



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 AM UTC

PDB ID : 3F3G / pdb_00003f3g
Title : Crystal structure of the nucleoporin pair Nup85-Seh1, space group P212121
Authors : Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.
Deposited on : 2008-10-30
Resolution : 3.75 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
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

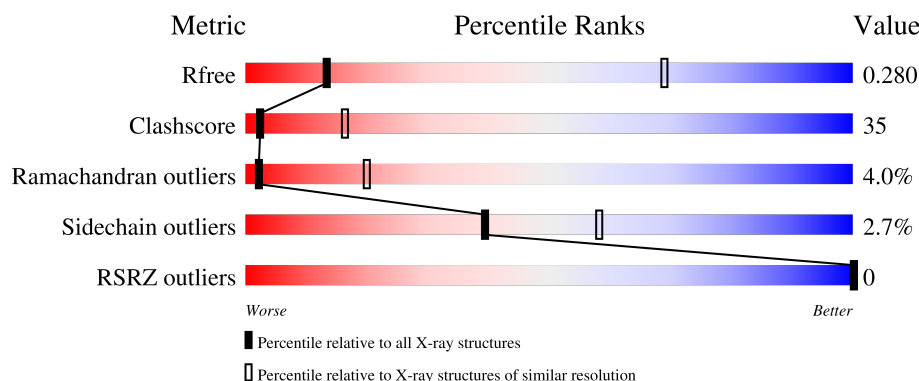
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

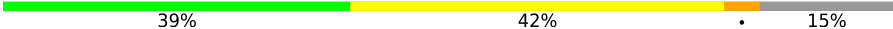
The reported resolution of this entry is 3.75 Å.

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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	351	
1	B	351	
1	E	351	
1	F	351	
2	C	570	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	570	34%44%5%16%
2	G	570	36%42%6%15%
2	H	570	35%44%7%14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25114 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2379	1506	410	452	11			
1	B	300	Total	C	N	O	S	0	0	0
			2379	1506	410	452	11			
1	E	300	Total	C	N	O	S	0	0	0
			2379	1506	410	452	11			
1	F	300	Total	C	N	O	S	0	0	0
			2379	1506	410	452	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	expression tag	UNP P53011
A	0	HIS	-	expression tag	UNP P53011
B	-1	PRO	-	expression tag	UNP P53011
B	0	HIS	-	expression tag	UNP P53011
E	-1	PRO	-	expression tag	UNP P53011
E	0	HIS	-	expression tag	UNP P53011
F	-1	PRO	-	expression tag	UNP P53011
F	0	HIS	-	expression tag	UNP P53011

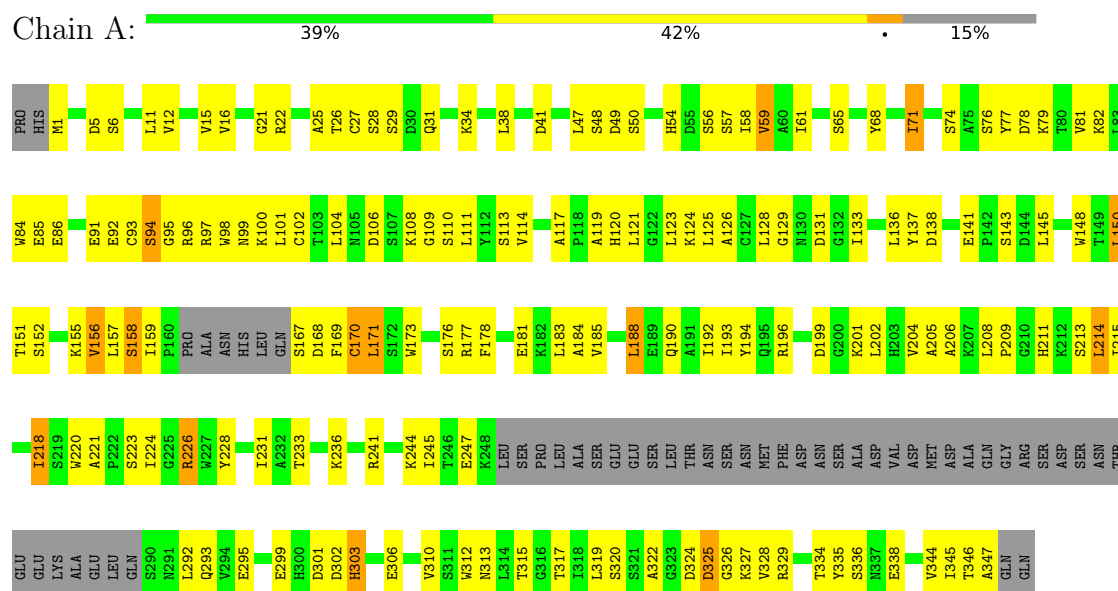
- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	492	Total	C	N	O	S	0	0	0
			3938	2526	634	756	22			
2	D	480	Total	C	N	O	S	0	0	0
			3850	2473	618	737	22			
2	G	482	Total	C	N	O	S	0	0	0
			3863	2482	620	739	22			
2	H	493	Total	C	N	O	S	0	0	0
			3947	2532	636	757	22			

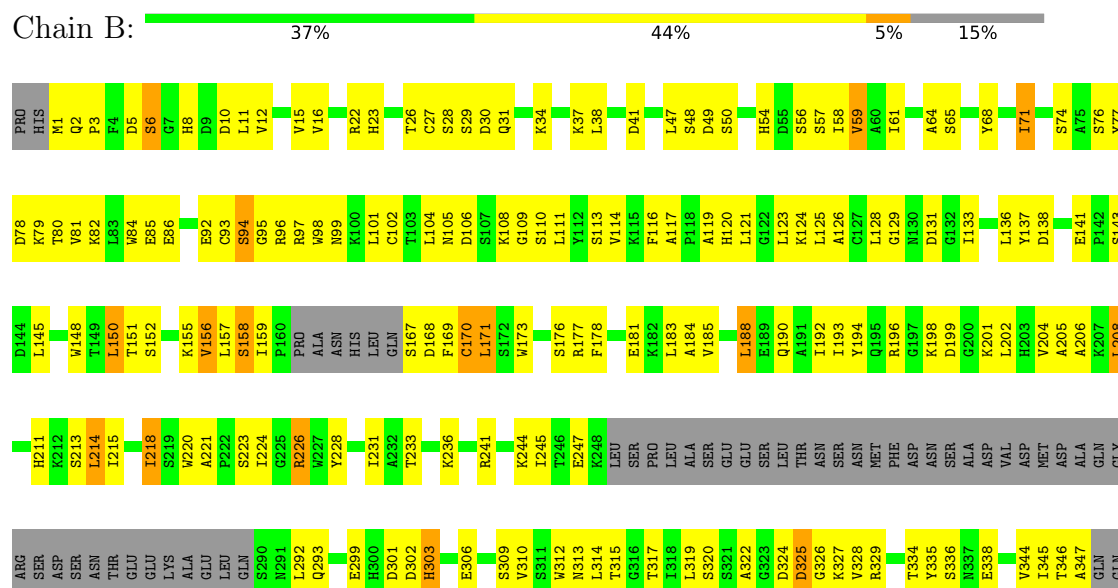
3 Residue-property plots

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: Nucleoporin SEH1

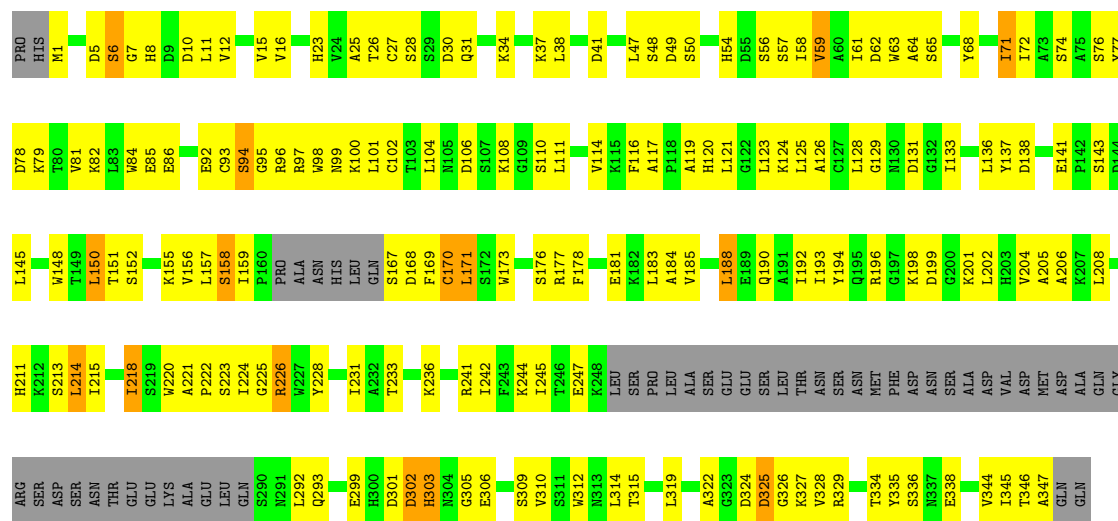


• Molecule 1: Nucleoporin SEH1



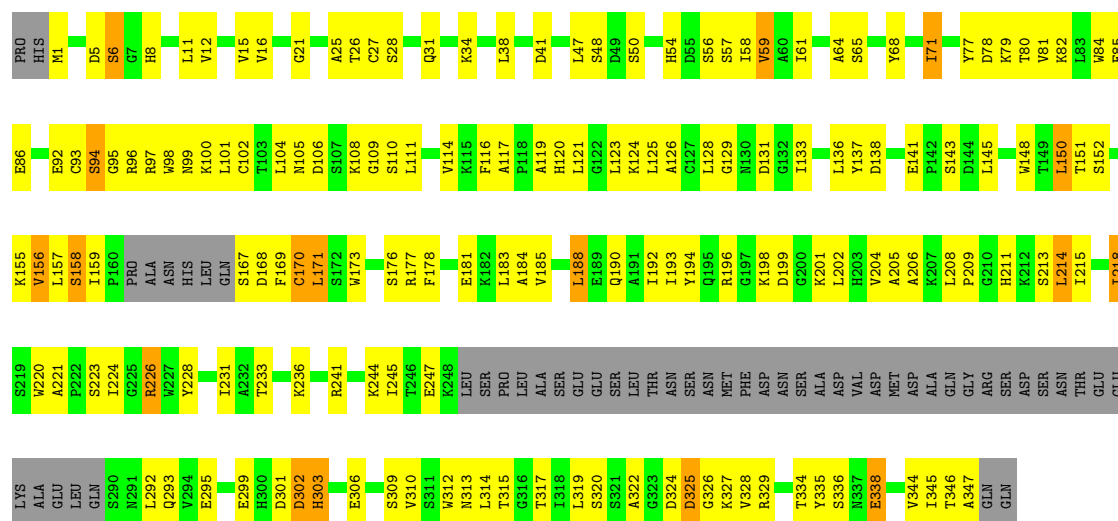
• Molecule 1: Nucleoporin SEH1

Chain E:  37% 44% 15%



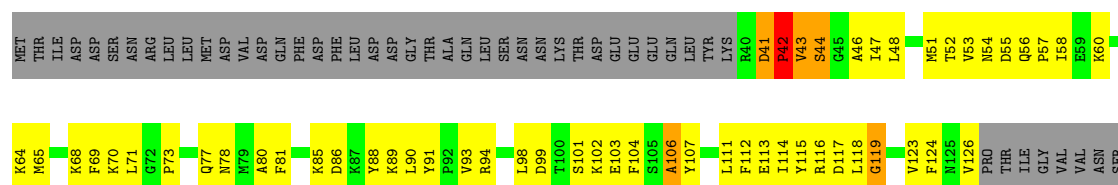
• Molecule 1: Nucleoporin SEH1

Chain F:  39% 42% 5% 15%



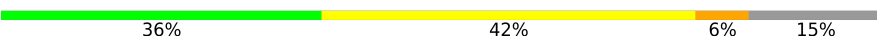
• Molecule 2: Nucleoporin NUP85

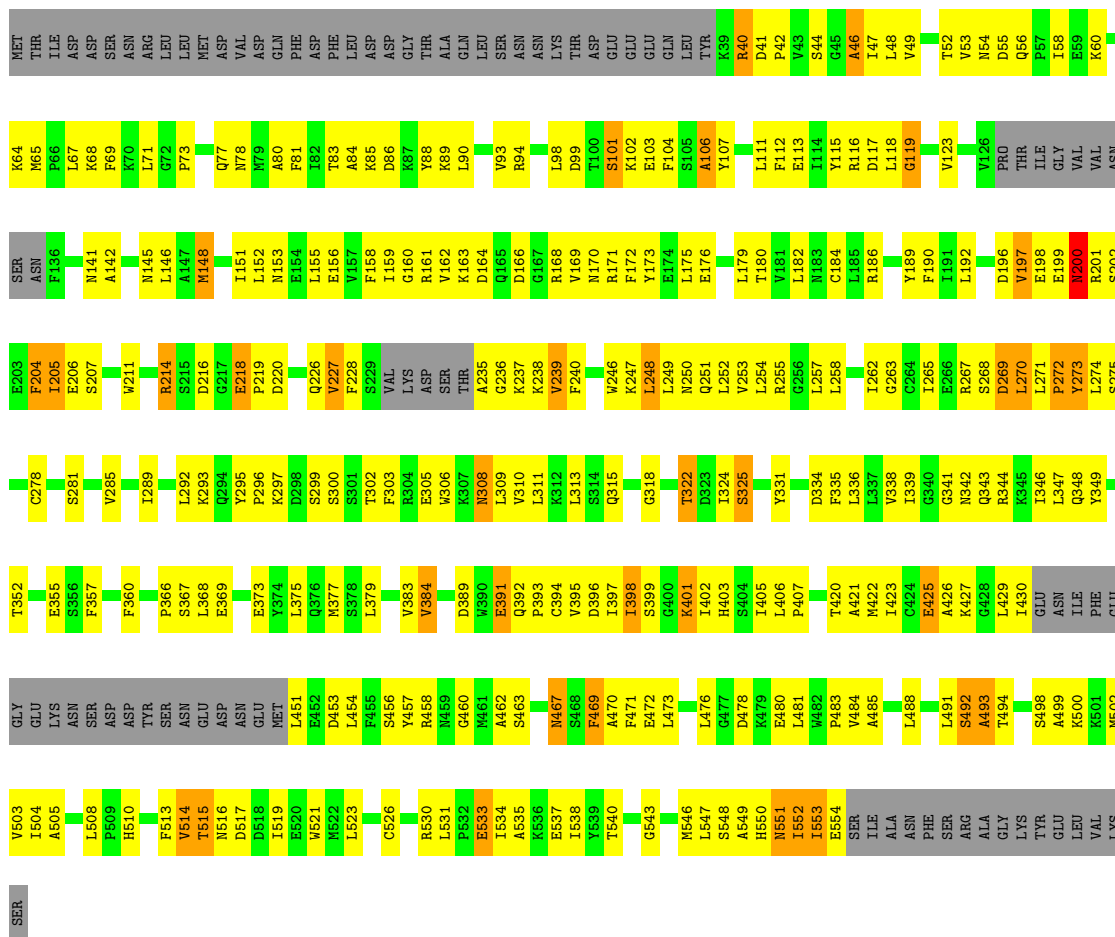
Chain C:  36% 44% 6% 14%



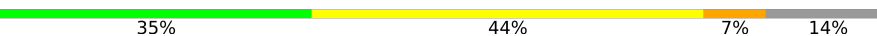


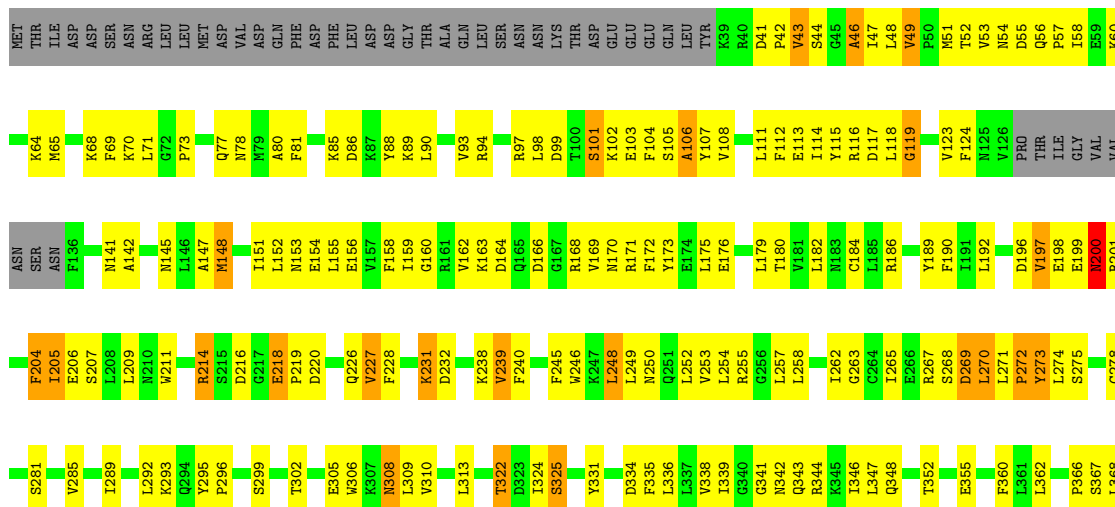
● Molecule 2: Nucleoporin NUP85

Chain G:  36% 42% 6% 15%



● Molecule 2: Nucleoporin NUP85

Chain H:  35% 44% 7% 14%



E369	ASN	E373	ASN	Y374	ASN	L375	GLU	Q376	MET	S377	LEU	S378	E452	D453	L454	F455	S456	Y457	R458	N459	G460	M461	S462	A462	S463	Y464	M465	L466	N467	S468	F469	A470	F471	E472	L473	C474	S475	L476	G477	D478	K479	E480	L481	W482	P483	V484	A485	I486	G487	L488	I489	A490	L491	S492	A493	T494	G495	T496	R497	S498	A499	K500	R501	M502	V503
L370	GLU	E374	ASN	Y375	ASN	Q376	GLU	M377	LEU	S378	E452	D453	L454	F455	S456	Y457	R458	N459	G460	M461	S462	A463	S463	Y464	M465	L466	N467	S468	F469	A470	F471	E472	L473	C474	S475	L476	G477	D478	K479	E480	L481	W482	P483	V484	A485	I486	G487	L488	I489	A490	L491	S492	A493	T494	G495	T496	R497	S498	A499	K500	R501	M502	V503		
L508	P509	H510	Y511	P512	F513	V514	T515	N516	D517	D518	I519	E520	W521	M522	L523	S524	I525	C526	V527	R530	L531	P532	E533	I534	A535	K536	E537	I538	T541	Q545	M546	L547	S548	A549	H550	N551	I552	I553	E554	S555	I556	A557	N558	F559	S560	R561	ALA	GLY	LYS	TYR	GLU	LEU	VAL	LYS	SER										
E369	ASN	E373	ASN	Y374	ASN	L375	GLU	Q376	MET	S377	LEU	S378	E452	D453	L454	F455	S456	Y457	R458	N459	G460	M461	S462	A462	S463	Y464	M465	L466	N467	S468	F469	A470	F471	E472	L473	C474	S475	L476	G477	D478	K479	E480	L481	W482	P483	V484	A485	I486	G487	L488	I489	A490	L491	S492	A493	T494	G495	T496	R497	S498	A499	K500	R501	M502	V503

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.38Å 106.49Å 358.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.75 50.00 – 3.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.75) 89.8 (50.00-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.272 0.254 , 0.280	Depositor DCC
R_{free} test set	2062 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 147.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.337 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25114	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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	0.49	0/2437	0.97	8/3301 (0.2%)
1	B	0.50	0/2437	0.97	11/3301 (0.3%)
1	E	0.49	0/2437	0.97	9/3301 (0.3%)
1	F	0.50	0/2437	0.96	9/3301 (0.3%)
2	C	0.72	9/4018 (0.2%)	1.04	20/5440 (0.4%)
2	D	0.67	8/3928 (0.2%)	1.06	24/5316 (0.5%)
2	G	0.63	4/3941 (0.1%)	1.08	22/5334 (0.4%)
2	H	0.73	6/4027 (0.1%)	1.11	24/5451 (0.4%)
All	All	0.62	27/25662 (0.1%)	1.03	127/34745 (0.4%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	552	ILE	CA-CB	9.97	1.64	1.55
2	H	552	ILE	CA-CB	9.28	1.64	1.54
2	C	552	ILE	CA-CB	9.12	1.66	1.54
2	D	553	ILE	CA-CB	8.20	1.65	1.54
2	C	556	ILE	CA-CB	7.94	1.65	1.54
2	H	43	VAL	CA-CB	7.77	1.65	1.54
2	H	553	ILE	CA-CB	7.13	1.62	1.54
2	C	553	ILE	CA-CB	7.08	1.64	1.54
2	C	42	PRO	CA-C	6.83	1.62	1.52
2	D	41	ASP	CA-C	6.63	1.60	1.52
2	C	560	SER	CA-C	6.60	1.59	1.52
2	D	553	ILE	N-CA	6.41	1.54	1.46
2	G	41	ASP	CA-C	5.92	1.59	1.52
2	D	40	ARG	N-CA	5.82	1.53	1.46
2	C	555	SER	CA-C	5.76	1.61	1.52
2	H	560	SER	CA-C	5.73	1.60	1.52
2	G	552	ILE	CA-C	5.61	1.59	1.52
2	C	558	ASN	C-O	5.59	1.31	1.24
2	C	44	SER	CA-CB	5.37	1.60	1.53
2	G	551	ASN	C-O	5.30	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	554	GLU	CA-C	5.23	1.59	1.52
2	G	553	ILE	CA-CB	5.20	1.61	1.54
2	D	41	ASP	C-N	5.17	1.40	1.33
2	C	43	VAL	N-CA	5.13	1.52	1.46
2	D	552	ILE	C-O	5.10	1.29	1.23
2	D	41	ASP	CA-CB	5.05	1.60	1.53
2	H	559	PHE	C-O	5.01	1.29	1.24

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	41	ASP	CA-C-N	15.30	134.90	120.21
2	G	41	ASP	C-N-CA	15.30	134.90	120.21
2	H	41	ASP	CA-C-N	14.63	134.25	120.21
2	H	41	ASP	C-N-CA	14.63	134.25	120.21
2	D	41	ASP	CA-C-N	11.34	131.10	119.76
2	D	41	ASP	C-N-CA	11.34	131.10	119.76
2	C	457	TYR	N-CA-C	-10.01	99.88	114.39
2	G	269	ASP	N-CA-C	9.84	124.34	111.75
2	H	269	ASP	N-CA-C	9.67	124.13	111.75
2	D	269	ASP	N-CA-C	9.63	124.08	111.75
2	C	269	ASP	N-CA-C	9.46	123.86	111.75
2	G	550	HIS	N-CA-C	-9.13	102.14	113.38
2	G	40	ARG	N-CA-C	8.97	123.87	107.99
2	D	43	VAL	N-CA-C	8.06	126.11	109.34
1	F	338	GLU	N-CA-C	-7.76	98.39	110.42
1	A	338	GLU	N-CA-C	-7.73	98.44	110.42
2	D	46	ALA	N-CA-C	7.72	122.60	112.72
2	D	102	LYS	N-CA-C	-7.70	102.89	111.82
1	E	338	GLU	N-CA-C	-7.68	98.51	110.42
1	B	338	GLU	N-CA-C	-7.67	98.53	110.42
2	G	526	CYS	N-CA-C	-7.44	104.17	113.18
2	C	102	LYS	N-CA-C	-7.36	103.28	111.82
2	G	102	LYS	N-CA-C	-7.25	103.40	111.82
2	H	102	LYS	N-CA-C	-7.18	103.49	111.82
2	C	497	ARG	N-CA-C	-7.07	104.12	112.89
2	C	425	GLU	N-CA-C	-7.05	103.67	112.90
2	H	552	ILE	CA-C-N	6.93	129.54	120.60
2	H	552	ILE	C-N-CA	6.93	129.54	120.60
2	H	425	GLU	N-CA-C	-6.92	103.84	112.90
2	G	40	ARG	CB-CA-C	-6.76	99.77	110.79
2	D	553	ILE	CA-C-N	-6.75	109.55	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	553	ILE	C-N-CA	-6.75	109.55	121.70
2	D	425	GLU	N-CA-C	-6.71	104.11	112.90
2	C	43	VAL	CB-CA-C	-6.70	100.30	111.29
2	C	55	ASP	N-CA-C	6.69	118.61	109.11
2	D	469	PHE	N-CA-C	-6.66	103.82	112.68
2	D	55	ASP	N-CA-C	6.66	118.56	109.11
2	C	43	VAL	N-CA-C	6.64	123.15	109.34
2	G	425	GLU	N-CA-C	-6.61	104.25	112.90
2	H	55	ASP	N-CA-C	6.58	118.46	109.11
1	B	106	ASP	N-CA-C	6.58	119.30	111.33
2	D	41	ASP	CB-CA-C	6.58	117.48	110.17
2	H	106	ALA	N-CA-C	-6.54	105.44	113.41
1	F	158	SER	N-CA-C	6.52	118.43	110.41
2	H	554	GLU	CA-C-N	6.50	129.64	120.28
2	H	554	GLU	C-N-CA	6.50	129.64	120.28
1	F	6	SER	N-CA-C	-6.49	104.30	111.82
2	D	550	HIS	N-CA-C	-6.45	104.67	112.54
1	A	158	SER	N-CA-C	6.45	118.34	110.41
2	G	389	ASP	N-CA-C	6.37	119.04	111.33
2	G	55	ASP	N-CA-C	6.37	118.16	109.11
1	B	6	SER	N-CA-C	-6.36	104.44	111.82
1	A	6	SER	N-CA-C	-6.35	104.45	111.82
1	E	6	SER	N-CA-C	-6.33	104.47	111.82
2	H	214	ARG	N-CA-C	-6.30	105.53	112.72
2	H	553	ILE	CB-CA-C	-6.30	103.81	111.88
1	B	59	VAL	N-CA-C	6.29	119.70	113.53
1	A	106	ASP	N-CA-C	6.28	118.92	111.33
2	G	49	VAL	N-CA-C	6.25	115.05	107.61
2	G	214	ARG	N-CA-C	-6.18	105.67	112.72
1	B	303	HIS	N-CA-C	6.16	120.53	112.89
1	E	106	ASP	N-CA-C	6.14	118.77	111.33
2	D	42	PRO	N-CA-C	6.14	120.83	111.19
1	F	71	ILE	N-CA-C	6.14	116.45	107.37
2	G	106	ALA	N-CA-C	-6.14	105.92	113.41
1	A	71	ILE	N-CA-C	6.12	116.42	107.37
1	F	106	ASP	N-CA-C	6.11	118.72	111.33
1	E	158	SER	N-CA-C	6.08	117.88	110.41
1	B	158	SER	N-CA-C	6.07	117.88	110.41
2	D	214	ARG	N-CA-C	-6.06	105.81	112.72
2	C	389	ASP	N-CA-C	6.02	118.61	111.33
1	A	59	VAL	N-CA-C	6.01	119.42	113.53
2	C	214	ARG	N-CA-C	-6.00	105.88	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	106	ALA	N-CA-C	-5.98	106.11	113.41
1	E	59	VAL	N-CA-C	5.96	119.38	113.53
1	E	71	ILE	N-CA-C	5.96	116.18	107.37
2	H	389	ASP	N-CA-C	5.96	118.54	111.33
2	G	420	THR	N-CA-C	-5.95	104.48	110.97
1	F	59	VAL	N-CA-C	5.91	119.32	113.53
2	H	469	PHE	N-CA-C	-5.91	104.83	112.68
2	H	457	TYR	N-CA-C	-5.90	104.76	113.61
1	E	303	HIS	N-CA-C	5.89	120.19	112.89
2	D	106	ALA	N-CA-C	-5.85	106.27	113.41
2	H	218	GLU	N-CA-C	5.82	116.30	109.60
1	E	198	LYS	N-CA-C	-5.79	105.06	111.71
2	D	420	THR	N-CA-C	-5.76	104.69	110.97
2	D	457	TYR	N-CA-C	-5.74	106.32	113.38
1	B	71	ILE	N-CA-C	5.72	115.83	107.37
2	G	467	ASN	N-CA-C	-5.72	105.41	112.90
2	H	462	ALA	N-CA-C	-5.70	102.20	111.04
2	G	218	GLU	N-CA-C	5.67	116.12	109.60
2	H	468	SER	N-CA-C	-5.63	106.76	113.97
1	A	303	HIS	N-CA-C	5.59	119.82	112.89
2	C	218	GLU	N-CA-C	5.56	116.00	109.60
2	D	218	GLU	N-CA-C	5.54	115.97	109.60
1	B	208	LEU	CA-C-N	5.51	125.99	120.14
1	B	208	LEU	C-N-CA	5.51	125.99	120.14
1	A	188	LEU	CB-CA-C	-5.49	109.76	117.23
1	F	303	HIS	N-CA-C	5.48	119.69	112.89
2	C	420	THR	N-CA-C	-5.43	105.06	110.97
1	B	198	LYS	N-CA-C	-5.42	105.48	111.71
1	E	188	LEU	CB-CA-C	-5.40	109.88	117.23
2	C	148	MET	N-CA-C	-5.40	105.31	111.14
2	D	497	ARG	N-CA-C	-5.39	105.40	111.28
2	H	391	GLU	N-CA-C	5.38	116.83	110.97
1	B	188	LEU	CB-CA-C	-5.37	109.93	117.23
2	C	551	ASN	CA-C-N	5.37	131.63	121.97
2	C	551	ASN	C-N-CA	5.37	131.63	121.97
2	H	519	ILE	N-CA-C	-5.35	105.50	110.53
2	G	469	PHE	N-CA-C	-5.34	105.57	112.68
2	D	49	VAL	N-CA-C	5.32	113.94	107.61
2	D	148	MET	N-CA-C	-5.29	105.43	111.14
2	D	526	CYS	N-CA-C	-5.28	106.54	112.87
2	C	41	ASP	CB-CA-C	-5.25	101.32	109.20
1	F	188	LEU	CB-CA-C	-5.24	110.10	117.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	148	MET	N-CA-C	-5.24	105.48	111.14
2	C	405	ILE	N-CA-C	-5.22	107.32	111.81
2	H	461	MET	N-CA-C	-5.21	106.76	113.01
2	C	469	PHE	N-CA-C	-5.19	105.77	112.68
2	G	47	ILE	N-CA-C	5.19	117.10	109.63
1	F	198	LYS	N-CA-C	-5.18	105.76	111.71
2	G	349	TYR	N-CA-C	5.09	119.36	113.20
2	G	391	GLU	N-CA-C	5.08	116.50	110.97
2	H	148	MET	N-CA-C	-5.06	105.67	111.14
2	H	49	VAL	N-CA-C	5.02	113.58	107.61
2	D	307	LYS	N-CA-C	-5.01	105.95	111.71
2	C	391	GLU	N-CA-C	5.01	116.43	110.97

There are no chirality outliers.

There are no planarity outliers.

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	2379	0	2319	171	0
1	B	2379	0	2319	173	0
1	E	2379	0	2319	176	0
1	F	2379	0	2319	176	0
2	C	3938	0	3892	291	0
2	D	3850	0	3807	279	0
2	G	3863	0	3823	280	0
2	H	3947	0	3905	304	0
All	All	25114	0	24703	1757	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 35.

All (1757) 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)
2:C:43:VAL:HG13	2:C:48:LEU:HD22	1.27	1.10
2:D:42:PRO:HB3	2:D:48:LEU:HD22	1.37	1.04
2:H:42:PRO:HB3	2:H:48:LEU:HD22	1.42	0.99
2:H:42:PRO:HD3	2:H:48:LEU:HB2	1.40	0.99
2:D:42:PRO:CG	2:D:48:LEU:HB2	1.94	0.98
2:D:515:THR:HG22	2:D:517:ASP:H	1.24	0.98
1:A:211:HIS:NE2	1:A:233:THR:HG21	1.79	0.97
2:C:43:VAL:CG1	2:C:48:LEU:HD22	1.94	0.97
1:F:211:HIS:NE2	1:F:233:THR:HG21	1.81	0.95
1:A:1:MET:HE3	2:C:94:ARG:HD2	1.49	0.94
1:B:211:HIS:NE2	1:B:233:THR:HG21	1.84	0.93
1:B:1:MET:HE3	2:D:94:ARG:HD2	1.51	0.92
2:H:42:PRO:CD	2:H:48:LEU:HB2	1.99	0.92
1:B:81:VAL:HG23	1:B:111:LEU:HD13	1.49	0.92
1:E:81:VAL:HG23	1:E:111:LEU:HD13	1.49	0.91
1:F:81:VAL:HG23	1:F:111:LEU:HD13	1.52	0.91
1:E:211:HIS:NE2	1:E:233:THR:HG21	1.84	0.91
2:G:42:PRO:HD3	2:G:48:LEU:HB2	1.51	0.91
1:E:1:MET:HE3	2:G:94:ARG:HD2	1.53	0.90
1:A:81:VAL:HG23	1:A:111:LEU:HD13	1.50	0.90
1:B:27:CYS:HB3	1:B:61:ILE:HD11	1.51	0.89
2:H:231:LYS:HE3	2:H:238:LYS:HG2	1.53	0.88
2:D:42:PRO:CB	2:D:48:LEU:HB2	2.03	0.88
1:F:220:TRP:HA	1:F:231:ILE:HG22	1.55	0.88
1:E:27:CYS:HB3	1:E:61:ILE:HD11	1.56	0.87
2:G:453:ASP:HB2	2:G:456:SER:HB2	1.54	0.87
1:F:1:MET:HE3	2:H:94:ARG:HD2	1.55	0.87
1:A:220:TRP:HA	1:A:231:ILE:HG22	1.57	0.86
2:D:42:PRO:HB3	2:D:48:LEU:HB2	1.58	0.85
2:C:515:THR:HG22	2:C:517:ASP:H	1.41	0.85
1:A:27:CYS:HB3	1:A:61:ILE:HD11	1.59	0.84
2:C:553:ILE:O	2:C:556:ILE:HB	1.77	0.83
2:D:515:THR:HG22	2:D:517:ASP:N	1.94	0.83
1:E:220:TRP:HA	1:E:231:ILE:HG22	1.61	0.83
2:G:515:THR:HG22	2:G:517:ASP:H	1.43	0.82
1:F:27:CYS:HB3	1:F:61:ILE:HD11	1.60	0.82
1:A:213:SER:HB3	1:A:236:LYS:HB3	1.62	0.82
1:A:12:VAL:HA	1:A:28:SER:HB3	1.61	0.81
2:D:422:MET:HB2	2:D:466:LEU:HD11	1.62	0.81
2:H:42:PRO:HD3	2:H:48:LEU:CB	2.09	0.81
1:A:11:LEU:O	1:A:28:SER:HB2	1.80	0.81
1:F:104:LEU:HD13	1:F:137:TYR:CD2	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HD13	1:B:137:TYR:CD2	2.16	0.80
2:H:499:ALA:O	2:H:503:VAL:HG23	1.80	0.80
1:E:104:LEU:HD13	1:E:137:TYR:CD2	2.15	0.80
2:D:249:LEU:O	2:D:253:VAL:HG23	1.80	0.80
1:B:220:TRP:HA	1:B:231:ILE:HG22	1.63	0.80
2:C:231:LYS:HE3	2:C:233:SER:HB3	1.64	0.80
1:B:213:SER:HB3	1:B:236:LYS:HB3	1.64	0.80
1:F:11:LEU:O	1:F:28:SER:HB2	1.82	0.80
1:F:12:VAL:HA	1:F:28:SER:HB3	1.62	0.80
1:E:11:LEU:O	1:E:28:SER:HB2	1.81	0.79
2:D:258:LEU:HD22	2:D:292:LEU:HD22	1.65	0.79
2:D:480:GLU:O	2:D:483:PRO:HD2	1.83	0.79
1:F:213:SER:HB3	1:F:236:LYS:HB3	1.65	0.79
1:A:104:LEU:HD13	1:A:137:TYR:CD2	2.17	0.79
1:B:27:CYS:CB	1:B:61:ILE:HD11	2.13	0.78
2:D:42:PRO:CD	2:D:48:LEU:HB2	2.13	0.78
1:E:213:SER:HB3	1:E:236:LYS:HB3	1.66	0.78
2:H:515:THR:HG22	2:H:516:ASN:H	1.47	0.78
2:H:521:TRP:CZ2	2:H:525:ILE:HD11	2.19	0.78
2:G:453:ASP:CB	2:G:456:SER:HB2	2.14	0.78
2:H:47:ILE:CD1	2:H:97:ARG:HE	1.96	0.78
2:D:42:PRO:HB3	2:D:48:LEU:CD2	2.13	0.78
2:G:249:LEU:O	2:G:253:VAL:HG23	1.83	0.78
2:D:296:PRO:HG3	2:D:302:THR:HG22	1.66	0.77
2:G:296:PRO:HG3	2:G:302:THR:HG22	1.65	0.77
2:C:249:LEU:O	2:C:253:VAL:HG23	1.83	0.77
2:C:258:LEU:HD22	2:C:292:LEU:HD22	1.66	0.77
2:H:553:ILE:CA	2:H:556:ILE:HG22	2.15	0.76
1:A:211:HIS:CD2	1:A:233:THR:HG21	2.21	0.76
2:G:258:LEU:HD22	2:G:292:LEU:HD22	1.67	0.76
2:H:69:PHE:HE1	2:H:71:LEU:HD23	1.50	0.75
2:C:478:ASP:OD1	2:C:480:GLU:HB2	1.85	0.75
1:E:27:CYS:CB	1:E:61:ILE:HD11	2.16	0.75
2:H:258:LEU:HD22	2:H:292:LEU:HD22	1.68	0.75
2:H:296:PRO:HG3	2:H:302:THR:HG22	1.69	0.75
1:F:211:HIS:CD2	1:F:233:THR:HG21	2.20	0.75
1:B:211:HIS:CD2	1:B:233:THR:HG21	2.21	0.75
2:C:406:LEU:HB2	2:C:407:PRO:HD3	1.67	0.75
2:C:296:PRO:HG3	2:C:302:THR:HG22	1.69	0.75
1:E:12:VAL:HA	1:E:28:SER:HB3	1.67	0.75
1:F:54:HIS:HB3	1:F:78:ASP:OD2	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:PRO:CD	2:G:48:LEU:HB2	2.16	0.75
2:G:344:ARG:HH11	2:G:344:ARG:HG3	1.51	0.75
2:H:344:ARG:HH11	2:H:344:ARG:HG3	1.51	0.75
2:C:69:PHE:HE1	2:C:71:LEU:HD23	1.51	0.75
2:D:454:LEU:HD23	2:D:503:VAL:HG21	1.69	0.75
1:B:11:LEU:O	1:B:28:SER:HB2	1.87	0.75
2:H:515:THR:HG22	2:H:516:ASN:N	2.01	0.75
2:D:42:PRO:HD3	2:D:48:LEU:N	2.02	0.74
2:G:278:CYS:HB2	2:G:324:ILE:HG23	1.68	0.74
1:E:324:ASP:HB3	2:G:64:LYS:HG2	1.70	0.74
1:A:208:LEU:HD11	1:A:231:ILE:CD1	2.16	0.74
1:B:54:HIS:HB3	1:B:78:ASP:OD2	1.88	0.74
1:E:211:HIS:CD2	1:E:233:THR:HG21	2.22	0.74
2:H:533:GLU:HA	2:H:533:GLU:OE1	1.88	0.74
2:C:344:ARG:HH11	2:C:344:ARG:HG3	1.50	0.74
1:E:208:LEU:HD11	1:E:231:ILE:CD1	2.17	0.74
1:F:208:LEU:HD11	1:F:231:ILE:CD1	2.18	0.74
2:H:454:LEU:HD23	2:H:503:VAL:HG21	1.70	0.74
2:H:553:ILE:C	2:H:556:ILE:HG22	2.13	0.74
2:C:550:HIS:HA	2:C:553:ILE:CD1	2.17	0.73
2:C:499:ALA:O	2:C:503:VAL:HG23	1.87	0.73
2:H:406:LEU:HB2	2:H:407:PRO:HD3	1.69	0.73
2:C:555:SER:HA	2:C:558:ASN:OD1	1.87	0.73
1:F:27:CYS:CB	1:F:61:ILE:HD11	2.18	0.73
2:D:344:ARG:HH11	2:D:344:ARG:HG3	1.52	0.73
2:H:249:LEU:O	2:H:253:VAL:HG23	1.87	0.73
1:A:27:CYS:CB	1:A:61:ILE:HD11	2.19	0.73
1:F:324:ASP:HB3	2:H:64:LYS:HG2	1.71	0.73
2:D:406:LEU:HB2	2:D:407:PRO:HD3	1.71	0.72
2:D:69:PHE:HE1	2:D:71:LEU:HD23	1.52	0.72
1:A:54:HIS:HB3	1:A:78:ASP:OD2	1.89	0.72
2:G:480:GLU:O	2:G:483:PRO:HD2	1.89	0.72
1:B:12:VAL:HA	1:B:28:SER:HB3	1.69	0.72
1:E:54:HIS:HB3	1:E:78:ASP:OD2	1.88	0.72
1:B:81:VAL:HG23	1:B:111:LEU:CD1	2.19	0.72
2:H:42:PRO:CG	2:H:48:LEU:HB2	2.18	0.72
2:G:69:PHE:HE1	2:G:71:LEU:HD23	1.55	0.72
2:G:335:PHE:O	2:G:339:ILE:HG13	1.89	0.72
2:H:184:CYS:HB2	2:H:211:TRP:NE1	2.05	0.72
2:H:278:CYS:HB2	2:H:324:ILE:HG23	1.71	0.72
2:H:478:ASP:OD1	2:H:480:GLU:HB2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:LYS:HG3	1:F:138:ASP:HB3	1.72	0.71
2:G:406:LEU:HB2	2:G:407:PRO:HD3	1.72	0.71
1:B:208:LEU:HD11	1:B:231:ILE:CD1	2.20	0.71
2:H:335:PHE:O	2:H:339:ILE:HG13	1.90	0.71
2:H:552:ILE:O	2:H:556:ILE:N	2.23	0.71
2:D:184:CYS:HB2	2:D:211:TRP:NE1	2.05	0.71
2:H:511:TYR:HD2	2:H:522:MET:SD	2.13	0.71
2:D:278:CYS:HB2	2:D:324:ILE:HG23	1.71	0.71
2:G:402:ILE:HD12	2:G:429:LEU:HB3	1.71	0.71
2:C:278:CYS:HB2	2:C:324:ILE:HG23	1.72	0.71
2:C:402:ILE:HD12	2:C:429:LEU:HB3	1.71	0.71
2:D:43:VAL:HG23	2:D:44:SER:H	1.56	0.71
1:E:334:THR:HG22	1:E:335:TYR:N	2.05	0.71
2:C:454:LEU:HD23	2:C:503:VAL:HG21	1.73	0.71
2:D:148:MET:HE1	2:D:182:LEU:HD22	1.72	0.71
2:C:148:MET:HE1	2:C:182:LEU:HD22	1.72	0.70
2:H:484:VAL:O	2:H:488:LEU:HB2	1.91	0.70
1:B:324:ASP:HB3	2:D:64:LYS:HG2	1.73	0.70
2:D:402:ILE:HD12	2:D:429:LEU:HB3	1.73	0.70
2:G:148:MET:HE1	2:G:182:LEU:HD22	1.71	0.70
1:B:334:THR:HG22	1:B:335:TYR:N	2.05	0.70
2:C:550:HIS:HA	2:C:553:ILE:HD12	1.72	0.70
2:G:523:LEU:HD21	2:G:538:ILE:HG21	1.73	0.70
1:A:124:LYS:HG3	1:A:138:ASP:HB3	1.74	0.70
2:C:335:PHE:O	2:C:339:ILE:HG13	1.91	0.70
1:F:326:GLY:HA3	2:H:58:ILE:HD12	1.73	0.70
1:E:81:VAL:HG23	1:E:111:LEU:CD1	2.21	0.70
1:F:214:LEU:H	1:F:214:LEU:HD12	1.57	0.70
1:F:334:THR:HG22	1:F:335:TYR:N	2.05	0.70
2:D:335:PHE:O	2:D:339:ILE:HG13	1.91	0.69
1:A:334:THR:HG22	1:A:335:TYR:N	2.06	0.69
1:F:345:ILE:HD13	2:H:93:VAL:HG11	1.74	0.69
2:G:98:LEU:HD11	2:G:476:LEU:HD11	1.73	0.69
2:G:454:LEU:HD23	2:G:503:VAL:HG21	1.74	0.69
2:G:515:THR:HG22	2:G:516:ASN:N	2.05	0.69
2:H:402:ILE:HD12	2:H:429:LEU:HB3	1.74	0.69
2:H:555:SER:HA	2:H:558:ASN:HB3	1.73	0.69
2:C:252:LEU:HD23	2:C:257:LEU:HD12	1.73	0.69
2:H:252:LEU:HD23	2:H:257:LEU:HD12	1.74	0.69
2:H:406:LEU:HD12	2:H:461:MET:HE3	1.74	0.69
2:H:553:ILE:HA	2:H:556:ILE:CG2	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:CYS:SG	1:F:61:ILE:HD11	2.34	0.68
2:G:184:CYS:HB2	2:G:211:TRP:NE1	2.08	0.68
2:C:184:CYS:HB2	2:C:211:TRP:NE1	2.08	0.68
2:C:196:ASP:O	2:C:198:GLU:N	2.27	0.68
2:H:231:LYS:HG3	2:H:232:ASP:H	1.57	0.68
1:A:324:ASP:HB3	2:C:64:LYS:HG2	1.75	0.68
2:G:196:ASP:O	2:G:198:GLU:N	2.26	0.68
2:H:148:MET:HE1	2:H:182:LEU:HD22	1.76	0.68
2:H:68:LYS:HB2	2:H:81:PHE:CE1	2.28	0.68
2:G:531:LEU:HD13	2:G:534:ILE:HD12	1.75	0.68
2:H:548:SER:O	2:H:552:ILE:HG13	1.94	0.68
2:C:265:ILE:HG21	2:C:289:ILE:HD11	1.76	0.68
2:C:515:THR:HG22	2:C:516:ASN:N	2.09	0.68
1:F:236:LYS:O	1:F:306:GLU:HG2	1.94	0.68
2:C:68:LYS:HB2	2:C:81:PHE:CE1	2.29	0.68
1:A:71:ILE:HD11	1:A:145:LEU:HD23	1.76	0.67
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.22	0.67
2:C:227:VAL:HG21	2:C:248:LEU:HD12	1.75	0.67
2:H:196:ASP:O	2:H:198:GLU:N	2.27	0.67
2:D:341:GLY:HA2	2:D:346:ILE:HD11	1.76	0.67
2:G:265:ILE:HG21	2:G:289:ILE:HD11	1.76	0.67
1:A:167:SER:HA	1:A:188:LEU:CD2	2.25	0.67
1:A:236:LYS:O	1:A:306:GLU:HG2	1.95	0.67
2:G:252:LEU:HD23	2:G:257:LEU:HD12	1.76	0.67
2:G:278:CYS:CB	2:G:324:ILE:HG23	2.24	0.67
1:F:11:LEU:O	1:F:11:LEU:HD12	1.94	0.67
1:A:177:ARG:HG2	1:A:177:ARG:O	1.95	0.67
1:F:71:ILE:HD11	1:F:145:LEU:HD23	1.77	0.67
1:B:85:GLU:HB3	1:B:101:LEU:HD21	1.77	0.67
2:H:403:HIS:HB2	2:H:461:MET:HE1	1.77	0.67
2:C:89:LYS:N	2:C:89:LYS:HD2	2.09	0.67
1:F:167:SER:HA	1:F:188:LEU:CD2	2.24	0.67
2:H:47:ILE:HD13	2:H:97:ARG:HE	1.60	0.67
1:A:65:SER:OG	1:A:119:ALA:HB2	1.95	0.67
2:C:118:LEU:HD21	2:C:147:ALA:HB2	1.77	0.67
1:E:236:LYS:O	1:E:306:GLU:HG2	1.94	0.67
2:D:89:LYS:N	2:D:89:LYS:HD2	2.09	0.66
1:B:124:LYS:HG3	1:B:138:ASP:HB3	1.77	0.66
2:G:89:LYS:HD2	2:G:89:LYS:N	2.10	0.66
2:H:541:THR:O	2:H:545:GLN:HG3	1.95	0.66
1:A:214:LEU:HD12	1:A:214:LEU:H	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:511:TYR:HD2	2:C:522:MET:SD	2.19	0.66
2:C:533:GLU:OE1	2:C:536:LYS:HD2	1.96	0.66
1:F:85:GLU:HB3	1:F:101:LEU:HD21	1.78	0.66
2:G:169:VAL:HG12	2:G:170:ASN:H	1.59	0.66
1:A:209:PRO:HG3	2:D:315:GLN:HA	1.77	0.66
1:B:214:LEU:H	1:B:214:LEU:HD12	1.61	0.66
2:H:89:LYS:HD2	2:H:89:LYS:N	2.11	0.66
2:D:196:ASP:O	2:D:198:GLU:N	2.29	0.66
2:G:341:GLY:HA2	2:G:346:ILE:HD11	1.77	0.66
2:G:552:ILE:C	2:G:554:GLU:H	2.04	0.66
2:H:240:PHE:CE2	2:H:269:ASP:HB3	2.31	0.66
2:D:42:PRO:HD3	2:D:48:LEU:HB2	1.75	0.66
1:E:241:ARG:HG2	1:E:241:ARG:HH11	1.60	0.66
1:B:11:LEU:O	1:B:11:LEU:HD12	1.96	0.66
1:E:27:CYS:SG	1:E:61:ILE:HD11	2.35	0.66
1:E:214:LEU:H	1:E:214:LEU:HD12	1.60	0.66
2:H:105:SER:HB2	2:H:481:LEU:HD21	1.77	0.66
2:H:454:LEU:HB2	2:H:499:ALA:HB1	1.78	0.66
2:D:42:PRO:HB3	2:D:48:LEU:CB	2.26	0.66
1:E:167:SER:HA	1:E:188:LEU:CD2	2.26	0.66
1:B:236:LYS:O	1:B:306:GLU:HG2	1.96	0.65
1:B:329:ARG:HG2	1:B:344:VAL:HG22	1.77	0.65
2:C:41:ASP:O	2:C:48:LEU:N	2.27	0.65
1:B:177:ARG:O	1:B:177:ARG:HG2	1.96	0.65
2:D:201:ARG:CZ	2:D:205:ILE:HD11	2.26	0.65
1:E:329:ARG:HH12	2:G:44:SER:HB2	1.62	0.65
1:A:326:GLY:HA3	2:C:58:ILE:HD12	1.78	0.65
2:D:523:LEU:HD21	2:D:538:ILE:HG21	1.77	0.65
2:G:42:PRO:HB3	2:G:48:LEU:HD22	1.79	0.65
1:B:159:ILE:HG22	1:B:159:ILE:O	1.97	0.65
2:D:42:PRO:HG3	2:D:48:LEU:HB2	1.77	0.65
1:E:124:LYS:HG3	1:E:138:ASP:HB3	1.77	0.65
1:F:81:VAL:HG23	1:F:111:LEU:CD1	2.25	0.65
1:F:177:ARG:O	1:F:177:ARG:HG2	1.95	0.65
2:H:265:ILE:HG21	2:H:289:ILE:HD11	1.78	0.65
2:C:418:ALA:HB1	2:C:466:LEU:HD23	1.78	0.65
2:H:255:ARG:HB2	2:H:257:LEU:HG	1.77	0.65
2:C:124:PHE:HB2	2:C:426:ALA:O	1.97	0.65
2:H:533:GLU:OE1	2:H:536:LYS:HD2	1.96	0.65
1:A:345:ILE:HD13	2:C:93:VAL:HG11	1.79	0.65
1:E:159:ILE:HG22	1:E:159:ILE:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ARG:O	1:E:177:ARG:HG2	1.97	0.65
1:B:27:CYS:SG	1:B:61:ILE:HD11	2.37	0.65
1:A:27:CYS:SG	1:A:61:ILE:HD11	2.37	0.64
2:D:278:CYS:CB	2:D:324:ILE:HG23	2.27	0.64
2:H:278:CYS:CB	2:H:324:ILE:HG23	2.27	0.64
2:H:335:PHE:CE2	2:H:339:ILE:HD11	2.32	0.64
2:H:546:MET:O	2:H:549:ALA:HB3	1.98	0.64
2:C:255:ARG:HB2	2:C:257:LEU:HG	1.78	0.64
1:B:241:ARG:HG2	1:B:241:ARG:HH11	1.62	0.64
2:C:201:ARG:CZ	2:C:205:ILE:HD11	2.27	0.64
2:C:278:CYS:HB3	2:C:281:SER:HB2	1.79	0.64
2:C:480:GLU:O	2:C:483:PRO:HD2	1.97	0.64
1:F:329:ARG:HG2	1:F:344:VAL:HG22	1.78	0.64
1:B:71:ILE:HD11	1:B:145:LEU:HD23	1.79	0.64
2:G:240:PHE:CE2	2:G:269:ASP:HB3	2.32	0.64
1:A:85:GLU:HB3	1:A:101:LEU:HD21	1.80	0.64
1:A:241:ARG:HG2	1:A:241:ARG:HH11	1.61	0.64
2:D:240:PHE:CE2	2:D:269:ASP:HB3	2.32	0.64
2:C:335:PHE:CE2	2:C:339:ILE:HD11	2.32	0.64
2:D:169:VAL:HG12	2:D:170:ASN:H	1.62	0.64
2:D:252:LEU:HD23	2:D:257:LEU:HD12	1.78	0.64
1:E:205:ALA:HB1	1:E:292:LEU:HD12	1.79	0.64
1:E:208:LEU:HD11	1:E:231:ILE:HD11	1.80	0.64
1:F:167:SER:HA	1:F:188:LEU:HD21	1.80	0.64
2:G:201:ARG:CZ	2:G:205:ILE:HD11	2.28	0.64
2:C:169:VAL:HG12	2:C:170:ASN:H	1.62	0.64
1:E:10:ASP:C	2:G:88:TYR:HE2	2.06	0.64
2:H:278:CYS:HB3	2:H:281:SER:HB2	1.80	0.64
2:C:240:PHE:CE2	2:C:269:ASP:HB3	2.33	0.63
2:H:201:ARG:CZ	2:H:205:ILE:HD11	2.28	0.63
1:A:11:LEU:O	1:A:11:LEU:HD12	1.98	0.63
2:C:114:ILE:HD11	2:C:154:GLU:HG3	1.81	0.63
2:H:118:LEU:HD21	2:H:147:ALA:HB2	1.80	0.63
1:A:167:SER:HA	1:A:188:LEU:HD21	1.81	0.63
1:F:65:SER:OG	1:F:119:ALA:HB2	1.98	0.63
1:F:159:ILE:O	1:F:159:ILE:HG22	1.97	0.63
1:A:12:VAL:HA	1:A:28:SER:CB	2.29	0.63
1:A:159:ILE:O	1:A:159:ILE:HG22	1.99	0.63
2:C:278:CYS:CB	2:C:324:ILE:HG23	2.28	0.63
1:E:85:GLU:HB3	1:E:101:LEU:HD21	1.79	0.63
2:G:402:ILE:CD1	2:G:429:LEU:HD13	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:VAL:HG12	2:H:170:ASN:H	1.64	0.63
2:D:68:LYS:HB2	2:D:81:PHE:CE1	2.34	0.63
1:E:11:LEU:O	1:E:11:LEU:HD12	1.98	0.63
1:E:329:ARG:HG2	1:E:344:VAL:HG22	1.80	0.63
1:F:301:ASP:O	1:F:303:HIS:N	2.32	0.63
2:C:546:MET:O	2:C:549:ALA:HB3	1.99	0.63
2:D:265:ILE:HG21	2:D:289:ILE:HD11	1.80	0.63
1:F:335:TYR:HB3	2:G:373:GLU:HG3	1.80	0.63
2:H:192:LEU:HD11	2:H:204:PHE:CD2	2.33	0.63
2:C:43:VAL:HG13	2:C:48:LEU:CD2	2.18	0.63
1:F:241:ARG:HG2	1:F:241:ARG:HH11	1.63	0.63
1:F:334:THR:HG22	1:F:336:SER:H	1.63	0.63
2:G:278:CYS:HB3	2:G:281:SER:HB2	1.80	0.62
2:G:543:GLY:O	2:G:547:LEU:HG	1.99	0.62
2:H:114:ILE:HD11	2:H:154:GLU:HG3	1.81	0.62
2:H:453:ASP:HB3	2:H:456:SER:HB2	1.81	0.62
2:C:192:LEU:HD11	2:C:204:PHE:CD2	2.35	0.62
2:D:531:LEU:HD13	2:D:534:ILE:HD12	1.81	0.62
2:D:335:PHE:CE2	2:D:339:ILE:HD11	2.33	0.62
1:E:71:ILE:HD11	1:E:145:LEU:HD23	1.80	0.62
2:G:240:PHE:CD2	2:G:268:SER:HB2	2.34	0.62
2:G:197:VAL:HG12	2:G:197:VAL:O	1.99	0.62
2:H:531:LEU:HD13	2:H:534:ILE:HD12	1.80	0.62
2:C:496:THR:HG22	2:C:497:ARG:H	1.65	0.62
2:H:341:GLY:HA2	2:H:346:ILE:HD11	1.82	0.62
1:A:334:THR:HG22	1:A:336:SER:H	1.65	0.62
2:G:68:LYS:HB2	2:G:81:PHE:CE1	2.34	0.62
2:H:480:GLU:O	2:H:483:PRO:HD2	1.98	0.62
1:E:65:SER:OG	1:E:119:ALA:HB2	2.00	0.62
1:A:208:LEU:HD11	1:A:231:ILE:HD11	1.80	0.62
1:B:31:GLN:HG2	1:B:56:SER:O	2.00	0.62
2:C:42:PRO:HB3	2:C:46:ALA:C	2.25	0.62
2:C:541:THR:O	2:C:545:GLN:HG3	2.00	0.62
2:D:42:PRO:HD3	2:D:48:LEU:CB	2.29	0.62
1:A:329:ARG:HH12	2:C:44:SER:HB2	1.64	0.61
2:D:255:ARG:HB2	2:D:257:LEU:HG	1.81	0.61
2:C:197:VAL:O	2:C:197:VAL:HG12	1.99	0.61
2:D:278:CYS:HB3	2:D:281:SER:HB2	1.81	0.61
2:D:402:ILE:CD1	2:D:429:LEU:HD13	2.30	0.61
1:F:12:VAL:HA	1:F:28:SER:CB	2.30	0.61
2:H:197:VAL:O	2:H:197:VAL:HG12	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:HA	1:B:188:LEU:CD2	2.30	0.61
1:B:345:ILE:HD13	2:D:93:VAL:HG11	1.83	0.61
2:D:197:VAL:O	2:D:197:VAL:HG12	2.00	0.61
2:D:240:PHE:CD2	2:D:269:ASP:HB3	2.35	0.61
2:G:255:ARG:HB2	2:G:257:LEU:HG	1.80	0.61
1:B:159:ILE:HD12	1:B:159:ILE:N	2.15	0.61
2:H:515:THR:HB	2:H:518:ASP:OD1	2.00	0.61
1:E:158:SER:C	1:E:159:ILE:HD12	2.26	0.61
1:B:208:LEU:HD11	1:B:231:ILE:HD11	1.82	0.61
1:F:168:ASP:H	1:F:188:LEU:HD23	1.64	0.61
2:C:240:PHE:CD2	2:C:268:SER:HB2	2.35	0.61
1:E:168:ASP:H	1:E:188:LEU:HD23	1.65	0.61
2:H:456:SER:OG	2:H:457:TYR:N	2.33	0.61
1:B:131:ASP:OD2	1:B:133:ILE:HD12	2.01	0.61
1:B:205:ALA:HB1	1:B:292:LEU:HD12	1.83	0.61
2:G:478:ASP:OD1	2:G:480:GLU:HB2	2.01	0.61
2:H:240:PHE:CD2	2:H:268:SER:HB2	2.35	0.61
2:C:523:LEU:O	2:C:526:CYS:HB2	2.00	0.61
2:G:107:TYR:CZ	2:G:111:LEU:HD11	2.36	0.61
1:A:301:ASP:O	1:A:303:HIS:N	2.34	0.60
1:A:329:ARG:HG2	1:A:344:VAL:HG22	1.81	0.60
1:E:226:ARG:HH11	1:E:226:ARG:HG3	1.64	0.60
1:B:158:SER:C	1:B:159:ILE:HD12	2.26	0.60
1:F:214:LEU:HD12	1:F:214:LEU:N	2.16	0.60
1:A:131:ASP:OD2	1:A:133:ILE:HD12	2.02	0.60
1:A:168:ASP:H	1:A:188:LEU:HD23	1.65	0.60
2:C:554:GLU:O	2:C:558:ASN:HB3	2.01	0.60
1:E:345:ILE:HD13	2:G:93:VAL:HG11	1.82	0.60
2:H:334:ASP:O	2:H:338:VAL:HG23	2.01	0.60
1:B:65:SER:OG	1:B:119:ALA:HB2	2.01	0.60
2:H:553:ILE:O	2:H:556:ILE:HG22	2.02	0.60
2:C:459:ASN:OD1	2:C:494:THR:HB	2.00	0.60
2:C:551:ASN:O	2:C:554:GLU:HB3	2.02	0.60
1:E:302:ASP:OD2	2:G:44:SER:HB3	2.01	0.60
1:A:312:TRP:CE2	1:A:319:LEU:HD13	2.36	0.60
2:C:515:THR:CG2	2:C:516:ASN:N	2.65	0.60
1:F:183:LEU:HD12	1:F:184:ALA:N	2.16	0.60
2:G:299:SER:HB3	2:G:302:THR:OG1	2.01	0.60
2:H:392:GLN:HB3	2:H:393:PRO:HD3	1.84	0.60
2:H:510:HIS:O	2:H:512:PRO:HD3	2.02	0.60
2:C:341:GLY:HA2	2:C:346:ILE:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:PHE:CD2	2:D:268:SER:HB2	2.36	0.60
1:E:334:THR:HG22	1:E:336:SER:H	1.67	0.60
2:H:240:PHE:CD2	2:H:269:ASP:HB3	2.37	0.60
2:H:553:ILE:HA	2:H:556:ILE:HG22	1.81	0.60
1:B:334:THR:HG22	1:B:336:SER:H	1.66	0.60
2:D:405:ILE:HG13	2:D:406:LEU:N	2.17	0.60
1:F:208:LEU:HD11	1:F:231:ILE:HD11	1.82	0.60
1:A:117:ALA:HB2	1:A:173:TRP:CZ2	2.37	0.59
1:B:145:LEU:H	1:B:145:LEU:HD12	1.67	0.59
2:D:299:SER:HB3	2:D:302:THR:OG1	2.01	0.59
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.66	0.59
1:E:131:ASP:OD2	1:E:133:ILE:HD12	2.02	0.59
1:E:231:ILE:CD1	1:E:245:ILE:HD11	2.32	0.59
2:G:240:PHE:CD2	2:G:269:ASP:HB3	2.37	0.59
1:E:159:ILE:HD12	1:E:159:ILE:N	2.17	0.59
1:F:312:TRP:CE2	1:F:319:LEU:HD13	2.36	0.59
1:E:12:VAL:HA	1:E:28:SER:CB	2.32	0.59
1:E:117:ALA:HB2	1:E:173:TRP:CZ2	2.37	0.59
1:E:225:GLY:HA2	2:G:503:VAL:HG22	1.85	0.59
2:G:335:PHE:CE2	2:G:339:ILE:HD11	2.38	0.59
2:G:383:VAL:HG12	2:G:384:VAL:N	2.17	0.59
2:H:108:VAL:HG22	2:H:469:PHE:HZ	1.67	0.59
2:C:107:TYR:CZ	2:C:111:LEU:HD11	2.38	0.59
1:A:31:GLN:HG2	1:A:56:SER:O	2.02	0.59
2:C:482:TRP:NE1	2:C:512:PRO:HD2	2.17	0.59
1:E:84:TRP:HA	1:E:99:ASN:O	2.03	0.59
1:B:324:ASP:C	1:B:326:GLY:H	2.09	0.59
2:C:392:GLN:HB3	2:C:393:PRO:HD3	1.85	0.59
2:G:515:THR:CG2	2:G:516:ASN:N	2.65	0.59
1:B:301:ASP:O	1:B:303:HIS:N	2.36	0.59
2:C:240:PHE:CD2	2:C:269:ASP:HB3	2.38	0.59
2:D:392:GLN:HB3	2:D:393:PRO:HD3	1.84	0.59
1:F:111:LEU:HA	1:F:129:GLY:HA2	1.85	0.59
1:F:159:ILE:HD12	1:F:159:ILE:N	2.18	0.59
1:F:226:ARG:HH11	1:F:226:ARG:HG3	1.68	0.59
2:G:192:LEU:HD11	2:G:204:PHE:CD2	2.37	0.59
2:G:196:ASP:C	2:G:198:GLU:H	2.11	0.59
1:B:117:ALA:HB2	1:B:173:TRP:CZ2	2.38	0.59
2:C:78:ASN:HB2	2:C:93:VAL:O	2.03	0.59
2:D:192:LEU:HD11	2:D:204:PHE:CD2	2.38	0.59
2:D:383:VAL:HG12	2:D:384:VAL:N	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:SER:HA	1:E:188:LEU:HD21	1.84	0.59
1:A:159:ILE:N	1:A:159:ILE:HD12	2.18	0.58
1:B:85:GLU:CB	1:B:101:LEU:HD21	2.32	0.58
2:C:231:LYS:CE	2:C:233:SER:HB3	2.30	0.58
1:E:77:TYR:HD1	1:E:110:SER:HB2	1.67	0.58
2:C:299:SER:HB3	2:C:302:THR:OG1	2.03	0.58
2:C:383:VAL:HG12	2:C:384:VAL:N	2.18	0.58
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.38	0.58
1:E:170:CYS:SG	1:E:218:ILE:HG22	2.42	0.58
2:G:274:LEU:HD22	2:G:281:SER:HB3	1.85	0.58
2:G:392:GLN:HB3	2:G:393:PRO:HD3	1.84	0.58
1:B:84:TRP:HA	1:B:99:ASN:O	2.03	0.58
2:D:306:TRP:O	2:D:310:VAL:HG23	2.03	0.58
1:F:85:GLU:CB	1:F:101:LEU:HD21	2.32	0.58
1:F:158:SER:C	1:F:159:ILE:HD12	2.28	0.58
1:F:171:LEU:N	1:F:171:LEU:HD23	2.18	0.58
2:G:103:GLU:CD	2:G:103:GLU:H	2.11	0.58
2:H:227:VAL:HG21	2:H:248:LEU:HD12	1.84	0.58
1:A:84:TRP:HA	1:A:99:ASN:O	2.04	0.58
2:C:295:TYR:HD1	2:C:296:PRO:HD2	1.68	0.58
2:C:334:ASP:O	2:C:338:VAL:HG23	2.03	0.58
1:E:171:LEU:HD23	1:E:171:LEU:N	2.18	0.58
1:E:194:TYR:CE1	1:E:204:VAL:HG22	2.39	0.58
1:F:325:ASP:O	1:F:327:LYS:HG3	2.03	0.58
1:B:168:ASP:H	1:B:188:LEU:HD23	1.68	0.58
1:E:325:ASP:O	1:E:327:LYS:HG3	2.03	0.58
2:G:113:GLU:O	2:G:116:ARG:HG2	2.04	0.58
2:G:451:LEU:CD2	2:G:458:ARG:HG3	2.33	0.58
2:G:546:MET:HE3	2:G:547:LEU:HD23	1.85	0.58
1:A:171:LEU:N	1:A:171:LEU:HD23	2.17	0.58
2:C:274:LEU:HD22	2:C:281:SER:HB3	1.85	0.58
2:H:107:TYR:CZ	2:H:111:LEU:HD11	2.38	0.58
2:H:197:VAL:O	2:H:197:VAL:CG1	2.52	0.58
2:D:227:VAL:HG21	2:D:248:LEU:HD12	1.86	0.58
2:D:454:LEU:CD2	2:D:503:VAL:HG21	2.33	0.58
1:E:31:GLN:HG2	1:E:56:SER:O	2.03	0.58
2:G:394:CYS:O	2:G:398:ILE:HG22	2.04	0.58
2:H:274:LEU:HD22	2:H:281:SER:HB3	1.85	0.58
1:B:12:VAL:HA	1:B:28:SER:CB	2.34	0.58
1:B:171:LEU:HD23	1:B:171:LEU:N	2.18	0.58
2:C:521:TRP:CZ2	2:C:525:ILE:HD11	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:GLU:HB2	1:F:101:LEU:HD11	1.86	0.58
1:A:158:SER:C	1:A:159:ILE:HD12	2.29	0.58
1:A:213:SER:CB	1:A:236:LYS:HB3	2.34	0.58
1:B:325:ASP:O	1:B:327:LYS:HG3	2.03	0.58
2:D:334:ASP:O	2:D:338:VAL:HG23	2.04	0.58
2:H:196:ASP:C	2:H:198:GLU:H	2.12	0.58
2:D:262:ILE:HG23	2:D:289:ILE:HG23	1.86	0.57
2:G:306:TRP:O	2:G:310:VAL:HG23	2.03	0.57
1:A:231:ILE:CD1	1:A:245:ILE:HD11	2.34	0.57
2:D:500:LYS:O	2:D:504:ILE:HG13	2.03	0.57
1:E:214:LEU:HD12	1:E:214:LEU:N	2.19	0.57
1:F:92:GLU:O	1:F:93:CYS:HB2	2.04	0.57
1:F:205:ALA:HB1	1:F:292:LEU:HD12	1.86	0.57
2:H:459:ASN:N	2:H:459:ASN:HD22	2.02	0.57
2:H:186:ARG:HG3	2:H:190:PHE:HB2	1.87	0.57
1:E:301:ASP:O	1:E:303:HIS:N	2.36	0.57
1:E:324:ASP:C	1:E:326:GLY:H	2.12	0.57
1:F:131:ASP:OD2	1:F:133:ILE:HD12	2.03	0.57
1:F:156:VAL:O	1:F:157:LEU:HG	2.03	0.57
2:G:42:PRO:HD3	2:G:48:LEU:CB	2.27	0.57
2:G:186:ARG:HG3	2:G:190:PHE:HB2	1.86	0.57
2:G:406:LEU:HD22	2:G:421:ALA:HB2	1.86	0.57
2:H:299:SER:HB3	2:H:302:THR:OG1	2.04	0.57
2:H:508:LEU:HD11	2:H:522:MET:HG3	1.85	0.57
1:A:183:LEU:HD12	1:A:184:ALA:N	2.20	0.57
1:B:156:VAL:O	1:B:157:LEU:HG	2.04	0.57
2:C:482:TRP:N	2:C:483:PRO:CD	2.67	0.57
2:D:524:SER:O	2:D:527:VAL:HB	2.03	0.57
2:H:166:ASP:HB3	2:H:169:VAL:CG2	2.35	0.57
2:C:478:ASP:O	2:C:480:GLU:N	2.37	0.57
1:E:176:SER:HB2	1:E:223:SER:OG	2.05	0.57
2:G:262:ILE:HG23	2:G:289:ILE:HG23	1.86	0.57
1:E:156:VAL:O	1:E:157:LEU:HG	2.04	0.57
1:E:183:LEU:HD12	1:E:184:ALA:N	2.20	0.57
1:F:77:TYR:HD1	1:F:110:SER:HB2	1.68	0.57
1:A:26:THR:HG22	1:A:27:CYS:H	1.68	0.57
1:A:85:GLU:CB	1:A:101:LEU:HD21	2.34	0.57
1:A:226:ARG:HH11	1:A:226:ARG:HG3	1.70	0.57
2:D:113:GLU:O	2:D:116:ARG:HG2	2.05	0.57
2:D:425:GLU:HB2	2:D:430:ILE:HD11	1.86	0.57
2:H:270:LEU:HG	2:H:271:LEU:N	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:HB1	1:A:292:LEU:HD12	1.87	0.57
1:B:176:SER:HB2	1:B:223:SER:OG	2.04	0.57
2:C:113:GLU:O	2:C:116:ARG:HG2	2.05	0.57
2:C:523:LEU:HD23	2:C:538:ILE:HD12	1.86	0.57
1:E:85:GLU:CB	1:E:101:LEU:HD21	2.35	0.57
1:F:84:TRP:HA	1:F:99:ASN:O	2.04	0.57
2:H:42:PRO:HG3	2:H:48:LEU:HB2	1.86	0.57
2:H:285:VAL:O	2:H:289:ILE:HG13	2.05	0.57
2:H:308:ASN:C	2:H:308:ASN:HD22	2.13	0.57
1:A:38:LEU:HD21	2:C:77:GLN:HG3	1.85	0.57
1:A:156:VAL:O	1:A:157:LEU:HG	2.05	0.57
1:B:231:ILE:CD1	1:B:245:ILE:HD11	2.35	0.57
1:F:117:ALA:HB2	1:F:173:TRP:CZ2	2.40	0.57
2:G:405:ILE:HG13	2:G:406:LEU:N	2.20	0.57
1:A:145:LEU:H	1:A:145:LEU:HD12	1.69	0.56
1:A:176:SER:HB2	1:A:223:SER:OG	2.05	0.56
1:A:324:ASP:C	1:A:326:GLY:H	2.13	0.56
2:C:196:ASP:C	2:C:198:GLU:H	2.12	0.56
2:C:197:VAL:O	2:C:197:VAL:CG1	2.53	0.56
2:C:394:CYS:O	2:C:398:ILE:HG22	2.05	0.56
2:C:496:THR:HG22	2:C:497:ARG:N	2.20	0.56
2:D:394:CYS:O	2:D:398:ILE:HG22	2.05	0.56
2:D:453:ASP:CB	2:D:456:SER:HB2	2.35	0.56
2:D:515:THR:CG2	2:D:516:ASN:N	2.67	0.56
1:F:324:ASP:C	1:F:326:GLY:H	2.13	0.56
1:A:214:LEU:HD12	1:A:214:LEU:N	2.19	0.56
1:B:213:SER:CB	1:B:236:LYS:HB3	2.35	0.56
2:D:515:THR:HG22	2:D:516:ASN:N	2.20	0.56
1:F:31:GLN:HG2	1:F:56:SER:O	2.05	0.56
2:G:425:GLU:HB2	2:G:430:ILE:HD11	1.87	0.56
2:C:163:LYS:HE3	2:C:168:ARG:HH21	1.70	0.56
2:C:550:HIS:O	2:C:553:ILE:HB	2.05	0.56
1:E:121:LEU:HD21	1:E:181:GLU:HB2	1.88	0.56
2:G:500:LYS:O	2:G:504:ILE:HG13	2.06	0.56
2:H:113:GLU:O	2:H:116:ARG:HG2	2.05	0.56
2:H:402:ILE:CD1	2:H:429:LEU:HD13	2.36	0.56
2:H:454:LEU:HD13	2:H:495:GLY:HA3	1.87	0.56
2:C:270:LEU:HG	2:C:271:LEU:N	2.19	0.56
2:C:534:ILE:O	2:C:538:ILE:HG13	2.06	0.56
2:D:42:PRO:CD	2:D:48:LEU:N	2.67	0.56
2:D:197:VAL:O	2:D:197:VAL:CG1	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:VAL:O	2:D:289:ILE:HG13	2.05	0.56
1:F:209:PRO:HG3	2:G:315:GLN:HA	1.88	0.56
2:H:272:PRO:O	2:H:273:TYR:C	2.49	0.56
1:B:194:TYR:CE1	1:B:204:VAL:HG22	2.40	0.56
1:B:322:ALA:HB2	1:B:328:VAL:HG22	1.87	0.56
2:C:554:GLU:O	2:C:558:ASN:N	2.35	0.56
2:D:199:GLU:HG2	2:D:199:GLU:O	2.06	0.56
2:H:231:LYS:HE3	2:H:238:LYS:CG	2.30	0.56
1:A:77:TYR:HD1	1:A:110:SER:HB2	1.69	0.56
2:C:393:PRO:O	2:C:397:ILE:HG13	2.05	0.56
2:D:196:ASP:C	2:D:198:GLU:H	2.13	0.56
2:H:103:GLU:H	2:H:103:GLU:CD	2.13	0.56
1:A:228:TYR:HD2	1:A:244:LYS:HG3	1.71	0.56
1:B:26:THR:HG22	1:B:27:CYS:H	1.70	0.56
1:B:167:SER:HA	1:B:188:LEU:HD21	1.88	0.56
2:C:186:ARG:HG3	2:C:190:PHE:HB2	1.88	0.56
2:H:240:PHE:HD2	2:H:268:SER:HB2	1.71	0.56
1:A:57:SER:HB2	1:A:77:TYR:HD2	1.71	0.56
1:A:209:PRO:HB2	2:D:318:GLY:HA3	1.88	0.56
2:D:470:ALA:HA	2:D:473:LEU:HD12	1.86	0.56
1:F:228:TYR:HD2	1:F:244:LYS:HG3	1.70	0.56
2:G:285:VAL:O	2:G:289:ILE:HG13	2.06	0.56
2:G:296:PRO:CG	2:G:302:THR:HG22	2.36	0.56
2:C:262:ILE:HG23	2:C:289:ILE:HG23	1.88	0.56
2:D:42:PRO:CD	2:D:47:ILE:C	2.79	0.56
2:D:270:LEU:HG	2:D:271:LEU:N	2.20	0.56
2:D:393:PRO:O	2:D:397:ILE:HG13	2.06	0.56
2:D:274:LEU:HD22	2:D:281:SER:HB3	1.88	0.56
1:E:312:TRP:CE2	1:E:319:LEU:HD13	2.41	0.56
1:F:71:ILE:HD11	1:F:145:LEU:CD2	2.36	0.56
1:F:231:ILE:CD1	1:F:245:ILE:HD11	2.36	0.56
2:H:496:THR:HG22	2:H:498:SER:H	1.71	0.56
1:E:26:THR:HG22	1:E:27:CYS:H	1.70	0.55
2:G:197:VAL:O	2:G:197:VAL:CG1	2.52	0.55
2:H:391:GLU:O	2:H:395:VAL:HG23	2.05	0.55
1:B:10:ASP:C	2:D:88:TYR:HE2	2.14	0.55
1:B:214:LEU:HD12	1:B:214:LEU:N	2.20	0.55
2:G:240:PHE:HD2	2:G:268:SER:HB2	1.70	0.55
2:G:295:TYR:HD1	2:G:296:PRO:HD2	1.72	0.55
2:G:492:SER:O	2:G:494:THR:N	2.38	0.55
2:H:515:THR:CG2	2:H:516:ASN:H	2.16	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HA	1:A:129:GLY:HA2	1.89	0.55
1:B:121:LEU:HD21	1:B:181:GLU:HB2	1.89	0.55
2:D:296:PRO:CG	2:D:302:THR:HG22	2.36	0.55
2:D:367:SER:C	2:D:369:GLU:H	2.14	0.55
1:F:26:THR:HG22	1:F:27:CYS:H	1.70	0.55
1:F:121:LEU:HD21	1:F:181:GLU:HB2	1.87	0.55
1:F:209:PRO:HB2	2:G:318:GLY:HA3	1.88	0.55
2:G:484:VAL:O	2:G:488:LEU:HB2	2.05	0.55
2:C:103:GLU:H	2:C:103:GLU:CD	2.14	0.55
1:F:145:LEU:HD12	1:F:145:LEU:H	1.71	0.55
2:G:235:ALA:C	2:G:237:LYS:H	2.14	0.55
2:G:513:PHE:C	2:G:513:PHE:CD1	2.85	0.55
1:A:335:TYR:HB3	2:D:373:GLU:HG3	1.88	0.55
1:B:77:TYR:HD1	1:B:110:SER:HB2	1.69	0.55
1:E:334:THR:CG2	1:E:335:TYR:N	2.70	0.55
2:G:42:PRO:HD2	2:G:46:ALA:O	2.07	0.55
2:H:406:LEU:HD22	2:H:421:ALA:HB2	1.88	0.55
1:A:325:ASP:O	1:A:327:LYS:HG3	2.06	0.55
1:B:57:SER:HB2	1:B:77:TYR:HD2	1.71	0.55
2:C:524:SER:O	2:C:527:VAL:HB	2.06	0.55
2:C:531:LEU:HD13	2:C:534:ILE:HD12	1.88	0.55
2:D:486:ILE:HD12	2:D:504:ILE:HG23	1.89	0.55
1:A:38:LEU:CD2	2:C:77:GLN:HG3	2.37	0.55
1:A:71:ILE:HD11	1:A:145:LEU:CD2	2.36	0.55
2:C:166:ASP:HB3	2:C:169:VAL:CG2	2.36	0.55
1:E:68:TYR:CG	1:E:123:LEU:HD13	2.42	0.55
1:F:38:LEU:HD21	2:H:77:GLN:HG3	1.88	0.55
2:H:383:VAL:HG12	2:H:384:VAL:N	2.20	0.55
2:H:553:ILE:HA	2:H:556:ILE:HG21	1.89	0.55
2:C:367:SER:C	2:C:369:GLU:H	2.15	0.55
2:C:515:THR:HB	2:C:518:ASP:OD1	2.06	0.55
2:D:537:GLU:O	2:D:540:THR:HB	2.07	0.55
1:E:322:ALA:HB2	1:E:328:VAL:HG22	1.88	0.55
2:G:393:PRO:O	2:G:397:ILE:HG13	2.07	0.55
2:H:68:LYS:HD2	2:H:81:PHE:HE1	1.71	0.55
2:H:295:TYR:HD1	2:H:296:PRO:HD2	1.70	0.55
1:F:57:SER:HB2	1:F:77:TYR:HD2	1.71	0.55
2:G:199:GLU:O	2:G:199:GLU:HG2	2.06	0.55
1:A:92:GLU:O	1:A:93:CYS:HB2	2.07	0.55
1:B:178:PHE:CD2	2:D:502:MET:HE3	2.42	0.55
2:D:484:VAL:O	2:D:488:LEU:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:THR:CG2	1:F:335:TYR:N	2.70	0.55
2:H:163:LYS:HE3	2:H:168:ARG:HH21	1.72	0.55
2:H:496:THR:HG22	2:H:497:ARG:N	2.22	0.55
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.71	0.54
1:B:241:ARG:NH1	1:B:299:GLU:OE2	2.40	0.54
2:D:197:VAL:HB	2:D:366:PRO:HB2	1.89	0.54
1:E:92:GLU:O	1:E:93:CYS:HB2	2.06	0.54
1:E:145:LEU:H	1:E:145:LEU:HD12	1.72	0.54
1:E:224:ILE:HD12	1:E:315:THR:HA	1.88	0.54
1:F:120:HIS:HB3	1:F:177:ARG:HG3	1.89	0.54
1:F:192:ILE:CG2	1:F:204:VAL:HG13	2.37	0.54
1:F:213:SER:CB	1:F:236:LYS:HB3	2.36	0.54
2:H:306:TRP:O	2:H:310:VAL:HG23	2.07	0.54
1:A:346:THR:OG1	1:A:347:ALA:N	2.39	0.54
1:B:312:TRP:CE2	1:B:319:LEU:HD13	2.41	0.54
1:B:326:GLY:HA3	2:D:58:ILE:HD12	1.88	0.54
2:C:240:PHE:HD2	2:C:268:SER:HB2	1.70	0.54
2:C:453:ASP:CB	2:C:456:SER:HB2	2.37	0.54
1:F:346:THR:OG1	1:F:347:ALA:N	2.38	0.54
1:B:71:ILE:HD11	1:B:145:LEU:CD2	2.37	0.54
2:C:425:GLU:HB2	2:C:430:ILE:HD11	1.89	0.54
2:D:186:ARG:HG3	2:D:190:PHE:HB2	1.88	0.54
2:D:379:LEU:HD22	2:D:384:VAL:HG22	1.90	0.54
1:E:336:SER:HA	2:H:370:LEU:HD22	1.89	0.54
2:H:394:CYS:O	2:H:398:ILE:HG22	2.07	0.54
2:H:534:ILE:O	2:H:538:ILE:HG13	2.08	0.54
1:A:26:THR:HG22	1:A:27:CYS:N	2.23	0.54
2:C:523:LEU:HD23	2:C:538:ILE:CD1	2.37	0.54
1:E:57:SER:HB2	1:E:77:TYR:HD2	1.72	0.54
1:A:85:GLU:HB2	1:A:101:LEU:HD11	1.88	0.54
1:B:336:SER:HA	2:C:370:LEU:HD22	1.88	0.54
1:F:104:LEU:HD13	1:F:137:TYR:CE2	2.42	0.54
1:F:181:GLU:OE1	1:F:196:ARG:HD3	2.07	0.54
2:G:52:THR:HG22	2:G:53:VAL:N	2.23	0.54
2:G:166:ASP:HB3	2:G:169:VAL:CG2	2.38	0.54
2:G:169:VAL:HG12	2:G:170:ASN:N	2.23	0.54
2:H:367:SER:C	2:H:369:GLU:H	2.16	0.54
1:B:92:GLU:O	1:B:93:CYS:HB2	2.06	0.54
2:C:405:ILE:HG13	2:C:406:LEU:N	2.21	0.54
2:C:406:LEU:HD22	2:C:421:ALA:HB2	1.89	0.54
2:D:103:GLU:CD	2:D:103:GLU:H	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:163:LYS:HE3	2:G:168:ARG:HH21	1.73	0.54
2:G:391:GLU:O	2:G:395:VAL:HG23	2.07	0.54
2:H:199:GLU:O	2:H:199:GLU:HG2	2.07	0.54
2:H:379:LEU:HD22	2:H:384:VAL:HG22	1.90	0.54
1:A:94:SER:OG	1:A:95:GLY:N	2.38	0.54
1:B:133:ILE:HG12	1:B:155:LYS:HG3	1.89	0.54
1:B:170:CYS:SG	1:B:218:ILE:HG22	2.48	0.54
1:E:85:GLU:HB2	1:E:101:LEU:HD11	1.88	0.54
1:E:104:LEU:HD13	1:E:137:TYR:CE2	2.42	0.54
1:F:194:TYR:CE1	1:F:204:VAL:HG22	2.43	0.54
1:F:324:ASP:HB3	2:H:64:LYS:CG	2.36	0.54
2:G:367:SER:C	2:G:369:GLU:H	2.15	0.54
2:G:379:LEU:HD22	2:G:384:VAL:HG22	1.90	0.54
1:B:38:LEU:HD21	2:D:77:GLN:HG3	1.89	0.54
1:B:334:THR:CG2	1:B:335:TYR:N	2.70	0.54
2:C:52:THR:HG22	2:C:53:VAL:N	2.23	0.54
2:C:285:VAL:O	2:C:289:ILE:HG13	2.08	0.54
2:C:296:PRO:CG	2:C:302:THR:HG22	2.37	0.54
2:D:163:LYS:HE3	2:D:168:ARG:HH21	1.72	0.54
2:H:405:ILE:HG13	2:H:406:LEU:N	2.22	0.54
1:A:121:LEU:HD21	1:A:181:GLU:HB2	1.90	0.54
1:A:192:ILE:CG2	1:A:204:VAL:HG13	2.37	0.54
2:C:486:ILE:HD12	2:C:504:ILE:HG23	1.90	0.54
2:D:429:LEU:O	2:D:430:ILE:HG23	2.08	0.54
2:G:344:ARG:HH11	2:G:344:ARG:CG	2.21	0.54
1:B:38:LEU:CD2	2:D:77:GLN:HG3	2.38	0.54
2:D:406:LEU:HD22	2:D:421:ALA:HB2	1.89	0.54
2:H:393:PRO:O	2:H:397:ILE:HG13	2.07	0.54
2:H:515:THR:CG2	2:H:516:ASN:N	2.70	0.54
1:A:334:THR:CG2	1:A:335:TYR:N	2.71	0.53
1:B:85:GLU:HB2	1:B:101:LEU:HD11	1.88	0.53
1:B:96:ARG:HG2	1:B:96:ARG:NH1	2.23	0.53
2:C:43:VAL:HG23	2:C:44:SER:N	2.22	0.53
2:D:272:PRO:O	2:D:273:TYR:C	2.50	0.53
1:F:224:ILE:HD12	1:F:315:THR:HA	1.90	0.53
1:B:111:LEU:HA	1:B:129:GLY:HA2	1.91	0.53
2:C:199:GLU:HG2	2:C:199:GLU:O	2.08	0.53
2:C:272:PRO:O	2:C:273:TYR:C	2.51	0.53
2:C:556:ILE:HG22	2:C:557:ALA:N	2.23	0.53
1:A:194:TYR:CE1	1:A:204:VAL:HG22	2.43	0.53
1:B:181:GLU:OE1	1:B:196:ARG:HD3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LEU:O	2:D:156:GLU:HG3	2.09	0.53
2:D:240:PHE:HD2	2:D:268:SER:HB2	1.72	0.53
1:E:326:GLY:HA3	2:G:58:ILE:HD12	1.90	0.53
2:H:52:THR:HG22	2:H:53:VAL:N	2.22	0.53
2:D:52:THR:HG22	2:D:53:VAL:N	2.23	0.53
2:D:158:PHE:O	2:D:162:VAL:HG23	2.08	0.53
2:D:274:LEU:HD11	2:D:285:VAL:HG21	1.88	0.53
2:H:270:LEU:HD13	2:H:289:ILE:HD12	1.90	0.53
1:B:68:TYR:CG	1:B:123:LEU:HD13	2.44	0.53
1:E:133:ILE:HG12	1:E:155:LYS:HG3	1.91	0.53
2:H:262:ILE:HG23	2:H:289:ILE:HG23	1.91	0.53
2:H:521:TRP:CH2	2:H:525:ILE:HD11	2.44	0.53
1:A:128:LEU:HD22	1:A:185:VAL:CG1	2.38	0.53
1:B:27:CYS:HB3	1:B:61:ILE:CD1	2.33	0.53
2:D:166:ASP:HB3	2:D:169:VAL:CG2	2.39	0.53
1:E:241:ARG:HG2	1:E:241:ARG:NH1	2.23	0.53
2:G:270:LEU:HG	2:G:271:LEU:N	2.23	0.53
2:G:274:LEU:HD11	2:G:285:VAL:HG21	1.90	0.53
2:H:78:ASN:HB2	2:H:93:VAL:O	2.08	0.53
2:H:124:PHE:HB2	2:H:426:ALA:O	2.08	0.53
1:A:181:GLU:OE1	1:A:196:ARG:HD3	2.09	0.53
2:C:402:ILE:CD1	2:C:429:LEU:HD13	2.39	0.53
1:E:86:GLU:HB2	1:E:98:TRP:CH2	2.44	0.53
2:G:270:LEU:HD13	2:G:289:ILE:HD12	1.91	0.53
2:H:482:TRP:N	2:H:483:PRO:CD	2.72	0.53
2:C:306:TRP:O	2:C:310:VAL:HG23	2.09	0.53
1:E:38:LEU:HD21	2:G:77:GLN:HG3	1.89	0.53
1:E:71:ILE:HD11	1:E:145:LEU:CD2	2.39	0.53
1:F:26:THR:HG22	1:F:27:CYS:N	2.24	0.53
2:G:197:VAL:HB	2:G:366:PRO:HB2	1.91	0.53
1:A:241:ARG:HG2	1:A:241:ARG:NH1	2.24	0.53
2:C:68:LYS:HD2	2:C:81:PHE:HE1	1.74	0.53
2:D:270:LEU:HD13	2:D:289:ILE:HD12	1.91	0.53
2:D:308:ASN:HD22	2:D:308:ASN:C	2.16	0.53
2:D:391:GLU:O	2:D:395:VAL:HG23	2.09	0.53
2:D:422:MET:SD	2:D:423:ILE:N	2.82	0.53
1:E:96:ARG:HG2	1:E:96:ARG:HH11	1.72	0.53
2:G:86:ASP:HA	2:G:88:TYR:HE1	1.74	0.53
1:A:104:LEU:HD13	1:A:137:TYR:CE2	2.43	0.53
1:A:133:ILE:HG12	1:A:155:LYS:HG3	1.90	0.53
2:C:270:LEU:HD13	2:C:289:ILE:HD12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:308:ASN:C	2:C:308:ASN:HD22	2.16	0.53
2:C:521:TRP:CE2	2:C:525:ILE:HD11	2.44	0.53
1:E:111:LEU:HA	1:E:129:GLY:HA2	1.90	0.53
1:F:236:LYS:HG2	1:F:306:GLU:OE1	2.09	0.53
2:H:274:LEU:HD11	2:H:285:VAL:HG21	1.90	0.53
2:H:508:LEU:HB3	2:H:509:PRO:HD3	1.90	0.53
2:C:166:ASP:HB3	2:C:169:VAL:HG23	1.92	0.52
1:E:128:LEU:HD22	1:E:185:VAL:CG1	2.38	0.52
1:A:120:HIS:HB3	1:A:177:ARG:HG3	1.91	0.52
1:A:224:ILE:HD12	1:A:315:THR:HA	1.91	0.52
1:A:241:ARG:NH1	1:A:299:GLU:OE2	2.42	0.52
1:E:194:TYR:HE1	1:E:204:VAL:HG22	1.74	0.52
1:F:326:GLY:CA	2:H:58:ILE:HD12	2.39	0.52
2:C:43:VAL:HG23	2:C:44:SER:H	1.74	0.52
2:C:274:LEU:HD11	2:C:285:VAL:HG21	1.90	0.52
2:C:379:LEU:HD22	2:C:384:VAL:HG22	1.91	0.52
2:C:470:ALA:O	2:C:473:LEU:HB2	2.09	0.52
2:D:313:LEU:HD23	2:D:313:LEU:C	2.35	0.52
1:E:15:VAL:HG21	2:G:90:LEU:HD21	1.91	0.52
1:E:213:SER:CB	1:E:236:LYS:HB3	2.37	0.52
1:F:120:HIS:CB	1:F:177:ARG:HG3	2.39	0.52
1:B:128:LEU:HD22	1:B:185:VAL:CG1	2.39	0.52
2:C:152:LEU:O	2:C:156:GLU:HG3	2.09	0.52
2:C:453:ASP:HB3	2:C:456:SER:HB2	1.90	0.52
1:E:26:THR:HG22	1:E:27:CYS:N	2.23	0.52
1:F:176:SER:HB2	1:F:223:SER:OG	2.09	0.52
2:H:379:LEU:CD2	2:H:384:VAL:HG22	2.39	0.52
2:H:453:ASP:CB	2:H:456:SER:HB2	2.39	0.52
2:C:391:GLU:O	2:C:395:VAL:HG23	2.09	0.52
2:D:118:LEU:O	2:D:119:GLY:C	2.53	0.52
1:E:141:GLU:HG2	1:E:143:SER:OG	2.08	0.52
1:F:190:GLN:O	1:F:215:ILE:HD12	2.10	0.52
1:F:241:ARG:NH1	1:F:299:GLU:OE2	2.43	0.52
2:G:117:ASP:C	2:G:119:GLY:H	2.18	0.52
2:H:166:ASP:HB3	2:H:169:VAL:HG23	1.92	0.52
2:H:425:GLU:HB2	2:H:430:ILE:HD11	1.91	0.52
2:G:42:PRO:CG	2:G:48:LEU:HB2	2.39	0.52
2:G:269:ASP:O	2:G:270:LEU:C	2.53	0.52
1:B:104:LEU:HD13	1:B:137:TYR:CE2	2.43	0.52
1:B:192:ILE:CG2	1:B:204:VAL:HG13	2.39	0.52
1:E:96:ARG:HG2	1:E:96:ARG:NH1	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:ILE:CG2	1:E:204:VAL:HG13	2.40	0.52
1:F:346:THR:O	2:H:51:MET:HE2	2.09	0.52
2:G:118:LEU:O	2:G:119:GLY:C	2.52	0.52
1:B:183:LEU:HD12	1:B:184:ALA:N	2.24	0.52
1:B:190:GLN:O	1:B:215:ILE:HD12	2.09	0.52
2:D:68:LYS:HD2	2:D:81:PHE:HE1	1.74	0.52
1:F:141:GLU:HG2	1:F:143:SER:OG	2.10	0.52
2:G:204:PHE:HD1	2:G:205:ILE:N	2.07	0.52
2:H:508:LEU:HD11	2:H:522:MET:CG	2.40	0.52
1:A:190:GLN:O	1:A:215:ILE:HD12	2.10	0.52
1:B:120:HIS:HB3	1:B:177:ARG:HG3	1.92	0.52
2:C:492:SER:O	2:C:500:LYS:NZ	2.37	0.52
1:F:128:LEU:HD22	1:F:185:VAL:CG1	2.40	0.52
1:F:322:ALA:HB2	1:F:328:VAL:HG22	1.91	0.52
1:A:322:ALA:HB2	1:A:328:VAL:HG22	1.91	0.52
1:A:334:THR:HG22	1:A:335:TYR:H	1.75	0.52
1:B:241:ARG:HG2	1:B:241:ARG:NH1	2.25	0.52
2:C:379:LEU:HD11	2:C:395:VAL:CG1	2.40	0.52
2:C:533:GLU:OE1	2:C:533:GLU:HA	2.10	0.52
2:D:104:PHE:C	2:D:106:ALA:H	2.18	0.52
2:D:269:ASP:O	2:D:270:LEU:C	2.52	0.52
2:D:379:LEU:CD2	2:D:384:VAL:HG22	2.40	0.52
1:F:38:LEU:CD2	2:H:77:GLN:HG3	2.39	0.52
2:D:295:TYR:HD1	2:D:296:PRO:HD2	1.74	0.51
1:F:324:ASP:HB3	2:H:64:LYS:HB3	1.92	0.51
1:A:120:HIS:CB	1:A:177:ARG:HG3	2.40	0.51
2:D:204:PHE:HD1	2:D:205:ILE:N	2.08	0.51
2:H:549:ALA:O	2:H:550:HIS:C	2.52	0.51
1:B:224:ILE:HD12	1:B:315:THR:HA	1.91	0.51
1:E:329:ARG:NH1	2:G:44:SER:HB2	2.25	0.51
2:G:457:TYR:C	2:G:457:TYR:CD1	2.89	0.51
2:H:152:LEU:O	2:H:156:GLU:HG3	2.10	0.51
2:H:296:PRO:CG	2:H:302:THR:HG22	2.37	0.51
1:B:346:THR:OG1	1:B:347:ALA:N	2.41	0.51
2:G:379:LEU:CD2	2:G:384:VAL:HG22	2.40	0.51
2:C:192:LEU:HD11	2:C:204:PHE:HD2	1.76	0.51
2:D:453:ASP:HB2	2:D:456:SER:HB2	1.91	0.51
1:F:214:LEU:H	1:F:214:LEU:CD1	2.22	0.51
2:G:537:GLU:O	2:G:540:THR:HB	2.10	0.51
2:H:335:PHE:CD2	2:H:339:ILE:HD11	2.46	0.51
1:B:26:THR:HG22	1:B:27:CYS:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:429:LEU:O	2:C:430:ILE:HG23	2.11	0.51
2:D:78:ASN:HB2	2:D:93:VAL:O	2.11	0.51
2:D:86:ASP:HA	2:D:88:TYR:HE1	1.75	0.51
1:F:94:SER:OG	1:F:95:GLY:N	2.41	0.51
2:G:272:PRO:O	2:G:273:TYR:C	2.53	0.51
2:H:461:MET:O	2:H:465:MET:HG3	2.11	0.51
1:A:136:LEU:HD11	1:A:202:LEU:HD11	1.93	0.51
2:C:478:ASP:C	2:C:480:GLU:N	2.69	0.51
2:D:97:ARG:HD2	2:D:174:GLU:OE2	2.11	0.51
2:C:478:ASP:C	2:C:480:GLU:H	2.19	0.51
2:D:534:ILE:O	2:D:538:ILE:HG13	2.10	0.51
1:E:94:SER:OG	1:E:95:GLY:N	2.43	0.51
1:F:133:ILE:HG12	1:F:155:LYS:HG3	1.92	0.51
2:G:429:LEU:O	2:G:430:ILE:HG23	2.11	0.51
1:B:86:GLU:HB2	1:B:98:TRP:CH2	2.46	0.51
1:B:94:SER:OG	1:B:95:GLY:N	2.44	0.51
1:B:334:THR:HG22	1:B:335:TYR:H	1.75	0.51
2:C:457:TYR:CD1	2:C:457:TYR:C	2.89	0.51
2:D:322:THR:HG23	2:D:324:ILE:HG12	1.92	0.51
1:E:190:GLN:O	1:E:215:ILE:HD12	2.11	0.51
1:F:241:ARG:HG2	1:F:241:ARG:NH1	2.26	0.51
2:G:369:GLU:HG2	2:H:457:TYR:O	2.11	0.51
1:A:108:LYS:HE2	1:A:133:ILE:CD1	2.40	0.51
1:B:228:TYR:HD2	1:B:244:LYS:HG3	1.76	0.51
2:C:56:GLN:HG3	2:C:56:GLN:O	2.11	0.51
2:C:269:ASP:O	2:C:270:LEU:C	2.53	0.51
2:D:42:PRO:CB	2:D:48:LEU:HD22	2.27	0.51
2:D:335:PHE:CD2	2:D:339:ILE:HD11	2.46	0.51
1:E:34:LYS:HE2	1:E:50:SER:OG	2.11	0.51
1:E:125:LEU:C	1:E:125:LEU:HD12	2.36	0.51
1:E:221:ALA:HB2	1:E:312:TRP:CE2	2.46	0.51
1:F:125:LEU:C	1:F:125:LEU:HD12	2.36	0.51
1:B:125:LEU:HD12	1:B:125:LEU:C	2.36	0.50
2:C:231:LYS:H	2:C:234:THR:HB	1.75	0.50
2:D:42:PRO:HB3	2:D:48:LEU:CG	2.40	0.50
1:E:241:ARG:NH1	1:E:299:GLU:OE2	2.43	0.50
1:E:245:ILE:HA	1:E:293:GLN:O	2.11	0.50
2:G:158:PHE:O	2:G:162:VAL:HG23	2.11	0.50
1:E:228:TYR:HD2	1:E:244:LYS:HG3	1.77	0.50
1:A:236:LYS:HG2	1:A:306:GLU:OE1	2.11	0.50
1:A:336:SER:HA	2:D:370:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:O	2:C:51:MET:HE2	2.12	0.50
2:C:373:GLU:O	2:C:377:MET:HG3	2.12	0.50
2:C:508:LEU:HB3	2:C:509:PRO:HD3	1.94	0.50
2:G:481:LEU:O	2:G:484:VAL:HB	2.12	0.50
2:C:423:ILE:O	2:C:426:ALA:HB3	2.11	0.50
2:D:117:ASP:C	2:D:119:GLY:H	2.19	0.50
1:E:310:VAL:HG13	1:E:310:VAL:O	2.11	0.50
1:F:34:LYS:HE2	1:F:50:SER:OG	2.12	0.50
1:B:108:LYS:HE2	1:B:133:ILE:CD1	2.41	0.50
2:D:246:TRP:CE2	2:D:331:TYR:HB3	2.47	0.50
1:E:231:ILE:HD11	1:E:245:ILE:HD11	1.93	0.50
1:F:295:GLU:HG2	2:G:311:LEU:HD21	1.94	0.50
2:G:313:LEU:HD23	2:G:313:LEU:C	2.36	0.50
2:G:422:MET:SD	2:G:423:ILE:N	2.85	0.50
2:C:375:LEU:HD11	2:C:395:VAL:HG13	1.94	0.50
2:C:557:ALA:O	2:C:561:ARG:N	2.39	0.50
2:G:246:TRP:CE2	2:G:331:TYR:HB3	2.47	0.50
2:H:492:SER:O	2:H:500:LYS:NZ	2.41	0.50
2:C:158:PHE:O	2:C:162:VAL:HG23	2.12	0.50
2:G:514:VAL:HG12	2:G:515:THR:N	2.27	0.50
1:B:34:LYS:HE2	1:B:50:SER:OG	2.12	0.50
2:C:204:PHE:HD1	2:C:205:ILE:N	2.09	0.50
2:D:42:PRO:HD2	2:D:47:ILE:CA	2.42	0.50
2:G:152:LEU:O	2:G:156:GLU:HG3	2.12	0.50
2:C:169:VAL:HG12	2:C:170:ASN:N	2.27	0.50
2:C:379:LEU:CD2	2:C:384:VAL:HG22	2.42	0.50
2:D:271:LEU:N	2:D:272:PRO:CD	2.75	0.50
1:E:38:LEU:CD2	2:G:77:GLN:HG3	2.41	0.50
2:H:344:ARG:HH11	2:H:344:ARG:CG	2.21	0.50
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.27	0.49
2:D:169:VAL:HG12	2:D:170:ASN:N	2.25	0.49
2:D:190:PHE:CZ	2:D:427:LYS:HG3	2.47	0.49
1:F:221:ALA:HB2	1:F:312:TRP:CE2	2.47	0.49
2:G:214:ARG:O	2:G:214:ARG:HG3	2.12	0.49
2:G:451:LEU:CD1	2:G:458:ARG:HG3	2.42	0.49
2:H:379:LEU:HD11	2:H:395:VAL:CG1	2.42	0.49
1:B:194:TYR:HE1	1:B:204:VAL:HG22	1.77	0.49
2:D:214:ARG:O	2:D:214:ARG:HG3	2.11	0.49
1:E:120:HIS:HB3	1:E:177:ARG:HG3	1.94	0.49
2:G:68:LYS:HD2	2:G:81:PHE:HE1	1.77	0.49
2:G:166:ASP:HB3	2:G:169:VAL:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:322:THR:HG23	2:G:324:ILE:HG12	1.92	0.49
2:H:94:ARG:HH21	2:H:98:LEU:HB3	1.76	0.49
2:H:98:LEU:HD11	2:H:476:LEU:CD1	2.42	0.49
2:H:429:LEU:O	2:H:430:ILE:HG23	2.12	0.49
2:H:482:TRP:O	2:H:486:ILE:HG12	2.12	0.49
1:B:141:GLU:HG2	1:B:143:SER:OG	2.12	0.49
2:C:173:TYR:HA	2:C:176:GLU:HB2	1.93	0.49
2:C:204:PHE:CD1	2:C:204:PHE:C	2.90	0.49
2:D:56:GLN:O	2:D:56:GLN:HG3	2.11	0.49
1:F:194:TYR:HE1	1:F:204:VAL:HG22	1.77	0.49
1:A:86:GLU:HB2	1:A:98:TRP:CH2	2.47	0.49
1:A:221:ALA:HB2	1:A:312:TRP:CE2	2.47	0.49
1:E:128:LEU:HD22	1:E:185:VAL:HG11	1.94	0.49
2:G:334:ASP:O	2:G:338:VAL:HG23	2.10	0.49
1:A:194:TYR:HE1	1:A:204:VAL:HG22	1.78	0.49
1:B:221:ALA:HB2	1:B:312:TRP:CE2	2.47	0.49
1:B:245:ILE:HA	1:B:293:GLN:O	2.11	0.49
2:C:69:PHE:HD2	2:C:80:ALA:HB2	1.76	0.49
2:C:69:PHE:CD2	2:C:80:ALA:HB2	2.47	0.49
1:E:27:CYS:HB3	1:E:61:ILE:CD1	2.37	0.49
2:G:192:LEU:HD11	2:G:204:PHE:HD2	1.77	0.49
2:G:227:VAL:HG21	2:G:248:LEU:HD12	1.93	0.49
2:G:308:ASN:HD22	2:G:308:ASN:C	2.19	0.49
2:H:118:LEU:O	2:H:119:GLY:C	2.56	0.49
1:A:141:GLU:HG2	1:A:143:SER:OG	2.12	0.49
2:C:42:PRO:HA	2:C:46:ALA:O	2.13	0.49
2:C:118:LEU:O	2:C:119:GLY:C	2.55	0.49
2:C:268:SER:O	2:C:272:PRO:HD2	2.12	0.49
2:C:482:TRP:N	2:C:483:PRO:HD3	2.25	0.49
2:D:204:PHE:CD1	2:D:204:PHE:C	2.90	0.49
1:E:10:ASP:C	2:G:88:TYR:CE2	2.90	0.49
1:F:136:LEU:HD11	1:F:202:LEU:HD11	1.94	0.49
2:G:204:PHE:CD1	2:G:204:PHE:C	2.90	0.49
2:C:86:ASP:HA	2:C:88:TYR:HE1	1.77	0.49
2:C:104:PHE:C	2:C:106:ALA:H	2.20	0.49
2:D:86:ASP:N	2:D:88:TYR:CE1	2.80	0.49
2:H:155:LEU:O	2:H:159:ILE:HG13	2.13	0.49
1:B:120:HIS:CB	1:B:177:ARG:HG3	2.43	0.49
2:C:335:PHE:CD2	2:C:339:ILE:HD11	2.48	0.49
1:F:334:THR:HG22	1:F:335:TYR:H	1.75	0.49
2:G:86:ASP:HA	2:G:88:TYR:CE1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:ASP:C	2:H:119:GLY:H	2.20	0.49
2:H:471:PHE:C	2:H:473:LEU:N	2.71	0.49
2:D:166:ASP:HB3	2:D:169:VAL:HG23	1.95	0.49
2:G:69:PHE:HD2	2:G:80:ALA:HB2	1.76	0.49
2:H:231:LYS:HG3	2:H:232:ASP:N	2.27	0.49
2:H:398:ILE:HG23	2:H:399:SER:N	2.28	0.49
2:H:549:ALA:O	2:H:551:ASN:N	2.45	0.49
1:A:193:ILE:CD1	1:A:245:ILE:HD13	2.43	0.49
1:A:247:GLU:HB3	1:A:292:LEU:HD23	1.94	0.49
1:B:236:LYS:HG2	1:B:306:GLU:OE1	2.13	0.49
2:D:423:ILE:O	2:D:426:ALA:HB3	2.12	0.49
1:E:11:LEU:N	2:G:88:TYR:HE2	2.10	0.49
1:E:236:LYS:HG2	1:E:306:GLU:OE1	2.12	0.49
2:H:104:PHE:O	2:H:107:TYR:N	2.46	0.49
1:A:79:LYS:HG2	1:A:110:SER:N	2.28	0.48
1:A:125:LEU:C	1:A:125:LEU:HD12	2.38	0.48
1:A:128:LEU:HD22	1:A:185:VAL:HG11	1.95	0.48
2:C:535:ALA:HA	2:C:538:ILE:HD12	1.95	0.48
2:D:508:LEU:C	2:D:510:HIS:H	2.19	0.48
1:F:79:LYS:HG2	1:F:110:SER:N	2.27	0.48
1:F:231:ILE:HD11	1:F:245:ILE:HD11	1.95	0.48
2:G:508:LEU:C	2:G:510:HIS:N	2.71	0.48
2:H:231:LYS:NZ	2:H:238:LYS:HD3	2.28	0.48
1:F:168:ASP:H	1:F:188:LEU:CD2	2.26	0.48
2:H:158:PHE:O	2:H:162:VAL:HG23	2.12	0.48
2:H:204:PHE:O	2:H:206:GLU:N	2.46	0.48
2:H:344:ARG:HG3	2:H:344:ARG:NH1	2.25	0.48
1:A:114:VAL:HG23	1:A:126:ALA:O	2.13	0.48
1:A:208:LEU:HD11	1:A:231:ILE:HD12	1.94	0.48
2:C:515:THR:HG22	2:C:517:ASP:N	2.20	0.48
2:H:173:TYR:HA	2:H:176:GLU:HB2	1.95	0.48
1:A:68:TYR:CG	1:A:123:LEU:HD13	2.49	0.48
1:B:247:GLU:HB3	1:B:292:LEU:HD23	1.95	0.48
2:G:515:THR:HG22	2:G:517:ASP:N	2.22	0.48
2:G:552:ILE:O	2:G:552:ILE:HG22	2.13	0.48
2:H:268:SER:O	2:H:272:PRO:HD2	2.13	0.48
1:A:138:ASP:HA	1:A:148:TRP:CE3	2.49	0.48
1:E:334:THR:HG22	1:E:335:TYR:H	1.74	0.48
2:G:56:GLN:HG3	2:G:56:GLN:O	2.13	0.48
2:G:69:PHE:CD2	2:G:80:ALA:HB2	2.49	0.48
2:C:322:THR:HG23	2:C:324:ILE:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:LEU:HD12	2:D:99:ASP:H	1.78	0.48
2:D:104:PHE:C	2:D:106:ALA:N	2.72	0.48
1:E:181:GLU:OE1	1:E:196:ARG:HD3	2.13	0.48
2:H:56:GLN:HG3	2:H:56:GLN:O	2.13	0.48
2:H:189:TYR:O	2:H:427:LYS:HE3	2.14	0.48
1:A:247:GLU:HB3	1:A:292:LEU:CD2	2.44	0.48
1:B:310:VAL:O	1:B:310:VAL:HG13	2.14	0.48
2:C:532:PRO:HG2	2:C:533:GLU:H	1.78	0.48
2:D:145:ASN:OD1	2:D:190:PHE:HA	2.14	0.48
2:D:525:ILE:C	2:D:527:VAL:N	2.71	0.48
1:E:214:LEU:H	1:E:214:LEU:CD1	2.25	0.48
1:E:324:ASP:HB3	2:G:64:LYS:CG	2.42	0.48
1:F:128:LEU:HD22	1:F:185:VAL:HG11	1.96	0.48
1:F:247:GLU:HB3	1:F:292:LEU:HD23	1.94	0.48
2:H:269:ASP:O	2:H:270:LEU:C	2.55	0.48
1:A:15:VAL:O	2:C:70:LYS:HD2	2.13	0.48
2:C:344:ARG:HH11	2:C:344:ARG:CG	2.20	0.48
2:D:344:ARG:HG3	2:D:344:ARG:NH1	2.26	0.48
2:D:478:ASP:O	2:D:480:GLU:N	2.47	0.48
2:G:398:ILE:HG23	2:G:399:SER:N	2.29	0.48
2:H:104:PHE:C	2:H:106:ALA:H	2.19	0.48
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.78	0.48
1:B:224:ILE:HG22	2:D:471:PHE:CZ	2.48	0.48
1:B:231:ILE:HD11	1:B:245:ILE:HD11	1.94	0.48
1:B:247:GLU:HB3	1:B:292:LEU:CD2	2.44	0.48
2:D:268:SER:O	2:D:272:PRO:HD2	2.13	0.48
1:F:86:GLU:HB2	1:F:98:TRP:CH2	2.48	0.48
2:G:103:GLU:CD	2:G:103:GLU:N	2.71	0.48
2:G:151:ILE:O	2:G:152:LEU:C	2.57	0.48
2:G:523:LEU:HD23	2:G:538:ILE:CD1	2.43	0.48
2:H:169:VAL:HG12	2:H:170:ASN:N	2.27	0.48
2:C:155:LEU:O	2:C:159:ILE:HG13	2.13	0.48
2:C:271:LEU:N	2:C:272:PRO:CD	2.77	0.48
2:C:508:LEU:HD11	2:C:522:MET:HG3	1.96	0.48
2:D:204:PHE:O	2:D:206:GLU:N	2.47	0.48
2:D:398:ILE:HG23	2:D:399:SER:N	2.29	0.48
2:D:492:SER:C	2:D:494:THR:H	2.22	0.48
1:E:226:ARG:HG3	1:E:226:ARG:NH1	2.28	0.48
1:F:96:ARG:NH1	1:F:96:ARG:HG2	2.29	0.48
1:F:151:THR:HG22	1:F:152:SER:N	2.29	0.48
2:G:78:ASN:HB2	2:G:93:VAL:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:190:PHE:CZ	2:G:427:LYS:HG3	2.48	0.48
2:H:52:THR:HG22	2:H:54:ASN:H	1.79	0.48
2:H:422:MET:SD	2:H:423:ILE:N	2.87	0.48
2:H:459:ASN:HB3	2:H:494:THR:CB	2.44	0.48
2:H:471:PHE:O	2:H:473:LEU:N	2.47	0.48
1:B:214:LEU:H	1:B:214:LEU:CD1	2.25	0.47
2:C:86:ASP:HA	2:C:88:TYR:CE1	2.49	0.47
2:C:226:GLN:C	2:C:228:PHE:H	2.21	0.47
2:C:460:GLY:C	2:C:462:ALA:N	2.69	0.47
2:D:52:THR:HG22	2:D:54:ASN:H	1.79	0.47
1:E:54:HIS:HD2	1:E:58:ILE:HG12	1.78	0.47
1:E:193:ILE:CD1	1:E:245:ILE:HD13	2.44	0.47
2:G:104:PHE:C	2:G:106:ALA:H	2.21	0.47
2:G:173:TYR:HA	2:G:176:GLU:HB2	1.95	0.47
2:G:268:SER:O	2:G:272:PRO:HD2	2.13	0.47
2:H:192:LEU:HD11	2:H:204:PHE:HD2	1.75	0.47
2:C:117:ASP:C	2:C:119:GLY:H	2.22	0.47
1:E:247:GLU:HB3	1:E:292:LEU:HD23	1.96	0.47
1:F:54:HIS:CE1	1:F:82:LYS:HB2	2.49	0.47
1:F:108:LYS:HE2	1:F:133:ILE:CD1	2.44	0.47
2:G:86:ASP:N	2:G:88:TYR:CE1	2.82	0.47
2:G:469:PHE:O	2:G:472:GLU:N	2.47	0.47
2:H:69:PHE:HD2	2:H:80:ALA:HB2	1.79	0.47
2:C:52:THR:HG22	2:C:54:ASN:H	1.79	0.47
2:D:502:MET:O	2:D:505:ALA:HB3	2.15	0.47
1:E:108:LYS:HE2	1:E:133:ILE:CD1	2.43	0.47
1:E:120:HIS:CB	1:E:177:ARG:HG3	2.44	0.47
1:E:247:GLU:HB3	1:E:292:LEU:CD2	2.45	0.47
2:G:505:ALA:HB2	2:G:531:LEU:HD22	1.95	0.47
2:H:153:ASN:O	2:H:156:GLU:N	2.46	0.47
1:B:128:LEU:HD22	1:B:185:VAL:HG11	1.97	0.47
2:D:226:GLN:C	2:D:228:PHE:H	2.21	0.47
1:F:247:GLU:HB3	1:F:292:LEU:CD2	2.44	0.47
2:G:250:ASN:O	2:G:254:LEU:HG	2.13	0.47
2:G:271:LEU:N	2:G:272:PRO:CD	2.77	0.47
2:H:81:PHE:CD1	2:H:81:PHE:C	2.92	0.47
2:H:204:PHE:HD1	2:H:205:ILE:N	2.12	0.47
2:H:470:ALA:O	2:H:473:LEU:HB2	2.15	0.47
2:C:103:GLU:CD	2:C:103:GLU:N	2.73	0.47
2:C:204:PHE:O	2:C:206:GLU:N	2.48	0.47
2:D:86:ASP:HA	2:D:88:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:GLU:HA	2:D:300:SER:OG	2.14	0.47
1:F:96:ARG:HG2	1:F:96:ARG:HH11	1.80	0.47
2:G:204:PHE:O	2:G:206:GLU:N	2.48	0.47
2:G:240:PHE:HD2	2:G:268:SER:CB	2.28	0.47
2:H:532:PRO:O	2:H:535:ALA:HB3	2.15	0.47
1:A:310:VAL:O	1:A:310:VAL:HG13	2.15	0.47
2:D:228:PHE:CE2	2:D:267:ARG:HG3	2.49	0.47
2:D:324:ILE:O	2:D:325:SER:C	2.58	0.47
2:G:112:PHE:O	2:G:115:TYR:HB3	2.14	0.47
1:A:97:ARG:HH11	1:A:97:ARG:HG3	1.80	0.47
1:A:214:LEU:H	1:A:214:LEU:CD1	2.26	0.47
1:A:324:ASP:HB3	2:C:64:LYS:CG	2.43	0.47
2:C:104:PHE:C	2:C:106:ALA:N	2.73	0.47
2:D:104:PHE:O	2:D:107:TYR:N	2.47	0.47
2:D:155:LEU:O	2:D:159:ILE:HG13	2.14	0.47
2:D:238:LYS:O	2:D:239:VAL:C	2.57	0.47
1:F:68:TYR:CG	1:F:123:LEU:HD13	2.49	0.47
2:G:155:LEU:O	2:G:159:ILE:HG13	2.14	0.47
2:G:505:ALA:HB2	2:G:531:LEU:CD2	2.45	0.47
2:H:98:LEU:HD12	2:H:99:ASP:H	1.79	0.47
2:H:104:PHE:C	2:H:106:ALA:N	2.72	0.47
2:H:184:CYS:HB2	2:H:211:TRP:CE2	2.49	0.47
2:H:204:PHE:CD1	2:H:204:PHE:C	2.92	0.47
2:H:226:GLN:C	2:H:228:PHE:H	2.22	0.47
2:H:322:THR:HG23	2:H:324:ILE:HG12	1.95	0.47
1:A:231:ILE:HD11	1:A:245:ILE:HD11	1.96	0.47
2:C:112:PHE:O	2:C:115:TYR:HB3	2.14	0.47
2:C:189:TYR:O	2:C:427:LYS:HE3	2.15	0.47
2:D:108:VAL:HG22	2:D:469:PHE:HZ	1.80	0.47
2:D:498:SER:O	2:D:499:ALA:C	2.57	0.47
1:E:346:THR:OG1	1:E:347:ALA:N	2.40	0.47
2:G:335:PHE:CD2	2:G:339:ILE:HD11	2.50	0.47
2:H:271:LEU:O	2:H:275:SER:HB3	2.15	0.47
2:H:375:LEU:HD11	2:H:395:VAL:HG13	1.96	0.47
1:A:168:ASP:H	1:A:188:LEU:CD2	2.27	0.47
2:C:398:ILE:HG23	2:C:399:SER:N	2.29	0.47
2:C:487:GLY:O	2:C:488:LEU:C	2.57	0.47
2:D:112:PHE:O	2:D:115:TYR:HB3	2.15	0.47
2:D:173:TYR:HA	2:D:176:GLU:HB2	1.95	0.47
1:E:81:VAL:CG2	1:E:111:LEU:HD13	2.33	0.47
2:G:98:LEU:HD12	2:G:99:ASP:H	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:344:ARG:CG	2:G:344:ARG:NH1	2.78	0.47
2:G:451:LEU:HD21	2:G:458:ARG:HG3	1.97	0.47
2:G:552:ILE:C	2:G:554:GLU:N	2.72	0.47
2:H:373:GLU:O	2:H:377:MET:HG3	2.15	0.47
1:B:138:ASP:HA	1:B:148:TRP:CE3	2.50	0.47
2:C:269:ASP:O	2:C:270:LEU:O	2.32	0.47
2:C:454:LEU:HD13	2:C:495:GLY:HA3	1.97	0.47
2:D:99:ASP:OD2	2:D:171:ARG:NE	2.48	0.47
2:D:103:GLU:CD	2:D:103:GLU:N	2.73	0.47
2:D:192:LEU:HD11	2:D:204:PHE:HD2	1.79	0.47
1:E:54:HIS:CE1	1:E:82:LYS:HB2	2.50	0.47
1:F:138:ASP:HA	1:F:148:TRP:CE3	2.50	0.47
1:F:193:ILE:CD1	1:F:245:ILE:HD13	2.44	0.47
2:G:508:LEU:O	2:G:510:HIS:N	2.48	0.47
2:H:103:GLU:CD	2:H:103:GLU:N	2.73	0.47
1:A:324:ASP:HB3	2:C:64:LYS:HB3	1.96	0.46
2:D:201:ARG:NH2	2:D:303:PHE:CD1	2.83	0.46
2:D:344:ARG:HH11	2:D:344:ARG:CG	2.22	0.46
1:E:168:ASP:H	1:E:188:LEU:CD2	2.28	0.46
1:F:328:VAL:HG11	2:H:69:PHE:CG	2.50	0.46
2:G:52:THR:HG22	2:G:54:ASN:H	1.80	0.46
2:G:454:LEU:HD12	2:G:454:LEU:O	2.15	0.46
2:H:69:PHE:CD2	2:H:80:ALA:HB2	2.49	0.46
2:H:342:ASN:O	2:H:343:GLN:C	2.58	0.46
1:A:27:CYS:HB3	1:A:61:ILE:CD1	2.39	0.46
1:B:324:ASP:HB3	2:D:64:LYS:CG	2.45	0.46
2:C:42:PRO:HB3	2:C:46:ALA:O	2.14	0.46
2:C:94:ARG:HH21	2:C:98:LEU:HB3	1.80	0.46
2:D:196:ASP:C	2:D:198:GLU:N	2.73	0.46
2:G:548:SER:HA	2:G:551:ASN:ND2	2.30	0.46
2:H:112:PHE:O	2:H:115:TYR:HB3	2.15	0.46
2:H:216:ASP:OD2	2:H:218:GLU:HB2	2.15	0.46
1:B:151:THR:CG2	1:B:196:ARG:HH22	2.29	0.46
2:C:81:PHE:CD1	2:C:81:PHE:C	2.93	0.46
2:C:344:ARG:HG3	2:C:344:ARG:NH1	2.24	0.46
1:E:16:VAL:HG21	1:E:61:ILE:O	2.15	0.46
2:H:86:ASP:HA	2:H:88:TYR:HE1	1.79	0.46
2:H:271:LEU:N	2:H:272:PRO:CD	2.78	0.46
2:H:457:TYR:CD1	2:H:457:TYR:C	2.93	0.46
2:H:469:PHE:O	2:H:470:ALA:C	2.58	0.46
1:A:34:LYS:HE2	1:A:50:SER:OG	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ASP:N	2:C:88:TYR:CE1	2.82	0.46
2:C:526:CYS:O	2:C:530:ARG:HA	2.15	0.46
1:E:86:GLU:HB2	1:E:98:TRP:CZ3	2.50	0.46
1:F:97:ARG:HH11	1:F:97:ARG:HG3	1.80	0.46
1:F:169:PHE:O	1:F:170:CYS:HB3	2.16	0.46
2:G:104:PHE:C	2:G:106:ALA:N	2.74	0.46
2:G:226:GLN:C	2:G:228:PHE:H	2.23	0.46
2:G:508:LEU:C	2:G:510:HIS:H	2.23	0.46
2:H:200:ASN:O	2:H:201:ARG:C	2.59	0.46
2:H:423:ILE:O	2:H:426:ALA:HB3	2.14	0.46
1:B:226:ARG:HG3	1:B:226:ARG:NH1	2.30	0.46
2:C:552:ILE:O	2:C:556:ILE:HG13	2.16	0.46
1:F:295:GLU:HG2	2:G:311:LEU:CD2	2.46	0.46
1:F:302:ASP:OD2	2:H:44:SER:HB3	2.16	0.46
2:G:305:GLU:O	2:G:309:LEU:HG	2.15	0.46
2:D:153:ASN:O	2:D:156:GLU:N	2.46	0.46
2:D:240:PHE:HD2	2:D:268:SER:CB	2.29	0.46
2:D:496:THR:HB	2:D:499:ALA:H	1.81	0.46
1:F:310:VAL:HG13	1:F:310:VAL:O	2.15	0.46
1:B:76:SER:OG	1:B:77:TYR:N	2.48	0.46
1:B:303:HIS:HD1	1:B:325:ASP:CG	2.24	0.46
2:C:271:LEU:O	2:C:275:SER:HB3	2.15	0.46
2:D:375:LEU:HD11	2:D:395:VAL:HG13	1.98	0.46
2:H:250:ASN:O	2:H:254:LEU:HG	2.16	0.46
2:D:184:CYS:HB2	2:D:211:TRP:CE2	2.50	0.46
2:G:216:ASP:OD2	2:G:218:GLU:HB2	2.16	0.46
2:G:289:ILE:O	2:G:293:LYS:HG3	2.15	0.46
2:G:423:ILE:O	2:G:426:ALA:HB3	2.16	0.46
1:A:169:PHE:O	1:A:170:CYS:HB3	2.16	0.46
1:B:48:SER:O	1:B:49:ASP:HB2	2.15	0.46
1:B:54:HIS:CE1	1:B:82:LYS:HB2	2.51	0.46
1:B:193:ILE:CD1	1:B:245:ILE:HD13	2.46	0.46
2:C:551:ASN:O	2:C:554:GLU:N	2.49	0.46
2:D:269:ASP:O	2:D:270:LEU:O	2.34	0.46
2:G:352:THR:OG1	2:G:355:GLU:HG3	2.15	0.46
2:H:86:ASP:N	2:H:88:TYR:CE1	2.82	0.46
2:H:478:ASP:C	2:H:480:GLU:N	2.74	0.46
1:A:54:HIS:CE1	1:A:82:LYS:HB2	2.51	0.46
1:A:178:PHE:CD2	2:C:502:MET:HE3	2.51	0.46
2:C:43:VAL:CG1	2:C:48:LEU:CD2	2.79	0.46
2:D:343:GLN:HA	2:D:360:PHE:HE1	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:LEU:HD11	1:E:202:LEU:HD11	1.97	0.46
1:E:138:ASP:HA	1:E:148:TRP:CE3	2.51	0.46
1:E:208:LEU:HD11	1:E:231:ILE:HD12	1.96	0.46
1:E:309:SER:HB3	2:G:68:LYS:HA	1.97	0.46
2:G:347:LEU:O	2:G:348:GLN:C	2.57	0.46
2:H:305:GLU:O	2:H:309:LEU:HG	2.16	0.46
2:H:313:LEU:C	2:H:313:LEU:HD23	2.41	0.46
2:H:344:ARG:CG	2:H:344:ARG:NH1	2.78	0.46
1:A:205:ALA:O	1:A:206:ALA:HB2	2.15	0.45
1:B:79:LYS:HG2	1:B:110:SER:N	2.31	0.45
2:C:480:GLU:O	2:C:483:PRO:CD	2.64	0.45
2:D:347:LEU:O	2:D:348:GLN:C	2.59	0.45
2:D:352:THR:OG1	2:D:355:GLU:HG3	2.16	0.45
2:G:171:ARG:O	2:G:175:LEU:HG	2.17	0.45
2:H:270:LEU:HD13	2:H:289:ILE:CD1	2.46	0.45
1:A:16:VAL:HG21	1:A:61:ILE:O	2.15	0.45
2:C:246:TRP:CE2	2:C:331:TYR:HB3	2.51	0.45
2:C:342:ASN:O	2:C:343:GLN:C	2.59	0.45
2:C:459:ASN:HD22	2:C:459:ASN:N	2.14	0.45
2:D:453:ASP:HB3	2:D:456:SER:HB2	1.97	0.45
2:D:482:TRP:O	2:D:485:ALA:HB3	2.16	0.45
2:D:523:LEU:HD23	2:D:538:ILE:CD1	2.47	0.45
1:E:101:LEU:O	1:E:102:CYS:HB2	2.16	0.45
1:F:208:LEU:HD11	1:F:231:ILE:HD12	1.96	0.45
2:G:104:PHE:O	2:G:107:TYR:N	2.49	0.45
2:G:379:LEU:HD11	2:G:395:VAL:CG1	2.47	0.45
2:G:515:THR:CG2	2:G:516:ASN:H	2.27	0.45
2:H:352:THR:OG1	2:H:355:GLU:HG3	2.16	0.45
1:A:326:GLY:CA	2:C:58:ILE:HD12	2.44	0.45
2:C:415:CYS:HB2	2:C:469:PHE:CE1	2.51	0.45
1:F:205:ALA:O	1:F:206:ALA:HB2	2.15	0.45
2:G:81:PHE:CD1	2:G:81:PHE:C	2.94	0.45
2:H:145:ASN:OD1	2:H:190:PHE:HA	2.15	0.45
2:H:406:LEU:O	2:H:407:PRO:C	2.59	0.45
1:A:151:THR:HG22	1:A:152:SER:N	2.30	0.45
1:B:136:LEU:HD11	1:B:202:LEU:HD11	1.98	0.45
2:C:41:ASP:HA	2:C:42:PRO:HD3	1.77	0.45
2:C:145:ASN:OD1	2:C:190:PHE:HA	2.16	0.45
2:C:184:CYS:HB2	2:C:211:TRP:CE2	2.51	0.45
2:C:324:ILE:O	2:C:325:SER:C	2.60	0.45
2:H:245:PHE:O	2:H:248:LEU:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:PHE:CE1	2:C:71:LEU:HD23	2.41	0.45
2:D:263:GLY:O	2:D:267:ARG:HG2	2.17	0.45
2:D:289:ILE:O	2:D:293:LYS:HG3	2.17	0.45
1:F:114:VAL:HG23	1:F:126:ALA:O	2.16	0.45
2:G:153:ASN:O	2:G:156:GLU:N	2.46	0.45
2:H:531:LEU:HD13	2:H:534:ILE:CD1	2.46	0.45
1:A:86:GLU:HB2	1:A:98:TRP:CZ3	2.52	0.45
2:C:406:LEU:O	2:C:407:PRO:C	2.60	0.45
2:D:379:LEU:HD11	2:D:395:VAL:CG1	2.46	0.45
1:F:347:ALA:HB1	2:H:57:PRO:HG2	1.99	0.45
2:G:460:GLY:C	2:G:462:ALA:N	2.72	0.45
1:B:54:HIS:HD2	1:B:58:ILE:HG12	1.81	0.45
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.81	0.45
2:D:200:ASN:O	2:D:201:ARG:C	2.60	0.45
2:D:250:ASN:O	2:D:254:LEU:HG	2.17	0.45
1:E:74:SER:O	1:E:81:VAL:HG13	2.17	0.45
1:F:137:TYR:HE1	1:F:150:LEU:HG	1.80	0.45
2:H:81:PHE:HB3	2:H:90:LEU:HD23	1.99	0.45
2:H:190:PHE:CD1	2:H:190:PHE:N	2.85	0.45
2:H:523:LEU:O	2:H:526:CYS:HB2	2.17	0.45
1:B:81:VAL:CG2	1:B:111:LEU:HD13	2.32	0.45
1:B:168:ASP:H	1:B:188:LEU:CD2	2.29	0.45
2:C:163:LYS:CE	2:C:168:ARG:HH21	2.29	0.45
2:C:558:ASN:CG	2:C:559:PHE:N	2.75	0.45
2:D:204:PHE:CD1	2:D:205:ILE:N	2.84	0.45
2:D:367:SER:C	2:D:369:GLU:N	2.75	0.45
1:F:336:SER:HB2	2:G:343:GLN:OE1	2.17	0.45
2:H:240:PHE:HD2	2:H:268:SER:CB	2.29	0.45
2:H:289:ILE:O	2:H:293:LYS:HG3	2.17	0.45
1:B:114:VAL:O	1:B:114:VAL:HG13	2.17	0.45
2:C:216:ASP:OD2	2:C:218:GLU:HB2	2.16	0.45
2:C:552:ILE:O	2:C:556:ILE:N	2.36	0.45
2:D:99:ASP:OD1	2:D:101:SER:HB2	2.17	0.45
2:D:492:SER:O	2:D:494:THR:N	2.50	0.45
1:E:47:LEU:HD12	1:E:48:SER:N	2.32	0.45
1:E:151:THR:HG22	1:E:152:SER:N	2.31	0.45
1:F:178:PHE:CD2	2:H:502:MET:HE3	2.52	0.45
2:G:336:LEU:HA	2:G:339:ILE:HD12	1.99	0.45
2:H:336:LEU:HA	2:H:339:ILE:HD12	1.99	0.45
2:C:98:LEU:HD12	2:C:99:ASP:H	1.81	0.45
2:C:153:ASN:O	2:C:156:GLU:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:VAL:O	2:H:70:LYS:HD2	2.17	0.45
2:G:269:ASP:O	2:G:270:LEU:O	2.35	0.45
2:G:324:ILE:O	2:G:325:SER:C	2.60	0.45
2:H:248:LEU:HD23	2:H:248:LEU:C	2.42	0.45
1:B:334:THR:CG2	1:B:335:TYR:H	2.30	0.44
2:C:118:LEU:HD21	2:C:147:ALA:CB	2.46	0.44
2:C:190:PHE:CD1	2:C:190:PHE:N	2.85	0.44
2:C:422:MET:SD	2:C:423:ILE:N	2.90	0.44
2:D:81:PHE:CD1	2:D:81:PHE:C	2.95	0.44
2:D:247:LYS:O	2:D:251:GLN:HG3	2.18	0.44
2:D:498:SER:O	2:D:501:LYS:HB3	2.17	0.44
1:F:183:LEU:HD12	1:F:184:ALA:H	1.82	0.44
2:G:204:PHE:CD1	2:G:205:ILE:N	2.84	0.44
2:G:383:VAL:CG1	2:G:384:VAL:N	2.80	0.44
2:G:396:ASP:OD1	2:G:401:LYS:HE3	2.16	0.44
2:G:500:LYS:C	2:G:502:MET:N	2.75	0.44
2:H:86:ASP:HA	2:H:88:TYR:CE1	2.52	0.44
2:H:482:TRP:N	2:H:483:PRO:HD3	2.32	0.44
1:A:334:THR:CG2	1:A:335:TYR:H	2.30	0.44
2:C:126:VAL:O	2:C:126:VAL:HG12	2.16	0.44
2:C:500:LYS:O	2:C:501:LYS:C	2.60	0.44
1:E:97:ARG:HH11	1:E:97:ARG:HG3	1.81	0.44
2:H:524:SER:O	2:H:527:VAL:N	2.50	0.44
2:C:179:LEU:O	2:C:182:LEU:N	2.50	0.44
2:C:240:PHE:HD2	2:C:268:SER:CB	2.29	0.44
2:C:523:LEU:CD2	2:C:538:ILE:CD1	2.95	0.44
2:D:305:GLU:O	2:D:309:LEU:HG	2.17	0.44
2:G:189:TYR:O	2:G:427:LYS:HE3	2.17	0.44
2:H:179:LEU:O	2:H:182:LEU:N	2.50	0.44
2:H:269:ASP:O	2:H:270:LEU:O	2.35	0.44
2:H:547:LEU:C	2:H:547:LEU:HD23	2.43	0.44
1:A:79:LYS:HG2	1:A:109:GLY:C	2.43	0.44
2:C:313:LEU:C	2:C:313:LEU:HD23	2.43	0.44
2:D:179:LEU:O	2:D:180:THR:C	2.58	0.44
2:D:189:TYR:O	2:D:427:LYS:HE3	2.16	0.44
1:E:151:THR:CG2	1:E:196:ARG:HH22	2.31	0.44
1:E:334:THR:CG2	1:E:335:TYR:H	2.29	0.44
2:G:492:SER:C	2:G:494:THR:N	2.75	0.44
2:H:343:GLN:HA	2:H:360:PHE:HE1	1.82	0.44
2:H:531:LEU:CD1	2:H:534:ILE:HD12	2.48	0.44
1:B:309:SER:HB3	2:D:68:LYS:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:THR:OG1	2:C:355:GLU:HG3	2.18	0.44
2:D:271:LEU:O	2:D:275:SER:HB3	2.18	0.44
2:D:373:GLU:O	2:D:377:MET:HG3	2.17	0.44
1:E:76:SER:OG	1:E:77:TYR:N	2.50	0.44
1:E:224:ILE:HG22	2:G:503:VAL:HG13	1.99	0.44
1:F:171:LEU:HB3	1:F:185:VAL:HG13	1.99	0.44
2:G:235:ALA:O	2:G:237:LYS:N	2.48	0.44
2:G:547:LEU:C	2:G:549:ALA:N	2.73	0.44
2:H:179:LEU:O	2:H:180:THR:C	2.61	0.44
1:B:16:VAL:HG21	1:B:61:ILE:O	2.18	0.44
2:C:42:PRO:CB	2:C:46:ALA:O	2.66	0.44
2:C:214:ARG:HG3	2:C:214:ARG:O	2.17	0.44
2:C:247:LYS:O	2:C:251:GLN:HG3	2.18	0.44
2:C:305:GLU:O	2:C:308:ASN:HB3	2.17	0.44
2:C:456:SER:OG	2:C:457:TYR:N	2.51	0.44
2:C:546:MET:O	2:C:547:LEU:C	2.60	0.44
1:E:137:TYR:HE1	1:E:150:LEU:HG	1.81	0.44
2:G:145:ASN:OD1	2:G:190:PHE:HA	2.18	0.44
2:H:214:ARG:HG3	2:H:214:ARG:O	2.17	0.44
2:H:555:SER:CA	2:H:558:ASN:HB3	2.46	0.44
2:C:171:ARG:O	2:C:175:LEU:HG	2.18	0.44
2:C:344:ARG:CG	2:C:344:ARG:NH1	2.77	0.44
1:E:205:ALA:O	1:E:206:ALA:HB2	2.18	0.44
1:E:315:THR:HB	2:G:471:PHE:HD2	1.82	0.44
1:F:309:SER:HB3	2:H:68:LYS:HA	1.99	0.44
2:H:523:LEU:HD23	2:H:538:ILE:HD12	2.00	0.44
1:A:124:LYS:HA	1:A:138:ASP:HB3	1.99	0.44
1:B:86:GLU:HB2	1:B:98:TRP:CZ3	2.52	0.44
1:B:114:VAL:HG23	1:B:126:ALA:O	2.17	0.44
2:C:343:GLN:HA	2:C:360:PHE:HE1	1.82	0.44
2:C:551:ASN:O	2:C:554:GLU:CB	2.65	0.44
1:F:228:TYR:CD2	1:F:244:LYS:HG3	2.52	0.44
2:G:163:LYS:CE	2:G:168:ARG:HH21	2.31	0.44
2:G:190:PHE:N	2:G:190:PHE:CD1	2.85	0.44
2:G:196:ASP:C	2:G:198:GLU:N	2.72	0.44
2:G:343:GLN:HA	2:G:360:PHE:HE1	1.82	0.44
2:G:478:ASP:C	2:G:480:GLU:H	2.25	0.44
2:H:163:LYS:CE	2:H:168:ARG:HH21	2.30	0.44
2:H:367:SER:C	2:H:369:GLU:N	2.75	0.44
1:A:59:VAL:O	1:A:59:VAL:HG12	2.18	0.44
1:A:108:LYS:HE2	1:A:133:ILE:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD12	1:B:48:SER:N	2.32	0.44
2:C:81:PHE:HB3	2:C:90:LEU:HD23	2.00	0.44
2:C:179:LEU:O	2:C:180:THR:C	2.60	0.44
2:D:171:ARG:O	2:D:175:LEU:HG	2.18	0.44
2:D:216:ASP:OD2	2:D:218:GLU:HB2	2.18	0.44
2:D:270:LEU:HD13	2:D:289:ILE:CD1	2.48	0.44
2:D:460:GLY:C	2:D:462:ALA:N	2.75	0.44
1:E:15:VAL:HB	2:G:81:PHE:CE2	2.53	0.44
1:F:334:THR:CG2	1:F:335:TYR:H	2.29	0.44
2:G:533:GLU:O	2:G:534:ILE:C	2.60	0.44
2:H:85:LYS:O	2:H:86:ASP:HB2	2.18	0.44
2:H:246:TRP:CE2	2:H:331:TYR:HB3	2.53	0.44
2:H:274:LEU:HD22	2:H:281:SER:CB	2.47	0.44
1:A:137:TYR:HE1	1:A:150:LEU:HG	1.82	0.43
1:B:15:VAL:HG21	2:D:90:LEU:HD21	2.00	0.43
1:B:137:TYR:HE1	1:B:150:LEU:HG	1.82	0.43
2:C:204:PHE:O	2:C:207:SER:N	2.51	0.43
2:C:289:ILE:O	2:C:293:LYS:HG3	2.17	0.43
2:D:336:LEU:HA	2:D:339:ILE:HD12	1.99	0.43
1:E:54:HIS:CD2	1:E:58:ILE:HG12	2.53	0.43
1:E:79:LYS:HG2	1:E:110:SER:N	2.33	0.43
1:E:178:PHE:CD2	2:G:502:MET:HE3	2.53	0.43
1:F:310:VAL:HA	1:F:320:SER:O	2.17	0.43
1:F:345:ILE:HA	2:H:49:VAL:O	2.18	0.43
2:G:367:SER:C	2:G:369:GLU:N	2.76	0.43
2:H:258:LEU:HD22	2:H:292:LEU:CD2	2.44	0.43
2:H:470:ALA:HB1	2:H:489:ILE:HG13	2.00	0.43
2:H:486:ILE:O	2:H:490:ALA:HB2	2.18	0.43
2:H:541:THR:HG22	2:H:545:GLN:NE2	2.33	0.43
1:B:74:SER:O	1:B:81:VAL:HG13	2.18	0.43
2:C:250:ASN:O	2:C:254:LEU:HG	2.17	0.43
2:C:367:SER:C	2:C:369:GLU:N	2.75	0.43
2:D:69:PHE:CD2	2:D:80:ALA:HB2	2.53	0.43
2:D:197:VAL:CB	2:D:366:PRO:HB2	2.48	0.43
1:E:6:SER:HB2	1:E:8:HIS:HD2	1.84	0.43
1:F:170:CYS:SG	1:F:218:ILE:HG22	2.59	0.43
2:G:457:TYR:C	2:G:457:TYR:HD1	2.25	0.43
2:H:324:ILE:O	2:H:325:SER:C	2.60	0.43
2:H:415:CYS:HB2	2:H:469:PHE:CE1	2.51	0.43
1:B:28:SER:OG	1:B:30:ASP:OD1	2.36	0.43
1:B:59:VAL:O	1:B:59:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ALA:O	1:B:206:ALA:HB2	2.17	0.43
1:E:314:LEU:CD2	2:G:73:PRO:O	2.67	0.43
2:H:481:LEU:O	2:H:484:VAL:HB	2.19	0.43
2:H:547:LEU:O	2:H:548:SER:C	2.61	0.43
1:A:25:ALA:O	1:A:61:ILE:HD12	2.18	0.43
1:B:145:LEU:HD12	1:B:145:LEU:N	2.33	0.43
1:B:169:PHE:O	1:B:170:CYS:HB3	2.19	0.43
2:C:200:ASN:O	2:C:201:ARG:C	2.61	0.43
2:C:515:THR:CG2	2:C:516:ASN:H	2.31	0.43
2:D:492:SER:C	2:D:494:THR:N	2.74	0.43
2:D:525:ILE:C	2:D:527:VAL:H	2.25	0.43
1:E:328:VAL:HG11	2:G:69:PHE:CG	2.53	0.43
2:G:238:LYS:O	2:G:239:VAL:C	2.61	0.43
2:H:526:CYS:O	2:H:530:ARG:N	2.47	0.43
1:A:170:CYS:SG	1:A:218:ILE:HG22	2.59	0.43
2:D:163:LYS:CE	2:D:168:ARG:HH21	2.29	0.43
2:D:344:ARG:NH1	2:D:344:ARG:CG	2.79	0.43
2:G:184:CYS:HB2	2:G:211:TRP:CE2	2.54	0.43
2:H:196:ASP:C	2:H:198:GLU:N	2.73	0.43
2:H:420:THR:O	2:H:421:ALA:C	2.60	0.43
1:A:47:LEU:HD12	1:A:48:SER:N	2.34	0.43
2:D:81:PHE:HB3	2:D:90:LEU:HD23	2.00	0.43
2:D:197:VAL:HB	2:D:366:PRO:O	2.19	0.43
1:E:48:SER:O	1:E:49:ASP:HB2	2.17	0.43
1:E:199:ASP:OD2	1:E:201:LYS:HB2	2.18	0.43
1:F:79:LYS:HG2	1:F:109:GLY:C	2.44	0.43
1:F:101:LEU:O	1:F:102:CYS:HB2	2.17	0.43
2:G:198:GLU:HA	2:G:300:SER:OG	2.17	0.43
2:G:200:ASN:O	2:G:201:ARG:C	2.60	0.43
2:G:253:VAL:HG21	2:G:335:PHE:CE1	2.54	0.43
2:G:263:GLY:O	2:G:267:ARG:HG2	2.19	0.43
2:G:274:LEU:HD22	2:G:281:SER:CB	2.47	0.43
2:H:478:ASP:O	2:H:480:GLU:N	2.51	0.43
2:C:167:GLY:O	2:C:168:ARG:HG3	2.18	0.43
2:C:218:GLU:HA	2:C:219:PRO:C	2.43	0.43
2:C:482:TRP:O	2:C:486:ILE:HG12	2.19	0.43
2:C:527:VAL:HG12	2:C:528:GLU:N	2.34	0.43
2:D:85:LYS:O	2:D:86:ASP:HB2	2.18	0.43
2:D:108:VAL:HG12	2:D:484:VAL:HG11	2.01	0.43
2:D:462:ALA:O	2:D:463:SER:C	2.61	0.43
1:E:117:ALA:HB2	1:E:173:TRP:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:40:ARG:O	2:G:42:PRO:HD3	2.19	0.43
2:G:218:GLU:HA	2:G:219:PRO:C	2.44	0.43
1:A:76:SER:OG	1:A:77:TYR:N	2.51	0.43
2:D:151:ILE:O	2:D:152:LEU:C	2.61	0.43
1:F:6:SER:HB2	1:F:8:HIS:HD2	1.84	0.43
2:H:218:GLU:HA	2:H:219:PRO:C	2.44	0.43
2:H:555:SER:HA	2:H:558:ASN:OD1	2.19	0.43
2:C:258:LEU:HD22	2:C:292:LEU:CD2	2.42	0.43
2:D:253:VAL:HG21	2:D:335:PHE:CE1	2.53	0.43
1:E:169:PHE:O	1:E:170:CYS:HB3	2.19	0.43
2:G:81:PHE:HB3	2:G:90:LEU:HD23	2.00	0.43
2:G:99:ASP:OD1	2:G:101:SER:HB2	2.18	0.43
2:G:547:LEU:C	2:G:549:ALA:H	2.27	0.43
2:H:197:VAL:HB	2:H:366:PRO:HB2	2.01	0.43
2:H:459:ASN:OD1	2:H:494:THR:HB	2.18	0.43
1:A:328:VAL:HG11	2:C:69:PHE:CG	2.54	0.43
1:B:11:LEU:N	2:D:88:TYR:HE2	2.17	0.43
1:B:324:ASP:C	1:B:326:GLY:N	2.74	0.43
2:C:47:ILE:HG22	2:C:48:LEU:N	2.33	0.43
2:D:515:THR:HB	2:D:518:ASP:OD1	2.18	0.43
2:D:533:GLU:OE1	2:D:533:GLU:HA	2.19	0.43
2:G:67:LEU:HD12	2:G:81:PHE:O	2.19	0.43
2:G:247:LYS:O	2:G:251:GLN:HG3	2.19	0.43
2:G:460:GLY:O	2:G:463:SER:N	2.52	0.43
2:G:508:LEU:HB3	2:G:534:ILE:HD13	2.01	0.43
2:H:89:LYS:HD2	2:H:89:LYS:H	1.82	0.43
2:H:201:ARG:HG3	2:H:201:ARG:NH1	2.33	0.43
2:H:305:GLU:O	2:H:308:ASN:HB3	2.19	0.43
2:C:104:PHE:O	2:C:107:TYR:N	2.51	0.42
2:C:270:LEU:HD13	2:C:289:ILE:CD1	2.49	0.42
2:C:406:LEU:HB2	2:C:407:PRO:CD	2.44	0.42
2:D:383:VAL:CG1	2:D:384:VAL:N	2.81	0.42
1:F:314:LEU:HD21	2:H:475:SER:OG	2.19	0.42
2:G:94:ARG:HH21	2:G:98:LEU:HB3	1.83	0.42
2:G:271:LEU:O	2:G:275:SER:HB3	2.19	0.42
2:G:519:ILE:O	2:G:523:LEU:HG	2.19	0.42
2:H:462:ALA:O	2:H:463:SER:C	2.60	0.42
2:H:553:ILE:O	2:H:556:ILE:CG2	2.67	0.42
1:A:82:LYS:HE3	1:A:100:LYS:HD3	2.00	0.42
2:C:252:LEU:HD23	2:C:252:LEU:HA	1.89	0.42
2:C:529:TRP:O	2:C:530:ARG:HB2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:GLU:HB2	1:F:98:TRP:CZ3	2.54	0.42
2:G:197:VAL:HB	2:G:366:PRO:O	2.19	0.42
2:H:160:GLY:C	2:H:162:VAL:N	2.76	0.42
2:H:204:PHE:O	2:H:207:SER:N	2.52	0.42
2:H:471:PHE:O	2:H:472:GLU:C	2.62	0.42
2:H:480:GLU:O	2:H:483:PRO:CD	2.66	0.42
2:H:496:THR:C	2:H:498:SER:N	2.75	0.42
1:A:303:HIS:ND1	1:A:325:ASP:OD1	2.53	0.42
2:C:89:LYS:HD2	2:C:89:LYS:H	1.80	0.42
1:E:114:VAL:O	1:E:114:VAL:HG13	2.19	0.42
1:A:77:TYR:C	1:A:79:LYS:H	2.28	0.42
1:B:314:LEU:CD2	2:D:73:PRO:O	2.67	0.42
2:C:204:PHE:CD1	2:C:205:ILE:N	2.87	0.42
2:C:238:LYS:O	2:C:239:VAL:C	2.62	0.42
2:D:406:LEU:O	2:D:407:PRO:C	2.62	0.42
2:D:508:LEU:C	2:D:510:HIS:N	2.75	0.42
1:E:183:LEU:HD12	1:E:184:ALA:H	1.85	0.42
1:F:27:CYS:HB3	1:F:61:ILE:CD1	2.40	0.42
1:F:77:TYR:C	1:F:79:LYS:H	2.28	0.42
2:G:85:LYS:O	2:G:86:ASP:HB2	2.18	0.42
2:H:231:LYS:CG	2:H:232:ASP:H	2.29	0.42
2:H:402:ILE:O	2:H:403:HIS:C	2.62	0.42
1:A:199:ASP:OD2	1:A:201:LYS:HD2	2.19	0.42
1:B:22:ARG:HA	1:B:22:ARG:HD3	1.83	0.42
1:B:151:THR:HG22	1:B:152:SER:N	2.32	0.42
2:C:305:GLU:O	2:C:309:LEU:HG	2.20	0.42
2:D:86:ASP:CA	2:D:88:TYR:CE1	3.03	0.42
2:D:202:SER:HA	2:D:297:LYS:O	2.19	0.42
2:H:526:CYS:O	2:H:530:ARG:HA	2.20	0.42
1:B:27:CYS:SG	1:B:27:CYS:O	2.78	0.42
2:D:69:PHE:HD2	2:D:80:ALA:HB2	1.83	0.42
2:D:179:LEU:O	2:D:182:LEU:N	2.52	0.42
2:D:218:GLU:HA	2:D:219:PRO:C	2.44	0.42
1:E:28:SER:OG	1:E:30:ASP:OD1	2.37	0.42
1:F:156:VAL:HG12	1:F:157:LEU:N	2.34	0.42
1:A:11:LEU:C	1:A:28:SER:HB2	2.44	0.42
1:A:22:ARG:HD3	1:A:22:ARG:HA	1.85	0.42
1:A:199:ASP:OD2	1:A:201:LYS:HB2	2.20	0.42
1:B:101:LEU:O	1:B:102:CYS:HB2	2.18	0.42
2:C:336:LEU:HA	2:C:339:ILE:HD12	2.00	0.42
2:D:89:LYS:HD2	2:D:89:LYS:H	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:ARG:HH21	2:D:98:LEU:HB3	1.83	0.42
2:D:112:PHE:CE1	2:D:488:LEU:HD13	2.54	0.42
2:D:342:ASN:O	2:D:343:GLN:C	2.62	0.42
1:E:59:VAL:O	1:E:59:VAL:HG12	2.19	0.42
1:F:80:THR:HG22	1:F:105:ASN:HA	2.01	0.42
1:F:199:ASP:OD2	1:F:201:LYS:HD2	2.19	0.42
2:G:141:ASN:O	2:G:142:ALA:C	2.62	0.42
2:G:145:ASN:O	2:G:148:MET:HB3	2.20	0.42
2:G:402:ILE:O	2:G:403:HIS:C	2.63	0.42
2:H:42:PRO:HD2	2:H:46:ALA:O	2.19	0.42
2:H:459:ASN:HB3	2:H:494:THR:HB	2.02	0.42
2:H:551:ASN:O	2:H:555:SER:HB2	2.20	0.42
1:B:117:ALA:HB2	1:B:173:TRP:CE2	2.55	0.42
1:B:178:PHE:CE2	2:D:502:MET:HG2	2.55	0.42
1:B:328:VAL:HG11	2:D:69:PHE:CG	2.55	0.42
2:C:141:ASN:O	2:C:142:ALA:C	2.63	0.42
2:D:396:ASP:OD1	2:D:401:LYS:HE3	2.19	0.42
1:F:116:PHE:HD1	1:F:124:LYS:O	2.03	0.42
2:G:478:ASP:C	2:G:480:GLU:N	2.77	0.42
1:A:91:GLU:O	1:A:97:ARG:HD2	2.20	0.42
1:B:80:THR:HG22	1:B:105:ASN:HA	2.02	0.42
2:D:167:GLY:O	2:D:168:ARG:HG3	2.20	0.42
1:E:82:LYS:HE3	1:E:100:LYS:HD3	2.02	0.42
1:F:245:ILE:HA	1:F:293:GLN:O	2.20	0.42
2:G:204:PHE:O	2:G:207:SER:N	2.53	0.42
2:G:218:GLU:HA	2:G:220:ASP:N	2.35	0.42
2:G:270:LEU:HD13	2:G:289:ILE:CD1	2.49	0.42
1:A:114:VAL:HG13	1:A:114:VAL:O	2.20	0.42
1:A:310:VAL:HA	1:A:320:SER:O	2.20	0.42
1:A:313:ASN:HB3	1:A:317:THR:H	1.84	0.42
1:B:320:SER:HB3	2:D:71:LEU:HD21	2.02	0.42
2:C:274:LEU:HD22	2:C:281:SER:CB	2.49	0.42
2:D:141:ASN:O	2:D:142:ALA:C	2.63	0.42
2:D:365:ILE:HB	2:D:374:TYR:OH	2.20	0.42
1:E:114:VAL:HG23	1:E:126:ALA:O	2.19	0.42
2:G:69:PHE:CE1	2:G:71:LEU:HD23	2.45	0.42
2:G:179:LEU:O	2:G:180:THR:C	2.63	0.42
2:G:373:GLU:O	2:G:377:MET:HG3	2.20	0.42
2:H:113:GLU:O	2:H:114:ILE:C	2.63	0.42
1:A:54:HIS:HD2	1:A:58:ILE:HG12	1.85	0.41
1:A:117:ALA:HB2	1:A:173:TRP:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:OD2	1:B:201:LYS:HB2	2.20	0.41
1:B:236:LYS:HG2	1:B:306:GLU:CD	2.45	0.41
2:D:258:LEU:HD22	2:D:292:LEU:CD2	2.42	0.41
1:E:23:HIS:HD2	1:E:37:LYS:HA	1.84	0.41
1:E:61:ILE:HG22	1:E:62:ASP:N	2.35	0.41
1:E:64:ALA:O	1:E:65:SER:C	2.63	0.41
1:E:124:LYS:HA	1:E:138:ASP:HB3	2.01	0.41
1:F:16:VAL:HG21	1:F:61:ILE:O	2.19	0.41
2:G:357:PHE:CE1	2:G:398:ILE:HD11	2.56	0.41
2:H:467:ASN:OD1	2:H:467:ASN:N	2.51	0.41
2:H:508:LEU:C	2:H:510:HIS:N	2.78	0.41
1:A:101:LEU:O	1:A:102:CYS:HB2	2.19	0.41
1:B:10:ASP:C	2:D:88:TYR:CE2	2.97	0.41
1:B:208:LEU:HD11	1:B:231:ILE:HD12	1.99	0.41
2:C:383:VAL:CG1	2:C:384:VAL:N	2.81	0.41
2:C:469:PHE:O	2:C:470:ALA:C	2.62	0.41
2:C:557:ALA:O	2:C:558:ASN:C	2.63	0.41
2:D:83:THR:O	2:D:84:ALA:HB2	2.20	0.41
1:F:301:ASP:C	1:F:303:HIS:N	2.78	0.41
2:G:197:VAL:CB	2:G:366:PRO:HB2	2.50	0.41
2:G:473:LEU:HB2	2:G:485:ALA:HB2	2.02	0.41
2:H:478:ASP:C	2:H:480:GLU:H	2.28	0.41
1:A:48:SER:O	1:A:49:ASP:HB2	2.20	0.41
1:B:64:ALA:O	1:B:65:SER:C	2.63	0.41
2:C:160:GLY:C	2:C:162:VAL:N	2.77	0.41
2:C:228:PHE:CE2	2:C:267:ARG:HG3	2.55	0.41
2:C:231:LYS:NZ	2:C:233:SER:HB3	2.35	0.41
2:D:142:ALA:O	2:D:146:LEU:HG	2.21	0.41
2:D:248:LEU:HD23	2:D:248:LEU:O	2.20	0.41
2:D:511:TYR:HA	2:D:512:PRO:HD3	1.81	0.41
1:F:47:LEU:HD12	1:F:48:SER:N	2.36	0.41
1:F:206:ALA:HB1	2:G:315:GLN:OE1	2.20	0.41
1:F:247:GLU:HG3	1:F:247:GLU:O	2.20	0.41
2:G:201:ARG:NH2	2:G:303:PHE:CD1	2.88	0.41
2:G:491:LEU:O	2:G:493:ALA:N	2.54	0.41
2:H:171:ARG:O	2:H:175:LEU:HG	2.20	0.41
2:H:253:VAL:HG21	2:H:335:PHE:CE1	2.55	0.41
2:H:557:ALA:O	2:H:561:ARG:N	2.40	0.41
1:A:171:LEU:HB3	1:A:185:VAL:HG13	2.01	0.41
1:A:347:ALA:HB1	2:C:57:PRO:HG2	2.03	0.41
1:B:124:LYS:HA	1:B:138:ASP:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:GLY:O	2:C:168:ARG:CG	2.68	0.41
2:D:305:GLU:O	2:D:308:ASN:HB3	2.20	0.41
1:E:156:VAL:HG12	1:E:157:LEU:N	2.36	0.41
1:E:242:ILE:HD11	1:E:319:LEU:CD2	2.50	0.41
1:F:124:LYS:HA	1:F:138:ASP:HB3	2.01	0.41
2:H:201:ARG:HG3	2:H:201:ARG:HH11	1.85	0.41
1:A:21:GLY:HA3	2:C:73:PRO:HD2	2.02	0.41
1:A:226:ARG:HG3	1:A:226:ARG:NH1	2.34	0.41
2:C:113:GLU:O	2:C:114:ILE:C	2.64	0.41
2:C:173:TYR:HD1	2:C:173:TYR:H	1.68	0.41
2:C:407:PRO:O	2:C:410:GLU:HB3	2.21	0.41
2:D:204:PHE:O	2:D:207:SER:N	2.53	0.41
1:E:199:ASP:OD2	1:E:201:LYS:HD2	2.20	0.41
1:E:236:LYS:HG2	1:E:306:GLU:CD	2.46	0.41
1:F:199:ASP:OD2	1:F:201:LYS:HB2	2.20	0.41
2:G:228:PHE:CE2	2:G:267:ARG:HG3	2.56	0.41
2:H:151:ILE:O	2:H:152:LEU:C	2.63	0.41
2:H:263:GLY:O	2:H:267:ARG:HG2	2.19	0.41
1:A:81:VAL:CG2	1:A:111:LEU:HD13	2.36	0.41
1:B:23:HIS:HD2	1:B:37:LYS:HA	1.85	0.41
2:C:296:PRO:HD3	2:C:306:TRP:CD1	2.55	0.41
2:C:461:MET:O	2:C:465:MET:HG3	2.21	0.41
2:C:550:HIS:HA	2:C:553:ILE:CG1	2.50	0.41
2:D:57:PRO:HG2	2:D:58:ILE:H	1.86	0.41
2:D:190:PHE:CE2	2:D:427:LYS:HG3	2.56	0.41
1:E:54:HIS:HE1	1:E:82:LYS:HB2	1.85	0.41
1:F:54:HIS:HE1	1:F:82:LYS:HB2	1.85	0.41
2:G:169:VAL:O	2:G:170:ASN:C	2.64	0.41
2:G:375:LEU:HD11	2:G:395:VAL:HG13	2.01	0.41
2:H:141:ASN:O	2:H:142:ALA:C	2.61	0.41
2:H:383:VAL:CG1	2:H:384:VAL:N	2.83	0.41
2:H:532:PRO:O	2:H:536:LYS:HG3	2.21	0.41
1:A:29:SER:C	1:A:31:GLN:H	2.28	0.41
2:C:245:PHE:O	2:C:248:LEU:HB3	2.20	0.41
2:D:190:PHE:N	2:D:190:PHE:CD1	2.87	0.41
2:D:402:ILE:O	2:D:403:HIS:C	2.63	0.41
1:E:117:ALA:HA	1:E:173:TRP:CG	2.55	0.41
2:G:142:ALA:O	2:G:146:LEU:HG	2.21	0.41
1:B:54:HIS:HE1	1:B:82:LYS:HB2	1.86	0.41
1:B:156:VAL:HG12	1:B:157:LEU:N	2.35	0.41
2:C:205:ILE:O	2:C:205:ILE:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:248:LEU:C	2:C:248:LEU:HD23	2.45	0.41
2:C:511:TYR:CE2	2:C:513:PHE:HB3	2.56	0.41
2:D:42:PRO:HG3	2:D:47:ILE:C	2.46	0.41
2:D:466:LEU:HD23	2:D:466:LEU:HA	1.92	0.41
1:E:170:CYS:C	1:E:171:LEU:HD23	2.46	0.41
1:E:221:ALA:HA	1:E:222:PRO:HD3	1.87	0.41
1:E:324:ASP:C	1:E:326:GLY:N	2.76	0.41
2:G:204:PHE:C	2:G:206:GLU:N	2.79	0.41
2:G:253:VAL:HG21	2:G:335:PHE:HE1	1.85	0.41
2:G:456:SER:OG	2:G:457:TYR:N	2.54	0.41
2:G:516:ASN:HA	2:G:519:ILE:HD12	2.01	0.41
2:H:99:ASP:OD1	2:H:101:SER:HB2	2.20	0.41
2:H:173:TYR:HD1	2:H:173:TYR:H	1.69	0.41
1:A:145:LEU:HD12	1:A:145:LEU:N	2.36	0.41
1:A:151:THR:CG2	1:A:196:ARG:HH22	2.33	0.41
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.36	0.41
1:B:108:LYS:HE2	1:B:133:ILE:HD12	2.01	0.41
1:B:116:PHE:HD1	1:B:124:LYS:O	2.03	0.41
1:B:301:ASP:C	1:B:303:HIS:N	2.79	0.41
2:D:204:PHE:C	2:D:206:GLU:N	2.79	0.41
2:D:218:GLU:HA	2:D:220:ASP:N	2.35	0.41
2:D:248:LEU:HD23	2:D:248:LEU:C	2.45	0.41
1:F:25:ALA:O	1:F:61:ILE:HD12	2.20	0.41
1:F:54:HIS:HD2	1:F:58:ILE:HG12	1.86	0.41
1:F:226:ARG:HG3	1:F:226:ARG:NH1	2.33	0.41
2:G:83:THR:O	2:G:84:ALA:HB2	2.20	0.41
2:G:248:LEU:HD23	2:G:248:LEU:C	2.45	0.41
2:G:296:PRO:HD3	2:G:306:TRP:CD1	2.55	0.41
2:H:204:PHE:CD1	2:H:205:ILE:N	2.89	0.41
2:H:209:LEU:HD21	2:H:362:LEU:HD11	2.02	0.41
2:H:347:LEU:O	2:H:348:GLN:C	2.64	0.41
2:H:511:TYR:CE2	2:H:513:PHE:HB3	2.56	0.41
1:A:113:SER:HB3	1:A:170:CYS:HA	2.03	0.41
1:A:228:TYR:CD2	1:A:244:LYS:HG3	2.53	0.41
1:A:245:ILE:HA	1:A:293:GLN:O	2.20	0.41
1:A:301:ASP:C	1:A:303:HIS:N	2.79	0.41
1:B:6:SER:HB2	1:B:8:HIS:HD2	1.86	0.41
1:B:199:ASP:OD2	1:B:201:LYS:HD2	2.21	0.41
2:D:42:PRO:HD2	2:D:47:ILE:HA	2.01	0.41
2:D:105:SER:HB2	2:D:481:LEU:HD21	2.03	0.41
2:D:253:VAL:HG21	2:D:335:PHE:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:THR:CG2	1:F:196:ARG:HH22	2.34	0.41
1:F:313:ASN:HB3	1:F:317:THR:H	1.86	0.41
1:F:338:GLU:HB3	2:G:377:MET:HE1	2.02	0.41
2:G:179:LEU:O	2:G:182:LEU:N	2.54	0.41
2:G:240:PHE:CE2	2:G:268:SER:HB2	2.56	0.41
2:G:305:GLU:O	2:G:308:ASN:HB3	2.21	0.41
2:G:523:LEU:HD23	2:G:538:ILE:HD12	2.02	0.41
2:H:467:ASN:HA	2:H:470:ALA:HB3	2.02	0.41
1:A:74:SER:O	1:A:81:VAL:HG13	2.21	0.40
1:B:15:VAL:HB	2:D:81:PHE:CE2	2.56	0.40
1:B:79:LYS:HG2	1:B:109:GLY:C	2.46	0.40
2:C:57:PRO:HG2	2:C:58:ILE:H	1.86	0.40
2:C:151:ILE:O	2:C:152:LEU:C	2.63	0.40
2:C:253:VAL:HG21	2:C:335:PHE:CE1	2.56	0.40
2:D:160:GLY:C	2:D:162:VAL:N	2.78	0.40
2:D:273:TYR:O	2:D:274:LEU:C	2.64	0.40
2:D:313:LEU:HD23	2:D:313:LEU:O	2.19	0.40
2:D:543:GLY:O	2:D:547:LEU:HG	2.21	0.40
1:F:21:GLY:HA3	2:H:73:PRO:HD2	2.02	0.40
1:F:108:LYS:HE2	1:F:133:ILE:HD12	2.04	0.40
1:F:324:ASP:C	1:F:326:GLY:N	2.77	0.40
2:G:483:PRO:HA	2:G:521:TRP:HZ2	1.86	0.40
2:C:91:TYR:CD1	2:C:91:TYR:N	2.89	0.40
2:C:201:ARG:NH1	2:C:201:ARG:HG3	2.36	0.40
2:C:218:GLU:HA	2:C:220:ASP:N	2.35	0.40
1:E:7:GLY:HA3	1:E:34:LYS:HZ2	1.86	0.40
1:F:303:HIS:ND1	1:F:325:ASP:OD1	2.54	0.40
2:G:202:SER:HA	2:G:297:LYS:O	2.21	0.40
2:G:248:LEU:HD23	2:G:248:LEU:O	2.21	0.40
2:H:218:GLU:HA	2:H:220:ASP:N	2.36	0.40
2:H:238:LYS:O	2:H:239:VAL:C	2.63	0.40
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.35	0.40
1:B:2:GLN:HA	1:B:3:PRO:HD3	1.95	0.40
2:C:86:ASP:CA	2:C:88:TYR:CE1	3.05	0.40
2:C:142:ALA:O	2:C:146:LEU:HG	2.22	0.40
2:C:467:ASN:O	2:C:471:PHE:CD1	2.74	0.40
2:D:113:GLU:O	2:D:114:ILE:C	2.65	0.40
1:E:177:ARG:HD2	1:E:178:PHE:CE1	2.57	0.40
1:E:305:GLY:HA3	1:E:324:ASP:HB2	2.03	0.40
1:F:82:LYS:HE3	1:F:100:LYS:HD3	2.02	0.40
1:F:97:ARG:HG3	1:F:97:ARG:NH1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:86:ASP:CA	2:G:88:TYR:CE1	3.03	0.40
2:G:342:ASN:O	2:G:343:GLN:C	2.64	0.40
2:G:492:SER:C	2:G:494:THR:H	2.29	0.40
2:G:535:ALA:O	2:G:538:ILE:HB	2.20	0.40
2:H:205:ILE:O	2:H:205:ILE:HG22	2.21	0.40
2:H:248:LEU:HD23	2:H:248:LEU:O	2.21	0.40
2:H:375:LEU:HB2	2:H:398:ILE:HD13	2.03	0.40
1:A:117:ALA:HA	1:A:173:TRP:CG	2.56	0.40
1:A:295:GLU:HG2	2:D:311:LEU:HD21	2.04	0.40
2:C:85:LYS:O	2:C:86:ASP:HB2	2.21	0.40
2:D:274:LEU:HD22	2:D:281:SER:CB	2.50	0.40
2:D:296:PRO:HD3	2:D:306:TRP:CD1	2.55	0.40
1:E:25:ALA:O	1:E:61:ILE:HD12	2.21	0.40
1:F:59:VAL:O	1:F:59:VAL:HG12	2.20	0.40
1:F:64:ALA:O	1:F:65:SER:C	2.64	0.40
1:F:117:ALA:HB2	1:F:173:TRP:CE2	2.56	0.40
1:F:236:LYS:HG2	1:F:306:GLU:CD	2.46	0.40
2:G:160:GLY:C	2:G:162:VAL:N	2.76	0.40
2:G:498:SER:O	2:G:499:ALA:C	2.65	0.40
1:B:29:SER:C	1:B:31:GLN:H	2.30	0.40
1:B:113:SER:HB3	1:B:170:CYS:HA	2.04	0.40
1:B:313:ASN:HB3	1:B:317:THR:H	1.86	0.40
2:C:204:PHE:C	2:C:206:GLU:N	2.79	0.40
2:D:67:LEU:HD12	2:D:81:PHE:O	2.22	0.40
2:D:93:VAL:HG12	2:D:94:ARG:N	2.36	0.40
2:D:240:PHE:CE2	2:D:268:SER:HB2	2.57	0.40
2:D:460:GLY:O	2:D:462:ALA:N	2.54	0.40
2:D:549:ALA:C	2:D:551:ASN:N	2.76	0.40
1:E:63:TRP:CH2	1:E:72:ILE:HD11	2.56	0.40
1:E:116:PHE:HD1	1:E:124:LYS:O	2.03	0.40
1:F:345:ILE:CD1	2:H:93:VAL:HG11	2.48	0.40
2:G:467:ASN:O	2:G:471:PHE:HD1	2.05	0.40
2:G:469:PHE:O	2:G:470:ALA:C	2.64	0.40
2:H:166:ASP:HB3	2:H:169:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/351 (84%)	240 (82%)	48 (16%)	6 (2%)	6	31
1	B	294/351 (84%)	243 (83%)	45 (15%)	6 (2%)	6	31
1	E	294/351 (84%)	242 (82%)	47 (16%)	5 (2%)	7	33
1	F	294/351 (84%)	242 (82%)	46 (16%)	6 (2%)	6	31
2	C	486/570 (85%)	378 (78%)	82 (17%)	26 (5%)	1	16
2	D	472/570 (83%)	371 (79%)	76 (16%)	25 (5%)	1	16
2	G	474/570 (83%)	370 (78%)	79 (17%)	25 (5%)	1	16
2	H	487/570 (85%)	384 (79%)	78 (16%)	25 (5%)	1	16
All	All	3095/3684 (84%)	2470 (80%)	501 (16%)	124 (4%)	2	20

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	B	302	ASP
2	C	197	VAL
2	C	200	ASN
2	C	270	LEU
2	C	273	TYR
2	D	43	VAL
2	D	197	VAL
2	D	200	ASN
2	D	270	LEU
2	D	273	TYR
2	D	515	THR
2	D	553	ILE
1	E	302	ASP
1	F	302	ASP
2	G	46	ALA
2	G	197	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	200	ASN
2	G	270	LEU
2	G	273	TYR
2	G	514	VAL
2	H	43	VAL
2	H	197	VAL
2	H	200	ASN
2	H	270	LEU
2	H	273	TYR
2	H	549	ALA
2	C	205	ILE
2	C	235	ALA
2	C	239	VAL
2	C	272	PRO
2	C	479	LYS
2	C	549	ALA
2	C	552	ILE
2	C	556	ILE
2	D	205	ILE
2	D	239	VAL
2	D	272	PRO
2	D	479	LYS
2	D	514	VAL
2	G	205	ILE
2	G	239	VAL
2	G	272	PRO
2	G	493	ALA
2	H	46	ALA
2	H	239	VAL
2	H	272	PRO
2	H	550	HIS
1	A	94	SER
1	A	170	CYS
1	B	170	CYS
1	B	325	ASP
2	C	60	LYS
2	C	101	SER
2	C	543	GLY
2	D	60	LYS
2	D	101	SER
2	D	204	PHE
2	D	461	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	493	ALA
1	E	94	SER
1	E	170	CYS
1	E	325	ASP
1	F	94	SER
1	F	170	CYS
1	F	325	ASP
2	G	60	LYS
2	G	101	SER
2	G	204	PHE
2	G	236	GLY
2	G	492	SER
2	G	515	THR
2	H	60	LYS
2	H	101	SER
2	H	204	PHE
2	H	205	ILE
2	H	460	GLY
2	H	479	LYS
1	A	41	ASP
1	A	325	ASP
1	B	41	ASP
1	B	94	SER
2	C	42	PRO
2	C	164	ASP
2	C	172	PHE
2	C	204	PHE
2	C	325	SER
2	C	368	LEU
2	D	164	ASP
2	D	325	SER
2	D	401	LYS
1	E	41	ASP
1	F	41	ASP
2	G	164	ASP
2	G	325	SER
2	G	368	LEU
2	H	164	ASP
2	H	172	PHE
2	H	325	SER
2	H	472	GLU
2	C	119	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	401	LYS
2	D	119	GLY
2	D	172	PHE
2	D	368	LEU
2	D	485	ALA
2	G	119	GLY
2	G	161	ARG
2	G	172	PHE
2	H	368	LEU
2	H	401	LYS
2	C	227	VAL
2	D	227	VAL
2	G	227	VAL
2	G	401	LYS
2	H	119	GLY
2	H	227	VAL
2	C	514	VAL
2	C	553	ILE
1	A	156	VAL
2	G	553	ILE
2	H	527	VAL
1	B	156	VAL
1	F	156	VAL

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	262/307 (85%)	256 (98%)	6 (2%)	44	62
1	B	262/307 (85%)	256 (98%)	6 (2%)	44	62
1	E	262/307 (85%)	256 (98%)	6 (2%)	44	62
1	F	262/307 (85%)	256 (98%)	6 (2%)	44	62
2	C	438/510 (86%)	425 (97%)	13 (3%)	36	56
2	D	428/510 (84%)	414 (97%)	14 (3%)	33	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	429/510 (84%)	419 (98%)	10 (2%)	44	62
2	H	439/510 (86%)	425 (97%)	14 (3%)	34	55
All	All	2782/3268 (85%)	2707 (97%)	75 (3%)	39	58

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	150	LEU
1	A	171	LEU
1	A	214	LEU
1	A	218	ILE
1	A	226	ARG
1	B	5	ASP
1	B	150	LEU
1	B	171	LEU
1	B	214	LEU
1	B	218	ILE
1	B	226	ARG
2	C	65	MET
2	C	123	VAL
2	C	200	ASN
2	C	248	LEU
2	C	308	ASN
2	C	322	THR
2	C	384	VAL
2	C	398	ILE
2	C	459	ASN
2	C	465	MET
2	C	488	LEU
2	C	497	ARG
2	C	558	ASN
2	D	65	MET
2	D	123	VAL
2	D	200	ASN
2	D	248	LEU
2	D	308	ASN
2	D	322	THR
2	D	384	VAL
2	D	398	ILE
2	D	416	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	476	LEU
2	D	497	ARG
2	D	530	ARG
2	D	533	GLU
2	D	553	ILE
1	E	5	ASP
1	E	150	LEU
1	E	171	LEU
1	E	214	LEU
1	E	218	ILE
1	E	226	ARG
1	F	5	ASP
1	F	150	LEU
1	F	171	LEU
1	F	214	LEU
1	F	218	ILE
1	F	226	ARG
2	G	65	MET
2	G	123	VAL
2	G	200	ASN
2	G	248	LEU
2	G	308	ASN
2	G	322	THR
2	G	384	VAL
2	G	398	ILE
2	G	530	ARG
2	G	533	GLU
2	H	65	MET
2	H	123	VAL
2	H	200	ASN
2	H	231	LYS
2	H	248	LEU
2	H	308	ASN
2	H	322	THR
2	H	384	VAL
2	H	398	ILE
2	H	459	ASN
2	H	467	ASN
2	H	497	ARG
2	H	533	GLU
2	H	558	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	B	44	ASN
1	B	90	GLN
1	B	203	HIS
2	C	183	ASN
2	C	308	ASN
2	C	315	GLN
2	C	348	GLN
2	C	545	GLN
2	D	140	HIS
2	D	308	ASN
2	D	348	GLN
1	E	90	GLN
1	E	203	HIS
1	F	90	GLN
1	F	190	GLN
2	G	308	ASN
2	G	348	GLN
2	G	551	ASN
2	H	308	ASN
2	H	315	GLN
2	H	348	GLN
2	H	545	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	300/351 (85%)	-1.16	0 100 100	97, 126, 151, 158	0
1	B	300/351 (85%)	-1.13	0 100 100	96, 125, 152, 160	0
1	E	300/351 (85%)	-1.13	0 100 100	97, 126, 152, 160	0
1	F	300/351 (85%)	-1.20	0 100 100	98, 126, 151, 158	0
2	C	492/570 (86%)	-1.20	0 100 100	90, 124, 170, 179	0
2	D	480/570 (84%)	-1.21	0 100 100	92, 122, 167, 180	0
2	G	482/570 (84%)	-1.18	0 100 100	92, 123, 167, 179	0
2	H	493/570 (86%)	-1.17	0 100 100	91, 125, 170, 183	0
All	All	3147/3684 (85%)	-1.18	0 100 100	90, 124, 162, 183	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.