



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 5AX8 / pdb_00005ax8
Title : Recombinant expression, purification and preliminary crystallographic studies of the mature form of human mitochondrial aspartate aminotransferase
Authors : Jiang, X.; Wang, J.; Chang, H.; Zhou, Y.
Deposited on : 2015-07-20
Resolution : 2.99 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

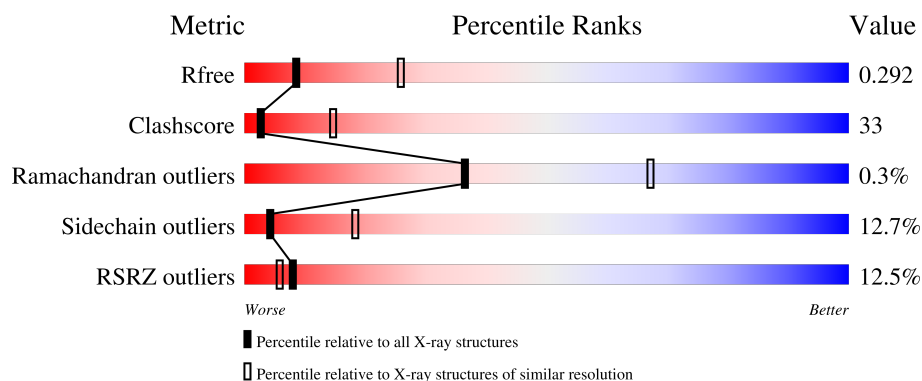
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	407	6% 32% 48% 16% ..
1	B	407	16% 58% 35%
1	C	407	12% 47% 40% 11% .
1	D	407	15% 44% 44% 9% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12580 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 Aspartate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			
1	B	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			
1	C	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			
1	D	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	GLY	VAL	engineered mutation	UNP P00505
A	431	HIS	-	expression tag	UNP P00505
A	432	HIS	-	expression tag	UNP P00505
A	433	HIS	-	expression tag	UNP P00505
A	434	HIS	-	expression tag	UNP P00505
A	435	HIS	-	expression tag	UNP P00505
A	436	HIS	-	expression tag	UNP P00505
B	346	GLY	VAL	engineered mutation	UNP P00505
B	431	HIS	-	expression tag	UNP P00505
B	432	HIS	-	expression tag	UNP P00505
B	433	HIS	-	expression tag	UNP P00505
B	434	HIS	-	expression tag	UNP P00505
B	435	HIS	-	expression tag	UNP P00505
B	436	HIS	-	expression tag	UNP P00505
C	346	GLY	VAL	engineered mutation	UNP P00505
C	431	HIS	-	expression tag	UNP P00505
C	432	HIS	-	expression tag	UNP P00505
C	433	HIS	-	expression tag	UNP P00505
C	434	HIS	-	expression tag	UNP P00505
C	435	HIS	-	expression tag	UNP P00505
C	436	HIS	-	expression tag	UNP P00505

Continued on next page...

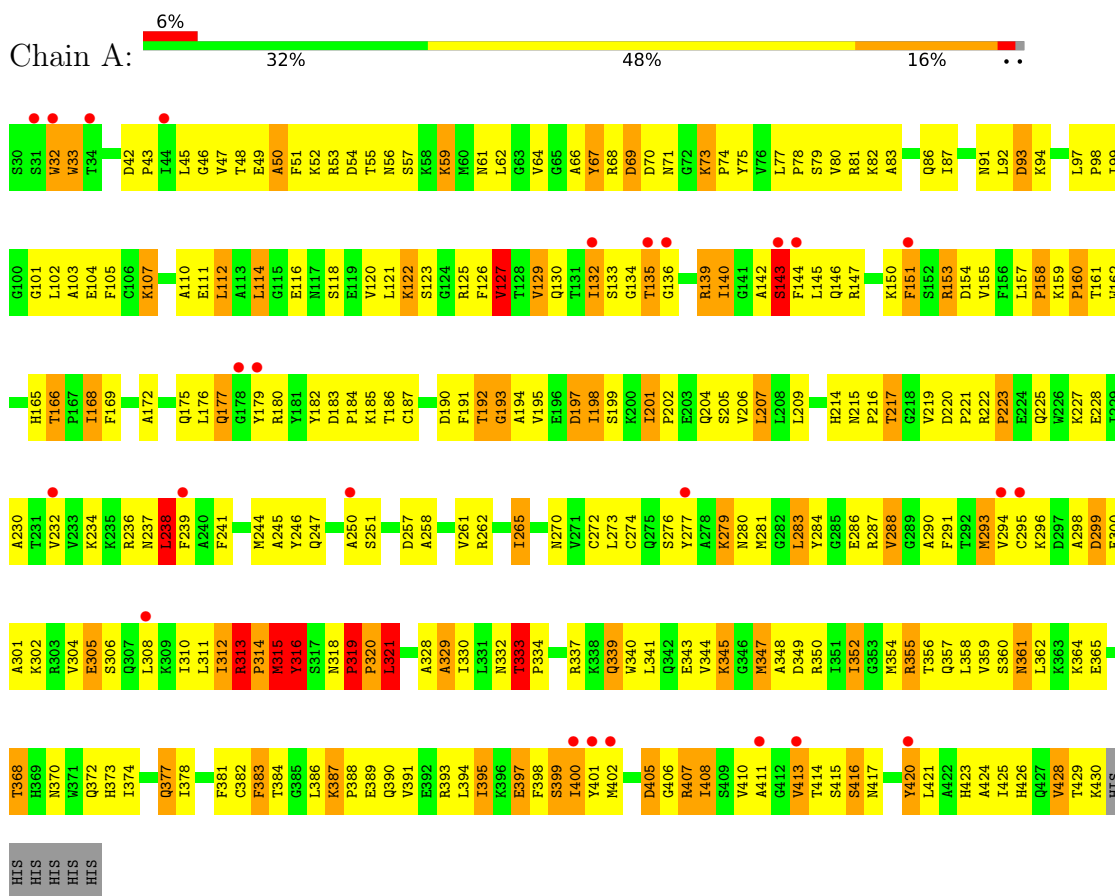
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	346	GLY	VAL	engineered mutation	UNP P00505
D	431	HIS	-	expression tag	UNP P00505
D	432	HIS	-	expression tag	UNP P00505
D	433	HIS	-	expression tag	UNP P00505
D	434	HIS	-	expression tag	UNP P00505
D	435	HIS	-	expression tag	UNP P00505
D	436	HIS	-	expression tag	UNP P00505

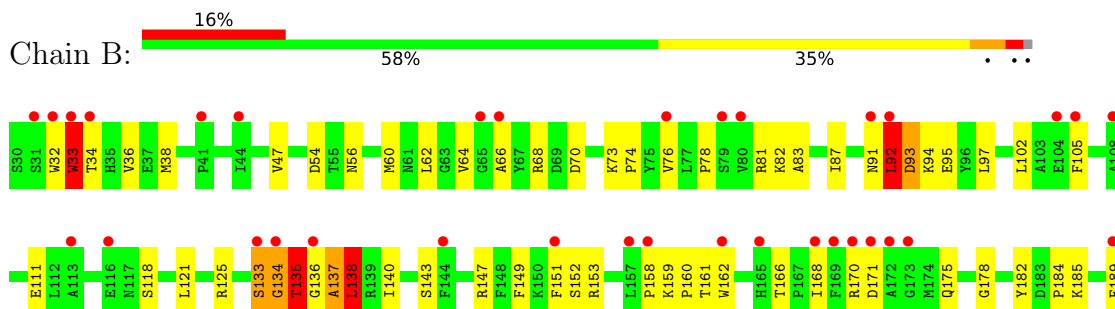
3 Residue-property plots

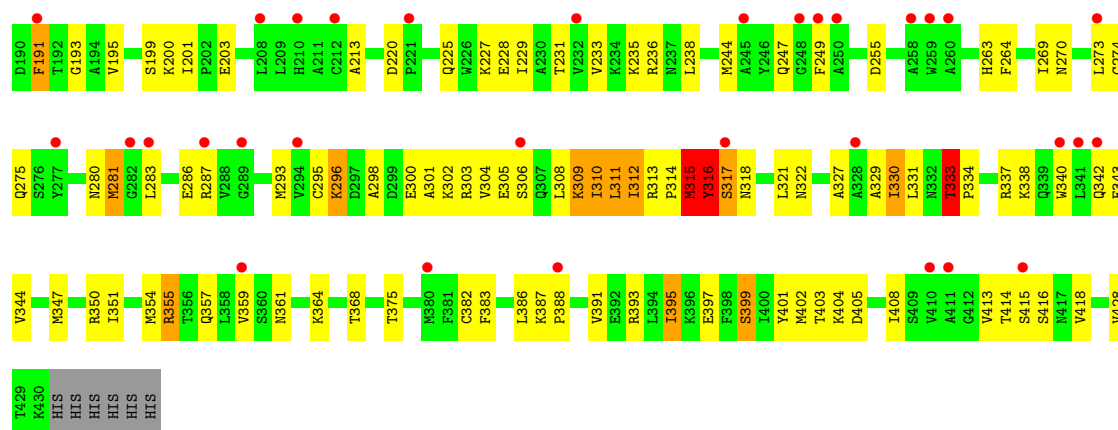
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

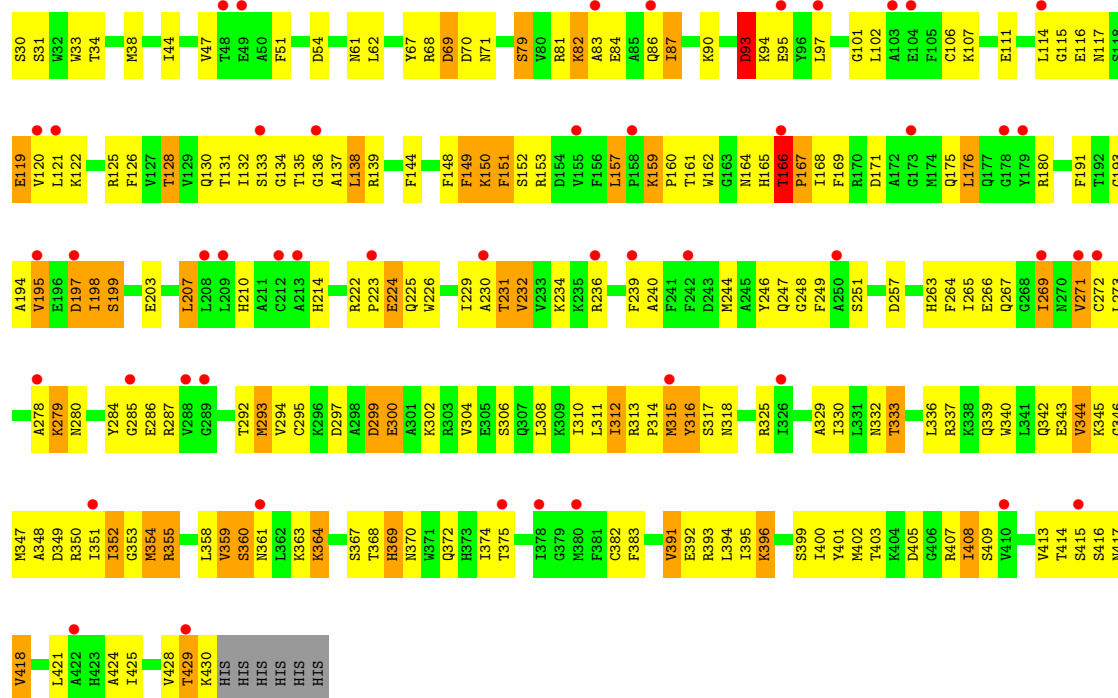


- Molecule 1: Aspartate aminotransferase, mitochondrial

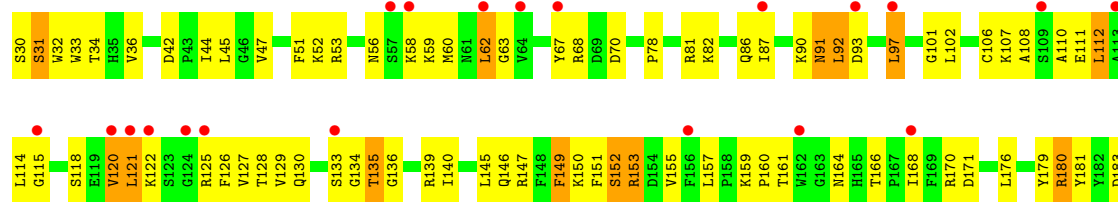
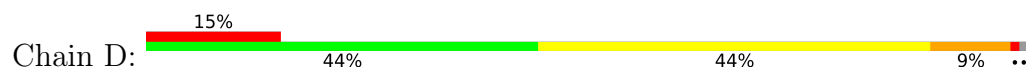


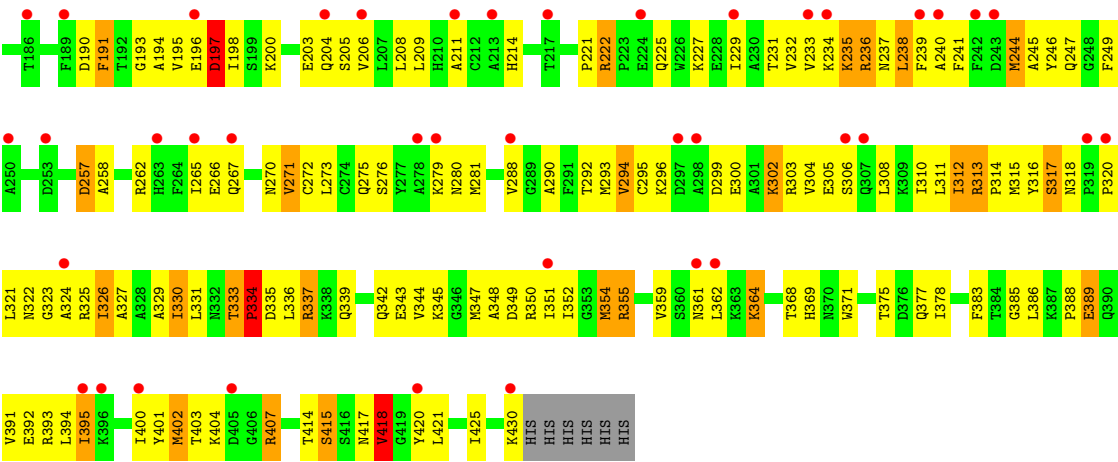


• Molecule 1: Aspartate aminotransferase, mitochondrial



• Molecule 1: Aspartate aminotransferase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.71Å 76.14Å 94.25Å 78.00° 85.65° 78.41°	Depositor
Resolution (Å)	48.31 – 2.99 48.31 – 2.99	Depositor EDS
% Data completeness (in resolution range)	88.2 (48.31-2.99) 84.4 (48.31-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.273 , 0.291 0.277 , 0.292	Depositor DCC
R_{free} test set	2000 reflections (7.42%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12580	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6868e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.96	49/3218 (1.5%)	1.49	64/4348 (1.5%)
1	B	0.96	7/3218 (0.2%)	1.08	20/4348 (0.5%)
1	C	0.99	4/3218 (0.1%)	1.08	20/4348 (0.5%)
1	D	0.87	4/3218 (0.1%)	1.12	23/4348 (0.5%)
All	All	1.28	64/12872 (0.5%)	1.20	127/17392 (0.7%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	LEU	CA-C	-7.59	1.44	1.52
1	D	195	VAL	C-O	-6.82	1.16	1.24
1	A	378	ILE	C-O	-6.33	1.17	1.24
1	A	129	VAL	C-O	-6.27	1.17	1.24
1	D	233	VAL	C-O	-6.23	1.16	1.24
1	A	197	ASP	C-O	-6.14	1.17	1.24
1	C	318	ASN	C-O	-5.95	1.18	1.24
1	A	201	ILE	C-N	5.90	1.40	1.33
1	A	143	SER	C-O	-5.77	1.17	1.24
1	B	137	ALA	C-O	-5.75	1.17	1.24
1	A	318	ASN	C-N	5.71	1.40	1.33
1	A	274	CYS	C-O	-5.70	1.17	1.24
1	A	313	ARG	C-O	-5.67	1.19	1.24
1	A	127	VAL	C-O	-5.66	1.18	1.24
1	A	305	GLU	CA-C	-5.65	1.45	1.52
1	A	112	LEU	C-O	-5.65	1.17	1.24
1	A	356	THR	C-O	-5.62	1.17	1.24
1	A	157	LEU	C-N	5.59	1.40	1.33
1	A	166	THR	C-N	5.54	1.40	1.34
1	A	103	ALA	C-O	-5.51	1.17	1.24
1	A	291	PHE	C-O	-5.46	1.17	1.24
1	A	86	GLN	C-O	-5.46	1.17	1.24
1	A	97	LEU	C-O	-5.45	1.18	1.24
1	A	381	PHE	CA-C	-5.43	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	PRO	N-CD	5.43	1.55	1.47
1	A	388	PRO	N-CD	5.42	1.55	1.47
1	A	408	ILE	N-CA	-5.36	1.40	1.46
1	B	333	THR	C-N	5.36	1.40	1.33
1	A	333	THR	C-N	5.35	1.40	1.34
1	A	183	ASP	C-N	5.34	1.40	1.34
1	A	230	ALA	CA-C	-5.33	1.45	1.52
1	A	207	LEU	C-O	-5.32	1.17	1.24
1	D	333	THR	C-N	5.32	1.40	1.34
1	A	319	PRO	N-CD	5.27	1.55	1.47
1	A	143	SER	CA-C	-5.26	1.46	1.52
1	C	167	PRO	N-CD	5.26	1.55	1.47
1	A	193	GLY	C-O	-5.25	1.17	1.23
1	B	314	PRO	N-CD	5.24	1.55	1.47
1	A	155	VAL	C-O	-5.23	1.18	1.24
1	B	316	TYR	CA-C	-5.22	1.46	1.52
1	A	162	TRP	CA-C	-5.21	1.46	1.52
1	A	223	PRO	N-CD	5.19	1.55	1.47
1	A	225	GLN	C-O	-5.18	1.18	1.24
1	A	313	ARG	C-N	5.17	1.40	1.33
1	D	334	PRO	N-CD	5.17	1.54	1.47
1	C	315	MET	C-O	-5.16	1.18	1.24
1	A	158	PRO	N-CD	5.15	1.54	1.47
1	A	157	LEU	C-O	-5.15	1.18	1.24
1	C	359	VAL	C-O	-5.14	1.18	1.24
1	A	209	LEU	N-CA	-5.14	1.39	1.46
1	A	129	VAL	CA-C	-5.12	1.46	1.52
1	A	64	VAL	C-O	-5.12	1.18	1.24
1	A	73	LYS	C-N	5.11	1.40	1.33
1	A	305	GLU	C-O	-5.11	1.18	1.24
1	B	193	GLY	C-O	-5.11	1.17	1.23
1	A	329	ALA	C-O	-5.09	1.18	1.24
1	B	118	SER	CA-C	-5.09	1.46	1.52
1	A	320	PRO	N-CD	5.06	1.54	1.47
1	A	140	ILE	C-O	-5.06	1.18	1.24
1	A	97	LEU	C-N	5.03	1.40	1.33
1	A	217	THR	C-O	-5.03	1.18	1.24
1	A	67	TYR	CA-C	-5.01	1.46	1.52
1	A	314	PRO	N-CD	5.00	1.54	1.47
1	A	177	GLN	C-O	-5.00	1.17	1.23

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	LEU	N-CA-C	12.29	124.41	111.14
1	D	315	MET	N-CA-C	9.27	121.47	111.36
1	A	313	ARG	N-CA-C	-8.81	100.76	112.75
1	D	312	ILE	N-CA-C	8.61	119.42	110.72
1	C	316	TYR	N-CA-C	-8.36	95.55	108.76
1	A	397	GLU	N-CA-C	8.31	120.41	111.36
1	D	316	TYR	N-CA-C	-8.06	96.02	108.76
1	D	153	ARG	N-CA-C	-7.94	101.35	113.89
1	B	33	TRP	N-CA-C	7.89	123.06	112.88
1	B	397	GLU	N-CA-C	7.79	119.85	111.36
1	A	315	MET	N-CA-C	7.76	119.81	111.36
1	B	312	ILE	N-CA-C	7.71	118.50	110.72
1	A	316	TYR	N-CA-C	-7.70	97.00	108.79
1	B	93	ASP	N-CA-C	7.66	121.05	109.41
1	B	315	MET	N-CA-C	7.57	119.32	111.14
1	A	347	MET	N-CA-C	7.45	119.48	111.36
1	A	312	ILE	N-CA-C	7.30	118.09	110.72
1	A	217	THR	N-CA-C	7.13	119.05	111.28
1	A	139	ARG	N-CA-C	7.10	119.10	111.36
1	A	32	TRP	N-CA-C	6.68	118.35	111.14
1	C	195	VAL	CB-CA-C	-6.67	103.13	112.14
1	A	53	ARG	N-CA-C	6.67	119.55	111.82
1	D	317	SER	N-CA-C	6.64	118.60	111.36
1	D	166	THR	CA-C-N	-6.60	112.90	119.56
1	D	166	THR	C-N-CA	-6.60	112.90	119.56
1	A	157	LEU	CA-C-N	-6.57	113.90	120.21
1	A	157	LEU	C-N-CA	-6.57	113.90	120.21
1	C	230	ALA	N-CA-C	6.50	118.36	111.28
1	A	359	VAL	N-CA-C	6.48	117.26	110.72
1	D	197	ASP	N-CA-C	-6.42	104.20	111.07
1	D	52	LYS	N-CA-C	6.40	119.24	111.82
1	B	316	TYR	N-CA-C	-6.31	99.08	108.99
1	A	361	ASN	N-CA-C	6.30	118.23	111.36
1	B	133	SER	N-CA-C	6.30	119.79	111.28
1	A	166	THR	CA-C-N	-6.30	113.32	119.87
1	A	166	THR	C-N-CA	-6.30	113.32	119.87
1	C	197	ASP	N-CA-C	6.28	118.21	111.36
1	B	138	LEU	N-CA-C	6.25	118.17	111.36
1	B	231	THR	CB-CA-C	-6.24	100.42	110.79
1	A	238	LEU	N-CA-C	-6.24	102.48	110.53
1	C	354	MET	N-CA-C	6.23	118.15	111.36
1	C	346	GLY	N-CA-C	-6.14	105.36	112.73
1	B	135	THR	N-CA-C	-6.09	104.64	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	TYR	N-CA-C	-6.08	104.65	111.28
1	B	166	THR	CA-C-N	-6.06	113.44	119.56
1	B	166	THR	C-N-CA	-6.06	113.44	119.56
1	D	32	TRP	N-CA-C	-6.04	104.81	111.82
1	C	344	VAL	N-CA-C	6.02	116.80	110.72
1	A	395	ILE	N-CA-C	5.99	116.16	110.53
1	A	201	ILE	CA-C-N	-5.97	114.12	120.03
1	A	201	ILE	C-N-CA	-5.97	114.12	120.03
1	C	344	VAL	CB-CA-C	-5.92	104.04	112.22
1	A	318	ASN	CA-C-N	-5.90	114.31	120.38
1	A	318	ASN	C-N-CA	-5.90	114.31	120.38
1	A	417	ASN	N-CA-C	5.87	120.46	112.88
1	D	318	ASN	N-CA-C	-5.83	102.98	108.22
1	A	166	THR	O-C-N	5.79	124.96	120.38
1	A	318	ASN	N-CA-C	-5.78	103.02	108.22
1	A	222	ARG	N-CA-C	-5.76	102.85	110.40
1	A	73	LYS	CA-C-N	-5.75	113.86	119.78
1	A	73	LYS	C-N-CA	-5.75	113.86	119.78
1	C	166	THR	O-C-N	5.75	124.92	120.38
1	A	97	LEU	CA-C-N	-5.70	113.82	119.92
1	A	97	LEU	C-N-CA	-5.70	113.82	119.92
1	A	299	ASP	N-CA-C	-5.61	105.17	111.28
1	A	184	PRO	N-CA-C	5.61	120.91	113.57
1	D	198	ILE	N-CA-C	5.61	116.38	110.72
1	A	132	ILE	N-CA-C	-5.60	99.42	107.37
1	C	300	GLU	N-CA-C	-5.59	105.28	111.71
1	B	314	PRO	N-CA-C	5.57	121.27	113.53
1	A	290	ALA	N-CA-C	5.55	117.71	108.99
1	D	299	ASP	N-CA-C	-5.54	105.24	111.28
1	A	147	ARG	N-CA-C	5.54	117.39	111.36
1	A	265	ILE	N-CA-C	5.51	116.29	110.72
1	D	62	LEU	N-CA-C	-5.50	106.15	112.92
1	A	400	ILE	CB-CA-C	-5.49	102.46	110.81
1	A	250	ALA	N-CA-C	5.49	116.94	111.07
1	B	191	PHE	N-CA-C	5.44	117.21	111.28
1	A	99	ILE	CB-CA-C	-5.44	104.80	112.14
1	A	190	ASP	N-CA-C	-5.43	99.11	108.56
1	D	344	VAL	N-CA-C	-5.42	105.09	110.62
1	C	312	ILE	N-CA-C	5.42	116.15	110.62
1	A	42	ASP	CA-C-N	-5.39	113.07	119.05
1	A	42	ASP	C-N-CA	-5.39	113.07	119.05
1	C	148	PHE	N-CA-C	5.38	119.82	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	ASN	N-CA-C	5.38	120.50	113.30
1	D	333	THR	CA-C-N	-5.36	113.00	118.85
1	D	333	THR	C-N-CA	-5.36	113.00	118.85
1	A	377	GLN	N-CA-C	5.36	118.05	110.50
1	A	192	THR	N-CA-C	-5.32	105.48	111.28
1	A	352	ILE	N-CA-C	-5.31	105.20	110.62
1	B	395	ILE	CB-CA-C	-5.29	105.09	112.02
1	A	288	VAL	CB-CA-C	-5.28	104.29	111.15
1	A	405	ASP	N-CA-C	-5.26	106.12	112.54
1	C	429	THR	N-CA-C	5.25	119.32	113.02
1	A	368	THR	N-CA-C	5.25	117.08	111.36
1	B	333	THR	CA-C-N	-5.24	113.51	119.28
1	B	333	THR	C-N-CA	-5.24	113.51	119.28
1	A	184	PRO	CA-N-CD	-5.22	104.69	112.00
1	C	352	ILE	N-CA-C	-5.22	105.29	110.62
1	A	320	PRO	N-CA-C	5.21	119.27	111.14
1	B	317	SER	N-CA-C	5.21	117.04	111.36
1	A	122	LYS	CA-C-N	5.20	127.25	120.28
1	A	122	LYS	C-N-CA	5.20	127.25	120.28
1	C	166	THR	CA-C-N	-5.20	113.28	119.05
1	C	166	THR	C-N-CA	-5.20	113.28	119.05
1	A	287	ARG	N-CA-C	5.17	118.72	111.74
1	A	428	VAL	N-CA-C	5.15	115.92	110.72
1	D	326	ILE	N-CA-C	5.15	115.92	110.72
1	A	202	PRO	CA-N-CD	-5.14	104.80	112.00
1	D	120	VAL	N-CA-C	5.13	115.85	110.62
1	C	159	LYS	C-N-CD	-5.13	109.31	120.60
1	D	418	VAL	CB-CA-C	-5.13	105.14	112.22
1	A	388	PRO	CB-CA-C	-5.11	104.19	112.62
1	C	318	ASN	N-CA-C	5.10	114.00	108.14
1	B	91	ASN	N-CA-C	5.08	117.53	109.50
1	A	362	LEU	N-CA-C	-5.08	105.75	111.28
1	D	385	GLY	N-CA-C	-5.08	108.24	115.30
1	A	334	PRO	CA-N-CD	-5.07	104.90	112.00
1	D	389	GLU	N-CA-C	-5.07	105.84	111.36
1	A	157	LEU	N-CA-C	-5.05	102.82	110.50
1	C	391	VAL	N-CA-C	-5.05	105.47	110.62
1	A	158	PRO	N-CA-C	5.05	118.29	111.22
1	A	97	LEU	O-C-N	5.04	125.48	121.55
1	A	50	ALA	N-CA-C	-5.03	105.80	111.28
1	B	92	LEU	N-CA-C	-5.03	102.66	109.54
1	D	395	ILE	CB-CA-C	-5.02	105.45	112.02

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	3145	0	3133	296	0
1	B	3145	0	3133	165	0
1	C	3145	0	3133	217	0
1	D	3145	0	3133	258	0
All	All	12580	0	12532	841	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 33.

All (841) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:CZ2	1:C:293:MET:HE1	1.56	1.38
1:B:32:TRP:CE3	1:D:151:PHE:CZ	2.21	1.29
1:D:333:THR:HG21	1:D:336:LEU:CD1	1.63	1.28
1:D:333:THR:HG23	1:D:336:LEU:CB	1.65	1.26
1:D:333:THR:CG2	1:D:336:LEU:HB2	1.65	1.25
1:B:33:TRP:HH2	1:D:149:PHE:CD1	1.54	1.24
1:B:32:TRP:CZ3	1:D:151:PHE:CZ	2.29	1.20
1:A:354:MET:HE1	1:A:414:THR:C	1.66	1.19
1:D:149:PHE:CZ	1:D:151:PHE:CE1	2.31	1.17
1:D:70:ASP:OD1	1:D:414:THR:HG23	1.41	1.17
1:A:78:PRO:HD2	1:A:343:GLU:OE2	1.44	1.14
1:B:33:TRP:CH2	1:D:149:PHE:CE1	2.34	1.14
1:B:33:TRP:HH2	1:D:149:PHE:CE1	1.65	1.14
1:D:149:PHE:CZ	1:D:151:PHE:HE1	1.66	1.13
1:A:140:ILE:CD1	1:A:315:MET:HE1	1.80	1.12
1:D:389:GLU:O	1:D:393:ARG:HG3	1.45	1.12
1:B:32:TRP:CZ3	1:D:151:PHE:CE1	2.39	1.11
1:C:354:MET:HE1	1:C:414:THR:C	1.74	1.10
1:D:333:THR:CG2	1:D:336:LEU:CB	2.25	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TRP:CH2	1:D:149:PHE:CD1	2.40	1.09
1:A:140:ILE:HD13	1:A:315:MET:HE1	1.35	1.08
1:C:354:MET:CE	1:C:414:THR:C	2.29	1.06
1:D:333:THR:CG2	1:D:336:LEU:HD12	1.85	1.06
1:B:306:SER:O	1:B:310:ILE:HG13	1.54	1.05
1:B:311:LEU:O	1:B:315:MET:HE3	1.57	1.04
1:C:349:ASP:HA	1:C:352:ILE:HD12	1.38	1.03
1:A:302:LYS:HG2	1:C:38:MET:HE1	1.39	1.02
1:B:33:TRP:NE1	1:D:293:MET:SD	2.33	1.01
1:A:354:MET:HE2	1:A:414:THR:CA	1.91	1.00
1:D:70:ASP:CB	1:D:350:ARG:NH2	2.24	1.00
1:C:180:ARG:HH11	1:C:193:GLY:HA2	1.24	1.00
1:B:344:VAL:HA	1:B:347:MET:HE3	1.40	1.00
1:C:339:GLN:O	1:C:343:GLU:HG3	1.60	0.99
1:D:229:ILE:O	1:D:232:VAL:HG12	1.60	0.99
1:A:33:TRP:CE2	1:C:293:MET:HE1	1.97	0.99
1:B:32:TRP:HZ3	1:D:151:PHE:CE1	1.77	0.99
1:C:308:LEU:O	1:C:312:ILE:HG13	1.63	0.99
1:A:355:ARG:NH2	1:A:377:GLN:HB2	1.78	0.98
1:A:140:ILE:CD1	1:A:315:MET:CE	2.42	0.97
1:A:293:MET:CE	1:C:33:TRP:HE1	1.78	0.96
1:A:354:MET:HE2	1:A:414:THR:HA	1.44	0.96
1:A:354:MET:CE	1:A:414:THR:CA	2.43	0.96
1:B:33:TRP:CH2	1:D:149:PHE:HE1	1.83	0.96
1:D:70:ASP:HB2	1:D:350:ARG:NH2	1.80	0.96
1:C:340:TRP:O	1:C:344:VAL:HG23	1.66	0.96
1:A:132:ILE:CD1	1:C:132:ILE:HD13	1.96	0.95
1:C:354:MET:HE2	1:C:414:THR:CA	1.96	0.95
1:A:354:MET:CE	1:A:414:THR:C	2.38	0.94
1:B:200:LYS:C	1:B:236:ARG:HH11	1.75	0.94
1:A:293:MET:CE	1:C:33:TRP:NE1	2.29	0.94
1:C:191:PHE:CD2	1:C:225:GLN:HG2	2.01	0.94
1:A:135:THR:HG21	1:C:317:SER:OG	1.69	0.93
1:B:93:ASP:OD1	1:B:94:LYS:N	2.00	0.93
1:B:32:TRP:HE3	1:D:151:PHE:CZ	1.73	0.93
1:D:128:THR:HG22	1:D:292:THR:HG23	1.51	0.93
1:A:140:ILE:HD11	1:A:315:MET:CE	1.99	0.93
1:A:48:THR:HG23	1:A:61:ASN:ND2	1.83	0.92
1:A:158:PRO:HG2	1:A:161:THR:HB	1.51	0.92
1:A:382:CYS:O	1:A:407:ARG:HA	1.70	0.91
1:B:354:MET:HE2	1:B:413:VAL:O	1.70	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:CZ2	1:C:293:MET:CE	2.52	0.91
1:B:92:LEU:HA	1:D:81:ARG:NH2	1.85	0.91
1:B:32:TRP:CE3	1:D:151:PHE:HZ	1.75	0.91
1:D:70:ASP:HB2	1:D:350:ARG:HH21	1.36	0.90
1:C:114:LEU:HD21	1:C:265:ILE:HD12	1.54	0.90
1:D:70:ASP:CB	1:D:350:ARG:HH22	1.84	0.89
1:C:354:MET:HE3	1:C:413:VAL:HG12	1.54	0.89
1:C:354:MET:HE2	1:C:414:THR:HA	1.52	0.89
1:C:344:VAL:HA	1:C:347:MET:HE2	1.55	0.89
1:D:354:MET:HE3	1:D:354:MET:HA	1.52	0.88
1:C:131:THR:OG1	1:C:137:ALA:HB2	1.73	0.88
1:D:70:ASP:CA	1:D:350:ARG:HH22	1.87	0.88
1:C:139:ARG:HB2	1:C:168:ILE:HG23	1.53	0.88
1:B:158:PRO:HG2	1:B:161:THR:HB	1.54	0.87
1:C:329:ALA:O	1:C:333:THR:HG23	1.73	0.87
1:A:354:MET:HE3	1:A:413:VAL:CG1	2.05	0.87
1:C:354:MET:HE1	1:C:414:THR:O	1.75	0.86
1:D:179:TYR:HA	1:D:197:ASP:OD2	1.74	0.86
1:D:333:THR:HG21	1:D:336:LEU:HD12	0.89	0.86
1:C:191:PHE:O	1:C:195:VAL:HG23	1.75	0.85
1:C:414:THR:O	1:C:418:VAL:HG22	1.77	0.85
1:B:200:LYS:C	1:B:236:ARG:NH1	2.35	0.85
1:B:168:ILE:HG12	1:D:314:PRO:O	1.77	0.85
1:D:70:ASP:OD1	1:D:414:THR:CG2	2.23	0.84
1:D:326:ILE:O	1:D:330:ILE:HG22	1.77	0.84
1:B:32:TRP:HE3	1:D:151:PHE:HZ	1.13	0.84
1:D:70:ASP:CA	1:D:350:ARG:NH2	2.39	0.84
1:D:149:PHE:CE2	1:D:151:PHE:CE1	2.66	0.83
1:D:414:THR:O	1:D:418:VAL:HG22	1.77	0.83
1:D:70:ASP:HA	1:D:350:ARG:HH22	1.42	0.83
1:A:33:TRP:HZ2	1:C:293:MET:CE	1.88	0.83
1:A:55:THR:OG1	1:D:153:ARG:HG3	1.78	0.83
1:A:33:TRP:HB2	1:C:300:GLU:CD	2.03	0.82
1:A:394:LEU:HD22	1:A:400:ILE:HD12	1.59	0.82
1:B:264:PHE:HD2	1:B:269:ILE:HD11	1.44	0.82
1:C:333:THR:OG1	1:C:336:LEU:HB2	1.80	0.82
1:A:394:LEU:HD23	1:A:424:ALA:HB1	1.62	0.81
1:A:228:GLU:O	1:A:232:VAL:HG23	1.79	0.81
1:B:329:ALA:O	1:B:333:THR:HG23	1.79	0.81
1:C:198:ILE:HD13	1:C:207:LEU:HD11	1.62	0.81
1:D:355:ARG:HH12	1:D:377:GLN:HB2	1.43	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:HZ2	1:C:293:MET:HE1	1.02	0.81
1:A:348:ALA:O	1:A:352:ILE:HG13	1.80	0.80
1:A:56:ASN:O	1:A:59:LYS:HD3	1.81	0.80
1:B:136:GLY:O	1:B:140:ILE:HG13	1.82	0.80
1:C:139:ARG:HB2	1:C:168:ILE:CG2	2.10	0.80
1:B:93:ASP:O	1:B:94:LYS:HG2	1.82	0.80
1:A:354:MET:HE1	1:A:414:THR:O	1.82	0.79
1:B:270:ASN:HD21	1:B:296:LYS:HD3	1.46	0.79
1:D:82:LYS:HB2	1:D:336:LEU:HD21	1.63	0.79
1:D:151:PHE:HD1	1:D:204:GLN:O	1.66	0.79
1:C:67:TYR:OH	1:C:350:ARG:HD3	1.83	0.78
1:B:391:VAL:HG22	1:B:402:MET:HE3	1.65	0.78
1:A:166:THR:HG23	1:A:176:LEU:CD1	2.13	0.78
1:A:387:LYS:O	1:A:390:GLN:HB2	1.84	0.78
1:A:354:MET:HE3	1:A:413:VAL:HG13	1.64	0.78
1:C:355:ARG:HH22	1:C:382:CYS:HB2	1.49	0.78
1:D:331:LEU:HD23	1:D:331:LEU:O	1.84	0.78
1:A:283:LEU:HD12	1:A:288:VAL:HG21	1.65	0.78
1:A:350:ARG:HG2	1:A:350:ARG:HH21	1.49	0.77
1:A:354:MET:CE	1:A:414:THR:N	2.48	0.77
1:A:279:LYS:HD2	1:A:284:TYR:HE1	1.50	0.77
1:A:293:MET:HE1	1:C:33:TRP:HE1	1.48	0.77
1:D:354:MET:HE3	1:D:354:MET:CA	2.14	0.77
1:C:224:GLU:CD	1:C:224:GLU:H	1.93	0.76
1:B:33:TRP:CH2	1:D:149:PHE:HD1	1.96	0.76
1:D:151:PHE:CD1	1:D:204:GLN:O	2.39	0.76
1:B:36:VAL:HG11	1:D:304:VAL:HA	1.69	0.75
1:C:355:ARG:HH11	1:C:355:ARG:HG2	1.51	0.75
1:D:92:LEU:HD12	1:D:92:LEU:H	1.51	0.75
1:A:283:LEU:N	1:A:283:LEU:HD23	2.01	0.75
1:B:315:MET:HE2	1:D:139:ARG:NH1	2.02	0.75
1:B:317:SER:OG	1:D:135:THR:HG21	1.87	0.75
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.51	0.75
1:B:388:PRO:HB3	1:B:404:LYS:HD2	1.67	0.75
1:A:33:TRP:NE1	1:C:293:MET:SD	2.57	0.75
1:A:306:SER:O	1:A:310:ILE:HG13	1.86	0.75
1:B:95:GLU:CD	1:D:68:ARG:HH12	1.94	0.75
1:A:48:THR:HG23	1:A:61:ASN:HD21	1.51	0.75
1:A:140:ILE:HD11	1:A:315:MET:HE2	1.68	0.75
1:D:327:ALA:HA	1:D:330:ILE:CG2	2.17	0.75
1:D:333:THR:HG23	1:D:336:LEU:HB2	0.81	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:MET:HA	1:D:354:MET:CE	2.13	0.74
1:A:382:CYS:HB3	1:A:408:ILE:HG12	1.68	0.74
1:C:359:VAL:HG21	1:C:375:THR:HG23	1.67	0.74
1:A:340:TRP:O	1:A:344:VAL:HG23	1.87	0.74
1:D:333:THR:HG21	1:D:336:LEU:CG	2.18	0.74
1:A:391:VAL:HG12	1:A:395:ILE:CD1	2.18	0.73
1:D:345:LYS:O	1:D:349:ASP:HB2	1.88	0.73
1:C:355:ARG:HG2	1:C:355:ARG:NH1	2.01	0.73
1:A:283:LEU:HB3	1:A:286:GLU:HB2	1.70	0.73
1:A:355:ARG:NH2	1:A:377:GLN:CB	2.52	0.73
1:B:200:LYS:HA	1:B:236:ARG:NH1	2.02	0.73
1:B:36:VAL:O	1:D:303:ARG:NH1	2.21	0.73
1:D:351:ILE:O	1:D:355:ARG:HG3	1.89	0.72
1:D:391:VAL:O	1:D:395:ILE:HG13	1.89	0.72
1:D:354:MET:HE3	1:D:354:MET:O	1.89	0.72
1:A:413:VAL:CG2	1:A:421:LEU:HD22	2.19	0.72
1:B:200:LYS:CA	1:B:236:ARG:HH11	2.02	0.72
1:D:414:THR:HG22	1:D:415:SER:N	2.04	0.72
1:D:275:GLN:NE2	1:D:290:ALA:HB3	2.05	0.72
1:C:354:MET:CE	1:C:414:THR:CA	2.63	0.72
1:A:70:ASP:O	1:A:414:THR:HG23	1.89	0.72
1:D:244:MET:HE2	1:D:273:LEU:HD11	1.72	0.72
1:A:82:LYS:CE	1:A:339:GLN:HE22	2.03	0.72
1:C:62:LEU:HD13	1:C:408:ILE:HG13	1.69	0.71
1:A:87:ILE:HG23	1:A:92:LEU:HD12	1.70	0.71
1:A:300:GLU:O	1:A:304:VAL:HG23	1.90	0.71
1:A:339:GLN:O	1:A:343:GLU:HG3	1.89	0.71
1:C:198:ILE:CD1	1:C:207:LEU:HD11	2.20	0.71
1:A:180:ARG:O	1:A:194:ALA:HB2	1.90	0.71
1:D:145:LEU:O	1:D:153:ARG:NH2	2.23	0.71
1:B:344:VAL:HA	1:B:347:MET:CE	2.18	0.71
1:C:295:CYS:HB3	1:C:300:GLU:HG2	1.73	0.71
1:D:350:ARG:O	1:D:354:MET:HB2	1.90	0.71
1:B:322:ASN:ND2	1:D:322:ASN:OD1	2.24	0.71
1:A:394:LEU:CD2	1:A:424:ALA:HB1	2.20	0.71
1:D:62:LEU:HB2	1:D:402:MET:HB3	1.73	0.71
1:B:133:SER:HB2	1:B:287:ARG:HA	1.71	0.70
1:C:355:ARG:HH11	1:C:355:ARG:CG	2.04	0.70
1:C:31:SER:HB3	1:C:34:THR:HG23	1.71	0.70
1:D:70:ASP:HA	1:D:350:ARG:NH2	2.04	0.70
1:D:82:LYS:NZ	1:D:339:GLN:OE1	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ALA:HB2	1:D:128:THR:HG21	1.72	0.70
1:A:33:TRP:HE1	1:C:293:MET:CE	2.04	0.70
1:A:83:ALA:O	1:A:87:ILE:HD12	1.91	0.70
1:D:82:LYS:CB	1:D:336:LEU:HD21	2.22	0.70
1:A:169:PHE:O	1:A:172:ALA:HB3	1.91	0.70
1:A:293:MET:HE3	1:C:33:TRP:NE1	2.07	0.70
1:C:151:PHE:HD1	1:C:151:PHE:H	1.38	0.70
1:D:149:PHE:CE2	1:D:206:VAL:CG1	2.75	0.70
1:A:140:ILE:HD11	1:A:315:MET:HE1	1.60	0.69
1:A:391:VAL:HG12	1:A:395:ILE:HD12	1.74	0.69
1:D:157:LEU:HD22	1:D:208:LEU:HD23	1.72	0.69
1:D:310:ILE:O	1:D:314:PRO:HD3	1.92	0.69
1:D:355:ARG:NH1	1:D:377:GLN:HB2	2.07	0.69
1:B:32:TRP:HZ3	1:D:151:PHE:CZ	1.88	0.69
1:B:355:ARG:HG2	1:B:355:ARG:NH1	2.06	0.69
1:D:191:PHE:HD2	1:D:225:GLN:HG2	1.55	0.69
1:D:327:ALA:O	1:D:330:ILE:HG23	1.92	0.69
1:C:106:CYS:HB3	1:C:128:THR:HB	1.73	0.69
1:C:198:ILE:HD13	1:C:207:LEU:CD1	2.22	0.69
1:A:350:ARG:HG2	1:A:350:ARG:NH2	2.03	0.69
1:D:63:GLY:HA2	1:D:407:ARG:HH21	1.57	0.69
1:B:170:ARG:HH12	1:B:175:GLN:HA	1.58	0.68
1:A:350:ARG:NH1	1:A:413:VAL:O	2.23	0.68
1:B:135:THR:HG23	1:B:162:TRP:HH2	1.57	0.68
1:C:117:ASN:O	1:C:122:LYS:HE3	1.94	0.68
1:A:70:ASP:O	1:A:414:THR:CG2	2.41	0.68
1:C:306:SER:O	1:C:310:ILE:HG13	1.92	0.68
1:D:322:ASN:O	1:D:326:ILE:HG13	1.94	0.68
1:B:200:LYS:CA	1:B:236:ARG:NH1	2.56	0.68
1:D:321:LEU:HD21	1:D:325:ARG:NH2	2.08	0.68
1:D:93:ASP:O	1:D:325:ARG:NH2	2.24	0.68
1:D:193:GLY:O	1:D:196:GLU:HB3	1.94	0.68
1:A:132:ILE:HD13	1:C:132:ILE:HD13	1.73	0.68
1:A:354:MET:HE3	1:A:413:VAL:HG12	1.74	0.68
1:A:33:TRP:NE1	1:C:293:MET:CE	2.57	0.67
1:D:333:THR:CG2	1:D:336:LEU:CD1	2.52	0.67
1:A:54:ASP:OD1	1:A:399:SER:HB3	1.93	0.67
1:A:33:TRP:CD1	1:C:304:VAL:HG21	2.29	0.67
1:D:333:THR:CG2	1:D:336:LEU:HB3	2.21	0.67
1:A:199:SER:O	1:A:236:ARG:NH1	2.27	0.67
1:A:311:LEU:O	1:A:314:PRO:HD2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ILE:O	1:C:337:ARG:HB2	1.95	0.67
1:A:391:VAL:O	1:A:395:ILE:HG13	1.94	0.67
1:A:393:ARG:O	1:A:397:GLU:HB2	1.95	0.66
1:C:115:GLY:C	1:C:117:ASN:H	2.03	0.66
1:B:33:TRP:CD1	1:D:293:MET:SD	2.88	0.66
1:A:191:PHE:CE1	1:A:195:VAL:HG21	2.30	0.66
1:A:201:ILE:O	1:A:236:ARG:NH1	2.29	0.66
1:D:333:THR:HG23	1:D:333:THR:O	1.94	0.66
1:A:191:PHE:CZ	1:A:195:VAL:HG21	2.30	0.66
1:D:311:LEU:O	1:D:314:PRO:HD2	1.96	0.66
1:A:198:ILE:HD13	1:A:207:LEU:HD21	1.78	0.66
1:D:211:ALA:HB3	1:D:244:MET:HG3	1.76	0.66
1:B:171:ASP:OD1	1:D:147:ARG:NH2	2.29	0.65
1:C:191:PHE:HD2	1:C:225:GLN:HG2	1.56	0.65
1:C:263:HIS:HA	1:C:266:GLU:HG2	1.78	0.65
1:A:102:LEU:HB3	1:A:105:PHE:HB3	1.78	0.65
1:A:258:ALA:O	1:A:262:ARG:HG3	1.96	0.65
1:A:312:ILE:O	1:A:313:ARG:C	2.35	0.65
1:C:311:LEU:O	1:C:314:PRO:HD2	1.95	0.65
1:A:364:LYS:NZ	1:B:151:PHE:O	2.30	0.65
1:B:264:PHE:CD2	1:B:269:ILE:HD11	2.28	0.65
1:B:338:LYS:O	1:B:342:GLN:HG3	1.96	0.65
1:A:391:VAL:CG1	1:A:395:ILE:HD11	2.27	0.65
1:A:382:CYS:HB3	1:A:408:ILE:CG1	2.26	0.65
1:B:92:LEU:CA	1:D:81:ARG:NH2	2.58	0.65
1:D:414:THR:HG22	1:D:415:SER:H	1.60	0.65
1:C:360:SER:HA	1:C:363:LYS:HG2	1.79	0.65
1:D:150:LYS:HG3	1:D:151:PHE:CD2	2.32	0.65
1:A:132:ILE:CD1	1:C:132:ILE:CD1	2.75	0.64
1:A:373:HIS:O	1:A:377:GLN:HG3	1.96	0.64
1:C:86:GLN:HE22	1:C:333:THR:HG21	1.63	0.64
1:C:93:ASP:O	1:C:325:ARG:NH2	2.28	0.64
1:A:293:MET:HE3	1:C:33:TRP:HE1	1.58	0.64
1:B:159:LYS:HE3	1:B:178:GLY:HA3	1.78	0.64
1:C:391:VAL:HG12	1:C:395:ILE:CD1	2.27	0.64
1:A:166:THR:HG23	1:A:176:LEU:HD12	1.78	0.64
1:D:120:VAL:HG22	1:D:125:ARG:NE	2.13	0.64
1:A:33:TRP:CE2	1:C:293:MET:CE	2.78	0.64
1:A:143:SER:O	1:A:146:GLN:N	2.29	0.64
1:C:382:CYS:HB3	1:C:408:ILE:HG23	1.80	0.64
1:D:231:THR:O	1:D:235:LYS:N	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ASN:HA	1:C:364:LYS:HB2	1.79	0.64
1:B:244:MET:HE2	1:B:273:LEU:HD11	1.80	0.63
1:A:54:ASP:HB2	1:A:401:TYR:OH	1.98	0.63
1:A:355:ARG:HH21	1:A:377:GLN:HB2	1.62	0.63
1:D:149:PHE:CE1	1:D:151:PHE:CE1	2.86	0.63
1:A:123:SER:OG	1:A:125:ARG:HG2	1.98	0.63
1:A:286:GLU:OE1	1:A:286:GLU:HA	1.97	0.63
1:A:329:ALA:O	1:A:333:THR:HG23	1.98	0.63
1:B:306:SER:O	1:B:310:ILE:CG1	2.39	0.63
1:A:394:LEU:CD2	1:A:424:ALA:CB	2.77	0.63
1:A:49:GLU:OE2	1:A:49:GLU:HA	1.98	0.63
1:A:205:SER:O	1:A:238:LEU:HB3	1.98	0.63
1:C:339:GLN:HG2	1:C:343:GLU:OE2	1.99	0.62
1:A:355:ARG:HH21	1:A:377:GLN:CB	2.12	0.62
1:A:166:THR:HG23	1:A:176:LEU:HD13	1.81	0.62
1:C:164:ASN:O	1:C:168:ILE:HG13	2.00	0.62
1:A:33:TRP:HB2	1:C:300:GLU:OE1	1.98	0.62
1:D:70:ASP:CG	1:D:350:ARG:HH22	2.07	0.62
1:A:176:LEU:O	1:A:177:GLN:NE2	2.33	0.62
1:B:350:ARG:O	1:B:354:MET:HG2	1.99	0.62
1:D:108:ALA:HB1	1:D:331:LEU:HD22	1.82	0.62
1:C:199:SER:O	1:C:236:ARG:CZ	2.48	0.61
1:C:249:PHE:HB2	1:C:280:ASN:HB3	1.80	0.61
1:D:112:LEU:HD13	1:D:331:LEU:HD11	1.82	0.61
1:B:227:LYS:HD2	1:B:263:HIS:CE1	2.35	0.61
1:B:304:VAL:O	1:B:308:LEU:HD23	2.00	0.61
1:A:62:LEU:HD11	1:A:421:LEU:HD11	1.80	0.61
1:C:354:MET:HE2	1:C:414:THR:C	2.14	0.61
1:D:231:THR:O	1:D:234:LYS:HB3	2.00	0.61
1:A:354:MET:HE2	1:A:414:THR:N	2.14	0.61
1:A:33:TRP:HD1	1:C:304:VAL:HG21	1.65	0.61
1:A:127:VAL:CG2	1:A:305:GLU:HG3	2.31	0.61
1:B:93:ASP:O	1:B:94:LYS:CG	2.49	0.60
1:B:351:ILE:O	1:B:355:ARG:HD2	2.01	0.60
1:A:33:TRP:CZ3	1:C:149:PHE:HE1	2.20	0.60
1:A:107:LYS:O	1:A:111:GLU:HG3	2.00	0.60
1:A:355:ARG:CG	1:A:355:ARG:HH11	2.14	0.60
1:B:354:MET:HE2	1:B:413:VAL:C	2.25	0.60
1:D:354:MET:HE3	1:D:354:MET:C	2.26	0.60
1:A:201:ILE:O	1:A:236:ARG:CZ	2.50	0.60
1:C:354:MET:CE	1:C:414:THR:O	2.44	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:CE1	1:D:151:PHE:CZ	2.89	0.60
1:A:355:ARG:NH1	1:A:355:ARG:HG2	2.17	0.60
1:B:357:GLN:O	1:B:361:ASN:ND2	2.23	0.60
1:D:331:LEU:HA	1:D:337:ARG:HG3	1.83	0.60
1:B:303:ARG:NH1	1:D:36:VAL:O	2.35	0.60
1:B:244:MET:HG2	1:B:247:GLN:HB2	1.84	0.60
1:C:244:MET:HE2	1:C:273:LEU:HD11	1.83	0.59
1:A:33:TRP:CH2	1:C:149:PHE:HE1	2.20	0.59
1:A:261:VAL:O	1:A:265:ILE:HG13	2.02	0.59
1:B:170:ARG:NH1	1:B:175:GLN:HA	2.17	0.59
1:C:349:ASP:CA	1:C:352:ILE:HD12	2.25	0.59
1:D:149:PHE:CE2	1:D:206:VAL:HG13	2.37	0.59
1:A:383:PHE:CD1	1:A:407:ARG:HB2	2.38	0.59
1:D:333:THR:CG2	1:D:333:THR:O	2.50	0.59
1:A:358:LEU:HD13	1:A:421:LEU:HD23	1.85	0.59
1:B:293:MET:HE1	1:D:33:TRP:CZ2	2.38	0.59
1:C:240:ALA:HB3	1:C:271:VAL:HG12	1.84	0.59
1:A:321:LEU:HB2	1:C:285:GLY:O	2.02	0.59
1:A:382:CYS:O	1:A:407:ARG:CA	2.49	0.59
1:A:244:MET:HB2	1:A:273:LEU:HD11	1.85	0.58
1:A:46:GLY:O	1:A:50:ALA:N	2.24	0.58
1:A:206:VAL:HG13	1:A:239:PHE:HD2	1.69	0.58
1:C:191:PHE:CE2	1:C:225:GLN:HG2	2.37	0.58
1:A:48:THR:O	1:A:51:PHE:HB3	2.04	0.58
1:A:330:ILE:O	1:A:337:ARG:HB2	2.04	0.58
1:C:247:GLN:O	1:C:280:ASN:ND2	2.34	0.58
1:B:73:LYS:HG2	1:B:74:PRO:HD2	1.85	0.58
1:B:33:TRP:HE3	1:B:33:TRP:HA	1.68	0.58
1:C:391:VAL:HG12	1:C:395:ILE:HD12	1.86	0.58
1:D:190:ASP:O	1:D:194:ALA:HB2	2.03	0.57
1:C:358:LEU:HD23	1:C:374:ILE:HG21	1.86	0.57
1:B:280:ASN:O	1:B:340:TRP:NE1	2.37	0.57
1:D:258:ALA:O	1:D:262:ARG:HG3	2.04	0.57
1:D:321:LEU:HG	1:D:325:ARG:NE	2.19	0.57
1:C:313:ARG:N	1:C:314:PRO:CD	2.67	0.57
1:D:118:SER:O	1:D:121:LEU:HD23	2.05	0.57
1:A:32:TRP:O	1:A:33:TRP:HE3	1.88	0.57
1:A:383:PHE:CE1	1:A:405:ASP:OD2	2.58	0.57
1:B:315:MET:HG3	1:B:316:TYR:CE1	2.40	0.57
1:B:33:TRP:HA	1:B:33:TRP:CE3	2.40	0.57
1:B:354:MET:CE	1:B:413:VAL:C	2.77	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:HE	1:C:193:GLY:HA3	1.69	0.57
1:B:293:MET:HE1	1:D:33:TRP:HZ2	1.70	0.57
1:D:86:GLN:OE1	1:D:90:LYS:NZ	2.38	0.57
1:D:348:ALA:HA	1:D:351:ILE:HD12	1.86	0.57
1:C:151:PHE:CD1	1:C:151:PHE:N	2.73	0.57
1:C:354:MET:HE1	1:C:415:SER:N	2.17	0.57
1:D:92:LEU:HD13	1:D:325:ARG:NH1	2.20	0.57
1:A:33:TRP:NE1	1:C:293:MET:HE1	2.16	0.56
1:A:293:MET:CE	1:C:33:TRP:CE2	2.88	0.56
1:D:70:ASP:OD2	1:D:415:SER:OG	2.22	0.56
1:A:127:VAL:HG23	1:A:305:GLU:HG3	1.87	0.56
1:A:151:PHE:CD1	1:A:151:PHE:N	2.73	0.56
1:D:227:LYS:O	1:D:231:THR:HG23	2.05	0.56
1:A:401:TYR:CD1	1:A:401:TYR:N	2.73	0.56
1:A:118:SER:O	1:A:122:LYS:HG3	2.05	0.56
1:A:398:PHE:O	1:A:420:TYR:OH	2.22	0.56
1:B:355:ARG:HH11	1:B:355:ARG:CG	2.16	0.56
1:C:180:ARG:NH1	1:C:193:GLY:HA2	2.08	0.56
1:D:321:LEU:HD21	1:D:325:ARG:HH21	1.69	0.56
1:B:32:TRP:HH2	1:D:204:GLN:HA	1.71	0.56
1:B:38:MET:HE2	1:D:303:ARG:HG2	1.87	0.56
1:B:47:VAL:HG13	1:B:401:TYR:HB3	1.86	0.56
1:D:245:ALA:HA	1:D:276:SER:HB3	1.88	0.56
1:D:342:GLN:O	1:D:345:LYS:HB3	2.05	0.56
1:D:159:LYS:HG3	1:D:179:TYR:O	2.06	0.56
1:B:315:MET:HE2	1:D:139:ARG:HH12	1.69	0.56
1:A:186:THR:O	1:A:187:CYS:HB2	2.05	0.55
1:A:139:ARG:HD3	1:C:315:MET:HA	1.88	0.55
1:B:249:PHE:HB2	1:B:280:ASN:HB3	1.89	0.55
1:A:74:PRO:HB3	1:C:95:GLU:OE2	2.06	0.55
1:A:279:LYS:HD2	1:A:284:TYR:CE1	2.37	0.55
1:B:137:ALA:CB	1:B:274:CYS:HB3	2.36	0.55
1:D:31:SER:OG	1:D:34:THR:HG23	2.06	0.55
1:D:271:VAL:O	1:D:294:VAL:HG13	2.06	0.55
1:A:345:LYS:O	1:A:349:ASP:HB2	2.06	0.55
1:C:223:PRO:O	1:C:226:TRP:HB2	2.07	0.55
1:D:120:VAL:HG22	1:D:125:ARG:HE	1.70	0.55
1:C:199:SER:O	1:C:236:ARG:NH1	2.39	0.55
1:D:271:VAL:N	1:D:294:VAL:HG22	2.22	0.55
1:A:45:LEU:C	1:A:45:LEU:HD23	2.32	0.55
1:D:362:LEU:HD13	1:D:371:TRP:CD2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:O	1:A:429:THR:HG23	2.07	0.55
1:B:140:ILE:O	1:B:143:SER:OG	2.24	0.55
1:D:67:TYR:CE2	1:D:347:MET:HB3	2.42	0.55
1:D:414:THR:N	1:D:417:ASN:OD1	2.25	0.55
1:A:310:ILE:O	1:A:314:PRO:HD3	2.07	0.54
1:D:58:LYS:HE2	1:D:420:TYR:CD2	2.43	0.54
1:A:236:ARG:HB2	1:A:238:LEU:HG	1.88	0.54
1:A:430:LYS:O	1:A:430:LYS:HG2	2.06	0.54
1:C:360:SER:O	1:C:363:LYS:HG2	2.06	0.54
1:A:82:LYS:HE2	1:A:339:GLN:HE22	1.71	0.54
1:A:191:PHE:O	1:A:195:VAL:HG23	2.07	0.54
1:A:354:MET:HE2	1:A:413:VAL:C	2.33	0.54
1:C:402:MET:HB2	1:C:407:ARG:O	2.07	0.54
1:D:62:LEU:N	1:D:401:TYR:O	2.31	0.54
1:D:191:PHE:CD1	1:D:191:PHE:C	2.85	0.54
1:A:398:PHE:O	1:A:420:TYR:CE1	2.61	0.54
1:D:180:ARG:HG3	1:D:197:ASP:OD1	2.06	0.54
1:D:265:ILE:HG13	1:D:266:GLU:N	2.22	0.54
1:A:245:ALA:HA	1:A:276:SER:HB3	1.89	0.54
1:B:34:THR:HA	1:D:303:ARG:HH22	1.72	0.54
1:A:32:TRP:C	1:A:33:TRP:CE3	2.85	0.54
1:A:43:PRO:O	1:A:47:VAL:HG23	2.07	0.54
1:A:280:ASN:OD1	1:A:281:MET:N	2.40	0.54
1:B:327:ALA:O	1:B:331:LEU:HG	2.08	0.54
1:D:222:ARG:HH12	1:D:378:ILE:HD11	1.73	0.54
1:D:386:LEU:HD21	1:D:425:ILE:HG23	1.88	0.54
1:A:93:ASP:OD1	1:A:93:ASP:N	2.29	0.54
1:D:270:ASN:OD1	1:D:296:LYS:HE2	2.08	0.53
1:A:56:ASN:ND2	1:A:399:SER:OG	2.24	0.53
1:B:83:ALA:O	1:B:87:ILE:HD12	2.08	0.53
1:B:354:MET:CE	1:B:413:VAL:O	2.52	0.53
1:D:310:ILE:O	1:D:314:PRO:CD	2.55	0.53
1:C:299:ASP:O	1:C:302:LYS:N	2.41	0.53
1:B:191:PHE:O	1:B:195:VAL:HG23	2.08	0.53
1:C:119:GLU:O	1:C:120:VAL:C	2.48	0.53
1:A:154:ASP:HA	1:A:175:GLN:HB2	1.91	0.53
1:C:83:ALA:O	1:C:87:ILE:HG23	2.08	0.53
1:A:176:LEU:C	1:A:177:GLN:HG2	2.33	0.53
1:B:92:LEU:HA	1:D:81:ARG:HH22	1.70	0.53
1:D:308:LEU:O	1:D:312:ILE:HG13	2.09	0.53
1:C:51:PHE:HD1	1:C:401:TYR:CD2	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:PRO:O	1:D:82:LYS:HG2	2.09	0.53
1:A:55:THR:HG1	1:D:153:ARG:HG3	1.70	0.52
1:D:70:ASP:CG	1:D:350:ARG:NH2	2.66	0.52
1:A:87:ILE:HG23	1:A:92:LEU:CD1	2.38	0.52
1:A:54:ASP:OD2	1:A:56:ASN:HB3	2.09	0.52
1:A:320:PRO:HA	1:C:287:ARG:HG2	1.91	0.52
1:A:125:ARG:HD2	1:A:295:CYS:O	2.09	0.52
1:A:146:GLN:O	1:A:153:ARG:NH2	2.42	0.52
1:D:414:THR:CG2	1:D:415:SER:N	2.73	0.52
1:A:299:ASP:O	1:A:302:LYS:HB3	2.09	0.52
1:C:400:ILE:HD13	1:C:421:LEU:HD12	1.92	0.52
1:D:208:LEU:HD12	1:D:209:LEU:N	2.25	0.52
1:D:389:GLU:C	1:D:393:ARG:HG3	2.30	0.52
1:D:267:GLN:O	1:D:267:GLN:HG3	2.08	0.52
1:A:130:GLN:NE2	1:A:319:PRO:HG2	2.25	0.52
1:B:233:VAL:HG13	1:B:238:LEU:HB2	1.91	0.52
1:C:180:ARG:HH11	1:C:193:GLY:CA	2.10	0.52
1:C:349:ASP:O	1:C:353:GLY:N	2.42	0.52
1:A:132:ILE:HD12	1:C:132:ILE:CD1	2.39	0.52
1:A:140:ILE:CD1	1:A:315:MET:HE2	2.30	0.52
1:A:354:MET:CE	1:A:413:VAL:C	2.83	0.52
1:A:413:VAL:HG21	1:A:421:LEU:HD22	1.91	0.52
1:C:157:LEU:HD11	1:C:176:LEU:HB3	1.91	0.52
1:C:273:LEU:HB3	1:C:292:THR:HB	1.91	0.52
1:D:262:ARG:HA	1:D:265:ILE:HG12	1.91	0.52
1:A:146:GLN:O	1:A:153:ARG:NH1	2.41	0.51
1:A:246:TYR:HE1	1:A:279:LYS:HE2	1.74	0.51
1:B:137:ALA:HB3	1:B:274:CYS:HB3	1.91	0.51
1:C:355:ARG:NH2	1:C:382:CYS:HB2	2.22	0.51
1:A:413:VAL:HG21	1:A:421:LEU:CD2	2.40	0.51
1:B:76:VAL:HG11	1:B:81:ARG:HH21	1.74	0.51
1:A:370:ASN:OD1	1:A:372:GLN:HG2	2.11	0.51
1:D:240:ALA:HB3	1:D:271:VAL:HG12	1.93	0.51
1:A:394:LEU:HD23	1:A:424:ALA:CB	2.36	0.51
1:C:68:ARG:O	1:C:350:ARG:NH1	2.44	0.51
1:C:115:GLY:C	1:C:117:ASN:N	2.65	0.51
1:D:149:PHE:HB3	1:D:153:ARG:HH21	1.76	0.51
1:A:101:GLY:HA3	1:A:130:GLN:HB3	1.92	0.51
1:A:105:PHE:CZ	1:A:288:VAL:HG12	2.46	0.51
1:D:155:VAL:HG22	1:D:206:VAL:HG21	1.92	0.51
1:D:246:TYR:HE1	1:D:279:LYS:HG2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD12	1:A:402:MET:HE2	1.92	0.51
1:A:135:THR:CG2	1:C:317:SER:OG	2.51	0.51
1:C:81:ARG:NH1	1:C:84:GLU:OE1	2.44	0.51
1:A:384:THR:HG23	1:A:406:GLY:O	2.10	0.51
1:D:321:LEU:HD11	1:D:325:ARG:HE	1.76	0.51
1:A:194:ALA:O	1:A:198:ILE:HG13	2.11	0.51
1:A:293:MET:HE1	1:C:33:TRP:NE1	2.13	0.51
1:A:314:PRO:HG3	1:C:167:PRO:HB2	1.93	0.51
1:B:171:ASP:CG	1:D:147:ARG:HH22	2.18	0.51
1:B:189:PHE:CE2	1:B:191:PHE:HD1	2.28	0.51
1:C:107:LYS:O	1:C:111:GLU:HG3	2.10	0.51
1:A:33:TRP:CH2	1:C:149:PHE:CE1	2.99	0.50
1:C:370:ASN:OD1	1:C:372:GLN:HG3	2.11	0.50
1:C:391:VAL:HG12	1:C:395:ILE:HD11	1.93	0.50
1:D:133:SER:OG	1:D:134:GLY:N	2.42	0.50
1:D:206:VAL:HG12	1:D:239:PHE:HB3	1.91	0.50
1:C:51:PHE:HD1	1:C:401:TYR:HD2	1.59	0.50
1:D:179:TYR:OH	1:D:208:LEU:O	2.24	0.50
1:A:140:ILE:HD13	1:A:315:MET:CE	2.17	0.50
1:C:239:PHE:HZ	1:C:272:CYS:HB3	1.75	0.50
1:C:394:LEU:CD2	1:C:424:ALA:HB1	2.40	0.50
1:D:145:LEU:O	1:D:149:PHE:HB2	2.12	0.50
1:A:328:ALA:O	1:A:332:ASN:HB2	2.12	0.50
1:C:79:SER:OG	1:C:343:GLU:OE1	2.28	0.50
1:A:68:ARG:HB2	1:A:411:ALA:O	2.12	0.50
1:A:118:SER:HB3	1:A:121:LEU:HD12	1.94	0.50
1:C:160:PRO:O	1:C:214:HIS:CE1	2.65	0.50
1:D:149:PHE:CZ	1:D:151:PHE:CZ	2.95	0.50
1:A:277:TYR:HB2	1:A:288:VAL:HB	1.94	0.50
1:A:135:THR:HG22	1:A:168:ILE:HD11	1.94	0.50
1:A:354:MET:HE2	1:A:413:VAL:O	2.12	0.50
1:A:414:THR:HG22	1:A:416:SER:H	1.77	0.50
1:C:82:LYS:HA	1:D:389:GLU:OE2	2.11	0.50
1:A:355:ARG:HH22	1:A:377:GLN:HB2	1.73	0.49
1:A:383:PHE:HD1	1:A:407:ARG:HB2	1.77	0.49
1:A:272:CYS:HB3	1:A:293:MET:SD	2.51	0.49
1:C:348:ALA:O	1:C:352:ILE:HD12	2.11	0.49
1:C:392:GLU:O	1:C:396:LYS:HG2	2.12	0.49
1:A:400:ILE:C	1:A:401:TYR:CD1	2.91	0.49
1:B:135:THR:HG23	1:B:162:TRP:CH2	2.44	0.49
1:B:264:PHE:O	1:B:269:ILE:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ARG:HH12	1:D:378:ILE:CD1	2.24	0.49
1:D:180:ARG:CG	1:D:197:ASP:OD1	2.60	0.49
1:D:295:CYS:HB3	1:D:300:GLU:HG2	1.95	0.49
1:B:199:SER:O	1:B:236:ARG:NE	2.46	0.49
1:B:295:CYS:HB3	1:B:300:GLU:HB3	1.95	0.49
1:A:355:ARG:HH21	1:A:377:GLN:C	2.20	0.49
1:C:349:ASP:HA	1:C:352:ILE:CD1	2.27	0.49
1:A:54:ASP:OD2	1:A:56:ASN:N	2.43	0.49
1:B:33:TRP:HB2	1:D:300:GLU:OE1	2.12	0.49
1:C:229:ILE:O	1:C:232:VAL:HG23	2.12	0.49
1:A:182:TYR:HD1	1:A:219:VAL:HG21	1.77	0.49
1:C:278:ALA:HB1	1:C:284:TYR:HA	1.95	0.49
1:C:311:LEU:C	1:C:314:PRO:HD2	2.38	0.49
1:D:60:MET:HE1	1:D:421:LEU:HB2	1.95	0.49
1:D:106:CYS:HB3	1:D:128:THR:OG1	2.12	0.49
1:A:67:TYR:HE2	1:A:75:TYR:CD2	2.31	0.49
1:D:97:LEU:HD21	1:D:102:LEU:HB2	1.94	0.49
1:A:121:LEU:HA	1:A:126:PHE:HE2	1.78	0.49
1:A:132:ILE:O	1:A:136:GLY:HA3	2.12	0.49
1:A:302:LYS:HG2	1:C:38:MET:CE	2.28	0.49
1:A:56:ASN:OD1	1:A:57:SER:N	2.46	0.48
1:A:102:LEU:HB3	1:A:105:PHE:CB	2.42	0.48
1:A:398:PHE:HB3	1:A:420:TYR:CE1	2.48	0.48
1:B:312:ILE:O	1:B:316:TYR:O	2.31	0.48
1:C:394:LEU:HG	1:C:428:VAL:HG11	1.95	0.48
1:A:355:ARG:HH11	1:A:355:ARG:HG2	1.73	0.48
1:A:143:SER:HB3	1:A:311:LEU:HD22	1.95	0.48
1:A:180:ARG:O	1:A:194:ALA:CB	2.58	0.48
1:C:222:ARG:O	1:C:225:GLN:HB2	2.13	0.48
1:A:54:ASP:OD2	1:A:56:ASN:CB	2.61	0.48
1:C:144:PHE:HA	1:C:311:LEU:HD11	1.95	0.48
1:C:166:THR:HA	1:C:176:LEU:HD22	1.95	0.48
1:D:42:ASP:HB3	1:D:45:LEU:HB3	1.94	0.48
1:A:33:TRP:CE3	1:A:33:TRP:HA	2.49	0.48
1:C:425:ILE:O	1:C:429:THR:OG1	2.27	0.48
1:D:107:LYS:O	1:D:111:GLU:HG3	2.14	0.48
1:D:271:VAL:H	1:D:294:VAL:HG22	1.79	0.48
1:A:94:LYS:NZ	1:C:286:GLU:OE2	2.46	0.48
1:A:349:ASP:OD1	1:A:352:ILE:HD12	2.14	0.48
1:B:287:ARG:HG2	1:D:320:PRO:HA	1.96	0.48
1:A:398:PHE:O	1:A:420:TYR:HE1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HD12	1:D:209:LEU:H	1.77	0.48
1:D:354:MET:CA	1:D:354:MET:CE	2.85	0.48
1:A:168:ILE:O	1:A:172:ALA:HB2	2.13	0.48
1:A:383:PHE:CZ	1:A:405:ASP:OD2	2.67	0.48
1:B:359:VAL:HG21	1:B:375:THR:HG23	1.94	0.48
1:C:68:ARG:O	1:C:350:ARG:CZ	2.61	0.48
1:C:153:ARG:NH2	1:C:175:GLN:OE1	2.47	0.48
1:D:127:VAL:HG21	1:D:305:GLU:HB2	1.96	0.48
1:A:77:LEU:O	1:A:80:VAL:HB	2.14	0.48
1:A:82:LYS:HE2	1:A:339:GLN:OE1	2.13	0.48
1:D:183:ASP:HB2	1:D:190:ASP:HB2	1.95	0.48
1:D:359:VAL:HG21	1:D:375:THR:HG23	1.95	0.48
1:A:159:LYS:HA	1:A:160:PRO:HA	1.73	0.48
1:D:321:LEU:CD1	1:D:325:ARG:HE	2.27	0.48
1:A:78:PRO:HD2	1:A:343:GLU:CD	2.30	0.47
1:D:389:GLU:O	1:D:393:ARG:CG	2.38	0.47
1:A:310:ILE:O	1:A:314:PRO:CD	2.62	0.47
1:B:149:PHE:O	1:B:153:ARG:NH2	2.46	0.47
1:B:386:LEU:HD13	1:B:402:MET:HE1	1.96	0.47
1:C:51:PHE:CE2	1:C:61:ASN:HB2	2.49	0.47
1:C:350:ARG:HG2	1:C:350:ARG:NH2	2.29	0.47
1:D:179:TYR:CA	1:D:197:ASP:OD2	2.56	0.47
1:D:330:ILE:HA	1:D:336:LEU:HD13	1.95	0.47
1:B:159:LYS:HA	1:B:160:PRO:HA	1.76	0.47
1:C:139:ARG:CB	1:C:168:ILE:CG2	2.88	0.47
1:A:33:TRP:HE3	1:A:33:TRP:HA	1.79	0.47
1:B:147:ARG:NH2	1:D:171:ASP:OD1	2.48	0.47
1:B:182:TYR:CE2	1:B:184:PRO:HA	2.50	0.47
1:B:225:GLN:O	1:B:229:ILE:HG12	2.15	0.47
1:D:135:THR:HG22	1:D:168:ILE:HD11	1.95	0.47
1:D:164:ASN:O	1:D:168:ILE:HG13	2.15	0.47
1:A:244:MET:HE3	1:A:247:GLN:OE1	2.14	0.47
1:B:203:GLU:HG2	1:B:236:ARG:O	2.14	0.47
1:C:114:LEU:HB2	1:C:121:LEU:HD11	1.95	0.47
1:A:298:ALA:O	1:A:301:ALA:HB3	2.15	0.47
1:D:190:ASP:O	1:D:194:ALA:CB	2.61	0.47
1:D:246:TYR:CE1	1:D:279:LYS:HG2	2.50	0.47
1:B:315:MET:HG3	1:B:316:TYR:CD1	2.49	0.47
1:B:316:TYR:CD1	1:B:316:TYR:N	2.81	0.47
1:D:101:GLY:HA3	1:D:130:GLN:HB3	1.96	0.47
1:D:160:PRO:O	1:D:214:HIS:CE1	2.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LEU:HD22	1:D:400:ILE:HD12	1.97	0.47
1:A:32:TRP:C	1:A:33:TRP:HE3	2.22	0.47
1:A:180:ARG:NH2	1:A:197:ASP:OD1	2.40	0.47
1:C:224:GLU:OE2	1:C:224:GLU:N	2.40	0.47
1:A:293:MET:HE2	1:C:33:TRP:CE2	2.49	0.47
1:C:279:LYS:HG3	1:C:284:TYR:HE1	1.80	0.47
1:D:122:LYS:HA	1:D:122:LYS:HD3	1.60	0.47
1:A:358:LEU:HD23	1:A:374:ILE:HG21	1.97	0.47
1:B:102:LEU:HB3	1:B:105:PHE:HB3	1.97	0.47
1:B:330:ILE:O	1:B:337:ARG:HB2	2.15	0.47
1:C:414:THR:HG1	1:C:417:ASN:CG	2.22	0.47
1:D:343:GLU:O	1:D:347:MET:HG3	2.14	0.47
1:A:142:ALA:O	1:A:145:LEU:HB2	2.15	0.46
1:A:158:PRO:CG	1:A:161:THR:HB	2.36	0.46
1:A:340:TRP:CE3	1:A:341:LEU:HG	2.50	0.46
1:B:78:PRO:O	1:B:82:LYS:HG2	2.14	0.46
1:B:133:SER:O	1:B:135:THR:N	2.41	0.46
1:B:354:MET:HE2	1:B:414:THR:HA	1.97	0.46
1:D:191:PHE:CD2	1:D:225:GLN:HG2	2.43	0.46
1:A:394:LEU:HD21	1:A:424:ALA:CB	2.45	0.46
1:B:305:GLU:O	1:B:309:LYS:HG3	2.15	0.46
1:C:44:ILE:O	1:C:47:VAL:HG12	2.15	0.46
1:D:125:ARG:HB2	1:D:295:CYS:O	2.15	0.46
1:D:271:VAL:H	1:D:294:VAL:CG2	2.27	0.46
1:D:414:THR:CG2	1:D:415:SER:H	2.27	0.46
1:C:403:THR:OG1	1:C:405:ASP:OD1	2.24	0.46
1:D:339:GLN:O	1:D:342:GLN:HG2	2.15	0.46
1:B:93:ASP:CG	1:B:94:LYS:N	2.72	0.46
1:D:149:PHE:CE2	1:D:151:PHE:HE1	2.14	0.46
1:A:321:LEU:HB2	1:C:285:GLY:C	2.40	0.46
1:B:149:PHE:HE2	1:B:152:SER:HB3	1.79	0.46
1:B:158:PRO:CG	1:B:161:THR:HB	2.36	0.46
1:B:247:GLN:O	1:B:280:ASN:ND2	2.49	0.46
1:C:121:LEU:HA	1:C:126:PHE:CE1	2.51	0.46
1:A:414:THR:HG22	1:A:415:SER:N	2.29	0.46
1:C:225:GLN:O	1:C:229:ILE:HG12	2.16	0.46
1:D:205:SER:O	1:D:238:LEU:HB3	2.15	0.46
1:A:33:TRP:CZ3	1:C:149:PHE:CE1	3.01	0.46
1:A:191:PHE:CE1	1:A:195:VAL:CG2	2.98	0.46
1:B:87:ILE:O	1:B:87:ILE:HG22	2.16	0.46
1:C:132:ILE:O	1:C:136:GLY:HA3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:GLY:HA3	1:D:262:ARG:HH12	1.81	0.46
1:D:155:VAL:HG22	1:D:206:VAL:CG2	2.46	0.46
1:D:347:MET:O	1:D:350:ARG:HB3	2.16	0.46
1:B:56:ASN:HD22	1:B:399:SER:HB2	1.81	0.46
1:C:395:ILE:HG23	1:C:401:TYR:CE1	2.51	0.46
1:D:333:THR:CG2	1:D:336:LEU:CG	2.76	0.46
1:A:110:ALA:O	1:A:114:LEU:HG	2.16	0.45
1:A:386:LEU:HD21	1:A:429:THR:HG21	1.98	0.45
1:B:81:ARG:NH2	1:D:92:LEU:O	2.49	0.45
1:C:408:ILE:HG12	1:C:409:SER:N	2.30	0.45
1:A:69:ASP:CG	1:A:71:ASN:H	2.23	0.45
1:B:111:GLU:HG2	1:B:121:LEU:HD13	1.99	0.45
1:A:82:LYS:HE2	1:A:339:GLN:NE2	2.31	0.45
1:B:298:ALA:O	1:B:301:ALA:HB3	2.16	0.45
1:D:265:ILE:HG22	1:D:271:VAL:HG22	1.98	0.45
1:A:144:PHE:CD1	1:A:144:PHE:C	2.95	0.45
1:C:166:THR:HB	1:C:167:PRO:CD	2.46	0.45
1:A:283:LEU:N	1:A:283:LEU:CD2	2.73	0.45
1:A:321:LEU:HD22	1:C:285:GLY:HA3	1.99	0.45
1:C:264:PHE:CD2	1:C:269:ILE:HD12	2.51	0.45
1:D:231:THR:HA	1:D:234:LYS:CB	2.47	0.45
1:A:127:VAL:HG21	1:A:305:GLU:HG3	1.99	0.45
1:C:54:ASP:OD2	1:C:399:SER:HB3	2.16	0.45
1:B:64:VAL:HG22	1:B:66:ALA:H	1.81	0.45
1:B:111:GLU:HA	1:B:121:LEU:HD11	1.97	0.45
1:C:134:GLY:O	1:C:138:LEU:HB2	2.16	0.45
1:D:257:ASP:OD1	1:D:257:ASP:N	2.49	0.45
1:A:214:HIS:CE1	1:A:217:THR:HG23	2.51	0.45
1:D:311:LEU:C	1:D:314:PRO:HD2	2.42	0.45
1:A:82:LYS:CE	1:A:339:GLN:NE2	2.78	0.45
1:B:70:ASP:CG	1:B:415:SER:HG	2.25	0.45
1:C:299:ASP:O	1:C:302:LYS:HB2	2.16	0.45
1:A:92:LEU:O	1:C:81:ARG:NH2	2.49	0.45
1:A:399:SER:O	1:A:401:TYR:CE1	2.70	0.45
1:B:393:ARG:HG2	1:B:428:VAL:HG12	1.98	0.45
1:C:161:THR:HG1	1:C:165:HIS:CE1	2.31	0.45
1:A:112:LEU:HD23	1:A:277:TYR:OH	2.17	0.44
1:A:204:GLN:HA	1:A:237:ASN:O	2.18	0.44
1:A:241:PHE:CD1	1:A:241:PHE:C	2.96	0.44
1:A:391:VAL:CG1	1:A:395:ILE:CD1	2.85	0.44
1:B:68:ARG:O	1:B:350:ARG:NH1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:THR:OG1	1:B:405:ASP:OD1	2.20	0.44
1:D:60:MET:HE2	1:D:62:LEU:HD21	1.98	0.44
1:A:357:GLN:O	1:A:361:ASN:ND2	2.32	0.44
1:B:340:TRP:O	1:B:344:VAL:HG23	2.17	0.44
1:D:329:ALA:O	1:D:333:THR:CG2	2.65	0.44
1:D:329:ALA:O	1:D:333:THR:HB	2.16	0.44
1:D:334:PRO:HG2	1:D:335:ASP:N	2.32	0.44
1:C:69:ASP:C	1:C:71:ASN:H	2.25	0.44
1:D:78:PRO:HD2	1:D:343:GLU:OE1	2.17	0.44
1:D:92:LEU:HD13	1:D:325:ARG:HH11	1.79	0.44
1:B:125:ARG:NH1	1:B:295:CYS:O	2.47	0.44
1:D:136:GLY:O	1:D:140:ILE:HG12	2.17	0.44
1:D:181:TYR:OH	1:D:221:PRO:HD3	2.18	0.44
1:A:284:TYR:HB2	1:C:94:LYS:O	2.17	0.44
1:C:115:GLY:O	1:C:117:ASN:N	2.50	0.44
1:C:165:HIS:O	1:C:169:PHE:HD2	2.00	0.44
1:A:70:ASP:O	1:A:414:THR:HG21	2.18	0.44
1:A:144:PHE:CD1	1:A:144:PHE:O	2.71	0.44
1:A:365:GLU:OE2	1:A:423:HIS:HD2	2.01	0.44
1:B:387:LYS:O	1:B:391:VAL:HG23	2.18	0.44
1:D:157:LEU:HG	1:D:176:LEU:HD22	1.99	0.44
1:A:399:SER:O	1:A:401:TYR:HE1	2.00	0.44
1:C:297:ASP:OD1	1:C:300:GLU:HB3	2.17	0.44
1:D:391:VAL:HG11	1:D:404:LYS:HA	1.99	0.44
1:C:248:GLY:N	1:C:257:ASP:OD2	2.50	0.43
1:C:316:TYR:O	1:C:316:TYR:CD1	2.70	0.43
1:D:121:LEU:HG	1:D:122:LYS:N	2.32	0.43
1:A:56:ASN:HB3	1:A:59:LYS:HB3	1.99	0.43
1:C:101:GLY:HA3	1:C:130:GLN:HB3	1.99	0.43
1:C:246:TYR:HE1	1:C:279:LYS:HD3	1.82	0.43
1:D:149:PHE:HE2	1:D:206:VAL:HG13	1.82	0.43
1:A:48:THR:CG2	1:A:61:ASN:HD21	2.26	0.43
1:B:60:MET:HE2	1:B:62:LEU:HD21	1.99	0.43
1:C:97:LEU:HD13	1:C:102:LEU:N	2.34	0.43
1:C:194:ALA:O	1:C:198:ILE:HG13	2.18	0.43
1:C:70:ASP:N	1:C:350:ARG:HE	2.17	0.43
1:C:313:ARG:N	1:C:314:PRO:HD2	2.33	0.43
1:D:334:PRO:HG2	1:D:335:ASP:H	1.84	0.43
1:A:215:ASN:HA	1:A:216:PRO:HA	1.62	0.43
1:A:343:GLU:O	1:A:347:MET:HG3	2.18	0.43
1:A:364:LYS:HE3	1:B:203:GLU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LYS:HA	1:D:160:PRO:HA	1.71	0.43
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.73	0.43
1:A:179:TYR:CD1	1:A:179:TYR:C	2.96	0.43
1:B:281:MET:HB3	1:B:283:LEU:HG	2.00	0.43
1:D:280:ASN:OD1	1:D:281:MET:N	2.52	0.43
1:A:32:TRP:O	1:A:33:TRP:CE3	2.70	0.43
1:A:261:VAL:HG11	1:A:273:LEU:HD22	1.99	0.43
1:A:270:ASN:HB3	1:A:294:VAL:O	2.19	0.43
1:C:267:GLN:HG3	1:C:267:GLN:O	2.19	0.43
1:C:360:SER:O	1:C:364:LYS:N	2.48	0.43
1:A:130:GLN:NE2	1:A:319:PRO:CG	2.82	0.43
1:D:155:VAL:HB	1:D:176:LEU:HD23	2.01	0.43
1:A:308:LEU:O	1:A:312:ILE:HD12	2.19	0.43
1:B:191:PHE:O	1:B:195:VAL:CG2	2.67	0.43
1:C:134:GLY:O	1:C:138:LEU:N	2.47	0.43
1:C:400:ILE:HD13	1:C:421:LEU:CD1	2.49	0.43
1:D:361:ASN:HA	1:D:364:LYS:HB3	2.00	0.43
1:A:413:VAL:HG22	1:A:421:LEU:HD22	1.98	0.42
1:A:421:LEU:O	1:A:425:ILE:HG13	2.18	0.42
1:D:53:ARG:O	1:D:53:ARG:HG3	2.19	0.42
1:D:191:PHE:CD2	1:D:225:GLN:CG	3.02	0.42
1:D:288:VAL:HG22	1:D:323:GLY:HA3	2.00	0.42
1:A:251:SER:OG	1:A:257:ASP:OD1	2.26	0.42
1:A:355:ARG:HH11	1:A:410:VAL:HG21	1.85	0.42
1:B:361:ASN:HA	1:B:364:LYS:HB2	2.00	0.42
1:D:130:GLN:NE2	1:D:324:ALA:HB2	2.35	0.42
1:A:66:ALA:HB1	1:A:284:TYR:CE2	2.55	0.42
1:A:321:LEU:N	1:C:285:GLY:O	2.46	0.42
1:A:394:LEU:HA	1:A:398:PHE:HD2	1.83	0.42
1:B:158:PRO:HG2	1:B:161:THR:CB	2.39	0.42
1:B:160:PRO:HD2	1:B:182:TYR:HB3	2.00	0.42
1:B:296:LYS:HA	1:B:296:LYS:HD2	1.79	0.42
1:D:149:PHE:CE2	1:D:151:PHE:CD1	3.08	0.42
1:A:165:HIS:O	1:A:169:PHE:HD2	2.02	0.42
1:C:139:ARG:NH1	1:C:171:ASP:HB3	2.34	0.42
1:D:155:VAL:HB	1:D:176:LEU:CD2	2.49	0.42
1:A:283:LEU:HD12	1:A:288:VAL:CG2	2.44	0.42
1:B:382:CYS:HB3	1:B:408:ILE:HG13	2.01	0.42
1:B:395:ILE:HG23	1:B:401:TYR:CE1	2.54	0.42
1:B:402:MET:SD	1:B:408:ILE:HG22	2.60	0.42
1:C:231:THR:HA	1:C:234:LYS:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:LYS:HG2	1:C:396:LYS:H	1.71	0.42
1:D:56:ASN:HB3	1:D:59:LYS:HG3	2.01	0.42
1:C:125:ARG:NH1	1:C:295:CYS:O	2.52	0.42
1:B:97:LEU:HG	1:B:321:LEU:HD13	2.02	0.42
1:C:150:LYS:HA	1:C:150:LYS:HD3	1.81	0.42
1:C:313:ARG:HB2	1:C:314:PRO:HD3	2.01	0.42
1:C:393:ARG:HH11	1:C:393:ARG:HD3	1.71	0.42
1:D:180:ARG:H	1:D:197:ASP:CG	2.28	0.42
1:A:365:GLU:O	1:A:426:HIS:NE2	2.53	0.42
1:C:102:LEU:H	1:C:130:GLN:NE2	2.17	0.42
1:C:120:VAL:HG21	1:C:265:ILE:HG21	2.01	0.42
1:C:239:PHE:CZ	1:C:272:CYS:HB3	2.53	0.42
1:C:343:GLU:O	1:C:347:MET:HB2	2.19	0.42
1:C:351:ILE:O	1:C:355:ARG:HG3	2.20	0.42
1:D:51:PHE:CE1	1:D:59:LYS:HB3	2.55	0.42
1:D:313:ARG:N	1:D:314:PRO:CD	2.83	0.42
1:D:388:PRO:O	1:D:392:GLU:HG2	2.19	0.42
1:A:220:ASP:HA	1:A:221:PRO:HD3	1.83	0.42
1:B:38:MET:HE1	1:D:302:LYS:HG2	2.02	0.42
1:D:191:PHE:HD2	1:D:225:GLN:CG	2.27	0.41
1:D:205:SER:O	1:D:239:PHE:N	2.45	0.41
1:A:81:ARG:HD3	1:A:81:ARG:HA	1.79	0.41
1:B:81:ARG:NH1	1:D:91:ASN:OD1	2.53	0.41
1:A:120:VAL:HG12	1:A:126:PHE:CD2	2.55	0.41
1:B:93:ASP:OD1	1:B:95:GLU:HG2	2.20	0.41
1:B:134:GLY:O	1:B:137:ALA:HB3	2.20	0.41
1:B:201:ILE:N	1:B:236:ARG:HH11	2.15	0.41
1:C:400:ILE:HG22	1:C:402:MET:HE3	2.02	0.41
1:A:413:VAL:CG2	1:A:421:LEU:CD2	2.95	0.41
1:B:283:LEU:HD22	1:B:286:GLU:HG3	2.01	0.41
1:B:391:VAL:O	1:B:395:ILE:HD12	2.21	0.41
1:D:152:SER:OG	1:D:205:SER:HA	2.20	0.41
1:A:192:THR:OG1	1:A:193:GLY:N	2.54	0.41
1:A:414:THR:CG2	1:A:416:SER:OG	2.68	0.41
1:A:414:THR:HG22	1:A:416:SER:OG	2.20	0.41
1:B:244:MET:O	1:B:275:GLN:HA	2.20	0.41
1:B:199:SER:O	1:B:236:ARG:CZ	2.68	0.41
1:D:236:ARG:O	1:D:237:ASN:HB3	2.20	0.41
1:D:296:LYS:HD3	1:D:296:LYS:HA	1.94	0.41
1:A:198:ILE:HA	1:A:201:ILE:HG13	2.02	0.41
1:B:33:TRP:CZ3	1:D:149:PHE:CD1	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:THR:OG1	1:C:162:TRP:HH2	2.04	0.41
1:D:149:PHE:CE2	1:D:206:VAL:HG12	2.53	0.41
1:D:300:GLU:O	1:D:304:VAL:HG23	2.21	0.41
1:D:369:HIS:HB2	1:D:371:TRP:CE2	2.56	0.41
1:A:51:PHE:CD1	1:A:51:PHE:C	2.98	0.41
1:A:105:PHE:CZ	1:A:288:VAL:CG1	3.03	0.41
1:A:394:LEU:CD2	1:A:424:ALA:HB3	2.51	0.41
1:C:139:ARG:O	1:C:139:ARG:HG3	2.19	0.41
1:C:159:LYS:HA	1:C:160:PRO:HA	1.69	0.41
1:C:339:GLN:O	1:C:342:GLN:HG2	2.21	0.41
1:D:87:ILE:HG23	1:D:92:LEU:HD11	2.03	0.41
1:A:133:SER:OG	1:A:134:GLY:N	2.54	0.41
1:A:236:ARG:HB3	1:A:238:LEU:HD21	2.03	0.41
1:C:203:GLU:HG3	1:C:236:ARG:HD3	2.03	0.41
1:C:360:SER:CA	1:C:363:LYS:HG2	2.47	0.41
1:C:400:ILE:HG22	1:C:402:MET:CE	2.51	0.41
1:D:120:VAL:HG13	1:D:125:ARG:HG3	2.03	0.41
1:A:214:HIS:ND1	1:A:217:THR:OG1	2.28	0.41
1:A:312:ILE:O	1:A:316:TYR:O	2.38	0.41
1:B:227:LYS:HD2	1:B:263:HIS:NE2	2.36	0.41
1:B:315:MET:CE	1:D:139:ARG:HH12	2.32	0.41
1:B:361:ASN:HA	1:B:364:LYS:HD2	2.03	0.41
1:C:87:ILE:HD12	1:C:325:ARG:HD3	2.03	0.41
1:C:161:THR:OG1	1:C:210:HIS:NE2	2.54	0.41
1:C:354:MET:HE1	1:C:418:VAL:HG22	2.03	0.41
1:D:306:SER:O	1:D:310:ILE:HG13	2.21	0.41
1:C:180:ARG:CZ	1:C:197:ASP:OD1	2.69	0.40
1:C:345:LYS:HA	1:C:348:ALA:HB3	2.02	0.40
1:D:241:PHE:HA	1:D:272:CYS:SG	2.61	0.40
1:A:354:MET:HE1	1:A:415:SER:N	2.26	0.40
1:B:140:ILE:CD1	1:B:316:TYR:OH	2.69	0.40
1:D:234:LYS:HD3	1:D:267:GLN:HG3	2.04	0.40
1:A:120:VAL:HG12	1:A:126:PHE:HD2	1.84	0.40
1:B:54:ASP:OD2	1:B:399:SER:OG	2.23	0.40
1:B:134:GLY:O	1:B:138:LEU:HD12	2.21	0.40
1:B:213:ALA:N	1:B:220:ASP:OD2	2.52	0.40
1:C:86:GLN:O	1:C:90:LYS:HG3	2.21	0.40
1:C:139:ARG:HA	1:C:168:ILE:HG22	2.04	0.40
1:C:369:HIS:ND1	1:C:369:HIS:N	2.69	0.40
1:B:317:SER:OG	1:D:135:THR:CG2	2.65	0.40
1:D:249:PHE:CZ	1:D:351:ILE:HD11	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:HH2	1:C:149:PHE:CE1	2.39	0.40
1:B:330:ILE:HG22	1:B:337:ARG:HA	2.04	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	399/407 (98%)	391 (98%)	7 (2%)	1 (0%)	36	67
1	B	399/407 (98%)	387 (97%)	10 (2%)	2 (0%)	24	58
1	C	399/407 (98%)	387 (97%)	10 (2%)	2 (0%)	24	58
1	D	399/407 (98%)	390 (98%)	9 (2%)	0	100	100
All	All	1596/1628 (98%)	1555 (97%)	36 (2%)	5 (0%)	36	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	GLU
1	B	281	MET
1	C	93	ASP
1	B	134	GLY
1	A	160	PRO

5.3.2 Protein sidechains [i](#)

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	333/339 (98%)	283 (85%)	50 (15%)	3	13
1	B	333/339 (98%)	307 (92%)	26 (8%)	11	37
1	C	333/339 (98%)	290 (87%)	43 (13%)	4	18
1	D	333/339 (98%)	283 (85%)	50 (15%)	3	13
All	All	1332/1356 (98%)	1163 (87%)	169 (13%)	4	18

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TRP
1	A	52	LYS
1	A	59	LYS
1	A	69	ASP
1	A	73	LYS
1	A	79	SER
1	A	91	ASN
1	A	93	ASP
1	A	98	PRO
1	A	104	GLU
1	A	107	LYS
1	A	114	LEU
1	A	116	GLU
1	A	127	VAL
1	A	129	VAL
1	A	135	THR
1	A	143	SER
1	A	150	LYS
1	A	151	PHE
1	A	153	ARG
1	A	168	ILE
1	A	185	LYS
1	A	198	ILE
1	A	223	PRO
1	A	227	LYS
1	A	234	LYS
1	A	238	LEU
1	A	279	LYS
1	A	283	LEU
1	A	293	MET
1	A	296	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	313	ARG
1	A	315	MET
1	A	316	TYR
1	A	319	PRO
1	A	321	LEU
1	A	333	THR
1	A	339	GLN
1	A	345	LYS
1	A	355	ARG
1	A	360	SER
1	A	368	THR
1	A	383	PHE
1	A	387	LYS
1	A	389	GLU
1	A	399	SER
1	A	407	ARG
1	A	413	VAL
1	A	416	SER
1	A	428	VAL
1	B	33	TRP
1	B	92	LEU
1	B	135	THR
1	B	138	LEU
1	B	185	LYS
1	B	228	GLU
1	B	235	LYS
1	B	255	ASP
1	B	296	LYS
1	B	302	LYS
1	B	309	LYS
1	B	310	ILE
1	B	311	LEU
1	B	313	ARG
1	B	315	MET
1	B	316	TYR
1	B	318	ASN
1	B	330	ILE
1	B	333	THR
1	B	343	GLU
1	B	355	ARG
1	B	368	THR
1	B	383	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	399	SER
1	B	416	SER
1	B	418	VAL
1	C	30	SER
1	C	69	ASP
1	C	79	SER
1	C	82	LYS
1	C	87	ILE
1	C	93	ASP
1	C	119	GLU
1	C	128	THR
1	C	133	SER
1	C	138	LEU
1	C	149	PHE
1	C	150	LYS
1	C	151	PHE
1	C	152	SER
1	C	157	LEU
1	C	166	THR
1	C	176	LEU
1	C	198	ILE
1	C	199	SER
1	C	207	LEU
1	C	224	GLU
1	C	231	THR
1	C	232	VAL
1	C	251	SER
1	C	269	ILE
1	C	271	VAL
1	C	279	LYS
1	C	293	MET
1	C	294	VAL
1	C	299	ASP
1	C	333	THR
1	C	355	ARG
1	C	360	SER
1	C	364	LYS
1	C	367	SER
1	C	368	THR
1	C	369	HIS
1	C	383	PHE
1	C	396	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	408	ILE
1	C	416	SER
1	C	418	VAL
1	C	430	LYS
1	D	30	SER
1	D	31	SER
1	D	44	ILE
1	D	47	VAL
1	D	91	ASN
1	D	92	LEU
1	D	97	LEU
1	D	112	LEU
1	D	114	LEU
1	D	121	LEU
1	D	126	PHE
1	D	129	VAL
1	D	135	THR
1	D	146	GLN
1	D	149	PHE
1	D	152	SER
1	D	161	THR
1	D	170	ARG
1	D	180	ARG
1	D	191	PHE
1	D	197	ASP
1	D	200	LYS
1	D	203	GLU
1	D	222	ARG
1	D	235	LYS
1	D	236	ARG
1	D	238	LEU
1	D	244	MET
1	D	247	GLN
1	D	257	ASP
1	D	271	VAL
1	D	294	VAL
1	D	302	LYS
1	D	313	ARG
1	D	317	SER
1	D	330	ILE
1	D	334	PRO
1	D	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	352	ILE
1	D	354	MET
1	D	355	ARG
1	D	364	LYS
1	D	368	THR
1	D	383	PHE
1	D	402	MET
1	D	403	THR
1	D	407	ARG
1	D	415	SER
1	D	418	VAL
1	D	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	270	ASN
1	A	275	GLN
1	A	318	ASN
1	A	322	ASN
1	A	339	GLN
1	A	423	HIS
1	B	130	GLN
1	B	270	ASN
1	B	322	ASN
1	C	86	GLN
1	C	322	ASN
1	D	165	HIS
1	D	177	GLN
1	D	426	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 ⓘ

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	401/407 (98%)	0.78	25 (6%) 26 16	38, 44, 58, 65	0
1	B	401/407 (98%)	1.24	66 (16%) 4 3	41, 49, 64, 77	0
1	C	401/407 (98%)	1.11	49 (12%) 8 6	41, 51, 58, 65	0
1	D	401/407 (98%)	1.26	60 (14%) 5 4	45, 62, 70, 75	0
All	All	1604/1628 (98%)	1.10	200 (12%) 8 6	38, 51, 68, 77	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	SER	5.6
1	B	134	GLY	4.6
1	C	361	ASN	4.6
1	B	342	GLN	4.3
1	B	34	THR	4.2
1	B	410	VAL	4.2
1	D	263	HIS	4.1
1	B	31	SER	4.1
1	C	114	LEU	4.0
1	C	269	ILE	4.0
1	B	212	CYS	3.8
1	B	172	ALA	3.8
1	D	242	PHE	3.8
1	C	271	VAL	3.7
1	B	66	ALA	3.7
1	B	245	ALA	3.7
1	B	32	TRP	3.7
1	D	298	ALA	3.6
1	B	65	GLY	3.6
1	C	315	MET	3.6
1	B	91	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	250	ALA	3.5
1	D	278	ALA	3.4
1	D	351	ILE	3.4
1	D	234	LYS	3.3
1	B	33	TRP	3.3
1	D	213	ALA	3.3
1	C	422	ALA	3.3
1	C	213	ALA	3.2
1	C	208	LEU	3.1
1	A	136	GLY	3.1
1	C	351	ILE	3.1
1	C	230	ALA	3.1
1	D	64	VAL	3.1
1	B	328	ALA	3.1
1	B	169	PHE	3.1
1	D	279	LYS	3.0
1	D	265	ILE	3.0
1	C	223	PRO	3.0
1	A	232	VAL	3.0
1	B	151	PHE	3.0
1	B	232	VAL	3.0
1	D	239	PHE	3.0
1	D	229	ILE	3.0
1	B	92	LEU	3.0
1	C	197	ASP	3.0
1	D	217	THR	3.0
1	B	173	GLY	2.9
1	C	289	GLY	2.9
1	D	93	ASP	2.9
1	B	259	TRP	2.9
1	C	410	VAL	2.9
1	D	133	SER	2.9
1	B	287	ARG	2.8
1	D	253	ASP	2.8
1	A	400	ILE	2.8
1	B	341	LEU	2.8
1	B	76	VAL	2.7
1	D	267	GLN	2.7
1	C	104	GLU	2.7
1	C	288	VAL	2.7
1	C	97	LEU	2.7
1	C	250	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	204	GLN	2.7
1	B	411	ALA	2.7
1	C	136	GLY	2.7
1	A	144	PHE	2.6
1	A	277	TYR	2.6
1	B	273	LEU	2.6
1	D	113	ALA	2.6
1	D	211	ALA	2.6
1	D	240	ALA	2.6
1	D	324	ALA	2.6
1	D	67	TYR	2.6
1	D	115	GLY	2.6
1	C	83	ALA	2.6
1	C	236	ARG	2.6
1	C	121	LEU	2.6
1	D	250	ALA	2.6
1	A	420	TYR	2.6
1	D	58	LYS	2.6
1	C	285	GLY	2.5
1	D	196	GLU	2.5
1	D	224	GLU	2.5
1	B	282	GLY	2.5
1	B	277	TYR	2.5
1	C	48	THR	2.5
1	C	158	PRO	2.5
1	B	248	GLY	2.5
1	D	400	ILE	2.5
1	D	288	VAL	2.5
1	D	156	PHE	2.5
1	B	208	LEU	2.5
1	D	120	VAL	2.5
1	C	278	ALA	2.5
1	D	121	LEU	2.4
1	D	297	ASP	2.4
1	D	405	ASP	2.4
1	A	151	PHE	2.4
1	B	144	PHE	2.4
1	B	189	PHE	2.4
1	A	132	ILE	2.4
1	B	171	ASP	2.4
1	B	79	SER	2.4
1	C	155	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	243	ASP	2.4
1	B	116	GLU	2.4
1	B	133	SER	2.4
1	C	242	PHE	2.4
1	A	135	THR	2.4
1	C	326	ILE	2.4
1	B	221	PRO	2.4
1	A	250	ALA	2.4
1	B	113	ALA	2.4
1	D	109	SER	2.4
1	B	168	ILE	2.4
1	D	206	VAL	2.3
1	D	233	VAL	2.3
1	D	124	GLY	2.3
1	B	249	PHE	2.3
1	B	306	SER	2.3
1	D	430	LYS	2.3
1	C	380	MET	2.3
1	D	361	ASN	2.3
1	C	103	ALA	2.3
1	D	396	LYS	2.3
1	B	415	SER	2.3
1	C	239	PHE	2.2
1	B	258	ALA	2.2
1	D	362	LEU	2.2
1	B	80	VAL	2.2
1	C	49	GLU	2.2
1	B	340	TRP	2.2
1	B	388	PRO	2.2
1	C	120	VAL	2.2
1	B	136	GLY	2.2
1	C	178	GLY	2.2
1	A	411	ALA	2.2
1	B	283	LEU	2.2
1	B	44	ILE	2.2
1	C	86	GLN	2.2
1	D	319	PRO	2.2
1	B	380	MET	2.2
1	A	44	ILE	2.2
1	B	170	ARG	2.2
1	D	395	ILE	2.2
1	B	165	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	2.2
1	C	133	SER	2.2
1	C	209	LEU	2.2
1	D	62	LEU	2.2
1	C	166	THR	2.1
1	D	186	THR	2.1
1	D	189	PHE	2.1
1	A	295	CYS	2.1
1	B	104	GLU	2.1
1	D	125	ARG	2.1
1	D	87	ILE	2.1
1	D	307	GLN	2.1
1	B	210	HIS	2.1
1	D	122	LYS	2.1
1	A	178	GLY	2.1
1	B	289	GLY	2.1
1	B	191	PHE	2.1
1	A	32	TRP	2.1
1	B	108	ALA	2.1
1	B	260	ALA	2.1
1	C	415	SER	2.1
1	D	57	SER	2.1
1	B	41	PRO	2.1
1	D	320	PRO	2.1
1	B	157	LEU	2.1
1	C	173	GLY	2.1
1	C	378	ILE	2.1
1	C	212	CYS	2.1
1	C	272	CYS	2.1
1	A	294	VAL	2.1
1	B	158	PRO	2.1
1	C	179	TYR	2.1
1	A	143	SER	2.0
1	B	317	SER	2.0
1	A	413	VAL	2.0
1	A	308	LEU	2.0
1	D	168	ILE	2.0
1	D	162	TRP	2.0
1	A	401	TYR	2.0
1	A	402	MET	2.0
1	C	195	VAL	2.0
1	D	306	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	97	LEU	2.0
1	A	239	PHE	2.0
1	A	34	THR	2.0
1	C	375	THR	2.0
1	C	429	THR	2.0
1	C	95	GLU	2.0
1	B	162	TRP	2.0
1	A	179	TYR	2.0
1	D	420	TYR	2.0
1	B	294	VAL	2.0
1	B	359	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.