



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 AM UTC

PDB ID : 2PFD / pdb_00002pfd
Title : Anisotropically refined structure of FTCD
Authors : Poon, B.K.; Chen, X.; Lu, M.; Quioco, F.A.; Wang, Q.; Ma, J.
Deposited on : 2007-04-04
Resolution : 3.42 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

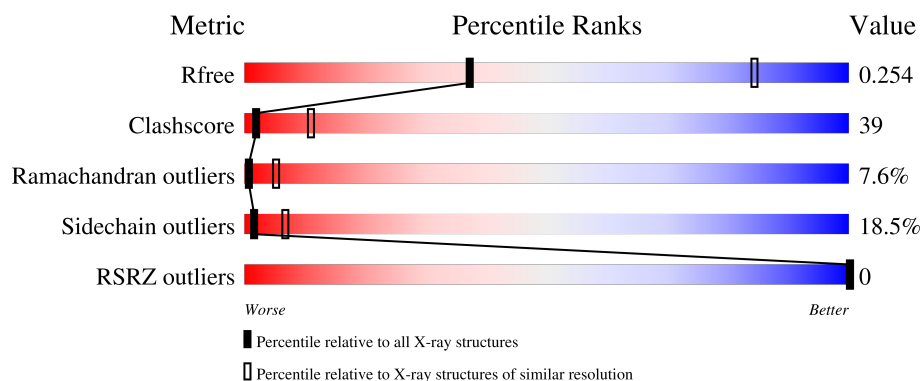
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

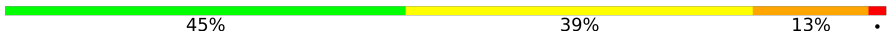
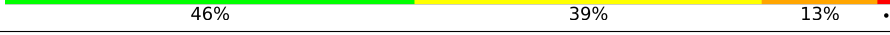
The reported resolution of this entry is 3.42 Å.

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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	541	 45% 39% 13% .
1	B	541	 42% 40% 15% .
1	C	541	 44% 39% 15% .
1	D	541	 46% 39% 13% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16524 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.

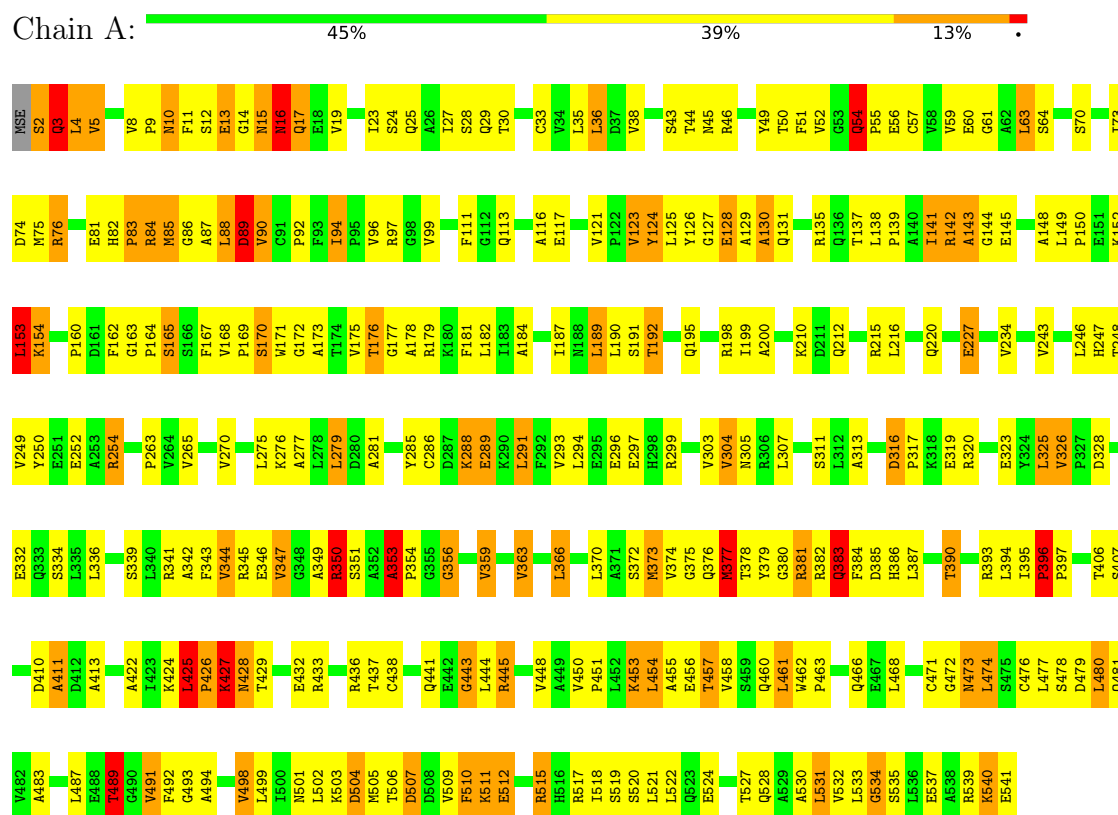
- Molecule 1 is a protein called Formimidoyltransferase-cyclodeaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	540	Total 4131	C 2602	N 731	O 779	S 11	Se 8	0	0	0
1	B	540	Total 4131	C 2602	N 731	O 779	S 11	Se 8	0	0	0
1	C	540	Total 4131	C 2602	N 731	O 779	S 11	Se 8	0	0	0
1	D	540	Total 4131	C 2602	N 731	O 779	S 11	Se 8	0	0	0

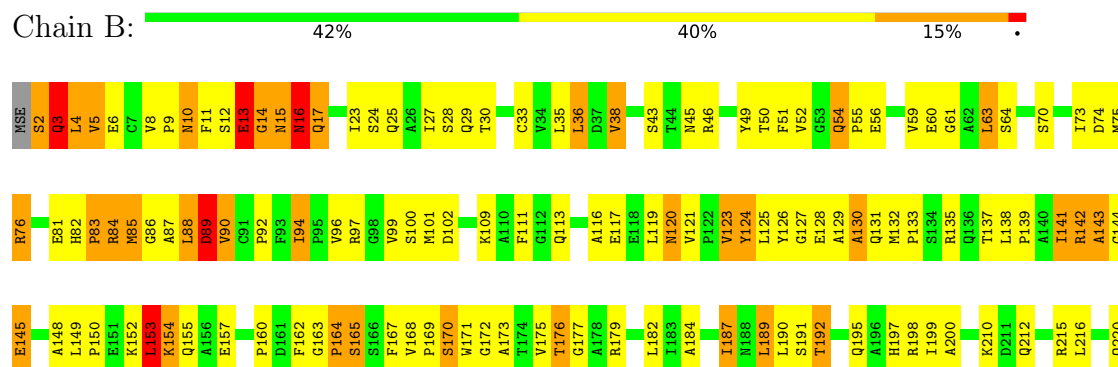
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Formimidoyltransferase-cyclodeaminase



• Molecule 1: Formimidoyltransferase-cyclodeaminase



V491	V498	L499	I500	N501	L502	K503	D504	M505	T506	D507	F509	F510	K511	E512	T514	R515	H516	R517	I518	S519	S520	L521	L522	G523	E524	T527	Q528	A529	A530	L531	V532	L533	G534	S535	L536	E537	A538	R539	K540	E541															
L335	L336	D337	A338	S339	L340	R341	A342	F343	N344	R345	E346	V347	G348	A349	R350	S351	A352	A353	P354	G355	G356	V359	V363	L366	L370	M373	V374	G375	Q376	M377	T378	Y379	G380	R381	R382	Q383	F384	D385	H386	L387	T390	R393	L394	I395	P396	P397	T406	S407	D410	A411					
D412	A413	A422	I423	K424	L425	P426	K427	N428	T429	E432	R433	R436	T437	C438	Q441	E442	G443	L444	R445	V448	A449	V450	K453	L454	A455	E456	T457	Q458	V459	Q460	L461	W462	P463	Q466	C471	Q472	N473	L474	L477	S478	D479	L480	Q481	V482	A483	L487	E488	T489	G490						
E81	H82	P83	R84	M85	G86	A87	L88	D89	V90	C91	P92	F93	I94	P95	V96	R97	G98	V99	F111	G112	Q113	A116	E117	E118	L119	N120	V121	P122	V123	Y124	L125	Y126	G127	E128	A129	A130	Q131	R135	Q136	T137	L138	P139	A140	T141	R142	A143	G144	E145	A148	L149	P150	E151	K152	L153	K154
P160	D161	F162	G163	S165	S166	F167	V168	P169	S170	W171	G172	T173	V175	T176	G177	A178	R179	K180	F181	L182	I183	A184	I187	N188	L189	L190	S191	T192	Q195	R198	I199	A200	K210	D211	Q212	R215	L216	Q220	E227	V234	V243	L246	H247	T248	V249	Y250									
E251	E252	A253	R254	L260	P263	V264	V265	V270	L279	D280	A281	F284	Y285	C286	D287	K288	E289	K290	L291	F292	V293	L294	E295	E296	E297	H298	R299	V303	V304	N305	E306	L307	S311	L312	A313	D316	P317	K318	E319	R320	E323	Y324	L325	V326	P327	D328	E332	Q333	S334						

4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	134.85Å 134.85Å 156.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.42 10.00 – 3.42	Depositor EDS
% Data completeness (in resolution range)	94.0 (10.00-3.42) 95.9 (10.00-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.249 0.242 , 0.254	Depositor DCC
R_{free} test set	1803 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.367 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16524	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.75	1/4195 (0.0%)	1.05	22/5674 (0.4%)
1	B	0.76	2/4195 (0.0%)	1.07	21/5674 (0.4%)
1	C	0.68	3/4195 (0.1%)	1.05	19/5674 (0.3%)
1	D	0.71	3/4195 (0.1%)	1.05	18/5674 (0.3%)
All	All	0.73	9/16780 (0.1%)	1.05	80/22696 (0.4%)

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
1	C	0	1
1	D	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	LEU	CG-CD2	-10.27	1.18	1.52
1	B	13	GLU	C-O	-9.48	1.12	1.24
1	B	153	LEU	CG-CD2	-9.14	1.22	1.52
1	D	13	GLU	CD-OE1	8.62	1.41	1.25
1	A	153	LEU	CG-CD2	-8.56	1.24	1.52
1	C	153	LEU	CG-CD2	-8.47	1.24	1.52
1	C	344	VAL	CA-CB	5.30	1.60	1.54
1	D	15	ASN	CG-OD1	5.14	1.33	1.23
1	C	457	THR	CA-CB	5.09	1.61	1.53

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	LEU	CD1-CG-CD2	-9.06	90.86	110.80
1	B	153	LEU	CD1-CG-CD2	-8.38	92.37	110.80
1	A	311	SER	N-CA-C	-7.26	106.34	114.62
1	D	15	ASN	OD1-CG-ND2	7.17	129.76	122.60
1	D	54	GLN	CA-C-N	7.13	128.75	119.84
1	D	54	GLN	C-N-CA	7.13	128.75	119.84
1	C	54	GLN	CA-C-N	7.10	128.72	119.84
1	C	54	GLN	C-N-CA	7.10	128.72	119.84
1	B	311	SER	N-CA-C	-7.04	106.59	114.62
1	C	311	SER	N-CA-C	-6.99	106.65	114.62
1	B	54	GLN	CA-C-N	6.99	128.57	119.84
1	B	54	GLN	C-N-CA	6.99	128.57	119.84
1	A	54	GLN	CA-C-N	6.85	128.41	119.84
1	A	54	GLN	C-N-CA	6.85	128.41	119.84
1	D	311	SER	N-CA-C	-6.74	106.94	114.62
1	B	435	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	A	377	MSE	CB-CG-SE	6.67	132.70	112.70
1	C	153	LEU	CD1-CG-CD2	-6.46	96.58	110.80
1	A	377	MSE	CG-SE-CE	6.43	113.06	98.92
1	D	153	LEU	CB-CG-CD1	6.34	129.73	110.70
1	A	153	LEU	CD1-CG-CD2	-6.33	96.86	110.80
1	C	352	ALA	N-CA-C	-6.30	104.85	112.54
1	D	163	GLY	CA-C-N	6.22	127.62	119.84
1	D	163	GLY	C-N-CA	6.22	127.62	119.84
1	A	163	GLY	CA-C-N	6.15	127.53	119.84
1	A	163	GLY	C-N-CA	6.15	127.53	119.84
1	A	313	ALA	CA-C-N	-6.13	114.30	120.31
1	A	313	ALA	C-N-CA	-6.13	114.30	120.31
1	B	435	ARG	CD-NE-CZ	6.11	132.96	124.40
1	B	153	LEU	CB-CG-CD1	6.08	128.95	110.70
1	B	313	ALA	CA-C-N	-5.99	114.44	120.31
1	B	313	ALA	C-N-CA	-5.99	114.44	120.31
1	D	353	ALA	CA-C-N	-5.96	114.13	120.03
1	D	353	ALA	C-N-CA	-5.96	114.13	120.03
1	C	313	ALA	CA-C-N	-5.88	114.55	120.31
1	C	313	ALA	C-N-CA	-5.88	114.55	120.31
1	B	163	GLY	CA-C-N	5.83	127.13	119.84
1	B	163	GLY	C-N-CA	5.83	127.13	119.84
1	B	396	PRO	N-CA-C	5.79	117.77	110.70
1	B	435	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	489	THR	N-CA-C	-5.71	105.58	112.54
1	B	13	GLU	O-C-N	-5.70	115.01	122.59
1	D	313	ALA	CA-C-N	-5.67	114.76	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	ALA	C-N-CA	-5.67	114.76	120.31
1	A	316	ASP	CA-C-N	-5.63	113.87	119.56
1	A	316	ASP	C-N-CA	-5.63	113.87	119.56
1	C	163	GLY	CA-C-N	5.56	126.80	119.84
1	C	163	GLY	C-N-CA	5.56	126.80	119.84
1	A	396	PRO	N-CA-C	5.52	117.44	110.70
1	A	366	LEU	N-CA-C	-5.51	105.37	111.71
1	B	468	LEU	N-CA-C	-5.46	105.49	111.82
1	A	425	LEU	CA-C-N	5.39	126.58	119.84
1	A	425	LEU	C-N-CA	5.39	126.58	119.84
1	A	153	LEU	CB-CG-CD1	5.38	126.83	110.70
1	C	468	LEU	N-CA-C	-5.34	105.63	111.82
1	A	353	ALA	CA-C-N	-5.30	114.25	119.92
1	A	353	ALA	C-N-CA	-5.30	114.25	119.92
1	C	396	PRO	N-CA-C	5.28	117.14	110.70
1	A	468	LEU	N-CA-C	-5.26	105.72	111.82
1	C	41	GLY	CA-C-N	5.22	126.37	119.84
1	C	41	GLY	C-N-CA	5.22	126.37	119.84
1	B	353	ALA	CA-C-N	-5.21	114.58	119.85
1	B	353	ALA	C-N-CA	-5.21	114.58	119.85
1	C	353	ALA	CA-C-N	-5.21	114.59	119.85
1	C	353	ALA	C-N-CA	-5.21	114.59	119.85
1	D	425	LEU	CA-C-N	5.14	126.27	119.84
1	D	425	LEU	C-N-CA	5.14	126.27	119.84
1	C	153	LEU	CB-CG-CD1	5.12	126.04	110.70
1	A	153	LEU	CB-CG-CD2	-5.09	95.43	110.70
1	B	425	LEU	CA-C-N	5.08	126.19	119.84
1	B	425	LEU	C-N-CA	5.08	126.19	119.84
1	B	352	ALA	N-CA-C	-5.07	106.36	112.54
1	C	425	LEU	CA-C-N	5.07	126.18	119.84
1	C	425	LEU	C-N-CA	5.07	126.18	119.84
1	D	316	ASP	CA-C-N	-5.04	114.47	119.56
1	D	316	ASP	C-N-CA	-5.04	114.47	119.56
1	C	145	GLU	N-CA-C	5.02	118.56	109.32
1	D	396	PRO	N-CA-C	5.01	116.81	110.70
1	D	489	THR	N-CA-C	-5.01	106.43	112.54
1	B	145	GLU	N-CA-C	5.00	118.53	109.32

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	LYS	Peptide
1	B	427	LYS	Peptide
1	C	427	LYS	Peptide
1	D	427	LYS	Peptide

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	4131	0	4175	337	0
1	B	4131	0	4175	350	0
1	C	4131	0	4175	339	0
1	D	4131	0	4175	332	0
All	All	16524	0	16700	1290	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 39.

All (1290) 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:C:351:SER:O	1:D:373:MSE:HE2	1.37	1.22
1:A:373:MSE:HE2	1:B:351:SER:O	1.44	1.18
1:C:427:LYS:HE3	1:C:436:ARG:NH1	1.63	1.14
1:B:426:PRO:O	1:B:427:LYS:HB2	1.48	1.13
1:B:2:SER:N	1:B:328:ASP:HB2	1.63	1.13
1:B:427:LYS:HE3	1:B:436:ARG:NH1	1.66	1.11
1:A:27:ILE:HD11	1:A:51:PHE:CD1	1.86	1.11
1:A:427:LYS:HE3	1:A:436:ARG:HH12	1.16	1.11
1:C:2:SER:N	1:C:328:ASP:HB2	1.64	1.11
1:C:347:VAL:O	1:D:373:MSE:HE3	1.52	1.10
1:C:489:THR:HG21	1:D:489:THR:HG21	1.11	1.10
1:A:2:SER:N	1:A:328:ASP:HB2	1.67	1.10
1:C:149:LEU:CD2	1:C:153:LEU:HD23	1.81	1.09
1:B:27:ILE:HD11	1:B:51:PHE:CD1	1.87	1.09
1:A:373:MSE:HE3	1:B:347:VAL:O	1.52	1.09
1:A:427:LYS:HE3	1:A:436:ARG:NH1	1.66	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:SER:N	1:D:328:ASP:HB2	1.67	1.09
1:C:427:LYS:HE3	1:C:436:ARG:HH12	1.10	1.08
1:B:359:VAL:O	1:B:363:VAL:HG23	1.54	1.08
1:C:359:VAL:O	1:C:363:VAL:HG23	1.54	1.07
1:D:427:LYS:HE3	1:D:436:ARG:NH1	1.67	1.07
1:C:425:LEU:HD22	1:C:426:PRO:HD2	1.35	1.07
1:C:149:LEU:HD22	1:C:153:LEU:HD23	1.16	1.07
1:C:27:ILE:HD11	1:C:51:PHE:CD1	1.89	1.07
1:D:27:ILE:HD11	1:D:51:PHE:CD1	1.90	1.06
1:C:426:PRO:O	1:C:427:LYS:HB2	1.50	1.06
1:D:426:PRO:O	1:D:427:LYS:HB2	1.52	1.06
1:D:531:LEU:HD23	1:D:531:LEU:H	1.20	1.06
1:A:426:PRO:O	1:A:427:LYS:HB2	1.52	1.06
1:D:425:LEU:HD22	1:D:426:PRO:HD2	1.37	1.05
1:D:427:LYS:HE3	1:D:436:ARG:HH12	1.16	1.05
1:A:359:VAL:O	1:A:363:VAL:HG23	1.56	1.05
1:D:359:VAL:O	1:D:363:VAL:HG23	1.55	1.05
1:A:5:VAL:HG23	1:A:99:VAL:HG11	1.34	1.05
1:D:5:VAL:HG23	1:D:99:VAL:HG11	1.34	1.05
1:A:489:THR:CG2	1:B:489:THR:HG21	1.88	1.04
1:B:425:LEU:HD22	1:B:426:PRO:HD2	1.33	1.04
1:D:149:LEU:O	1:D:153:LEU:HD12	1.57	1.04
1:A:425:LEU:HD22	1:A:426:PRO:HD2	1.37	1.02
1:B:5:VAL:HG23	1:B:99:VAL:HG11	1.38	1.02
1:A:351:SER:O	1:B:373:MSE:HE2	1.58	1.02
1:C:5:VAL:HG23	1:C:99:VAL:HG11	1.38	1.01
1:A:531:LEU:H	1:A:531:LEU:HD23	1.21	1.01
1:A:27:ILE:HD11	1:A:51:PHE:CE1	1.96	1.01
1:B:27:ILE:HD11	1:B:51:PHE:CE1	1.95	1.00
1:D:153:LEU:HD23	1:D:165:SER:O	1.61	1.00
1:B:427:LYS:HE3	1:B:436:ARG:HH12	1.14	0.99
1:C:502:LEU:HA	1:C:505:MSE:HG3	1.42	0.99
1:B:531:LEU:HD23	1:B:531:LEU:H	1.27	0.98
1:C:27:ILE:HD11	1:C:51:PHE:CE1	1.97	0.98
1:A:489:THR:HG21	1:B:489:THR:HG21	1.00	0.98
1:C:458:VAL:HG11	1:C:491:VAL:HG22	1.42	0.98
1:C:531:LEU:H	1:C:531:LEU:HD23	1.27	0.97
1:A:489:THR:HG21	1:B:489:THR:CG2	1.95	0.96
1:D:502:LEU:HA	1:D:505:MSE:HG3	1.48	0.95
1:C:373:MSE:HE2	1:D:351:SER:O	1.67	0.94
1:B:13:GLU:HG2	1:B:13:GLU:O	1.68	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:THR:HG21	1:D:489:THR:CG2	1.97	0.94
1:D:27:ILE:HD11	1:D:51:PHE:CE1	2.01	0.94
1:C:445:ARG:HG3	1:C:445:ARG:HH11	1.32	0.93
1:A:373:MSE:HE1	1:B:354:PRO:O	1.68	0.93
1:A:502:LEU:HA	1:A:505:MSE:HG3	1.51	0.93
1:A:422:ALA:O	1:A:425:LEU:HB2	1.69	0.93
1:D:153:LEU:CD2	1:D:165:SER:O	2.17	0.93
1:B:502:LEU:HA	1:B:505:MSE:HG3	1.48	0.93
1:A:149:LEU:CD2	1:A:153:LEU:HD23	1.99	0.92
1:D:422:ALA:O	1:D:425:LEU:HB2	1.69	0.92
1:B:422:ALA:O	1:B:425:LEU:HB2	1.69	0.92
1:C:15:ASN:O	1:C:16:ASN:HB3	1.70	0.91
1:A:363:VAL:HG13	1:B:363:VAL:HG13	1.50	0.91
1:D:227:GLU:OE1	1:D:227:GLU:HA	1.70	0.91
1:D:15:ASN:O	1:D:16:ASN:HB3	1.71	0.91
1:D:445:ARG:HG3	1:D:445:ARG:HH11	1.35	0.91
1:B:483:ALA:O	1:B:487:LEU:HD12	1.71	0.90
1:A:370:LEU:HD11	1:B:359:VAL:HG11	1.52	0.90
1:B:445:ARG:HG3	1:B:445:ARG:HH11	1.36	0.90
1:B:15:ASN:O	1:B:16:ASN:HB3	1.70	0.90
1:C:422:ALA:O	1:C:425:LEU:HB2	1.69	0.89
1:A:15:ASN:O	1:A:16:ASN:HB3	1.70	0.89
1:D:149:LEU:O	1:D:153:LEU:CD1	2.21	0.89
1:A:390:THR:HG22	1:A:393:ARG:HH21	1.37	0.88
1:A:149:LEU:HB3	1:A:153:LEU:HD21	1.56	0.88
1:A:356:GLY:H	1:B:370:LEU:HD21	1.38	0.88
1:C:113:GLN:O	1:C:117:GLU:HG2	1.74	0.87
1:C:149:LEU:HD22	1:C:153:LEU:CD2	2.05	0.87
1:C:359:VAL:HG11	1:D:370:LEU:HD11	1.55	0.87
1:A:349:ALA:C	1:A:351:SER:H	1.81	0.87
1:C:483:ALA:O	1:C:487:LEU:HD12	1.75	0.86
1:C:349:ALA:C	1:C:351:SER:H	1.79	0.86
1:B:113:GLN:O	1:B:117:GLU:HG2	1.75	0.85
1:C:445:ARG:HH11	1:C:445:ARG:CG	1.89	0.85
1:A:445:ARG:HG3	1:A:445:ARG:HH11	1.38	0.85
1:C:390:THR:HG22	1:C:393:ARG:HH21	1.42	0.85
1:D:445:ARG:HH11	1:D:445:ARG:CG	1.89	0.84
1:A:370:LEU:HD21	1:B:356:GLY:H	1.40	0.84
1:A:113:GLN:O	1:A:117:GLU:HG2	1.78	0.83
1:D:483:ALA:O	1:D:487:LEU:HD12	1.78	0.83
1:B:153:LEU:C	1:B:153:LEU:HD23	2.03	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:PRO:O	1:D:373:MSE:HE1	1.78	0.83
1:A:149:LEU:HB3	1:A:153:LEU:CD2	2.08	0.83
1:C:345:ARG:HH21	1:D:406:THR:HB	1.43	0.82
1:D:390:THR:HG22	1:D:393:ARG:HH21	1.41	0.82
1:B:349:ALA:C	1:B:351:SER:H	1.84	0.82
1:A:227:GLU:OE1	1:A:227:GLU:HA	1.76	0.82
1:A:373:MSE:CE	1:B:351:SER:OG	2.27	0.82
1:A:90:VAL:HA	1:A:175:VAL:HG23	1.60	0.82
1:C:227:GLU:HA	1:C:227:GLU:OE1	1.79	0.82
1:C:351:SER:OG	1:D:373:MSE:CE	2.26	0.82
1:A:445:ARG:HH11	1:A:445:ARG:CG	1.92	0.81
1:B:445:ARG:HH11	1:B:445:ARG:CG	1.93	0.81
1:D:15:ASN:HB2	1:D:45:ASN:OD1	1.80	0.81
1:C:2:SER:N	1:C:328:ASP:CB	2.43	0.81
1:A:15:ASN:HB2	1:A:45:ASN:OD1	1.81	0.81
1:B:15:ASN:HB2	1:B:45:ASN:OD1	1.80	0.81
1:B:153:LEU:HG	1:B:165:SER:O	1.80	0.81
1:B:227:GLU:OE1	1:B:227:GLU:HA	1.80	0.81
1:B:390:THR:HG22	1:B:393:ARG:HH21	1.46	0.81
1:B:2:SER:N	1:B:328:ASP:CB	2.43	0.81
1:C:90:VAL:HA	1:C:175:VAL:HG23	1.62	0.81
1:D:113:GLN:O	1:D:117:GLU:HG2	1.80	0.81
1:B:458:VAL:HG11	1:B:491:VAL:HG22	1.61	0.81
1:A:483:ALA:O	1:A:487:LEU:HD12	1.81	0.80
1:A:97:ARG:NH2	1:A:328:ASP:HB3	1.96	0.80
1:D:90:VAL:HA	1:D:175:VAL:HG23	1.62	0.80
1:D:349:ALA:C	1:D:351:SER:H	1.88	0.80
1:D:427:LYS:HB3	1:D:428:ASN:HD22	1.46	0.80
1:C:15:ASN:HB2	1:C:45:ASN:OD1	1.81	0.80
1:A:427:LYS:HB3	1:A:428:ASN:HD22	1.47	0.80
1:A:149:LEU:HD22	1:A:153:LEU:CD2	2.11	0.79
1:B:149:LEU:HD23	1:B:153:LEU:HB3	1.64	0.79
1:B:149:LEU:CD2	1:B:153:LEU:HB3	2.11	0.79
1:D:97:ARG:NH2	1:D:328:ASP:HB3	1.98	0.79
1:D:515:ARG:O	1:D:518:ILE:HG22	1.83	0.78
1:B:90:VAL:HA	1:B:175:VAL:HG23	1.63	0.78
1:B:471:CYS:SG	1:B:472:GLY:N	2.55	0.78
1:A:363:VAL:CG1	1:B:363:VAL:HG13	2.14	0.77
1:D:149:LEU:HD23	1:D:153:LEU:HB3	1.66	0.77
1:B:190:LEU:HB2	1:B:263:PRO:HG2	1.67	0.77
1:A:2:SER:N	1:A:328:ASP:CB	2.46	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HD22	1:D:153:LEU:HG	1.66	0.77
1:D:2:SER:N	1:D:328:ASP:CB	2.47	0.77
1:A:515:ARG:O	1:A:518:ILE:HG22	1.84	0.77
1:C:373:MSE:HE3	1:D:347:VAL:O	1.84	0.77
1:C:351:SER:OG	1:D:373:MSE:HE2	1.85	0.76
1:C:370:LEU:HD21	1:D:356:GLY:H	1.50	0.76
1:B:13:GLU:O	1:B:15:ASN:N	2.18	0.76
1:C:363:VAL:HG13	1:D:363:VAL:HG13	1.66	0.76
1:B:97:ARG:NH2	1:B:328:ASP:HB3	2.00	0.76
1:D:494:ALA:O	1:D:498:VAL:HG23	1.84	0.76
1:C:97:ARG:NH2	1:C:328:ASP:HB3	2.00	0.76
1:C:458:VAL:HG11	1:C:491:VAL:CG2	2.17	0.75
1:D:25:GLN:HB3	1:D:29:GLN:NE2	2.01	0.75
1:A:342:ALA:O	1:A:346:GLU:HB2	1.87	0.74
1:C:25:GLN:HB3	1:C:29:GLN:NE2	2.01	0.74
1:C:471:CYS:SG	1:C:472:GLY:N	2.60	0.74
1:A:494:ALA:O	1:A:498:VAL:HG23	1.86	0.74
1:C:356:GLY:H	1:D:370:LEU:HD21	1.53	0.74
1:D:473:ASN:O	1:D:474:LEU:HB2	1.87	0.74
1:B:25:GLN:HB3	1:B:29:GLN:NE2	2.03	0.73
1:B:396:PRO:HB2	1:B:397:PRO:CD	2.18	0.73
1:C:116:ALA:HB2	1:C:123:VAL:HG12	1.69	0.73
1:C:454:LEU:HD12	1:C:454:LEU:O	1.87	0.73
1:D:116:ALA:HB2	1:D:123:VAL:HG12	1.71	0.73
1:C:148:ALA:C	1:C:150:PRO:HD2	2.13	0.73
1:D:148:ALA:C	1:D:150:PRO:HD2	2.14	0.73
1:A:116:ALA:HB2	1:A:123:VAL:HG12	1.70	0.73
1:C:494:ALA:O	1:C:498:VAL:HG23	1.88	0.73
1:A:25:GLN:HB3	1:A:29:GLN:NE2	2.04	0.72
1:D:216:LEU:HD21	1:D:252:GLU:HG2	1.71	0.72
1:D:342:ALA:O	1:D:346:GLU:HB2	1.88	0.72
1:B:116:ALA:HB2	1:B:123:VAL:HG12	1.69	0.72
1:D:382:ARG:O	1:D:383:GLN:HB3	1.88	0.72
1:B:148:ALA:C	1:B:150:PRO:HD2	2.14	0.72
1:A:458:VAL:HG11	1:A:491:VAL:HG22	1.71	0.72
1:A:373:MSE:HE3	1:B:351:SER:OG	1.89	0.71
1:A:347:VAL:O	1:B:373:MSE:HE3	1.90	0.71
1:C:190:LEU:HB2	1:C:263:PRO:HG2	1.72	0.71
1:C:427:LYS:HB3	1:C:428:ASN:HD22	1.54	0.71
1:B:494:ALA:O	1:B:498:VAL:HG23	1.89	0.71
1:D:149:LEU:CD2	1:D:153:LEU:HB3	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:O	1:B:346:GLU:HB2	1.91	0.71
1:C:342:ALA:O	1:C:346:GLU:HB2	1.90	0.71
1:C:396:PRO:HB2	1:C:397:PRO:CD	2.20	0.71
1:C:515:ARG:O	1:C:518:ILE:HG22	1.91	0.71
1:A:135:ARG:HG2	1:A:141:ILE:HD11	1.73	0.71
1:A:406:THR:HB	1:B:345:ARG:HH21	1.55	0.71
1:B:135:ARG:HG2	1:B:141:ILE:HD11	1.73	0.71
1:B:149:LEU:HB3	1:B:153:LEU:HD13	1.73	0.71
1:C:382:ARG:O	1:C:383:GLN:HB3	1.90	0.71
1:D:11:PHE:CE1	1:D:88:LEU:HD12	2.26	0.71
1:C:135:ARG:HG2	1:C:141:ILE:HD11	1.72	0.70
1:A:148:ALA:C	1:A:150:PRO:HD2	2.15	0.70
1:B:427:LYS:HB3	1:B:428:ASN:HD22	1.55	0.70
1:C:13:GLU:HG2	1:C:15:ASN:N	2.06	0.70
1:A:386:HIS:CD2	1:A:387:LEU:HD12	2.26	0.70
1:A:13:GLU:HG2	1:A:15:ASN:N	2.06	0.70
1:C:473:ASN:O	1:C:474:LEU:HB2	1.91	0.70
1:D:190:LEU:HB2	1:D:263:PRO:HG2	1.74	0.70
1:C:116:ALA:HB2	1:C:123:VAL:CG1	2.22	0.70
1:A:149:LEU:CD2	1:A:153:LEU:CD2	2.68	0.70
1:A:149:LEU:HD23	1:A:153:LEU:HD23	1.72	0.70
1:D:458:VAL:HG11	1:D:491:VAL:HG22	1.73	0.70
1:A:216:LEU:HD21	1:A:252:GLU:HG2	1.72	0.69
1:B:454:LEU:O	1:B:454:LEU:HD12	1.91	0.69
1:A:190:LEU:HB2	1:A:263:PRO:HG2	1.74	0.69
1:D:76:ARG:NH2	1:D:169:PRO:HB3	2.08	0.69
1:B:515:ARG:O	1:B:518:ILE:HG22	1.92	0.69
1:A:471:CYS:SG	1:A:472:GLY:N	2.65	0.69
1:D:13:GLU:H	1:D:46:ARG:HA	1.57	0.69
1:D:424:LYS:HG3	1:D:424:LYS:O	1.93	0.69
1:D:458:VAL:HG23	1:D:487:LEU:HD23	1.74	0.69
1:B:176:THR:CG2	1:B:177:GLY:N	2.56	0.69
1:C:148:ALA:N	1:C:150:PRO:HD2	2.08	0.69
1:D:149:LEU:C	1:D:153:LEU:HD12	2.18	0.69
1:C:76:ARG:NH2	1:C:169:PRO:HB3	2.08	0.68
1:A:473:ASN:O	1:A:474:LEU:HB2	1.93	0.68
1:B:76:ARG:NH2	1:B:169:PRO:HB3	2.08	0.68
1:B:116:ALA:HB2	1:B:123:VAL:CG1	2.23	0.68
1:D:13:GLU:HG2	1:D:15:ASN:N	2.08	0.68
1:D:25:GLN:HB3	1:D:29:GLN:HE21	1.59	0.68
1:A:424:LYS:HG3	1:A:424:LYS:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:HB2	1:A:397:PRO:CD	2.24	0.68
1:A:427:LYS:HB3	1:A:428:ASN:ND2	2.09	0.68
1:B:473:ASN:O	1:B:474:LEU:HB2	1.92	0.68
1:C:489:THR:CG2	1:D:489:THR:HG21	2.07	0.68
1:C:445:ARG:HG3	1:C:445:ARG:NH1	2.07	0.68
1:D:471:CYS:SG	1:D:472:GLY:N	2.67	0.68
1:A:116:ALA:HB2	1:A:123:VAL:CG1	2.24	0.67
1:A:373:MSE:HE2	1:B:351:SER:OG	1.93	0.67
1:A:382:ARG:O	1:A:383:GLN:HB3	1.92	0.67
1:B:374:VAL:HG21	1:B:480:LEU:HD22	1.76	0.67
1:D:11:PHE:CZ	1:D:88:LEU:HD11	2.29	0.67
1:D:116:ALA:HB2	1:D:123:VAL:CG1	2.24	0.67
1:B:148:ALA:N	1:B:150:PRO:HD2	2.09	0.67
1:C:427:LYS:HG3	1:C:436:ARG:HH11	1.60	0.67
1:D:316:ASP:O	1:D:320:ARG:HG2	1.95	0.67
1:C:374:VAL:HG21	1:C:480:LEU:HD22	1.77	0.67
1:A:11:PHE:CE1	1:A:88:LEU:HD12	2.29	0.67
1:A:531:LEU:H	1:A:531:LEU:CD2	2.01	0.67
1:D:427:LYS:HB3	1:D:428:ASN:ND2	2.08	0.67
1:A:111:PHE:HD2	1:A:176:THR:HG1	1.40	0.67
1:A:176:THR:CG2	1:A:177:GLY:N	2.58	0.67
1:B:299:ARG:O	1:B:303:VAL:HG12	1.95	0.67
1:D:8:VAL:HG12	1:D:8:VAL:O	1.95	0.67
1:A:76:ARG:NH2	1:A:169:PRO:HB3	2.10	0.67
1:C:351:SER:OG	1:D:373:MSE:HE3	1.95	0.67
1:C:386:HIS:CD2	1:C:387:LEU:HD12	2.30	0.67
1:D:299:ARG:O	1:D:303:VAL:HG12	1.95	0.67
1:D:396:PRO:HB2	1:D:397:PRO:CD	2.25	0.67
1:C:25:GLN:HB3	1:C:29:GLN:HE21	1.58	0.66
1:A:149:LEU:HD22	1:A:153:LEU:HD22	1.75	0.66
1:C:299:ARG:O	1:C:303:VAL:HG12	1.95	0.66
1:D:148:ALA:N	1:D:150:PRO:HD2	2.10	0.66
1:A:373:MSE:CE	1:B:354:PRO:O	2.43	0.66
1:C:76:ARG:CZ	1:C:169:PRO:HB2	2.24	0.66
1:B:13:GLU:O	1:B:13:GLU:CG	2.36	0.66
1:A:76:ARG:CZ	1:A:169:PRO:HB2	2.26	0.66
1:D:386:HIS:CD2	1:D:387:LEU:HD12	2.31	0.66
1:B:76:ARG:CZ	1:B:169:PRO:HB2	2.25	0.66
1:B:386:HIS:CD2	1:B:387:LEU:HD12	2.30	0.66
1:C:349:ALA:C	1:C:351:SER:N	2.51	0.66
1:B:382:ARG:O	1:B:383:GLN:HB3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LYS:HG3	1:B:436:ARG:HH11	1.61	0.66
1:B:531:LEU:H	1:B:531:LEU:CD2	2.05	0.66
1:D:531:LEU:H	1:D:531:LEU:CD2	1.99	0.66
1:A:13:GLU:H	1:A:46:ARG:HA	1.61	0.66
1:A:374:VAL:HG21	1:A:480:LEU:CD2	2.26	0.66
1:A:148:ALA:N	1:A:150:PRO:HD2	2.10	0.65
1:A:374:VAL:HG21	1:A:480:LEU:HD22	1.78	0.65
1:B:25:GLN:HB3	1:B:29:GLN:HE21	1.61	0.65
1:C:13:GLU:H	1:C:46:ARG:HA	1.60	0.65
1:D:76:ARG:CZ	1:D:169:PRO:HB2	2.25	0.65
1:D:46:ARG:CZ	1:D:82:HIS:HD2	2.10	0.65
1:A:299:ARG:O	1:A:303:VAL:HG12	1.97	0.65
1:B:458:VAL:CG1	1:B:491:VAL:HG22	2.27	0.65
1:B:502:LEU:HA	1:B:505:MSE:CG	2.26	0.65
1:C:8:VAL:HG12	1:C:8:VAL:O	1.96	0.65
1:D:374:VAL:HG21	1:D:480:LEU:HD22	1.78	0.65
1:A:189:LEU:HD12	1:A:234:VAL:HG23	1.79	0.65
1:A:247:HIS:CD2	1:A:281:ALA:HA	2.32	0.65
1:A:316:ASP:O	1:A:320:ARG:HG2	1.97	0.65
1:C:46:ARG:CZ	1:C:82:HIS:HD2	2.10	0.65
1:A:25:GLN:HB3	1:A:29:GLN:HE21	1.61	0.64
1:A:344:VAL:HG22	1:A:345:ARG:HG2	1.78	0.64
1:C:11:PHE:CZ	1:C:88:LEU:HD11	2.32	0.64
1:C:502:LEU:HA	1:C:505:MSE:CG	2.24	0.64
1:D:189:LEU:HD12	1:D:234:VAL:HG23	1.79	0.64
1:D:247:HIS:CD2	1:D:281:ALA:HA	2.31	0.64
1:B:374:VAL:HG21	1:B:480:LEU:CD2	2.27	0.64
1:C:247:HIS:CD2	1:C:281:ALA:HA	2.32	0.64
1:D:176:THR:CG2	1:D:177:GLY:N	2.60	0.64
1:B:46:ARG:CZ	1:B:82:HIS:HD2	2.10	0.64
1:C:189:LEU:HD12	1:C:234:VAL:HG23	1.80	0.64
1:C:316:ASP:O	1:C:320:ARG:HG2	1.98	0.64
1:D:351:SER:HB2	1:D:354:PRO:HD2	1.80	0.64
1:A:46:ARG:CZ	1:A:82:HIS:HD2	2.10	0.64
1:C:374:VAL:HG21	1:C:480:LEU:CD2	2.27	0.64
1:B:426:PRO:O	1:B:427:LYS:CB	2.35	0.64
1:D:11:PHE:CE1	1:D:88:LEU:CD1	2.81	0.64
1:D:441:GLN:OE1	1:D:505:MSE:HA	1.97	0.64
1:A:11:PHE:CZ	1:A:88:LEU:HD11	2.33	0.64
1:A:373:MSE:CE	1:B:351:SER:O	2.36	0.64
1:A:386:HIS:CD2	1:A:387:LEU:CD1	2.81	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLN:OE1	1:A:505:MSE:HA	1.98	0.64
1:A:458:VAL:HG23	1:A:487:LEU:HD23	1.80	0.64
1:B:13:GLU:HG2	1:B:15:ASN:N	2.13	0.64
1:D:502:LEU:HA	1:D:505:MSE:CG	2.25	0.63
1:B:8:VAL:HG12	1:B:8:VAL:O	1.97	0.63
1:B:441:GLN:OE1	1:B:505:MSE:HA	1.99	0.63
1:C:285:TYR:O	1:C:289:GLU:HB2	1.98	0.63
1:B:247:HIS:CD2	1:B:281:ALA:HA	2.33	0.63
1:C:427:LYS:HB3	1:C:428:ASN:ND2	2.12	0.63
1:D:454:LEU:HD12	1:D:454:LEU:O	1.98	0.63
1:C:424:LYS:O	1:C:424:LYS:HG3	1.97	0.63
1:A:127:GLY:C	1:A:129:ALA:H	2.06	0.63
1:C:363:VAL:HG13	1:D:363:VAL:CG1	2.27	0.63
1:C:427:LYS:CE	1:C:436:ARG:HH12	2.00	0.63
1:D:425:LEU:HB3	1:D:436:ARG:HG3	1.80	0.63
1:D:285:TYR:O	1:D:289:GLU:HB2	1.98	0.63
1:C:176:THR:CG2	1:C:177:GLY:N	2.61	0.63
1:B:171:TRP:CD1	1:B:172:GLY:H	2.16	0.63
1:B:424:LYS:O	1:B:424:LYS:HG3	1.98	0.63
1:D:382:ARG:O	1:D:383:GLN:CB	2.46	0.63
1:A:8:VAL:O	1:A:8:VAL:HG12	1.97	0.62
1:A:111:PHE:HD2	1:A:176:THR:OG1	1.82	0.62
1:A:200:ALA:HB2	1:A:234:VAL:HG13	1.81	0.62
1:B:13:GLU:O	1:B:14:GLY:C	2.36	0.62
1:D:374:VAL:HG21	1:D:480:LEU:CD2	2.30	0.62
1:C:111:PHE:HD2	1:C:176:THR:OG1	1.83	0.62
1:D:171:TRP:CD1	1:D:172:GLY:H	2.17	0.62
1:C:425:LEU:HB3	1:C:436:ARG:HG3	1.81	0.62
1:A:425:LEU:HB3	1:A:436:ARG:HG3	1.81	0.62
1:B:427:LYS:HB3	1:B:428:ASN:ND2	2.13	0.62
1:B:453:LYS:O	1:B:457:THR:HG22	1.99	0.62
1:C:149:LEU:HB3	1:C:153:LEU:CD2	2.30	0.62
1:C:458:VAL:HG22	1:C:487:LEU:HD23	1.82	0.62
1:D:200:ALA:HB2	1:D:234:VAL:HG13	1.80	0.62
1:B:189:LEU:HD11	1:B:199:ILE:HD12	1.82	0.62
1:B:425:LEU:HB3	1:B:436:ARG:HG3	1.81	0.62
1:A:370:LEU:HD11	1:B:359:VAL:CG1	2.27	0.62
1:D:127:GLY:C	1:D:129:ALA:H	2.08	0.62
1:B:200:ALA:HB2	1:B:234:VAL:HG13	1.82	0.62
1:B:285:TYR:O	1:B:289:GLU:HB2	1.99	0.62
1:B:506:THR:O	1:B:507:ASP:CB	2.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:HG3	1:A:436:ARG:HH11	1.65	0.62
1:C:254:ARG:HH11	1:C:254:ARG:HB3	1.65	0.62
1:C:351:SER:O	1:D:373:MSE:CE	2.30	0.62
1:C:386:HIS:CD2	1:C:387:LEU:CD1	2.83	0.62
1:C:171:TRP:CD1	1:C:172:GLY:H	2.17	0.61
1:C:200:ALA:HB2	1:C:234:VAL:HG13	1.81	0.61
1:D:111:PHE:HD2	1:D:176:THR:OG1	1.83	0.61
1:B:11:PHE:CE1	1:B:88:LEU:HD12	2.34	0.61
1:D:111:PHE:HD2	1:D:176:THR:HG1	1.47	0.61
1:A:11:PHE:CE1	1:A:88:LEU:CD1	2.83	0.61
1:C:149:LEU:HB3	1:C:153:LEU:HD21	1.82	0.61
1:C:441:GLN:OE1	1:C:505:MSE:HA	2.00	0.61
1:B:189:LEU:HD12	1:B:234:VAL:HG23	1.82	0.61
1:B:386:HIS:CD2	1:B:387:LEU:CD1	2.83	0.61
1:B:458:VAL:HG23	1:B:487:LEU:HD23	1.82	0.61
1:C:9:PRO:HG2	1:C:49:TYR:HB2	1.83	0.61
1:D:82:HIS:O	1:D:84:ARG:N	2.34	0.61
1:B:111:PHE:HD2	1:B:176:THR:OG1	1.84	0.61
1:A:2:SER:O	1:A:3:GLN:HB2	2.01	0.61
1:A:534:GLY:O	1:A:535:SER:C	2.43	0.61
1:C:506:THR:O	1:C:507:ASP:CB	2.49	0.61
1:D:478:SER:OG	1:D:479:ASP:N	2.33	0.61
1:A:390:THR:HG22	1:A:393:ARG:NH2	2.14	0.61
1:A:458:VAL:CG2	1:A:487:LEU:HD23	2.31	0.61
1:B:458:VAL:CG2	1:B:487:LEU:HD23	2.31	0.61
1:C:462:TRP:HB3	1:C:528:GLN:HG2	1.83	0.61
1:A:35:LEU:HD12	1:A:51:PHE:HB3	1.83	0.61
1:D:254:ARG:HH11	1:D:254:ARG:HB3	1.65	0.61
1:B:11:PHE:CZ	1:B:88:LEU:HD11	2.36	0.60
1:C:215:ARG:CZ	1:C:252:GLU:OE2	2.49	0.60
1:A:382:ARG:O	1:A:383:GLN:CB	2.49	0.60
1:A:454:LEU:HD12	1:A:454:LEU:O	2.01	0.60
1:B:127:GLY:C	1:B:129:ALA:H	2.09	0.60
1:B:9:PRO:HG2	1:B:49:TYR:HB2	1.83	0.60
1:C:11:PHE:CE1	1:C:88:LEU:HD12	2.35	0.60
1:D:506:THR:O	1:D:507:ASP:CB	2.48	0.60
1:A:502:LEU:HA	1:A:505:MSE:CG	2.28	0.60
1:A:506:THR:O	1:A:507:ASP:CB	2.49	0.60
1:C:453:LYS:O	1:C:457:THR:HG22	2.00	0.60
1:A:82:HIS:O	1:A:84:ARG:N	2.34	0.60
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:CB	1:A:153:LEU:CD2	2.78	0.60
1:A:215:ARG:CZ	1:A:252:GLU:OE2	2.49	0.60
1:C:351:SER:HB2	1:C:354:PRO:HD2	1.84	0.60
1:D:189:LEU:HD11	1:D:199:ILE:HD12	1.84	0.60
1:D:386:HIS:CD2	1:D:387:LEU:CD1	2.84	0.60
1:A:326:VAL:CG2	1:A:326:VAL:O	2.49	0.60
1:C:354:PRO:O	1:D:373:MSE:CE	2.50	0.60
1:A:499:LEU:CD2	1:A:515:ARG:HH11	2.14	0.60
1:D:427:LYS:HG3	1:D:436:ARG:HH11	1.67	0.60
1:D:453:LYS:O	1:D:457:THR:HG22	2.02	0.60
1:A:153:LEU:HD12	1:A:165:SER:O	2.02	0.60
1:A:363:VAL:HG13	1:B:363:VAL:CG1	2.27	0.60
1:A:171:TRP:CD1	1:A:172:GLY:H	2.19	0.59
1:B:82:HIS:O	1:B:84:ARG:N	2.36	0.59
1:B:351:SER:HB2	1:B:354:PRO:HD2	1.83	0.59
1:C:382:ARG:O	1:C:383:GLN:CB	2.50	0.59
1:A:353:ALA:HB3	1:A:354:PRO:HD2	1.84	0.59
1:C:10:ASN:OD1	1:C:46:ARG:NH1	2.35	0.59
1:C:248:THR:O	1:C:252:GLU:HB2	2.03	0.59
1:D:135:ARG:HG2	1:D:141:ILE:HD11	1.84	0.59
1:A:499:LEU:HD21	1:A:515:ARG:HH11	1.68	0.59
1:B:316:ASP:O	1:B:320:ARG:HG2	2.02	0.59
1:C:141:ILE:O	1:C:143:ALA:N	2.34	0.59
1:D:2:SER:O	1:D:3:GLN:HB2	2.01	0.59
1:B:102:ASP:CG	1:C:109:LYS:HZ1	2.09	0.59
1:C:142:ARG:O	1:C:144:GLY:N	2.35	0.59
1:C:349:ALA:O	1:C:351:SER:N	2.35	0.59
1:A:138:LEU:HD21	1:A:142:ARG:HH12	1.68	0.59
1:A:142:ARG:O	1:A:144:GLY:N	2.36	0.59
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.67	0.59
1:B:215:ARG:CZ	1:B:252:GLU:OE2	2.50	0.59
1:B:349:ALA:C	1:B:351:SER:N	2.54	0.59
1:D:35:LEU:HD12	1:D:51:PHE:HB3	1.85	0.59
1:B:27:ILE:CD1	1:B:51:PHE:CE1	2.81	0.59
1:D:143:ALA:O	1:D:152:LYS:NZ	2.35	0.59
1:C:359:VAL:CG1	1:D:370:LEU:HD11	2.31	0.59
1:D:248:THR:O	1:D:252:GLU:HB2	2.02	0.59
1:D:534:GLY:O	1:D:535:SER:C	2.46	0.59
1:C:11:PHE:CE1	1:C:88:LEU:CD1	2.86	0.59
1:C:138:LEU:HD21	1:C:142:ARG:HH12	1.68	0.59
1:D:215:ARG:CZ	1:D:252:GLU:OE2	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:O	1:A:252:GLU:HB2	2.03	0.58
1:A:363:VAL:CG1	1:B:363:VAL:CG1	2.80	0.58
1:B:138:LEU:HD21	1:B:142:ARG:HH12	1.68	0.58
1:B:141:ILE:O	1:B:143:ALA:N	2.34	0.58
1:D:326:VAL:CG2	1:D:326:VAL:O	2.50	0.58
1:B:142:ARG:O	1:B:144:GLY:N	2.34	0.58
1:B:455:ALA:O	1:B:456:GLU:C	2.46	0.58
1:B:499:LEU:CD2	1:B:515:ARG:HH11	2.17	0.58
1:C:35:LEU:HD12	1:C:51:PHE:HB3	1.83	0.58
1:C:43:SER:O	1:C:81:GLU:HB2	2.04	0.58
1:D:445:ARG:HG3	1:D:445:ARG:NH1	2.10	0.58
1:A:4:LEU:HD12	1:A:52:VAL:HB	1.85	0.58
1:A:12:SER:HB2	1:A:87:ALA:HA	1.85	0.58
1:A:351:SER:HB2	1:A:354:PRO:HD2	1.85	0.58
1:B:153:LEU:HD22	1:B:153:LEU:H	1.68	0.58
1:B:248:THR:O	1:B:252:GLU:HB2	2.04	0.58
1:D:83:PRO:HA	1:D:145:GLU:OE1	2.03	0.58
1:A:376:GLN:HG2	1:A:395:ILE:HD13	1.85	0.58
1:A:453:LYS:O	1:A:457:THR:HG22	2.03	0.58
1:D:12:SER:HB2	1:D:87:ALA:HA	1.86	0.58
1:D:462:TRP:HB3	1:D:528:GLN:HG2	1.84	0.58
1:A:458:VAL:CG1	1:A:491:VAL:HG22	2.34	0.58
1:D:376:GLN:HG2	1:D:395:ILE:HD13	1.85	0.58
1:A:189:LEU:HD11	1:A:199:ILE:HD12	1.86	0.58
1:B:304:VAL:HG12	1:B:305:ASN:N	2.18	0.58
1:C:82:HIS:O	1:C:84:ARG:N	2.36	0.58
1:D:527:THR:O	1:D:531:LEU:HD23	2.03	0.58
1:A:13:GLU:HB2	1:A:46:ARG:C	2.28	0.58
1:B:216:LEU:HD21	1:B:252:GLU:HG2	1.85	0.58
1:B:254:ARG:HB3	1:B:254:ARG:HH11	1.69	0.58
1:B:2:SER:O	1:B:3:GLN:HB2	2.03	0.58
1:B:382:ARG:O	1:B:383:GLN:CB	2.52	0.58
1:D:9:PRO:HG2	1:D:49:TYR:HB2	1.86	0.58
1:D:138:LEU:HD21	1:D:142:ARG:HH12	1.69	0.58
1:B:462:TRP:HB3	1:B:528:GLN:HG2	1.86	0.57
1:C:15:ASN:O	1:C:16:ASN:CB	2.49	0.57
1:A:427:LYS:CE	1:A:436:ARG:HH12	2.04	0.57
1:B:373:MSE:O	1:B:373:MSE:HG2	1.95	0.57
1:D:499:LEU:HD21	1:D:515:ARG:HH11	1.69	0.57
1:A:254:ARG:HH11	1:A:254:ARG:HB3	1.69	0.57
1:C:189:LEU:HD11	1:C:199:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD12	1:B:51:PHE:HB3	1.84	0.57
1:B:143:ALA:O	1:B:152:LYS:NZ	2.38	0.57
1:D:4:LEU:HD12	1:D:52:VAL:HB	1.86	0.57
1:C:2:SER:O	1:C:3:GLN:HB2	2.03	0.57
1:C:458:VAL:CG1	1:C:491:VAL:HG22	2.27	0.57
1:D:142:ARG:O	1:D:144:GLY:N	2.37	0.57
1:A:9:PRO:HG2	1:A:49:TYR:HB2	1.86	0.57
1:A:462:TRP:HB3	1:A:528:GLN:HG2	1.85	0.57
1:C:4:LEU:HD23	1:C:97:ARG:NH2	2.19	0.57
1:C:127:GLY:C	1:C:129:ALA:H	2.11	0.57
1:A:143:ALA:O	1:A:152:LYS:NZ	2.37	0.57
1:A:285:TYR:O	1:A:289:GLU:HB2	2.04	0.57
1:A:343:PHE:O	1:A:346:GLU:HB3	2.05	0.57
1:D:458:VAL:CG1	1:D:491:VAL:HG22	2.34	0.57
1:A:349:ALA:C	1:A:351:SER:N	2.54	0.57
1:B:149:LEU:HD22	1:B:153:LEU:HB3	1.86	0.57
1:A:510:PHE:C	1:A:510:PHE:CD2	2.83	0.57
1:B:10:ASN:OD1	1:B:46:ARG:NH1	2.38	0.57
1:B:376:GLN:HG2	1:B:395:ILE:HD13	1.87	0.57
1:C:4:LEU:HB3	1:C:96:VAL:HB	1.87	0.57
1:C:135:ARG:HG3	1:C:135:ARG:HH11	1.68	0.57
1:C:143:ALA:O	1:C:152:LYS:NZ	2.38	0.57
1:D:344:VAL:HG22	1:D:345:ARG:HG2	1.85	0.57
1:D:458:VAL:CG2	1:D:487:LEU:HD23	2.34	0.57
1:A:478:SER:OG	1:A:479:ASP:N	2.34	0.56
1:A:527:THR:O	1:A:531:LEU:HD23	2.05	0.56
1:B:13:GLU:H	1:B:46:ARG:HA	1.70	0.56
1:A:83:PRO:HA	1:A:145:GLU:OE1	2.04	0.56
1:A:141:ILE:HG21	1:A:175:VAL:HG11	1.88	0.56
1:A:326:VAL:O	1:A:326:VAL:HG22	2.05	0.56
1:B:11:PHE:CE1	1:B:88:LEU:CD1	2.88	0.56
1:B:425:LEU:CD2	1:B:426:PRO:HD2	2.23	0.56
1:C:487:LEU:O	1:C:491:VAL:HG23	2.04	0.56
1:C:517:ARG:O	1:C:520:SER:OG	2.23	0.56
1:A:149:LEU:CB	1:A:153:LEU:HD23	2.36	0.56
1:C:376:GLN:HG2	1:C:395:ILE:HD13	1.88	0.56
1:D:191:SER:HB2	1:D:195:GLN:OE1	2.06	0.56
1:C:12:SER:HB2	1:C:87:ALA:HA	1.88	0.56
1:C:348:GLY:HA2	1:D:373:MSE:HB2	1.88	0.56
1:B:30:THR:HG21	1:B:61:GLY:N	2.21	0.56
1:D:498:VAL:HG12	1:D:502:LEU:CD1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:LEU:CD2	1:D:515:ARG:HH11	2.19	0.56
1:B:153:LEU:N	1:B:153:LEU:CD2	2.68	0.56
1:C:13:GLU:HB2	1:C:46:ARG:C	2.31	0.56
1:C:390:THR:HG22	1:C:393:ARG:NH2	2.17	0.56
1:B:4:LEU:HB3	1:B:96:VAL:HB	1.87	0.56
1:B:43:SER:O	1:B:81:GLU:HB2	2.06	0.56
1:B:344:VAL:HG22	1:B:345:ARG:HG2	1.86	0.56
1:A:304:VAL:HG12	1:A:305:ASN:N	2.20	0.56
1:A:455:ALA:O	1:A:456:GLU:C	2.49	0.56
1:A:36:LEU:HD22	1:A:325:LEU:HD22	1.87	0.56
1:A:428:ASN:H	1:A:433:ARG:HB2	1.71	0.55
1:B:4:LEU:HD12	1:B:52:VAL:HB	1.88	0.55
1:B:498:VAL:HG12	1:B:502:LEU:CD1	2.36	0.55
1:C:111:PHE:HD2	1:C:176:THR:HG1	1.52	0.55
1:B:390:THR:HG22	1:B:393:ARG:NH2	2.18	0.55
1:C:326:VAL:O	1:C:326:VAL:CG2	2.53	0.55
1:D:36:LEU:HD22	1:D:325:LEU:HD22	1.88	0.55
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.70	0.55
1:A:141:ILE:O	1:A:143:ALA:N	2.38	0.55
1:C:4:LEU:HD12	1:C:52:VAL:HB	1.89	0.55
1:D:15:ASN:O	1:D:16:ASN:CB	2.49	0.55
1:A:349:ALA:O	1:A:351:SER:N	2.39	0.55
1:A:492:PHE:CD2	1:A:522:LEU:HD11	2.42	0.55
1:B:499:LEU:HD21	1:B:515:ARG:HH11	1.71	0.55
1:A:517:ARG:O	1:A:520:SER:OG	2.24	0.55
1:B:109:LYS:HZ1	1:C:102:ASP:CG	2.15	0.55
1:B:111:PHE:HD2	1:B:176:THR:HG1	1.54	0.55
1:D:141:ILE:O	1:D:143:ALA:N	2.38	0.55
1:D:353:ALA:HB3	1:D:354:PRO:HD2	1.87	0.55
1:B:4:LEU:HD23	1:B:97:ARG:NH2	2.21	0.55
1:B:76:ARG:NH2	1:B:169:PRO:CB	2.69	0.55
1:C:510:PHE:C	1:C:510:PHE:CD2	2.85	0.55
1:C:534:GLY:O	1:C:535:SER:C	2.49	0.55
1:A:124:TYR:HD2	1:A:160:PRO:HA	1.71	0.55
1:B:8:VAL:HG22	1:B:50:THR:HG23	1.89	0.55
1:B:216:LEU:HD13	1:B:249:VAL:HG22	1.89	0.55
1:D:4:LEU:HB3	1:D:96:VAL:HB	1.89	0.55
1:A:498:VAL:HG12	1:A:502:LEU:CD1	2.36	0.55
1:C:138:LEU:N	1:C:139:PRO:HD2	2.22	0.55
1:A:84:ARG:O	1:A:145:GLU:HB2	2.06	0.55
1:B:176:THR:HG22	1:B:177:GLY:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:ARG:CG	1:D:445:ARG:NH1	2.60	0.55
1:A:27:ILE:CD1	1:A:51:PHE:CE1	2.81	0.55
1:B:124:TYR:HD2	1:B:160:PRO:HA	1.72	0.55
1:C:455:ALA:O	1:C:456:GLU:C	2.48	0.55
1:D:84:ARG:O	1:D:145:GLU:HB2	2.07	0.55
1:D:428:ASN:H	1:D:433:ARG:HB2	1.72	0.55
1:B:343:PHE:O	1:B:347:VAL:HG13	2.07	0.54
1:B:510:PHE:C	1:B:510:PHE:CD2	2.85	0.54
1:C:76:ARG:NH2	1:C:169:PRO:CB	2.70	0.54
1:C:425:LEU:CD2	1:C:426:PRO:HD2	2.24	0.54
1:C:477:LEU:O	1:C:481:GLN:HG3	2.07	0.54
1:D:390:THR:HG22	1:D:393:ARG:NH2	2.17	0.54
1:A:359:VAL:HG11	1:B:370:LEU:HD11	1.88	0.54
1:C:124:TYR:HD2	1:C:160:PRO:HA	1.72	0.54
1:C:215:ARG:NH2	1:C:252:GLU:OE2	2.39	0.54
1:C:141:ILE:HG21	1:C:175:VAL:HG11	1.88	0.54
1:C:499:LEU:HD21	1:C:515:ARG:HH11	1.72	0.54
1:D:510:PHE:C	1:D:510:PHE:CD2	2.85	0.54
1:A:10:ASN:OD1	1:A:46:ARG:NH1	2.39	0.54
1:B:12:SER:HB2	1:B:87:ALA:HA	1.89	0.54
1:B:141:ILE:HG21	1:B:175:VAL:HG11	1.89	0.54
1:C:216:LEU:HD21	1:C:252:GLU:HG2	1.89	0.54
1:C:498:VAL:HG12	1:C:502:LEU:CD1	2.36	0.54
1:D:76:ARG:NH2	1:D:169:PRO:CB	2.70	0.54
1:A:148:ALA:H	1:A:150:PRO:HD2	1.73	0.54
1:B:143:ALA:HB1	1:B:152:LYS:NZ	2.23	0.54
1:D:4:LEU:HD23	1:D:97:ARG:NH2	2.23	0.54
1:D:125:LEU:O	1:D:130:ALA:HB2	2.07	0.54
1:B:149:LEU:N	1:B:150:PRO:HD2	2.23	0.54
1:B:445:ARG:HG3	1:B:445:ARG:NH1	2.11	0.54
1:C:323:GLU:N	1:C:323:GLU:OE1	2.41	0.54
1:D:10:ASN:OD1	1:D:46:ARG:NH1	2.41	0.54
1:D:531:LEU:HD23	1:D:531:LEU:N	2.05	0.54
1:A:215:ARG:NH2	1:A:252:GLU:OE2	2.40	0.54
1:B:380:GLY:O	1:B:381:ARG:C	2.51	0.54
1:C:30:THR:HG21	1:C:61:GLY:N	2.22	0.54
1:C:83:PRO:HA	1:C:145:GLU:OE1	2.08	0.54
1:C:326:VAL:O	1:C:326:VAL:HG22	2.07	0.54
1:D:30:THR:HG21	1:D:61:GLY:N	2.23	0.54
1:D:141:ILE:HG21	1:D:175:VAL:HG11	1.89	0.54
1:D:326:VAL:O	1:D:326:VAL:HG22	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:HB2	1:A:195:GLN:OE1	2.07	0.54
1:C:125:LEU:O	1:C:130:ALA:HB2	2.08	0.54
1:D:143:ALA:HB1	1:D:152:LYS:NZ	2.23	0.54
1:A:531:LEU:HD23	1:A:531:LEU:N	2.06	0.53
1:B:527:THR:O	1:B:531:LEU:HD23	2.08	0.53
1:C:143:ALA:HB1	1:C:152:LYS:NZ	2.23	0.53
1:D:8:VAL:HG22	1:D:50:THR:HG23	1.90	0.53
1:D:382:ARG:HG2	1:D:383:GLN:N	2.23	0.53
1:D:427:LYS:CE	1:D:436:ARG:HH12	2.05	0.53
1:A:510:PHE:C	1:A:510:PHE:HD2	2.16	0.53
1:B:349:ALA:O	1:B:351:SER:N	2.42	0.53
1:A:4:LEU:HB3	1:A:96:VAL:HB	1.89	0.53
1:A:30:THR:HG21	1:A:61:GLY:N	2.23	0.53
1:A:125:LEU:O	1:A:130:ALA:HB2	2.08	0.53
1:C:345:ARG:HH21	1:D:406:THR:CB	2.18	0.53
1:D:304:VAL:HG12	1:D:305:ASN:N	2.22	0.53
1:B:138:LEU:N	1:B:139:PRO:HD2	2.22	0.53
1:D:215:ARG:NH2	1:D:252:GLU:OE2	2.40	0.53
1:D:343:PHE:O	1:D:347:VAL:HG13	2.09	0.53
1:B:36:LEU:HD22	1:B:325:LEU:HD22	1.91	0.53
1:C:148:ALA:H	1:C:150:PRO:HD2	1.72	0.53
1:A:127:GLY:C	1:A:129:ALA:N	2.67	0.53
1:B:427:LYS:CE	1:B:436:ARG:HH12	2.03	0.53
1:A:143:ALA:HB1	1:A:152:LYS:NZ	2.23	0.53
1:C:124:TYR:CD2	1:C:160:PRO:HA	2.44	0.53
1:D:11:PHE:CZ	1:D:88:LEU:CD1	2.90	0.53
1:D:43:SER:O	1:D:81:GLU:HB2	2.09	0.53
1:A:124:TYR:CD2	1:A:160:PRO:HA	2.44	0.53
1:A:149:LEU:N	1:A:150:PRO:HD2	2.24	0.53
1:B:124:TYR:CD2	1:B:160:PRO:HA	2.44	0.53
1:D:349:ALA:C	1:D:351:SER:N	2.59	0.53
1:D:477:LEU:O	1:D:481:GLN:HG3	2.08	0.53
1:B:83:PRO:HA	1:B:145:GLU:OE1	2.09	0.52
1:D:323:GLU:OE1	1:D:323:GLU:N	2.41	0.52
1:B:428:ASN:H	1:B:433:ARG:HB2	1.74	0.52
1:D:149:LEU:N	1:D:150:PRO:HD2	2.24	0.52
1:D:487:LEU:O	1:D:491:VAL:HG23	2.09	0.52
1:A:353:ALA:HB3	1:A:354:PRO:CD	2.38	0.52
1:B:125:LEU:O	1:B:130:ALA:HB2	2.09	0.52
1:B:527:THR:O	1:B:530:ALA:HB3	2.09	0.52
1:C:36:LEU:HD22	1:C:325:LEU:HD22	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:PHE:C	1:C:510:PHE:HD2	2.17	0.52
1:D:13:GLU:HB2	1:D:46:ARG:C	2.33	0.52
1:A:138:LEU:N	1:A:139:PRO:HD2	2.25	0.52
1:A:445:ARG:CG	1:A:445:ARG:NH1	2.61	0.52
1:B:126:TYR:O	1:B:129:ALA:HB3	2.10	0.52
1:C:17:GLN:OE1	1:C:17:GLN:HA	2.09	0.52
1:C:531:LEU:H	1:C:531:LEU:CD2	2.06	0.52
1:A:8:VAL:HG22	1:A:50:THR:HG23	1.92	0.52
1:B:326:VAL:CG2	1:B:326:VAL:O	2.57	0.52
1:C:8:VAL:HG22	1:C:50:THR:HG23	1.92	0.52
1:C:149:LEU:N	1:C:150:PRO:HD2	2.24	0.52
1:D:527:THR:O	1:D:530:ALA:HB3	2.10	0.52
1:A:445:ARG:HG3	1:A:445:ARG:NH1	2.12	0.52
1:A:487:LEU:O	1:A:491:VAL:HG23	2.09	0.52
1:B:153:LEU:H	1:B:153:LEU:CD2	2.22	0.52
1:B:517:ARG:O	1:B:520:SER:OG	2.28	0.52
1:A:76:ARG:NH2	1:A:169:PRO:CB	2.71	0.52
1:B:382:ARG:HA	1:B:385:ASP:OD1	2.09	0.52
1:D:425:LEU:CD2	1:D:426:PRO:HD2	2.26	0.52
1:B:506:THR:O	1:B:507:ASP:HB2	2.10	0.52
1:C:13:GLU:HG2	1:C:15:ASN:CA	2.40	0.52
1:C:36:LEU:HD22	1:C:325:LEU:CD2	2.40	0.52
1:D:124:TYR:HD2	1:D:160:PRO:HA	1.74	0.52
1:B:176:THR:HG23	1:B:177:GLY:H	1.75	0.52
1:D:148:ALA:H	1:D:150:PRO:HD2	1.72	0.52
1:A:11:PHE:CZ	1:A:88:LEU:CD1	2.93	0.52
1:A:43:SER:O	1:A:81:GLU:HB2	2.10	0.52
1:A:176:THR:HG22	1:A:177:GLY:N	2.25	0.52
1:B:510:PHE:C	1:B:510:PHE:HD2	2.18	0.52
1:C:216:LEU:HD13	1:C:249:VAL:HG22	1.91	0.52
1:C:499:LEU:CD2	1:C:515:ARG:HH11	2.22	0.52
1:C:13:GLU:HG2	1:C:15:ASN:H	1.75	0.51
1:D:13:GLU:OE1	1:D:45:ASN:HA	2.10	0.51
1:D:227:GLU:OE1	1:D:227:GLU:CA	2.50	0.51
1:A:176:THR:HG23	1:A:177:GLY:H	1.76	0.51
1:D:27:ILE:CD1	1:D:51:PHE:CE1	2.87	0.51
1:D:123:VAL:HG13	1:D:162:PHE:HB2	1.92	0.51
1:A:265:VAL:HG23	1:A:265:VAL:O	2.10	0.51
1:A:506:THR:O	1:A:507:ASP:HB2	2.11	0.51
1:B:148:ALA:H	1:B:150:PRO:HD2	1.73	0.51
1:C:84:ARG:O	1:C:145:GLU:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:O	1:B:145:GLU:HB2	2.10	0.51
1:B:353:ALA:HB3	1:B:354:PRO:HD2	1.92	0.51
1:B:476:CYS:O	1:B:477:LEU:C	2.54	0.51
1:A:4:LEU:HD23	1:A:97:ARG:NH2	2.26	0.51
1:B:382:ARG:HG2	1:B:383:GLN:N	2.25	0.51
1:C:396:PRO:HB2	1:C:397:PRO:HD2	1.92	0.51
1:D:124:TYR:CD2	1:D:160:PRO:HA	2.46	0.51
1:D:129:ALA:O	1:D:130:ALA:C	2.53	0.51
1:D:216:LEU:HD13	1:D:249:VAL:HG22	1.92	0.51
1:A:84:ARG:O	1:A:145:GLU:CB	2.59	0.51
1:A:378:THR:HG22	1:A:378:THR:O	2.11	0.51
1:B:378:THR:O	1:B:378:THR:HG22	2.10	0.51
1:B:487:LEU:O	1:B:491:VAL:HG23	2.10	0.51
1:C:382:ARG:HA	1:C:385:ASP:OD1	2.10	0.51
1:C:528:GLN:O	1:C:532:VAL:HG23	2.11	0.51
1:A:123:VAL:HG13	1:A:162:PHE:HB2	1.93	0.51
1:A:376:GLN:HB3	1:B:350:ARG:HD2	1.91	0.51
1:C:76:ARG:CZ	1:C:169:PRO:CB	2.89	0.51
1:D:380:GLY:O	1:D:381:ARG:C	2.53	0.51
1:D:455:ALA:O	1:D:456:GLU:C	2.51	0.51
1:B:296:GLU:O	1:B:297:GLU:C	2.51	0.51
1:B:534:GLY:O	1:B:535:SER:C	2.52	0.51
1:C:350:ARG:HD2	1:D:376:GLN:O	2.11	0.51
1:C:380:GLY:O	1:C:381:ARG:C	2.53	0.51
1:C:382:ARG:HG2	1:C:383:GLN:N	2.25	0.51
1:C:13:GLU:HB3	1:C:45:ASN:C	2.36	0.51
1:C:304:VAL:HG12	1:C:305:ASN:N	2.27	0.51
1:C:444:LEU:HD11	1:C:504:ASP:HB2	1.93	0.51
1:D:127:GLY:C	1:D:129:ALA:N	2.68	0.51
1:D:149:LEU:CA	1:D:153:LEU:HD12	2.40	0.51
1:A:249:VAL:HG12	1:A:250:TYR:N	2.25	0.50
1:A:382:ARG:HG2	1:A:383:GLN:N	2.25	0.50
1:B:191:SER:HB2	1:B:195:GLN:OE1	2.10	0.50
1:D:97:ARG:HH21	1:D:328:ASP:HB3	1.74	0.50
1:B:410:ASP:O	1:B:411:ALA:C	2.53	0.50
1:C:129:ALA:O	1:C:130:ALA:C	2.54	0.50
1:C:373:MSE:O	1:C:373:MSE:HG2	2.03	0.50
1:A:373:MSE:HB2	1:B:348:GLY:HA2	1.93	0.50
1:B:76:ARG:CZ	1:B:169:PRO:CB	2.89	0.50
1:B:395:ILE:N	1:B:396:PRO:CD	2.74	0.50
1:C:11:PHE:CZ	1:C:88:LEU:CD1	2.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:O	1:C:64:SER:N	2.35	0.50
1:C:428:ASN:H	1:C:433:ARG:HB2	1.76	0.50
1:D:192:THR:HG22	1:D:195:GLN:OE1	2.10	0.50
1:A:379:TYR:CG	1:A:380:GLY:N	2.80	0.50
1:B:444:LEU:HD11	1:B:504:ASP:HB2	1.93	0.50
1:C:478:SER:OG	1:C:479:ASP:N	2.43	0.50
1:D:73:ILE:HG21	1:D:75:MSE:HE3	1.93	0.50
1:D:353:ALA:HB3	1:D:354:PRO:CD	2.41	0.50
1:A:25:GLN:O	1:A:28:SER:N	2.45	0.50
1:C:378:THR:HG22	1:C:378:THR:O	2.11	0.50
1:A:126:TYR:O	1:A:129:ALA:HB3	2.12	0.50
1:A:425:LEU:CD2	1:A:426:PRO:HD2	2.27	0.50
1:D:84:ARG:O	1:D:145:GLU:CB	2.59	0.50
1:D:138:LEU:N	1:D:139:PRO:HD2	2.27	0.50
1:D:454:LEU:HG	1:D:494:ALA:HB2	1.94	0.50
1:D:510:PHE:C	1:D:510:PHE:HD2	2.18	0.50
1:A:15:ASN:O	1:A:16:ASN:CB	2.48	0.50
1:B:127:GLY:C	1:B:129:ALA:N	2.70	0.50
1:B:326:VAL:O	1:B:326:VAL:HG22	2.12	0.50
1:C:527:THR:O	1:C:531:LEU:HD23	2.11	0.50
1:D:76:ARG:CZ	1:D:169:PRO:CB	2.90	0.50
1:A:73:ILE:HG21	1:A:75:MSE:HE3	1.92	0.50
1:B:192:THR:HG22	1:B:195:GLN:OE1	2.10	0.50
1:C:383:GLN:HG3	1:C:384:PHE:N	2.27	0.50
1:D:530:ALA:O	1:D:533:LEU:HB2	2.12	0.50
1:B:36:LEU:HD22	1:B:325:LEU:CD2	2.41	0.50
1:C:153:LEU:HD13	1:C:165:SER:O	2.12	0.50
1:D:506:THR:O	1:D:507:ASP:HB2	2.12	0.50
1:A:531:LEU:O	1:A:532:VAL:C	2.55	0.49
1:B:323:GLU:OE1	1:B:323:GLU:N	2.44	0.49
1:C:395:ILE:N	1:C:396:PRO:CD	2.75	0.49
1:A:13:GLU:HG2	1:A:15:ASN:CA	2.41	0.49
1:C:506:THR:O	1:C:507:ASP:HB2	2.11	0.49
1:B:17:GLN:HA	1:B:17:GLN:OE1	2.11	0.49
1:B:383:GLN:HG3	1:B:384:PHE:N	2.26	0.49
1:D:25:GLN:O	1:D:28:SER:N	2.45	0.49
1:D:176:THR:HG22	1:D:177:GLY:N	2.27	0.49
1:B:129:ALA:O	1:B:130:ALA:C	2.55	0.49
1:A:97:ARG:CZ	1:A:328:ASP:HB3	2.42	0.49
1:B:60:GLU:O	1:B:64:SER:N	2.34	0.49
1:B:97:ARG:HH21	1:B:328:ASP:HB3	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:TYR:HD1	1:B:175:VAL:HG12	1.76	0.49
1:D:247:HIS:HD2	1:D:281:ALA:HA	1.77	0.49
1:A:54:GLN:HB2	1:A:57:CYS:SG	2.52	0.49
1:A:76:ARG:CZ	1:A:169:PRO:CB	2.90	0.49
1:A:537:GLU:O	1:A:540:LYS:HB2	2.13	0.49
1:B:215:ARG:NH2	1:B:252:GLU:OE2	2.44	0.49
1:B:379:TYR:CG	1:B:380:GLY:N	2.81	0.49
1:C:353:ALA:HB3	1:C:354:PRO:HD2	1.93	0.49
1:C:448:VAL:HG13	1:C:498:VAL:HG13	1.94	0.49
1:D:13:GLU:HB3	1:D:45:ASN:C	2.37	0.49
1:A:124:TYR:HD1	1:A:175:VAL:HG12	1.78	0.49
1:C:344:VAL:HG22	1:C:345:ARG:HG2	1.94	0.49
1:D:265:VAL:HG23	1:D:265:VAL:O	2.13	0.49
1:B:249:VAL:HG12	1:B:250:TYR:N	2.27	0.49
1:B:427:LYS:O	1:B:428:ASN:HB2	2.12	0.49
1:B:444:LEU:O	1:B:445:ARG:C	2.56	0.49
1:C:191:SER:HB2	1:C:195:GLN:OE1	2.13	0.49
1:C:247:HIS:HD2	1:C:281:ALA:HA	1.76	0.49
1:A:13:GLU:HG2	1:A:15:ASN:H	1.76	0.49
1:B:511:LYS:O	1:B:514:THR:N	2.46	0.49
1:C:370:LEU:HD11	1:D:359:VAL:HG11	1.95	0.49
1:A:323:GLU:OE1	1:A:323:GLU:N	2.42	0.48
1:B:477:LEU:O	1:B:481:GLN:HG3	2.13	0.48
1:C:124:TYR:HD1	1:C:175:VAL:HG12	1.77	0.48
1:D:303:VAL:HG22	1:D:303:VAL:O	2.12	0.48
1:A:353:ALA:CB	1:A:354:PRO:CD	2.91	0.48
1:A:527:THR:O	1:A:530:ALA:HB3	2.13	0.48
1:D:153:LEU:HD23	1:D:165:SER:C	2.35	0.48
1:A:345:ARG:HH21	1:B:406:THR:HB	1.77	0.48
1:C:192:THR:HG22	1:C:195:GLN:OE1	2.12	0.48
1:C:530:ALA:O	1:C:533:LEU:HB2	2.12	0.48
1:A:192:THR:HG22	1:A:195:GLN:OE1	2.13	0.48
1:A:383:GLN:N	1:A:385:ASP:OD1	2.47	0.48
1:B:149:LEU:O	1:B:153:LEU:HD22	2.13	0.48
1:B:530:ALA:O	1:B:533:LEU:HB2	2.13	0.48
1:C:126:TYR:O	1:C:129:ALA:HB3	2.13	0.48
1:C:427:LYS:O	1:C:428:ASN:HB2	2.13	0.48
1:B:383:GLN:N	1:B:385:ASP:OD1	2.46	0.48
1:C:176:THR:HG22	1:C:177:GLY:N	2.29	0.48
1:C:343:PHE:O	1:C:347:VAL:HG13	2.13	0.48
1:D:135:ARG:HH11	1:D:135:ARG:CG	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:O	1:D:531:LEU:CD2	2.60	0.48
1:A:84:ARG:HG2	1:A:85:MSE:N	2.28	0.48
1:A:374:VAL:HA	1:A:377:MSE:HB2	1.95	0.48
1:A:390:THR:CG2	1:A:393:ARG:HH21	2.19	0.48
1:A:410:ASP:O	1:A:413:ALA:N	2.46	0.48
1:B:13:GLU:HB3	1:B:46:ARG:HA	1.96	0.48
1:B:478:SER:OG	1:B:479:ASP:N	2.43	0.48
1:D:153:LEU:HD22	1:D:153:LEU:C	2.38	0.48
1:A:97:ARG:HH21	1:A:328:ASP:HB3	1.74	0.48
1:B:97:ARG:CZ	1:B:328:ASP:HB3	2.44	0.48
1:B:353:ALA:HB3	1:B:354:PRO:CD	2.44	0.48
1:C:84:ARG:O	1:C:145:GLU:CB	2.62	0.48
1:C:527:THR:O	1:C:530:ALA:HB3	2.14	0.48
1:D:13:GLU:HG2	1:D:15:ASN:CA	2.44	0.48
1:D:492:PHE:CD2	1:D:522:LEU:HD11	2.49	0.48
1:A:13:GLU:HB3	1:A:45:ASN:C	2.38	0.48
1:B:25:GLN:O	1:B:28:SER:N	2.47	0.48
1:C:13:GLU:C	1:C:15:ASN:H	2.21	0.48
1:D:379:TYR:CG	1:D:380:GLY:N	2.81	0.48
1:A:303:VAL:O	1:A:303:VAL:HG22	2.14	0.48
1:A:383:GLN:HG3	1:A:384:PHE:N	2.29	0.48
1:A:444:LEU:CD1	1:A:504:ASP:HB2	2.44	0.48
1:B:11:PHE:CZ	1:B:88:LEU:CD1	2.96	0.48
1:C:444:LEU:O	1:C:445:ARG:C	2.56	0.48
1:D:90:VAL:HG11	1:D:138:LEU:HD21	1.95	0.48
1:D:427:LYS:O	1:D:428:ASN:HB2	2.13	0.48
1:C:76:ARG:HH21	1:C:169:PRO:HB3	1.79	0.48
1:D:84:ARG:HG2	1:D:85:MSE:N	2.29	0.48
1:A:216:LEU:HD13	1:A:249:VAL:HG22	1.95	0.47
1:A:454:LEU:HG	1:A:494:ALA:HB2	1.96	0.47
1:A:530:ALA:O	1:A:533:LEU:HB2	2.14	0.47
1:B:10:ASN:HB2	1:B:90:VAL:O	2.14	0.47
1:C:27:ILE:CD1	1:C:51:PHE:CE1	2.83	0.47
1:C:127:GLY:C	1:C:129:ALA:N	2.71	0.47
1:D:76:ARG:NE	1:D:169:PRO:HB2	2.29	0.47
1:B:143:ALA:HB1	1:B:152:LYS:HZ3	1.79	0.47
1:C:13:GLU:HB2	1:C:46:ARG:CA	2.44	0.47
1:C:288:LYS:HG3	1:C:289:GLU:N	2.29	0.47
1:B:84:ARG:O	1:B:145:GLU:CB	2.63	0.47
1:B:528:GLN:O	1:B:532:VAL:HG23	2.15	0.47
1:D:97:ARG:CZ	1:D:328:ASP:HB3	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:GLN:HG3	1:D:384:PHE:N	2.26	0.47
1:A:350:ARG:HD2	1:B:376:GLN:HB3	1.95	0.47
1:A:380:GLY:O	1:A:381:ARG:C	2.58	0.47
1:D:126:TYR:O	1:D:129:ALA:HB3	2.14	0.47
1:A:90:VAL:HG11	1:A:138:LEU:HD21	1.96	0.47
1:A:370:LEU:CD1	1:B:359:VAL:HG11	2.36	0.47
1:A:463:PRO:O	1:A:466:GLN:HB3	2.13	0.47
1:B:343:PHE:O	1:B:346:GLU:HB3	2.14	0.47
1:C:171:TRP:CD1	1:C:172:GLY:N	2.83	0.47
1:C:425:LEU:O	1:C:426:PRO:C	2.58	0.47
1:A:17:GLN:OE1	1:A:17:GLN:HA	2.14	0.47
1:A:76:ARG:NE	1:A:169:PRO:HB2	2.29	0.47
1:A:153:LEU:CD1	1:A:165:SER:O	2.62	0.47
1:B:76:ARG:HH21	1:B:169:PRO:HB3	1.79	0.47
1:B:410:ASP:O	1:B:413:ALA:N	2.47	0.47
1:B:445:ARG:CG	1:B:445:ARG:NH1	2.62	0.47
1:C:90:VAL:HG11	1:C:138:LEU:HD21	1.96	0.47
1:C:97:ARG:HH21	1:C:328:ASP:HB3	1.79	0.47
1:C:406:THR:HB	1:D:345:ARG:HH21	1.79	0.47
1:D:60:GLU:O	1:D:64:SER:N	2.36	0.47
1:D:74:ASP:OD1	1:D:170:SER:HB3	2.15	0.47
1:D:124:TYR:HD1	1:D:175:VAL:HG12	1.78	0.47
1:D:378:THR:O	1:D:378:THR:HG22	2.14	0.47
1:B:90:VAL:HG11	1:B:138:LEU:HD21	1.96	0.47
1:B:176:THR:HG23	1:B:177:GLY:N	2.29	0.47
1:A:74:ASP:OD1	1:A:170:SER:HB3	2.14	0.47
1:A:443:GLY:O	1:A:444:LEU:C	2.58	0.47
1:B:347:VAL:HA	1:B:354:PRO:HG2	1.96	0.47
1:B:425:LEU:O	1:B:426:PRO:C	2.58	0.47
1:C:347:VAL:HA	1:C:354:PRO:HG2	1.96	0.47
1:A:395:ILE:N	1:A:396:PRO:CD	2.78	0.47
1:B:396:PRO:HB2	1:B:397:PRO:HD2	1.93	0.47
1:C:76:ARG:NE	1:C:169:PRO:HB2	2.29	0.47
1:D:176:THR:HG23	1:D:177:GLY:H	1.80	0.47
1:C:265:VAL:O	1:C:265:VAL:HG23	2.14	0.46
1:C:351:SER:O	1:C:351:SER:OG	2.32	0.46
1:D:76:ARG:HH21	1:D:169:PRO:HB3	1.79	0.46
1:D:94:ILE:HG22	1:D:179:ARG:O	2.15	0.46
1:D:426:PRO:O	1:D:427:LYS:CB	2.39	0.46
1:A:13:GLU:HB2	1:A:46:ARG:CA	2.45	0.46
1:A:60:GLU:O	1:A:64:SER:N	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:VAL:HG11	1:B:480:LEU:HD23	1.97	0.46
1:C:97:ARG:CZ	1:C:328:ASP:HB3	2.44	0.46
1:C:454:LEU:HG	1:C:494:ALA:HB2	1.97	0.46
1:C:10:ASN:HB2	1:C:90:VAL:O	2.15	0.46
1:D:288:LYS:HG3	1:D:289:GLU:N	2.30	0.46
1:B:76:ARG:NE	1:B:169:PRO:HB2	2.30	0.46
1:B:84:ARG:HG2	1:B:85:MSE:N	2.30	0.46
1:B:123:VAL:HG13	1:B:162:PHE:HB2	1.96	0.46
1:B:537:GLU:O	1:B:540:LYS:HB2	2.16	0.46
1:C:123:VAL:HG13	1:C:162:PHE:HB2	1.96	0.46
1:C:522:LEU:O	1:C:525:ALA:HB3	2.16	0.46
1:D:353:ALA:CB	1:D:354:PRO:CD	2.93	0.46
1:A:8:VAL:O	1:A:92:PRO:HD2	2.15	0.46
1:A:46:ARG:CZ	1:A:82:HIS:CD2	2.96	0.46
1:A:129:ALA:O	1:A:130:ALA:C	2.57	0.46
1:A:527:THR:O	1:A:531:LEU:CD2	2.64	0.46
1:D:349:ALA:O	1:D:351:SER:N	2.49	0.46
1:C:353:ALA:HB3	1:C:354:PRO:CD	2.46	0.46
1:C:383:GLN:N	1:C:385:ASP:OD1	2.45	0.46
1:C:537:GLU:O	1:C:540:LYS:HB2	2.16	0.46
1:D:387:LEU:CD2	1:D:471:CYS:SG	3.04	0.46
1:A:448:VAL:O	1:A:451:PRO:HD2	2.16	0.46
1:C:84:ARG:HG2	1:C:85:MSE:N	2.30	0.46
1:D:131:GLN:HE21	1:D:131:GLN:HB2	1.58	0.46
1:A:111:PHE:CD2	1:A:176:THR:OG1	2.67	0.46
1:A:176:THR:HG23	1:A:177:GLY:N	2.30	0.46
1:A:347:VAL:HA	1:A:354:PRO:HG2	1.98	0.46
1:A:427:LYS:O	1:A:428:ASN:HB2	2.15	0.46
1:B:132:MSE:HA	1:B:133:PRO:HD3	1.76	0.46
1:C:4:LEU:HD23	1:C:97:ARG:HH21	1.80	0.46
1:C:379:TYR:CG	1:C:380:GLY:N	2.84	0.46
1:D:517:ARG:O	1:D:520:SER:OG	2.33	0.46
1:A:184:ALA:HB3	1:A:270:VAL:HB	1.98	0.46
1:A:343:PHE:O	1:A:347:VAL:HG13	2.15	0.46
1:B:167:PHE:HD1	1:B:168:VAL:N	2.14	0.46
1:B:530:ALA:O	1:B:533:LEU:N	2.48	0.46
1:C:281:ALA:O	1:C:284:PHE:HB3	2.16	0.46
1:C:410:ASP:O	1:C:411:ALA:C	2.59	0.46
1:D:334:SER:OG	1:D:336:LEU:HB2	2.15	0.46
1:D:463:PRO:O	1:D:466:GLN:HB3	2.16	0.46
1:D:498:VAL:O	1:D:499:LEU:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:CYS:O	1:A:477:LEU:C	2.59	0.46
1:A:531:LEU:O	1:A:535:SER:N	2.44	0.46
1:B:13:GLU:HB3	1:B:46:ARG:CA	2.46	0.46
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.80	0.46
1:B:531:LEU:O	1:B:535:SER:N	2.44	0.46
1:D:17:GLN:HA	1:D:17:GLN:OE1	2.15	0.46
1:D:249:VAL:HG12	1:D:250:TYR:N	2.29	0.46
1:A:10:ASN:HB2	1:A:90:VAL:O	2.16	0.45
1:A:334:SER:OG	1:A:336:LEU:HB2	2.16	0.45
1:B:171:TRP:CD1	1:B:172:GLY:N	2.82	0.45
1:B:265:VAL:HG23	1:B:265:VAL:O	2.16	0.45
1:C:167:PHE:HD1	1:C:168:VAL:N	2.14	0.45
1:C:296:GLU:O	1:C:297:GLU:C	2.59	0.45
1:C:343:PHE:O	1:C:346:GLU:HB3	2.17	0.45
1:D:13:GLU:C	1:D:15:ASN:H	2.24	0.45
1:D:448:VAL:HG13	1:D:498:VAL:HG13	1.99	0.45
1:D:531:LEU:O	1:D:532:VAL:C	2.57	0.45
1:B:444:LEU:CD1	1:B:504:ASP:HB2	2.47	0.45
1:C:303:VAL:O	1:C:303:VAL:HG22	2.16	0.45
1:D:143:ALA:HB1	1:D:152:LYS:HZ3	1.80	0.45
1:A:498:VAL:O	1:A:499:LEU:C	2.59	0.45
1:B:247:HIS:HD2	1:B:281:ALA:HA	1.77	0.45
1:B:339:SER:O	1:B:340:LEU:C	2.59	0.45
1:C:227:GLU:OE1	1:C:227:GLU:CA	2.58	0.45
1:D:537:GLU:O	1:D:540:LYS:HB2	2.16	0.45
1:A:444:LEU:O	1:A:445:ARG:C	2.57	0.45
1:C:90:VAL:HG23	1:C:92:PRO:HD3	1.99	0.45
1:C:337:ASP:OD1	1:D:341:ARG:NH1	2.28	0.45
1:C:448:VAL:O	1:C:451:PRO:HD2	2.16	0.45
1:D:10:ASN:HB2	1:D:90:VAL:O	2.17	0.45
1:D:524:GLU:O	1:D:528:GLN:HB2	2.16	0.45
1:A:74:ASP:HA	1:A:170:SER:CB	2.46	0.45
1:A:76:ARG:HH21	1:A:169:PRO:HB3	1.81	0.45
1:D:167:PHE:HD1	1:D:168:VAL:N	2.14	0.45
1:D:347:VAL:HA	1:D:354:PRO:HG2	1.99	0.45
1:A:354:PRO:O	1:B:373:MSE:HE1	2.17	0.45
1:A:410:ASP:O	1:A:411:ALA:C	2.59	0.45
1:B:450:VAL:HG22	1:B:451:PRO:HD3	1.99	0.45
1:D:410:ASP:O	1:D:413:ALA:N	2.49	0.45
1:D:444:LEU:CD1	1:D:504:ASP:HB2	2.47	0.45
1:A:184:ALA:CB	1:A:270:VAL:HB	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:O	1:A:297:GLU:C	2.59	0.45
1:A:373:MSE:O	1:A:373:MSE:HG2	2.08	0.45
1:B:12:SER:O	1:B:73:ILE:HD13	2.16	0.45
1:B:303:VAL:O	1:B:303:VAL:HG22	2.14	0.45
1:B:448:VAL:HG13	1:B:498:VAL:HG13	1.98	0.45
1:C:350:ARG:HD2	1:D:376:GLN:HB3	1.98	0.45
1:C:374:VAL:HG11	1:C:480:LEU:HD23	1.99	0.45
1:D:184:ALA:CB	1:D:270:VAL:HB	2.46	0.45
1:D:184:ALA:HB3	1:D:270:VAL:HB	1.99	0.45
1:A:86:GLY:HA3	1:A:173:ALA:O	2.16	0.45
1:A:89:ASP:HB3	1:A:90:VAL:H	1.64	0.45
1:C:476:CYS:O	1:C:477:LEU:C	2.60	0.45
1:D:395:ILE:N	1:D:396:PRO:CD	2.79	0.45
1:D:474:LEU:HD23	1:D:477:LEU:HD13	1.98	0.45
1:A:444:LEU:HD11	1:A:504:ASP:HB2	1.99	0.45
1:C:25:GLN:O	1:C:28:SER:N	2.49	0.45
1:D:425:LEU:O	1:D:426:PRO:C	2.60	0.45
1:A:127:GLY:O	1:A:129:ALA:N	2.50	0.45
1:B:94:ILE:HG22	1:B:179:ARG:O	2.17	0.45
1:C:23:ILE:O	1:C:27:ILE:HG22	2.17	0.45
1:C:179:ARG:HH12	1:C:182:LEU:HB3	1.82	0.45
1:C:445:ARG:CG	1:C:445:ARG:NH1	2.58	0.45
1:C:458:VAL:CG2	1:C:487:LEU:HD23	2.47	0.45
1:C:531:LEU:O	1:C:535:SER:N	2.42	0.45
1:D:531:LEU:O	1:D:535:SER:N	2.44	0.45
1:A:511:LYS:O	1:A:512:GLU:C	2.60	0.44
1:B:6:GLU:OE1	1:B:94:ILE:HG13	2.17	0.44
1:B:74:ASP:OD1	1:B:170:SER:HB3	2.17	0.44
1:D:444:LEU:HD11	1:D:504:ASP:HB2	1.99	0.44
1:A:167:PHE:HD1	1:A:168:VAL:N	2.15	0.44
1:A:396:PRO:O	1:A:397:PRO:C	2.58	0.44
1:B:111:PHE:CD2	1:B:176:THR:OG1	2.69	0.44
1:B:454:LEU:HG	1:B:494:ALA:HB2	1.98	0.44
1:C:179:ARG:NH1	1:C:182:LEU:HB3	2.32	0.44
1:D:129:ALA:O	1:D:130:ALA:O	2.35	0.44
1:D:383:GLN:N	1:D:385:ASP:OD1	2.47	0.44
1:A:73:ILE:CG2	1:A:75:MSE:HE3	2.47	0.44
1:A:382:ARG:HA	1:A:385:ASP:OD1	2.18	0.44
1:A:474:LEU:HD11	1:A:541:GLU:OE2	2.17	0.44
1:B:3:GLN:HA	1:B:3:GLN:OE1	2.17	0.44
1:B:307:LEU:O	1:B:308:GLY:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:VAL:O	1:B:499:LEU:C	2.58	0.44
1:C:249:VAL:HG12	1:C:250:TYR:N	2.32	0.44
1:A:462:TRP:HA	1:A:462:TRP:CE3	2.53	0.44
1:B:198:ARG:O	1:B:199:ILE:C	2.60	0.44
1:C:176:THR:HG23	1:C:177:GLY:H	1.81	0.44
1:C:379:TYR:CE1	1:C:388:ASP:OD2	2.70	0.44
1:C:539:ARG:O	1:C:541:GLU:N	2.51	0.44
1:A:12:SER:O	1:A:73:ILE:HD13	2.18	0.44
1:B:86:GLY:HA3	1:B:173:ALA:O	2.17	0.44
1:A:477:LEU:O	1:A:481:GLN:HG3	2.18	0.44
1:B:23:ILE:O	1:B:27:ILE:HG22	2.17	0.44
1:B:458:VAL:HA	1:B:461:LEU:HD22	2.00	0.44
1:C:461:LEU:N	1:C:461:LEU:CD1	2.79	0.44
1:D:8:VAL:O	1:D:92:PRO:HD2	2.16	0.44
1:D:198:ARG:HD3	1:D:260:LEU:HD11	2.00	0.44
1:D:373:MSE:O	1:D:373:MSE:HG2	2.09	0.44
1:A:492:PHE:CE2	1:A:522:LEU:HD11	2.53	0.44
1:B:281:ALA:O	1:B:284:PHE:HB3	2.17	0.44
1:B:443:GLY:O	1:B:444:LEU:C	2.60	0.44
1:B:492:PHE:CD2	1:B:522:LEU:HD11	2.53	0.44
1:C:6:GLU:OE1	1:C:94:ILE:HG13	2.17	0.44
1:D:46:ARG:CZ	1:D:82:HIS:CD2	2.95	0.44
1:D:86:GLY:HA3	1:D:173:ALA:O	2.17	0.44
1:D:171:TRP:CD1	1:D:172:GLY:N	2.84	0.44
1:D:410:ASP:O	1:D:411:ALA:C	2.61	0.44
1:A:247:HIS:HD2	1:A:281:ALA:HA	1.79	0.44
1:B:149:LEU:O	1:B:153:LEU:CD2	2.66	0.44
1:C:73:ILE:HG21	1:C:75:MSE:HE3	1.99	0.44
1:D:74:ASP:HA	1:D:170:SER:CB	2.47	0.44
1:D:187:ILE:HD11	1:D:249:VAL:HG12	1.99	0.44
1:D:377:MSE:HE3	1:D:377:MSE:HA	2.00	0.44
1:A:13:GLU:C	1:A:15:ASN:H	2.25	0.44
1:A:128:GLU:HB2	1:A:178:ALA:O	2.17	0.44
1:A:171:TRP:CD1	1:A:172:GLY:N	2.85	0.44
1:A:336:LEU:O	1:B:339:SER:HB2	2.18	0.44
1:B:25:GLN:O	1:B:29:GLN:N	2.50	0.44
1:B:184:ALA:CB	1:B:270:VAL:HB	2.48	0.44
1:C:74:ASP:OD1	1:C:170:SER:HB3	2.18	0.44
1:C:86:GLY:HA3	1:C:173:ALA:O	2.18	0.44
1:C:94:ILE:HG22	1:C:179:ARG:O	2.18	0.44
1:D:128:GLU:HB2	1:D:178:ALA:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:VAL:HG11	1:D:480:LEU:HD23	2.00	0.44
1:D:443:GLY:O	1:D:444:LEU:C	2.61	0.44
1:D:511:LYS:O	1:D:512:GLU:C	2.61	0.44
1:A:341:ARG:NH1	1:B:337:ASP:OD1	2.34	0.43
1:A:493:GLY:HA2	1:B:482:VAL:HG22	2.00	0.43
1:B:8:VAL:O	1:B:92:PRO:HD2	2.18	0.43
1:B:15:ASN:O	1:B:16:ASN:CB	2.49	0.43
1:B:46:ARG:CZ	1:B:82:HIS:CD2	2.95	0.43
1:D:176:THR:HG23	1:D:177:GLY:N	2.33	0.43
1:A:288:LYS:HG3	1:A:289:GLU:N	2.33	0.43
1:A:425:LEU:O	1:A:426:PRO:C	2.61	0.43
1:B:276:LYS:HE2	1:B:280:ASP:OD1	2.19	0.43
1:D:127:GLY:O	1:D:129:ALA:N	2.52	0.43
1:B:4:LEU:HD23	1:B:97:ARG:HH21	1.82	0.43
1:C:13:GLU:HG2	1:C:15:ASN:HA	2.01	0.43
1:D:351:SER:O	1:D:351:SER:OG	2.35	0.43
1:A:458:VAL:HA	1:A:461:LEU:HD22	2.00	0.43
1:B:13:GLU:HG2	1:B:15:ASN:H	1.83	0.43
1:B:73:ILE:HG21	1:B:75:MSE:HE3	1.99	0.43
1:B:461:LEU:N	1:B:461:LEU:CD1	2.81	0.43
1:B:511:LYS:O	1:B:512:GLU:C	2.61	0.43
1:C:59:VAL:O	1:C:63:LEU:HG	2.18	0.43
1:C:511:LYS:O	1:C:512:GLU:C	2.62	0.43
1:D:3:GLN:HA	1:D:3:GLN:OE1	2.18	0.43
1:D:76:ARG:H	1:D:76:ARG:HG3	1.48	0.43
1:D:462:TRP:HA	1:D:462:TRP:CE3	2.54	0.43
1:B:288:LYS:HG3	1:B:289:GLU:N	2.33	0.43
1:C:113:GLN:O	1:C:117:GLU:CG	2.57	0.43
1:C:531:LEU:HD23	1:C:531:LEU:N	2.12	0.43
1:D:23:ILE:O	1:D:27:ILE:HG22	2.18	0.43
1:D:296:GLU:O	1:D:297:GLU:C	2.59	0.43
1:A:14:GLY:O	1:A:15:ASN:HB3	2.18	0.43
1:B:13:GLU:C	1:B:15:ASN:N	2.75	0.43
1:B:396:PRO:CB	1:B:397:PRO:CD	2.92	0.43
1:C:184:ALA:CB	1:C:270:VAL:HB	2.48	0.43
1:C:458:VAL:HA	1:C:461:LEU:HD22	2.00	0.43
1:B:385:ASP:C	1:B:387:LEU:H	2.26	0.43
1:C:443:GLY:O	1:C:444:LEU:C	2.61	0.43
1:C:482:VAL:HG22	1:D:493:GLY:HA2	2.01	0.43
1:D:111:PHE:CD2	1:D:176:THR:OG1	2.68	0.43
1:D:432:GLU:HG2	1:D:432:GLU:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:VAL:HG13	1:A:498:VAL:HG13	2.01	0.43
1:B:478:SER:HA	1:B:481:GLN:HE21	1.83	0.43
1:B:524:GLU:O	1:B:528:GLN:HB2	2.18	0.43
1:C:378:THR:OG1	1:C:473:ASN:N	2.47	0.43
1:D:382:ARG:HA	1:D:385:ASP:OD1	2.19	0.43
1:C:46:ARG:CZ	1:C:82:HIS:CD2	2.95	0.43
1:A:154:LYS:HB3	1:A:154:LYS:HE2	1.70	0.43
1:A:286:CYS:HA	1:A:291:LEU:CD1	2.49	0.43
1:A:477:LEU:O	1:A:478:SER:C	2.62	0.43
1:C:135:ARG:HH11	1:C:135:ARG:CG	2.31	0.43
1:D:12:SER:O	1:D:73:ILE:HD13	2.19	0.43
1:A:432:GLU:O	1:A:432:GLU:HG2	2.19	0.42
1:B:74:ASP:HA	1:B:170:SER:CB	2.49	0.42
1:C:3:GLN:OE1	1:C:3:GLN:HA	2.18	0.42
1:C:8:VAL:O	1:C:92:PRO:HD2	2.18	0.42
1:C:38:VAL:O	1:C:38:VAL:HG22	2.18	0.42
1:C:375:GLY:HA3	1:C:395:ILE:HG12	1.99	0.42
1:C:444:LEU:CD1	1:C:504:ASP:HB2	2.49	0.42
1:D:461:LEU:N	1:D:461:LEU:CD1	2.82	0.42
1:A:377:MSE:HA	1:A:377:MSE:CE	2.49	0.42
1:A:406:THR:CB	1:B:345:ARG:HH21	2.27	0.42
1:C:12:SER:HB3	1:C:75:MSE:HE1	2.00	0.42
1:D:36:LEU:HD22	1:D:325:LEU:CD2	2.49	0.42
1:A:317:PRO:C	1:A:319:GLU:H	2.27	0.42
1:A:375:GLY:HA3	1:A:395:ILE:HG12	2.00	0.42
1:A:524:GLU:O	1:A:528:GLN:HB2	2.19	0.42
1:B:12:SER:HB3	1:B:75:MSE:HE1	2.00	0.42
1:B:240:ASP:OD1	1:B:240:ASP:C	2.62	0.42
1:B:432:GLU:O	1:B:432:GLU:HG2	2.18	0.42
1:B:518:ILE:HD12	1:B:518:ILE:HA	1.89	0.42
1:D:13:GLU:CB	1:D:46:ARG:HA	2.50	0.42
1:A:94:ILE:HG22	1:A:179:ARG:O	2.19	0.42
1:B:312:LEU:HD23	1:B:312:LEU:HA	1.81	0.42
1:D:82:HIS:ND1	1:D:83:PRO:HD2	2.35	0.42
1:D:498:VAL:HG12	1:D:502:LEU:HD13	2.01	0.42
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.89	0.42
1:A:346:GLU:HG3	1:A:354:PRO:HG3	2.01	0.42
1:B:59:VAL:O	1:B:63:LEU:HG	2.19	0.42
1:C:187:ILE:HD11	1:C:249:VAL:HG12	2.01	0.42
1:C:531:LEU:O	1:C:532:VAL:C	2.63	0.42
1:D:73:ILE:CG2	1:D:75:MSE:HE3	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:OE1	1:A:3:GLN:HA	2.18	0.42
1:A:149:LEU:CD2	1:A:153:LEU:HB3	2.49	0.42
1:A:275:LEU:HG	1:A:279:LEU:HD12	2.01	0.42
1:B:520:SER:O	1:B:523:GLN:HB3	2.19	0.42
1:B:522:LEU:O	1:B:525:ALA:HB3	2.19	0.42
1:C:74:ASP:HA	1:C:170:SER:CB	2.49	0.42
1:C:82:HIS:ND1	1:C:83:PRO:HD2	2.35	0.42
1:C:275:LEU:HG	1:C:279:LEU:HD12	2.01	0.42
1:C:511:LYS:O	1:C:514:THR:N	2.53	0.42
1:C:524:GLU:O	1:C:528:GLN:HB2	2.19	0.42
1:D:149:LEU:HB3	1:D:153:LEU:HD12	2.00	0.42
1:A:36:LEU:HD22	1:A:325:LEU:CD2	2.50	0.42
1:A:90:VAL:HG12	1:A:138:LEU:HD11	2.01	0.42
1:B:113:GLN:HA	1:B:162:PHE:CD2	2.55	0.42
1:A:461:LEU:N	1:A:461:LEU:CD1	2.82	0.42
1:B:154:LYS:HE2	1:B:154:LYS:HB3	1.80	0.42
1:B:373:MSE:O	1:B:377:MSE:HB2	2.19	0.42
1:B:480:LEU:O	1:B:483:ALA:HB3	2.20	0.42
1:C:14:GLY:O	1:C:15:ASN:HB3	2.20	0.42
1:C:190:LEU:CB	1:C:263:PRO:HG2	2.47	0.42
1:C:339:SER:HB2	1:D:336:LEU:O	2.19	0.42
1:D:54:GLN:HB2	1:D:57:CYS:SG	2.60	0.42
1:D:343:PHE:O	1:D:346:GLU:HB3	2.20	0.42
1:D:472:GLY:O	1:D:473:ASN:C	2.62	0.42
1:A:13:GLU:CB	1:A:46:ARG:HA	2.50	0.42
1:A:344:VAL:HG21	1:B:406:THR:OG1	2.20	0.42
1:B:38:VAL:O	1:B:38:VAL:HG22	2.20	0.42
1:B:353:ALA:CB	1:B:354:PRO:CD	2.97	0.42
1:C:13:GLU:O	1:C:15:ASN:N	2.51	0.42
1:C:132:MSE:HA	1:C:133:PRO:HD3	1.76	0.42
1:C:334:SER:OG	1:C:336:LEU:HB2	2.19	0.42
1:D:444:LEU:O	1:D:445:ARG:C	2.62	0.42
1:A:23:ILE:O	1:A:27:ILE:HG22	2.19	0.42
1:B:155:GLN:C	1:B:157:GLU:N	2.77	0.42
1:B:275:LEU:HG	1:B:279:LEU:HD12	2.01	0.42
1:B:539:ARG:O	1:B:541:GLU:N	2.53	0.42
1:C:25:GLN:O	1:C:29:GLN:N	2.52	0.42
1:C:492:PHE:CD2	1:C:522:LEU:HD11	2.55	0.42
1:C:498:VAL:O	1:C:499:LEU:C	2.62	0.42
1:D:317:PRO:C	1:D:319:GLU:H	2.28	0.42
1:A:143:ALA:HB1	1:A:152:LYS:HZ2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLY:O	1:A:473:ASN:C	2.62	0.41
1:B:13:GLU:HG2	1:B:15:ASN:CA	2.50	0.41
1:B:184:ALA:HB3	1:B:270:VAL:HB	2.01	0.41
1:B:492:PHE:O	1:B:493:GLY:C	2.63	0.41
1:C:16:ASN:O	1:C:17:GLN:C	2.63	0.41
1:C:176:THR:HG23	1:C:177:GLY:N	2.34	0.41
1:C:454:LEU:HD12	1:C:454:LEU:C	2.44	0.41
1:D:4:LEU:HD23	1:D:97:ARG:HH21	1.85	0.41
1:D:25:GLN:O	1:D:29:GLN:N	2.51	0.41
1:D:335:LEU:C	1:D:337:ASP:N	2.78	0.41
1:B:119:LEU:O	1:B:120:ASN:CB	2.68	0.41
1:C:154:LYS:HB3	1:C:154:LYS:HE2	1.79	0.41
1:C:240:ASP:CG	1:C:243:VAL:HG23	2.45	0.41
1:C:353:ALA:CB	1:C:354:PRO:CD	2.98	0.41
1:C:390:THR:CG2	1:C:393:ARG:HH21	2.23	0.41
1:A:12:SER:HB3	1:A:75:MSE:HE1	2.02	0.41
1:A:376:GLN:O	1:B:350:ARG:HD2	2.20	0.41
1:B:82:HIS:ND1	1:B:83:PRO:HD2	2.34	0.41
1:C:254:ARG:HH11	1:C:254:ARG:CB	2.32	0.41
1:A:227:GLU:OE1	1:A:227:GLU:CA	2.54	0.41
1:B:13:GLU:OE1	1:B:45:ASN:HA	2.20	0.41
1:B:127:GLY:O	1:B:129:ALA:N	2.53	0.41
1:B:135:ARG:HH11	1:B:135:ARG:CG	2.29	0.41
1:C:13:GLU:C	1:C:15:ASN:N	2.79	0.41
1:C:129:ALA:O	1:C:130:ALA:O	2.39	0.41
1:C:474:LEU:HD23	1:C:477:LEU:HD13	2.02	0.41
1:D:154:LYS:HB3	1:D:154:LYS:HE2	1.78	0.41
1:A:82:HIS:ND1	1:A:83:PRO:HD2	2.35	0.41
1:A:518:ILE:HA	1:A:521:LEU:HD12	2.02	0.41
1:B:375:GLY:HA3	1:B:395:ILE:HG12	2.02	0.41
1:C:13:GLU:CB	1:C:46:ARG:HA	2.50	0.41
1:A:14:GLY:O	1:A:15:ASN:CB	2.69	0.41
1:A:150:PRO:HD3	1:A:167:PHE:CE2	2.56	0.41
1:B:135:ARG:CG	1:B:141:ILE:HD11	2.48	0.41
1:B:187:ILE:HD11	1:B:249:VAL:HG12	2.02	0.41
1:B:454:LEU:HD12	1:B:454:LEU:C	2.46	0.41
1:C:12:SER:O	1:C:73:ILE:HD13	2.19	0.41
1:C:111:PHE:CD2	1:C:176:THR:OG1	2.67	0.41
1:C:335:LEU:C	1:C:337:ASP:N	2.79	0.41
1:C:340:LEU:O	1:C:344:VAL:HG12	2.21	0.41
1:C:432:GLU:O	1:C:432:GLU:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:GLN:HA	1:D:162:PHE:CD2	2.55	0.41
1:D:149:LEU:CD2	1:D:153:LEU:HG	2.45	0.41
1:D:375:GLY:HA3	1:D:395:ILE:HG12	2.01	0.41
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.32	0.41
1:A:351:SER:O	1:A:351:SER:OG	2.38	0.41
1:B:70:SER:HA	1:B:171:TRP:HZ3	1.85	0.41
1:C:155:GLN:C	1:C:157:GLU:N	2.77	0.41
1:C:307:LEU:O	1:C:308:GLY:C	2.64	0.41
1:D:6:GLU:OE1	1:D:94:ILE:HG13	2.20	0.41
1:A:13:GLU:OE1	1:A:45:ASN:HA	2.21	0.41
1:A:25:GLN:O	1:A:29:GLN:N	2.51	0.41
1:A:303:VAL:O	1:A:303:VAL:CG2	2.69	0.41
1:B:4:LEU:HB2	1:B:97:ARG:HG2	2.03	0.41
1:B:149:LEU:N	1:B:150:PRO:CD	2.84	0.41
1:B:197:HIS:HB2	1:B:223:GLY:HA3	2.02	0.41
1:B:276:LYS:O	1:B:277:ALA:C	2.64	0.41
1:A:181:PHE:CD1	1:A:181:PHE:C	2.99	0.41
1:A:198:ARG:O	1:A:199:ILE:C	2.64	0.41
1:A:406:THR:OG1	1:B:344:VAL:HG21	2.21	0.41
1:A:501:ASN:C	1:A:503:LYS:N	2.78	0.41
1:B:153:LEU:HD23	1:B:153:LEU:N	2.23	0.41
1:B:164:PRO:HB2	1:B:165:SER:H	1.60	0.41
1:B:249:VAL:O	1:B:250:TYR:C	2.64	0.41
1:B:531:LEU:O	1:B:532:VAL:C	2.64	0.41
1:C:76:ARG:H	1:C:76:ARG:HG3	1.48	0.41
1:C:89:ASP:HB3	1:C:90:VAL:H	1.63	0.41
1:C:113:GLN:HA	1:C:162:PHE:CD2	2.55	0.41
1:C:149:LEU:HB3	1:C:153:LEU:HD23	2.03	0.41
1:C:184:ALA:HB3	1:C:270:VAL:HB	2.02	0.41
1:C:187:ILE:HD12	1:C:253:ALA:CB	2.51	0.41
1:C:363:VAL:CG1	1:D:363:VAL:CG1	2.97	0.41
1:C:385:ASP:C	1:C:387:LEU:H	2.29	0.41
1:C:426:PRO:O	1:C:427:LYS:CB	2.37	0.41
1:C:461:LEU:N	1:C:461:LEU:HD13	2.36	0.41
1:D:90:VAL:HG12	1:D:138:LEU:HD11	2.03	0.41
1:D:119:LEU:O	1:D:120:ASN:CB	2.69	0.41
1:D:373:MSE:O	1:D:377:MSE:HB2	2.21	0.41
1:D:378:THR:OG1	1:D:473:ASN:N	2.49	0.41
1:D:458:VAL:HA	1:D:461:LEU:HD22	2.02	0.41
1:D:502:LEU:HD21	1:D:514:THR:HB	2.03	0.41
1:A:113:GLN:HA	1:A:162:PHE:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:SER:O	1:A:376:GLN:HG3	2.21	0.41
1:B:16:ASN:O	1:B:17:GLN:C	2.64	0.41
1:C:131:GLN:HE21	1:C:131:GLN:HB2	1.59	0.41
1:C:312:LEU:HD23	1:C:312:LEU:HA	1.81	0.41
1:C:485:LYS:HD3	1:C:485:LYS:HA	1.96	0.41
1:C:492:PHE:O	1:C:493:GLY:C	2.63	0.41
1:C:539:ARG:O	1:C:540:LYS:C	2.64	0.41
1:D:164:PRO:HB2	1:D:165:SER:H	1.59	0.41
1:D:454:LEU:HD12	1:D:454:LEU:C	2.46	0.41
1:A:124:TYR:CD1	1:A:124:TYR:N	2.89	0.40
1:B:286:CYS:HA	1:B:291:LEU:CD1	2.52	0.40
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.89	0.40
1:D:501:ASN:C	1:D:503:LYS:N	2.78	0.40
1:B:100:SER:O	1:B:101:MSE:C	2.65	0.40
1:B:474:LEU:HD23	1:B:477:LEU:HD13	2.02	0.40
1:B:485:LYS:HD3	1:B:485:LYS:HA	1.97	0.40
1:C:198:ARG:O	1:C:199:ILE:C	2.63	0.40
1:D:12:SER:HB3	1:D:75:MSE:HE1	2.02	0.40
1:D:125:LEU:HD12	1:D:129:ALA:HB1	2.04	0.40
1:D:303:VAL:O	1:D:303:VAL:CG2	2.70	0.40
1:D:518:ILE:HD12	1:D:518:ILE:HA	1.89	0.40
1:A:70:SER:HA	1:A:171:TRP:HZ3	1.86	0.40
1:A:276:LYS:O	1:A:277:ALA:C	2.63	0.40
1:A:395:ILE:HB	1:A:396:PRO:HD3	2.04	0.40
1:B:89:ASP:HB3	1:B:90:VAL:H	1.63	0.40
1:C:135:ARG:HG2	1:C:141:ILE:CD1	2.47	0.40
1:D:2:SER:HA	1:D:97:ARG:HE	1.86	0.40
1:D:198:ARG:O	1:D:199:ILE:C	2.63	0.40
1:D:281:ALA:O	1:D:284:PHE:HB3	2.21	0.40
1:A:377:MSE:HA	1:A:377:MSE:HE3	2.03	0.40
1:B:334:SER:OG	1:B:336:LEU:HB2	2.22	0.40
1:B:351:SER:O	1:B:351:SER:OG	2.38	0.40
1:C:149:LEU:N	1:C:150:PRO:CD	2.85	0.40
1:D:124:TYR:CD1	1:D:124:TYR:N	2.88	0.40
1:D:286:CYS:HA	1:D:291:LEU:CD1	2.52	0.40
1:D:385:ASP:C	1:D:387:LEU:H	2.29	0.40
1:A:19:VAL:HG11	1:A:73:ILE:HD11	2.03	0.40
1:A:59:VAL:O	1:A:63:LEU:HG	2.21	0.40
1:A:498:VAL:HG12	1:A:502:LEU:HD13	2.03	0.40
1:B:240:ASP:CG	1:B:243:VAL:HG23	2.47	0.40
1:C:125:LEU:HD12	1:C:129:ALA:HB1	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ASN:O	1:D:17:GLN:C	2.65	0.40
1:D:181:PHE:C	1:D:181:PHE:CD1	3.00	0.40
1:D:396:PRO:O	1:D:397:PRO:C	2.65	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	538/541 (99%)	401 (74%)	97 (18%)	40 (7%)	1	5
1	B	538/541 (99%)	407 (76%)	88 (16%)	43 (8%)	1	4
1	C	538/541 (99%)	404 (75%)	94 (18%)	40 (7%)	1	5
1	D	538/541 (99%)	404 (75%)	94 (18%)	40 (7%)	1	5
All	All	2152/2164 (99%)	1616 (75%)	373 (17%)	163 (8%)	1	5

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	89	ASP
1	A	142	ARG
1	A	164	PRO
1	A	350	ARG
1	A	353	ALA
1	A	383	GLN
1	A	426	PRO
1	A	427	LYS
1	A	428	ASN
1	A	473	ASN
1	A	507	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	511	LYS
1	A	540	LYS
1	B	13	GLU
1	B	14	GLY
1	B	16	ASN
1	B	89	ASP
1	B	142	ARG
1	B	143	ALA
1	B	164	PRO
1	B	350	ARG
1	B	383	GLN
1	B	426	PRO
1	B	427	LYS
1	B	428	ASN
1	B	473	ASN
1	B	507	ASP
1	B	511	LYS
1	B	540	LYS
1	C	16	ASN
1	C	89	ASP
1	C	130	ALA
1	C	142	ARG
1	C	143	ALA
1	C	164	PRO
1	C	350	ARG
1	C	353	ALA
1	C	383	GLN
1	C	426	PRO
1	C	427	LYS
1	C	428	ASN
1	C	473	ASN
1	C	507	ASP
1	C	511	LYS
1	C	540	LYS
1	D	16	ASN
1	D	89	ASP
1	D	130	ALA
1	D	142	ARG
1	D	143	ALA
1	D	164	PRO
1	D	350	ARG
1	D	353	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	383	GLN
1	D	426	PRO
1	D	427	LYS
1	D	428	ASN
1	D	473	ASN
1	D	507	ASP
1	D	511	LYS
1	D	540	LYS
1	A	13	GLU
1	A	83	PRO
1	A	128	GLU
1	A	130	ALA
1	A	143	ALA
1	A	210	LYS
1	A	356	GLY
1	A	381	ARG
1	A	411	ALA
1	A	474	LEU
1	B	83	PRO
1	B	128	GLU
1	B	130	ALA
1	B	165	SER
1	B	210	LYS
1	B	304	VAL
1	B	353	ALA
1	B	356	GLY
1	B	381	ARG
1	B	411	ALA
1	B	474	LEU
1	C	13	GLU
1	C	83	PRO
1	C	128	GLU
1	C	165	SER
1	C	210	LYS
1	C	356	GLY
1	C	381	ARG
1	C	411	ALA
1	C	474	LEU
1	D	13	GLU
1	D	83	PRO
1	D	128	GLU
1	D	210	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	356	GLY
1	D	381	ARG
1	D	411	ALA
1	D	474	LEU
1	A	3	GLN
1	A	17	GLN
1	A	165	SER
1	A	304	VAL
1	A	339	SER
1	B	3	GLN
1	C	3	GLN
1	C	17	GLN
1	D	3	GLN
1	D	17	GLN
1	D	165	SER
1	D	332	GLU
1	D	336	LEU
1	D	339	SER
1	A	15	ASN
1	A	212	GLN
1	B	17	GLN
1	B	512	GLU
1	C	15	ASN
1	C	304	VAL
1	C	332	GLU
1	C	339	SER
1	D	15	ASN
1	D	212	GLN
1	D	304	VAL
1	D	512	GLU
1	A	84	ARG
1	A	85	MSE
1	A	332	GLU
1	A	396	PRO
1	A	512	GLU
1	B	15	ASN
1	B	55	PRO
1	B	84	ARG
1	B	85	MSE
1	B	212	GLN
1	B	332	GLU
1	B	339	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	530	ALA
1	C	84	ARG
1	C	85	MSE
1	C	212	GLN
1	C	530	ALA
1	D	84	ARG
1	D	85	MSE
1	D	509	VAL
1	A	55	PRO
1	A	443	GLY
1	A	509	VAL
1	B	120	ASN
1	B	396	PRO
1	C	55	PRO
1	C	396	PRO
1	C	509	VAL
1	D	55	PRO
1	D	396	PRO
1	D	443	GLY
1	B	249	VAL
1	B	443	GLY
1	C	443	GLY
1	B	509	VAL
1	C	249	VAL
1	A	534	GLY

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	437/429 (102%)	357 (82%)	80 (18%)	2	7
1	B	437/429 (102%)	355 (81%)	82 (19%)	1	6
1	C	437/429 (102%)	355 (81%)	82 (19%)	1	6
1	D	437/429 (102%)	357 (82%)	80 (18%)	2	7
All	All	1748/1716 (102%)	1424 (82%)	324 (18%)	1	7

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	GLN
1	A	4	LEU
1	A	5	VAL
1	A	10	ASN
1	A	16	ASN
1	A	24	SER
1	A	33	CYS
1	A	36	LEU
1	A	38	VAL
1	A	44	THR
1	A	54	GLN
1	A	56	GLU
1	A	63	LEU
1	A	76	ARG
1	A	88	LEU
1	A	89	ASP
1	A	90	VAL
1	A	94	ILE
1	A	121	VAL
1	A	123	VAL
1	A	124	TYR
1	A	131	GLN
1	A	137	THR
1	A	141	ILE
1	A	153	LEU
1	A	154	LYS
1	A	170	SER
1	A	176	THR
1	A	182	LEU
1	A	187	ILE
1	A	189	LEU
1	A	192	THR
1	A	220	GLN
1	A	227	GLU
1	A	243	VAL
1	A	246	LEU
1	A	254	ARG
1	A	279	LEU
1	A	288	LYS
1	A	289	GLU
1	A	291	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	VAL
1	A	294	LEU
1	A	307	LEU
1	A	325	LEU
1	A	326	VAL
1	A	344	VAL
1	A	347	VAL
1	A	350	ARG
1	A	359	VAL
1	A	363	VAL
1	A	366	LEU
1	A	373	MSE
1	A	377	MSE
1	A	383	GLN
1	A	390	THR
1	A	394	LEU
1	A	407	SER
1	A	425	LEU
1	A	429	THR
1	A	437	THR
1	A	438	CYS
1	A	445	ARG
1	A	450	VAL
1	A	453	LYS
1	A	454	LEU
1	A	457	THR
1	A	460	GLN
1	A	461	LEU
1	A	480	LEU
1	A	489	THR
1	A	491	VAL
1	A	498	VAL
1	A	504	ASP
1	A	510	PHE
1	A	515	ARG
1	A	519	SER
1	A	531	LEU
1	A	539	ARG
1	B	2	SER
1	B	3	GLN
1	B	4	LEU
1	B	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	10	ASN
1	B	16	ASN
1	B	24	SER
1	B	33	CYS
1	B	36	LEU
1	B	38	VAL
1	B	54	GLN
1	B	56	GLU
1	B	63	LEU
1	B	76	ARG
1	B	88	LEU
1	B	89	ASP
1	B	90	VAL
1	B	94	ILE
1	B	121	VAL
1	B	123	VAL
1	B	124	TYR
1	B	131	GLN
1	B	137	THR
1	B	141	ILE
1	B	153	LEU
1	B	154	LYS
1	B	170	SER
1	B	176	THR
1	B	182	LEU
1	B	187	ILE
1	B	189	LEU
1	B	192	THR
1	B	220	GLN
1	B	227	GLU
1	B	243	VAL
1	B	246	LEU
1	B	254	ARG
1	B	279	LEU
1	B	288	LYS
1	B	289	GLU
1	B	291	LEU
1	B	293	VAL
1	B	294	LEU
1	B	297	GLU
1	B	300	ILE
1	B	325	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	326	VAL
1	B	344	VAL
1	B	347	VAL
1	B	350	ARG
1	B	359	VAL
1	B	363	VAL
1	B	366	LEU
1	B	373	MSE
1	B	383	GLN
1	B	390	THR
1	B	394	LEU
1	B	407	SER
1	B	425	LEU
1	B	429	THR
1	B	435	ARG
1	B	437	THR
1	B	438	CYS
1	B	445	ARG
1	B	450	VAL
1	B	452	LEU
1	B	453	LYS
1	B	454	LEU
1	B	457	THR
1	B	460	GLN
1	B	461	LEU
1	B	480	LEU
1	B	489	THR
1	B	491	VAL
1	B	498	VAL
1	B	504	ASP
1	B	510	PHE
1	B	515	ARG
1	B	519	SER
1	B	527	THR
1	B	531	LEU
1	B	539	ARG
1	C	2	SER
1	C	3	GLN
1	C	4	LEU
1	C	5	VAL
1	C	10	ASN
1	C	16	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	24	SER
1	C	33	CYS
1	C	36	LEU
1	C	38	VAL
1	C	54	GLN
1	C	56	GLU
1	C	63	LEU
1	C	76	ARG
1	C	88	LEU
1	C	89	ASP
1	C	90	VAL
1	C	94	ILE
1	C	121	VAL
1	C	123	VAL
1	C	124	TYR
1	C	131	GLN
1	C	137	THR
1	C	141	ILE
1	C	153	LEU
1	C	154	LYS
1	C	170	SER
1	C	176	THR
1	C	182	LEU
1	C	187	ILE
1	C	189	LEU
1	C	192	THR
1	C	220	GLN
1	C	227	GLU
1	C	243	VAL
1	C	246	LEU
1	C	254	ARG
1	C	279	LEU
1	C	288	LYS
1	C	289	GLU
1	C	291	LEU
1	C	293	VAL
1	C	294	LEU
1	C	297	GLU
1	C	307	LEU
1	C	325	LEU
1	C	326	VAL
1	C	344	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	347	VAL
1	C	350	ARG
1	C	359	VAL
1	C	363	VAL
1	C	366	LEU
1	C	370	LEU
1	C	373	MSE
1	C	383	GLN
1	C	390	THR
1	C	394	LEU
1	C	407	SER
1	C	420	LEU
1	C	425	LEU
1	C	429	THR
1	C	437	THR
1	C	438	CYS
1	C	445	ARG
1	C	450	VAL
1	C	453	LYS
1	C	454	LEU
1	C	457	THR
1	C	458	VAL
1	C	460	GLN
1	C	461	LEU
1	C	480	LEU
1	C	489	THR
1	C	491	VAL
1	C	498	VAL
1	C	504	ASP
1	C	510	PHE
1	C	515	ARG
1	C	519	SER
1	C	531	LEU
1	C	539	ARG
1	D	2	SER
1	D	3	GLN
1	D	4	LEU
1	D	5	VAL
1	D	10	ASN
1	D	16	ASN
1	D	24	SER
1	D	33	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	36	LEU
1	D	38	VAL
1	D	44	THR
1	D	54	GLN
1	D	56	GLU
1	D	63	LEU
1	D	76	ARG
1	D	88	LEU
1	D	89	ASP
1	D	90	VAL
1	D	94	ILE
1	D	121	VAL
1	D	123	VAL
1	D	124	TYR
1	D	131	GLN
1	D	137	THR
1	D	141	ILE
1	D	153	LEU
1	D	154	LYS
1	D	170	SER
1	D	176	THR
1	D	182	LEU
1	D	187	ILE
1	D	189	LEU
1	D	192	THR
1	D	220	GLN
1	D	227	GLU
1	D	243	VAL
1	D	246	LEU
1	D	254	ARG
1	D	279	LEU
1	D	288	LYS
1	D	289	GLU
1	D	291	LEU
1	D	293	VAL
1	D	294	LEU
1	D	307	LEU
1	D	325	LEU
1	D	326	VAL
1	D	344	VAL
1	D	347	VAL
1	D	350	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	359	VAL
1	D	363	VAL
1	D	366	LEU
1	D	373	MSE
1	D	383	GLN
1	D	390	THR
1	D	394	LEU
1	D	407	SER
1	D	425	LEU
1	D	429	THR
1	D	437	THR
1	D	438	CYS
1	D	445	ARG
1	D	450	VAL
1	D	453	LYS
1	D	454	LEU
1	D	457	THR
1	D	460	GLN
1	D	461	LEU
1	D	474	LEU
1	D	480	LEU
1	D	489	THR
1	D	498	VAL
1	D	504	ASP
1	D	509	VAL
1	D	510	PHE
1	D	515	ARG
1	D	519	SER
1	D	531	LEU
1	D	539	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	29	GLN
1	A	78	HIS
1	A	82	HIS
1	A	131	GLN
1	A	155	GLN
1	A	186	ASN
1	A	202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	ASN
1	A	386	HIS
1	A	428	ASN
1	A	466	GLN
1	A	470	GLN
1	A	481	GLN
1	A	497	ASN
1	A	528	GLN
1	B	25	GLN
1	B	29	GLN
1	B	78	HIS
1	B	82	HIS
1	B	131	GLN
1	B	155	GLN
1	B	202	ASN
1	B	261	ASN
1	B	404	GLN
1	B	428	ASN
1	B	466	GLN
1	B	481	GLN
1	B	497	ASN
1	B	528	GLN
1	C	25	GLN
1	C	29	GLN
1	C	78	HIS
1	C	82	HIS
1	C	131	GLN
1	C	155	GLN
1	C	202	ASN
1	C	261	ASN
1	C	404	GLN
1	C	428	ASN
1	C	466	GLN
1	C	481	GLN
1	C	497	ASN
1	C	528	GLN
1	D	25	GLN
1	D	29	GLN
1	D	78	HIS
1	D	82	HIS
1	D	131	GLN
1	D	155	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	202	ASN
1	D	261	ASN
1	D	404	GLN
1	D	428	ASN
1	D	466	GLN
1	D	470	GLN
1	D	481	GLN
1	D	497	ASN
1	D	528	GLN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	532/541 (98%)	-1.13	0 100 100	29, 53, 164, 213	0
1	B	532/541 (98%)	-1.18	0 100 100	30, 53, 158, 222	0
1	C	532/541 (98%)	-1.09	0 100 100	31, 60, 149, 194	0
1	D	532/541 (98%)	-1.06	0 100 100	33, 60, 159, 199	0
All	All	2128/2164 (98%)	-1.11	0 100 100	29, 56, 157, 222	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.