F:188:SER:HB3	1.78	0.49
2:B:323:SER:HB2	2:B:333:TYR:CZ	2.47	0.49
2:B:11:VAL:HA	2:B:112:THR:O	2.12	0.49
2:H:323:SER:HB3	2:H:333:TYR:CE2	2.47	0.49
1:E:118:ALA:HB1	1:E:207:LEU:HD23	1.95	0.49
1:A:172:GLN:HA	1:A:178:THR:O	2.13	0.49
2:F:5:VAL:HG23	2:F:23:LYS:HB3	1.92	0.49
2:D:186:VAL:HG11	2:D:196:TYR:CE1	2.47	0.49
1:A:114:ARG:HH12	1:A:115:THR:HG22	1.72	0.49
2:F:140:LEU:HD21	2:F:184:VAL:HG13	1.95	0.49
1:G:6:GLN:NE2	1:G:94:CYS:N	2.60	0.49
2:B:247:THR:O	2:B:248:LEU:HD23	2.11	0.49
1:G:30:LEU:HD12	1:G:36:LYS:O	2.12	0.49
1:G:204:HIS:CG	1:G:205:GLN:N	2.80	0.49
1:G:43:GLN:HG3	1:G:92:TYR:CZ	2.47	0.49
2:B:121:PRO:HA	2:B:147:TYR:HB3	1.94	0.49
1:E:12:ALA:HA	1:E:111:GLU:O	2.12	0.49
2:D:36:TRP:CZ3	2:D:96:CYS:HB3	2.47	0.49
2:H:130:SER:CB	2:H:133:THR:HB	2.26	0.49
2:H:324:VAL:O	2:H:325:MET:CG	2.61	0.49
1:E:204:HIS:H	1:E:207:LEU:HD12	1.77	0.49
2:H:338:LEU:HD22	2:H:338:LEU:C	2.33	0.49
1:G:148:ARG:HB2	1:G:179:TYR:CE1	2.48	0.49
1:E:216:ASN:O	1:E:218:GLY:N	2.46	0.49
2:D:245:VAL:HG22	2:D:266:VAL:CG1	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LYS:CD	1:C:196:LYS:C	2.81	0.49
2:H:243:PRO:HD2	2:H:329:LEU:HD21	1.93	0.49
1:C:95:GLN:HE22	2:D:102:MET:HE3	1.78	0.49
1:G:68:PHE:HE2	1:G:81:ILE:HG12	1.77	0.49
2:H:55:ASN:ND2	2:H:57:ASP:HB3	2.28	0.49
1:A:109:LYS:NZ	1:A:109:LYS:CB	2.74	0.49
1:G:44:GLN:CD	1:G:50:PRO:HG3	2.32	0.49
1:C:147:PRO:O	1:C:204:HIS:HE1	1.96	0.49
2:F:172:LEU:HB2	2:F:178:TYR:CE1	2.48	0.49
2:F:147:TYR:HD2	2:F:147:TYR:H	1.59	0.49
1:C:60:ARG:HD2	1:C:64:VAL:O	2.13	0.49
2:B:184:VAL:HG22	2:B:185:THR:N	2.28	0.49
2:D:325:MET:O	2:D:326:HIS:HB2	2.11	0.49
2:B:242:GLU:HG2	2:B:329:LEU:HD23	1.94	0.49
2:F:172:LEU:HB2	2:F:178:TYR:HE1	1.77	0.49
1:G:198:TYR:O	1:G:214:SER:HB2	2.13	0.49
2:H:145:LYS:HG2	2:H:146:ASP:N	2.28	0.49
1:A:128:ASP:HA	1:A:131:LEU:HD12	1.94	0.49
1:E:67:ARG:HG2	1:E:67:ARG:HH11	1.78	0.48
1:E:167:GLU:HG3	1:E:183:SER:HA	1.95	0.48
1:G:181:LEU:CA	2:H:168:PHE:HE2	2.26	0.48
2:H:243:PRO:CG	2:H:329:LEU:HD21	2.43	0.48
2:B:255:LEU:O	2:B:311:LYS:HE3	2.13	0.48
1:G:195:HIS:O	1:G:218:GLY:HA3	2.13	0.48
2:F:131:LYS:O	2:F:133:THR:N	2.46	0.48
1:E:31:TYR:HD2	1:E:34:ASN:ND2	2.12	0.48
2:F:249:PRO:HB2	2:F:250:PRO:HD2	1.95	0.48
2:H:7:SER:HB3	2:H:21:SER:OG	2.12	0.48
1:E:15:LEU:HD23	1:E:15:LEU:C	2.34	0.48
1:G:19:VAL:CG2	1:G:81:ILE:HD12	2.42	0.48
1:C:122:PHE:CD2	2:D:139:ALA:HB3	2.49	0.48
2:D:125:PRO:HB3	2:D:213:VAL:HG22	1.94	0.48
1:A:97:TYR:HA	1:A:102:LEU:HD22	1.95	0.48
1:C:145:PHE:CD2	1:C:145:PHE:N	2.81	0.48
1:E:164:ASN:ND2	1:E:185:LEU:HD12	2.28	0.48
1:E:2:ILE:O	1:E:103:THR:HG21	2.12	0.48
2:D:36:TRP:CD1	2:D:70:LEU:HD22	2.47	0.48
2:F:131:LYS:C	2:F:133:THR:N	2.64	0.48
1:G:148:ARG:HH21	1:G:169:VAL:CG2	2.26	0.48
1:G:12:ALA:HA	1:G:111:GLU:O	2.12	0.48
2:H:36:TRP:CZ3	2:H:96:CYS:HB3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:TYR:HB3	1:C:147:PRO:HD2	1.95	0.48
1:A:169:VAL:HG22	1:A:181:LEU:HB2	1.93	0.48
2:D:60:TYR:OH	2:D:69:THR:HA	2.14	0.48
1:A:141:LEU:HD22	2:B:183:VAL:HG11	1.95	0.48
2:D:324:VAL:C	2:D:325:MET:HG3	2.33	0.48
1:C:156:VAL:HG23	1:C:161:GLN:OE1	2.14	0.48
1:E:123:ILE:HD11	1:E:138:VAL:CG2	2.44	0.48
1:C:211:VAL:HG12	1:C:212:THR:N	2.27	0.48
1:E:143:ASN:HD22	1:E:144:ASN:HD21	1.60	0.48
1:E:193:GLU:HA	1:E:217:ARG:CD	2.42	0.48
2:F:243:PRO:CB	2:F:269:PHE:HB3	2.43	0.48
1:G:176:ASP:OD2	1:G:178:THR:HG23	2.13	0.48
1:C:109:LYS:HD2	1:C:110:LEU:H	1.77	0.48
2:D:123:VAL:O	2:D:211:LYS:HE3	2.14	0.48
2:F:251:SER:CB	2:H:246:TYR:HB3	2.43	0.48
1:C:114:ARG:NH1	1:C:115:THR:O	2.47	0.48
2:B:76:ALA:O	2:B:77:SER:CB	2.61	0.48
2:D:152:VAL:CG2	2:D:153:THR:N	2.77	0.48
1:A:125:PRO:HD2	2:B:216:LYS:NZ	2.27	0.48
1:E:156:VAL:CG1	1:E:198:TYR:HE2	2.26	0.48
1:G:19:VAL:HG22	1:G:81:ILE:HB	1.95	0.48
1:G:51:LYS:HE2	1:G:52:LEU:H	1.78	0.48
2:H:40:ASN:CB	2:H:41:PRO:HD2	2.38	0.48
2:F:110:LEU:HD12	2:F:111:VAL:N	2.29	0.48
2:B:323:SER:HB2	2:B:333:TYR:CE2	2.49	0.48
1:E:24:LYS:HB3	1:E:24:LYS:HZ3	1.78	0.48
1:C:42:TYR:CE1	1:C:95:GLN:NE2	2.80	0.48
2:F:60:TYR:OH	2:F:69:THR:HA	2.14	0.48
2:F:265:LEU:HD12	2:F:266:VAL:N	2.29	0.48
1:G:198:TYR:CB	1:G:215:PHE:CE1	2.97	0.47
2:F:27:TYR:CE1	2:F:29:PHE:HA	2.48	0.47
2:H:28:THR:HB	2:H:31:ASP:OD1	2.14	0.47
1:A:43:GLN:HB2	1:A:53:LEU:HD11	1.95	0.47
2:F:59:LYS:HD2	2:F:60:TYR:N	2.29	0.47
1:G:217:ARG:CG	1:G:220:CYS:H	2.27	0.47
2:B:148:PHE:CE1	2:B:149:PRO:HB3	2.49	0.47
2:D:73:ASP:C	2:D:73:ASP:OD2	2.52	0.47
1:G:148:ARG:HA	1:G:179:TYR:HD1	1.80	0.47
2:F:177:LEU:N	2:F:177:LEU:CD1	2.78	0.47
1:C:131:LEU:O	1:C:189:LYS:HD2	2.14	0.47
2:H:259:GLN:HG2	2:H:310:ASP:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:GLU:HG3	2:B:328:ALA:O	2.14	0.47
2:B:40:ASN:HB2	2:B:43:GLN:CG	2.44	0.47
2:D:125:PRO:HG3	2:D:211:LYS:HD2	1.97	0.47
2:B:5:VAL:HA	2:B:107:GLN:HE22	1.79	0.47
2:B:197:ILE:HG13	2:B:197:ILE:O	2.15	0.47
1:C:127:SER:HB2	1:C:129:GLU:OE1	2.15	0.47
2:B:40:ASN:CB	2:B:43:GLN:HG2	2.44	0.47
1:G:164:ASN:N	1:G:164:ASN:ND2	2.61	0.47
2:D:318:ASN:N	2:D:318:ASN:HD22	2.13	0.47
1:C:60:ARG:CG	1:C:64:VAL:HB	2.44	0.47
1:E:102:LEU:HD11	2:F:100:LEU:CD2	2.45	0.47
1:A:196:LYS:HG3	1:A:196:LYS:O	2.15	0.47
1:G:217:ARG:HD3	1:G:220:CYS:HB3	1.96	0.47
2:H:148:PHE:CE2	2:H:149:PRO:HB3	2.49	0.47
1:C:85:GLN:HB3	1:C:87:GLU:HG2	1.97	0.47
1:A:121:VAL:HG11	1:A:202:VAL:HG21	1.97	0.47
2:D:320:PHE:N	2:D:320:PHE:CD1	2.83	0.47
1:C:193:GLU:O	1:C:217:ARG:NH2	2.48	0.47
1:E:214:SER:OG	1:E:215:PHE:N	2.47	0.47
2:F:86:LEU:HB3	2:F:113:VAL:HG21	1.96	0.47
2:H:279:GLU:HA	2:H:285:GLU:N	2.29	0.47
2:H:280:SER:OG	2:H:281:ASN:N	2.44	0.47
1:G:13:VAL:HG12	1:G:84:VAL:HG21	1.96	0.47
2:F:290:THR:HG23	2:F:303:LEU:HD13	1.97	0.47
2:H:86:LEU:HD22	2:H:90:ASP:HB3	1.97	0.47
1:E:18:ARG:HG3	1:E:18:ARG:NH1	2.29	0.47
2:F:91:THR:O	2:F:92:ALA:HB2	2.14	0.47
1:G:100:TYR:HA	1:G:101:PRO:C	2.35	0.47
1:C:151:LYS:CE	1:C:151:LYS:HA	2.45	0.47
1:G:198:TYR:HB2	1:G:215:PHE:CE1	2.49	0.47
2:B:315:GLN:C	2:B:317:GLY:N	2.68	0.47
1:A:45:LYS:O	1:A:48:GLN:HB2	2.15	0.47
2:F:161:LEU:CD1	2:F:184:VAL:HG21	2.44	0.47
1:E:144:ASN:HA	1:E:179:TYR:O	2.15	0.47
2:D:283:GLN:HA	2:D:284:PRO:HD3	1.65	0.47
1:A:128:ASP:O	1:A:131:LEU:HB2	2.15	0.47
1:E:121:VAL:C	1:E:122:PHE:CD1	2.88	0.47
1:E:72:GLY:HA3	1:E:77:PHE:HA	1.97	0.47
1:E:198:TYR:HD1	1:E:215:PHE:CE1	2.33	0.47
2:H:259:GLN:HA	2:H:309:VAL:O	2.15	0.47
2:B:81:VAL:HG22	2:B:83:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:VAL:O	1:G:90:ALA:HB2	2.14	0.47
2:F:207:THR:C	2:F:208:LYS:HD2	2.36	0.47
2:B:248:LEU:CD2	2:D:251:SER:HB2	2.44	0.47
1:A:35:GLN:HA	1:A:35:GLN:OE1	2.14	0.47
1:C:195:HIS:O	1:C:217:ARG:NE	2.45	0.46
2:F:326:HIS:O	2:F:332:HIS:HA	2.15	0.46
1:G:60:ARG:HD3	1:G:68:PHE:O	2.15	0.46
2:F:285:GLU:HB3	2:F:307:LEU:HD11	1.97	0.46
1:G:15:LEU:HD12	1:G:113:LYS:O	2.15	0.46
2:B:13:LYS:O	2:B:16:ALA:HB3	2.14	0.46
1:E:158:ASN:O	1:E:158:ASN:CG	2.54	0.46
1:C:204:HIS:H	1:C:207:LEU:HD12	1.80	0.46
2:D:146:ASP:HB3	2:D:177:LEU:HD13	1.96	0.46
2:F:2:VAL:O	2:F:3:GLN:HG2	2.16	0.46
1:G:217:ARG:HD3	2:H:218:CYS:SG	2.55	0.46
2:B:315:GLN:HA	2:B:340:LEU:HD22	1.96	0.46
1:E:97:TYR:HA	1:E:102:LEU:HD22	1.96	0.46
1:G:55:TYR:HD2	1:G:56:TRP:CD1	2.34	0.46
2:H:330:HIS:O	2:H:330:HIS:ND1	2.48	0.46
2:F:36:TRP:CH2	2:F:96:CYS:HB3	2.49	0.46
2:H:288:TYR:HB3	2:H:307:LEU:HD12	1.98	0.46
2:F:60:TYR:CE2	2:F:70:LEU:HD23	2.50	0.46
1:G:157:ASP:OD2	1:G:195:HIS:HB3	2.16	0.46
2:H:241:ARG:HH11	2:H:300:SER:HB3	1.80	0.46
1:G:131:LEU:O	1:G:189:LYS:HD2	2.14	0.46
1:A:188:SER:OG	1:A:191:ASP:HB2	2.15	0.46
2:H:157:ASN:ND2	2:H:196:TYR:HA	2.20	0.46
1:C:89:VAL:CG1	1:C:89:VAL:O	2.64	0.46
1:G:51:LYS:CE	1:G:52:LEU:H	2.28	0.46
1:A:11:LEU:HD21	1:A:110:LEU:HD13	1.98	0.46
2:H:259:GLN:H	2:H:311:LYS:H	1.64	0.46
1:A:2:ILE:O	1:A:103:THR:HG21	2.16	0.46
2:H:240:PRO:HA	2:H:270:TYR:HB3	1.97	0.46
1:E:95:GLN:HB2	1:E:104:PHE:CD1	2.51	0.46
1:C:114:ARG:HG2	1:C:146:TYR:CD2	2.50	0.46
1:C:67:ARG:HG2	1:C:67:ARG:HH11	1.80	0.46
2:H:303:LEU:CD1	2:H:303:LEU:C	2.84	0.46
2:B:121:PRO:HB3	2:B:147:TYR:HB3	1.98	0.46
1:G:124:PHE:HB2	2:H:126:LEU:CD2	2.37	0.46
2:F:340:LEU:HD12	2:F:341:SER:N	2.30	0.46
1:A:115:THR:HG21	2:D:340:LEU:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:THR:HG23	2:F:163:SER:N	2.31	0.46
2:B:255:LEU:O	2:B:311:LYS:CE	2.64	0.46
2:D:254:GLU:HG3	2:D:260:VAL:HG12	1.96	0.46
1:A:20:THR:HG22	1:A:80:THR:HG23	1.98	0.46
2:F:254:GLU:O	2:F:254:GLU:HG2	2.15	0.46
1:A:67:ARG:NH1	1:A:88:ASP:OD1	2.48	0.46
2:B:303:LEU:CD1	2:B:303:LEU:C	2.83	0.46
2:B:251:SER:HB2	2:D:246:TYR:HB3	1.98	0.46
1:G:39:LEU:HG	1:G:40:ALA:N	2.31	0.46
2:F:263:THR:HG22	2:F:264:CYS:N	2.31	0.46
1:C:60:ARG:CD	1:C:64:VAL:HB	2.46	0.46
1:C:142:LEU:HD11	1:C:202:VAL:HG13	1.98	0.46
2:D:141:GLY:O	2:D:213:VAL:HG21	2.16	0.46
1:A:45:LYS:HE3	1:A:90:ALA:HB2	1.97	0.46
1:G:2:ILE:HD12	1:G:96:GLN:CD	2.36	0.46
1:C:169:VAL:CG2	1:C:181:LEU:HD12	2.46	0.45
2:B:154:VAL:HG11	2:B:182:SER:CB	2.46	0.45
2:D:291:THR:HG23	2:D:304:TYR:O	2.16	0.45
1:G:21:LEU:HD23	1:G:21:LEU:HA	1.65	0.45
2:B:243:PRO:CB	2:B:269:PHE:HB3	2.41	0.45
1:E:167:GLU:HG3	1:E:183:SER:CB	2.46	0.45
1:C:67:ARG:HG2	1:C:67:ARG:NH1	2.30	0.45
2:H:145:LYS:HG2	2:H:146:ASP:H	1.82	0.45
2:D:327:GLU:HA	2:D:332:HIS:CE1	2.51	0.45
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.34	0.45
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.30	0.45
1:E:190:ALA:O	1:E:193:GLU:HG2	2.17	0.45
2:D:128:PRO:C	2:D:130:SER:N	2.68	0.45
1:E:124:PHE:HB2	1:E:139:VAL:HB	1.99	0.45
1:G:217:ARG:HG3	1:G:219:GLU:HG3	1.99	0.45
1:G:217:ARG:HG3	1:G:220:CYS:H	1.81	0.45
2:F:243:PRO:HG2	2:F:329:LEU:HD21	1.98	0.45
2:H:76:ALA:O	2:H:77:SER:CB	2.65	0.45
2:B:251:SER:HB3	2:D:246:TYR:HB3	1.97	0.45
1:G:19:VAL:HG23	1:G:81:ILE:HG13	1.97	0.45
2:B:76:ALA:HB3	2:B:78:THR:HG23	1.97	0.45
2:B:134:SER:O	2:B:136:GLY:N	2.44	0.45
1:E:13:VAL:O	1:E:112:LEU:HD22	2.17	0.45
1:E:158:ASN:O	1:E:158:ASN:ND2	2.50	0.45
2:D:156:TRP:CH2	2:D:198:CYS:HB3	2.52	0.45
2:F:316:GLN:OE1	2:F:316:GLN:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:VAL:HG22	1:G:109:LYS:HD3	1.97	0.45
2:H:264:CYS:HB2	2:H:278:TRP:CZ2	2.51	0.45
1:C:155:LYS:HD2	1:C:159:ALA:C	2.37	0.45
1:C:43:GLN:HB2	1:C:53:LEU:HD11	1.97	0.45
2:H:292:PRO:O	2:H:293:PRO:C	2.55	0.45
2:H:134:SER:HB3	2:H:138:ALA:HB2	1.98	0.45
2:B:172:LEU:HA	2:B:178:TYR:CD1	2.52	0.45
2:F:245:VAL:HG22	2:F:266:VAL:HG13	1.99	0.45
2:H:241:ARG:HG2	2:H:268:GLY:O	2.17	0.45
1:G:4:MET:HE2	1:G:96:GLN:N	2.32	0.45
1:C:56:TRP:O	1:C:58:SER:N	2.50	0.45
2:H:127:ALA:HA	2:H:128:PRO:HD3	1.81	0.45
1:C:114:ARG:HG3	1:C:114:ARG:NH1	2.30	0.45
1:C:146:TYR:CB	1:C:147:PRO:CD	2.95	0.45
2:D:252:ARG:CG	2:D:252:ARG:NH1	2.80	0.45
2:B:161:LEU:HD21	2:B:184:VAL:HG21	1.99	0.45
2:H:146:ASP:HB3	2:H:177:LEU:HD13	1.99	0.45
2:D:259:GLN:HA	2:D:309:VAL:O	2.17	0.45
1:E:124:PHE:O	1:E:138:VAL:HG23	2.17	0.45
1:G:156:VAL:HG22	1:G:198:TYR:CD2	2.52	0.45
1:G:30:LEU:HA	1:G:36:LYS:O	2.16	0.45
1:G:152:VAL:HG21	1:G:183:SER:HB2	1.99	0.45
2:D:145:LYS:HG2	2:D:146:ASP:H	1.82	0.44
2:D:148:PHE:HB2	2:D:177:LEU:HD23	1.99	0.44
2:D:132:SER:C	2:D:134:SER:N	2.63	0.44
2:B:58:PHE:C	2:B:58:PHE:CD1	2.89	0.44
2:F:11:VAL:HG12	2:F:12:VAL:N	2.32	0.44
1:G:196:LYS:HG2	1:G:216:ASN:OD1	2.17	0.44
1:A:29:LEU:HD12	1:A:39:LEU:HB2	1.98	0.44
1:G:141:LEU:HD12	1:G:142:LEU:N	2.32	0.44
2:H:241:ARG:H	2:H:270:TYR:HB3	1.82	0.44
2:H:150:GLU:HG3	2:H:151:PRO:CB	2.47	0.44
2:D:150:GLU:HG2	2:D:178:TYR:CD1	2.52	0.44
2:F:86:LEU:H	2:F:86:LEU:HD12	1.82	0.44
1:E:88:ASP:O	1:E:110:LEU:HD23	2.17	0.44
2:B:264:CYS:HB2	2:B:278:TRP:CZ2	2.51	0.44
1:C:176:ASP:OD2	1:C:176:ASP:C	2.56	0.44
1:E:154:TRP:CD2	1:E:185:LEU:HD22	2.52	0.44
1:A:100:TYR:CD2	2:B:59:LYS:HD3	2.52	0.44
2:F:259:GLN:H	2:F:311:LYS:H	1.65	0.44
2:F:11:VAL:CG2	2:F:149:PRO:HG3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:O	1:C:11:LEU:HD23	2.17	0.44
1:E:141:LEU:HD12	1:E:142:LEU:N	2.32	0.44
2:B:63:ARG:HD2	2:B:64:PHE:CE1	2.53	0.44
1:C:121:VAL:CG2	1:C:202:VAL:HG21	2.47	0.44
2:H:243:PRO:CD	2:H:329:LEU:HD21	2.48	0.44
2:F:184:VAL:HG22	2:F:185:THR:N	2.33	0.44
2:B:251:SER:O	2:B:252:ARG:C	2.54	0.44
2:B:190:SER:HA	2:B:193:THR:CG2	2.48	0.44
2:D:48:ILE:HG12	2:D:64:PHE:CE1	2.51	0.44
2:D:290:THR:HG23	2:D:303:LEU:HD13	1.99	0.44
1:A:220:CYS:O	2:B:218:CYS:SG	2.76	0.44
1:C:186:THR:O	1:C:186:THR:HG22	2.16	0.44
2:D:243:PRO:CA	2:D:269:PHE:HB3	2.48	0.44
2:D:243:PRO:HG2	2:D:329:LEU:HD21	2.00	0.44
1:G:125:PRO:HB3	1:G:215:PHE:CE2	2.53	0.44
1:A:13:VAL:HG13	1:A:84:VAL:HG11	1.99	0.44
2:F:141:GLY:HA2	2:F:156:TRP:CH2	2.53	0.44
1:A:187:LEU:CD2	1:A:187:LEU:N	2.81	0.44
2:D:143:LEU:HD12	2:D:143:LEU:C	2.38	0.44
2:B:195:THR:CG2	2:B:212:LYS:HE3	2.44	0.44
2:H:243:PRO:HD2	2:H:329:LEU:CD2	2.48	0.44
2:B:60:TYR:OH	2:B:69:THR:HA	2.18	0.44
1:A:67:ARG:HG3	1:A:81:ILE:CG2	2.46	0.44
2:H:124:PHE:HA	2:H:125:PRO:HD3	1.78	0.44
2:D:48:ILE:HG23	2:D:64:PHE:CB	2.47	0.44
2:F:70:LEU:HD22	2:F:70:LEU:H	1.83	0.44
1:G:19:VAL:O	1:G:80:THR:HG23	2.17	0.44
1:A:42:TYR:HB2	1:A:93:TYR:HB2	1.99	0.44
2:F:136:GLY:O	2:F:187:PRO:HA	2.17	0.44
1:G:6:GLN:HE21	1:G:94:CYS:H	1.59	0.44
2:F:150:GLU:HG2	2:F:178:TYR:CD2	2.53	0.44
1:C:2:ILE:CG2	1:C:96:GLN:HG2	2.48	0.44
2:H:241:ARG:NH1	2:H:300:SER:HB3	2.32	0.44
2:D:156:TRP:O	2:D:157:ASN:C	2.56	0.44
1:A:46:PRO:HD2	1:A:171:GLU:OE2	2.18	0.44
1:C:15:LEU:CD2	1:C:15:LEU:C	2.84	0.44
1:G:145:PHE:O	1:G:178:THR:HB	2.17	0.44
1:C:187:LEU:N	1:C:187:LEU:CD2	2.80	0.44
1:C:142:LEU:HD21	1:C:152:VAL:CG2	2.48	0.44
2:B:39:GLN:HB3	2:B:93:VAL:HG13	1.99	0.44
1:G:58:SER:CB	1:G:70:GLY:O	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ASP:CG	1:E:175:LYS:H	2.20	0.44
2:D:148:PHE:CD1	2:D:149:PRO:HA	2.53	0.43
2:H:32:HIS:CD2	2:H:99:SER:HB2	2.53	0.43
2:H:150:GLU:HG3	2:H:151:PRO:CA	2.48	0.43
2:B:147:TYR:CE1	2:B:152:VAL:HG13	2.53	0.43
2:B:327:GLU:HA	2:B:332:HIS:ND1	2.33	0.43
2:D:23:LYS:HE3	2:D:77:SER:HB3	2.00	0.43
2:F:241:ARG:HH11	2:F:241:ARG:HG3	1.82	0.43
1:E:192:TYR:CE1	1:E:198:TYR:HE1	2.36	0.43
2:D:252:ARG:O	2:D:252:ARG:HG3	2.18	0.43
1:C:129:GLU:O	1:C:132:LYS:HB2	2.18	0.43
2:H:35:HIS:CD2	2:H:50:TYR:HB3	2.53	0.43
2:H:33:ALA:HB1	2:H:50:TYR:CD2	2.53	0.43
2:B:70:LEU:O	2:B:71:THR:HG23	2.18	0.43
1:E:173:ASP:OD2	1:E:176:ASP:N	2.37	0.43
1:E:176:ASP:C	1:E:176:ASP:OD2	2.57	0.43
1:E:45:LYS:HB2	1:E:48:GLN:OE1	2.18	0.43
2:B:265:LEU:HD12	2:B:266:VAL:N	2.33	0.43
2:B:28:THR:O	2:B:30:THR:N	2.51	0.43
2:D:154:VAL:HG12	2:D:155:SER:N	2.32	0.43
1:C:204:HIS:HB3	1:C:207:LEU:HG	2.00	0.43
1:E:29:LEU:O	1:E:37:ASN:HA	2.18	0.43
2:B:258:ASN:O	2:B:259:GLN:CB	2.65	0.43
1:E:13:VAL:HG21	1:E:19:VAL:CG1	2.48	0.43
1:G:20:THR:HG22	1:G:80:THR:CG2	2.48	0.43
2:B:265:LEU:HD11	2:B:267:LYS:HB3	2.00	0.43
1:C:204:HIS:CG	1:C:205:GLN:N	2.86	0.43
2:F:60:TYR:CZ	2:F:70:LEU:CD2	3.00	0.43
2:B:250:PRO:HB3	2:B:261:SER:O	2.18	0.43
2:B:36:TRP:CD1	2:B:70:LEU:HD22	2.53	0.43
1:E:6:GLN:OE1	1:E:93:TYR:HA	2.18	0.43
2:H:329:LEU:HD13	2:H:334:THR:HG22	2.00	0.43
1:C:204:HIS:CG	1:C:205:GLN:H	2.35	0.43
2:F:44:ARG:C	2:F:45:LEU:HD12	2.39	0.43
2:H:212:LYS:HZ3	2:H:214:GLU:HB3	1.81	0.43
1:G:141:LEU:CD2	2:H:183:VAL:HG21	2.48	0.43
2:B:254:GLU:CG	2:B:254:GLU:O	2.66	0.43
2:B:254:GLU:OE2	2:B:261:SER:OG	2.37	0.43
2:H:190:SER:HB2	2:H:194:GLN:HB3	2.01	0.43
2:F:209:VAL:HG12	2:F:210:ASP:N	2.33	0.43
2:B:279:GLU:HA	2:B:284:PRO:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:VAL:O	1:G:197:VAL:CG2	2.66	0.43
2:F:290:THR:HA	2:F:305:SER:HA	2.01	0.43
2:H:41:PRO:O	2:H:43:GLN:NE2	2.51	0.43
2:F:243:PRO:CA	2:F:269:PHE:HB3	2.48	0.43
2:B:246:TYR:HB3	2:D:251:SER:HB3	2.00	0.43
2:B:58:PHE:O	2:B:58:PHE:CD1	2.72	0.43
2:F:52:SER:HB2	2:F:55:ASN:OD1	2.19	0.43
2:F:194:GLN:HA	2:F:194:GLN:NE2	2.33	0.43
1:C:129:GLU:CD	1:C:129:GLU:N	2.70	0.43
1:G:85:GLN:CD	1:G:86:ALA:H	2.22	0.43
1:E:64:VAL:HA	1:E:65:PRO:HD2	1.82	0.43
1:E:18:ARG:HG3	1:E:18:ARG:HH11	1.84	0.43
2:H:213:VAL:HG12	2:H:214:GLU:N	2.34	0.43
1:E:68:PHE:CE1	1:E:81:ILE:HG12	2.54	0.43
1:A:217:ARG:HG2	1:A:217:ARG:NH1	2.30	0.43
2:B:23:LYS:HE2	2:B:78:THR:HG22	2.00	0.43
2:B:275:ALA:HB3	2:B:325:MET:HB2	2.00	0.43
2:D:44:ARG:HB3	2:D:44:ARG:HE	1.66	0.43
1:E:61:GLU:OE1	1:E:61:GLU:HA	2.19	0.43
2:B:6:GLN:HA	2:B:21:SER:O	2.18	0.43
1:C:137:SER:HA	1:C:185:LEU:O	2.17	0.43
1:C:164:ASN:OD1	1:C:164:ASN:N	2.51	0.43
1:E:123:ILE:HD11	1:E:138:VAL:HG22	2.01	0.43
2:B:40:ASN:HB2	2:B:43:GLN:HG2	2.01	0.43
2:F:279:GLU:HA	2:F:284:PRO:HA	2.00	0.43
2:B:36:TRP:CZ3	2:B:96:CYS:HB3	2.54	0.43
1:A:187:LEU:N	1:A:187:LEU:HD23	2.34	0.43
2:D:101:ASN:O	2:D:103:ALA:N	2.49	0.43
2:F:73:ASP:OD1	2:F:73:ASP:C	2.56	0.43
2:H:19:LYS:HG3	2:H:82:GLU:HB2	2.00	0.43
2:F:12:VAL:CG1	2:F:16:ALA:HB3	2.49	0.43
2:H:47:TRP:CE2	2:H:49:GLY:HA2	2.54	0.43
2:D:153:THR:HG23	2:D:201:ASN:HB3	2.01	0.43
1:A:155:LYS:HA	1:A:159:ALA:O	2.18	0.43
2:D:87:ARG:O	2:D:88:SER:C	2.56	0.43
2:D:326:HIS:CD2	2:D:328:ALA:HB3	2.54	0.42
2:B:172:LEU:HA	2:B:178:TYR:HD1	1.83	0.42
2:D:279:GLU:HA	2:D:285:GLU:N	2.32	0.42
1:G:156:VAL:O	1:G:159:ALA:HB3	2.18	0.42
1:E:114:ARG:O	1:E:115:THR:CB	2.67	0.42
2:H:27:TYR:CE2	2:H:98:ARG:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:LYS:HG3	1:G:75:THR:HG22	2.01	0.42
1:G:60:ARG:HD2	1:G:64:VAL:HG12	2.01	0.42
2:H:12:VAL:HG11	2:H:86:LEU:HD12	2.01	0.42
1:A:193:GLU:HA	1:A:217:ARG:HD2	2.00	0.42
1:E:66:ASP:C	1:E:68:PHE:H	2.22	0.42
1:G:121:VAL:C	1:G:122:PHE:CD1	2.92	0.42
2:F:291:THR:HG22	2:H:294:VAL:HG21	2.01	0.42
2:D:254:GLU:OE2	2:D:261:SER:OG	2.31	0.42
2:H:271:PRO:C	2:H:273:ASP:H	2.23	0.42
2:H:319:VAL:CG2	2:H:319:VAL:O	2.67	0.42
2:F:309:VAL:HG11	2:F:320:PHE:CE2	2.54	0.42
1:E:164:ASN:ND2	1:E:185:LEU:HD11	2.33	0.42
2:B:190:SER:O	2:B:191:LEU:C	2.58	0.42
1:E:17:GLU:O	1:E:83:SER:HA	2.18	0.42
1:G:93:TYR:CE1	1:G:107:GLY:HA3	2.55	0.42
2:H:18:VAL:HG12	2:H:86:LEU:HD11	2.02	0.42
1:A:6:GLN:OE1	1:A:93:TYR:HA	2.19	0.42
2:H:241:ARG:N	2:H:270:TYR:HB3	2.34	0.42
1:G:2:ILE:HB	1:G:96:GLN:NE2	2.34	0.42
2:B:134:SER:HB2	2:B:188:SER:OG	2.18	0.42
1:E:11:LEU:HD21	1:E:110:LEU:HD13	2.00	0.42
2:F:140:LEU:HD12	2:F:213:VAL:CG1	2.49	0.42
2:F:11:VAL:HG22	2:F:149:PRO:CG	2.49	0.42
2:F:149:PRO:HD2	2:F:204:PRO:CB	2.49	0.42
1:G:137:SER:HA	1:G:185:LEU:O	2.18	0.42
2:B:172:LEU:CB	2:B:178:TYR:HE1	2.24	0.42
2:F:51:PHE:HB2	2:F:70:LEU:HB3	2.01	0.42
2:H:241:ARG:HH12	2:H:298:ASP:CG	2.22	0.42
2:D:290:THR:HA	2:D:305:SER:HA	2.02	0.42
1:E:122:PHE:N	1:E:122:PHE:CD1	2.87	0.42
2:D:271:PRO:C	2:D:273:ASP:H	2.22	0.42
1:G:143:ASN:ND2	1:G:144:ASN:ND2	2.68	0.42
1:A:157:ASP:HA	1:A:197:VAL:CG2	2.27	0.42
2:B:132:SER:O	2:B:135:GLY:N	2.52	0.42
2:H:37:VAL:HG22	2:H:47:TRP:HA	2.01	0.42
1:G:211:VAL:CG1	1:G:212:THR:N	2.82	0.42
2:F:288:TYR:CB	2:F:307:LEU:HA	2.49	0.42
2:B:76:ALA:HB1	2:B:78:THR:CG2	2.49	0.42
1:C:72:GLY:HA3	1:C:77:PHE:HA	2.01	0.42
2:F:138:ALA:HB3	2:F:191:LEU:HD12	2.02	0.42
2:B:73:ASP:OD2	2:B:73:ASP:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:239:GLN:N	2:H:239:GLN:OE1	2.53	0.42
1:E:23:CYS:HB2	1:E:41:TRP:CH2	2.54	0.42
1:E:139:VAL:HG21	2:F:126:LEU:HD21	2.02	0.42
1:C:20:THR:HG22	1:C:80:THR:HG23	1.95	0.42
2:H:141:GLY:O	2:H:213:VAL:HG21	2.20	0.42
2:F:60:TYR:OH	2:F:70:LEU:N	2.41	0.42
1:E:13:VAL:HG22	1:E:17:GLU:OE1	2.19	0.42
1:E:34:ASN:ND2	1:E:34:ASN:N	2.66	0.42
2:D:254:GLU:C	2:D:256:THR:H	2.22	0.42
2:B:76:ALA:HB1	2:B:78:THR:HG23	2.00	0.42
1:G:30:LEU:HD11	1:G:35:GLN:C	2.40	0.42
2:H:162:THR:C	2:H:165:VAL:HG23	2.40	0.42
1:A:125:PRO:HD2	2:B:216:LYS:HZ1	1.83	0.42
2:D:313:ARG:O	2:D:316:GLN:CB	2.68	0.42
1:C:66:ASP:OD1	1:C:66:ASP:N	2.52	0.42
2:F:140:LEU:CD2	2:F:184:VAL:HG13	2.50	0.42
2:F:11:VAL:HA	2:F:112:THR:O	2.20	0.42
2:H:141:GLY:HA2	2:H:156:TRP:CZ2	2.55	0.42
1:E:141:LEU:HD21	1:E:143:ASN:OD1	2.19	0.42
2:F:263:THR:CG2	2:F:264:CYS:N	2.82	0.42
1:G:51:LYS:NZ	1:G:52:LEU:HB3	2.34	0.42
1:C:45:LYS:HB2	1:C:48:GLN:HE21	1.85	0.42
2:F:201:ASN:OD1	2:F:208:LYS:HE3	2.19	0.42
2:D:152:VAL:CG2	2:D:153:THR:H	2.33	0.42
2:B:250:PRO:HD3	2:B:262:LEU:CD2	2.50	0.42
2:B:150:GLU:HG2	2:B:151:PRO:HA	2.01	0.42
2:B:319:VAL:HG22	2:B:339:SER:HB3	2.02	0.42
1:C:102:LEU:HD23	1:C:102:LEU:HA	1.73	0.42
2:F:209:VAL:CG1	2:F:210:ASP:N	2.82	0.42
2:F:274:ILE:CG1	2:F:326:HIS:HB2	2.43	0.42
1:G:39:LEU:HD22	1:G:77:PHE:CD2	2.54	0.42
2:H:43:GLN:HG2	2:H:44:ARG:N	2.35	0.42
2:F:20:ILE:CG2	2:F:21:SER:N	2.83	0.42
2:F:248:LEU:HD23	2:H:251:SER:HB2	2.01	0.42
1:C:39:LEU:CD1	1:C:39:LEU:C	2.88	0.42
2:H:326:HIS:O	2:H:332:HIS:HA	2.19	0.42
2:H:32:HIS:HD2	2:H:99:SER:HB2	1.85	0.42
1:A:61:GLU:O	1:A:64:VAL:HG23	2.19	0.42
1:G:121:VAL:HG22	1:G:202:VAL:HG21	1.99	0.42
1:G:124:PHE:N	1:G:124:PHE:HD1	2.17	0.41
2:F:45:LEU:H	2:F:45:LEU:HD12	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:LYS:HA	1:E:146:TYR:OH	2.20	0.41
2:H:278:TRP:HZ3	2:H:338:LEU:HD11	1.85	0.41
1:A:121:VAL:CG1	1:A:202:VAL:HG21	2.50	0.41
2:D:264:CYS:HB2	2:D:278:TRP:CZ2	2.55	0.41
2:B:20:ILE:HG22	2:B:21:SER:N	2.35	0.41
1:E:100:TYR:HA	1:E:101:PRO:C	2.40	0.41
1:C:147:PRO:O	1:C:148:ARG:C	2.58	0.41
2:B:243:PRO:HB3	2:B:269:PHE:CB	2.47	0.41
1:C:169:VAL:HG22	1:C:181:LEU:CB	2.47	0.41
2:D:279:GLU:CB	2:D:284:PRO:HA	2.50	0.41
2:H:43:GLN:HE21	2:H:43:GLN:HB3	1.64	0.41
1:A:153:GLN:HG2	1:A:160:LEU:HD21	2.02	0.41
2:D:41:PRO:C	2:D:43:GLN:H	2.21	0.41
1:C:8:PRO:O	1:C:108:THR:HG23	2.20	0.41
2:H:306:LYS:NZ	2:H:306:LYS:HB3	2.35	0.41
2:B:309:VAL:HG13	2:B:313:ARG:HB2	2.02	0.41
2:D:201:ASN:OD1	2:D:208:LYS:HG2	2.20	0.41
2:D:264:CYS:HB2	2:D:278:TRP:CH2	2.54	0.41
1:C:188:SER:OG	1:C:191:ASP:HB2	2.20	0.41
2:H:333:TYR:CD1	2:H:334:THR:N	2.89	0.41
1:E:189:LYS:HB3	1:E:189:LYS:HE2	1.87	0.41
1:C:44:GLN:HE21	1:C:93:TYR:HE1	1.68	0.41
1:G:130:GLN:OE1	1:G:137:SER:N	2.54	0.41
2:H:99:SER:OG	2:H:100:LEU:N	2.53	0.41
1:A:109:LYS:HZ3	1:A:109:LYS:HB2	1.80	0.41
2:B:288:TYR:C	2:B:289:LYS:HG2	2.41	0.41
1:G:181:LEU:HA	2:H:168:PHE:HE2	1.83	0.41
2:F:6:GLN:HE21	2:F:6:GLN:HB3	1.72	0.41
2:H:298:ASP:C	2:H:298:ASP:OD2	2.59	0.41
1:G:192:TYR:CD1	1:G:198:TYR:CE1	3.09	0.41
2:F:191:LEU:HD23	2:F:215:PRO:HG3	2.01	0.41
1:E:150:ALA:C	1:E:151:LYS:HD2	2.40	0.41
2:B:333:TYR:CE1	2:B:335:GLN:HG3	2.56	0.41
2:D:11:VAL:HG22	2:D:149:PRO:CG	2.40	0.41
1:E:181:LEU:HD23	1:E:182:SER:N	2.35	0.41
1:G:53:LEU:HD11	1:G:92:TYR:HE1	1.85	0.41
2:F:190:SER:O	2:F:191:LEU:C	2.58	0.41
2:D:129:SER:O	2:D:130:SER:HB3	2.19	0.41
1:C:21:LEU:CD2	1:C:108:THR:HG21	2.50	0.41
2:H:333:TYR:CD1	2:H:333:TYR:C	2.94	0.41
1:G:77:PHE:C	1:G:78:THR:HG22	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ARG:O	2:B:63:ARG:HD3	2.20	0.41
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.56	0.41
2:D:32:HIS:HB2	2:D:98:ARG:HG3	2.02	0.41
2:B:280:SER:HB3	2:B:281:ASN:H	1.71	0.41
2:F:243:PRO:HB3	2:F:269:PHE:CB	2.46	0.41
2:B:29:PHE:CD1	2:B:77:SER:HA	2.56	0.41
1:C:18:ARG:HG2	1:C:18:ARG:NH1	2.34	0.41
1:G:38:TYR:CE2	1:G:56:TRP:HZ3	2.38	0.41
2:H:330:HIS:C	2:H:330:HIS:ND1	2.73	0.41
2:B:304:TYR:OH	2:D:263:THR:HG23	2.21	0.41
1:A:122:PHE:N	1:A:122:PHE:CD1	2.88	0.41
2:H:147:TYR:CD1	2:H:178:TYR:O	2.73	0.41
2:D:150:GLU:HA	2:D:151:PRO:HA	1.81	0.41
2:B:252:ARG:HH11	2:B:255:LEU:CD1	2.34	0.41
1:A:112:LEU:C	1:A:112:LEU:HD23	2.41	0.41
1:E:114:ARG:O	1:E:115:THR:OG1	2.34	0.41
2:F:36:TRP:CZ3	2:F:96:CYS:HB3	2.56	0.41
1:E:194:LYS:HD2	1:E:194:LYS:O	2.19	0.41
1:E:165:SER:HA	1:E:184:THR:O	2.21	0.41
2:D:309:VAL:HG11	2:D:320:PHE:HE2	1.85	0.41
2:H:186:VAL:HG11	2:H:196:TYR:CZ	2.56	0.41
1:E:89:VAL:CG2	1:E:112:LEU:HB2	2.51	0.41
1:E:68:PHE:CD1	1:E:81:ILE:HG12	2.55	0.41
1:G:85:GLN:CD	1:G:86:ALA:N	2.74	0.41
1:G:40:ALA:O	1:G:94:CYS:HA	2.20	0.41
1:G:211:VAL:HG12	1:G:212:THR:N	2.35	0.41
2:B:48:ILE:HG23	2:B:64:PHE:CB	2.50	0.41
1:C:18:ARG:HG3	1:C:82:SER:HA	2.02	0.41
2:F:55:ASN:HD21	2:F:57:ASP:HB3	1.86	0.41
2:D:13:LYS:O	2:D:16:ALA:HB3	2.21	0.41
1:E:38:TYR:CE2	1:E:56:TRP:CH2	3.09	0.41
1:A:34:ASN:H	1:A:34:ASN:ND2	2.19	0.41
2:D:50:TYR:HE1	2:D:59:LYS:HB2	1.75	0.41
2:H:47:TRP:CE3	2:H:61:ASN:HB2	2.56	0.41
1:G:64:VAL:HG13	1:G:65:PRO:HD2	2.02	0.41
1:G:51:LYS:HZ3	1:G:52:LEU:N	2.20	0.41
2:F:121:PRO:HB2	2:F:144:VAL:CG1	2.51	0.41
2:B:46:GLU:OE1	2:B:64:PHE:CZ	2.73	0.41
1:G:198:TYR:HB3	1:G:215:PHE:CE1	2.56	0.41
2:B:262:LEU:HD12	2:B:307:LEU:HD23	2.03	0.41
2:B:331:ASN:O	2:B:332:HIS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:H	1:A:187:LEU:HD23	1.86	0.41
2:D:27:TYR:CE1	2:D:98:ARG:HD2	2.56	0.41
1:A:17:GLU:HG3	1:A:18:ARG:H	1.86	0.41
2:F:1:GLN:CA	2:F:1:GLN:OE1	2.69	0.41
2:B:157:ASN:HD21	2:B:196:TYR:HA	1.86	0.40
1:G:67:ARG:HH11	1:G:67:ARG:HG2	1.86	0.40
2:B:295:LEU:HD13	2:B:301:PHE:CE2	2.55	0.40
2:B:304:TYR:HB2	2:D:304:TYR:CD1	2.57	0.40
2:D:13:LYS:HA	2:D:14:PRO:HD3	1.86	0.40
2:F:168:PHE:CD2	2:F:168:PHE:N	2.89	0.40
2:B:94:TYR:CD2	2:B:94:TYR:N	2.89	0.40
2:H:194:GLN:CG	2:H:196:TYR:CE2	3.04	0.40
1:E:154:TRP:CG	1:E:185:LEU:HD22	2.56	0.40
2:B:132:SER:C	2:B:135:GLY:H	2.25	0.40
2:H:50:TYR:C	2:H:50:TYR:CD2	2.94	0.40
2:H:263:THR:HG22	2:H:264:CYS:N	2.36	0.40
2:B:316:GLN:HE21	2:B:316:GLN:HA	1.86	0.40
1:G:126:PRO:HB2	1:G:131:LEU:CD1	2.52	0.40
2:D:291:THR:HB	2:D:292:PRO:HD2	2.03	0.40
2:F:140:LEU:H	2:F:140:LEU:HD23	1.85	0.40
1:C:11:LEU:HD11	1:C:19:VAL:HG23	1.99	0.40
2:H:43:GLN:CG	2:H:44:ARG:N	2.84	0.40
2:B:61:ASN:OD1	2:B:63:ARG:N	2.41	0.40
1:E:117:ALA:HB1	2:H:315:GLN:NE2	2.37	0.40
2:D:321:SER:HB3	2:D:337:SER:HA	2.04	0.40
1:A:87:GLU:HG3	1:A:87:GLU:H	1.53	0.40
2:F:255:LEU:HD22	2:F:315:GLN:HE22	1.86	0.40
2:B:259:GLN:H	2:B:311:LYS:H	1.68	0.40
1:A:109:LYS:HZ3	1:A:109:LYS:CB	2.34	0.40
2:H:110:LEU:O	2:H:110:LEU:HD13	2.21	0.40
2:F:147:TYR:HE1	2:F:152:VAL:HB	1.82	0.40
2:F:29:PHE:CD2	2:F:77:SER:HA	2.56	0.40
1:A:164:ASN:N	1:A:164:ASN:OD1	2.48	0.40
2:H:55:ASN:HD21	2:H:57:ASP:HB3	1.86	0.40
1:G:16:GLY:O	1:G:83:SER:HA	2.21	0.40
1:A:72:GLY:HA3	1:A:77:PHE:HA	2.03	0.40
2:H:324:VAL:C	2:H:325:MET:HG3	2.42	0.40
2:B:190:SER:O	2:B:193:THR:N	2.55	0.40
2:H:33:ALA:HB1	2:H:50:TYR:HD2	1.87	0.40
1:C:4:MET:HE2	1:C:96:GLN:N	2.37	0.40
1:G:25:SER:O	1:G:75:THR:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HB	2:H:104:TYR:CE2	2.56	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	218/220 (99%)	196 (90%)	16 (7%)	6 (3%)	6	21
1	C	218/220 (99%)	202 (93%)	10 (5%)	6 (3%)	6	21
1	E	218/220 (99%)	198 (91%)	16 (7%)	4 (2%)	11	34
1	G	218/220 (99%)	196 (90%)	15 (7%)	7 (3%)	5	17
2	B	320/344 (93%)	279 (87%)	33 (10%)	8 (2%)	7	24
2	D	320/344 (93%)	272 (85%)	36 (11%)	12 (4%)	4	13
2	F	320/344 (93%)	285 (89%)	24 (8%)	11 (3%)	5	16
2	H	320/344 (93%)	277 (87%)	34 (11%)	9 (3%)	6	21
All	All	2152/2256 (95%)	1905 (88%)	184 (9%)	63 (3%)	6	19

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	THR
2	B	43	GLN
1	C	146	TYR
2	D	43	GLN
2	D	130	SER
2	D	132	SER
1	E	115	THR
1	E	146	TYR
1	E	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	41	PRO
2	F	318	ASN
1	G	217	ARG
2	H	41	PRO
2	H	128	PRO
2	H	318	ASN
1	A	46	PRO
2	B	29	PHE
2	B	281	ASN
2	B	311	LYS
1	C	17	GLU
1	C	57	ALA
1	C	147	PRO
2	D	217	SER
2	F	40	ASN
2	F	44	ARG
2	F	135	GLY
2	H	281	ASN
2	H	297	SER
1	A	158	ASN
1	A	219	GLU
2	D	44	ARG
2	F	132	SER
2	F	191	LEU
1	G	57	ALA
1	G	90	ALA
1	A	217	ARG
2	B	297	SER
1	C	90	ALA
2	D	41	PRO
2	D	62	GLU
2	D	272	SER
2	D	281	ASN
2	F	128	PRO
1	G	62	SER
2	H	43	GLN
2	H	270	TYR
2	B	259	GLN
2	B	330	HIS
2	D	29	PHE
2	D	216	LYS
2	F	29	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	32	SER
2	F	259	GLN
2	H	191	LEU
1	E	46	PRO
1	A	50	PRO
2	B	135	GLY
1	G	46	PRO
1	G	84	VAL
1	C	46	PRO
2	H	151	PRO
2	D	151	PRO
2	F	151	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	193/193 (100%)	161 (83%)	32 (17%)	3	8
1	C	193/193 (100%)	167 (86%)	26 (14%)	5	14
1	E	193/193 (100%)	171 (89%)	22 (11%)	7	21
1	G	193/193 (100%)	175 (91%)	18 (9%)	11	32
2	B	284/296 (96%)	244 (86%)	40 (14%)	4	12
2	D	284/296 (96%)	250 (88%)	34 (12%)	6	19
2	F	284/296 (96%)	239 (84%)	45 (16%)	3	9
2	H	284/296 (96%)	252 (89%)	32 (11%)	7	22
All	All	1908/1956 (98%)	1659 (87%)	249 (13%)	5	15

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	13	VAL
1	A	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	ASN
1	A	39	LEU
1	A	46	PRO
1	A	60	ARG
1	A	66	ASP
1	A	75	THR
1	A	78	THR
1	A	79	LEU
1	A	85	GLN
1	A	95	GLN
1	A	109	LYS
1	A	115	THR
1	A	119	PRO
1	A	135	THR
1	A	138	VAL
1	A	146	TYR
1	A	151	LYS
1	A	153	GLN
1	A	160	LEU
1	A	161	GLN
1	A	167	GLU
1	A	181	LEU
1	A	187	LEU
1	A	197	VAL
1	A	203	THR
1	A	209	SER
1	A	214	SER
1	A	216	ASN
1	A	219	GLU
2	B	2	VAL
2	B	18	VAL
2	B	25	SER
2	B	39	GLN
2	B	41	PRO
2	B	59	LYS
2	B	63	ARG
2	B	74	THR
2	B	78	THR
2	B	98	ARG
2	B	107	GLN
2	B	110	LEU
2	B	117	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	118	THR
2	B	125	PRO
2	B	131	LYS
2	B	140	LEU
2	B	150	GLU
2	B	151	PRO
2	B	152	VAL
2	B	153	THR
2	B	180	LEU
2	B	185	THR
2	B	193	THR
2	B	197	ILE
2	B	204	PRO
2	B	239	GLN
2	B	256	THR
2	B	257	LYS
2	B	261	SER
2	B	277	GLU
2	B	286	ASN
2	B	303	LEU
2	B	305	SER
2	B	307	LEU
2	B	315	GLN
2	B	321	SER
2	B	327	GLU
2	B	335	GLN
2	B	344	LYS
1	C	11	LEU
1	C	27	GLN
1	C	39	LEU
1	C	46	PRO
1	C	48	GLN
1	C	49	SER
1	C	66	ASP
1	C	80	THR
1	C	85	GLN
1	C	89	VAL
1	C	95	GLN
1	C	101	PRO
1	C	111	GLU
1	C	112	LEU
1	C	115	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	133	SER
1	C	142	LEU
1	C	148	ARG
1	C	151	LYS
1	C	161	GLN
1	C	162	SER
1	C	186	THR
1	C	187	LEU
1	C	196	LYS
1	C	201	GLU
1	C	203	THR
2	D	34	ILE
2	D	38	LYS
2	D	41	PRO
2	D	46	GLU
2	D	61	ASN
2	D	63	ARG
2	D	65	LYS
2	D	102	MET
2	D	107	GLN
2	D	113	VAL
2	D	143	LEU
2	D	151	PRO
2	D	153	THR
2	D	162	THR
2	D	172	LEU
2	D	180	LEU
2	D	190	SER
2	D	193	THR
2	D	199	ASN
2	D	207	THR
2	D	252	ARG
2	D	254	GLU
2	D	261	SER
2	D	266	VAL
2	D	286	ASN
2	D	298	ASP
2	D	311	LYS
2	D	312	SER
2	D	318	ASN
2	D	319	VAL
2	D	321	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	338	LEU
2	D	339	SER
2	D	340	LEU
1	E	6	GLN
1	E	14	SER
1	E	18	ARG
1	E	20	THR
1	E	24	LYS
1	E	34	ASN
1	E	61	GLU
1	E	66	ASP
1	E	69	SER
1	E	76	ASP
1	E	84	VAL
1	E	85	GLN
1	E	87	GLU
1	E	115	THR
1	E	129	GLU
1	E	145	PHE
1	E	148	ARG
1	E	153	GLN
1	E	187	LEU
1	E	194	LYS
1	E	196	LYS
1	E	220	CYS
2	F	1	GLN
2	F	2	VAL
2	F	5	VAL
2	F	17	SER
2	F	18	VAL
2	F	23	LYS
2	F	44	ARG
2	F	48	ILE
2	F	63	ARG
2	F	78	THR
2	F	82	GLU
2	F	87	ARG
2	F	98	ARG
2	F	99	SER
2	F	102	MET
2	F	107	GLN
2	F	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	118	THR
2	F	125	PRO
2	F	147	TYR
2	F	149	PRO
2	F	151	PRO
2	F	161	LEU
2	F	162	THR
2	F	180	LEU
2	F	181	SER
2	F	197	ILE
2	F	199	ASN
2	F	239	GLN
2	F	252	ARG
2	F	253	ASP
2	F	259	GLN
2	F	276	VAL
2	F	277	GLU
2	F	279	GLU
2	F	281	ASN
2	F	289	LYS
2	F	295	LEU
2	F	296	ASP
2	F	298	ASP
2	F	311	LYS
2	F	313	ARG
2	F	315	GLN
2	F	323	SER
2	F	338	LEU
1	G	39	LEU
1	G	51	LYS
1	G	66	ASP
1	G	78	THR
1	G	84	VAL
1	G	115	THR
1	G	124	PHE
1	G	127	SER
1	G	148	ARG
1	G	152	VAL
1	G	161	GLN
1	G	164	ASN
1	G	166	GLN
1	G	185	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	197	VAL
1	G	208	SER
1	G	210	PRO
1	G	217	ARG
2	H	11	VAL
2	H	43	GLN
2	H	52	SER
2	H	63	ARG
2	H	70	LEU
2	H	78	THR
2	H	81	VAL
2	H	87	ARG
2	H	97	THR
2	H	101	ASN
2	H	102	MET
2	H	107	GLN
2	H	140	LEU
2	H	144	VAL
2	H	151	PRO
2	H	180	LEU
2	H	185	THR
2	H	194	GLN
2	H	197	ILE
2	H	199	ASN
2	H	239	GLN
2	H	252	ARG
2	H	255	LEU
2	H	256	THR
2	H	258	ASN
2	H	267	LYS
2	H	303	LEU
2	H	318	ASN
2	H	320	PHE
2	H	331	ASN
2	H	338	LEU
2	H	344	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	GLN
1	A	158	ASN
2	B	35	HIS
2	B	40	ASN
2	B	107	GLN
2	B	157	ASN
2	B	166	HIS
2	B	201	ASN
2	B	202	HIS
2	B	239	GLN
2	B	316	GLN
2	B	330	HIS
2	B	335	GLN
1	C	27	GLN
1	C	35	GLN
1	C	43	GLN
1	C	48	GLN
1	C	85	GLN
1	C	95	GLN
1	C	172	GLN
1	C	204	HIS
2	D	32	HIS
2	D	239	GLN
2	D	259	GLN
2	D	281	ASN
2	D	286	ASN
2	D	316	GLN
2	D	318	ASN
2	D	326	HIS
1	E	34	ASN
1	E	43	GLN
1	E	144	ASN
1	E	153	GLN
1	E	164	ASN
1	E	204	HIS
1	E	205	GLN
2	F	32	HIS
2	F	43	GLN
2	F	173	GLN
2	F	194	GLN
2	F	259	GLN
2	F	281	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	287	ASN
2	F	315	GLN
2	F	335	GLN
1	G	6	GLN
1	G	44	GLN
1	G	95	GLN
1	G	143	ASN
1	G	144	ASN
1	G	164	ASN
1	G	166	GLN
1	G	172	GLN
1	G	195	HIS
1	G	205	GLN
2	H	35	HIS
2	H	107	GLN
2	H	157	ASN
2	H	166	HIS
2	H	194	GLN
2	H	239	GLN
2	H	258	ASN
2	H	287	ASN
2	H	318	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

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/220 (100%)	-0.30	1 (0%) 91 88	5, 28, 50, 97	0
1	C	220/220 (100%)	-0.21	2 (0%) 85 79	3, 35, 57, 100	0
1	E	220/220 (100%)	0.03	4 (1%) 71 61	9, 43, 75, 113	0
1	G	220/220 (100%)	0.05	6 (2%) 58 45	7, 49, 76, 112	0
2	B	324/344 (94%)	-0.22	5 (1%) 76 68	4, 29, 60, 96	0
2	D	324/344 (94%)	-0.14	8 (2%) 61 48	7, 29, 74, 100	0
2	F	324/344 (94%)	0.16	11 (3%) 49 36	13, 52, 92, 120	0
2	H	324/344 (94%)	0.29	22 (6%) 20 12	15, 50, 91, 121	0
All	All	2176/2256 (96%)	-0.03	59 (2%) 58 45	3, 38, 80, 121	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	220	CYS	6.4
2	H	131	LYS	5.9
2	F	344	LYS	5.8
2	F	130	SER	5.7
2	F	218	CYS	5.4
2	F	343	GLY	5.2
1	E	220	CYS	5.0
2	D	217	SER	4.9
2	F	217	SER	4.7
2	F	134	SER	4.4
2	H	132	SER	4.2
2	B	134	SER	3.9
2	H	327	GLU	3.8
2	D	343	GLY	3.6
2	H	342	PRO	3.5
2	H	129	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	134	SER	3.2
1	C	220	CYS	3.2
2	F	131	LYS	3.1
2	H	324	VAL	2.9
2	H	344	LYS	2.9
2	B	218	CYS	2.8
2	D	344	LYS	2.8
2	H	270	TYR	2.8
2	H	134	SER	2.7
1	G	198	TYR	2.7
1	E	187	LEU	2.7
2	D	218	CYS	2.7
2	B	216	LYS	2.7
2	F	135	GLY	2.6
2	H	139	ALA	2.6
1	G	215	PHE	2.6
2	H	328	ALA	2.5
2	H	276	VAL	2.5
2	D	130	SER	2.5
1	G	216	ASN	2.5
2	H	329	LEU	2.4
2	F	133	THR	2.4
2	H	218	CYS	2.4
1	A	220	CYS	2.3
2	H	239	GLN	2.3
1	G	197	VAL	2.3
2	D	131	LYS	2.3
2	H	241	ARG	2.2
2	F	213	VAL	2.2
2	H	240	PRO	2.2
2	H	343	GLY	2.2
1	E	156	VAL	2.2
2	F	193	THR	2.1
2	H	140	LEU	2.1
1	G	219	GLU	2.1
2	H	211	LYS	2.1
2	B	132	SER	2.1
2	H	128	PRO	2.1
1	E	19	VAL	2.1
2	H	269	PHE	2.1
2	B	344	LYS	2.1
1	C	156	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	342	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.