



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:30 PM UTC

PDB ID : 4LJZ / pdb_00004ljz
Title : Crystal Structure Analysis of the E.coli holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-05
Resolution : 3.59 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:

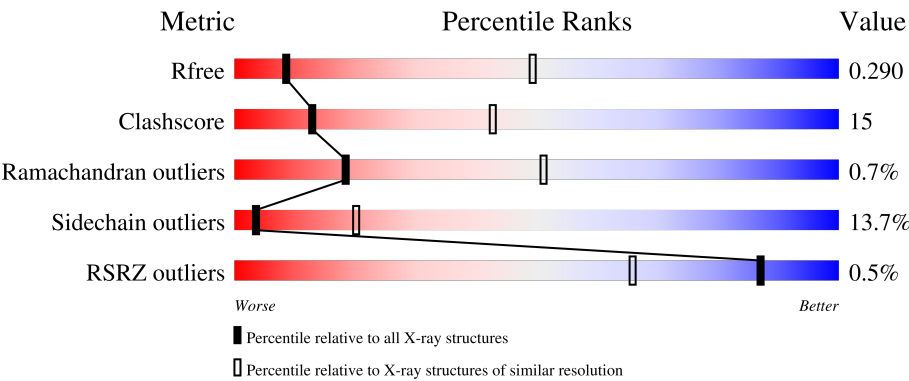
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.59 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	239	59%29%6%6%
1	B	239	47%40%5%8%
1	G	239	60%28%7%5%
1	H	239	45%40%5%9%
2	C	1342	61%32%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1342	% 62%31%6%
3	D	1407	48%29%6%17%
3	J	1407	% 54%33%7%6%
4	E	91	60%31%5%
4	K	91	52%27%8%13%
5	F	522	% 57%25%6%10%
5	L	522	56%26%6%10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56339 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP C9QXI7
A	236	VAL	-	expression tag	UNP C9QXI7
A	237	LEU	-	expression tag	UNP C9QXI7
A	238	PHE	-	expression tag	UNP C9QXI7
A	239	GLN	-	expression tag	UNP C9QXI7
B	235	GLU	-	expression tag	UNP C9QXI7
B	236	VAL	-	expression tag	UNP C9QXI7
B	237	LEU	-	expression tag	UNP C9QXI7
B	238	PHE	-	expression tag	UNP C9QXI7
B	239	GLN	-	expression tag	UNP C9QXI7
G	235	GLU	-	expression tag	UNP C9QXI7
G	236	VAL	-	expression tag	UNP C9QXI7
G	237	LEU	-	expression tag	UNP C9QXI7
G	238	PHE	-	expression tag	UNP C9QXI7
G	239	GLN	-	expression tag	UNP C9QXI7
H	235	GLU	-	expression tag	UNP C9QXI7
H	236	VAL	-	expression tag	UNP C9QXI7
H	237	LEU	-	expression tag	UNP C9QXI7
H	238	PHE	-	expression tag	UNP C9QXI7
H	239	GLN	-	expression tag	UNP C9QXI7

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	49			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	470	Total	C	N	O	S	0	0	0
			3822	2394	680	725	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

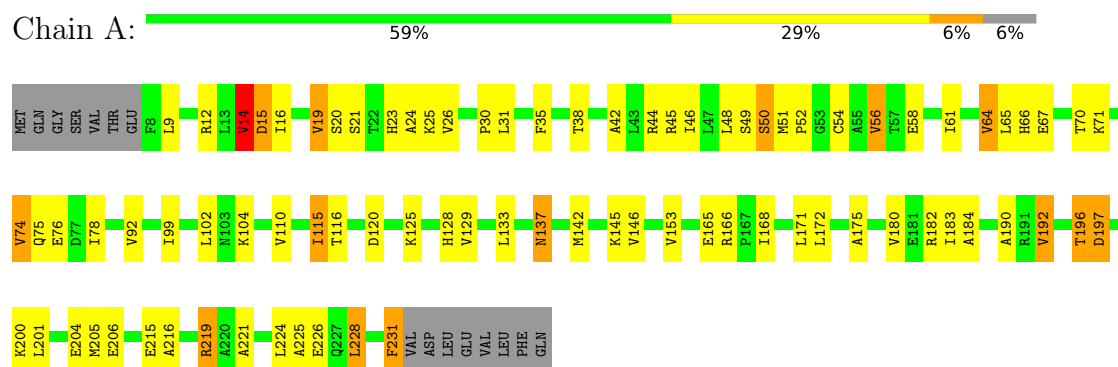
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total 2	Zn 2	0	0
7	J	2	Total 2	Zn 2	0	0

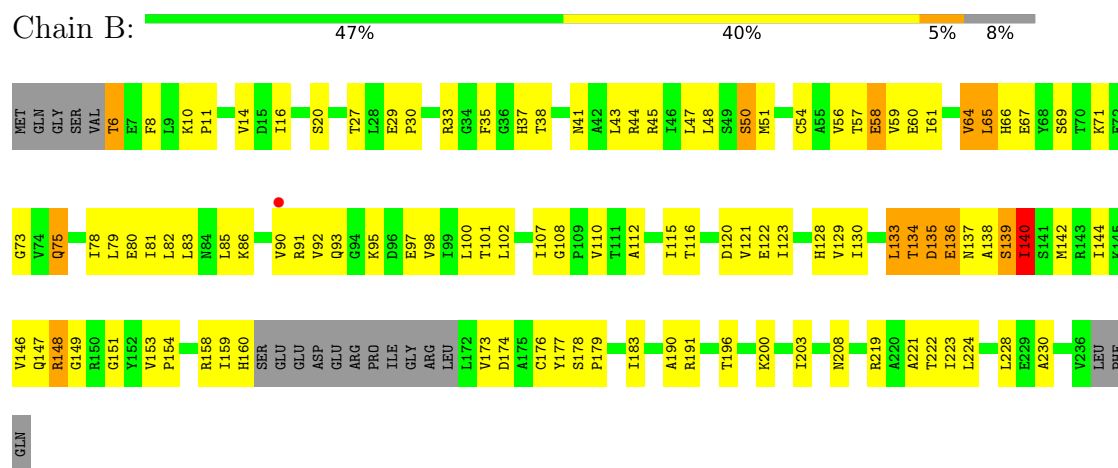
3 Residue-property plots

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

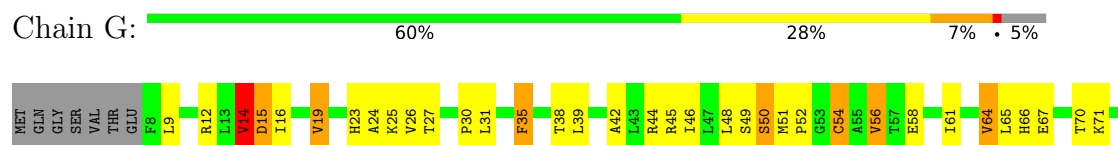
• Molecule 1: DNA-directed RNA polymerase subunit alpha

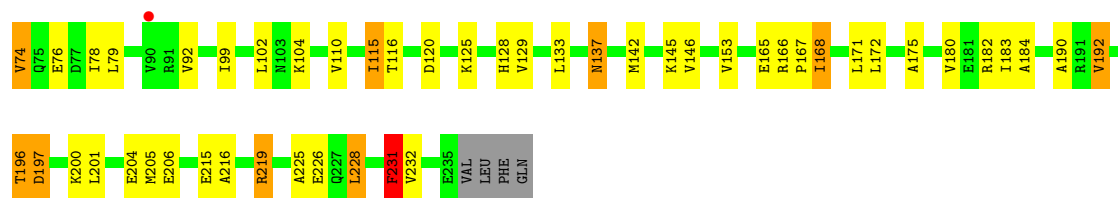


• Molecule 1: DNA-directed RNA polymerase subunit alpha



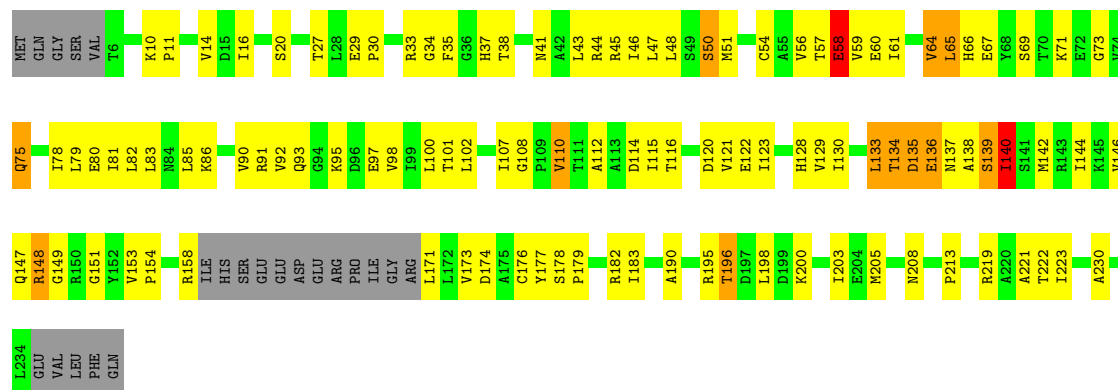
• Molecule 1: DNA-directed RNA polymerase subunit alpha





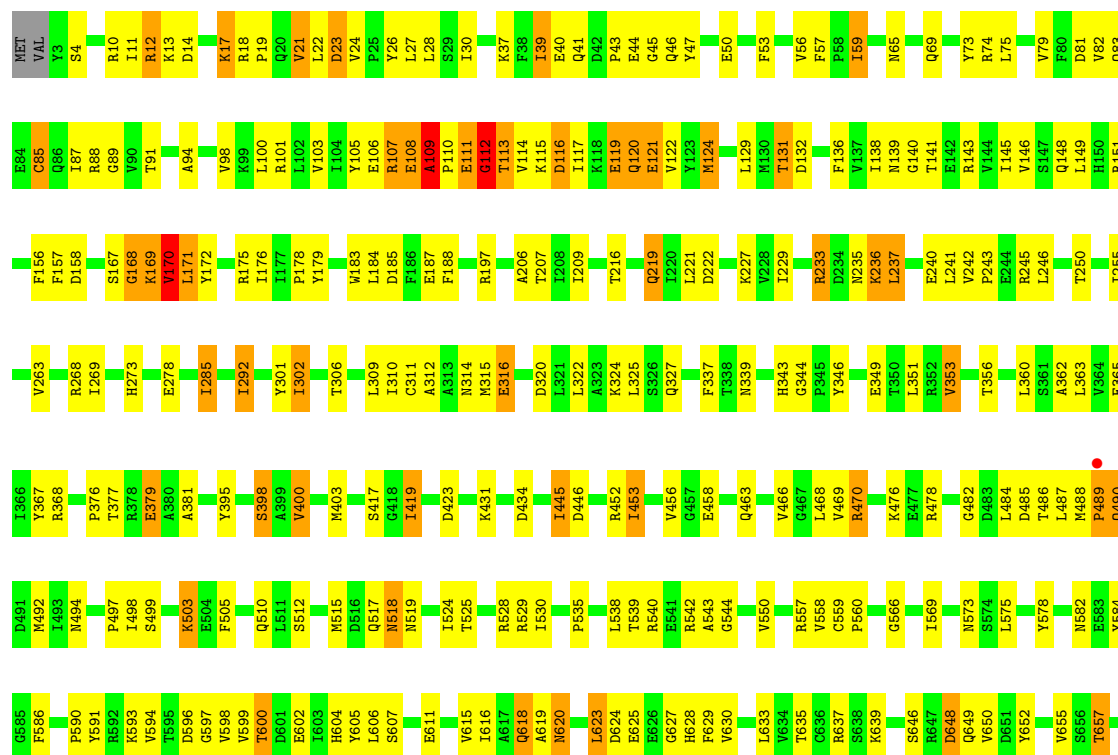
• Molecule 1: DNA-directed RNA polymerase subunit alpha

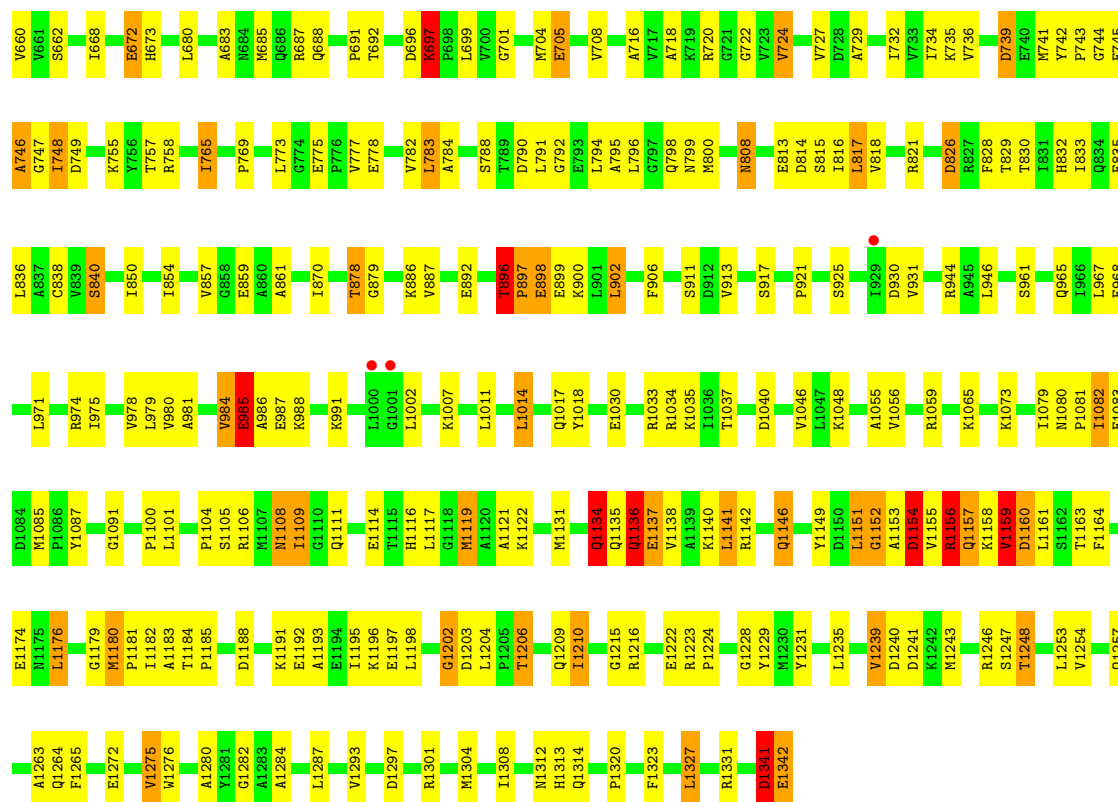
Chain H: 45% 40% 5% 9%



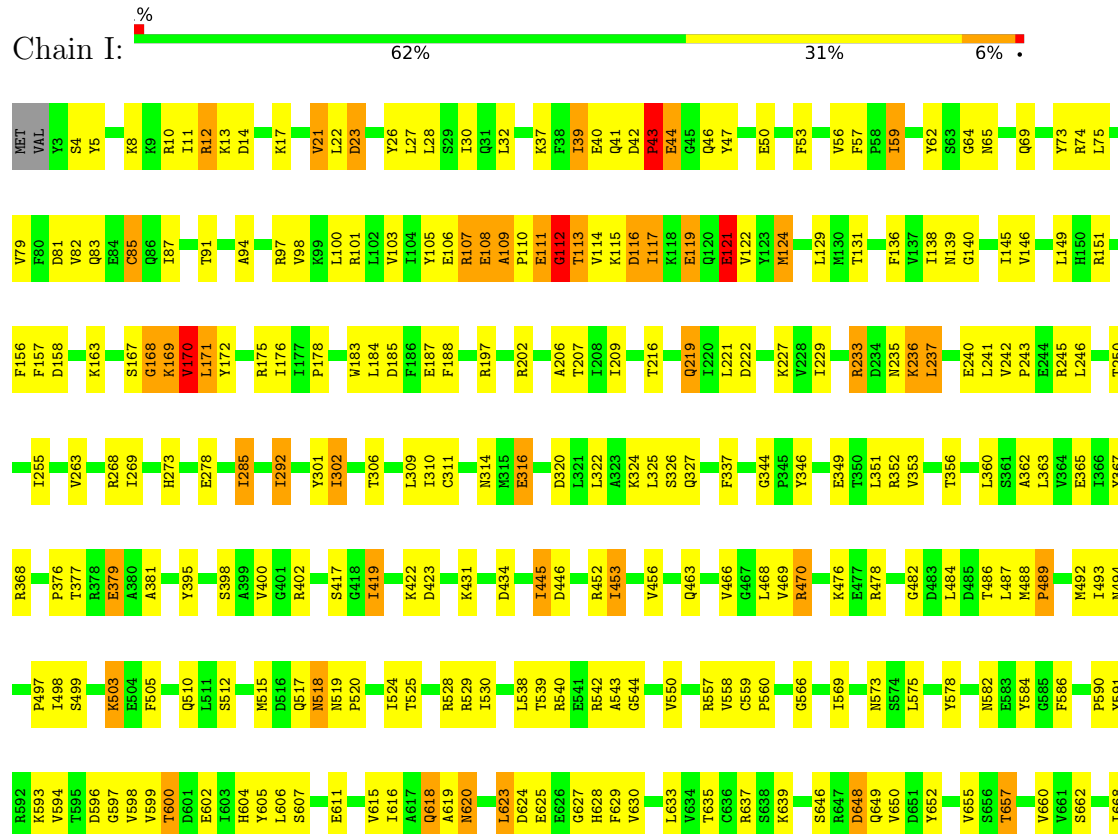
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 61% 32% 6%



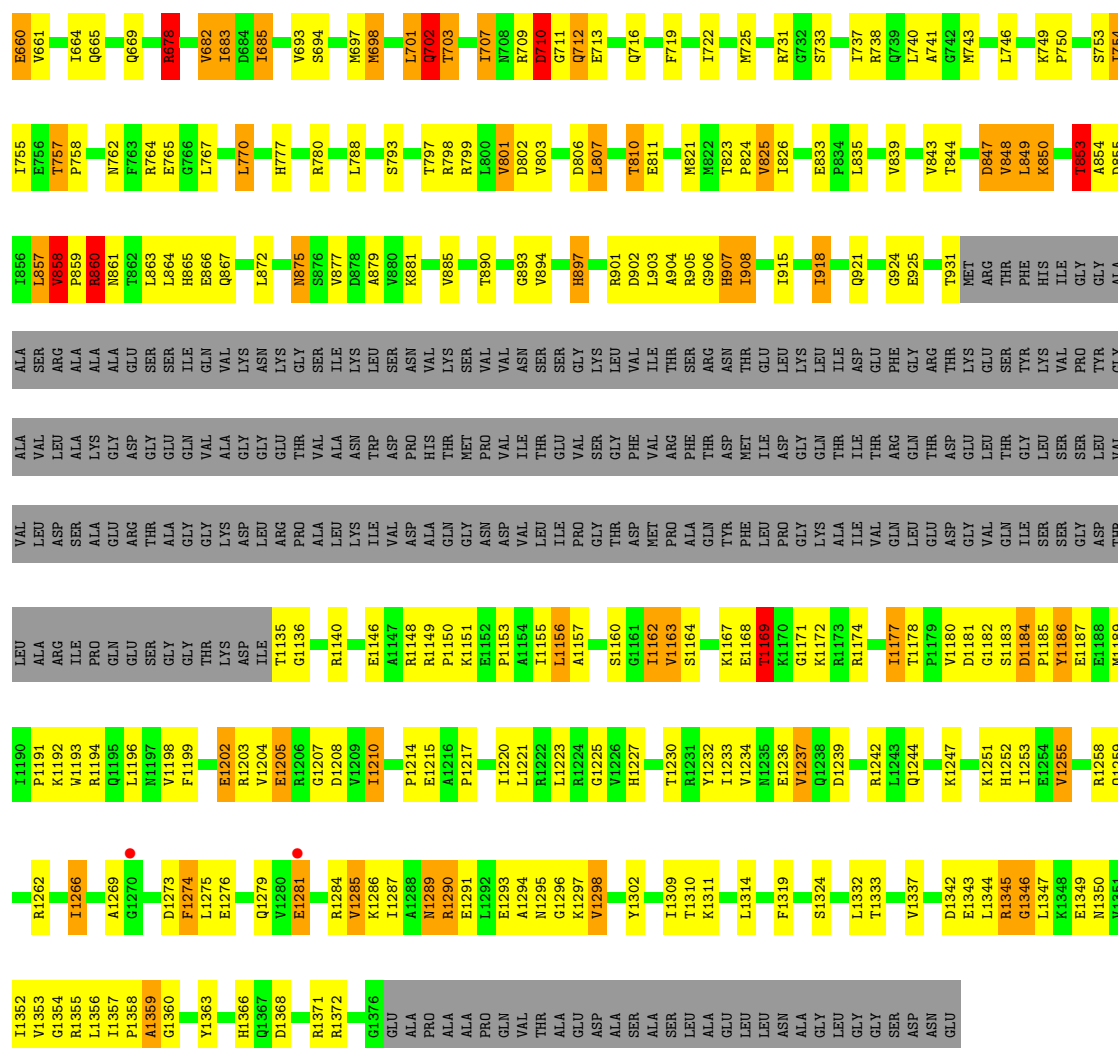


• Molecule 2: DNA-directed RNA polymerase subunit beta

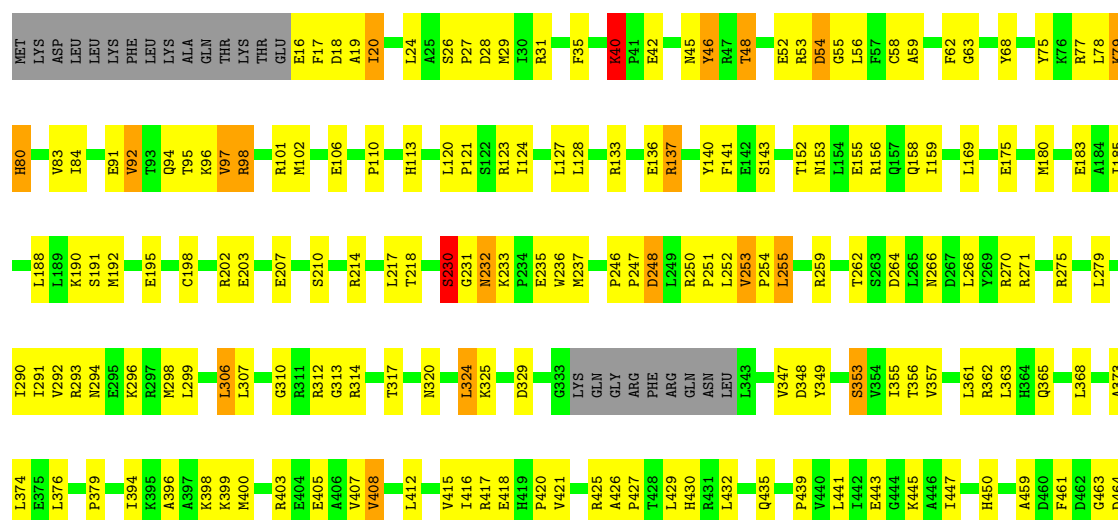




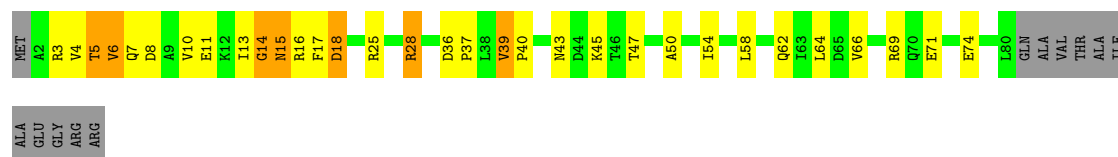
L569	Q477	K296	L188	V92	MET
T573	A452	K297	L189	T93	LYS
V574	L483	K298	K190	Q94	ASP
G575	M484	K395	S191	T95	LEU
R576	M485	L306	M192	K96	LEU
A577		L307	E203	V97	LYS
L578	M488	M400		R98	PHE
L579	M489	G310	E207	R101	L8
	L490	R311		M102	K9
I582	L491	E404	S210		Q11
		E405		E106	T12
K585	E497	A406	R214		
G586	P498	V407		P110	D18
L587	L499	V408	L217		A19
	I500	V409	T218	H113	I20
N593	V501	R320			
Q594		L412	S236	L120	L24
L596	Q504		G231	P121	A25
	D505	V415	S232	S122	S26
V506		L416	R233	R123	P27
		R417	P234		D28
K599	M513	E418	E235	L127	N29
A600	T514	R419	E236	L128	T30
	R515	P420	K237		R31
K603	D516	V421		R133	
	C517	R425	P246		F35
G608	V518	R338	P247	E136	
R610	M519	R339	D248	R137	K40
I611		P427	L249		P41
L612	E523	T428	R250	Y140	E42
G613	G524	L429	P251	F141	
K614	M525	H430	L252	E142	N45
G615	V526	R431	V253	S143	Y46
P616	L527	L432	P254	R47	
T617	T528	D348	L255	T152	T48
	G529	R349		N153	
F620			R259	L154	E52
I624	E532	R353		E155	R53
	R535	V354	T262	R156	D54
G628	L536	G444	S263	Q157	G55
		K445	D264	Q158	
		V357	L265	I159	
A632	L544	L447	K266	L160	C58
A633	H545		D267	T161	A59
S635	V548	H450	V269	Q164	F62
	K549	A459	R270		G63
I641	V550	D460	R271	L169	
		F461			Y68
V645	E556	D462	R275	F172	Y75
I646	K557	G463			K76
P647	D558	D464	L279	E175	R77
	A559	G465			L78
K650	M560	M466	A373	M180	K79
			L374		H80
I654	L563	L472	L376	E183	
					V63
E658	T567	T473	P379	I185	I84
S659		L474	R390		



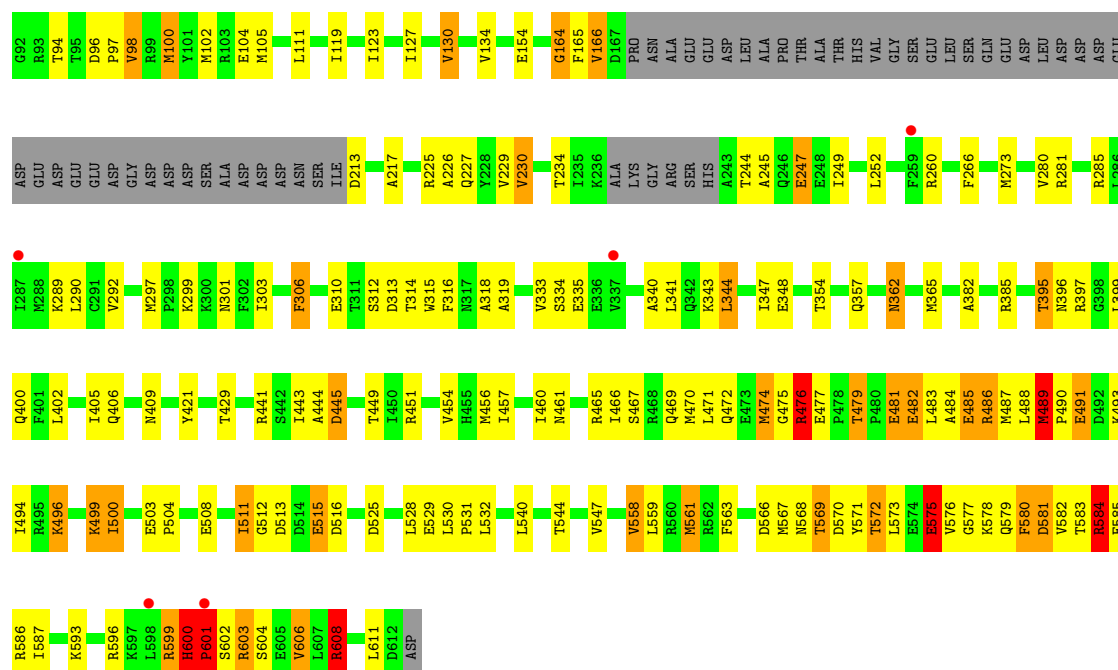
• Molecule 3: DNA-directed RNA polymerase subunit beta'



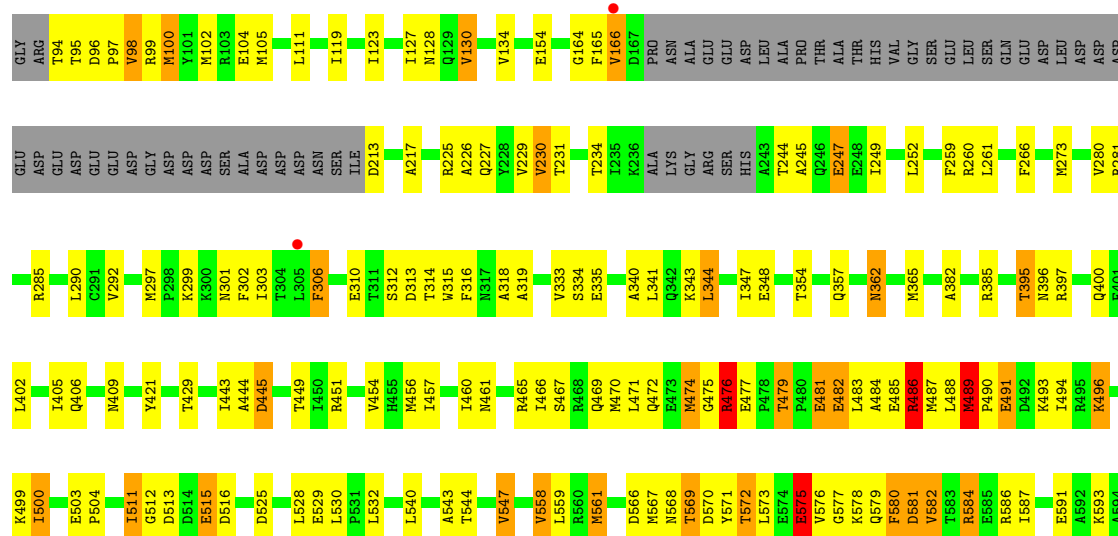




• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD



L595	R596	R597	L598	R599	H600	R601	S602	R603	V606	L607	R608	L611	D612	D613
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.37Å 206.74Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.59 29.88 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.88-3.59) 99.1 (29.88-3.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.246 , 0.288 0.244 , 0.290	Depositor DCC
R_{free} test set	6979 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56339	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.39	0/1751	0.93	4/2373 (0.2%)
1	B	0.39	0/1707	0.93	7/2314 (0.3%)
1	G	0.42	1/1771 (0.1%)	0.94	4/2401 (0.2%)
1	H	0.40	0/1686	0.94	7/2285 (0.3%)
2	C	0.40	0/10739	0.96	42/14489 (0.3%)
2	I	0.40	0/10735	0.94	35/14484 (0.2%)
3	D	0.40	0/9246	0.93	35/12478 (0.3%)
3	J	0.38	0/10450	0.90	29/14112 (0.2%)
4	E	0.38	0/693	0.89	1/935 (0.1%)
4	K	0.39	0/629	0.87	0/847
5	F	0.48	4/3873 (0.1%)	0.97	17/5206 (0.3%)
5	L	0.48	2/3872 (0.1%)	0.97	13/5205 (0.2%)
All	All	0.41	7/57152 (0.0%)	0.94	194/77129 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
1	H	0	1
2	C	0	14
2	I	0	15
3	D	0	5
3	J	0	6
4	K	0	1
5	F	0	4
5	L	0	2
All	All	0	50

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	600	HIS	CA-C	7.35	1.62	1.52
5	F	600	HIS	N-CA	6.30	1.57	1.45
1	G	231	PHE	CA-C	5.89	1.60	1.52
5	F	600	HIS	CA-C	5.61	1.61	1.53
5	F	601	PRO	CA-CB	-5.26	1.46	1.53
5	L	128	ASN	N-CA	5.15	1.52	1.46
5	F	599	ARG	CA-C	5.13	1.59	1.52

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	747	GLY	N-CA-C	21.85	142.76	112.17
2	C	109	ALA	CA-C-N	15.46	136.52	119.83
2	C	109	ALA	C-N-CA	15.46	136.52	119.83
2	C	747	GLY	N-CA-C	15.37	149.61	113.18
2	C	490	GLN	N-CA-C	12.74	128.28	112.23
2	C	896	THR	CA-C-N	10.18	132.57	119.84
2	C	896	THR	C-N-CA	10.18	132.57	119.84
2	C	1138	VAL	N-CA-C	10.08	120.90	110.72
2	C	112	GLY	N-CA-C	9.99	125.57	112.18
2	I	1134	GLN	CA-C-N	9.30	134.34	121.05
2	I	1134	GLN	C-N-CA	9.30	134.34	121.05
2	I	896	THR	CA-C-N	9.29	131.46	119.84
2	I	896	THR	C-N-CA	9.29	131.46	119.84
5	L	166	VAL	N-CA-C	-8.97	97.00	108.84
3	D	172	PHE	N-CA-C	8.80	122.51	112.57
5	F	166	VAL	N-CA-C	-8.77	97.09	108.93
3	D	858	VAL	CA-C-N	8.33	130.25	119.84
3	D	858	VAL	C-N-CA	8.33	130.25	119.84
3	J	858	VAL	CA-C-N	8.18	130.07	119.84
3	J	858	VAL	C-N-CA	8.18	130.07	119.84
1	G	232	VAL	N-CA-C	7.93	125.83	109.34
2	C	45	GLY	N-CA-C	7.92	125.70	115.32
2	I	812	PHE	N-CA-C	7.83	120.51	111.11
2	C	985	GLU	N-CA-C	7.80	122.55	112.41
3	D	853	THR	N-CA-C	7.67	120.07	109.18
2	I	1157	GLN	N-CA-C	7.60	119.56	111.28
3	D	1171	GLY	N-CA-C	-7.55	105.70	114.69
2	I	236	LYS	N-CA-C	7.45	119.63	110.91
2	C	236	LYS	N-CA-C	7.39	119.56	110.91
3	J	853	THR	N-CA-C	7.33	119.58	109.18
2	I	112	GLY	N-CA-C	7.19	130.22	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	601	PRO	CA-C-N	7.13	135.15	121.54
5	F	601	PRO	C-N-CA	7.13	135.15	121.54
5	F	164	GLY	N-CA-C	-7.10	104.33	112.29
2	C	1152	GLY	CA-C-N	7.06	135.03	121.54
2	C	1152	GLY	C-N-CA	7.06	135.03	121.54
5	L	213	ASP	CA-C-N	7.04	126.87	119.05
5	L	213	ASP	C-N-CA	7.04	126.87	119.05
5	F	213	ASP	CA-C-N	7.00	126.82	119.05
5	F	213	ASP	C-N-CA	7.00	126.82	119.05
3	D	230	SER	N-CA-C	7.00	125.70	110.80
2	C	512	SER	CA-C-N	-6.98	111.29	122.53
2	C	512	SER	C-N-CA	-6.98	111.29	122.53
1	G	192	VAL	N-CA-C	-6.96	99.94	109.55
2	C	237	LEU	N-CA-C	6.95	125.60	110.80
2	C	1264	GLN	N-CA-C	-6.92	97.45	108.73
2	I	237	LEU	N-CA-C	6.91	125.53	110.80
1	A	192	VAL	N-CA-C	-6.91	100.02	109.55
2	I	1264	GLN	N-CA-C	-6.90	97.28	108.52
3	D	231	GLY	N-CA-C	6.88	129.50	113.18
5	L	584	ARG	N-CA-C	6.87	125.44	110.80
2	C	1134	GLN	O-C-N	6.87	129.40	122.12
3	D	1225	GLY	N-CA-C	6.80	118.95	112.08
1	A	166	ARG	CA-C-N	-6.78	111.37	119.84
1	A	166	ARG	C-N-CA	-6.78	111.37	119.84
5	F	486	ARG	CB-CG-CD	6.76	126.85	111.30
2	C	1157	GLN	N-CA-C	6.71	119.45	111.33
3	J	711	GLY	N-CA-C	-6.68	103.41	112.57
3	J	678	ARG	CA-CB-CG	6.67	127.43	114.10
2	I	1136	GLN	CA-C-N	6.39	133.74	121.54
2	I	1136	GLN	C-N-CA	6.39	133.74	121.54
3	J	1210	ILE	N-CA-C	-6.38	106.51	112.83
3	D	678	ARG	CA-CB-CG	6.38	126.85	114.10
1	B	75	GLN	CA-CB-CG	6.26	126.62	114.10
5	L	600	HIS	CA-C-N	6.26	127.67	119.84
5	L	600	HIS	C-N-CA	6.26	127.67	119.84
1	B	108	GLY	CA-C-N	6.22	126.24	119.90
1	B	108	GLY	C-N-CA	6.22	126.24	119.90
3	D	335	GLN	N-CA-C	-6.20	105.67	113.23
3	D	1210	ILE	N-CA-C	-6.20	106.69	112.83
1	H	108	GLY	CA-C-N	6.16	126.18	119.90
1	H	108	GLY	C-N-CA	6.16	126.18	119.90
3	J	1021	ASP	CA-C-N	6.12	125.34	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1021	ASP	C-N-CA	6.12	125.34	118.97
5	L	575	GLU	CA-CB-CG	6.11	126.31	114.10
3	D	850	LYS	CA-C-N	-6.06	112.32	119.05
3	D	850	LYS	C-N-CA	-6.06	112.32	119.05
2	C	398	SER	CB-CA-C	-6.06	107.89	115.89
3	D	1346	GLY	N-CA-C	5.96	120.23	112.25
2	I	398	SER	CB-CA-C	-5.94	108.05	115.89
3	J	40	LYS	CA-C-N	5.90	125.52	119.56
3	J	40	LYS	C-N-CA	5.90	125.52	119.56
5	F	575	GLU	CA-CB-CG	5.86	125.81	114.10
1	H	75	GLN	CA-CB-CG	5.84	125.78	114.10
2	C	1154	ASP	N-CA-C	5.82	123.19	110.80
5	L	486	ARG	CB-CG-CD	5.81	124.66	111.30
3	D	40	LYS	CA-C-N	5.78	125.40	119.56
3	D	40	LYS	C-N-CA	5.78	125.40	119.56
3	D	207	GLU	N-CA-C	5.78	117.44	111.03
3	D	529	GLY	CA-C-N	5.78	125.90	119.32
3	D	529	GLY	C-N-CA	5.78	125.90	119.32
3	J	850	LYS	CA-C-N	-5.77	112.65	119.05
3	J	850	LYS	C-N-CA	-5.77	112.65	119.05
2	I	1138	VAL	N-CA-C	5.73	117.25	111.00
3	D	1359	ALA	N-CA-C	-5.72	98.62	110.80
2	C	1156	ARG	N-CA-C	5.72	120.38	113.17
3	J	313	GLY	N-CA-C	5.71	122.80	115.32
1	G	54	CYS	N-CA-C	5.69	119.00	112.57
4	E	15	ASN	N-CA-CB	-5.67	100.91	110.49
3	J	529	GLY	CA-C-N	5.67	125.79	119.32
3	J	529	GLY	C-N-CA	5.67	125.79	119.32
3	D	586	GLY	N-CA-C	5.65	120.67	114.40
2	C	1341	ASP	N-CA-C	5.63	116.34	108.00
5	F	489	MET	CA-C-N	5.63	126.87	119.84
5	F	489	MET	C-N-CA	5.63	126.87	119.84
3	D	253	VAL	CA-C-N	5.62	125.59	120.03
3	D	253	VAL	C-N-CA	5.62	125.59	120.03
2	I	44	GLU	N-CA-C	5.61	122.74	110.80
3	D	515	ARG	N-CA-C	-5.60	99.80	108.42
3	J	586	GLY	N-CA-C	5.59	120.61	114.40
2	C	485	ASP	N-CA-C	5.59	118.89	112.57
2	I	1341	ASP	N-CA-C	5.59	116.27	108.00
5	F	601	PRO	N-CA-C	5.58	123.97	112.47
2	C	573	ASN	CB-CA-C	-5.58	108.53	116.34
2	I	1162	SER	N-CA-C	-5.56	104.12	111.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1235	LEU	CA-C-N	-5.56	114.55	122.77
2	I	1235	LEU	C-N-CA	-5.56	114.55	122.77
2	I	573	ASN	CB-CA-C	-5.55	108.58	116.34
2	I	1156	ARG	N-CA-C	5.55	120.16	113.17
5	F	608	ARG	CG-CD-NE	5.54	124.20	112.00
2	C	1341	ASP	CB-CA-C	-5.54	108.58	116.34
3	D	48	THR	N-CA-C	-5.54	101.45	109.59
2	C	1179	GLY	N-CA-C	-5.54	103.73	111.09
1	B	58	GLU	N-CA-C	5.53	117.25	108.79
2	C	1137	GLU	N-CA-C	-5.53	99.03	110.80
3	J	48	THR	N-CA-C	-5.53	101.47	109.59
3	D	450	HIS	CA-C-N	5.50	125.59	119.32
3	D	450	HIS	C-N-CA	5.50	125.59	119.32
2	I	1341	ASP	CB-CA-C	-5.50	108.64	116.34
3	J	253	VAL	CA-C-N	5.50	125.47	120.03
3	J	253	VAL	C-N-CA	5.50	125.47	120.03
2	I	997	TRP	N-CA-C	-5.49	105.69	112.72
2	I	1179	GLY	N-CA-C	-5.49	103.80	111.09
2	C	1160	ASP	CA-C-N	5.48	131.57	121.70
2	C	1160	ASP	C-N-CA	5.48	131.57	121.70
5	L	489	MET	CA-C-N	5.47	126.68	119.84
5	L	489	MET	C-N-CA	5.47	126.68	119.84
5	F	584	ARG	N-CA-CB	5.46	119.73	110.49
1	B	66	HIS	N-CA-C	5.45	117.97	109.52
3	J	515	ARG	N-CA-C	-5.45	100.03	108.42
1	G	64	VAL	N-CA-C	5.45	115.74	108.11
5	F	600	HIS	CA-C-N	5.43	126.63	119.84
5	F	600	HIS	C-N-CA	5.43	126.63	119.84
2	I	1153	ALA	N-CA-C	-5.43	99.24	110.80
5	F	608	ARG	CB-CG-CD	5.41	123.74	111.30
2	I	1263	ALA	N-CA-C	-5.40	106.65	113.23
3	J	450	HIS	CA-C-N	5.39	125.47	119.32
3	J	450	HIS	C-N-CA	5.39	125.47	119.32
1	B	136	GLU	N-CA-C	5.38	115.97	108.00
2	C	697	LYS	N-CA-C	-5.38	97.93	109.81
1	B	20	SER	CB-CA-C	-5.36	109.94	117.23
2	I	1241	ASP	N-CA-C	-5.36	99.39	110.80
3	J	1169	THR	CA-C-N	-5.34	115.83	123.20
3	J	1169	THR	C-N-CA	-5.34	115.83	123.20
2	C	1263	ALA	N-CA-C	-5.33	106.73	113.23
2	I	43	PRO	CA-C-N	5.32	131.71	121.54
2	I	43	PRO	C-N-CA	5.32	131.71	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	20	SER	CB-CA-C	-5.30	110.02	117.23
1	H	58	GLU	N-CA-C	5.30	116.58	108.42
1	A	64	VAL	N-CA-C	5.29	115.51	108.11
2	C	171	LEU	N-CA-C	-5.26	100.74	108.79
3	J	1167	LYS	CB-CA-C	-5.26	109.53	115.79
3	J	207	GLU	N-CA-C	5.26	116.86	111.03
3	D	1167	LYS	CB-CA-C	-5.25	109.54	115.79
2	I	171	LEU	N-CA-C	-5.24	100.77	108.79
5	L	476	ARG	CB-CA-C	-5.22	104.83	115.27
3	J	713	GLU	N-CA-C	5.22	117.12	109.24
2	C	1235	LEU	CA-C-N	-5.19	115.09	122.77
2	C	1235	LEU	C-N-CA	-5.19	115.09	122.77
2	C	1241	ASP	N-CA-C	-5.18	105.18	112.12
3	D	713	GLU	N-CA-C	5.16	117.04	109.24
2	C	112	GLY	CA-C-O	5.16	125.90	121.88
1	H	66	HIS	N-CA-C	5.15	117.99	109.85
2	I	1135	GLN	N-CA-CB	-5.14	101.51	109.48
2	C	1136	GLN	CA-C-N	5.13	131.33	121.54
2	C	1136	GLN	C-N-CA	5.13	131.33	121.54
2	C	1202	GLY	CA-C-N	5.13	131.34	121.54
2	C	1202	GLY	C-N-CA	5.13	131.34	121.54
5	L	601	PRO	CA-CB-CG	-5.11	94.80	104.50
3	D	702	GLN	N-CA-C	5.09	116.68	111.03
1	H	136	GLU	N-CA-C	5.09	115.53	108.00
2	I	856	ASN	N-CA-C	5.08	118.14	111.28
5	L	608	ARG	CG-CD-NE	5.07	123.15	112.00
3	D	362	ARG	N-CA-C	-5.06	103.37	110.50
3	D	860	ARG	CB-CA-C	-5.05	110.37	117.23
3	D	1269	ALA	N-CA-C	5.05	114.95	108.34
5	F	476	ARG	CB-CG-CD	5.04	122.90	111.30
2	I	1106	ARG	CA-C-N	-5.04	115.00	122.41
2	I	1106	ARG	C-N-CA	-5.04	115.00	122.41
2	C	1159	VAL	N-CA-CB	5.02	119.52	111.23
3	J	1269	ALA	N-CA-C	5.02	114.92	108.34
3	D	501	VAL	CA-C-N	5.02	125.02	119.90
3	D	501	VAL	C-N-CA	5.02	125.02	119.90
3	J	362	ARG	N-CA-C	-5.00	103.44	110.50

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ILE	Peptide
2	C	109	ALA	Peptide
2	C	111	GLU	Peptide
2	C	112	GLY	Peptide
2	C	1134	GLN	Peptide
2	C	1152	GLY	Mainchain
2	C	1202	GLY	Peptide,Mainchain
2	C	168	GLY	Mainchain
2	C	236	LYS	Peptide
2	C	43	PRO	Mainchain
2	C	489	PRO	Peptide
2	C	648	ASP	Peptide
2	C	746	ALA	Peptide
2	C	985	GLU	Mainchain
3	D	1168	GLU	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
3	D	172	PHE	Mainchain
3	D	230	SER	Peptide
5	F	474	MET	Peptide,Mainchain
5	F	601	PRO	Peptide
5	F	602	SER	Mainchain
1	G	231	PHE	Peptide
1	H	140	ILE	Peptide
2	I	109	ALA	Peptide
2	I	111	GLU	Peptide
2	I	112	GLY	Peptide
2	I	1134	GLN	Peptide
2	I	1136	GLN	Peptide
2	I	1152	GLY	Mainchain
2	I	1153	ALA	Peptide
2	I	1202	GLY	Peptide,Mainchain
2	I	1236	ASN	Peptide
2	I	168	GLY	Mainchain
2	I	236	LYS	Peptide
2	I	43	PRO	Mainchain
2	I	489	PRO	Peptide
2	I	648	ASP	Peptide
3	J	1168	GLU	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
3	J	1359	ALA	Mainchain
3	J	230	SER	Peptide,Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	K	14	GLY	Mainchain
5	L	474	MET	Mainchain
5	L	601	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	56	0
1	B	1687	0	1700	70	0
1	G	1750	0	1764	54	0
1	H	1667	0	1689	71	0
2	C	10570	0	10582	317	1
2	I	10566	0	10576	297	1
3	D	9107	0	9308	338	0
3	J	10295	0	10511	398	0
4	E	691	0	695	23	0
4	K	627	0	634	19	0
5	F	3822	0	3885	104	0
5	L	3821	0	3884	112	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	56339	0	56984	1715	1

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 15.

All (1715) 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:233:ARG:HH11	2:C:233:ARG:HG3	1.24	1.02
3:D:26:SER:HA	3:D:236:TRP:HE1	1.30	0.96
3:J:98:ARG:HG2	3:J:98:ARG:HH11	1.32	0.94
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.51	0.92
3:D:98:ARG:HH11	3:D:98:ARG:HG2	1.35	0.89
2:C:898:GLU:HB3	5:F:544:THR:HG21	1.57	0.87
3:D:418:GLU:HG3	4:E:45:LYS:H	1.40	0.86
3:J:26:SER:HA	3:J:236:TRP:HE1	1.39	0.86
3:D:26:SER:HA	3:D:236:TRP:NE1	1.89	0.85
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.57	0.85
2:I:119:GLU:HB2	2:I:489:PRO:HD2	1.57	0.85
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.59	0.84
3:J:26:SER:HA	3:J:236:TRP:NE1	1.91	0.84
3:J:418:GLU:HG3	4:K:45:LYS:H	1.40	0.84
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.84
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.61	0.82
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.61	0.82
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.61	0.82
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.60	0.81
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.62	0.81
2:I:452:ARG:NH1	2:I:584:TYR:O	2.13	0.81
2:C:452:ARG:NH1	2:C:584:TYR:O	2.14	0.80
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.62	0.80
1:A:231:PHE:HZ	1:B:221:ALA:HB3	1.45	0.80
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.45	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.64	0.79
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.63	0.79
5:L:474:MET:O	5:L:476:ARG:N	2.15	0.79
2:I:112:GLY:HA3	2:I:113:THR:HG23	1.65	0.78
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.64	0.78
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.66	0.78
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.49	0.77
5:F:474:MET:O	5:F:476:ARG:N	2.14	0.77
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.67	0.77
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.66	0.77
2:C:620:ASN:C	2:C:620:ASN:HD22	1.93	0.76
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.66	0.76
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.51	0.76
2:I:685:MET:HA	2:I:688:GLN:HE21	1.51	0.75
5:F:569:THR:OG1	5:F:570:ASP:N	2.14	0.75
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.68	0.75
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.52	0.75
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.69	0.75
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:893:GLY:O	3:J:1258:ARG:NH1	2.18	0.75
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.51	0.75
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.68	0.74
3:J:310:GLY:HA2	3:J:314:ARG:HG2	1.69	0.74
5:L:569:THR:OG1	5:L:570:ASP:N	2.09	0.74
3:D:310:GLY:HA2	3:D:314:ARG:HG2	1.69	0.74
2:C:685:MET:HA	2:C:688:GLN:HE21	1.52	0.74
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.69	0.74
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.69	0.74
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.67	0.74
2:C:168:GLY:O	2:C:170:VAL:N	2.20	0.74
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.74
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.70	0.74
2:I:168:GLY:O	2:I:170:VAL:N	2.19	0.74
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.53	0.74
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.68	0.74
3:J:1108:GLN:NE2	3:J:1120:THR:OG1	2.21	0.73
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.24	0.73
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.70	0.73
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.21	0.73
3:J:79:LYS:HB2	5:L:569:THR:H	1.53	0.73
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.70	0.73
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.54	0.73
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.24	0.72
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.70	0.72
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.71	0.72
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.71	0.72
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.71	0.72
2:C:23:ASP:OD1	2:C:23:ASP:N	2.21	0.72
2:C:739:ASP:OD1	2:C:739:ASP:N	2.21	0.72
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.54	0.72
2:I:23:ASP:OD1	2:I:23:ASP:N	2.21	0.72
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.71	0.72
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.72	0.72
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.72	0.72
2:I:560:PRO:O	3:J:780:ARG:NH2	2.23	0.72
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.70	0.71
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.55	0.71
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.23	0.71
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.23	0.71
1:G:196:THR:OG1	1:G:197:ASP:OD1	2.08	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:560:PRO:O	3:D:780:ARG:NH2	2.24	0.71
3:D:893:GLY:O	3:D:1258:ARG:NH1	2.19	0.71
2:I:898:GLU:HB3	5:L:544:THR:HG21	1.72	0.71
1:A:196:THR:OG1	1:A:197:ASP:OD1	2.09	0.71
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.71	0.71
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.72	0.70
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.55	0.70
3:J:16:GLU:HG3	3:J:17:PHE:H	1.56	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.74	0.70
3:J:1359:ALA:O	3:J:1363:TYR:HB2	1.92	0.70
3:D:710:ASP:OD1	3:D:711:GLY:N	2.25	0.70
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.22	0.70
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.73	0.70
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.72	0.69
3:J:233:LYS:H	3:J:236:TRP:HE3	1.40	0.69
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.72	0.69
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.75	0.69
1:B:93:GLN:HB2	1:B:120:ASP:HB3	1.74	0.69
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.73	0.69
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.75	0.69
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.75	0.69
3:D:233:LYS:H	3:D:236:TRP:HE3	1.39	0.69
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.73	0.69
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.75	0.69
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.18	0.69
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.22	0.69
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.25	0.69
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.74	0.69
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.75	0.69
3:J:1034:PHE:HA	3:J:1114:GLN:HA	1.75	0.69
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.27	0.68
1:G:56:VAL:HG23	1:G:146:VAL:HG22	1.76	0.68
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.25	0.68
3:J:1064:SER:HA	3:J:1067:ARG:HD2	1.74	0.68
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.59	0.68
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.75	0.68
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.59	0.68
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.76	0.68
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.73	0.68
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.75	0.67
3:J:140:TYR:OH	3:J:312:ARG:NH1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.27	0.67
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.76	0.67
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.77	0.67
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.76	0.67
5:L:97:PRO:HA	5:L:100:MET:HG3	1.76	0.67
5:F:97:PRO:HA	5:F:100:MET:HG3	1.77	0.67
3:J:27:PRO:HD3	3:J:236:TRP:HE1	1.58	0.67
1:A:196:THR:OG1	1:A:197:ASP:N	2.28	0.67
1:A:56:VAL:HG23	1:A:146:VAL:HG22	1.76	0.67
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.75	0.67
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.67
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.76	0.67
2:I:739:ASP:OD1	2:I:739:ASP:N	2.22	0.67
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.77	0.67
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.76	0.67
2:I:620:ASN:C	2:I:620:ASN:HD22	2.03	0.67
2:C:233:ARG:HG3	2:C:233:ARG:NH1	2.03	0.67
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.76	0.66
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.59	0.66
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.78	0.66
2:C:237:LEU:HD11	2:C:292:ILE:HD11	1.76	0.66
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.77	0.66
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.28	0.66
1:G:215:GLU:OE2	1:G:219:ARG:NH2	2.28	0.66
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.59	0.66
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.76	0.66
2:I:237:LEU:HD11	2:I:292:ILE:HD11	1.76	0.65
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.78	0.65
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.60	0.65
3:D:573:THR:H	3:D:576:ARG:HG3	1.62	0.65
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.60	0.65
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.77	0.65
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.19	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.79	0.65
3:D:1297:LYS:HG2	3:J:1302:TYR:O	1.97	0.65
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.77	0.65
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.79	0.65
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.22	0.65
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.78	0.65
1:A:231:PHE:CZ	1:B:221:ALA:HB3	2.29	0.65
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.79	0.65
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.22	0.65
3:J:573:THR:H	3:J:576:ARG:HG3	1.61	0.65
3:D:9:LYS:HE3	3:D:12:THR:HG23	1.80	0.64
3:D:54:ASP:OD1	3:D:54:ASP:N	2.30	0.64
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.78	0.64
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.79	0.64
3:J:674:THR:O	3:J:678:ARG:HB3	1.97	0.64
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.30	0.64
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.79	0.64
3:D:576:ARG:NH1	3:D:593:ASN:O	2.31	0.64
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.28	0.64
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.78	0.63
2:I:39:ILE:HD11	2:I:75:LEU:HG	1.79	0.63
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.80	0.63
3:J:613:GLY:O	3:J:617:THR:OG1	2.17	0.63
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.79	0.63
2:C:250:THR:HA	2:C:268:ARG:HA	1.81	0.63
3:J:576:ARG:NH1	3:J:593:ASN:O	2.31	0.63
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.30	0.63
5:L:543:ALA:HB1	5:L:607:LEU:HD22	1.80	0.63
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.80	0.63
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.28	0.63
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.79	0.63
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.81	0.63
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.80	0.63
3:D:1297:LYS:HB3	3:J:1303:SER:HA	1.79	0.63
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.81	0.63
3:J:741:ALA:O	3:J:762:ASN:ND2	2.32	0.63
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.80	0.63
3:J:54:ASP:OD1	3:J:54:ASP:N	2.30	0.63
5:L:577:GLY:O	5:L:581:ASP:N	2.32	0.63
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.32	0.62
1:H:182:ARG:NH1	3:J:581:MET:SD	2.72	0.62
2:I:250:THR:HA	2:I:268:ARG:HA	1.81	0.62
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.32	0.62
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.80	0.62
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.62
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.82	0.62
3:D:27:PRO:HD3	3:D:236:TRP:HE1	1.63	0.62
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.80	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.64	0.62
3:J:821:MET:HE2	3:J:879:ALA:HB1	1.81	0.62
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.32	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.80	0.62
2:C:136:PHE:O	2:C:143:ARG:N	2.26	0.62
1:H:93:GLN:HB2	1:H:120:ASP:HB3	1.80	0.62
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.80	0.62
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.80	0.62
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.81	0.62
2:C:701:GLY:O	2:C:1184:THR:N	2.28	0.62
2:I:980:VAL:HA	2:I:984:VAL:HA	1.82	0.62
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.33	0.62
5:L:561:MET:HA	5:L:567:MET:HE1	1.82	0.62
2:C:40:GLU:O	2:C:73:TYR:OH	2.16	0.62
5:F:310:GLU:O	5:F:344:LEU:HD21	2.00	0.62
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.65	0.62
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.33	0.62
3:D:821:MET:HE2	3:D:879:ALA:HB1	1.82	0.62
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.80	0.62
2:I:705:GLU:HB2	2:I:794:LEU:H	1.64	0.62
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.80	0.62
5:L:310:GLU:O	5:L:344:LEU:HD21	2.00	0.62
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.32	0.62
2:C:705:GLU:HB2	2:C:794:LEU:H	1.65	0.62
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.33	0.61
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.33	0.61
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.82	0.61
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.27	0.61
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.82	0.61
5:L:94:THR:OG1	5:L:95:THR:N	2.33	0.61
5:L:600:HIS:HD2	5:L:601:PRO:HD3	1.65	0.61
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.82	0.61
2:I:40:GLU:O	2:I:73:TYR:OH	2.17	0.61
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.80	0.61
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.34	0.61
3:J:698:MET:O	3:J:702:GLN:HB3	2.01	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.65	0.61
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.34	0.61
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.81	0.61
2:I:886:LYS:H	2:I:917:SER:HB3	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.65	0.61
3:D:613:GLY:O	3:D:617:THR:OG1	2.18	0.61
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.82	0.61
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.33	0.61
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.83	0.61
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.61
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.82	0.61
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.64	0.61
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.32	0.61
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.32	0.61
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.82	0.61
3:J:79:LYS:HG3	3:J:80:HIS:ND1	2.16	0.61
5:L:479:THR:HG23	5:L:481:GLU:H	1.66	0.61
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	1.83	0.61
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.34	0.61
1:A:51:MET:HE3	1:A:52:PRO:HD2	1.83	0.60
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.65	0.60
2:C:41:GLN:NE2	2:C:73:TYR:O	2.35	0.60
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.83	0.60
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.34	0.60
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.83	0.60
5:F:577:GLY:O	5:F:581:ASP:N	2.31	0.60
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.17	0.60
2:I:324:LYS:O	2:I:327:GLN:NE2	2.35	0.60
1:A:23:HIS:HB2	1:A:205:MET:O	2.01	0.60
3:D:848:VAL:HG22	3:D:857:LEU:HD11	1.83	0.60
3:D:931:THR:OG1	3:D:1244:GLN:NE2	2.34	0.60
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.82	0.60
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.83	0.60
5:F:479:THR:HG23	5:F:481:GLU:H	1.66	0.60
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.66	0.60
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.82	0.60
1:G:196:THR:OG1	1:G:197:ASP:N	2.29	0.60
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	1.83	0.60
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.84	0.60
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.82	0.60
2:I:41:GLN:NE2	2:I:73:TYR:O	2.35	0.60
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.82	0.60
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.84	0.60
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.31	0.60
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.36	0.60
1:G:23:HIS:HB2	1:G:205:MET:O	2.01	0.60
3:J:722:ILE:HA	3:J:725:MET:HE3	1.83	0.60
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.82	0.60
2:I:735:LYS:HA	2:I:748:ILE:HG22	1.83	0.60
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.82	0.60
4:K:14:GLY:O	4:K:16:ARG:N	2.34	0.60
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.84	0.59
1:G:51:MET:HE3	1:G:52:PRO:HD2	1.83	0.59
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.84	0.59
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.66	0.59
2:C:620:ASN:C	2:C:620:ASN:ND2	2.58	0.59
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.83	0.59
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.67	0.59
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.82	0.59
3:D:698:MET:O	3:D:702:GLN:HB3	2.02	0.59
5:F:561:MET:HA	5:F:567:MET:HE1	1.83	0.59
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.83	0.59
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.84	0.59
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.84	0.59
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.84	0.59
2:I:975:ILE:HG13	2:I:1014:LEU:HD22	1.84	0.59
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.84	0.59
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.84	0.59
2:C:324:LYS:O	2:C:327:GLN:NE2	2.34	0.59
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.02	0.59
3:J:75:TYR:CD2	3:J:80:HIS:HD2	2.20	0.59
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.41	0.59
3:D:722:ILE:HA	3:D:725:MET:HE3	1.83	0.59
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.85	0.59
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.03	0.59
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.85	0.59
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.68	0.59
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.83	0.59
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.84	0.59
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.83	0.59
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.85	0.59
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.85	0.59
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.31	0.59
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.02	0.59
2:C:980:VAL:HA	2:C:984:VAL:HA	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.85	0.58
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.85	0.58
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.85	0.58
3:D:75:TYR:CD2	3:D:80:HIS:HD2	2.20	0.58
3:D:325:LYS:HG3	3:D:329:ASP:HB2	1.85	0.58
3:D:857:LEU:HD12	3:D:858:VAL:H	1.67	0.58
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.84	0.58
3:J:860:ARG:HG3	3:J:860:ARG:HH11	1.69	0.58
3:J:1067:ARG:HD3	3:J:1072:LYS:HA	1.84	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.69	0.58
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.85	0.58
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.86	0.58
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.37	0.58
5:L:600:HIS:CD2	5:L:601:PRO:HD3	2.37	0.58
2:C:207:THR:HG21	2:C:351:LEU:HG	1.86	0.58
5:F:312:SER:OG	5:F:313:ASP:N	2.37	0.58
5:F:395:THR:OG1	5:F:396:ASN:N	2.37	0.58
3:J:519:ASN:HB2	3:J:709:ARG:HD3	1.86	0.58
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.85	0.58
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.39	0.58
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.86	0.58
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.85	0.58
5:L:127:ILE:O	5:L:130:VAL:HG22	2.03	0.58
5:L:395:THR:OG1	5:L:396:ASN:N	2.37	0.58
5:L:483:LEU:HD12	5:L:483:LEU:H	1.68	0.58
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.67	0.58
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.03	0.58
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.85	0.58
3:D:519:ASN:HB2	3:D:709:ARG:HD3	1.85	0.58
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.86	0.57
2:C:746:ALA:HA	2:C:974:ARG:HE	1.68	0.57
5:F:466:ILE:CG2	5:F:486:ARG:HG3	2.34	0.57
2:I:13:LYS:HZ1	2:I:1151:LEU:HB2	1.68	0.57
2:I:696:ASP:O	2:I:697:LYS:HB3	2.04	0.57
2:I:896:THR:HB	2:I:897:PRO:HD2	1.86	0.57
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.57
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.38	0.57
1:A:197:ASP:OD1	1:A:197:ASP:N	2.37	0.57
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.37	0.57
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.86	0.57
2:C:1313:HIS:N	4:E:31:GLN:OE1	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:514:THR:HG22	3:D:596:LEU:HB2	1.86	0.57
1:G:74:VAL:HG22	1:G:76:GLU:H	1.70	0.57
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.87	0.57
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.39	0.57
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.85	0.57
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.70	0.57
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.38	0.57
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.38	0.57
1:G:197:ASP:OD1	1:G:197:ASP:N	2.37	0.57
2:I:499:SER:O	2:I:503:LYS:HB2	2.05	0.57
2:I:620:ASN:C	2:I:620:ASN:ND2	2.62	0.57
2:I:1142:ARG:HD3	2:I:1161:LEU:HD22	1.87	0.57
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.05	0.57
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.86	0.57
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.37	0.57
1:A:74:VAL:HG22	1:A:76:GLU:H	1.70	0.57
2:C:170:VAL:HG23	2:C:171:LEU:N	2.20	0.57
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.57
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.40	0.57
2:I:207:THR:HG21	2:I:351:LEU:HG	1.85	0.57
2:C:696:ASP:O	2:C:697:LYS:HB3	2.05	0.57
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.04	0.57
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.87	0.57
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.85	0.57
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.39	0.57
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.85	0.56
2:C:27:LEU:O	2:C:528:ARG:NH1	2.37	0.56
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.87	0.56
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.85	0.56
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.69	0.56
3:D:843:VAL:HG11	3:D:897:HIS:O	2.05	0.56
5:F:466:ILE:HG21	5:F:486:ARG:HG3	1.86	0.56
2:C:896:THR:HB	2:C:897:PRO:HD2	1.86	0.56
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.86	0.56
5:F:483:LEU:H	5:F:483:LEU:HD12	1.69	0.56
2:I:21:VAL:HG13	2:I:655:VAL:HG13	1.86	0.56
2:I:170:VAL:HG23	2:I:171:LEU:N	2.19	0.56
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.87	0.56
3:J:514:THR:HG22	3:J:596:LEU:HB2	1.87	0.56
3:J:843:VAL:HG11	3:J:897:HIS:O	2.05	0.56
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:THR:O	1:B:6:THR:OG1	2.19	0.56
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.41	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.70	0.56
2:I:27:LEU:O	2:I:528:ARG:NH1	2.37	0.56
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.88	0.56
2:I:741:MET:SD	2:I:974:ARG:NH2	2.78	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.56
3:J:961:SER:HB2	3:J:981:GLU:HB3	1.88	0.56
2:C:499:SER:O	2:C:503:LYS:HB2	2.05	0.56
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.56
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.87	0.56
3:J:678:ARG:O	3:J:682:VAL:HG23	2.06	0.56
5:L:312:SER:OG	5:L:313:ASP:N	2.37	0.56
2:C:138:ILE:HD13	2:C:143:ARG:HD3	1.87	0.56
3:D:425:ARG:HG2	3:D:426:ALA:H	1.70	0.56
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.41	0.56
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.38	0.56
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.87	0.56
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.88	0.56
3:D:712:GLN:H	3:D:712:GLN:CD	2.14	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.88	0.56
2:C:606:LEU:HD23	2:C:611:GLU:HA	1.88	0.56
3:J:1079:LYS:HZ2	3:J:1079:LYS:HB3	1.71	0.56
3:D:27:PRO:O	3:D:31:ARG:HG3	2.05	0.56
3:J:152:THR:OG1	3:J:153:ASN:N	2.38	0.56
3:J:425:ARG:HG2	3:J:426:ALA:H	1.70	0.56
3:J:755:ILE:HG22	3:J:757:THR:H	1.71	0.56
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:755:ILE:HG22	3:D:757:THR:H	1.72	0.55
3:J:746:LEU:HG	3:J:758:PRO:HG3	1.88	0.55
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.38	0.55
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.89	0.55
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.87	0.55
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.88	0.55
1:B:64:VAL:HG12	1:B:65:LEU:H	1.72	0.55
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.89	0.55
3:J:27:PRO:O	3:J:31:ARG:HG3	2.05	0.55
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.89	0.55
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.87	0.55
3:J:26:SER:HB3	3:J:29:MET:HB3	1.89	0.55
3:D:250:ARG:HH11	3:D:250:ARG:HG3	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:860:ARG:HH11	3:D:860:ARG:HG3	1.70	0.55
5:F:575:GLU:O	5:F:579:GLN:HG2	2.07	0.55
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.22	0.55
3:D:26:SER:HB3	3:D:29:MET:HB3	1.87	0.55
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.88	0.55
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.87	0.55
2:I:1131:MET:O	2:I:1134:GLN:HB2	2.06	0.55
2:I:1239:VAL:HG13	3:J:445:LYS:HB2	1.89	0.55
3:D:746:LEU:HG	3:D:758:PRO:HG3	1.88	0.55
3:D:857:LEU:HD13	3:D:858:VAL:HG13	1.89	0.55
5:F:134:VAL:HA	5:F:273:MET:HE1	1.88	0.55
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.87	0.55
1:H:71:LYS:NZ	1:H:139:SER:O	2.36	0.55
2:C:1239:VAL:HG13	3:D:445:LYS:HB2	1.89	0.55
2:I:255:ILE:HB	2:I:263:VAL:HB	1.89	0.55
2:C:255:ILE:HB	2:C:263:VAL:HB	1.89	0.54
2:I:897:PRO:O	2:I:900:LYS:N	2.40	0.54
3:J:682:VAL:O	3:J:685:ILE:HG12	2.06	0.54
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.89	0.54
1:G:231:PHE:N	1:G:231:PHE:CD2	2.75	0.54
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.88	0.54
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.88	0.54
3:J:857:LEU:HD12	3:J:858:VAL:H	1.71	0.54
3:J:1040:MET:HE3	3:J:1076:PRO:HB2	1.89	0.54
2:C:498:ILE:H	2:C:498:ILE:HD12	1.72	0.54
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.88	0.54
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.23	0.54
3:D:62:PHE:O	3:D:101:ARG:HD2	2.07	0.54
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.90	0.54
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.43	0.54
5:L:134:VAL:HA	5:L:273:MET:HE1	1.88	0.54
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.90	0.54
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.89	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.88	0.54
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.88	0.54
2:C:832:HIS:O	2:C:1055:ALA:HA	2.08	0.54
3:D:317:THR:HB	3:D:324:LEU:HB3	1.90	0.54
3:J:557:LYS:HA	3:J:563:LEU:HA	1.90	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.72	0.54
5:L:575:GLU:O	5:L:579:GLN:HG2	2.08	0.54
2:C:46:GLN:OE1	2:C:47:TYR:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.90	0.54
3:D:678:ARG:O	3:D:682:VAL:HG23	2.08	0.54
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.35	0.54
2:I:826:ASP:OD1	2:I:829:THR:OG1	2.24	0.54
3:J:317:THR:HB	3:J:324:LEU:HB3	1.89	0.54
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.90	0.54
2:C:624:ASP:OD1	2:C:625:GLU:N	2.41	0.54
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.89	0.54
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.90	0.54
3:D:557:LYS:HA	3:D:563:LEU:HA	1.90	0.54
3:D:901:ARG:HA	3:D:908:ILE:HA	1.89	0.54
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.88	0.54
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.90	0.54
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.89	0.54
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.89	0.54
2:I:498:ILE:H	2:I:498:ILE:HD12	1.73	0.54
2:I:620:ASN:ND2	2:I:620:ASN:O	2.41	0.54
2:I:624:ASP:OD1	2:I:625:GLU:N	2.41	0.54
1:H:35:PHE:HA	1:H:38:THR:HG22	1.89	0.53
2:I:322:LEU:O	2:I:326:SER:OG	2.21	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.44	0.53
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.90	0.53
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.53
3:J:62:PHE:O	3:J:101:ARG:HD2	2.07	0.53
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.90	0.53
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.43	0.53
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.56	0.53
2:I:219:GLN:HA	2:I:222:ASP:HB3	1.89	0.53
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.91	0.53
3:J:712:GLN:CD	3:J:712:GLN:H	2.15	0.53
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.39	0.53
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.43	0.53
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.23	0.53
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.91	0.53
1:G:182:ARG:H	1:G:206:GLU:HB3	1.74	0.53
1:G:226:GLU:HG2	1:H:10:LYS:HE3	1.91	0.53
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.39	0.53
3:J:1357:ILE:HG22	3:J:1359:ALA:H	1.73	0.53
2:I:46:GLN:OE1	2:I:47:TYR:N	2.41	0.53
3:J:514:THR:HG21	3:J:596:LEU:HD23	1.90	0.53
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.90	0.53
3:D:156:ARG:NH2	3:D:191:SER:OG	2.42	0.53
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.90	0.53
2:C:219:GLN:HA	2:C:222:ASP:HB3	1.89	0.53
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.91	0.53
5:F:164:GLY:O	5:F:260:ARG:HB2	2.08	0.53
2:I:724:VAL:HG23	2:I:775:GLU:H	1.74	0.53
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.90	0.53
3:J:857:LEU:HD13	3:J:858:VAL:HG13	1.90	0.53
3:J:901:ARG:HA	3:J:908:ILE:HA	1.91	0.53
1:A:182:ARG:H	1:A:206:GLU:HB3	1.74	0.53
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.90	0.53
2:C:741:MET:SD	2:C:974:ARG:NH2	2.82	0.53
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.90	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.73	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.57	0.53
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.90	0.53
3:D:1174:ARG:HE	3:D:1189:MET:HE2	1.74	0.53
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.74	0.53
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.90	0.53
3:J:230:SER:OG	3:J:231:GLY:N	2.42	0.53
2:C:821:ARG:HH21	2:C:1082:ILE:HG21	1.74	0.53
2:C:897:PRO:O	2:C:899:GLU:N	2.42	0.53
1:H:58:GLU:HB3	1:H:171:LEU:O	2.09	0.53
2:I:56:VAL:HG11	2:I:468:LEU:HB3	1.90	0.53
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.45	0.53
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.90	0.52
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.91	0.52
5:F:474:MET:C	5:F:476:ARG:H	2.07	0.52
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.44	0.52
3:J:79:LYS:HB2	5:L:569:THR:N	2.21	0.52
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.39	0.52
1:B:35:PHE:HA	1:B:38:THR:HG22	1.89	0.52
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.56	0.52
3:D:361:LEU:HD22	3:D:365:GLN:HG3	1.92	0.52
3:J:697:MET:O	3:J:701:LEU:HB2	2.09	0.52
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.90	0.52
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.90	0.52
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.74	0.52
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.36	0.52
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.90	0.52
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.52
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.92	0.52
2:I:1134:GLN:OE1	2:I:1134:GLN:HA	2.09	0.52
5:L:130:VAL:HB	5:L:365:MET:HG3	1.92	0.52
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.91	0.52
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.55	0.52
3:J:156:ARG:NH2	3:J:191:SER:OG	2.42	0.52
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.45	0.52
3:D:514:THR:HG21	3:D:596:LEU:HD23	1.90	0.52
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.08	0.52
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.91	0.52
3:J:1174:ARG:HE	3:J:1189:MET:HE2	1.74	0.52
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.45	0.52
3:D:579:LEU:HD12	3:D:582:ILE:HD12	1.91	0.52
2:I:233:ARG:HG3	2:I:233:ARG:HH11	1.73	0.52
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.92	0.52
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.10	0.52
5:L:513:ASP:C	5:L:515:GLU:H	2.18	0.52
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.92	0.52
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.45	0.52
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.91	0.52
2:C:724:VAL:HG23	2:C:775:GLU:H	1.75	0.52
3:D:682:VAL:O	3:D:685:ILE:HG12	2.10	0.52
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.92	0.52
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.92	0.52
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.92	0.51
3:D:1372:ARG:HE	3:J:854:ALA:CB	2.22	0.51
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.43	0.51
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.92	0.51
3:J:27:PRO:HD3	3:J:236:TRP:NE1	2.25	0.51
3:J:860:ARG:HH11	3:J:860:ARG:CG	2.23	0.51
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.91	0.51
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.92	0.51
2:C:826:ASP:OD1	2:C:829:THR:OG1	2.23	0.51
3:D:697:MET:O	3:D:701:LEU:HB2	2.10	0.51
3:J:844:THR:OG1	3:J:860:ARG:O	2.18	0.51
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.74	0.51
1:G:12:ARG:H	1:G:30:PRO:HD2	1.76	0.51
3:J:210:SER:O	3:J:214:ARG:HG2	2.10	0.51
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:314:ASN:O	2:I:352:ARG:NH1	2.44	0.51
3:J:654:ILE:O	3:J:658:GLU:HB2	2.10	0.51
1:B:136:GLU:HG2	1:B:137:ASN:H	1.75	0.51
2:C:179:TYR:OH	2:C:458:GLU:OE2	2.20	0.51
2:C:829:THR:HA	2:C:1059:ARG:HA	1.93	0.51
2:I:701:GLY:O	2:I:1184:THR:N	2.34	0.51
3:J:27:PRO:CD	3:J:236:TRP:HE1	2.23	0.51
3:J:1100:PHE:HB2	3:J:1200:GLU:CD	2.35	0.51
2:C:1119:MET:HE1	2:C:1210:ILE:HD11	1.93	0.51
3:D:860:ARG:HH11	3:D:860:ARG:CG	2.23	0.51
1:G:231:PHE:HZ	1:H:221:ALA:HB3	1.75	0.51
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.45	0.51
2:I:873:ILE:HG13	2:I:944:ARG:NH2	2.20	0.51
3:J:579:LEU:HD12	3:J:582:ILE:HD12	1.91	0.51
1:A:12:ARG:H	1:A:30:PRO:HD2	1.76	0.51
1:B:102:LEU:HB2	1:B:142:MET:H	1.76	0.51
1:B:134:THR:HG23	1:B:135:ASP:OD1	2.10	0.51
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.92	0.51
2:C:758:ARG:HD3	2:C:835:GLU:HB2	1.93	0.51
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.92	0.51
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.92	0.51
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.51
1:H:134:THR:HG23	1:H:135:ASP:OD1	2.10	0.51
2:I:138:ILE:HG22	2:I:139:ASN:HD22	1.75	0.51
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.93	0.51
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.91	0.51
2:C:138:ILE:HG22	2:C:139:ASN:HD22	1.75	0.51
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.93	0.51
3:D:210:SER:O	3:D:214:ARG:HG2	2.11	0.51
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.35	0.51
1:G:166:ARG:O	1:G:168:ILE:N	2.44	0.51
2:I:1119:MET:HE1	2:I:1210:ILE:HD11	1.92	0.51
3:J:94:GLN:O	3:J:97:VAL:HG23	2.11	0.51
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.92	0.51
3:D:654:ILE:O	3:D:658:GLU:HB2	2.11	0.51
3:D:1368:ASP:OD1	3:J:854:ALA:HB1	2.11	0.51
2:I:782:VAL:HG11	2:I:792:GLY:HA2	1.93	0.51
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.93	0.51
2:C:906:PHE:CE2	5:F:608:ARG:HB2	2.46	0.51
3:D:844:THR:OG1	3:D:860:ARG:O	2.18	0.50
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:348:GLU:HG2	5:F:354:THR:HA	1.92	0.50
2:I:59:ILE:HG22	2:I:476:LYS:HE3	1.92	0.50
2:I:594:VAL:HG22	2:I:599:VAL:HA	1.92	0.50
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.74	0.50
1:B:79:LEU:HD23	1:B:79:LEU:H	1.76	0.50
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.11	0.50
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.74	0.50
3:J:356:THR:OG1	3:J:357:VAL:N	2.44	0.50
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.92	0.50
5:L:482:GLU:HG2	5:L:486:ARG:HH12	1.77	0.50
2:C:59:ILE:HG22	2:C:476:LYS:HE3	1.93	0.50
3:D:94:GLN:O	3:D:97:VAL:HG23	2.12	0.50
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.77	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HA	1.92	0.50
3:D:27:PRO:HD3	3:D:236:TRP:NE1	2.26	0.50
3:D:75:TYR:HD2	3:D:80:HIS:HD2	1.59	0.50
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.77	0.50
5:F:580:PHE:O	5:F:581:ASP:HB3	2.11	0.50
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.93	0.50
3:J:963:VAL:HB	3:J:980:THR:HG23	1.94	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.12	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.92	0.50
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.93	0.50
1:H:102:LEU:HB2	1:H:142:MET:H	1.76	0.50
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.94	0.50
5:L:348:GLU:HG2	5:L:354:THR:HA	1.92	0.50
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.26	0.50
2:C:47:TYR:OH	2:C:398:SER:HB2	2.12	0.50
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.93	0.50
2:C:120:GLN:HG3	2:C:121:GLU:N	2.26	0.50
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.94	0.50
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.93	0.50
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.94	0.50
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.94	0.50
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.92	0.50
2:I:1085:MET:HE2	2:I:1085:MET:HA	1.93	0.50
3:J:75:TYR:HD2	3:J:80:HIS:HD2	1.59	0.50
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.94	0.50
5:F:513:ASP:C	5:F:515:GLU:H	2.18	0.50
2:I:138:ILE:C	2:I:139:ASN:HD22	2.19	0.50
2:I:1134:GLN:CB	2:I:1136:GLN:HG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.92	0.50
1:B:101:THR:H	1:B:116:THR:HG22	1.77	0.50
4:E:8:ASP:O	4:E:11:GLU:HB2	2.11	0.50
5:F:525:ASP:OD1	5:F:528:LEU:N	2.45	0.50
1:H:101:THR:H	1:H:116:THR:HG22	1.76	0.50
2:I:518:ASN:OD1	2:I:518:ASN:N	2.45	0.50
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.94	0.50
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.50
1:B:134:THR:HG23	1:B:135:ASP:H	1.77	0.50
2:C:840:SER:HB3	2:C:1048:LYS:HG2	1.94	0.50
2:I:98:VAL:HG21	2:I:124:MET:HE3	1.93	0.50
2:I:829:THR:HA	2:I:1059:ARG:HA	1.92	0.50
2:C:518:ASN:O	2:C:691:PRO:HD3	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.77	0.49
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.10	0.49
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.41	0.49
2:C:13:LYS:HZ1	2:C:1151:LEU:HB2	1.77	0.49
2:C:582:ASN:HB3	2:C:586:PHE:H	1.78	0.49
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.94	0.49
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.78	0.49
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.77	0.49
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.93	0.49
5:L:580:PHE:O	5:L:581:ASP:HB3	2.12	0.49
1:B:54:CYS:SG	1:B:148:ARG:HG3	2.53	0.49
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.93	0.49
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.49
4:E:36:ASP:HB2	4:E:37:PRO:HD2	1.94	0.49
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.94	0.49
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.12	0.49
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.93	0.49
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.94	0.49
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.94	0.49
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.93	0.49
2:C:316:GLU:H	2:C:316:GLU:CD	2.20	0.49
2:C:1257:GLN:HE22	3:D:340:GLN:HE21	1.60	0.49
3:D:290:ILE:H	3:D:290:ILE:HD12	1.78	0.49
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.93	0.49
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.49
1:G:51:MET:HE1	1:G:216:ALA:HA	1.95	0.49
2:I:518:ASN:O	2:I:691:PRO:HD3	2.12	0.49
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.93	0.49
2:I:285:ILE:O	2:I:285:ILE:HG13	2.13	0.49
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.12	0.49
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.95	0.49
3:J:872:LEU:O	3:J:877:VAL:HG12	2.12	0.49
2:C:620:ASN:ND2	2:C:620:ASN:O	2.46	0.49
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.94	0.49
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.95	0.49
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.94	0.49
3:J:63:GLY:O	3:J:98:ARG:HD2	2.12	0.49
3:J:694:SER:OG	3:J:738:ARG:NE	2.46	0.49
3:J:733:SER:O	3:J:737:ILE:HG12	2.12	0.49
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.93	0.49
5:L:511:ILE:HG13	5:L:512:GLY:H	1.77	0.49
1:B:11:PRO:HB3	1:B:30:PRO:O	2.13	0.49
3:D:872:LEU:O	3:D:877:VAL:HG12	2.11	0.49
2:I:316:GLU:H	2:I:316:GLU:CD	2.21	0.49
1:A:49:SER:OG	1:A:50:SER:N	2.46	0.49
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.12	0.49
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.49
5:F:130:VAL:HB	5:F:365:MET:HG3	1.95	0.49
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.43	0.49
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.78	0.49
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.34	0.49
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.95	0.49
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.94	0.49
3:D:137:ARG:HD3	3:D:143:SER:OG	2.12	0.49
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.94	0.49
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.93	0.49
2:C:69:GLN:HG3	2:C:101:ARG:HB3	1.95	0.49
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.48	0.49
1:H:67:GLU:HG3	1:H:171:LEU:HD13	1.95	0.49
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.43	0.49
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.94	0.49
3:J:1170:LYS:C	3:J:1172:LYS:H	2.20	0.49
1:A:137:ASN:N	1:A:137:ASN:OD1	2.46	0.48
1:B:151:GLY:O	1:B:177:TYR:HD2	1.96	0.48
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.93	0.48
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.76	0.48
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.95	0.48
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.48	0.48
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.48
3:J:956:GLY:O	3:J:1011:VAL:HG22	2.13	0.48
3:D:392:THR:HG21	5:F:606:VAL:HA	1.94	0.48
3:D:694:SER:OG	3:D:738:ARG:NE	2.46	0.48
1:H:151:GLY:O	1:H:177:TYR:HD2	1.96	0.48
2:I:206:ALA:O	2:I:209:ILE:HG22	2.13	0.48
2:I:896:THR:O	2:I:900:LYS:HB2	2.13	0.48
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.77	0.48
3:J:709:ARG:O	3:J:711:GLY:N	2.38	0.48
3:J:825:VAL:C	3:J:826:ILE:HG13	2.39	0.48
5:L:343:LYS:H	5:L:343:LYS:HD2	1.77	0.48
1:B:81:ILE:O	1:B:85:LEU:HG	2.13	0.48
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.77	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.94	0.48
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.95	0.48
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.95	0.48
5:L:456:MET:O	5:L:460:ILE:HG13	2.13	0.48
2:C:206:ALA:O	2:C:209:ILE:HG22	2.14	0.48
3:D:770:LEU:H	3:D:770:LEU:HD22	1.79	0.48
1:H:54:CYS:SG	1:H:148:ARG:HG3	2.52	0.48
1:H:79:LEU:HD23	1:H:79:LEU:H	1.77	0.48
1:H:134:THR:HG23	1:H:135:ASP:H	1.78	0.48
2:I:840:SER:HB3	2:I:1048:LYS:HG2	1.95	0.48
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.18	0.48
3:J:1041:ILE:C	3:J:1046:ILE:HG12	2.39	0.48
2:C:896:THR:O	2:C:900:LYS:HB2	2.13	0.48
2:I:582:ASN:HB3	2:I:586:PHE:H	1.78	0.48
2:I:1243:MET:HA	3:J:353:SER:HB3	1.95	0.48
3:J:697:MET:HE1	3:J:737:ILE:HG22	1.96	0.48
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.95	0.48
5:L:227:GLN:HG2	5:L:252:LEU:HA	1.94	0.48
2:C:1243:MET:HA	3:D:353:SER:HB3	1.95	0.48
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.78	0.48
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.96	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.94	0.48
5:L:306:PHE:CE1	5:L:310:GLU:HG3	2.49	0.48
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.95	0.48
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.96	0.48
1:G:49:SER:OG	1:G:50:SER:N	2.46	0.48
1:H:51:MET:HB3	1:H:178:SER:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG2	1:B:38:THR:HB	1.95	0.48
1:B:78:ILE:O	1:B:82:LEU:HG	2.14	0.48
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.49	0.48
2:C:445:ILE:HG22	2:C:446:ASP:OD1	2.14	0.48
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.96	0.48
2:C:1257:GLN:HE22	3:D:340:GLN:NE2	2.11	0.48
3:D:27:PRO:CD	3:D:236:TRP:HE1	2.27	0.48
3:D:98:ARG:HG2	3:D:98:ARG:NH1	2.13	0.48
3:D:847:ASP:HB3	3:D:859:PRO:HA	1.94	0.48
3:J:847:ASP:HB3	3:J:859:PRO:HA	1.95	0.48
5:L:314:THR:O	5:L:318:ALA:HB3	2.14	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.96	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.48
3:D:797:THR:O	3:D:801:VAL:HG13	2.13	0.48
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.95	0.48
3:D:1297:LYS:HE3	3:J:1302:TYR:H	1.79	0.48
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.95	0.48
3:D:1359:ALA:O	3:D:1363:TYR:N	2.46	0.48
5:F:511:ILE:HG13	5:F:512:GLY:H	1.78	0.48
1:H:81:ILE:O	1:H:85:LEU:HG	2.13	0.48
2:I:616:ILE:HG13	2:I:652:TYR:HB2	1.96	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.96	0.48
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.94	0.48
3:J:797:THR:O	3:J:801:VAL:HG13	2.14	0.48
5:L:96:ASP:O	5:L:98:VAL:N	2.47	0.48
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	1.96	0.48
3:J:770:LEU:H	3:J:770:LEU:HD22	1.79	0.48
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.78	0.48
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.96	0.47
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.79	0.47
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.96	0.47
1:G:137:ASN:N	1:G:137:ASN:OD1	2.46	0.47
2:I:107:ARG:HA	2:I:108:GLU:HA	1.54	0.47
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.49	0.47
3:J:950:ILE:HD12	3:J:1020:TRP:CZ3	2.49	0.47
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.49	0.47
2:C:285:ILE:O	2:C:285:ILE:HG13	2.14	0.47
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.45	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.46	0.47
2:I:168:GLY:C	2:I:170:VAL:H	2.15	0.47
4:K:25:ARG:HD3	4:K:64:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:525:ASP:OD1	5:L:528:LEU:N	2.44	0.47
1:A:172:LEU:H	1:A:172:LEU:HD12	1.79	0.47
2:C:12:ARG:NH1	2:C:1182:ILE:O	2.43	0.47
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.55	0.47
2:C:515:MET:HE3	2:C:517:GLN:HB2	1.97	0.47
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.49	0.47
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.94	0.47
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.44	0.47
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.79	0.47
2:I:897:PRO:O	2:I:899:GLU:N	2.47	0.47
3:J:16:GLU:CG	3:J:17:PHE:H	2.25	0.47
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.96	0.47
1:A:51:MET:HE1	1:A:216:ALA:HA	1.96	0.47
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.96	0.47
2:C:349:GLU:O	2:C:353:VAL:HG23	2.14	0.47
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.95	0.47
3:D:1290:ARG:HG3	3:D:1298:VAL:HG12	1.96	0.47
1:H:11:PRO:HB3	1:H:30:PRO:O	2.15	0.47
1:H:149:GLY:HA3	1:H:177:TYR:CD2	2.48	0.47
2:I:233:ARG:HG3	2:I:233:ARG:NH1	2.30	0.47
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.14	0.47
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.97	0.47
3:D:709:ARG:HD2	3:D:710:ASP:N	2.30	0.47
3:D:825:VAL:C	3:D:826:ILE:HG13	2.39	0.47
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.49	0.47
1:G:172:LEU:HD12	1:G:172:LEU:H	1.80	0.47
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.96	0.47
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.96	0.47
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.97	0.47
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.96	0.47
3:J:984:LEU:HB3	3:J:993:GLU:HB2	1.96	0.47
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.95	0.47
4:K:8:ASP:O	4:K:11:GLU:HB2	2.15	0.47
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.96	0.47
2:C:356:THR:HG21	2:C:362:ALA:HA	1.96	0.47
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.97	0.47
2:C:623:LEU:HB2	2:C:627:GLY:HA2	1.97	0.47
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.96	0.47
3:D:264:ASP:N	3:D:264:ASP:OD2	2.48	0.47
3:D:518:VAL:N	3:D:716:GLN:OE1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:574:VAL:O	3:D:578:ILE:HG13	2.15	0.47
3:D:875:ASN:OD1	3:D:875:ASN:N	2.48	0.47
5:F:456:MET:O	5:F:460:ILE:HG13	2.14	0.47
2:I:1140:LYS:HZ3	2:I:1140:LYS:HG3	1.56	0.47
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.97	0.47
3:J:1290:ARG:HG3	3:J:1298:VAL:HG12	1.97	0.47
3:D:519:ASN:CG	3:D:709:ARG:HD3	2.40	0.47
2:I:466:VAL:O	2:I:469:VAL:HG22	2.15	0.47
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.50	0.47
3:J:665:GLN:HG3	3:J:669:GLN:HE21	1.80	0.47
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.95	0.47
1:B:71:LYS:NZ	1:B:139:SER:O	2.41	0.47
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.80	0.47
4:E:7:GLN:O	4:E:11:GLU:HG2	2.15	0.47
1:H:61:ILE:HB	1:H:64:VAL:O	2.14	0.47
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.50	0.47
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.30	0.47
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.96	0.47
3:J:702:GLN:HG2	3:J:703:THR:N	2.30	0.47
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.97	0.47
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.30	0.47
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.15	0.47
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.80	0.47
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.97	0.47
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.55	0.47
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.97	0.47
3:J:1061:VAL:HG21	3:J:1101:LEU:HB3	1.96	0.47
1:B:147:GLN:HG3	1:B:148:ARG:N	2.29	0.46
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.45	0.46
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.97	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
2:C:185:ASP:HB2	2:C:197:ARG:HG3	1.97	0.46
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.50	0.46
3:D:632:ALA:O	3:D:635:SER:OG	2.30	0.46
5:F:314:THR:O	5:F:318:ALA:HB3	2.15	0.46
2:I:349:GLU:O	2:I:353:VAL:HG23	2.14	0.46
2:I:445:ILE:HG22	2:I:446:ASP:OD1	2.15	0.46
2:I:557:ARG:HH21	2:I:607:SER:C	2.23	0.46
3:J:137:ARG:HD3	3:J:143:SER:OG	2.14	0.46
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.97	0.46
3:J:568:SER:OG	3:J:569:LEU:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.96	0.46
4:K:7:GLN:O	4:K:11:GLU:HG2	2.15	0.46
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.46	0.46
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.50	0.46
2:C:1136:GLN:HE21	2:C:1136:GLN:HA	1.80	0.46
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.51	0.46
1:H:78:ILE:O	1:H:82:LEU:HG	2.14	0.46
2:I:169:LYS:O	2:I:170:VAL:HG22	2.16	0.46
2:I:1182:ILE:HG22	2:I:1183:ALA:N	2.30	0.46
3:J:264:ASP:OD2	3:J:264:ASP:N	2.48	0.46
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.98	0.46
3:J:519:ASN:CG	3:J:709:ARG:HD3	2.40	0.46
3:J:560:ASN:O	3:J:560:ASN:ND2	2.47	0.46
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.51	0.46
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.96	0.46
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.97	0.46
3:D:127:LEU:HD22	3:D:237:MET:HE3	1.97	0.46
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.96	0.46
1:H:136:GLU:HG2	1:H:137:ASN:H	1.80	0.46
3:J:230:SER:CB	3:J:232:ASN:H	2.28	0.46
3:J:266:ASN:O	3:J:270:ARG:HB2	2.15	0.46
3:J:518:VAL:N	3:J:716:GLN:OE1	2.47	0.46
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.97	0.46
3:J:875:ASN:N	3:J:875:ASN:OD1	2.47	0.46
3:J:902:ASP:OD1	3:J:903:LEU:N	2.48	0.46
2:C:138:ILE:C	2:C:139:ASN:HD22	2.24	0.46
2:C:339:ASN:HB3	2:C:343:HIS:H	1.81	0.46
2:C:466:VAL:O	2:C:469:VAL:HG22	2.15	0.46
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.48	0.46
3:D:266:ASN:O	3:D:270:ARG:HB2	2.15	0.46
3:D:560:ASN:O	3:D:560:ASN:ND2	2.47	0.46
3:D:600:ALA:O	3:D:603:LYS:HG2	2.15	0.46
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.97	0.46
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.96	0.46
3:J:600:ALA:O	3:J:603:LYS:HG2	2.15	0.46
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.97	0.46
3:J:973:LEU:HD23	3:J:1003:LEU:HD12	1.98	0.46
3:J:1321:SER:HB2	3:J:1349:GLU:OE2	2.14	0.46
5:L:316:PHE:HZ	5:L:334:SER:HA	1.80	0.46
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.96	0.46
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.97	0.46
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.98	0.46
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.45	0.46
3:D:902:ASP:OD1	3:D:903:LEU:N	2.48	0.46
5:F:96:ASP:O	5:F:98:VAL:N	2.48	0.46
1:G:45:ARG:NH1	1:H:34:GLY:O	2.45	0.46
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.50	0.46
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.98	0.46
3:J:110:PRO:HD2	3:J:183:GLU:HG2	1.97	0.46
3:J:1067:ARG:HG3	3:J:1067:ARG:H	1.54	0.46
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.98	0.46
2:C:518:ASN:OD1	2:C:518:ASN:N	2.45	0.46
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.43	0.46
5:F:244:THR:O	5:F:247:GLU:HG2	2.15	0.46
5:F:281:ARG:O	5:F:285:ARG:HG3	2.15	0.46
5:F:601:PRO:C	5:F:603:ARG:H	2.23	0.46
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.46
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.98	0.46
3:J:250:ARG:HH11	3:J:250:ARG:HG3	1.80	0.46
2:C:672:GLU:HB3	3:D:767:LEU:O	2.16	0.46
3:D:63:GLY:O	3:D:98:ARG:HD2	2.15	0.46
3:D:293:ARG:NH1	5:F:104:GLU:OE2	2.47	0.46
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.97	0.46
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.98	0.46
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.96	0.46
1:H:147:GLN:HG3	1:H:148:ARG:N	2.30	0.46
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.45	0.46
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.97	0.46
3:J:1108:GLN:HE22	3:J:1123:ARG:NH2	2.13	0.46
3:J:1108:GLN:HE22	3:J:1123:ARG:HH22	1.64	0.46
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.51	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.15	0.46
1:B:61:ILE:HB	1:B:64:VAL:O	2.16	0.46
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.50	0.46
2:C:744:GLY:C	2:C:746:ALA:H	2.23	0.46
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.30	0.46
4:E:50:ALA:O	4:E:54:ILE:HG12	2.16	0.46
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.71	0.46
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.81	0.46
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.97	0.46
2:C:216:THR:H	2:C:219:GLN:HE22	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.46
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.50	0.46
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.81	0.46
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.51	0.46
2:I:356:THR:HG21	2:I:362:ALA:HA	1.97	0.46
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.30	0.46
2:I:672:GLU:HB3	3:J:767:LEU:O	2.16	0.46
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.46	0.46
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.97	0.46
3:J:574:VAL:O	3:J:578:ILE:HG13	2.15	0.46
3:J:1183:SER:HB3	3:J:1185:PRO:HD3	1.98	0.46
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.56	0.46
5:L:493:LYS:HA	5:L:496:LYS:HG3	1.98	0.46
3:D:485:MET:HB3	3:D:488:ASN:ND2	2.31	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.98	0.46
5:L:281:ARG:O	5:L:285:ARG:HG3	2.16	0.46
3:D:645:VAL:HB	3:D:701:LEU:HD23	1.97	0.45
3:J:45:ASN:HB3	3:J:48:THR:O	2.16	0.45
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.46	0.45
5:L:244:THR:O	5:L:247:GLU:HG2	2.16	0.45
1:A:14:VAL:HG13	1:A:15:ASP:N	2.31	0.45
3:D:45:ASN:HB3	3:D:48:THR:O	2.16	0.45
3:D:291:ILE:HD13	5:F:409:ASN:HB3	1.97	0.45
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.98	0.45
3:D:793:SER:O	3:D:797:THR:HG23	2.16	0.45
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.97	0.45
1:H:219:ARG:O	1:H:223:ILE:HG13	2.17	0.45
2:I:623:LEU:HB2	2:I:627:GLY:HA2	1.98	0.45
1:B:102:LEU:HD12	1:B:142:MET:HG2	1.98	0.45
2:C:107:ARG:HA	2:C:108:GLU:HA	1.49	0.45
1:H:102:LEU:HD12	1:H:142:MET:HG2	1.98	0.45
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.98	0.45
3:J:127:LEU:HD22	3:J:237:MET:HE3	1.97	0.45
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.98	0.45
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.42	0.45
2:C:17:LYS:NZ	2:C:1154:ASP:O	2.48	0.45
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.96	0.45
5:F:119:ILE:O	5:F:123:ILE:HG13	2.16	0.45
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.80	0.45
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.38	0.45
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1209:GLN:HB3	2:I:1224:PRO:HB2	1.98	0.45
3:J:19:ALA:O	3:J:20:ILE:HG13	2.17	0.45
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.79	0.45
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.81	0.45
2:C:107:ARG:H	2:C:107:ARG:HG3	1.61	0.45
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.99	0.45
3:D:53:ARG:HA	3:D:54:ASP:HA	1.56	0.45
4:E:14:GLY:O	4:E:16:ARG:N	2.50	0.45
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.45
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.70	0.45
2:I:816:ILE:HG22	2:I:818:VAL:HG23	1.97	0.45
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.97	0.45
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.31	0.45
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.99	0.45
1:G:14:VAL:HG13	1:G:15:ASP:N	2.31	0.45
2:I:30:ILE:HD12	2:I:30:ILE:H	1.81	0.45
2:I:69:GLN:HG3	2:I:101:ARG:HB3	1.97	0.45
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.45
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.99	0.45
2:C:722:GLY:O	2:C:777:VAL:HG22	2.16	0.45
3:D:19:ALA:O	3:D:20:ILE:HG13	2.17	0.45
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.99	0.45
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.45
2:I:744:GLY:C	2:I:746:ALA:H	2.23	0.45
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.87	0.45
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.71	0.45
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.32	0.45
3:J:485:MET:HB3	3:J:488:ASN:ND2	2.31	0.45
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.16	0.45
1:A:228:LEU:HA	1:A:228:LEU:HD13	1.68	0.45
3:D:519:ASN:CB	3:D:709:ARG:HD3	2.47	0.45
3:J:355:ILE:HG22	3:J:447:ILE:HB	1.99	0.45
3:J:484:MET:HE2	3:J:484:MET:HB3	1.81	0.45
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.99	0.45
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.52	0.45
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.30	0.45
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.47	0.45
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.99	0.45
3:D:347:VAL:HG12	3:D:348:ASP:O	2.17	0.45
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.42	0.45
2:I:722:GLY:O	2:I:777:VAL:HG22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.47	0.45
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.99	0.45
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.99	0.45
3:D:77:ARG:HG3	3:D:79:LYS:H	1.82	0.45
3:D:271:ARG:HE	3:D:271:ARG:HB2	1.41	0.45
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.63	0.45
5:F:225:ARG:O	5:F:229:VAL:HG13	2.17	0.45
5:F:482:GLU:HG3	5:F:486:ARG:HH22	1.82	0.45
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.98	0.45
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.99	0.45
3:J:1186:TYR:HD2	3:J:1186:TYR:HA	1.63	0.45
5:L:119:ILE:O	5:L:123:ILE:HG13	2.17	0.45
5:L:613:ASP:OD1	5:L:613:ASP:N	2.50	0.45
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.81	0.44
1:B:219:ARG:O	1:B:223:ILE:HG13	2.16	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
3:D:1262:ARG:HH11	3:D:1262:ARG:HD3	1.62	0.44
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.46	0.44
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.17	0.44
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.52	0.44
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.25	0.44
3:J:347:VAL:HG12	3:J:348:ASP:O	2.18	0.44
5:L:580:PHE:C	5:L:582:VAL:H	2.25	0.44
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.32	0.44
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.77	0.44
3:D:568:SER:OG	3:D:569:LEU:N	2.47	0.44
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.98	0.44
5:F:561:MET:HB2	5:F:561:MET:HE3	1.76	0.44
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.71	0.44
3:J:620:PHE:O	3:J:624:ILE:HG13	2.17	0.44
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.84	0.44
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.99	0.44
2:I:1182:ILE:HG22	2:I:1183:ALA:H	1.82	0.44
3:J:128:LEU:HA	3:J:192:MET:HE1	1.99	0.44
3:J:491:LEU:HD11	3:J:610:ARG:HH12	1.83	0.44
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.99	0.44
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.52	0.44
1:B:57:THR:O	1:B:173:VAL:HB	2.17	0.44
2:C:566:GLY:O	2:C:569:ILE:HG13	2.17	0.44
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.99	0.44
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:702:GLN:HG2	3:D:703:THR:N	2.31	0.44
3:D:1183:SER:HB3	3:D:1185:PRO:HD3	1.98	0.44
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.99	0.44
5:F:558:VAL:HG23	5:F:580:PHE:CE2	2.53	0.44
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.99	0.44
2:I:566:GLY:O	2:I:569:ILE:HG13	2.17	0.44
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.17	0.44
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.82	0.44
3:J:1273:ASP:HB3	3:J:1276:GLU:HG3	1.99	0.44
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.33	0.44
2:C:81:ASP:O	2:C:85:CYS:HB2	2.18	0.44
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.25	0.44
2:C:902:LEU:HD21	5:F:611:LEU:HD21	1.98	0.44
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.99	0.44
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.15	0.44
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.44
3:D:516:ASP:HB3	3:D:573:THR:HG21	2.00	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG22	2.18	0.44
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.85	0.44
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.99	0.44
5:L:225:ARG:O	5:L:229:VAL:HG13	2.18	0.44
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.52	0.44
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.99	0.44
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.44
5:F:485:GLU:H	5:F:485:GLU:HG3	1.61	0.44
5:F:496:LYS:O	5:F:500:ILE:HG12	2.17	0.44
2:I:81:ASP:O	2:I:85:CYS:HB2	2.18	0.44
2:I:930:ASP:OD2	2:I:931:VAL:N	2.50	0.44
3:J:45:ASN:O	3:J:46:TYR:HD2	2.01	0.44
3:J:660:GLU:O	3:J:664:ILE:HG12	2.18	0.44
3:J:903:LEU:HD12	3:J:903:LEU:HA	1.89	0.44
5:L:496:LYS:O	5:L:500:ILE:HG12	2.17	0.44
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.17	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.52	0.44
3:D:894:VAL:HB	3:D:915:ILE:HD11	2.00	0.44
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.31	0.44
3:D:1186:TYR:HD2	3:D:1186:TYR:HA	1.62	0.44
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.44
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.99	0.44
2:I:902:LEU:HD21	5:L:611:LEU:HD21	1.99	0.44
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:860:ARG:HG3	3:J:860:ARG:NH1	2.33	0.44
1:B:51:MET:HB3	1:B:178:SER:HA	1.98	0.44
2:C:83:GLN:O	2:C:87:ILE:HG13	2.18	0.44
2:C:1182:ILE:HG22	2:C:1183:ALA:H	1.83	0.44
2:C:1246:ARG:HG2	2:C:1247:SER:N	2.33	0.44
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.18	0.44
3:D:128:LEU:HA	3:D:192:MET:HE1	2.00	0.44
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.52	0.44
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.99	0.44
3:J:650:LYS:O	3:J:654:ILE:HG13	2.18	0.44
3:J:793:SER:O	3:J:797:THR:HG23	2.17	0.44
3:J:1061:VAL:HG21	3:J:1101:LEU:CB	2.48	0.44
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.99	0.44
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.99	0.44
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.99	0.44
3:D:333:GLY:O	3:D:334:LYS:HB2	2.17	0.44
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.83	0.44
5:F:111:LEU:HG	5:F:382:ALA:HB1	2.00	0.44
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.72	0.44
1:G:44:ARG:HG3	1:G:183:ILE:HG22	2.00	0.44
2:I:117:ILE:H	2:I:117:ILE:HG12	1.68	0.44
3:J:77:ARG:HG3	3:J:79:LYS:H	1.83	0.44
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.99	0.44
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.99	0.44
2:C:898:GLU:OE1	2:C:898:GLU:N	2.50	0.43
3:D:80:HIS:ND1	3:D:80:HIS:N	2.66	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.98	0.43
5:F:457:ILE:HA	5:F:460:ILE:HD12	1.99	0.43
2:I:243:PRO:HB2	2:I:278:GLU:HG3	1.99	0.43
3:J:516:ASP:HB3	3:J:573:THR:HG21	2.00	0.43
5:L:476:ARG:HH11	5:L:476:ARG:CG	2.31	0.43
5:L:479:THR:HG22	5:L:482:GLU:HB2	2.00	0.43
1:A:226:GLU:HG2	1:B:10:LYS:HE3	2.01	0.43
3:D:55:GLY:H	3:D:58:CYS:HB2	1.83	0.43
3:D:810:THR:HG23	3:D:811:GLU:H	1.83	0.43
5:F:461:ASN:O	5:F:465:ARG:HG2	2.17	0.43
5:F:476:ARG:CG	5:F:477:GLU:H	2.31	0.43
5:F:584:ARG:HB3	5:F:585:GLU:H	1.56	0.43
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.33	0.43
2:I:600:THR:HB	2:I:602:GLU:HG2	2.01	0.43
2:I:720:ARG:HB2	2:I:749:ASP:OD1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:53:ARG:HA	3:J:54:ASP:HA	1.56	0.43
3:J:894:VAL:HB	3:J:915:ILE:HD11	2.00	0.43
5:L:299:LYS:O	5:L:303:ILE:HG12	2.18	0.43
3:D:620:PHE:O	3:D:624:ILE:HG13	2.18	0.43
1:H:56:VAL:HG22	1:H:144:ILE:HD11	2.00	0.43
2:I:736:VAL:HG23	2:I:748:ILE:HA	2.00	0.43
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	2.00	0.43
3:J:133:ARG:O	3:J:137:ARG:HB2	2.18	0.43
3:J:1230:THR:O	3:J:1234:VAL:HG22	2.18	0.43
5:L:226:ALA:O	5:L:230:VAL:HG12	2.18	0.43
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.43
5:L:561:MET:HE3	5:L:561:MET:HB2	1.75	0.43
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.39	0.43
2:C:403:MET:HE3	2:C:403:MET:HB3	1.87	0.43
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.99	0.43
2:I:145:ILE:HG13	2:I:512:SER:HA	2.00	0.43
2:I:367:TYR:CE2	2:I:376:PRO:HA	2.53	0.43
3:J:810:THR:HG23	3:J:811:GLU:H	1.83	0.43
3:J:1040:MET:HB3	3:J:1046:ILE:HG21	2.00	0.43
2:C:720:ARG:HB2	2:C:749:ASP:OD1	2.19	0.43
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.70	0.43
3:D:484:MET:HE2	3:D:484:MET:HB3	1.80	0.43
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.86	0.43
3:D:1150:PRO:HG2	3:D:1153:PRO:HG3	2.00	0.43
5:F:496:LYS:HB2	5:F:496:LYS:HE3	1.71	0.43
1:G:42:ALA:O	1:G:46:ILE:HG12	2.19	0.43
1:G:125:LYS:HG3	1:G:128:HIS:HB2	2.00	0.43
1:G:228:LEU:HD12	1:G:231:PHE:CZ	2.54	0.43
2:I:1151:LEU:HD23	2:I:1197:GLU:OE2	2.19	0.43
3:J:997:VAL:HA	3:J:998:PRO:HD3	1.85	0.43
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.84	0.43
1:A:115:ILE:HG22	1:A:116:THR:H	1.83	0.43
2:C:30:ILE:H	2:C:30:ILE:HD12	1.83	0.43
2:C:175:ARG:HD3	2:C:183:TRP:CZ3	2.54	0.43
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.34	0.43
2:C:1146:GLN:HE21	2:C:1146:GLN:HB3	1.50	0.43
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.99	0.43
3:D:1160:SER:HA	3:D:1204:VAL:O	2.17	0.43
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	2.00	0.43
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.67	0.43
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:GLN:O	2:I:87:ILE:HG13	2.17	0.43
2:I:122:VAL:HG21	2:I:493:ILE:HG23	2.01	0.43
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.53	0.43
3:J:1163:VAL:HG22	3:J:1164:SER:H	1.84	0.43
3:J:1262:ARG:HD2	3:J:1279:GLN:OE1	2.19	0.43
1:B:50:SER:HA	1:B:151:GLY:HA2	2.00	0.43
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.33	0.43
2:C:600:THR:HB	2:C:602:GLU:HG2	2.01	0.43
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.19	0.43
3:D:45:ASN:O	3:D:46:TYR:HD2	2.01	0.43
3:D:339:ARG:O	3:D:340:GLN:HB3	2.19	0.43
1:H:67:GLU:O	1:H:78:ILE:HB	2.19	0.43
2:I:69:GLN:NE2	2:I:101:ARG:HD2	2.30	0.43
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.53	0.43
2:I:269:ILE:HA	2:I:273:HIS:ND1	2.33	0.43
3:J:75:TYR:HD2	3:J:80:HIS:CD2	2.35	0.43
3:J:271:ARG:HE	3:J:271:ARG:HB2	1.41	0.43
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	2.01	0.43
2:C:112:GLY:HA2	2:C:113:THR:HG23	2.00	0.43
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.54	0.43
2:C:245:ARG:HG2	2:C:337:PHE:CZ	2.53	0.43
2:C:453:ILE:HD11	2:C:530:ILE:HD12	2.00	0.43
2:C:886:LYS:HB3	2:C:917:SER:HA	2.01	0.43
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.54	0.43
3:D:847:ASP:OD1	3:D:847:ASP:N	2.51	0.43
5:F:513:ASP:C	5:F:515:GLU:N	2.77	0.43
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.43
1:H:41:ASN:O	1:H:45:ARG:HG3	2.18	0.43
3:J:255:LEU:N	3:J:259:ARG:O	2.50	0.43
3:J:519:ASN:CB	3:J:709:ARG:HD3	2.48	0.43
3:J:1150:PRO:HG2	3:J:1153:PRO:HG3	2.00	0.43
3:J:1295:ASN:CB	3:J:1298:VAL:HB	2.46	0.43
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.44	0.43
5:L:593:LYS:O	5:L:596:ARG:HB3	2.19	0.43
1:A:46:ILE:HD11	1:B:38:THR:HG21	2.01	0.43
2:C:87:ILE:HG13	2:C:87:ILE:H	1.70	0.43
2:C:88:ARG:NH2	2:C:1035:LYS:O	2.52	0.43
2:C:896:THR:OG1	2:C:899:GLU:OE2	2.30	0.43
2:C:930:ASP:OD2	2:C:931:VAL:N	2.51	0.43
2:C:1134:GLN:OE1	2:C:1134:GLN:HA	2.19	0.43
3:D:860:ARG:HB3	3:D:861:ASN:H	1.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.53	0.43
5:F:299:LYS:O	5:F:303:ILE:HG12	2.18	0.43
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.87	0.43
1:G:58:GLU:HB2	1:G:145:LYS:HB3	2.00	0.43
2:I:151:ARG:HH21	2:I:445:ILE:HD11	1.84	0.43
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.53	0.43
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.99	0.43
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.84	0.43
3:J:349:TYR:CD1	3:J:472:LEU:HD11	2.54	0.43
3:J:525:MET:O	3:J:548:VAL:HG13	2.19	0.43
3:J:1034:PHE:CE2	3:J:1114:GLN:HB2	2.54	0.43
3:J:1160:SER:HA	3:J:1204:VAL:O	2.19	0.43
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	2.00	0.43
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.19	0.43
1:B:102:LEU:HA	1:B:102:LEU:HD23	1.80	0.43
2:C:736:VAL:HG23	2:C:748:ILE:HA	2.01	0.43
2:C:1248:THR:HG21	5:F:531:PRO:HG3	2.00	0.43
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.54	0.43
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.54	0.43
3:D:905:ARG:NH1	4:E:16:ARG:HB2	2.34	0.43
3:D:1184:ASP:O	3:D:1186:TYR:N	2.52	0.43
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.01	0.43
1:G:102:LEU:HD12	1:G:142:MET:HE3	2.01	0.43
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.31	0.43
2:I:151:ARG:NH2	2:I:445:ILE:HD11	2.34	0.43
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.54	0.43
2:I:886:LYS:HB3	2:I:917:SER:HA	2.00	0.43
2:I:1007:LYS:O	2:I:1011:LEU:HG	2.19	0.43
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.19	0.43
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.43
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.81	0.43
5:L:111:LEU:HG	5:L:382:ALA:HB1	2.00	0.43
1:B:67:GLU:O	1:B:78:ILE:HB	2.18	0.42
1:B:158:ARG:HD2	1:B:158:ARG:HA	1.78	0.42
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.01	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.54	0.42
2:C:367:TYR:CE2	2:C:376:PRO:HA	2.53	0.42
2:C:1297:ASP:O	2:C:1301:ARG:HG2	2.18	0.42
3:D:128:LEU:HD23	3:D:192:MET:HE3	2.01	0.42
3:D:185:ILE:HD13	3:D:188:LEU:HD12	2.01	0.42
3:D:650:LYS:O	3:D:654:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:62:GLN:O	4:E:66:VAL:HG23	2.19	0.42
1:H:151:GLY:O	1:H:177:TYR:HB2	2.18	0.42
2:I:543:ALA:HA	2:I:544:GLY:HA3	1.87	0.42
3:J:710:ASP:OD1	3:J:710:ASP:C	2.61	0.42
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.49	0.42
1:B:115:ILE:HD11	1:B:130:ILE:HD11	2.01	0.42
2:C:596:ASP:OD2	2:C:597:GLY:N	2.51	0.42
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.84	0.42
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.19	0.42
3:D:133:ARG:O	3:D:137:ARG:HB2	2.18	0.42
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.02	0.42
3:D:1151:LYS:C	3:D:1153:PRO:HD3	2.45	0.42
1:G:92:VAL:HA	1:G:120:ASP:O	2.19	0.42
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.83	0.42
2:I:854:ILE:HB	2:I:857:VAL:HG21	2.01	0.42
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.50	0.42
3:J:55:GLY:H	3:J:58:CYS:HB2	1.83	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.18	0.42
3:D:232:ASN:OD1	3:D:232:ASN:N	2.51	0.42
3:D:418:GLU:O	3:D:420:PRO:HD3	2.20	0.42
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.78	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB3	1.84	0.42
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.01	0.42
2:I:216:THR:H	2:I:219:GLN:HE22	1.66	0.42
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.34	0.42
3:J:80:HIS:ND1	3:J:80:HIS:N	2.67	0.42
3:J:683:ILE:HD11	3:J:754:ILE:HG12	2.02	0.42
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.99	0.42
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.72	0.42
1:B:90:VAL:HG11	1:B:146:VAL:HG11	2.02	0.42
2:C:974:ARG:O	2:C:978:VAL:HG23	2.20	0.42
3:D:660:GLU:O	3:D:664:ILE:HG12	2.18	0.42
5:F:226:ALA:O	5:F:230:VAL:HG12	2.19	0.42
1:H:50:SER:HA	1:H:151:GLY:HA2	2.01	0.42
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.34	0.42
2:I:379:GLU:CD	2:I:379:GLU:H	2.27	0.42
2:I:1136:GLN:O	2:I:1137:GLU:HG2	2.19	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HB2	2.01	0.42
5:L:476:ARG:HB3	5:L:477:GLU:H	1.24	0.42
5:L:532:LEU:H	5:L:532:LEU:HD12	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HG3	1:A:183:ILE:HG22	2.00	0.42
1:A:125:LYS:HG3	1:A:128:HIS:HB2	2.01	0.42
1:B:136:GLU:CG	1:B:137:ASN:H	2.30	0.42
2:C:854:ILE:HB	2:C:857:VAL:HG21	2.01	0.42
2:C:961:SER:O	2:C:965:GLN:HG3	2.20	0.42
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.19	0.42
3:D:298:MET:SD	5:F:402:LEU:HB3	2.58	0.42
3:D:807:LEU:HD23	3:D:915:ILE:HG13	2.02	0.42
3:D:1163:VAL:HG22	3:D:1164:SER:H	1.85	0.42
3:D:1302:TYR:CZ	3:J:1297:LYS:HE2	2.55	0.42
2:I:619:ALA:HB1	2:I:657:THR:HA	2.01	0.42
3:J:298:MET:SD	5:L:402:LEU:HB3	2.59	0.42
1:A:92:VAL:HA	1:A:120:ASP:O	2.20	0.42
3:D:75:TYR:CE2	3:D:83:VAL:HG21	2.54	0.42
3:D:848:VAL:HG13	3:D:858:VAL:HG22	2.02	0.42
3:D:860:ARG:HG3	3:D:860:ARG:NH1	2.35	0.42
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.85	0.42
3:J:292:VAL:O	3:J:296:LYS:HG3	2.20	0.42
3:J:984:LEU:CB	3:J:993:GLU:HB2	2.50	0.42
3:J:1060:VAL:HG13	3:J:1106:ILE:HA	2.02	0.42
5:L:474:MET:C	5:L:476:ARG:H	2.12	0.42
1:A:42:ALA:O	1:A:46:ILE:HG12	2.19	0.42
1:B:43:LEU:HG	1:B:221:ALA:HB2	2.01	0.42
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.85	0.42
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.49	0.42
3:D:338:PHE:CB	3:D:343:LEU:HB2	2.49	0.42
1:G:115:ILE:HG22	1:G:116:THR:H	1.84	0.42
2:I:417:SER:OG	2:I:419:ILE:HG13	2.20	0.42
3:J:59:ALA:HA	3:J:63:GLY:O	2.20	0.42
3:J:1151:LYS:C	3:J:1153:PRO:HD3	2.45	0.42
1:B:147:GLN:HG3	1:B:148:ARG:H	1.85	0.42
2:C:148:GLN:NE2	2:C:535:PRO:O	2.46	0.42
2:C:417:SER:OG	2:C:419:ILE:HG13	2.20	0.42
2:C:494:ASN:HB3	2:C:497:PRO:CD	2.49	0.42
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.00	0.42
3:D:491:LEU:HD11	3:D:610:ARG:HH12	1.83	0.42
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.55	0.42
1:H:57:THR:O	1:H:173:VAL:HB	2.19	0.42
1:H:115:ILE:HD11	1:H:130:ILE:HD11	2.01	0.42
2:I:27:LEU:HB2	2:I:524:ILE:HD11	2.02	0.42
2:I:53:PHE:O	2:I:57:PHE:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:HG2	3:J:426:ALA:N	2.35	0.42
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.02	0.42
3:J:849:LEU:HB2	3:J:850:LYS:O	2.20	0.42
3:J:850:LYS:HE2	3:J:855:ASP:HB3	2.02	0.42
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.33	0.42
1:B:41:ASN:O	1:B:45:ARG:HG3	2.19	0.42
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.30	0.42
2:C:379:GLU:CD	2:C:379:GLU:H	2.27	0.42
2:C:1121:ALA:HB1	2:C:1180:MET:O	2.20	0.42
3:D:292:VAL:O	3:D:296:LYS:HG3	2.20	0.42
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.02	0.42
3:D:903:LEU:HD12	3:D:903:LEU:HA	1.90	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.85	0.42
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.85	0.42
4:E:86:ILE:C	4:E:88:GLU:N	2.78	0.42
2:I:138:ILE:HG22	2:I:139:ASN:ND2	2.35	0.42
3:J:632:ALA:O	3:J:635:SER:OG	2.30	0.42
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.20	0.42
3:J:1332:LEU:HD13	3:J:1332:LEU:HA	1.88	0.42
1:A:231:PHE:N	1:A:231:PHE:CD2	2.88	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.87	0.42
3:D:255:LEU:N	3:D:259:ARG:O	2.51	0.42
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.19	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HB	2.19	0.42
5:F:421:TYR:H	5:F:421:TYR:HD2	1.67	0.42
5:F:532:LEU:H	5:F:532:LEU:HD12	1.85	0.42
1:H:158:ARG:HD2	1:H:158:ARG:HA	1.82	0.42
2:I:961:SER:O	2:I:965:GLN:HG3	2.20	0.42
3:J:185:ILE:HD13	3:J:188:LEU:HD12	2.01	0.42
3:J:396:ALA:O	3:J:400:MET:HG3	2.19	0.42
3:J:527:LEU:HB2	3:J:550:VAL:HG12	2.02	0.42
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.84	0.41
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.35	0.41
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.89	0.41
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.02	0.41
2:I:202:ARG:H	2:I:202:ARG:HG3	1.71	0.41
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.19	0.41
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.50	0.41
3:J:128:LEU:HD23	3:J:192:MET:HE3	2.01	0.41
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.86	0.41
3:J:709:ARG:HD2	3:J:710:ASP:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:849:LEU:HB3	3:J:853:THR:HG23	2.02	0.41
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.54	0.41
3:J:1037:PHE:N	3:J:1111:ASP:OD2	2.53	0.41
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.85	0.41
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.75	0.41
5:L:582:VAL:HG23	5:L:586:ARG:HG2	2.00	0.41
1:B:56:VAL:HG22	1:B:144:ILE:HD11	2.01	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.83	0.41
3:D:863:LEU:CD1	3:D:901:ARG:HB3	2.50	0.41
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.20	0.41
2:I:97:ARG:HB3	2:I:121:GLU:HB2	2.01	0.41
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.50	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.76	0.41
3:J:310:GLY:HA2	3:J:314:ARG:CG	2.47	0.41
3:J:1192:LYS:HE3	3:J:1192:LYS:HB2	1.90	0.41
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.35	0.41
5:L:606:VAL:HG13	5:L:607:LEU:HD23	2.03	0.41
2:C:53:PHE:O	2:C:57:PHE:HB2	2.20	0.41
2:C:109:ALA:HB1	2:C:110:PRO:C	2.46	0.41
3:D:665:GLN:HG3	3:D:669:GLN:NE2	2.36	0.41
3:D:709:ARG:O	3:D:711:GLY:N	2.53	0.41
3:D:901:ARG:HD2	3:D:906:GLY:O	2.20	0.41
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.20	0.41
1:G:71:LYS:HB2	1:G:78:ILE:HD11	2.02	0.41
2:I:494:ASN:HB3	2:I:497:PRO:CD	2.49	0.41
2:I:718:ALA:HB2	2:I:783:LEU:HD23	2.03	0.41
2:I:898:GLU:OE1	2:I:898:GLU:N	2.53	0.41
3:J:1184:ASP:O	3:J:1186:TYR:N	2.52	0.41
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.83	0.41
5:L:513:ASP:C	5:L:515:GLU:N	2.77	0.41
1:A:48:LEU:HA	1:A:180:VAL:HG21	2.02	0.41
2:C:100:LEU:HD12	2:C:122:VAL:HG11	2.02	0.41
2:C:172:TYR:O	2:C:188:PHE:HD2	2.04	0.41
2:C:242:VAL:HA	2:C:243:PRO:HD3	1.87	0.41
2:C:718:ALA:HB2	2:C:783:LEU:HD23	2.02	0.41
3:D:230:SER:CB	3:D:232:ASN:H	2.33	0.41
3:D:1181:ASP:HA	3:J:202:ARG:HD3	2.01	0.41
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.20	0.41
1:H:83:LEU:HA	1:H:86:LYS:HE2	2.02	0.41
1:H:110:VAL:HG12	1:H:114:ASP:HB3	2.03	0.41
2:I:227:LYS:O	2:I:245:ARG:NH2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:596:ASP:OD2	2:I:597:GLY:N	2.52	0.41
3:J:56:LEU:HD12	3:J:56:LEU:H	1.85	0.41
3:J:403:ARG:HB3	3:J:405:GLU:HG3	2.02	0.41
3:J:807:LEU:HD23	3:J:915:ILE:HG13	2.02	0.41
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.21	0.41
1:A:228:LEU:HD12	1:A:231:PHE:CZ	2.56	0.41
2:C:131:THR:HG22	2:C:132:ASP:H	1.85	0.41
2:C:1134:GLN:CB	2:C:1136:GLN:HG2	2.51	0.41
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.41
3:D:527:LEU:HB2	3:D:550:VAL:HG12	2.02	0.41
5:F:593:LYS:O	5:F:596:ARG:HB3	2.20	0.41
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.03	0.41
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.80	0.41
2:I:453:ILE:HD11	2:I:530:ILE:HD12	2.01	0.41
2:I:710:VAL:HA	2:I:715:THR:HG21	2.02	0.41
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.20	0.41
3:J:514:THR:HG23	3:J:594:GLN:O	2.20	0.41
3:J:967:VAL:HG13	3:J:971:GLY:HA2	2.02	0.41
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.20	0.41
3:J:1311:LYS:O	3:J:1314:LEU:HB3	2.20	0.41
5:L:490:PRO:HG2	5:L:493:LYS:HE3	2.03	0.41
1:B:83:LEU:HA	1:B:86:LYS:HE2	2.02	0.41
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.86	0.41
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.60	0.41
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.21	0.41
3:D:59:ALA:HA	3:D:63:GLY:O	2.21	0.41
3:D:500:ILE:HG22	3:D:500:ILE:O	2.20	0.41
3:D:1311:LYS:O	3:D:1314:LEU:HB3	2.20	0.41
2:I:5:TYR:O	2:I:8:LYS:HG2	2.20	0.41
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.01	0.41
3:J:581:MET:HE2	3:J:581:MET:HB3	2.01	0.41
3:J:702:GLN:HB3	3:J:702:GLN:HE21	1.65	0.41
3:J:1079:LYS:HB3	3:J:1079:LYS:NZ	2.35	0.41
3:J:1105:ALA:HA	3:J:1125:PRO:HD2	2.03	0.41
3:J:1185:PRO:O	3:J:1187:GLU:HG2	2.20	0.41
5:L:603:ARG:HH11	5:L:603:ARG:HA	1.85	0.41
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.01	0.41
1:B:60:GLU:H	1:B:60:GLU:HG3	1.71	0.41
2:C:619:ALA:HB1	2:C:657:THR:HA	2.02	0.41
2:C:878:THR:OG1	2:C:879:GLY:N	2.54	0.41
2:C:899:GLU:O	2:C:902:LEU:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:925:SER:O	2:C:1056:VAL:HG13	2.21	0.41
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.21	0.41
3:D:702:GLN:HB3	3:D:702:GLN:HE21	1.67	0.41
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.85	0.41
5:F:292:VAL:HG21	5:F:299:LYS:CG	2.51	0.41
5:F:315:TRP:O	5:F:319:ALA:HB3	2.21	0.41
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.49	0.41
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.29	0.41
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.20	0.41
3:J:827:GLU:O	3:J:829:GLY:N	2.36	0.41
3:J:988:PHE:HD2	3:J:990:ARG:HH21	1.69	0.41
3:J:1281:GLU:O	3:J:1285:VAL:HB	2.20	0.41
5:L:245:ALA:O	5:L:249:ILE:HG13	2.21	0.41
5:L:461:ASN:O	5:L:465:ARG:HG2	2.20	0.41
5:L:489:MET:H	5:L:489:MET:HG2	1.60	0.41
5:L:572:THR:O	5:L:575:GLU:HB3	2.20	0.41
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.02	0.41
5:F:245:ALA:O	5:F:249:ILE:HG13	2.21	0.41
1:G:231:PHE:CZ	1:H:221:ALA:HB3	2.54	0.41
1:H:90:VAL:HG11	1:H:146:VAL:HG11	2.03	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.88	0.41
3:J:665:GLN:HG3	3:J:669:GLN:NE2	2.36	0.41
3:J:1290:ARG:HD3	3:J:1290:ARG:HA	1.74	0.41
5:L:489:MET:CB	5:L:490:PRO:HD2	2.50	0.41
1:A:20:SER:OG	1:A:21:SER:N	2.54	0.41
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.41
1:B:43:LEU:O	1:B:47:LEU:HB2	2.21	0.41
2:C:151:ARG:NE	2:C:445:ILE:HD11	2.36	0.41
2:C:227:LYS:O	2:C:245:ARG:NH2	2.53	0.41
2:C:365:GLU:CD	2:C:368:ARG:HH21	2.29	0.41
2:C:524:ILE:HG21	2:C:708:VAL:HG13	2.02	0.41
2:C:757:THR:O	2:C:833:ILE:HD12	2.21	0.41
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.21	0.41
2:C:1313:HIS:O	4:E:28:ARG:NH1	2.53	0.41
3:D:343:LEU:HD12	3:D:343:LEU:HA	1.85	0.41
3:D:514:THR:HG23	3:D:594:GLN:O	2.20	0.41
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.21	0.41
3:D:1372:ARG:HB2	3:J:854:ALA:HB2	2.03	0.41
5:F:105:MET:HE2	5:F:105:MET:HB2	1.92	0.41
5:F:134:VAL:HG22	5:F:273:MET:HE1	2.03	0.41
5:F:289:LYS:HB3	5:F:289:LYS:HE2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.20	0.41
5:F:559:LEU:O	5:F:563:PHE:HD2	2.04	0.41
5:F:572:THR:O	5:F:575:GLU:HB2	2.21	0.41
1:H:153:VAL:HA	1:H:154:PRO:HD3	1.90	0.41
1:H:205:MET:HE3	1:H:213:PRO:HB3	2.03	0.41
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.56	0.41
2:I:109:ALA:HB1	2:I:110:PRO:C	2.46	0.41
2:I:172:TYR:O	2:I:188:PHE:HD2	2.04	0.41
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.21	0.41
3:J:195:GLU:O	3:J:198:CYS:HB2	2.21	0.41
3:J:418:GLU:O	3:J:420:PRO:HD3	2.20	0.41
3:J:840:LEU:HG	3:J:841:GLY:N	2.35	0.41
3:J:905:ARG:NH1	4:K:10:VAL:HG11	2.35	0.41
3:J:1156:LEU:HG	3:J:1224:ARG:HH21	1.86	0.41
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.21	0.41
4:K:62:GLN:O	4:K:66:VAL:HG23	2.20	0.41
5:L:261:LEU:HD12	5:L:261:LEU:H	1.86	0.41
5:L:315:TRP:O	5:L:319:ALA:HB3	2.21	0.41
5:L:421:TYR:H	5:L:421:TYR:HD2	1.68	0.41
5:L:482:GLU:CG	5:L:486:ARG:HH12	2.34	0.41
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.86	0.41
1:A:75:GLN:HA	2:C:729:ALA:H	1.86	0.41
1:A:102:LEU:HD12	1:A:142:MET:HE3	2.02	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.91	0.41
2:C:18:ARG:HA	2:C:19:PRO:HD3	1.96	0.41
3:D:77:ARG:HD2	3:D:78:LEU:H	1.85	0.41
3:D:334:LYS:HG3	3:D:335:GLN:H	1.86	0.41
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	2.02	0.41
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.97	0.41
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.02	0.41
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.21	0.41
5:L:105:MET:HE2	5:L:105:MET:HB2	1.93	0.41
5:L:165:PHE:HE1	5:L:259:PHE:CD2	2.39	0.41
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.65	0.40
1:A:221:ALA:HB1	1:B:228:LEU:HD22	2.02	0.40
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.50	0.40
2:C:782:VAL:HG11	2:C:792:GLY:HA2	2.03	0.40
3:D:161:THR:H	3:D:164:GLN:HB2	1.86	0.40
3:D:849:LEU:HB3	3:D:853:THR:HG23	2.02	0.40
3:D:1185:PRO:O	3:D:1187:GLU:HG2	2.21	0.40
3:D:1371:ARG:HE	3:J:854:ALA:HA	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:340:ALA:HA	5:F:343:LYS:NZ	2.36	0.40
5:F:489:MET:CB	5:F:490:PRO:HD2	2.52	0.40
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.40
2:I:62:TYR:C	2:I:64:GLY:H	2.29	0.40
2:I:100:LEU:HD12	2:I:122:VAL:HG11	2.03	0.40
2:I:402:ARG:NH2	2:I:419:ILE:O	2.54	0.40
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.61	0.40
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.57	0.40
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.54	0.40
3:J:349:TYR:CG	3:J:472:LEU:HD21	2.57	0.40
3:J:901:ARG:HD2	3:J:906:GLY:O	2.21	0.40
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.36	0.40
5:L:231:THR:HG23	5:L:249:ILE:HG12	2.04	0.40
5:L:292:VAL:HG21	5:L:299:LYS:CG	2.51	0.40
1:A:153:VAL:HB	1:A:175:ALA:HB3	2.03	0.40
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.90	0.40
2:C:24:VAL:HG21	2:C:704:MET:SD	2.62	0.40
3:D:369:PRO:HB3	3:D:444:GLY:O	2.22	0.40
3:D:850:LYS:HE2	3:D:855:ASP:HB3	2.03	0.40
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.36	0.40
1:H:195:ARG:HB3	1:H:198:LEU:HD21	2.03	0.40
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.51	0.40
3:J:1024:THR:HG23	3:J:1123:ARG:HG2	2.03	0.40
3:J:1108:GLN:HE21	3:J:1120:THR:HG1	1.60	0.40
5:L:591:GLU:O	5:L:595:LEU:HG	2.22	0.40
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.66	0.40
2:C:13:LYS:HZ1	2:C:1151:LEU:HD12	1.85	0.40
2:C:857:VAL:HB	2:C:861:ALA:HB3	2.03	0.40
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.88	0.40
4:E:86:ILE:C	4:E:88:GLU:H	2.29	0.40
5:F:583:THR:O	5:F:584:ARG:HB2	2.21	0.40
1:H:136:GLU:CG	1:H:137:ASN:H	2.34	0.40
2:I:582:ASN:HB3	2:I:586:PHE:N	2.35	0.40
3:J:83:VAL:O	3:J:91:GLU:HA	2.22	0.40
3:J:124:ILE:H	3:J:124:ILE:HG13	1.65	0.40
3:J:800:LEU:HB3	3:J:920:ALA:HB1	2.04	0.40
3:J:1348:LYS:HD2	3:J:1348:LYS:HA	1.92	0.40
1:A:71:LYS:HB2	1:A:78:ILE:HD11	2.03	0.40
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.02	0.40
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.56	0.40
3:D:349:TYR:CG	3:D:472:LEU:HD21	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:853:THR:CG2	3:J:1375:ALA:HB1	2.45	0.40
5:F:482:GLU:HG2	5:F:486:ARG:HH12	1.86	0.40
1:H:43:LEU:O	1:H:47:LEU:HB2	2.20	0.40
1:H:147:GLN:HG3	1:H:148:ARG:H	1.86	0.40
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.95	0.40
2:I:524:ILE:HG21	2:I:708:VAL:HG13	2.02	0.40
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.85	0.40
2:I:974:ARG:O	2:I:978:VAL:HG23	2.21	0.40
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.90	0.40
3:J:294:ASN:HD22	5:L:406:GLN:HE21	1.69	0.40
3:J:417:ARG:HH21	4:K:43:ASN:C	2.30	0.40
3:J:780:ARG:HE	3:J:780:ARG:HB2	1.71	0.40
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	2.02	0.40
2:C:139:ASN:C	2:C:141:THR:N	2.78	0.40
2:C:312:ALA:HB3	2:C:315:MET:HE3	2.03	0.40
3:D:26:SER:HB3	3:D:29:MET:CB	2.50	0.40
3:D:396:ALA:O	3:D:400:MET:HG3	2.21	0.40
3:D:1153:PRO:HA	3:D:1214:PRO:O	2.21	0.40
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.36	0.40
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.03	0.40
5:F:604:SER:O	5:F:608:ARG:HB3	2.22	0.40
3:J:77:ARG:HD2	3:J:78:LEU:H	1.85	0.40
3:J:248:ASP:O	3:J:251:PRO:HG3	2.22	0.40
3:J:405:GLU:O	3:J:408:VAL:HG13	2.22	0.40
3:J:515:ARG:NH2	3:J:717:VAL:O	2.54	0.40
3:J:863:LEU:CD1	3:J:901:ARG:HB3	2.51	0.40
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.37	0.40
3:J:1265:THR:N	3:J:1305:ASP:OD2	2.55	0.40
5:L:134:VAL:HG22	5:L:273:MET:HE1	2.03	0.40
5:L:299:LYS:HA	5:L:302:PHE:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:GLU:OE2	2:I:422:LYS:NZ[3_554]	2.19	0.01

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	222/239 (93%)	195 (88%)	26 (12%)	1 (0%)	24	57
1	B	216/239 (90%)	192 (89%)	23 (11%)	1 (0%)	24	57
1	G	226/239 (95%)	197 (87%)	27 (12%)	2 (1%)	14	46
1	H	213/239 (89%)	191 (90%)	21 (10%)	1 (0%)	24	57
2	C	1338/1342 (100%)	1224 (92%)	100 (8%)	14 (1%)	12	44
2	I	1338/1342 (100%)	1228 (92%)	97 (7%)	13 (1%)	12	44
3	D	1162/1407 (83%)	1078 (93%)	78 (7%)	6 (0%)	24	57
3	J	1317/1407 (94%)	1225 (93%)	87 (7%)	5 (0%)	30	60
4	E	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	11	43
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	9	39
5	F	464/522 (89%)	420 (90%)	41 (9%)	3 (1%)	21	54
5	L	463/522 (89%)	422 (91%)	36 (8%)	5 (1%)	11	43
All	All	7123/7680 (93%)	6520 (92%)	550 (8%)	53 (1%)	18	51

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	44	GLU
2	C	169	LYS
2	C	697	LYS
2	C	897	PRO
2	C	898	GLU
2	C	1137	GLU
2	C	1159	VAL
2	C	1203	ASP
3	D	230	SER
5	F	584	ARG
1	H	138	ALA
2	I	169	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	170	VAL
2	I	897	PRO
2	I	1159	VAL
3	J	230	SER
4	K	15	ASN
2	C	170	VAL
4	E	15	ASN
5	F	475	GLY
2	I	898	GLU
2	I	1153	ALA
3	J	1360	GLY
5	L	584	ARG
5	L	602	SER
1	B	138	ALA
2	C	1153	ALA
2	C	1154	ASP
3	D	710	ASP
2	I	44	GLU
2	I	986	ALA
2	I	1137	GLU
1	A	14	VAL
3	D	1169	THR
2	I	697	LYS
3	J	710	ASP
5	L	475	GLY
5	L	603	ARG
2	C	986	ALA
2	C	1135	GLN
3	D	1345	ARG
1	G	14	VAL
2	I	121	GLU
3	J	1169	THR
5	L	601	PRO
2	C	896	THR
2	I	896	THR
2	I	140	GLY
3	D	1180	VAL
3	D	1360	GLY
5	F	601	PRO
3	J	1180	VAL
1	G	167	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/206 (93%)	164 (86%)	27 (14%)	3	19
1	B	184/206 (89%)	154 (84%)	30 (16%)	2	14
1	G	191/206 (93%)	164 (86%)	27 (14%)	3	19
1	H	183/206 (89%)	156 (85%)	27 (15%)	3	17
2	C	1155/1157 (100%)	1007 (87%)	148 (13%)	4	22
2	I	1154/1157 (100%)	1006 (87%)	148 (13%)	4	22
3	D	975/1168 (84%)	842 (86%)	133 (14%)	3	20
3	J	1110/1168 (95%)	961 (87%)	149 (13%)	4	21
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	23
4	K	67/75 (89%)	58 (87%)	9 (13%)	4	21
5	F	417/462 (90%)	352 (84%)	65 (16%)	2	16
5	L	418/462 (90%)	351 (84%)	67 (16%)	2	15
All	All	6117/6548 (93%)	5278 (86%)	839 (14%)	3	20

All (839) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	VAL
1	A	15	ASP
1	A	16	ILE
1	A	19	VAL
1	A	26	VAL
1	A	35	PHE
1	A	50	SER
1	A	54	CYS
1	A	56	VAL
1	A	61	ILE
1	A	64	VAL
1	A	65	LEU
1	A	67	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	74	VAL
1	A	115	ILE
1	A	129	VAL
1	A	133	LEU
1	A	137	ASN
1	A	165	GLU
1	A	168	ILE
1	A	192	VAL
1	A	196	THR
1	A	197	ASP
1	A	219	ARG
1	A	228	LEU
1	A	231	PHE
1	B	6	THR
1	B	8	PHE
1	B	14	VAL
1	B	16	ILE
1	B	27	THR
1	B	50	SER
1	B	58	GLU
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	80	GLU
1	B	92	VAL
1	B	97	GLU
1	B	107	ILE
1	B	110	VAL
1	B	123	ILE
1	B	129	VAL
1	B	133	LEU
1	B	134	THR
1	B	135	ASP
1	B	139	SER
1	B	140	ILE
1	B	148	ARG
1	B	159	ILE
1	B	160	HIS
1	B	176	CYS
1	B	183	ILE
1	B	196	THR
1	B	203	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	THR
2	C	4	SER
2	C	11	ILE
2	C	12	ARG
2	C	17	LYS
2	C	21	VAL
2	C	22	LEU
2	C	23	ASP
2	C	39	ILE
2	C	59	ILE
2	C	79	VAL
2	C	82	VAL
2	C	85	CYS
2	C	91	THR
2	C	106	GLU
2	C	107	ARG
2	C	108	GLU
2	C	111	GLU
2	C	113	THR
2	C	114	VAL
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	124	MET
2	C	131	THR
2	C	167	SER
2	C	170	VAL
2	C	219	GLN
2	C	233	ARG
2	C	235	ASN
2	C	285	ILE
2	C	292	ILE
2	C	302	ILE
2	C	306	THR
2	C	316	GLU
2	C	320	ASP
2	C	353	VAL
2	C	360	LEU
2	C	377	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	379	GLU
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	453	ILE
2	C	470	ARG
2	C	484	LEU
2	C	486	THR
2	C	490	GLN
2	C	492	MET
2	C	503	LYS
2	C	510	GLN
2	C	518	ASN
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	550	VAL
2	C	558	VAL
2	C	575	LEU
2	C	600	THR
2	C	604	HIS
2	C	615	VAL
2	C	618	GLN
2	C	620	ASN
2	C	623	LEU
2	C	630	VAL
2	C	633	LEU
2	C	635	THR
2	C	639	LYS
2	C	648	ASP
2	C	657	THR
2	C	660	VAL
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	724	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	783	LEU
2	C	788	SER
2	C	791	LEU
2	C	800	MET
2	C	808	ASN
2	C	815	SER
2	C	817	LEU
2	C	826	ASP
2	C	830	THR
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	892	GLU
2	C	902	LEU
2	C	911	SER
2	C	946	LEU
2	C	979	LEU
2	C	984	VAL
2	C	1002	LEU
2	C	1014	LEU
2	C	1034	ARG
2	C	1037	THR
2	C	1046	VAL
2	C	1073	LYS
2	C	1079	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1119	MET
2	C	1134	GLN
2	C	1136	GLN
2	C	1140	LYS
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1174	GLU
2	C	1176	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1204	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1222	GLU
2	C	1239	VAL
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1265	PHE
2	C	1275	VAL
2	C	1293	VAL
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	40	LYS
3	D	46	TYR
3	D	52	GLU
3	D	54	ASP
3	D	79	LYS
3	D	80	HIS
3	D	84	ILE
3	D	92	VAL
3	D	95	THR
3	D	96	LYS
3	D	97	VAL
3	D	98	ARG
3	D	106	GLU
3	D	137	ARG
3	D	159	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	169	LEU
3	D	175	GLU
3	D	203	GLU
3	D	217	LEU
3	D	218	THR
3	D	232	ASN
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	299	LEU
3	D	306	LEU
3	D	324	LEU
3	D	334	LYS
3	D	339	ARG
3	D	353	SER
3	D	363	LEU
3	D	374	LEU
3	D	376	LEU
3	D	394	ILE
3	D	407	VAL
3	D	408	VAL
3	D	416	ILE
3	D	429	LEU
3	D	435	GLN
3	D	490	ILE
3	D	501	VAL
3	D	506	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	544	LEU
3	D	545	HIS
3	D	560	ASN
3	D	567	THR
3	D	568	SER
3	D	573	THR
3	D	574	VAL
3	D	576	ARG
3	D	594	GLN
3	D	617	THR
3	D	641	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	682	VAL
3	D	683	ILE
3	D	685	ILE
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	703	THR
3	D	707	ILE
3	D	710	ASP
3	D	712	GLN
3	D	740	LEU
3	D	749	LYS
3	D	753	SER
3	D	754	ILE
3	D	757	THR
3	D	765	GLU
3	D	770	LEU
3	D	788	LEU
3	D	801	VAL
3	D	803	VAL
3	D	807	LEU
3	D	810	THR
3	D	823	THR
3	D	825	VAL
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	875	ASN
3	D	881	LYS
3	D	890	THR
3	D	897	HIS
3	D	907	HIS
3	D	908	ILE
3	D	918	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1155	ILE
3	D	1156	LEU
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1178	THR
3	D	1186	TYR
3	D	1196	LEU
3	D	1202	GLU
3	D	1205	GLU
3	D	1221	LEU
3	D	1223	LEU
3	D	1237	VAL
3	D	1251	LYS
3	D	1255	VAL
3	D	1266	ILE
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1290	ARG
3	D	1298	VAL
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1355	ARG
4	E	3	ARG
4	E	5	THR
4	E	6	VAL
4	E	13	ILE
4	E	18	ASP
4	E	28	ARG
4	E	39	VAL
4	E	47	THR
4	E	58	LEU
5	F	94	THR
5	F	98	VAL
5	F	100	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	102	MET
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	166	VAL
5	F	230	VAL
5	F	247	GLU
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	344	LEU
5	F	357	GLN
5	F	362	ASN
5	F	395	THR
5	F	400	GLN
5	F	429	THR
5	F	445	ASP
5	F	449	THR
5	F	467	SER
5	F	469	GLN
5	F	470	MET
5	F	471	LEU
5	F	472	GLN
5	F	476	ARG
5	F	479	THR
5	F	481	GLU
5	F	482	GLU
5	F	485	GLU
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	494	ILE
5	F	496	LYS
5	F	499	LYS
5	F	500	ILE
5	F	511	ILE
5	F	515	GLU
5	F	516	ASP
5	F	529	GLU
5	F	530	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	540	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	573	LEU
5	F	575	GLU
5	F	578	LYS
5	F	580	PHE
5	F	581	ASP
5	F	587	ILE
5	F	599	ARG
5	F	600	HIS
5	F	601	PRO
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	14	VAL
1	G	15	ASP
1	G	16	ILE
1	G	19	VAL
1	G	26	VAL
1	G	35	PHE
1	G	50	SER
1	G	54	CYS
1	G	56	VAL
1	G	61	ILE
1	G	64	VAL
1	G	65	LEU
1	G	67	GLU
1	G	74	VAL
1	G	115	ILE
1	G	129	VAL
1	G	133	LEU
1	G	137	ASN
1	G	165	GLU
1	G	168	ILE
1	G	192	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	196	THR
1	G	197	ASP
1	G	219	ARG
1	G	228	LEU
1	G	231	PHE
1	H	14	VAL
1	H	16	ILE
1	H	27	THR
1	H	50	SER
1	H	58	GLU
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	80	GLU
1	H	92	VAL
1	H	97	GLU
1	H	107	ILE
1	H	110	VAL
1	H	123	ILE
1	H	129	VAL
1	H	133	LEU
1	H	134	THR
1	H	135	ASP
1	H	139	SER
1	H	140	ILE
1	H	148	ARG
1	H	176	CYS
1	H	183	ILE
1	H	196	THR
1	H	203	ILE
1	H	222	THR
2	I	4	SER
2	I	11	ILE
2	I	12	ARG
2	I	17	LYS
2	I	21	VAL
2	I	22	LEU
2	I	23	ASP
2	I	39	ILE
2	I	59	ILE
2	I	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	82	VAL
2	I	85	CYS
2	I	91	THR
2	I	106	GLU
2	I	107	ARG
2	I	108	GLU
2	I	111	GLU
2	I	113	THR
2	I	114	VAL
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	119	GLU
2	I	121	GLU
2	I	124	MET
2	I	131	THR
2	I	167	SER
2	I	170	VAL
2	I	219	GLN
2	I	233	ARG
2	I	235	ASN
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	306	THR
2	I	316	GLU
2	I	320	ASP
2	I	360	LEU
2	I	377	THR
2	I	379	GLU
2	I	400	VAL
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	453	ILE
2	I	470	ARG
2	I	484	LEU
2	I	486	THR
2	I	492	MET
2	I	503	LYS
2	I	510	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	518	ASN
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	542	ARG
2	I	550	VAL
2	I	558	VAL
2	I	575	LEU
2	I	600	THR
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	620	ASN
2	I	623	LEU
2	I	630	VAL
2	I	633	LEU
2	I	635	THR
2	I	639	LYS
2	I	648	ASP
2	I	657	THR
2	I	660	VAL
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	750	ILE
2	I	765	ILE
2	I	773	LEU
2	I	778	GLU
2	I	783	LEU
2	I	788	SER
2	I	791	LEU
2	I	800	MET
2	I	808	ASN
2	I	815	SER
2	I	817	LEU
2	I	826	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	830	THR
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	892	GLU
2	I	902	LEU
2	I	911	SER
2	I	946	LEU
2	I	979	LEU
2	I	984	VAL
2	I	1002	LEU
2	I	1014	LEU
2	I	1034	ARG
2	I	1037	THR
2	I	1046	VAL
2	I	1073	LYS
2	I	1079	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1119	MET
2	I	1134	GLN
2	I	1135	GLN
2	I	1136	GLN
2	I	1140	LYS
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1155	VAL
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1174	GLU
2	I	1176	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1204	LEU
2	I	1206	THR
2	I	1210	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1222	GLU
2	I	1239	VAL
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1254	VAL
2	I	1265	PHE
2	I	1275	VAL
2	I	1293	VAL
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	40	LYS
3	J	46	TYR
3	J	52	GLU
3	J	54	ASP
3	J	79	LYS
3	J	80	HIS
3	J	84	ILE
3	J	92	VAL
3	J	95	THR
3	J	96	LYS
3	J	97	VAL
3	J	98	ARG
3	J	106	GLU
3	J	137	ARG
3	J	159	ILE
3	J	169	LEU
3	J	175	GLU
3	J	203	GLU
3	J	217	LEU
3	J	218	THR
3	J	232	ASN
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	299	LEU
3	J	306	LEU
3	J	324	LEU
3	J	353	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	394	ILE
3	J	398	LYS
3	J	399	LYS
3	J	407	VAL
3	J	408	VAL
3	J	416	ILE
3	J	429	LEU
3	J	435	GLN
3	J	490	ILE
3	J	501	VAL
3	J	506	VAL
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	544	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	574	VAL
3	J	576	ARG
3	J	594	GLN
3	J	617	THR
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	682	VAL
3	J	683	ILE
3	J	685	ILE
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	703	THR
3	J	707	ILE
3	J	710	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	712	GLN
3	J	740	LEU
3	J	749	LYS
3	J	753	SER
3	J	754	ILE
3	J	757	THR
3	J	765	GLU
3	J	770	LEU
3	J	788	LEU
3	J	801	VAL
3	J	803	VAL
3	J	807	LEU
3	J	810	THR
3	J	823	THR
3	J	825	VAL
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	875	ASN
3	J	881	LYS
3	J	890	THR
3	J	897	HIS
3	J	898	CYS
3	J	907	HIS
3	J	908	ILE
3	J	918	ILE
3	J	950	ILE
3	J	951	GLN
3	J	960	LEU
3	J	963	VAL
3	J	967	VAL
3	J	972	LYS
3	J	987	GLU
3	J	994	SER
3	J	1027	VAL
3	J	1053	LEU
3	J	1062	LEU
3	J	1063	ASP
3	J	1064	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	J	1067	ARG
3	J	1079	LYS
3	J	1089	LEU
3	J	1113	VAL
3	J	1121	LEU
3	J	1155	ILE
3	J	1156	LEU
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1177	ILE
3	J	1178	THR
3	J	1186	TYR
3	J	1196	LEU
3	J	1202	GLU
3	J	1205	GLU
3	J	1221	LEU
3	J	1237	VAL
3	J	1251	LYS
3	J	1255	VAL
3	J	1266	ILE
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1290	ARG
3	J	1293	GLU
3	J	1298	VAL
3	J	1310	THR
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
3	J	1355	ARG
4	K	3	ARG
4	K	5	THR
4	K	6	VAL
4	K	13	ILE
4	K	18	ASP
4	K	28	ARG
4	K	39	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	47	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	130	VAL
5	L	154	GLU
5	L	166	VAL
5	L	230	VAL
5	L	247	GLU
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	335	GLU
5	L	341	LEU
5	L	344	LEU
5	L	357	GLN
5	L	362	ASN
5	L	395	THR
5	L	400	GLN
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	467	SER
5	L	469	GLN
5	L	470	MET
5	L	471	LEU
5	L	472	GLN
5	L	476	ARG
5	L	479	THR
5	L	481	GLU
5	L	482	GLU
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	494	ILE
5	L	496	LYS
5	L	499	LYS
5	L	500	ILE
5	L	511	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	515	GLU
5	L	516	ASP
5	L	529	GLU
5	L	530	LEU
5	L	540	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	575	GLU
5	L	578	LYS
5	L	580	PHE
5	L	581	ASP
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	601	PRO
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
5	L	608	ARG
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	117	HIS
1	B	66	HIS
2	C	69	GLN
2	C	139	ASN
2	C	513	GLN
2	C	620	ASN
2	C	628	HIS
2	C	659	GLN
2	C	677	ASN
2	C	688	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	799	ASN
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN
2	C	1209	GLN
2	C	1237	HIS
2	C	1268	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	200	GLN
3	D	340	GLN
3	D	469	HIS
3	D	488	ASN
3	D	489	ASN
3	D	669	GLN
3	D	702	GLN
3	D	739	GLN
3	D	897	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1227	HIS
3	D	1244	GLN
3	D	1259	GLN
3	D	1295	ASN
4	E	7	GLN
4	E	61	ASN
4	E	62	GLN
5	F	258	GLN
5	F	301	ASN
5	F	396	ASN
5	F	406	GLN
5	F	446	GLN
5	F	579	GLN
5	F	600	HIS
1	G	103	ASN
1	G	117	HIS
1	H	66	HIS
2	I	69	GLN
2	I	139	ASN
2	I	513	GLN
2	I	620	ASN
2	I	628	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	658	GLN
2	I	677	ASN
2	I	688	GLN
2	I	799	ASN
2	I	1017	GLN
2	I	1116	HIS
2	I	1136	GLN
2	I	1146	GLN
2	I	1209	GLN
2	I	1237	HIS
2	I	1314	GLN
3	J	200	GLN
3	J	469	HIS
3	J	488	ASN
3	J	489	ASN
3	J	669	GLN
3	J	702	GLN
3	J	739	GLN
3	J	897	HIS
3	J	910	ASN
3	J	954	ASN
3	J	1023	HIS
3	J	1049	GLN
3	J	1108	GLN
3	J	1227	HIS
3	J	1244	GLN
3	J	1259	GLN
3	J	1268	ASN
4	K	7	GLN
4	K	61	ASN
4	K	62	GLN
5	L	258	GLN
5	L	301	ASN
5	L	396	ASN
5	L	406	GLN
5	L	446	GLN
5	L	579	GLN
5	L	600	HIS

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	224/239 (93%)	-0.44	0 100 100	59, 91, 130, 167	0
1	B	220/239 (92%)	-0.21	1 (0%) 87 66	63, 125, 155, 166	0
1	G	228/239 (95%)	-0.30	1 (0%) 88 70	85, 121, 148, 164	0
1	H	217/239 (90%)	-0.22	0 100 100	90, 130, 156, 165	0
2	C	1340/1342 (99%)	-0.36	4 (0%) 90 74	33, 84, 134, 170	0
2	I	1340/1342 (99%)	-0.31	9 (0%) 84 60	48, 101, 149, 179	0
3	D	1166/1407 (82%)	-0.40	4 (0%) 90 74	28, 77, 137, 168	0
3	J	1325/1407 (94%)	-0.33	8 (0%) 85 63	40, 96, 152, 176	0
4	E	89/91 (97%)	-0.53	0 100 100	44, 84, 114, 133	0
4	K	79/91 (86%)	-0.38	0 100 100	63, 97, 136, 150	0
5	F	470/522 (90%)	-0.21	5 (1%) 78 51	53, 119, 159, 181	0
5	L	469/522 (89%)	-0.29	2 (0%) 88 70	61, 117, 159, 173	0
All	All	7167/7680 (93%)	-0.33	34 (0%) 87 66	28, 97, 150, 181	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1017	VAL	3.5
5	F	287	ILE	3.3
3	D	341	ASN	3.3
3	D	340	GLN	3.3
2	C	1000	LEU	3.1
3	J	1198	VAL	3.0
3	J	1121	LEU	3.0
3	J	1059	LEU	2.9
2	I	1050	VAL	2.9
5	F	601	PRO	2.9
2	I	1052	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	259	PHE	2.8
3	D	1281	GLU	2.5
2	I	1334	GLY	2.4
5	L	166	VAL	2.4
3	J	903	LEU	2.4
5	L	305	LEU	2.4
2	I	975	ILE	2.3
1	G	90	VAL	2.2
5	F	337	VAL	2.2
2	C	929	ILE	2.1
2	C	1001	GLY	2.1
2	I	882	ILE	2.1
2	C	489	PRO	2.1
5	F	598	LEU	2.1
3	J	1054	THR	2.1
2	I	931	VAL	2.1
3	J	913	GLU	2.1
2	I	865	LEU	2.0
1	B	90	VAL	2.0
2	I	928	VAL	2.0
3	J	1215	GLU	2.0
2	I	725	GLN	2.0
3	D	1270	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	1501	1/1	0.84	0.14	78,78,78,78	0
6	MG	J	1501	1/1	0.87	0.09	89,89,89,89	0
7	ZN	J	1503	1/1	0.90	0.24	316,316,316,316	0
7	ZN	J	1502	1/1	0.95	0.19	314,314,314,314	0
7	ZN	D	1503	1/1	0.97	0.14	114,114,114,114	0
7	ZN	D	1502	1/1	0.98	0.15	198,198,198,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.