



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:27 AM UTC

PDB ID : 2G4C / pdb_00002g4c
Title : Crystal Structure of human DNA polymerase gamma accessory subunit
Authors : Fan, L.; Farr, C.L.; Kaguni, L.S.; Tainer, J.A.
Deposited on : 2006-02-22
Resolution : 3.15 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

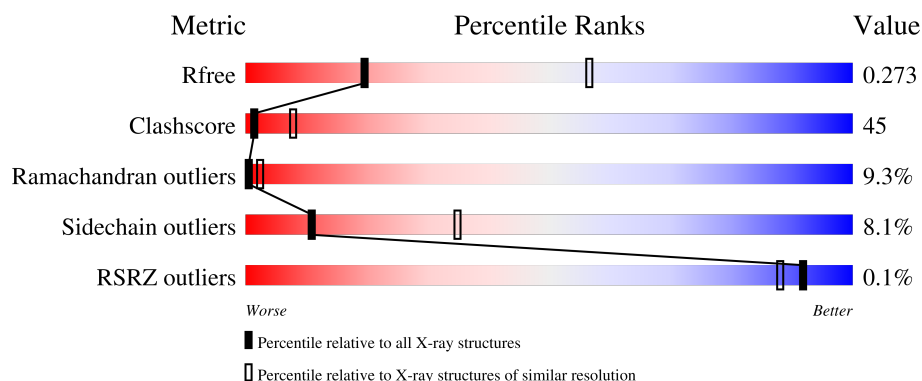
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	474	31% 41% 11% • 16%
1	B	474	31% 41% 11% • 16%
1	C	474	27% 44% 12% • 16%
1	D	474	29% 43% 11% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12847 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 polymerase gamma subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3202	2050	558	578	16			
1	B	397	Total	C	N	O	S	0	0	0
			3202	2050	558	578	16			
1	C	397	Total	C	N	O	S	0	0	0
			3206	2053	560	577	16			
1	D	397	Total	C	N	O	S	0	0	0
			3206	2053	560	577	16			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP Q9UHN1
A	13	ARG	-	cloning artifact	UNP Q9UHN1
A	14	GLY	-	cloning artifact	UNP Q9UHN1
A	15	SER	-	cloning artifact	UNP Q9UHN1
A	16	HIS	-	expression tag	UNP Q9UHN1
A	17	HIS	-	expression tag	UNP Q9UHN1
A	18	HIS	-	expression tag	UNP Q9UHN1
A	19	HIS	-	expression tag	UNP Q9UHN1
A	20	HIS	-	expression tag	UNP Q9UHN1
A	21	HIS	-	expression tag	UNP Q9UHN1
A	22	GLY	-	cloning artifact	UNP Q9UHN1
A	23	SER	-	cloning artifact	UNP Q9UHN1
A	24	THR	-	cloning artifact	UNP Q9UHN1
A	25	MET	-	cloning artifact	UNP Q9UHN1
A	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
B	12	MET	-	initiating methionine	UNP Q9UHN1
B	13	ARG	-	cloning artifact	UNP Q9UHN1
B	14	GLY	-	cloning artifact	UNP Q9UHN1
B	15	SER	-	cloning artifact	UNP Q9UHN1
B	16	HIS	-	expression tag	UNP Q9UHN1
B	17	HIS	-	expression tag	UNP Q9UHN1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	HIS	-	expression tag	UNP Q9UHN1
B	19	HIS	-	expression tag	UNP Q9UHN1
B	20	HIS	-	expression tag	UNP Q9UHN1
B	21	HIS	-	expression tag	UNP Q9UHN1
B	22	GLY	-	cloning artifact	UNP Q9UHN1
B	23	SER	-	cloning artifact	UNP Q9UHN1
B	24	THR	-	cloning artifact	UNP Q9UHN1
B	25	MET	-	cloning artifact	UNP Q9UHN1
B	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
C	12	MET	-	initiating methionine	UNP Q9UHN1
C	13	ARG	-	cloning artifact	UNP Q9UHN1
C	14	GLY	-	cloning artifact	UNP Q9UHN1
C	15	SER	-	cloning artifact	UNP Q9UHN1
C	16	HIS	-	expression tag	UNP Q9UHN1
C	17	HIS	-	expression tag	UNP Q9UHN1
C	18	HIS	-	expression tag	UNP Q9UHN1
C	19	HIS	-	expression tag	UNP Q9UHN1
C	20	HIS	-	expression tag	UNP Q9UHN1
C	21	HIS	-	expression tag	UNP Q9UHN1
C	22	GLY	-	cloning artifact	UNP Q9UHN1
C	23	SER	-	cloning artifact	UNP Q9UHN1
C	24	THR	-	cloning artifact	UNP Q9UHN1
C	25	MET	-	cloning artifact	UNP Q9UHN1
C	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
D	12	MET	-	initiating methionine	UNP Q9UHN1
D	13	ARG	-	cloning artifact	UNP Q9UHN1
D	14	GLY	-	cloning artifact	UNP Q9UHN1
D	15	SER	-	cloning artifact	UNP Q9UHN1
D	16	HIS	-	expression tag	UNP Q9UHN1
D	17	HIS	-	expression tag	UNP Q9UHN1
D	18	HIS	-	expression tag	UNP Q9UHN1
D	19	HIS	-	expression tag	UNP Q9UHN1
D	20	HIS	-	expression tag	UNP Q9UHN1
D	21	HIS	-	expression tag	UNP Q9UHN1
D	22	GLY	-	cloning artifact	UNP Q9UHN1
D	23	SER	-	cloning artifact	UNP Q9UHN1
D	24	THR	-	cloning artifact	UNP Q9UHN1
D	25	MET	-	cloning artifact	UNP Q9UHN1
D	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1

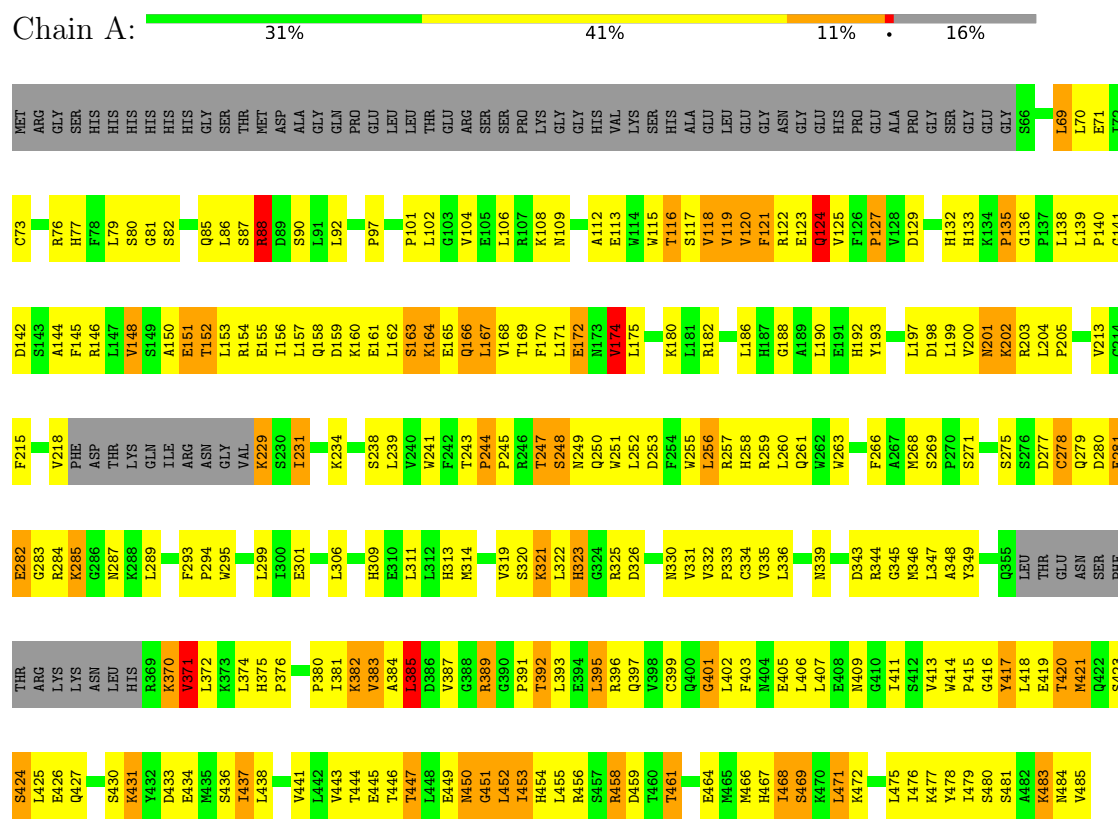
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total 12	O 12	0	0
2	B	5	Total 5	O 5	0	0
2	C	5	Total 5	O 5	0	0
2	D	9	Total 9	O 9	0	0

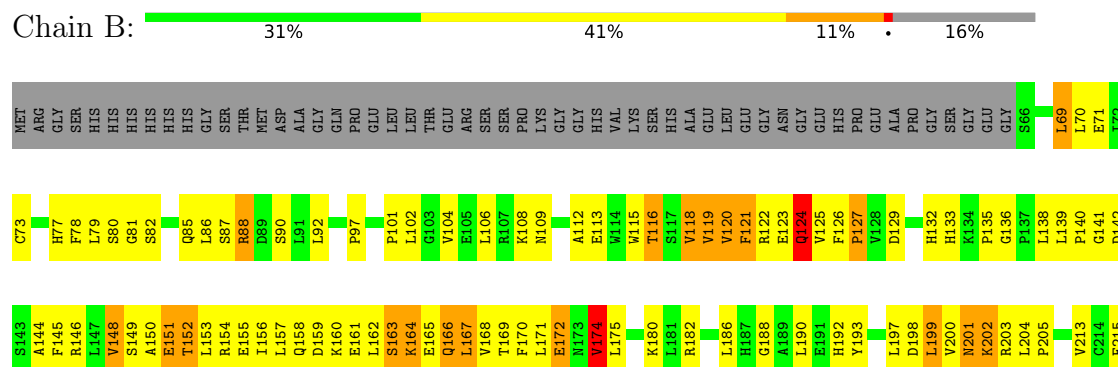
3 Residue-property plots

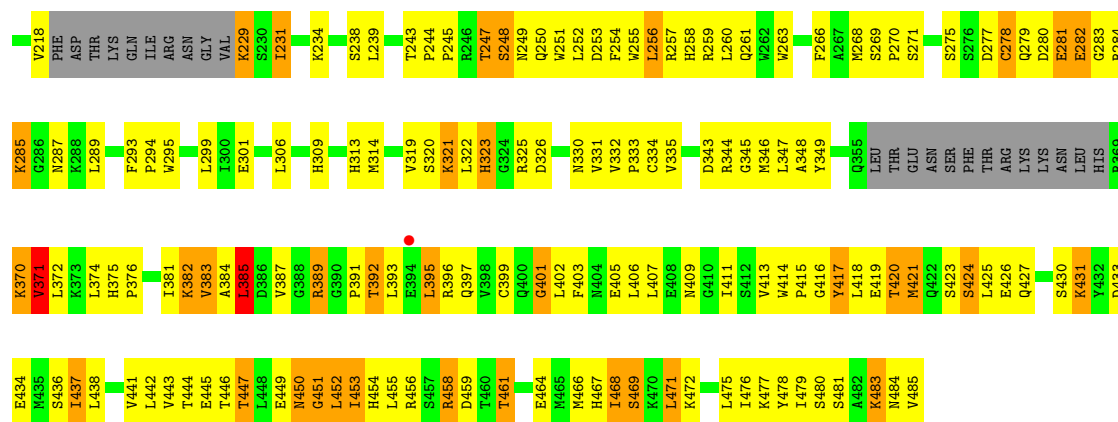
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 polymerase gamma subunit 2

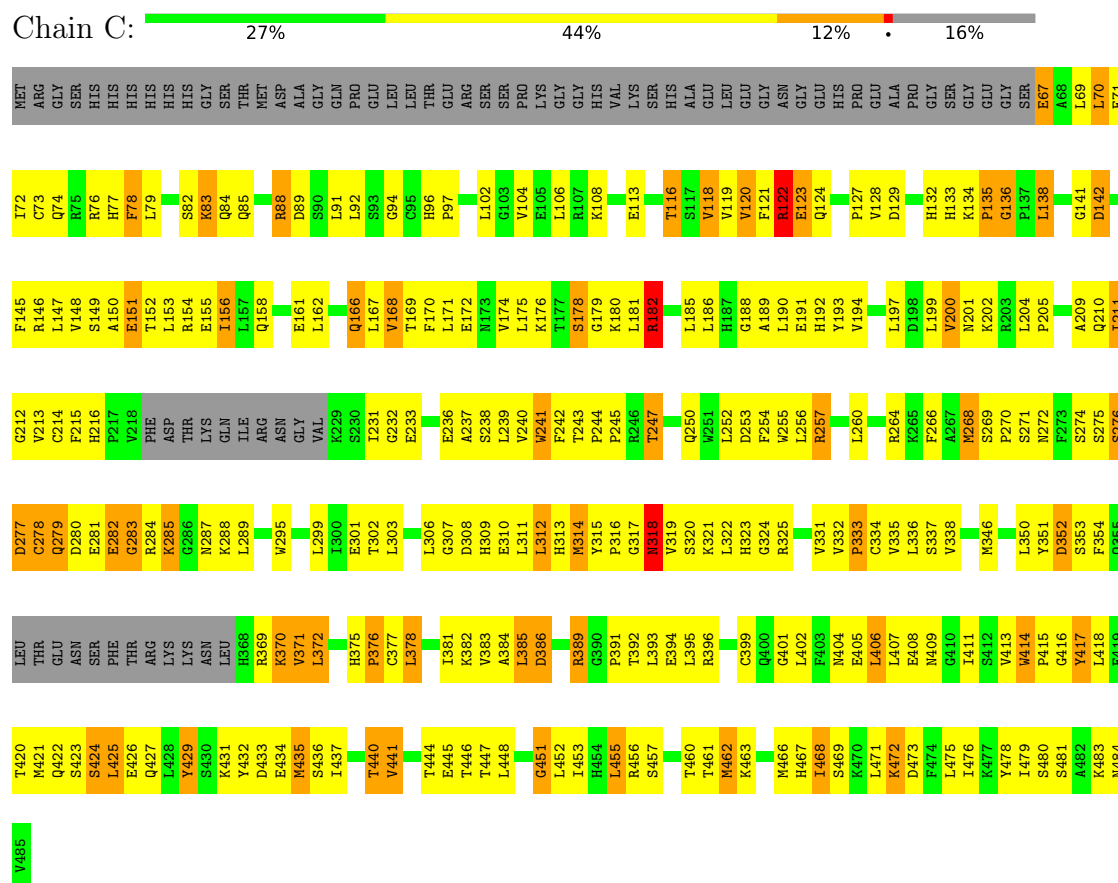


• Molecule 1: DNA polymerase gamma subunit 2

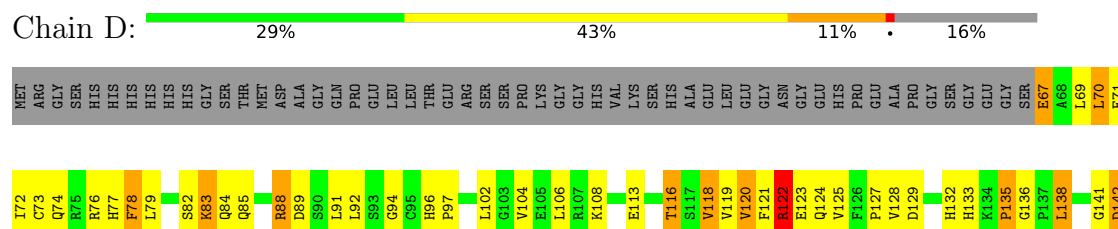




- Molecule 1: DNA polymerase gamma subunit 2



- Molecule 1: DNA polymerase gamma subunit 2



S423	S424	L425	E426	Q427	L428	Y429	S430	K431	Y432	D433	E434	M435	S436	I437	T440	V441	T444	E445	T446	T447	L448	G451	L452	L453	H454	L455	R456	S457	T460	T461	M462	K463	M466	H467	L468	S469	K470	L471	K472	D473	F474	L475	L476	K477	Y478	I479	S480	S481	A482	K483	M484	V485				
ASN	SER	PHE	THR	ARG	LYS	LYS	ASN	ASN	LEU	H368	R369	K370	V371	L372	H375	P376	G377	L378	I381	K382	V383	A384	L385	D386	R389	G390	P391	T392	L393	E394	L395	R396	Q399	Q400	G401	L402	F403	N404	E405	L406	L407	E408	N409	G410	I411	S412	V413	W414	P415	G416	Y417	L418	E419	T420	M421	Q422
D280	E281	E282	G283	R284	K285	G286	M287	K288	L289	W295	L299	I300	E301	T302	L303	L306	G307	D308	H309	E310	L311	L312	H313	M314	Y315	P316	G317	R318	V319	S320	K321	L322	H323	G324	R325	V331	V332	P333	C334	V335	L336	V338	M346	L350	Y351	D352	S353	F354	Q355	LEU	THR	GLU				
V213	C214	F215	H216	P217	V218	PHE	ASP	THR	LYS	GLN	ILE	ARG	ASN	GLY	VAL	K229	S230	I231	Q232	E233	E236	A237	S238	L239	W240	V241	F242	T243	P244	T247	Q250	W251	L252	D253	F254	W255	L256	R257	L260	R264	K265	F266	A267	M268	S269	P270	S271	N272	S275	S276	D277	C278	Q279			
R146	L147	V148	S149	A150	E151	T152	L153	R154	E155	I156	L157	Q158	D159	K160	E161	L162	S163	K164	E165	Q166	L167	V168	T169	F170	L171	E172	L175	S178	G179	K180	L181	R182	L186	A189	L190	E191	H192	Y193	V194	L197	D198	L199	V200	N201	K202	R203	L204	P205	A209	Q210	I211	G212				

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	101.79Å 101.79Å 170.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.15 50.00 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.15) 95.9 (50.00-3.17)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.285 0.222 , 0.273	Depositor DCC
R_{free} test set	1667 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 122.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.054 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12847	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/3278	1.07	25/4432 (0.6%)
1	B	0.49	0/3278	1.07	26/4432 (0.6%)
1	C	0.47	0/3283	1.05	19/4439 (0.4%)
1	D	0.46	0/3283	1.05	20/4439 (0.5%)
All	All	0.48	0/13122	1.06	90/17742 (0.5%)

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	GLN	N-CA-C	-10.88	99.72	113.43
1	D	124	GLN	N-CA-C	-10.61	100.06	113.43
1	B	124	GLN	N-CA-C	-10.41	98.00	113.61
1	A	124	GLN	N-CA-C	-10.23	98.26	113.61
1	C	283	GLY	N-CA-C	-8.68	98.56	110.80
1	D	283	GLY	N-CA-C	-8.52	98.83	111.19
1	A	88	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	C	279	GLN	N-CA-C	8.10	118.64	108.19
1	D	279	GLN	N-CA-C	7.92	118.42	108.45
1	A	88	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	A	152	THR	N-CA-C	-7.79	103.73	113.55
1	B	152	THR	N-CA-C	-7.74	103.80	113.55
1	B	119	VAL	N-CA-C	7.53	117.59	110.74
1	A	119	VAL	N-CA-C	7.41	117.48	110.74
1	A	401	GLY	N-CA-C	-6.91	106.09	114.66
1	A	244	PRO	CA-C-N	6.72	128.24	119.84
1	A	244	PRO	C-N-CA	6.72	128.24	119.84
1	B	279	GLN	N-CA-C	6.63	118.64	108.42
1	B	244	PRO	CA-C-N	6.61	128.10	119.84
1	B	244	PRO	C-N-CA	6.61	128.10	119.84
1	B	401	GLY	N-CA-C	-6.61	106.46	114.66
1	A	279	GLN	N-CA-C	6.49	118.42	108.42
1	A	345	GLY	N-CA-C	-6.47	104.70	113.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	GLU	N-CA-C	-6.46	104.09	112.23
1	B	345	GLY	N-CA-C	-6.45	104.73	113.37
1	B	169	THR	N-CA-C	-6.42	105.75	113.97
1	A	169	THR	N-CA-C	-6.40	105.78	113.97
1	B	88	ARG	CD-NE-CZ	6.39	133.35	124.40
1	B	426	GLU	N-CA-C	-6.36	104.22	112.23
1	B	69	LEU	N-CA-C	-6.33	105.21	113.12
1	B	256	LEU	N-CA-C	-6.32	104.39	111.28
1	A	69	LEU	N-CA-C	-6.28	105.28	113.12
1	A	127	PRO	N-CA-C	-6.18	100.75	111.32
1	A	88	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	255	TRP	N-CA-C	6.12	117.95	111.28
1	B	88	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	A	256	LEU	N-CA-C	-6.09	104.64	111.28
1	A	335	VAL	N-CA-C	6.08	116.12	106.88
1	B	321	LYS	N-CA-C	-6.08	106.02	113.50
1	A	321	LYS	N-CA-C	-6.06	106.04	113.50
1	D	414	TRP	CA-C-N	6.01	127.36	119.84
1	D	414	TRP	C-N-CA	6.01	127.36	119.84
1	B	255	TRP	N-CA-C	6.00	117.83	111.28
1	C	414	TRP	CA-C-N	5.99	127.33	119.84
1	C	414	TRP	C-N-CA	5.99	127.33	119.84
1	C	151	GLU	N-CA-C	-5.92	106.03	113.20
1	D	151	GLU	N-CA-C	-5.91	106.06	113.20
1	D	378	LEU	N-CA-C	-5.90	107.31	114.75
1	B	127	PRO	N-CA-C	-5.87	101.29	111.32
1	C	282	GLU	N-CA-C	-5.79	106.55	113.21
1	D	382	LYS	N-CA-C	5.78	119.44	112.38
1	D	268	MET	N-CA-C	-5.73	104.41	111.40
1	D	282	GLU	N-CA-C	-5.67	106.41	113.15
1	C	378	LEU	N-CA-C	-5.66	107.62	114.75
1	D	178	SER	N-CA-C	5.65	118.42	110.23
1	A	458	ARG	N-CA-C	-5.61	106.57	113.41
1	B	78	PHE	N-CA-C	-5.59	103.01	111.56
1	A	371	VAL	N-CA-C	5.57	120.93	109.34
1	B	371	VAL	N-CA-C	5.56	120.90	109.34
1	B	458	ARG	N-CA-C	-5.54	106.65	113.41
1	C	194	VAL	N-CA-C	5.53	116.17	110.36
1	C	78	PHE	N-CA-C	-5.49	105.62	112.93
1	C	178	SER	N-CA-C	5.49	118.19	110.23
1	D	169	THR	N-CA-C	-5.48	105.73	112.90
1	C	425	LEU	N-CA-C	-5.45	106.68	113.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333	PRO	N-CA-C	5.45	119.12	111.33
1	C	372	LEU	N-CA-C	-5.45	100.30	108.96
1	D	425	LEU	N-CA-C	-5.44	106.70	113.55
1	C	182	ARG	N-CA-C	5.43	117.90	110.24
1	C	169	THR	N-CA-C	-5.41	105.81	112.90
1	A	447	THR	N-CA-C	-5.39	106.75	113.55
1	D	372	LEU	N-CA-C	-5.37	100.42	108.96
1	D	182	ARG	N-CA-C	5.36	117.79	110.24
1	B	326	ASP	N-CA-C	-5.33	105.05	112.45
1	B	447	THR	N-CA-C	-5.32	106.84	113.55
1	B	172	GLU	N-CA-C	-5.32	106.84	113.38
1	C	268	MET	N-CA-C	-5.31	104.39	111.24
1	B	88	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	C	382	LYS	N-CA-C	5.30	119.00	112.54
1	A	172	GLU	N-CA-C	-5.25	106.92	113.38
1	B	238	SER	N-CA-C	5.23	117.60	108.76
1	D	435	MET	N-CA-C	-5.23	106.86	113.18
1	D	78	PHE	N-CA-C	-5.22	105.99	112.93
1	D	194	VAL	N-CA-C	5.21	115.83	110.36
1	D	333	PRO	N-CA-C	5.21	118.78	111.33
1	A	326	ASP	N-CA-C	-5.17	105.26	112.45
1	B	335	VAL	N-CA-C	5.14	114.70	106.88
1	A	238	SER	N-CA-C	5.10	117.38	108.76
1	D	441	VAL	N-CA-C	5.09	115.92	108.58
1	C	435	MET	N-CA-C	-5.08	107.03	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3202	0	3209	295	0
1	B	3202	0	3209	288	0
1	C	3206	0	3211	309	0
1	D	3206	0	3211	298	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	9	0	0	0	0
All	All	12847	0	12840	1143	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ASN:HD22	1:B:452:LEU:HD23	1.11	1.08
1:A:450:ASN:HD22	1:A:452:LEU:HD23	1.11	1.07
1:A:88:ARG:H	1:A:88:ARG:HD2	1.24	0.98
1:D:306:LEU:HB2	1:D:335:VAL:HG23	1.46	0.98
1:C:306:LEU:HB2	1:C:335:VAL:HG23	1.43	0.95
1:C:73:CYS:HB3	1:C:79:LEU:HD23	1.48	0.94
1:D:73:CYS:HB3	1:D:79:LEU:HD23	1.49	0.94
1:A:158:GLN:HG2	1:A:159:ASP:H	1.37	0.89
1:C:260:LEU:HD13	1:C:289:LEU:HD22	1.56	0.87
1:D:260:LEU:HD13	1:D:289:LEU:HD22	1.55	0.87
1:C:96:HIS:HB2	1:C:97:PRO:HD2	1.56	0.87
1:B:158:GLN:HG2	1:B:159:ASP:H	1.38	0.86
1:A:87:SER:HB2	1:A:90:SER:HB2	1.57	0.86
1:B:87:SER:HB2	1:B:90:SER:HB2	1.56	0.86
1:B:257:ARG:O	1:B:261:GLN:HG3	1.73	0.86
1:B:257:ARG:HB3	1:C:316:PRO:HG3	1.58	0.85
1:D:385:LEU:HB3	1:D:441:VAL:HG22	1.58	0.85
1:B:231:ILE:HD12	1:B:231:ILE:H	1.40	0.85
1:A:231:ILE:H	1:A:231:ILE:HD12	1.39	0.85
1:D:96:HIS:HB2	1:D:97:PRO:HD2	1.56	0.84
1:A:257:ARG:O	1:A:261:GLN:HG3	1.76	0.84
1:C:385:LEU:HB3	1:C:441:VAL:HG22	1.60	0.84
1:A:88:ARG:H	1:A:88:ARG:CD	1.91	0.84
1:C:77:HIS:O	1:C:102:LEU:HB2	1.78	0.83
1:B:450:ASN:HD22	1:B:452:LEU:CD2	1.91	0.83
1:A:201:ASN:HD22	1:A:203:ARG:HH22	1.23	0.82
1:B:201:ASN:HD22	1:B:203:ARG:HH22	1.23	0.82
1:B:401:GLY:O	1:B:405:GLU:HB2	1.80	0.82
1:A:450:ASN:HD22	1:A:452:LEU:CD2	1.91	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ARG:HH22	1:C:158:GLN:NE2	1.77	0.82
1:D:153:LEU:HD12	1:D:170:PHE:HE2	1.45	0.82
1:C:153:LEU:HD12	1:C:170:PHE:HE2	1.44	0.81
1:A:231:ILE:HD13	1:C:133:HIS:NE2	1.95	0.81
1:A:401:GLY:O	1:A:405:GLU:HB2	1.81	0.81
1:B:437:ILE:HG22	1:B:438:LEU:H	1.45	0.81
1:D:253:ASP:O	1:D:257:ARG:HG2	1.81	0.81
1:C:253:ASP:O	1:C:257:ARG:HG2	1.81	0.81
1:D:154:ARG:HH22	1:D:158:GLN:NE2	1.77	0.81
1:A:450:ASN:ND2	1:A:452:LEU:HD23	1.95	0.80
1:D:77:HIS:O	1:D:102:LEU:HB2	1.80	0.80
1:A:393:LEU:O	1:A:397:GLN:HG2	1.81	0.80
1:B:231:ILE:HD13	1:D:133:HIS:NE2	1.97	0.80
1:A:437:ILE:HG22	1:A:438:LEU:H	1.46	0.79
1:B:161:GLU:HG2	1:B:166:GLN:HG3	1.64	0.79
1:B:393:LEU:O	1:B:397:GLN:HG2	1.82	0.79
1:A:385:LEU:HD23	1:A:385:LEU:O	1.80	0.79
1:C:383:VAL:HG13	1:C:413:VAL:HG22	1.65	0.79
1:B:450:ASN:ND2	1:B:452:LEU:HD23	1.95	0.78
1:B:385:LEU:HD23	1:B:385:LEU:O	1.81	0.78
1:D:254:PHE:O	1:D:257:ARG:HG3	1.82	0.78
1:D:260:LEU:HD22	1:D:275:SER:HB3	1.66	0.78
1:A:161:GLU:HG2	1:A:166:GLN:HG3	1.64	0.78
1:C:254:PHE:O	1:C:257:ARG:HG3	1.83	0.77
1:C:260:LEU:HD22	1:C:275:SER:HB3	1.66	0.77
1:A:389:ARG:H	1:A:389:ARG:HD2	1.50	0.77
1:A:113:GLU:HG2	1:A:266:PHE:CZ	2.20	0.77
1:D:383:VAL:HG13	1:D:413:VAL:HG22	1.67	0.77
1:A:201:ASN:HD22	1:A:203:ARG:NH2	1.82	0.76
1:B:201:ASN:HD22	1:B:203:ARG:NH2	1.82	0.76
1:B:323:HIS:HB2	1:B:331:VAL:C	2.11	0.76
1:B:113:GLU:HG2	1:B:266:PHE:CZ	2.20	0.76
1:B:73:CYS:HB3	1:B:79:LEU:HD23	1.68	0.75
1:D:279:GLN:HB2	1:D:284:ARG:HG3	1.68	0.75
1:C:153:LEU:HD12	1:C:170:PHE:CE2	2.21	0.75
1:A:323:HIS:HB2	1:A:331:VAL:C	2.11	0.75
1:C:279:GLN:HB2	1:C:284:ARG:HG3	1.68	0.75
1:B:455:LEU:H	1:B:455:LEU:HD23	1.52	0.75
1:A:73:CYS:HB3	1:A:79:LEU:HD23	1.68	0.75
1:B:389:ARG:H	1:B:389:ARG:HD2	1.51	0.75
1:D:153:LEU:HD12	1:D:170:PHE:CE2	2.21	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HD12	1:A:231:ILE:N	2.02	0.74
1:B:254:PHE:CE1	1:C:316:PRO:HB3	2.23	0.74
1:A:455:LEU:HD23	1:A:455:LEU:H	1.53	0.73
1:D:451:GLY:C	1:D:452:LEU:HD22	2.14	0.73
1:A:129:ASP:HB2	1:C:104:VAL:HG22	1.71	0.73
1:B:231:ILE:HD12	1:B:231:ILE:N	2.03	0.73
1:B:441:VAL:HG11	1:B:471:LEU:HD21	1.71	0.73
1:D:204:LEU:HD21	1:D:324:GLY:HA3	1.72	0.72
1:B:437:ILE:HG22	1:B:438:LEU:N	2.05	0.72
1:C:451:GLY:C	1:C:452:LEU:HD22	2.14	0.72
1:A:139:LEU:HB2	1:A:140:PRO:HD2	1.71	0.72
1:B:200:VAL:O	1:B:202:LYS:N	2.23	0.72
1:B:280:ASP:HA	1:B:283:GLY:O	1.90	0.72
1:C:88:ARG:HD2	1:C:89:ASP:H	1.54	0.72
1:A:437:ILE:HG22	1:A:438:LEU:N	2.05	0.72
1:B:229:LYS:HB2	1:B:229:LYS:HZ2	1.55	0.71
1:A:441:VAL:HG11	1:A:471:LEU:HD21	1.72	0.71
1:D:76:ARG:NH2	1:D:431:LYS:HG3	2.05	0.71
1:D:254:PHE:HA	1:D:257:ARG:HD2	1.72	0.71
1:A:201:ASN:O	1:A:202:LYS:HB2	1.90	0.71
1:B:139:LEU:HB2	1:B:140:PRO:HD2	1.71	0.71
1:D:395:LEU:HD21	1:D:444:THR:HA	1.73	0.71
1:B:129:ASP:HB2	1:D:104:VAL:HG22	1.72	0.71
1:C:241:TRP:CD1	1:C:255:TRP:HE1	2.09	0.71
1:D:88:ARG:HD2	1:D:89:ASP:H	1.54	0.71
1:C:306:LEU:HB2	1:C:335:VAL:CG2	2.21	0.71
1:B:201:ASN:O	1:B:202:LYS:HB2	1.89	0.70
1:A:280:ASP:HA	1:A:283:GLY:O	1.91	0.70
1:C:76:ARG:NH2	1:C:431:LYS:HG3	2.06	0.70
1:C:395:LEU:HD21	1:C:444:THR:HA	1.72	0.70
1:D:76:ARG:HH21	1:D:431:LYS:HG3	1.56	0.70
1:B:204:LEU:HD13	1:B:333:PRO:HB3	1.72	0.70
1:D:241:TRP:CD1	1:D:255:TRP:HE1	2.09	0.70
1:C:204:LEU:HD21	1:C:324:GLY:HA3	1.74	0.70
1:B:231:ILE:HD13	1:D:133:HIS:HE2	1.55	0.69
1:C:146:ARG:HH11	1:C:146:ARG:HG2	1.57	0.69
1:A:186:LEU:HD11	1:A:306:LEU:HD11	1.75	0.69
1:B:409:ASN:ND2	1:B:472:LYS:HD2	2.07	0.69
1:A:200:VAL:O	1:A:202:LYS:N	2.24	0.69
1:A:229:LYS:HZ2	1:A:229:LYS:HB2	1.58	0.68
1:C:455:LEU:C	1:C:455:LEU:HD12	2.18	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG12	1:A:175:LEU:N	2.09	0.68
1:D:256:LEU:HD22	1:D:287:ASN:CG	2.18	0.68
1:D:260:LEU:HD13	1:D:289:LEU:CD2	2.23	0.68
1:D:306:LEU:HB2	1:D:335:VAL:CG2	2.23	0.68
1:A:284:ARG:O	1:A:285:LYS:HB2	1.92	0.68
1:B:186:LEU:HD11	1:B:306:LEU:HD11	1.76	0.68
1:C:254:PHE:HA	1:C:257:ARG:HD2	1.73	0.68
1:D:455:LEU:C	1:D:455:LEU:HD12	2.18	0.68
1:B:284:ARG:O	1:B:285:LYS:HB2	1.92	0.68
1:C:256:LEU:HD22	1:C:287:ASN:CG	2.19	0.68
1:A:409:ASN:ND2	1:A:472:LYS:HD2	2.09	0.68
1:B:174:VAL:HG12	1:B:175:LEU:N	2.09	0.68
1:C:199:LEU:O	1:C:200:VAL:HG13	1.93	0.67
1:A:471:LEU:HD12	1:A:471:LEU:O	1.93	0.67
1:C:76:ARG:HG3	1:C:434:GLU:HB3	1.76	0.67
1:D:307:GLY:HA2	1:D:334:CYS:SG	2.34	0.67
1:C:76:ARG:HH21	1:C:431:LYS:HG3	1.59	0.67
1:D:281:GLU:HG2	1:D:282:GLU:H	1.60	0.67
1:D:69:LEU:HB2	1:D:354:PHE:CD2	2.30	0.67
1:A:204:LEU:HD13	1:A:333:PRO:HB3	1.74	0.67
1:B:81:GLY:HA3	1:B:97:PRO:HG3	1.77	0.67
1:B:471:LEU:O	1:B:471:LEU:HD12	1.94	0.67
1:C:260:LEU:HD13	1:C:289:LEU:CD2	2.25	0.67
1:B:277:ASP:O	1:B:278:CYS:HB3	1.93	0.67
1:C:69:LEU:HB2	1:C:354:PHE:CD2	2.29	0.67
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.60	0.67
1:B:372:LEU:HD13	1:B:434:GLU:O	1.95	0.66
1:A:277:ASP:O	1:A:278:CYS:HB3	1.94	0.66
1:D:202:LYS:O	1:D:325:ARG:N	2.27	0.66
1:A:82:SER:HB2	1:A:85:GLN:HG2	1.76	0.66
1:B:453:ILE:HG12	1:B:468:ILE:HB	1.78	0.66
1:D:370:LYS:O	1:D:371:VAL:HG12	1.95	0.66
1:D:456:ARG:HG2	1:D:457:SER:H	1.61	0.66
1:A:81:GLY:HA3	1:A:97:PRO:HG3	1.78	0.66
1:C:154:ARG:HH22	1:C:158:GLN:HE21	1.42	0.66
1:C:281:GLU:HG2	1:C:282:GLU:H	1.59	0.66
1:D:147:LEU:HD21	1:D:181:LEU:HD21	1.75	0.66
1:C:370:LYS:O	1:C:371:VAL:HG12	1.96	0.66
1:C:456:ARG:HG2	1:C:457:SER:H	1.60	0.65
1:A:466:MET:HE1	1:A:471:LEU:HD13	1.78	0.65
1:B:145:PHE:HD1	1:D:149:SER:HA	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:VAL:HG23	1:B:433:ASP:HB3	1.78	0.65
1:D:154:ARG:HH22	1:D:158:GLN:HE21	1.42	0.65
1:D:467:HIS:C	1:D:469:SER:H	2.05	0.65
1:A:157:LEU:HD21	1:C:171:LEU:HB3	1.79	0.65
1:D:76:ARG:HG3	1:D:434:GLU:HB3	1.78	0.65
1:B:82:SER:HB2	1:B:85:GLN:HG2	1.77	0.65
1:C:307:GLY:HA2	1:C:334:CYS:SG	2.37	0.65
1:B:323:HIS:HB3	1:B:332:VAL:HA	1.78	0.65
1:B:157:LEU:HD21	1:D:171:LEU:HB3	1.79	0.65
1:B:451:GLY:C	1:B:452:LEU:HD22	2.22	0.65
1:C:202:LYS:O	1:C:325:ARG:N	2.26	0.65
1:A:293:PHE:O	1:A:295:TRP:N	2.30	0.64
1:C:147:LEU:HD21	1:C:181:LEU:HD21	1.77	0.64
1:B:466:MET:HE1	1:B:471:LEU:HD13	1.78	0.64
1:B:293:PHE:O	1:B:295:TRP:N	2.30	0.64
1:C:445:GLU:C	1:C:447:THR:H	2.05	0.64
1:A:371:VAL:HG23	1:A:433:ASP:HB3	1.79	0.64
1:A:323:HIS:HB3	1:A:332:VAL:HA	1.79	0.64
1:B:445:GLU:C	1:B:447:THR:H	2.05	0.64
1:C:467:HIS:C	1:C:469:SER:H	2.05	0.64
1:A:145:PHE:HD1	1:C:149:SER:HA	1.62	0.64
1:A:229:LYS:HZ2	1:A:229:LYS:CB	2.11	0.63
1:C:308:ASP:HB2	1:C:312:LEU:HD12	1.81	0.63
1:D:104:VAL:O	1:D:108:LYS:HB2	1.98	0.63
1:A:451:GLY:C	1:A:452:LEU:HD22	2.22	0.63
1:D:199:LEU:O	1:D:200:VAL:HG13	1.98	0.63
1:B:293:PHE:C	1:B:295:TRP:H	2.06	0.63
1:C:479:ILE:C	1:C:481:SER:H	2.06	0.63
1:D:479:ILE:C	1:D:481:SER:H	2.06	0.63
1:D:116:THR:HA	1:D:120:VAL:HG23	1.80	0.63
1:D:445:GLU:C	1:D:447:THR:H	2.05	0.63
1:B:163:SER:O	1:B:164:LYS:HG3	1.99	0.63
1:A:293:PHE:C	1:A:295:TRP:H	2.06	0.63
1:A:395:LEU:HD21	1:A:444:THR:C	2.24	0.63
1:A:445:GLU:C	1:A:447:THR:H	2.05	0.63
1:D:202:LYS:N	1:D:202:LYS:HD2	2.14	0.63
1:A:266:PHE:HA	1:A:375:HIS:HD2	1.62	0.62
1:A:163:SER:O	1:A:164:LYS:HG3	1.98	0.62
1:A:453:ILE:HG12	1:A:468:ILE:HB	1.81	0.62
1:A:133:HIS:CD2	1:C:231:ILE:HD12	2.33	0.62
1:A:372:LEU:HD13	1:A:434:GLU:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:THR:HA	1:C:120:VAL:HG23	1.81	0.62
1:C:243:THR:HB	1:C:244:PRO:HD2	1.81	0.62
1:D:385:LEU:CB	1:D:441:VAL:HG22	2.29	0.62
1:A:385:LEU:HB2	1:A:441:VAL:CG2	2.30	0.62
1:C:121:PHE:O	1:C:122:ARG:C	2.42	0.62
1:D:82:SER:C	1:D:84:GLN:H	2.07	0.62
1:D:308:ASP:HB2	1:D:312:LEU:HD12	1.81	0.62
1:A:162:LEU:C	1:A:164:LYS:H	2.07	0.62
1:B:266:PHE:HA	1:B:375:HIS:HD2	1.65	0.62
1:C:231:ILE:CG2	1:C:232:GLY:N	2.63	0.62
1:A:375:HIS:ND1	1:A:376:PRO:HD2	2.14	0.62
1:C:202:LYS:HD2	1:C:202:LYS:N	2.14	0.62
1:C:427:GLN:O	1:C:431:LYS:HE3	2.00	0.62
1:A:395:LEU:HD11	1:A:443:VAL:O	2.00	0.62
1:D:331:VAL:HG22	1:D:332:VAL:N	2.15	0.62
1:A:284:ARG:O	1:A:285:LYS:CB	2.48	0.62
1:D:121:PHE:O	1:D:122:ARG:C	2.43	0.62
1:D:331:VAL:HG22	1:D:332:VAL:H	1.66	0.61
1:B:395:LEU:HD21	1:B:444:THR:C	2.25	0.61
1:B:385:LEU:HA	1:B:441:VAL:O	1.99	0.61
1:C:190:LEU:C	1:C:192:HIS:H	2.08	0.61
1:B:395:LEU:HD11	1:B:443:VAL:O	2.00	0.61
1:B:403:PHE:HE1	1:B:415:PRO:HD3	1.65	0.61
1:B:269:SER:C	1:B:271:SER:H	2.07	0.61
1:B:344:ARG:HA	1:B:347:LEU:HD12	1.80	0.61
1:C:82:SER:C	1:C:84:GLN:H	2.07	0.61
1:D:113:GLU:HG2	1:D:266:PHE:CZ	2.36	0.61
1:A:417:TYR:CD1	1:A:418:LEU:HG	2.35	0.61
1:C:307:GLY:O	1:C:335:VAL:HG22	2.01	0.61
1:D:88:ARG:CD	1:D:89:ASP:H	2.14	0.61
1:D:372:LEU:HD22	1:D:434:GLU:O	2.00	0.61
1:A:344:ARG:HA	1:A:347:LEU:HD12	1.81	0.61
1:C:372:LEU:HD22	1:C:434:GLU:O	2.01	0.61
1:B:162:LEU:C	1:B:164:LYS:H	2.08	0.61
1:B:229:LYS:HZ2	1:B:229:LYS:CB	2.13	0.61
1:D:190:LEU:C	1:D:192:HIS:H	2.07	0.61
1:A:129:ASP:HB2	1:C:104:VAL:CG2	2.31	0.60
1:B:284:ARG:O	1:B:285:LYS:CB	2.48	0.60
1:B:323:HIS:HB2	1:B:331:VAL:O	2.00	0.60
1:C:385:LEU:CB	1:C:441:VAL:HG22	2.29	0.60
1:B:385:LEU:HB2	1:B:441:VAL:CG2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:SER:O	1:A:433:ASP:HB2	2.01	0.60
1:B:259:ARG:HE	1:B:301:GLU:CD	2.08	0.60
1:C:113:GLU:HG2	1:C:266:PHE:CZ	2.36	0.60
1:C:303:LEU:HG	1:C:338:VAL:HG13	1.83	0.60
1:D:150:ALA:O	1:D:154:ARG:HB2	2.02	0.60
1:A:174:VAL:HG11	1:C:153:LEU:HD21	1.84	0.60
1:B:133:HIS:CD2	1:D:231:ILE:HD12	2.36	0.60
1:B:466:MET:CE	1:B:471:LEU:HD22	2.32	0.60
1:C:88:ARG:CD	1:C:89:ASP:H	2.14	0.60
1:D:427:GLN:O	1:D:431:LYS:HE3	2.01	0.60
1:A:420:THR:HG23	1:A:421:MET:H	1.67	0.60
1:B:417:TYR:CD1	1:B:418:LEU:HG	2.36	0.60
1:C:104:VAL:O	1:C:108:LYS:HB2	2.00	0.60
1:A:385:LEU:HA	1:A:441:VAL:O	2.01	0.60
1:C:135:PRO:O	1:C:138:LEU:HD21	2.02	0.60
1:C:155:GLU:O	1:C:156:ILE:HG13	2.02	0.60
1:D:307:GLY:O	1:D:335:VAL:HG22	2.01	0.60
1:A:266:PHE:HA	1:A:375:HIS:CD2	2.37	0.59
1:C:456:ARG:CG	1:C:457:SER:H	2.15	0.59
1:A:259:ARG:HE	1:A:301:GLU:CD	2.10	0.59
1:A:466:MET:CE	1:A:471:LEU:HD22	2.32	0.59
1:B:129:ASP:HB2	1:D:104:VAL:CG2	2.32	0.59
1:A:269:SER:C	1:A:271:SER:H	2.09	0.59
1:A:420:THR:HG23	1:A:421:MET:N	2.17	0.59
1:A:392:THR:HG22	1:A:393:LEU:N	2.16	0.59
1:B:420:THR:HG23	1:B:421:MET:H	1.67	0.59
1:C:383:VAL:CG1	1:C:413:VAL:HG22	2.32	0.59
1:D:243:THR:HB	1:D:244:PRO:HD2	1.83	0.59
1:D:456:ARG:CG	1:D:457:SER:H	2.15	0.59
1:B:392:THR:HG22	1:B:393:LEU:N	2.16	0.59
1:C:331:VAL:HG22	1:C:332:VAL:N	2.16	0.59
1:B:434:GLU:C	1:B:436:SER:H	2.10	0.59
1:C:331:VAL:HG22	1:C:332:VAL:H	1.67	0.59
1:C:150:ALA:O	1:C:154:ARG:HB2	2.02	0.59
1:D:204:LEU:HD13	1:D:333:PRO:HB3	1.85	0.59
1:D:303:LEU:HG	1:D:338:VAL:HG13	1.85	0.59
1:B:430:SER:O	1:B:433:ASP:HB2	2.02	0.59
1:C:96:HIS:HB2	1:C:97:PRO:CD	2.30	0.59
1:A:434:GLU:C	1:A:436:SER:H	2.09	0.58
1:B:266:PHE:HA	1:B:375:HIS:CD2	2.38	0.58
1:C:275:SER:O	1:C:276:SER:HB3	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:HIS:ND1	1:B:376:PRO:HD2	2.17	0.58
1:D:135:PRO:O	1:D:138:LEU:HD21	2.04	0.58
1:D:254:PHE:HA	1:D:257:ARG:CD	2.32	0.58
1:B:371:VAL:HG23	1:B:433:ASP:CB	2.34	0.58
1:B:420:THR:HG23	1:B:421:MET:N	2.17	0.58
1:B:165:GLU:HA	1:B:165:GLU:OE1	2.03	0.58
1:D:155:GLU:O	1:D:156:ILE:HG13	2.02	0.58
1:D:471:LEU:O	1:D:475:LEU:HG	2.04	0.58
1:A:152:THR:O	1:A:156:ILE:HG13	2.04	0.58
1:B:370:LYS:O	1:B:371:VAL:HG12	2.04	0.58
1:C:204:LEU:HD13	1:C:333:PRO:HB3	1.86	0.58
1:D:231:ILE:CG2	1:D:232:GLY:N	2.67	0.58
1:D:275:SER:O	1:D:276:SER:HB3	2.03	0.58
1:C:106:LEU:HD23	1:C:346:MET:SD	2.44	0.58
1:C:231:ILE:HG22	1:C:232:GLY:N	2.16	0.58
1:B:452:LEU:CD1	1:B:467:HIS:HA	2.34	0.58
1:C:254:PHE:HA	1:C:257:ARG:CD	2.33	0.58
1:A:325:ARG:NH1	1:A:330:ASN:HD21	2.02	0.58
1:A:403:PHE:HE1	1:A:415:PRO:HD3	1.67	0.58
1:C:471:LEU:O	1:C:475:LEU:HG	2.04	0.58
1:D:146:ARG:HB3	1:D:178:SER:OG	2.03	0.58
1:A:452:LEU:CD1	1:A:467:HIS:HA	2.34	0.57
1:C:116:THR:HA	1:C:120:VAL:CG2	2.34	0.57
1:C:284:ARG:O	1:C:285:LYS:HB2	2.04	0.57
1:B:260:LEU:HD13	1:B:289:LEU:HD12	1.86	0.57
1:C:371:VAL:HG23	1:C:433:ASP:HB3	1.86	0.57
1:A:323:HIS:HB2	1:A:331:VAL:O	2.03	0.57
1:D:462:MET:O	1:D:463:LYS:HG3	2.04	0.57
1:A:371:VAL:HG23	1:A:433:ASP:CB	2.35	0.57
1:B:152:THR:O	1:B:156:ILE:HG13	2.04	0.57
1:B:467:HIS:O	1:B:469:SER:N	2.38	0.57
1:C:385:LEU:HD12	1:C:385:LEU:O	2.04	0.57
1:C:462:MET:O	1:C:463:LYS:HG3	2.05	0.57
1:A:165:GLU:OE1	1:A:165:GLU:HA	2.04	0.57
1:A:403:PHE:O	1:A:407:LEU:HG	2.04	0.57
1:B:257:ARG:HH21	1:B:257:ARG:HG3	1.70	0.57
1:B:385:LEU:HB2	1:B:441:VAL:HG23	1.86	0.57
1:D:284:ARG:O	1:D:285:LYS:HB2	2.05	0.57
1:D:371:VAL:HG23	1:D:433:ASP:HB3	1.86	0.57
1:A:452:LEU:HD13	1:A:467:HIS:HA	1.86	0.57
1:B:372:LEU:HB2	1:B:436:SER:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ILE:CG1	1:B:468:ILE:HB	2.34	0.57
1:D:447:THR:HG21	1:D:453:ILE:CG2	2.35	0.57
1:B:325:ARG:NH1	1:B:330:ASN:HD21	2.02	0.57
1:A:186:LEU:HD23	1:A:190:LEU:HG	1.87	0.57
1:D:167:LEU:O	1:D:168:VAL:HB	2.05	0.57
1:A:370:LYS:O	1:A:371:VAL:HG12	2.05	0.56
1:A:466:MET:HE3	1:A:471:LEU:HB2	1.86	0.56
1:C:422:GLN:HG3	1:C:423:SER:N	2.20	0.56
1:D:116:THR:HA	1:D:120:VAL:CG2	2.34	0.56
1:A:148:VAL:HG21	1:C:148:VAL:HG21	1.87	0.56
1:A:281:GLU:O	1:A:282:GLU:HG3	2.04	0.56
1:D:73:CYS:SG	1:D:350:LEU:HD22	2.46	0.56
1:D:383:VAL:CG1	1:D:413:VAL:HG22	2.34	0.56
1:D:422:GLN:HG3	1:D:423:SER:N	2.20	0.56
1:A:403:PHE:HZ	1:C:123:GLU:HG2	1.69	0.56
1:A:421:MET:HG3	1:A:423:SER:H	1.70	0.56
1:B:77:HIS:CD2	1:D:199:LEU:HD22	2.41	0.56
1:C:441:VAL:HG11	1:C:471:LEU:HD21	1.88	0.56
1:D:106:LEU:HD23	1:D:346:MET:SD	2.45	0.56
1:D:385:LEU:HD12	1:D:385:LEU:O	2.05	0.56
1:A:243:THR:HG1	1:A:251:TRP:CD1	2.24	0.56
1:B:403:PHE:HZ	1:D:123:GLU:HG2	1.69	0.56
1:A:257:ARG:HG3	1:A:257:ARG:HH21	1.71	0.56
1:B:323:HIS:HB3	1:B:332:VAL:CA	2.35	0.56
1:C:151:GLU:N	1:C:151:GLU:OE1	2.38	0.56
1:C:212:GLY:O	1:C:236:GLU:N	2.34	0.56
1:C:447:THR:HG21	1:C:453:ILE:CG2	2.35	0.56
1:D:151:GLU:OE1	1:D:151:GLU:N	2.38	0.56
1:D:455:LEU:HD12	1:D:455:LEU:O	2.06	0.56
1:A:413:VAL:HG12	1:A:414:TRP:N	2.21	0.56
1:B:413:VAL:HG12	1:B:414:TRP:N	2.20	0.56
1:B:159:ASP:C	1:B:161:GLU:H	2.13	0.56
1:B:403:PHE:O	1:B:407:LEU:HG	2.06	0.56
1:D:423:SER:O	1:D:424:SER:HB3	2.06	0.56
1:A:467:HIS:O	1:A:469:SER:N	2.38	0.56
1:C:281:GLU:HG2	1:C:282:GLU:N	2.20	0.56
1:C:455:LEU:HD12	1:C:455:LEU:O	2.05	0.56
1:A:158:GLN:HG2	1:A:159:ASP:N	2.16	0.56
1:A:159:ASP:C	1:A:161:GLU:H	2.14	0.56
1:A:385:LEU:HB2	1:A:441:VAL:HG23	1.86	0.56
1:A:399:CYS:HB3	1:A:417:TYR:CD2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD23	1:B:190:LEU:HG	1.88	0.56
1:C:420:THR:HG23	1:C:421:MET:N	2.21	0.56
1:C:427:GLN:O	1:C:431:LYS:HB2	2.06	0.56
1:A:471:LEU:HD12	1:A:475:LEU:HG	1.88	0.56
1:B:323:HIS:CB	1:B:331:VAL:C	2.79	0.56
1:C:76:ARG:HG3	1:C:434:GLU:CB	2.36	0.56
1:C:214:CYS:HB2	1:C:216:HIS:HE1	1.71	0.56
1:A:323:HIS:HB3	1:A:332:VAL:CA	2.35	0.55
1:B:162:LEU:O	1:B:164:LYS:N	2.37	0.55
1:B:260:LEU:HD13	1:B:289:LEU:CD1	2.36	0.55
1:C:167:LEU:O	1:C:168:VAL:HB	2.05	0.55
1:D:82:SER:O	1:D:84:GLN:N	2.37	0.55
1:D:281:GLU:HG2	1:D:282:GLU:N	2.20	0.55
1:A:77:HIS:CD2	1:C:199:LEU:HD22	2.41	0.55
1:B:452:LEU:HD13	1:B:467:HIS:HA	1.87	0.55
1:B:455:LEU:H	1:B:455:LEU:CD2	2.19	0.55
1:C:154:ARG:HD3	1:C:154:ARG:C	2.31	0.55
1:D:73:CYS:CB	1:D:79:LEU:HD23	2.31	0.55
1:D:420:THR:HG23	1:D:421:MET:N	2.21	0.55
1:A:156:ILE:HG23	1:A:167:LEU:HD11	1.88	0.55
1:A:480:SER:O	1:A:483:LYS:HB3	2.07	0.55
1:D:152:THR:HG22	1:D:170:PHE:HE1	1.70	0.55
1:D:214:CYS:HB2	1:D:216:HIS:HE1	1.71	0.55
1:A:453:ILE:CG1	1:A:468:ILE:HB	2.35	0.55
1:B:243:THR:HG1	1:B:251:TRP:CD1	2.24	0.55
1:C:119:VAL:O	1:C:121:PHE:N	2.40	0.55
1:D:422:GLN:HG3	1:D:423:SER:H	1.71	0.55
1:D:427:GLN:O	1:D:431:LYS:HB2	2.05	0.55
1:A:323:HIS:CB	1:A:331:VAL:C	2.79	0.55
1:C:423:SER:O	1:C:424:SER:HB3	2.06	0.55
1:D:154:ARG:HD3	1:D:154:ARG:C	2.32	0.55
1:D:231:ILE:HG22	1:D:232:GLY:N	2.21	0.55
1:D:441:VAL:HG11	1:D:471:LEU:HD21	1.88	0.55
1:B:399:CYS:HB3	1:B:417:TYR:CD2	2.41	0.55
1:B:416:GLY:C	1:B:418:LEU:H	2.14	0.55
1:A:138:LEU:HD21	1:A:180:LYS:HD3	1.87	0.55
1:C:152:THR:HG22	1:C:170:PHE:HE1	1.70	0.55
1:A:372:LEU:HB2	1:A:436:SER:HB2	1.87	0.55
1:C:384:ALA:O	1:C:385:LEU:HB3	2.07	0.55
1:A:407:LEU:C	1:A:409:ASN:H	2.14	0.55
1:B:281:GLU:O	1:B:282:GLU:HG3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:MET:HG3	1:B:423:SER:H	1.71	0.55
1:B:471:LEU:HD12	1:B:475:LEU:HG	1.87	0.55
1:C:346:MET:O	1:C:350:LEU:HD12	2.06	0.55
1:B:162:LEU:HD22	1:B:166:GLN:HG2	1.89	0.55
1:D:119:VAL:O	1:D:121:PHE:N	2.39	0.55
1:A:162:LEU:HD22	1:A:166:GLN:HG2	1.89	0.54
1:B:403:PHE:CE1	1:B:415:PRO:HD3	2.42	0.54
1:A:416:GLY:C	1:A:418:LEU:H	2.14	0.54
1:C:422:GLN:HG3	1:C:423:SER:H	1.70	0.54
1:A:260:LEU:HD13	1:A:289:LEU:HD12	1.89	0.54
1:A:447:THR:HG23	1:A:452:LEU:O	2.07	0.54
1:B:383:VAL:HG22	1:B:384:ALA:O	2.08	0.54
1:C:149:SER:O	1:C:153:LEU:HB2	2.07	0.54
1:D:472:LYS:HD3	1:D:473:ASP:N	2.23	0.54
1:A:186:LEU:HD23	1:A:186:LEU:O	2.06	0.54
1:B:154:ARG:C	1:B:156:ILE:H	2.15	0.54
1:B:447:THR:HG23	1:B:452:LEU:O	2.08	0.54
1:C:76:ARG:HD2	1:C:435:MET:HG3	1.90	0.54
1:A:190:LEU:HB2	1:A:314:MET:HE1	1.89	0.54
1:A:455:LEU:H	1:A:455:LEU:CD2	2.20	0.54
1:A:198:ASP:O	1:A:200:VAL:N	2.41	0.54
1:A:383:VAL:HG22	1:A:384:ALA:O	2.08	0.54
1:B:116:THR:HA	1:B:120:VAL:CG2	2.38	0.54
1:B:252:LEU:HD11	1:B:287:ASN:HD21	1.73	0.54
1:C:146:ARG:HB3	1:C:178:SER:OG	2.07	0.54
1:D:76:ARG:HG3	1:D:434:GLU:CB	2.37	0.54
1:D:149:SER:O	1:D:153:LEU:HB2	2.07	0.54
1:B:148:VAL:HG21	1:D:148:VAL:HG21	1.90	0.54
1:C:182:ARG:HG2	1:C:182:ARG:HH11	1.72	0.54
1:D:92:LEU:C	1:D:94:GLY:H	2.16	0.54
1:D:460:THR:OG1	1:D:462:MET:HE2	2.08	0.54
1:B:198:ASP:O	1:B:200:VAL:N	2.41	0.54
1:B:407:LEU:C	1:B:409:ASN:H	2.14	0.54
1:D:191:GLU:HA	1:D:314:MET:HE1	1.90	0.54
1:A:320:SER:HA	1:A:323:HIS:NE2	2.23	0.54
1:C:122:ARG:HH11	1:C:122:ARG:HB3	1.73	0.54
1:C:460:THR:OG1	1:C:462:MET:HE2	2.08	0.54
1:C:472:LYS:HD3	1:C:473:ASP:N	2.23	0.54
1:D:122:ARG:HH11	1:D:122:ARG:HB3	1.73	0.54
1:A:193:TYR:CZ	1:A:197:LEU:HD22	2.43	0.54
1:B:269:SER:C	1:B:271:SER:N	2.66	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ARG:HG2	1:C:264:ARG:HH11	1.73	0.54
1:D:189:ALA:O	1:D:192:HIS:HB2	2.07	0.54
1:D:323:HIS:HA	1:D:331:VAL:O	2.08	0.54
1:A:162:LEU:HB2	1:A:166:GLN:CG	2.37	0.53
1:B:174:VAL:HG11	1:D:153:LEU:HD21	1.89	0.53
1:B:437:ILE:CG2	1:B:438:LEU:H	2.16	0.53
1:B:162:LEU:HB2	1:B:166:GLN:CG	2.38	0.53
1:C:73:CYS:SG	1:C:350:LEU:HD22	2.48	0.53
1:C:323:HIS:HA	1:C:331:VAL:O	2.07	0.53
1:B:320:SER:HA	1:B:323:HIS:NE2	2.23	0.53
1:C:252:LEU:HA	1:C:336:LEU:HD11	1.90	0.53
1:A:437:ILE:CG2	1:A:438:LEU:H	2.17	0.53
1:B:156:ILE:HG23	1:B:167:LEU:HD11	1.89	0.53
1:C:189:ALA:O	1:C:192:HIS:HB2	2.08	0.53
1:D:280:ASP:CG	1:D:284:ARG:HH21	2.16	0.53
1:A:260:LEU:HD13	1:A:289:LEU:CD1	2.39	0.53
1:A:434:GLU:C	1:A:436:SER:N	2.66	0.53
1:B:423:SER:O	1:B:424:SER:HB3	2.09	0.53
1:C:92:LEU:C	1:C:94:GLY:H	2.16	0.53
1:D:411:ILE:HD11	1:D:476:ILE:HG13	1.90	0.53
1:A:116:THR:HA	1:A:120:VAL:CG2	2.39	0.53
1:A:154:ARG:C	1:A:156:ILE:H	2.15	0.53
1:B:193:TYR:CZ	1:B:197:LEU:HD22	2.44	0.53
1:C:186:LEU:HD12	1:C:240:VAL:HG22	1.91	0.53
1:D:252:LEU:HA	1:D:336:LEU:HD11	1.91	0.53
1:A:120:VAL:O	1:A:121:PHE:C	2.52	0.53
1:C:67:GLU:CD	1:C:67:GLU:N	2.67	0.53
1:D:384:ALA:O	1:D:385:LEU:HB3	2.08	0.53
1:D:182:ARG:HG2	1:D:182:ARG:HH11	1.74	0.53
1:D:416:GLY:C	1:D:418:LEU:H	2.17	0.53
1:A:313:HIS:O	1:A:313:HIS:CD2	2.62	0.52
1:A:403:PHE:CE1	1:A:415:PRO:HD3	2.44	0.52
1:B:480:SER:O	1:B:483:LYS:HB3	2.09	0.52
1:B:190:LEU:HB2	1:B:314:MET:HE1	1.90	0.52
1:B:434:GLU:C	1:B:436:SER:N	2.67	0.52
1:C:280:ASP:CG	1:C:284:ARG:HH21	2.17	0.52
1:C:411:ILE:HD11	1:C:476:ILE:HG13	1.91	0.52
1:A:269:SER:C	1:A:271:SER:N	2.66	0.52
1:A:423:SER:O	1:A:424:SER:HB3	2.08	0.52
1:B:382:LYS:O	1:B:438:LEU:HB2	2.09	0.52
1:B:466:MET:HE3	1:B:471:LEU:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:CYS:CB	1:C:79:LEU:HD23	2.30	0.52
1:C:416:GLY:C	1:C:418:LEU:H	2.18	0.52
1:D:67:GLU:N	1:D:67:GLU:CD	2.67	0.52
1:D:76:ARG:O	1:D:102:LEU:HD22	2.09	0.52
1:D:212:GLY:O	1:D:236:GLU:N	2.36	0.52
1:A:382:LYS:O	1:A:438:LEU:HB2	2.10	0.52
1:C:76:ARG:O	1:C:102:LEU:HD22	2.10	0.52
1:D:154:ARG:NH1	1:D:158:GLN:HB2	2.24	0.52
1:D:281:GLU:CG	1:D:282:GLU:H	2.20	0.52
1:A:468:ILE:O	1:A:468:ILE:HG23	2.10	0.52
1:D:92:LEU:C	1:D:94:GLY:N	2.65	0.52
1:A:375:HIS:ND1	1:A:376:PRO:N	2.58	0.52
1:A:384:ALA:O	1:A:385:LEU:HB3	2.09	0.52
1:A:252:LEU:HD11	1:A:287:ASN:HD21	1.75	0.52
1:A:116:THR:HA	1:A:120:VAL:HG23	1.91	0.52
1:A:122:ARG:HG3	1:A:122:ARG:O	2.10	0.52
1:B:158:GLN:C	1:B:160:LYS:H	2.18	0.52
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.73	0.52
1:D:281:GLU:C	1:D:283:GLY:H	2.17	0.52
1:B:186:LEU:HD23	1:B:186:LEU:O	2.09	0.52
1:B:437:ILE:CG2	1:B:438:LEU:N	2.73	0.52
1:C:154:ARG:NH1	1:C:158:GLN:HB2	2.24	0.52
1:C:191:GLU:HA	1:C:314:MET:HE1	1.91	0.52
1:D:122:ARG:HB3	1:D:122:ARG:NH1	2.25	0.52
1:C:135:PRO:O	1:C:138:LEU:CD2	2.58	0.52
1:B:258:HIS:HB2	1:C:316:PRO:HB2	1.92	0.51
1:B:263:TRP:O	1:B:349:TYR:OH	2.28	0.51
1:C:122:ARG:HB3	1:C:122:ARG:NH1	2.25	0.51
1:C:133:HIS:CG	1:C:133:HIS:O	2.64	0.51
1:C:313:HIS:O	1:C:316:PRO:HD3	2.10	0.51
1:D:92:LEU:HD11	1:D:295:TRP:HZ2	1.76	0.51
1:A:158:GLN:C	1:A:160:LYS:H	2.19	0.51
1:C:456:ARG:HG2	1:C:457:SER:N	2.24	0.51
1:A:387:VAL:HB	1:A:395:LEU:HD12	1.92	0.51
1:B:116:THR:HA	1:B:120:VAL:HG23	1.91	0.51
1:B:414:TRP:O	1:B:414:TRP:CD1	2.63	0.51
1:D:128:VAL:HG12	1:D:209:ALA:O	2.10	0.51
1:D:371:VAL:HG13	1:D:371:VAL:O	2.09	0.51
1:D:392:THR:C	1:D:394:GLU:H	2.19	0.51
1:A:375:HIS:ND1	1:A:376:PRO:CD	2.73	0.51
1:B:120:VAL:O	1:B:121:PHE:C	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:HB2	1:D:437:ILE:HD13	1.93	0.51
1:B:313:HIS:CD2	1:B:313:HIS:O	2.63	0.51
1:C:182:ARG:HG2	1:C:182:ARG:NH1	2.25	0.51
1:C:281:GLU:C	1:C:283:GLY:H	2.17	0.51
1:D:279:GLN:OE1	1:D:284:ARG:HD3	2.11	0.51
1:D:456:ARG:HG2	1:D:457:SER:N	2.24	0.51
1:B:443:VAL:HG22	1:B:453:ILE:HG21	1.93	0.51
1:B:138:LEU:HD21	1:B:180:LYS:HD3	1.92	0.51
1:B:387:VAL:HB	1:B:395:LEU:HD12	1.93	0.51
1:C:279:GLN:OE1	1:C:284:ARG:HD3	2.11	0.51
1:D:314:MET:HE3	1:D:315:TYR:CE2	2.46	0.51
1:B:393:LEU:O	1:B:393:LEU:HD23	2.11	0.51
1:D:384:ALA:HB3	1:D:440:THR:HG23	1.93	0.51
1:C:152:THR:HG22	1:C:170:PHE:CE1	2.46	0.51
1:D:76:ARG:HD2	1:D:435:MET:HG3	1.93	0.51
1:A:484:ASN:O	1:A:485:VAL:C	2.54	0.50
1:D:186:LEU:HD12	1:D:240:VAL:HG22	1.92	0.50
1:D:346:MET:O	1:D:350:LEU:HD12	2.10	0.50
1:A:437:ILE:CG2	1:A:438:LEU:N	2.74	0.50
1:B:106:LEU:HD12	1:B:106:LEU:O	2.11	0.50
1:C:92:LEU:HD11	1:C:295:TRP:HZ2	1.77	0.50
1:C:252:LEU:CA	1:C:336:LEU:HD11	2.41	0.50
1:C:453:ILE:HG23	1:C:468:ILE:HB	1.93	0.50
1:D:453:ILE:HD12	1:D:453:ILE:C	2.36	0.50
1:D:468:ILE:HG12	1:D:468:ILE:O	2.11	0.50
1:B:406:LEU:HB3	1:B:411:ILE:HB	1.92	0.50
1:B:115:TRP:CZ2	1:B:119:VAL:HG11	2.46	0.50
1:C:384:ALA:HB2	1:C:437:ILE:HD13	1.94	0.50
1:D:96:HIS:HB2	1:D:97:PRO:CD	2.29	0.50
1:C:371:VAL:HG13	1:C:371:VAL:O	2.10	0.50
1:C:468:ILE:O	1:C:468:ILE:HG12	2.11	0.50
1:D:69:LEU:HD21	1:D:351:TYR:HA	1.92	0.50
1:D:453:ILE:HG23	1:D:468:ILE:HB	1.94	0.50
1:A:393:LEU:O	1:A:393:LEU:HD23	2.12	0.50
1:B:122:ARG:O	1:B:122:ARG:HG3	2.11	0.50
1:B:484:ASN:O	1:B:485:VAL:C	2.55	0.50
1:C:392:THR:C	1:C:394:GLU:H	2.18	0.50
1:D:133:HIS:O	1:D:133:HIS:CG	2.65	0.50
1:A:158:GLN:O	1:A:160:LYS:N	2.38	0.50
1:A:406:LEU:HD12	1:A:475:LEU:HD12	1.94	0.50
1:A:414:TRP:O	1:A:414:TRP:CD1	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LEU:C	1:B:71:GLU:H	2.20	0.50
1:B:402:LEU:O	1:B:403:PHE:C	2.54	0.50
1:C:314:MET:HE3	1:C:315:TYR:CE2	2.47	0.50
1:D:152:THR:HG22	1:D:170:PHE:CE1	2.45	0.50
1:D:182:ARG:HG2	1:D:182:ARG:NH1	2.26	0.50
1:D:445:GLU:C	1:D:447:THR:N	2.70	0.50
1:A:118:VAL:HG21	1:A:239:LEU:HD22	1.93	0.50
1:A:402:LEU:O	1:A:403:PHE:C	2.55	0.50
1:A:406:LEU:HB3	1:A:411:ILE:HB	1.93	0.50
1:B:384:ALA:HB2	1:B:437:ILE:HD13	1.94	0.50
1:D:135:PRO:O	1:D:138:LEU:CD2	2.60	0.50
1:D:254:PHE:HD1	1:D:257:ARG:HD2	1.76	0.50
1:D:313:HIS:O	1:D:316:PRO:HD3	2.12	0.50
1:D:375:HIS:ND1	1:D:376:PRO:HD2	2.26	0.50
1:A:162:LEU:O	1:A:164:LYS:N	2.36	0.50
1:A:445:GLU:C	1:A:447:THR:N	2.70	0.50
1:C:384:ALA:HB3	1:C:440:THR:HG23	1.93	0.50
1:C:453:ILE:C	1:C:453:ILE:HD12	2.36	0.50
1:D:252:LEU:CA	1:D:336:LEU:HD11	2.42	0.50
1:D:270:PRO:C	1:D:272:ASN:H	2.20	0.50
1:A:106:LEU:HD12	1:A:106:LEU:O	2.12	0.49
1:B:168:VAL:HG12	1:B:168:VAL:O	2.11	0.49
1:C:254:PHE:HD1	1:C:257:ARG:HD2	1.77	0.49
1:A:384:ALA:HB2	1:A:437:ILE:HD13	1.94	0.49
1:B:104:VAL:HG11	1:D:127:PRO:HB2	1.93	0.49
1:B:213:VAL:HG21	1:D:132:HIS:CE1	2.47	0.49
1:B:277:ASP:O	1:B:278:CYS:CB	2.60	0.49
1:B:375:HIS:ND1	1:B:376:PRO:N	2.60	0.49
1:D:404:ASN:O	1:D:408:GLU:HG3	2.11	0.49
1:A:69:LEU:C	1:A:71:GLU:H	2.20	0.49
1:A:109:ASN:O	1:A:112:ALA:HB3	2.12	0.49
1:A:252:LEU:HD13	1:A:252:LEU:C	2.36	0.49
1:A:443:VAL:HG22	1:A:453:ILE:HG21	1.94	0.49
1:C:69:LEU:HD21	1:C:351:TYR:HA	1.93	0.49
1:C:420:THR:OG1	1:C:421:MET:N	2.45	0.49
1:D:154:ARG:NH2	1:D:158:GLN:HE21	2.10	0.49
1:B:213:VAL:HG21	1:D:132:HIS:HE1	1.78	0.49
1:A:133:HIS:HB2	1:A:180:LYS:O	2.12	0.49
1:B:375:HIS:ND1	1:B:376:PRO:CD	2.76	0.49
1:B:406:LEU:HD12	1:B:475:LEU:HD12	1.94	0.49
1:B:468:ILE:HG23	1:B:468:ILE:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:PHE:HB3	1:D:79:LEU:HD22	1.94	0.49
1:D:118:VAL:O	1:D:118:VAL:CG2	2.61	0.49
1:A:395:LEU:HD11	1:A:443:VAL:C	2.38	0.49
1:B:77:HIS:HB3	1:B:101:PRO:HD2	1.95	0.49
1:B:156:ILE:HD13	1:B:170:PHE:CE2	2.48	0.49
1:B:269:SER:O	1:B:271:SER:N	2.45	0.49
1:D:120:VAL:HG12	1:D:120:VAL:O	2.11	0.49
1:D:190:LEU:C	1:D:192:HIS:N	2.71	0.49
1:A:481:SER:C	1:A:483:LYS:N	2.69	0.49
1:B:477:LYS:O	1:B:481:SER:N	2.45	0.49
1:C:82:SER:O	1:C:84:GLN:N	2.37	0.49
1:C:92:LEU:C	1:C:94:GLY:N	2.66	0.49
1:C:381:ILE:HG21	1:C:414:TRP:HB2	1.95	0.49
1:D:155:GLU:C	1:D:156:ILE:HG13	2.38	0.49
1:A:459:ASP:C	1:A:461:THR:H	2.21	0.49
1:A:468:ILE:O	1:A:468:ILE:HG12	2.11	0.49
1:A:77:HIS:HB3	1:A:101:PRO:HD2	1.95	0.49
1:A:162:LEU:HD23	1:A:165:GLU:HB2	1.95	0.49
1:A:213:VAL:HG21	1:C:132:HIS:CE1	2.48	0.49
1:A:260:LEU:HD22	1:A:275:SER:HB3	1.94	0.49
1:C:155:GLU:C	1:C:156:ILE:HG13	2.37	0.49
1:C:391:PRO:HG2	1:C:395:LEU:HB2	1.95	0.49
1:C:402:LEU:O	1:C:406:LEU:HB2	2.13	0.49
1:D:420:THR:OG1	1:D:421:MET:N	2.46	0.49
1:A:168:VAL:HG12	1:A:168:VAL:O	2.12	0.48
1:A:263:TRP:O	1:A:349:TYR:OH	2.29	0.48
1:A:323:HIS:HA	1:A:333:PRO:HD3	1.94	0.48
1:B:384:ALA:O	1:B:385:LEU:HB3	2.12	0.48
1:C:270:PRO:C	1:C:272:ASN:H	2.21	0.48
1:D:381:ILE:HG21	1:D:414:TRP:HB2	1.95	0.48
1:A:104:VAL:HG11	1:C:127:PRO:HB2	1.94	0.48
1:A:423:SER:O	1:A:427:GLN:HB2	2.13	0.48
1:B:133:HIS:HB2	1:B:180:LYS:O	2.13	0.48
1:B:323:HIS:HA	1:B:333:PRO:HD3	1.94	0.48
1:B:423:SER:O	1:B:427:GLN:HB2	2.13	0.48
1:C:447:THR:HG21	1:C:453:ILE:HG23	1.95	0.48
1:D:82:SER:C	1:D:84:GLN:N	2.72	0.48
1:C:146:ARG:HG2	1:C:146:ARG:NH1	2.25	0.48
1:C:154:ARG:NH2	1:C:158:GLN:HE21	2.10	0.48
1:D:467:HIS:O	1:D:469:SER:N	2.46	0.48
1:B:252:LEU:C	1:B:252:LEU:HD13	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:PHE:HB3	1:C:378:LEU:HD22	1.95	0.48
1:C:281:GLU:CG	1:C:282:GLU:H	2.20	0.48
1:C:404:ASN:O	1:C:408:GLU:HG3	2.13	0.48
1:A:269:SER:O	1:A:271:SER:N	2.47	0.48
1:A:293:PHE:C	1:A:295:TRP:N	2.69	0.48
1:B:389:ARG:HD2	1:B:389:ARG:N	2.26	0.48
1:C:78:PHE:HB3	1:C:79:LEU:HD22	1.95	0.48
1:A:80:SER:O	1:A:86:LEU:HD21	2.13	0.48
1:A:407:LEU:C	1:A:409:ASN:N	2.71	0.48
1:B:109:ASN:O	1:B:112:ALA:HB3	2.14	0.48
1:B:395:LEU:HD11	1:B:443:VAL:C	2.38	0.48
1:C:186:LEU:HD13	1:C:337:SER:OG	2.13	0.48
1:D:453:ILE:HD11	1:D:466:MET:HB3	1.95	0.48
1:A:156:ILE:HD13	1:A:170:PHE:CE2	2.48	0.48
1:A:157:LEU:HD21	1:C:171:LEU:CB	2.42	0.48
1:B:80:SER:O	1:B:86:LEU:HD21	2.14	0.48
1:B:374:LEU:HB2	1:B:436:SER:OG	2.13	0.48
1:B:419:GLU:HG2	1:B:420:THR:HG22	1.96	0.48
1:C:118:VAL:O	1:C:118:VAL:CG2	2.62	0.48
1:C:369:ARG:HG3	1:C:369:ARG:HH11	1.79	0.48
1:A:188:GLY:O	1:A:192:HIS:HD2	1.96	0.48
1:B:450:ASN:CG	1:B:451:GLY:H	2.21	0.48
1:B:293:PHE:C	1:B:295:TRP:N	2.69	0.48
1:B:459:ASP:C	1:B:461:THR:H	2.22	0.48
1:C:82:SER:C	1:C:84:GLN:N	2.71	0.48
1:A:419:GLU:HG2	1:A:420:THR:HG22	1.96	0.47
1:B:118:VAL:HG21	1:B:239:LEU:HD22	1.95	0.47
1:B:260:LEU:HD22	1:B:275:SER:HB3	1.95	0.47
1:B:468:ILE:O	1:B:468:ILE:HG12	2.13	0.47
1:D:391:PRO:HG2	1:D:395:LEU:HB2	1.96	0.47
1:A:162:LEU:C	1:A:164:LYS:N	2.72	0.47
1:A:343:ASP:O	1:A:346:MET:HB2	2.14	0.47
1:B:481:SER:C	1:B:483:LYS:H	2.21	0.47
1:C:190:LEU:C	1:C:192:HIS:N	2.72	0.47
1:C:445:GLU:C	1:C:447:THR:N	2.69	0.47
1:A:381:ILE:O	1:A:437:ILE:HG23	2.13	0.47
1:B:162:LEU:C	1:B:164:LYS:N	2.73	0.47
1:D:447:THR:HG21	1:D:453:ILE:HG22	1.96	0.47
1:D:447:THR:HG21	1:D:453:ILE:HG23	1.95	0.47
1:A:450:ASN:CG	1:A:451:GLY:H	2.21	0.47
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:GLY:O	1:B:192:HIS:HD2	1.96	0.47
1:B:389:ARG:H	1:B:389:ARG:CD	2.24	0.47
1:B:419:GLU:HG3	1:D:201:ASN:ND2	2.29	0.47
1:C:467:HIS:C	1:C:469:SER:N	2.69	0.47
1:D:146:ARG:HG2	1:D:146:ARG:NH1	2.27	0.47
1:D:186:LEU:HD13	1:D:337:SER:OG	2.15	0.47
1:D:254:PHE:HA	1:D:257:ARG:CG	2.44	0.47
1:D:455:LEU:C	1:D:455:LEU:CD1	2.86	0.47
1:A:115:TRP:CZ2	1:A:119:VAL:HG11	2.49	0.47
1:A:146:ARG:HG2	1:A:146:ARG:HH11	1.80	0.47
1:B:481:SER:C	1:B:483:LYS:N	2.69	0.47
1:C:120:VAL:HG12	1:C:120:VAL:O	2.14	0.47
1:C:214:CYS:HB2	1:C:216:HIS:CE1	2.50	0.47
1:C:455:LEU:C	1:C:455:LEU:CD1	2.86	0.47
1:C:467:HIS:O	1:C:469:SER:N	2.46	0.47
1:D:351:TYR:O	1:D:353:SER:N	2.48	0.47
1:A:249:ASN:HD21	1:A:285:LYS:HE2	1.79	0.47
1:A:481:SER:C	1:A:483:LYS:H	2.21	0.47
1:B:106:LEU:HG	1:B:346:MET:SD	2.54	0.47
1:D:392:THR:HG22	1:D:396:ARG:HD3	1.97	0.47
1:A:381:ILE:HG13	1:A:437:ILE:HG12	1.96	0.47
1:A:419:GLU:HG3	1:C:201:ASN:ND2	2.29	0.47
1:B:158:GLN:O	1:B:160:LYS:N	2.38	0.47
1:B:204:LEU:CD1	1:B:333:PRO:HB3	2.42	0.47
1:B:213:VAL:HA	1:B:234:LYS:O	2.15	0.47
1:B:451:GLY:O	1:B:452:LEU:HD13	2.15	0.47
1:C:447:THR:HG21	1:C:453:ILE:HG22	1.97	0.47
1:A:477:LYS:O	1:A:481:SER:N	2.44	0.47
1:B:249:ASN:HD21	1:B:285:LYS:HE2	1.79	0.47
1:C:453:ILE:HD11	1:C:466:MET:HB3	1.97	0.47
1:D:369:ARG:HG3	1:D:369:ARG:HH11	1.80	0.47
1:C:405:GLU:O	1:C:409:ASN:ND2	2.47	0.47
1:B:104:VAL:HG22	1:D:129:ASP:HB2	1.96	0.47
1:B:343:ASP:O	1:B:346:MET:HB2	2.15	0.47
1:C:479:ILE:C	1:C:481:SER:N	2.73	0.47
1:D:289:LEU:HD12	1:D:301:GLU:HG2	1.97	0.47
1:A:76:ARG:HA	1:A:76:ARG:HD3	1.72	0.46
1:B:145:PHE:CD1	1:D:149:SER:HA	2.47	0.46
1:D:405:GLU:O	1:D:409:ASN:ND2	2.47	0.46
1:D:448:LEU:HD23	1:D:448:LEU:O	2.15	0.46
1:B:396:ARG:HA	1:B:399:CYS:SG	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:MET:C	1:B:423:SER:H	2.23	0.46
1:D:266:PHE:HB3	1:D:378:LEU:HD22	1.97	0.46
1:A:451:GLY:O	1:A:452:LEU:HD13	2.15	0.46
1:B:381:ILE:O	1:B:437:ILE:HG23	2.14	0.46
1:C:254:PHE:HA	1:C:257:ARG:CG	2.44	0.46
1:C:289:LEU:HD12	1:C:301:GLU:HG2	1.96	0.46
1:D:389:ARG:H	1:D:389:ARG:HD2	1.81	0.46
1:D:467:HIS:C	1:D:469:SER:N	2.69	0.46
1:A:399:CYS:HB3	1:A:417:TYR:CE2	2.51	0.46
1:C:128:VAL:HG12	1:C:209:ALA:O	2.16	0.46
1:C:448:LEU:O	1:C:448:LEU:HD23	2.15	0.46
1:D:384:ALA:HB2	1:D:437:ILE:CD1	2.45	0.46
1:A:145:PHE:CD1	1:C:149:SER:HA	2.48	0.46
1:A:396:ARG:HA	1:A:399:CYS:SG	2.55	0.46
1:B:347:LEU:O	1:B:348:ALA:C	2.58	0.46
1:C:389:ARG:H	1:C:389:ARG:HD2	1.81	0.46
1:D:118:VAL:CG2	1:D:239:LEU:HD22	2.45	0.46
1:D:162:LEU:HB2	1:D:166:GLN:NE2	2.30	0.46
1:D:317:GLY:O	1:D:319:VAL:N	2.48	0.46
1:A:148:VAL:HG21	1:C:148:VAL:CG2	2.45	0.46
1:A:154:ARG:C	1:A:156:ILE:N	2.74	0.46
1:A:471:LEU:HD12	1:A:471:LEU:C	2.40	0.46
1:B:157:LEU:HD21	1:D:171:LEU:CB	2.43	0.46
1:B:381:ILE:HG13	1:B:437:ILE:HG12	1.97	0.46
1:B:399:CYS:HB3	1:B:417:TYR:CE2	2.50	0.46
1:B:402:LEU:HA	1:B:405:GLU:HB3	1.97	0.46
1:C:384:ALA:HB2	1:C:437:ILE:CD1	2.46	0.46
1:A:250:GLN:HA	1:A:253:ASP:OD2	2.16	0.46
1:B:471:LEU:HD12	1:B:471:LEU:C	2.40	0.46
1:A:277:ASP:O	1:A:278:CYS:CB	2.60	0.46
1:B:162:LEU:HD23	1:B:165:GLU:HB2	1.98	0.46
1:B:323:HIS:HB3	1:B:332:VAL:N	2.30	0.46
1:C:353:SER:O	1:C:372:LEU:HA	2.15	0.46
1:D:211:ILE:HA	1:D:237:ALA:HA	1.98	0.46
1:D:353:SER:O	1:D:372:LEU:HA	2.16	0.46
1:A:323:HIS:HB3	1:A:332:VAL:N	2.30	0.46
1:C:308:ASP:HB2	1:C:312:LEU:CD1	2.45	0.46
1:C:392:THR:HG22	1:C:396:ARG:HD3	1.97	0.46
1:D:69:LEU:CD2	1:D:351:TYR:HA	2.45	0.46
1:D:147:LEU:HD21	1:D:181:LEU:CD2	2.46	0.46
1:D:242:PHE:CE1	1:D:335:VAL:HG12	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:O	1:A:375:HIS:C	2.59	0.46
1:A:402:LEU:HA	1:A:405:GLU:HB3	1.98	0.45
1:B:402:LEU:O	1:B:405:GLU:N	2.50	0.45
1:B:158:GLN:HG2	1:B:159:ASP:N	2.17	0.45
1:C:162:LEU:HB2	1:C:166:GLN:NE2	2.31	0.45
1:C:211:ILE:HA	1:C:237:ALA:HA	1.98	0.45
1:C:317:GLY:O	1:C:319:VAL:N	2.48	0.45
1:C:351:TYR:O	1:C:353:SER:N	2.49	0.45
1:A:421:MET:C	1:A:423:SER:N	2.73	0.45
1:B:119:VAL:HG22	1:B:125:VAL:HG11	1.98	0.45
1:B:154:ARG:C	1:B:156:ILE:N	2.74	0.45
1:B:407:LEU:C	1:B:409:ASN:N	2.71	0.45
1:C:199:LEU:O	1:C:200:VAL:CG1	2.64	0.45
1:C:200:VAL:O	1:C:201:ASN:C	2.60	0.45
1:D:72:ILE:HG12	1:D:434:GLU:OE1	2.17	0.45
1:D:256:LEU:HD22	1:D:287:ASN:OD1	2.15	0.45
1:A:104:VAL:HG22	1:C:129:ASP:HB2	1.97	0.45
1:A:402:LEU:HA	1:A:402:LEU:HD23	1.78	0.45
1:A:420:THR:CG2	1:A:421:MET:H	2.27	0.45
1:A:421:MET:C	1:A:423:SER:H	2.23	0.45
1:B:122:ARG:O	1:B:124:GLN:HG3	2.15	0.45
1:B:437:ILE:O	1:B:458:ARG:HD3	2.16	0.45
1:C:69:LEU:HD13	1:C:354:PHE:CG	2.52	0.45
1:C:118:VAL:CG2	1:C:239:LEU:HD22	2.47	0.45
1:C:299:LEU:HD21	1:C:302:THR:HG22	1.98	0.45
1:D:352:ASP:O	1:D:352:ASP:CG	2.59	0.45
1:B:247:THR:O	1:B:250:GLN:HB3	2.17	0.45
1:B:403:PHE:HZ	1:D:123:GLU:CG	2.30	0.45
1:B:459:ASP:C	1:B:461:THR:N	2.73	0.45
1:D:375:HIS:CG	1:D:376:PRO:HD2	2.51	0.45
1:A:213:VAL:HA	1:A:234:LYS:O	2.17	0.45
1:A:374:LEU:HB2	1:A:436:SER:OG	2.16	0.45
1:A:402:LEU:O	1:A:405:GLU:N	2.50	0.45
1:B:250:GLN:HA	1:B:253:ASP:OD2	2.16	0.45
1:B:472:LYS:O	1:B:476:ILE:HG13	2.17	0.45
1:C:205:PRO:HB3	1:C:243:THR:HG22	1.98	0.45
1:A:106:LEU:HG	1:A:346:MET:SD	2.56	0.45
1:A:313:HIS:CD2	1:A:313:HIS:C	2.95	0.45
1:A:472:LYS:O	1:A:476:ILE:HG13	2.17	0.45
1:C:352:ASP:O	1:C:352:ASP:CG	2.60	0.45
1:D:479:ILE:C	1:D:481:SER:N	2.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LYS:HG3	1:B:479:ILE:HD11	1.98	0.45
1:D:146:ARG:HA	1:D:179:GLY:O	2.17	0.45
1:A:150:ALA:C	1:A:152:THR:H	2.25	0.45
1:B:132:HIS:CE1	1:D:213:VAL:HG21	2.52	0.45
1:D:247:THR:HG22	1:D:250:GLN:CB	2.47	0.45
1:A:403:PHE:HZ	1:C:123:GLU:CG	2.30	0.45
1:C:69:LEU:CD2	1:C:351:TYR:HA	2.47	0.45
1:D:200:VAL:O	1:D:201:ASN:C	2.60	0.45
1:A:132:HIS:CE1	1:C:213:VAL:HG21	2.51	0.44
1:A:459:ASP:C	1:A:461:THR:N	2.72	0.44
1:D:154:ARG:CZ	1:D:158:GLN:HB2	2.48	0.44
1:B:150:ALA:C	1:B:152:THR:H	2.25	0.44
1:C:247:THR:HG22	1:C:250:GLN:CB	2.47	0.44
1:A:88:ARG:CD	1:A:88:ARG:N	2.68	0.44
1:A:319:VAL:C	1:A:321:LYS:H	2.24	0.44
1:A:382:LYS:HG3	1:A:479:ILE:HD11	1.99	0.44
1:B:319:VAL:C	1:B:321:LYS:H	2.25	0.44
1:C:242:PHE:CE1	1:C:335:VAL:HG12	2.52	0.44
1:C:375:HIS:ND1	1:C:376:PRO:HD2	2.32	0.44
1:D:71:GLU:O	1:D:74:GLN:HB3	2.17	0.44
1:D:82:SER:HB3	1:D:85:GLN:HG2	1.99	0.44
1:D:320:SER:HA	1:D:323:HIS:CD2	2.52	0.44
1:C:71:GLU:O	1:C:74:GLN:HB3	2.18	0.44
1:C:72:ILE:HG12	1:C:434:GLU:OE1	2.16	0.44
1:C:154:ARG:CZ	1:C:158:GLN:HB2	2.48	0.44
1:D:260:LEU:CD2	1:D:275:SER:HB3	2.43	0.44
1:B:170:PHE:C	1:B:172:GLU:H	2.26	0.44
1:B:441:VAL:HG12	1:B:455:LEU:HB3	1.99	0.44
1:B:477:LYS:O	1:B:478:TYR:C	2.61	0.44
1:C:320:SER:C	1:C:322:LEU:H	2.26	0.44
1:A:170:PHE:C	1:A:172:GLU:H	2.26	0.44
1:A:204:LEU:CD1	1:A:333:PRO:HB3	2.44	0.44
1:B:154:ARG:O	1:B:156:ILE:N	2.50	0.44
1:D:69:LEU:HD13	1:D:354:PHE:CG	2.53	0.44
1:D:288:LYS:HG2	1:D:302:THR:HG22	2.00	0.44
1:A:119:VAL:HG22	1:A:125:VAL:HG11	2.00	0.44
1:A:215:PHE:CD1	1:A:215:PHE:N	2.86	0.44
1:A:347:LEU:O	1:A:348:ALA:C	2.60	0.44
1:B:313:HIS:CD2	1:B:313:HIS:C	2.95	0.44
1:B:421:MET:C	1:B:423:SER:N	2.73	0.44
1:C:70:LEU:HD13	1:C:70:LEU:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:GLY:O	1:C:142:ASP:CB	2.65	0.44
1:D:141:GLY:O	1:D:142:ASP:CB	2.65	0.44
1:D:205:PRO:HB3	1:D:243:THR:HG22	1.99	0.44
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.18	0.44
1:A:431:LYS:O	1:A:434:GLU:HB2	2.18	0.44
1:B:92:LEU:HD22	1:B:344:ARG:NE	2.33	0.44
1:C:256:LEU:HD22	1:C:287:ASN:OD1	2.18	0.44
1:C:420:THR:HG23	1:C:421:MET:H	1.82	0.44
1:D:214:CYS:HB2	1:D:216:HIS:CE1	2.50	0.44
1:A:154:ARG:O	1:A:156:ILE:N	2.51	0.44
1:B:200:VAL:C	1:B:202:LYS:N	2.75	0.44
1:B:374:LEU:O	1:B:375:HIS:C	2.60	0.44
1:D:351:TYR:C	1:D:353:SER:H	2.26	0.44
1:A:174:VAL:CG1	1:C:153:LEU:HD21	2.47	0.43
1:B:151:GLU:OE1	1:B:151:GLU:HA	2.18	0.43
1:C:320:SER:HA	1:C:323:HIS:CD2	2.53	0.43
1:D:71:GLU:HG2	1:D:83:LYS:NZ	2.32	0.43
1:D:299:LEU:HD21	1:D:302:THR:HG22	1.99	0.43
1:D:308:ASP:HB2	1:D:312:LEU:CD1	2.46	0.43
1:D:399:CYS:HB3	1:D:417:TYR:CD2	2.53	0.43
1:A:375:HIS:CE1	1:A:376:PRO:HD2	2.53	0.43
1:A:452:LEU:HD22	1:A:452:LEU:N	2.33	0.43
1:A:477:LYS:O	1:A:478:TYR:C	2.61	0.43
1:B:148:VAL:HG21	1:D:148:VAL:CG2	2.48	0.43
1:B:455:LEU:HD23	1:B:455:LEU:N	2.24	0.43
1:C:82:SER:HB3	1:C:85:GLN:HG2	1.99	0.43
1:D:190:LEU:HB2	1:D:314:MET:HE2	2.01	0.43
1:A:174:VAL:CG1	1:A:175:LEU:N	2.79	0.43
1:A:200:VAL:C	1:A:202:LYS:N	2.76	0.43
1:A:449:GLU:C	1:A:450:ASN:OD1	2.61	0.43
1:B:153:LEU:HA	1:B:156:ILE:HD12	2.00	0.43
1:C:71:GLU:HG2	1:C:83:LYS:NZ	2.33	0.43
1:D:420:THR:HG23	1:D:421:MET:H	1.82	0.43
1:A:122:ARG:O	1:A:124:GLN:HG3	2.18	0.43
1:A:395:LEU:C	1:A:397:GLN:H	2.27	0.43
1:B:159:ASP:C	1:B:161:GLU:N	2.77	0.43
1:B:424:SER:HB3	1:B:427:GLN:HB2	1.99	0.43
1:C:190:LEU:HB2	1:C:314:MET:HE2	2.00	0.43
1:D:402:LEU:O	1:D:406:LEU:HB2	2.18	0.43
1:A:153:LEU:HA	1:A:156:ILE:HD12	2.01	0.43
1:A:247:THR:O	1:A:250:GLN:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ARG:H	1:A:389:ARG:CD	2.23	0.43
1:A:424:SER:HB3	1:A:427:GLN:HB2	1.99	0.43
1:C:146:ARG:HA	1:C:179:GLY:O	2.18	0.43
1:D:460:THR:C	1:D:462:MET:H	2.27	0.43
1:A:437:ILE:O	1:A:458:ARG:HD3	2.18	0.43
1:B:162:LEU:HB2	1:B:166:GLN:HB2	2.00	0.43
1:B:395:LEU:C	1:B:397:GLN:H	2.27	0.43
1:C:188:GLY:O	1:C:192:HIS:HD2	2.02	0.43
1:C:415:PRO:HB2	1:C:418:LEU:HD13	2.01	0.43
1:D:429:TYR:HD2	1:D:429:TYR:HA	1.73	0.43
1:A:133:HIS:O	1:A:135:PRO:HD3	2.18	0.43
1:A:142:ASP:C	1:A:144:ALA:H	2.27	0.43
1:A:162:LEU:HB2	1:A:166:GLN:HB2	1.99	0.43
1:A:385:LEU:O	1:A:385:LEU:CD2	2.60	0.43
1:B:431:LYS:O	1:B:434:GLU:HB2	2.19	0.43
1:C:205:PRO:CB	1:C:243:THR:HG22	2.48	0.43
1:C:375:HIS:CG	1:C:376:PRO:HD2	2.53	0.43
1:D:371:VAL:O	1:D:371:VAL:CG1	2.67	0.43
1:D:418:LEU:HD12	1:D:418:LEU:N	2.33	0.43
1:B:245:PRO:HG3	1:B:334:CYS:SG	2.59	0.43
1:B:322:LEU:O	1:B:323:HIS:O	2.36	0.43
1:D:320:SER:C	1:D:322:LEU:H	2.26	0.43
1:B:454:HIS:ND1	1:B:454:HIS:N	2.67	0.43
1:C:288:LYS:HG2	1:C:302:THR:HG22	2.01	0.43
1:A:313:HIS:O	1:A:313:HIS:HD2	2.02	0.43
1:B:69:LEU:C	1:B:71:GLU:N	2.77	0.43
1:B:449:GLU:C	1:B:450:ASN:OD1	2.62	0.43
1:C:147:LEU:HD21	1:C:181:LEU:CD2	2.48	0.43
1:C:386:ASP:HB3	1:C:416:GLY:C	2.44	0.43
1:C:399:CYS:HB3	1:C:417:TYR:CD2	2.54	0.43
1:C:424:SER:OG	1:C:425:LEU:N	2.51	0.43
1:D:182:ARG:NE	1:D:213:VAL:O	2.48	0.43
1:D:318:ASN:HD22	1:D:318:ASN:HA	1.55	0.43
1:D:351:TYR:C	1:D:353:SER:N	2.77	0.43
1:D:415:PRO:HB2	1:D:418:LEU:HD13	2.01	0.43
1:A:122:ARG:HD3	1:A:124:GLN:NE2	2.34	0.42
1:A:213:VAL:HG21	1:C:132:HIS:HE1	1.82	0.42
1:A:241:TRP:HB3	1:A:336:LEU:HB3	2.00	0.42
1:B:144:ALA:O	1:B:146:ARG:NH1	2.52	0.42
1:B:402:LEU:HA	1:B:402:LEU:HD23	1.79	0.42
1:C:313:HIS:O	1:C:313:HIS:CD2	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:TYR:C	1:C:353:SER:N	2.77	0.42
1:C:432:TYR:CD1	1:C:437:ILE:HD12	2.54	0.42
1:D:424:SER:OG	1:D:425:LEU:N	2.51	0.42
1:A:92:LEU:HD22	1:A:344:ARG:NE	2.34	0.42
1:B:431:LYS:HB2	1:B:431:LYS:NZ	2.34	0.42
1:C:479:ILE:O	1:C:483:LYS:HB2	2.18	0.42
1:B:142:ASP:C	1:B:144:ALA:H	2.27	0.42
1:C:308:ASP:O	1:C:312:LEU:HD12	2.19	0.42
1:C:314:MET:HE3	1:C:315:TYR:CZ	2.54	0.42
1:D:460:THR:C	1:D:462:MET:N	2.77	0.42
1:D:479:ILE:O	1:D:483:LYS:HB2	2.18	0.42
1:A:73:CYS:CB	1:A:79:LEU:HD23	2.42	0.42
1:A:159:ASP:C	1:A:161:GLU:N	2.77	0.42
1:B:413:VAL:CG1	1:B:414:TRP:N	2.81	0.42
1:B:452:LEU:HD22	1:B:452:LEU:N	2.34	0.42
1:C:289:LEU:HD12	1:C:301:GLU:CG	2.50	0.42
1:D:118:VAL:O	1:D:118:VAL:HG23	2.19	0.42
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.86	0.42
1:D:477:LYS:HD3	1:D:477:LYS:HA	1.94	0.42
1:A:141:GLY:O	1:A:142:ASP:HB2	2.19	0.42
1:A:245:PRO:O	1:A:248:SER:HB3	2.19	0.42
1:C:351:TYR:C	1:C:353:SER:H	2.27	0.42
1:D:205:PRO:CB	1:D:243:THR:HG22	2.49	0.42
1:A:104:VAL:O	1:A:108:LYS:HB2	2.20	0.42
1:A:281:GLU:OE2	1:A:282:GLU:HB2	2.20	0.42
1:B:141:GLY:O	1:B:142:ASP:HB2	2.18	0.42
1:B:153:LEU:O	1:B:156:ILE:HB	2.19	0.42
1:B:170:PHE:C	1:B:172:GLU:N	2.78	0.42
1:B:417:TYR:HD1	1:B:417:TYR:O	2.03	0.42
1:B:456:ARG:NH1	1:B:456:ARG:HG2	2.35	0.42
1:C:182:ARG:NE	1:C:213:VAL:O	2.49	0.42
1:C:318:ASN:HD22	1:C:318:ASN:HA	1.54	0.42
1:D:118:VAL:HG21	1:D:239:LEU:HD22	2.01	0.42
1:D:313:HIS:O	1:D:313:HIS:CD2	2.72	0.42
1:D:386:ASP:HB3	1:D:416:GLY:C	2.45	0.42
1:A:153:LEU:O	1:A:156:ILE:HB	2.20	0.42
1:A:186:LEU:HD23	1:A:186:LEU:C	2.45	0.42
1:A:322:LEU:O	1:A:323:HIS:O	2.38	0.42
1:A:325:ARG:NH1	1:A:330:ASN:ND2	2.67	0.42
1:A:387:VAL:CB	1:A:395:LEU:HD12	2.49	0.42
1:B:231:ILE:HD13	1:D:133:HIS:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:HIS:CB	1:C:97:PRO:HD2	2.37	0.42
1:C:215:PHE:CD2	1:C:233:GLU:HG2	2.55	0.42
1:C:231:ILE:CG2	1:C:232:GLY:H	2.32	0.42
1:C:241:TRP:NE1	1:C:255:TRP:HE1	2.17	0.42
1:C:278:CYS:O	1:C:285:LYS:HA	2.19	0.42
1:A:301:GLU:HG3	1:A:339:ASN:O	2.20	0.42
1:B:126:PHE:CE2	1:B:199:LEU:HD21	2.55	0.42
1:B:215:PHE:CD1	1:B:215:PHE:N	2.88	0.42
1:B:442:LEU:C	1:B:442:LEU:HD23	2.45	0.42
1:C:418:LEU:N	1:C:418:LEU:HD12	2.34	0.42
1:C:423:SER:O	1:C:427:GLN:HB2	2.19	0.42
1:D:204:LEU:CD2	1:D:324:GLY:HA3	2.47	0.42
1:A:245:PRO:HG3	1:A:334:CYS:SG	2.59	0.42
1:A:441:VAL:HG12	1:A:455:LEU:HB3	2.02	0.42
1:A:456:ARG:NH1	1:A:456:ARG:HG2	2.35	0.42
1:B:186:LEU:HD23	1:B:186:LEU:C	2.45	0.42
1:B:281:GLU:OE2	1:B:282:GLU:HB2	2.20	0.42
1:B:445:GLU:O	1:B:447:THR:N	2.53	0.42
1:C:154:ARG:HG2	1:C:154:ARG:HH11	1.85	0.42
1:C:268:MET:O	1:C:270:PRO:HD2	2.20	0.42
1:C:401:GLY:O	1:C:405:GLU:HB2	2.20	0.42
1:C:411:ILE:O	1:C:413:VAL:HG23	2.20	0.42
1:D:82:SER:H	1:D:85:GLN:CG	2.33	0.42
1:D:308:ASP:OD2	1:D:308:ASP:N	2.52	0.42
1:A:144:ALA:O	1:A:146:ARG:NH1	2.53	0.42
1:B:73:CYS:CB	1:B:79:LEU:HD23	2.42	0.42
1:B:320:SER:HA	1:B:323:HIS:CE1	2.55	0.42
1:B:387:VAL:CB	1:B:395:LEU:HD12	2.49	0.42
1:B:416:GLY:C	1:B:418:LEU:N	2.78	0.42
1:C:82:SER:H	1:C:85:GLN:CG	2.33	0.42
1:C:260:LEU:CD2	1:C:275:SER:HB3	2.44	0.42
1:C:407:LEU:C	1:C:409:ASN:H	2.28	0.42
1:C:460:THR:C	1:C:462:MET:H	2.27	0.42
1:A:454:HIS:ND1	1:A:454:HIS:N	2.68	0.41
1:B:245:PRO:O	1:B:248:SER:HB3	2.20	0.41
1:B:325:ARG:NH1	1:B:330:ASN:ND2	2.67	0.41
1:C:170:PHE:C	1:C:172:GLU:N	2.77	0.41
1:C:371:VAL:O	1:C:371:VAL:CG1	2.68	0.41
1:C:375:HIS:CE1	1:C:377:CYS:SG	3.13	0.41
1:C:386:ASP:OD1	1:C:386:ASP:N	2.53	0.41
1:C:455:LEU:HD13	1:C:456:ARG:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:THR:O	1:D:462:MET:N	2.52	0.41
1:A:417:TYR:HD1	1:A:417:TYR:O	2.03	0.41
1:B:122:ARG:HD3	1:B:124:GLN:NE2	2.35	0.41
1:B:420:THR:CG2	1:B:421:MET:N	2.81	0.41
1:C:175:LEU:N	1:C:175:LEU:HD22	2.35	0.41
1:D:70:LEU:HD13	1:D:70:LEU:O	2.20	0.41
1:D:175:LEU:N	1:D:175:LEU:HD22	2.35	0.41
1:D:186:LEU:HD12	1:D:240:VAL:CG2	2.51	0.41
1:D:278:CYS:O	1:D:285:LYS:HA	2.19	0.41
1:D:314:MET:HE3	1:D:315:TYR:CZ	2.55	0.41
1:D:423:SER:O	1:D:427:GLN:HB2	2.19	0.41
1:D:435:MET:O	1:D:436:SER:OG	2.34	0.41
1:A:115:TRP:CZ2	1:A:127:PRO:HB3	2.55	0.41
1:A:117:SER:OG	1:A:258:HIS:CE1	2.73	0.41
1:B:256:LEU:HD22	1:B:287:ASN:CG	2.46	0.41
1:C:197:LEU:HD12	1:C:197:LEU:HA	1.88	0.41
1:C:252:LEU:N	1:C:336:LEU:HD11	2.35	0.41
1:D:386:ASP:OD1	1:D:386:ASP:N	2.54	0.41
1:D:483:LYS:HD2	1:D:484:ASN:OD1	2.20	0.41
1:A:162:LEU:HB2	1:A:166:GLN:CB	2.50	0.41
1:B:445:GLU:C	1:B:447:THR:N	2.70	0.41
1:C:243:THR:O	1:C:333:PRO:HA	2.20	0.41
1:C:268:MET:H	1:C:352:ASP:CG	2.28	0.41
1:C:308:ASP:OD2	1:C:308:ASP:N	2.53	0.41
1:C:429:TYR:HD2	1:C:429:TYR:HA	1.73	0.41
1:C:457:SER:HB2	1:C:462:MET:HG2	2.02	0.41
1:D:411:ILE:O	1:D:413:VAL:HG23	2.20	0.41
1:A:148:VAL:CG2	1:C:148:VAL:CG2	2.98	0.41
1:A:289:LEU:HD13	1:A:289:LEU:HA	1.91	0.41
1:A:453:ILE:HD11	1:A:471:LEU:HD22	2.03	0.41
1:B:161:GLU:O	1:B:162:LEU:C	2.63	0.41
1:C:476:ILE:O	1:C:476:ILE:HG22	2.21	0.41
1:D:215:PHE:CD1	1:D:215:PHE:N	2.89	0.41
1:D:289:LEU:HD12	1:D:301:GLU:CG	2.51	0.41
1:D:455:LEU:HD13	1:D:456:ARG:O	2.20	0.41
1:B:421:MET:HG3	1:B:423:SER:N	2.36	0.41
1:C:141:GLY:O	1:C:142:ASP:HB3	2.21	0.41
1:D:146:ARG:HD2	1:D:178:SER:OG	2.20	0.41
1:D:414:TRP:HA	1:D:415:PRO:HD2	1.80	0.41
1:A:156:ILE:CG2	1:A:167:LEU:HD11	2.51	0.41
1:A:383:VAL:HG13	1:A:383:VAL:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LYS:HA	1:B:163:SER:OG	2.21	0.41
1:C:186:LEU:HD12	1:C:240:VAL:CG2	2.51	0.41
1:C:193:TYR:OH	1:C:333:PRO:HG3	2.20	0.41
1:C:254:PHE:O	1:C:257:ARG:CG	2.61	0.41
1:C:483:LYS:HD2	1:C:484:ASN:OD1	2.21	0.41
1:D:119:VAL:HG13	1:D:125:VAL:CG1	2.51	0.41
1:D:161:GLU:O	1:D:163:SER:N	2.47	0.41
1:D:202:LYS:N	1:D:202:LYS:CD	2.84	0.41
1:D:401:GLY:O	1:D:405:GLU:HB2	2.20	0.41
1:A:413:VAL:CG1	1:A:414:TRP:N	2.82	0.41
1:C:118:VAL:O	1:C:118:VAL:HG23	2.21	0.41
1:C:186:LEU:HD21	1:C:306:LEU:HD11	2.02	0.41
1:C:460:THR:O	1:C:462:MET:N	2.53	0.41
1:A:156:ILE:C	1:A:158:GLN:H	2.29	0.41
1:A:385:LEU:HD21	1:A:417:TYR:CD2	2.56	0.41
1:A:389:ARG:HD2	1:A:389:ARG:N	2.25	0.41
1:B:385:LEU:O	1:B:385:LEU:CD2	2.61	0.41
1:C:167:LEU:N	1:C:167:LEU:HD22	2.36	0.41
1:C:435:MET:O	1:C:436:SER:OG	2.36	0.41
1:D:78:PHE:CZ	1:D:102:LEU:HD23	2.56	0.41
1:D:154:ARG:HG2	1:D:154:ARG:HH11	1.85	0.41
1:D:254:PHE:O	1:D:257:ARG:CG	2.62	0.41
1:D:264:ARG:HG2	1:D:264:ARG:NH1	2.35	0.41
1:D:381:ILE:HG22	1:D:437:ILE:HG23	2.02	0.41
1:D:407:LEU:C	1:D:409:ASN:H	2.27	0.41
1:D:457:SER:HB2	1:D:462:MET:HG2	2.02	0.41
1:D:481:SER:C	1:D:483:LYS:N	2.77	0.41
1:A:145:PHE:CE2	1:A:231:ILE:HG13	2.56	0.41
1:A:256:LEU:HD22	1:A:287:ASN:CG	2.46	0.41
1:B:104:VAL:O	1:B:108:LYS:HB2	2.21	0.41
1:B:113:GLU:HG2	1:B:266:PHE:HZ	1.79	0.41
1:C:135:PRO:HB2	1:C:136:GLY:H	1.70	0.41
1:C:174:VAL:C	1:C:176:LYS:N	2.79	0.41
1:C:270:PRO:C	1:C:272:ASN:N	2.79	0.41
1:C:392:THR:C	1:C:394:GLU:N	2.79	0.41
1:D:141:GLY:O	1:D:142:ASP:HB3	2.20	0.41
1:D:190:LEU:CB	1:D:314:MET:HE2	2.51	0.41
1:D:381:ILE:HG22	1:D:381:ILE:O	2.21	0.41
1:A:201:ASN:HB2	1:A:203:ARG:NH2	2.36	0.40
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.73	0.40
1:B:145:PHE:CE2	1:B:231:ILE:HG13	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:HIS:O	1:B:313:HIS:HD2	2.04	0.40
1:C:134:LYS:HA	1:C:135:PRO:HD2	1.95	0.40
1:C:269:SER:C	1:C:271:SER:N	2.79	0.40
1:C:460:THR:C	1:C:462:MET:N	2.78	0.40
1:D:170:PHE:C	1:D:172:GLU:N	2.78	0.40
1:D:268:MET:H	1:D:352:ASP:CG	2.29	0.40
1:D:299:LEU:C	1:D:299:LEU:HD13	2.46	0.40
1:D:429:TYR:O	1:D:433:ASP:OD2	2.39	0.40
1:A:323:HIS:O	1:A:323:HIS:HD2	2.03	0.40
1:B:453:ILE:HD11	1:B:471:LEU:HD22	2.03	0.40
1:C:119:VAL:C	1:C:121:PHE:N	2.80	0.40
1:C:277:ASP:N	1:C:277:ASP:OD2	2.54	0.40
1:C:432:TYR:HD2	1:C:440:THR:HG21	1.87	0.40
1:D:119:VAL:C	1:D:121:PHE:N	2.79	0.40
1:D:157:LEU:C	1:D:159:ASP:H	2.30	0.40
1:D:164:LYS:HB2	1:D:165:GLU:H	1.66	0.40
1:D:215:PHE:CD2	1:D:233:GLU:HG2	2.56	0.40
1:D:331:VAL:CG2	1:D:332:VAL:N	2.83	0.40
1:A:69:LEU:C	1:A:71:GLU:N	2.77	0.40
1:A:421:MET:HG3	1:A:423:SER:N	2.35	0.40
1:A:431:LYS:NZ	1:A:431:LYS:HB2	2.36	0.40
1:C:122:ARG:O	1:C:122:ARG:HG3	2.21	0.40
1:C:136:GLY:O	1:C:138:LEU:HD22	2.22	0.40
1:C:185:LEU:HD13	1:C:210:GLN:HG2	2.03	0.40
1:C:186:LEU:HD21	1:C:306:LEU:CD1	2.52	0.40
1:C:264:ARG:HG2	1:C:264:ARG:NH1	2.35	0.40
1:C:478:TYR:C	1:C:478:TYR:CD1	3.00	0.40
1:D:420:THR:CG2	1:D:421:MET:H	2.34	0.40
1:D:432:TYR:CD1	1:D:437:ILE:HD12	2.56	0.40
1:A:385:LEU:HB2	1:A:441:VAL:HG22	2.02	0.40
1:B:162:LEU:HB2	1:B:166:GLN:CB	2.51	0.40
1:B:323:HIS:O	1:B:323:HIS:HD2	2.04	0.40
1:C:69:LEU:HD13	1:C:354:PHE:HB2	2.02	0.40
1:C:70:LEU:HD22	1:C:70:LEU:HA	1.94	0.40
1:C:138:LEU:HD13	1:C:138:LEU:HA	1.91	0.40
1:C:148:VAL:HG11	1:C:153:LEU:HD13	2.03	0.40
1:C:244:PRO:HA	1:C:245:PRO:HD3	1.91	0.40
1:D:247:THR:HG22	1:D:250:GLN:HB3	2.03	0.40
1:A:170:PHE:C	1:A:172:GLU:N	2.78	0.40
1:A:244:PRO:HA	1:A:245:PRO:HD3	1.87	0.40
1:A:380:PRO:HG2	1:A:381:ILE:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:TRP:CZ2	1:B:127:PRO:HB3	2.57	0.40
1:B:156:ILE:C	1:B:158:GLN:H	2.29	0.40
1:C:145:PHE:O	1:C:180:LYS:HA	2.22	0.40
1:D:193:TYR:OH	1:D:333:PRO:HG3	2.22	0.40
1:D:241:TRP:NE1	1:D:255:TRP:HE1	2.19	0.40
1:D:451:GLY:O	1:D:452:LEU:HD13	2.22	0.40
1:D:476:ILE:O	1:D:476:ILE:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/474 (82%)	284 (73%)	66 (17%)	41 (10%)	0	2
1	B	391/474 (82%)	284 (73%)	64 (16%)	43 (11%)	0	1
1	C	391/474 (82%)	288 (74%)	72 (18%)	31 (8%)	1	4
1	D	391/474 (82%)	288 (74%)	73 (19%)	30 (8%)	1	4
All	All	1564/1896 (82%)	1144 (73%)	275 (18%)	145 (9%)	0	2

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	199	LEU
1	A	202	LYS
1	A	282	GLU
1	A	309	HIS
1	A	323	HIS
1	A	370	LYS
1	A	450	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	461	THR
1	A	464	GLU
1	A	468	ILE
1	A	469	SER
1	B	121	PHE
1	B	199	LEU
1	B	202	LYS
1	B	282	GLU
1	B	309	HIS
1	B	323	HIS
1	B	370	LYS
1	B	450	ASN
1	B	461	THR
1	B	464	GLU
1	B	468	ILE
1	B	469	SER
1	C	168	VAL
1	C	200	VAL
1	C	318	ASN
1	D	168	VAL
1	D	200	VAL
1	D	318	ASN
1	D	462	MET
1	A	136	GLY
1	A	163	SER
1	A	278	CYS
1	A	285	LYS
1	A	294	PRO
1	A	371	VAL
1	A	382	LYS
1	A	391	PRO
1	A	392	THR
1	A	424	SER
1	A	425	LEU
1	B	136	GLY
1	B	163	SER
1	B	248	SER
1	B	278	CYS
1	B	285	LYS
1	B	294	PRO
1	B	371	VAL
1	B	382	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	391	PRO
1	B	392	THR
1	B	424	SER
1	B	425	LEU
1	C	120	VAL
1	C	135	PRO
1	C	156	ILE
1	C	161	GLU
1	C	309	HIS
1	C	370	LYS
1	C	371	VAL
1	C	461	THR
1	C	462	MET
1	C	468	ILE
1	D	120	VAL
1	D	135	PRO
1	D	156	ILE
1	D	161	GLU
1	D	309	HIS
1	D	370	LYS
1	D	371	VAL
1	D	417	TYR
1	D	461	THR
1	D	468	ILE
1	A	135	PRO
1	A	155	GLU
1	A	171	LEU
1	A	248	SER
1	A	446	THR
1	B	155	GLU
1	B	171	LEU
1	B	446	THR
1	C	83	LYS
1	C	122	ARG
1	C	276	SER
1	C	278	CYS
1	C	352	ASP
1	C	385	LEU
1	C	417	TYR
1	C	451	GLY
1	D	83	LYS
1	D	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	276	SER
1	D	278	CYS
1	D	352	ASP
1	D	385	LEU
1	D	451	GLY
1	A	120	VAL
1	A	151	GLU
1	A	385	LEU
1	A	417	TYR
1	B	120	VAL
1	B	123	GLU
1	B	135	PRO
1	B	151	GLU
1	C	136	GLY
1	C	393	LEU
1	C	424	SER
1	C	446	THR
1	D	393	LEU
1	D	424	SER
1	D	446	THR
1	A	123	GLU
1	A	420	THR
1	A	421	MET
1	B	174	VAL
1	B	201	ASN
1	B	385	LEU
1	B	417	TYR
1	B	420	THR
1	C	142	ASP
1	C	285	LYS
1	C	321	LYS
1	C	480	SER
1	D	142	ASP
1	D	285	LYS
1	D	480	SER
1	A	164	LYS
1	A	174	VAL
1	A	201	ASN
1	A	383	VAL
1	A	437	ILE
1	A	451	GLY
1	B	149	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	LYS
1	B	383	VAL
1	B	421	MET
1	B	437	ILE
1	B	451	GLY
1	C	123	GLU
1	C	166	GLN
1	D	136	GLY
1	D	166	GLN
1	D	321	LYS
1	B	270	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	356/419 (85%)	328 (92%)	28 (8%)	11	36
1	B	356/419 (85%)	328 (92%)	28 (8%)	11	36
1	C	356/419 (85%)	325 (91%)	31 (9%)	9	32
1	D	356/419 (85%)	327 (92%)	29 (8%)	11	35
All	All	1424/1676 (85%)	1308 (92%)	116 (8%)	11	35

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	88	ARG
1	A	102	LEU
1	A	116	THR
1	A	118	VAL
1	A	124	GLN
1	A	148	VAL
1	A	166	GLN
1	A	167	LEU
1	A	174	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	ARG
1	A	205	PRO
1	A	218	VAL
1	A	229	LYS
1	A	231	ILE
1	A	247	THR
1	A	268	MET
1	A	281	GLU
1	A	299	LEU
1	A	371	VAL
1	A	385	LEU
1	A	389	ARG
1	A	395	LEU
1	A	431	LYS
1	A	452	LEU
1	A	453	ILE
1	A	471	LEU
1	A	483	LYS
1	B	70	LEU
1	B	88	ARG
1	B	102	LEU
1	B	116	THR
1	B	118	VAL
1	B	124	GLN
1	B	148	VAL
1	B	166	GLN
1	B	167	LEU
1	B	174	VAL
1	B	182	ARG
1	B	205	PRO
1	B	218	VAL
1	B	229	LYS
1	B	231	ILE
1	B	247	THR
1	B	268	MET
1	B	281	GLU
1	B	299	LEU
1	B	371	VAL
1	B	385	LEU
1	B	389	ARG
1	B	395	LEU
1	B	431	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	452	LEU
1	B	453	ILE
1	B	471	LEU
1	B	483	LYS
1	C	67	GLU
1	C	70	LEU
1	C	88	ARG
1	C	91	LEU
1	C	116	THR
1	C	118	VAL
1	C	122	ARG
1	C	138	LEU
1	C	182	ARG
1	C	211	ILE
1	C	238	SER
1	C	241	TRP
1	C	247	THR
1	C	257	ARG
1	C	274	SER
1	C	277	ASP
1	C	310	GLU
1	C	311	LEU
1	C	312	LEU
1	C	314	MET
1	C	318	ASN
1	C	376	PRO
1	C	386	ASP
1	C	389	ARG
1	C	406	LEU
1	C	426	GLU
1	C	429	TYR
1	C	440	THR
1	C	441	VAL
1	C	455	LEU
1	C	472	LYS
1	D	67	GLU
1	D	70	LEU
1	D	88	ARG
1	D	91	LEU
1	D	116	THR
1	D	118	VAL
1	D	122	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	138	LEU
1	D	182	ARG
1	D	238	SER
1	D	241	TRP
1	D	247	THR
1	D	257	ARG
1	D	277	ASP
1	D	310	GLU
1	D	311	LEU
1	D	312	LEU
1	D	314	MET
1	D	318	ASN
1	D	376	PRO
1	D	386	ASP
1	D	389	ARG
1	D	406	LEU
1	D	426	GLU
1	D	429	TYR
1	D	440	THR
1	D	441	VAL
1	D	455	LEU
1	D	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	84	GLN
1	A	124	GLN
1	A	133	HIS
1	A	166	GLN
1	A	173	ASN
1	A	187	HIS
1	A	192	HIS
1	A	201	ASN
1	A	249	ASN
1	A	258	HIS
1	A	287	ASN
1	A	292	ASN
1	A	313	HIS
1	A	318	ASN
1	A	323	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	400	GLN
1	A	409	ASN
1	A	427	GLN
1	A	450	ASN
1	B	77	HIS
1	B	84	GLN
1	B	133	HIS
1	B	166	GLN
1	B	173	ASN
1	B	187	HIS
1	B	192	HIS
1	B	201	ASN
1	B	249	ASN
1	B	258	HIS
1	B	287	ASN
1	B	313	HIS
1	B	318	ASN
1	B	323	HIS
1	B	400	GLN
1	B	409	ASN
1	B	427	GLN
1	B	450	ASN
1	C	124	GLN
1	C	132	HIS
1	C	158	GLN
1	C	192	HIS
1	C	216	HIS
1	C	318	ASN
1	C	330	ASN
1	C	400	GLN
1	C	467	HIS
1	D	158	GLN
1	D	192	HIS
1	D	216	HIS
1	D	292	ASN
1	D	313	HIS
1	D	318	ASN
1	D	323	HIS
1	D	330	ASN
1	D	400	GLN
1	D	467	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/474 (83%)	-1.26	0 100 100	23, 73, 155, 193	0
1	B	397/474 (83%)	-1.19	1 (0%) 90 81	26, 74, 161, 194	0
1	C	397/474 (83%)	-1.22	0 100 100	28, 80, 163, 202	0
1	D	397/474 (83%)	-1.22	1 (0%) 90 81	26, 78, 169, 202	0
All	All	1588/1896 (83%)	-1.22	2 (0%) 92 88	23, 77, 162, 202	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	GLU	3.4
1	D	448	LEU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.