



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:31 AM UTC

PDB ID : 4LDS / pdb_00004lds
Title : The inward-facing structure of the glucose transporter from *Staphylococcus epidermidis*
Authors : Choe, J.; Aleshin, A.; Iancu, C.V.
Deposited on : 2013-06-25
Resolution : 3.20 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

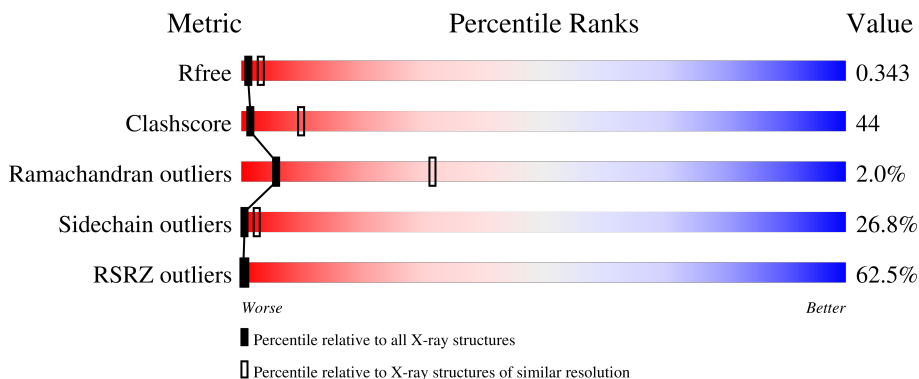
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	446	59% 25% 45% 21% • 6%
1	B	446	59% 31% 46% 14% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6388 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.

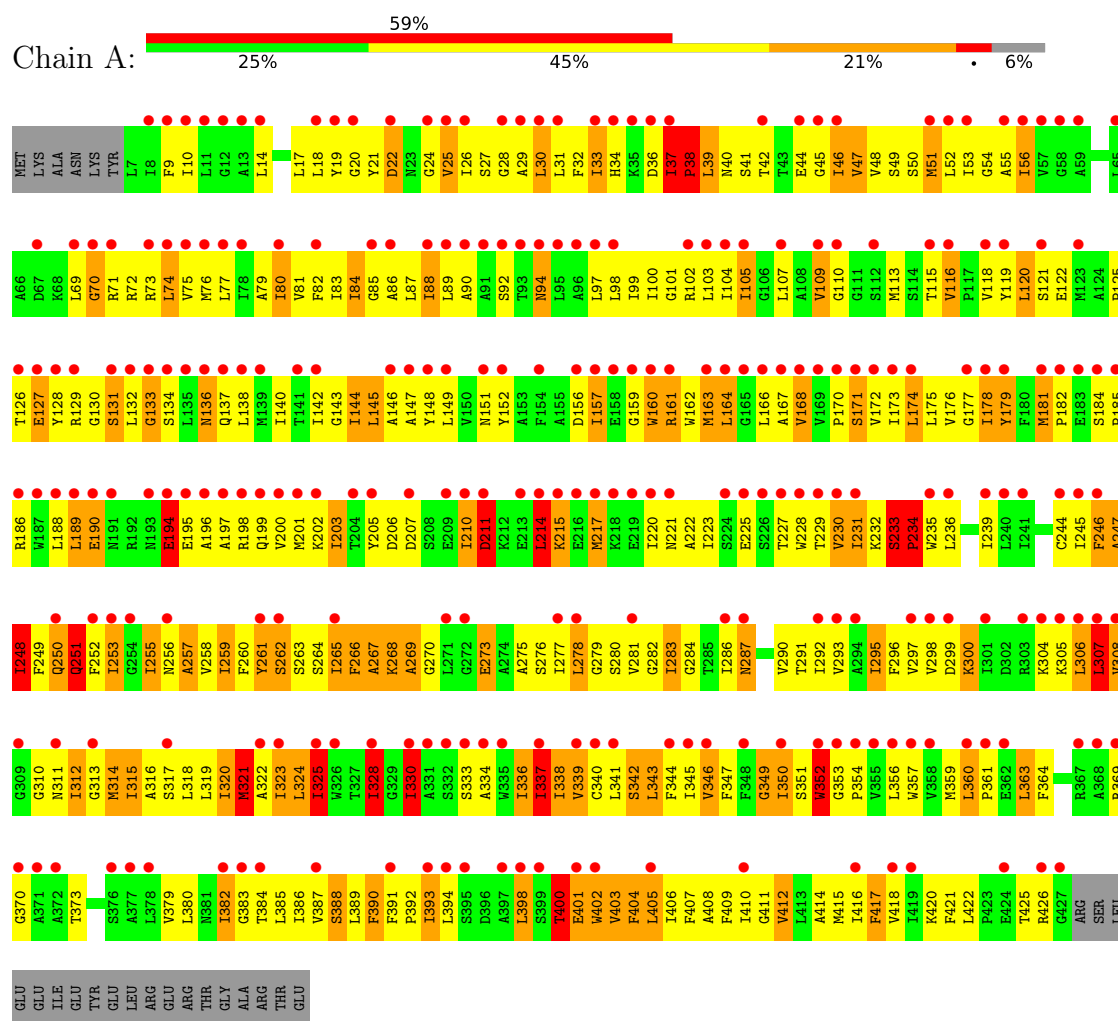
- Molecule 1 is a protein called Glucose transporter GlcP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3194	2127	503	548	16			
1	B	421	Total	C	N	O	S	0	0	0
			3194	2127	503	548	16			

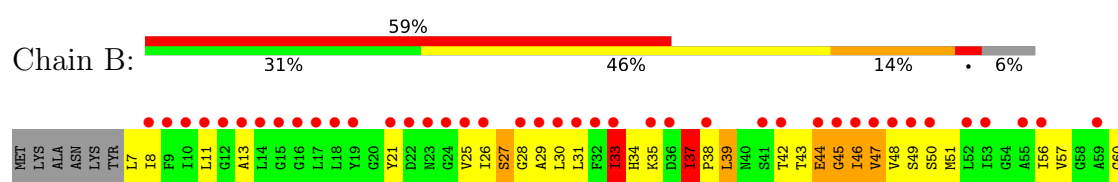
3 Residue-property plots

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: Glucose transporter GlcP



• Molecule 1: Glucose transporter GlcP



ARG	R367	L307	A247	S184	G124	S61
SER	A366	V308	I248	P185	P125	S62
LEU	R369	G309	F249	R186	T126	G63
GLU	G370	G310	Q250	W187	E127	P64
GLU	A371	N311	Q251	L188	Y128	L65
ILE	A372	I312	F252	L189	R129	A66
GLU	T373	G313	I253	E190	G130	D67
TTR	G374	M314	G254	N191	S131	K68
GLU	I375	I315	I255	R192	L132	L69
LEU	S376	A316	N256	N193	G133	G70
ARG	A377	S317	A257	E194	S134	R71
GLU	L378	L318	V258	E195	L135	R72
ARG	V379	I319	I259	A196	M136	R73
THR	L380	I320	F260	A197	Q137	L74
GLY	M381	M321	Y261	R198	L138	V75
ALA	I382	A322	S262	Q199	M139	M76
ARG	G383	I323	S263	V200	I140	L77
THR	I386	L324	S264	M201	T141	I78
GLU	V387	I325	I265	K202	I142	A79
	S388	T327	F266	I203	G143	I80
	L389	I328	K268	T204	I144	V81
GLU	F390	G329	A269	Y205	L145	F82
GLU	F391	I330	G270	D206	A146	I83
GLU	P392	A331	L271	S208	A147	I84
	I393	S332	G272	E209	Y148	G85
	L394	S333	E273	I210	L149	A86
	S395	A334	A274	D211	V150	L87
	D396	W335	A275	K212	N151	I88
LEU	A397	I336	S276	E213	Y152	L89
	L398	I337	I277	L214	A153	A90
	S399	I338	L278	L215	F154	A91
GLU	T400	V339	G279	M217	A155	S92
	W401	C340	S280	K218	D156	T93
GLU	W402	L341	V281	E219	I157	L97
GLU	F403	S342	G282	I220	E158	L98
F404	L343	L343	I283	N221	G159	I99
L405	F344	F344	G284	E225	R161	I100
L406	I345	I345	T285	S226	M162	G101
F407	V346	V346	I286	M163	M163	G102
A408	F347	F347	N287	L164	L164	L103
F409	F348	F348	V288	G165	G165	I104
I410	G349	G349	L289	T229	L166	I105
G411	I350	I350	V290	V230	A167	G106
ARG	S351	S351	T291	I231	V168	L107
	W352	W352	I292	K232	V169	A108
	G353	G353	V293	S233	P170	V109
	P354	P354	A294	P234	S171	G112
	V355	V355	I295	W235	W172	M113
	L356	L356	F296	L236	L173	S114
	W357	W357	V297	G237	L174	T115
	V358	V358	V298	R238	L175	V116
	M359	M359	D299	L239	V176	P117
	L360	L360	K300	G177	G177	V118
	P361	P361	I301	L241	I178	Y119
	F362	F362	D302	V242	V179	L120
	L363	L363	R303	G243	F180	S121
	F364	F364	K304	C244	M181	I122
	P365	P365	K305	L245	P182	M123
	M366	M366	L306	F246	E183	

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.07Å 118.85Å 160.05Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	19.90 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.90-3.20) 97.9 (19.90-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.302 , 0.341 0.302 , 0.343	Depositor DCC
R_{free} test set	1948 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 17.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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	1.03	6/3258 (0.2%)	1.48	58/4431 (1.3%)
1	B	0.79	0/3258	1.35	51/4431 (1.2%)
All	All	0.92	6/6516 (0.1%)	1.42	109/8862 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	ALA	CA-CB	-6.18	1.44	1.53
1	A	266	PHE	CA-C	6.13	1.61	1.52
1	A	253	ILE	CA-CB	5.98	1.62	1.54
1	A	37	ILE	CA-C	5.76	1.58	1.52
1	A	267	ALA	CA-C	5.75	1.58	1.53
1	A	251	GLN	CA-C	5.21	1.59	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ILE	N-CA-C	12.83	122.48	110.42
1	B	416	ILE	N-CA-C	-11.58	98.38	111.00
1	A	402	TRP	N-CA-C	11.07	124.67	111.82
1	A	338	ILE	N-CA-C	-10.99	98.82	110.36
1	A	401	GLU	N-CA-C	-10.81	99.28	111.71
1	A	251	GLN	N-CA-C	9.78	125.42	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ALA	N-CA-C	-9.74	100.25	112.72
1	B	270	GLY	N-CA-C	9.66	132.61	115.80
1	A	300	LYS	N-CA-C	9.61	121.69	111.03
1	B	205	TYR	N-CA-C	9.56	124.67	112.92
1	B	231	ILE	N-CA-C	9.49	121.35	111.00
1	A	337	ILE	N-CA-C	9.25	121.39	111.58
1	A	205	TYR	N-CA-C	9.06	124.07	112.92
1	B	175	LEU	N-CA-C	-8.87	101.19	111.03
1	B	56	ILE	N-CA-C	8.80	118.80	110.53
1	A	400	THR	N-CA-C	8.74	123.15	108.20
1	A	227	THR	N-CA-C	8.63	124.04	113.17
1	A	418	VAL	N-CA-C	8.37	118.42	110.30
1	A	370	GLY	N-CA-C	8.30	122.69	112.64
1	A	325	ILE	N-CA-C	8.13	120.20	111.58
1	B	233	SER	CA-C-N	7.93	129.75	119.84
1	B	233	SER	C-N-CA	7.93	129.75	119.84
1	A	349	GLY	N-CA-C	7.88	122.17	112.64
1	B	27	SER	N-CA-C	-7.77	102.76	111.07
1	B	399	SER	N-CA-C	-7.47	101.68	111.02
1	A	206	ASP	N-CA-C	7.43	121.88	111.92
1	B	155	ALA	N-CA-C	7.43	122.53	113.17
1	A	330	ILE	N-CA-C	7.38	122.13	112.76
1	B	69	LEU	N-CA-C	7.30	122.37	113.17
1	A	229	THR	N-CA-C	7.12	120.45	111.69
1	B	277	ILE	N-CA-C	7.06	117.67	110.82
1	A	299	ASP	N-CA-C	6.89	122.03	112.45
1	A	248	ILE	N-CA-C	6.89	118.51	111.00
1	A	398	LEU	N-CA-C	6.88	121.84	113.17
1	A	352	TRP	N-CA-C	6.85	121.34	112.92
1	B	276	SER	N-CA-C	-6.76	104.51	112.89
1	A	353	GLY	CA-C-N	6.74	128.26	119.84
1	A	353	GLY	C-N-CA	6.74	128.26	119.84
1	B	208	SER	N-CA-C	6.72	118.49	111.03
1	B	199	GLN	N-CA-C	6.63	118.20	110.97
1	B	45	GLY	N-CA-C	-6.62	104.78	112.73
1	A	38	PRO	N-CA-C	6.49	125.85	112.47
1	A	307	LEU	N-CA-C	-6.47	104.31	111.36
1	B	343	LEU	N-CA-C	-6.46	104.16	111.07
1	B	422	LEU	CA-C-N	6.45	127.90	119.84
1	B	422	LEU	C-N-CA	6.45	127.90	119.84
1	B	33	ILE	N-CA-C	6.40	116.89	110.23
1	A	194	GLU	N-CA-C	6.37	120.52	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ILE	N-CA-C	-6.36	97.81	107.73
1	B	422	LEU	N-CA-C	6.35	119.95	109.79
1	B	252	PHE	N-CA-C	6.35	120.23	112.23
1	B	71	ARG	N-CA-C	6.29	119.08	111.40
1	A	184	SER	CA-C-N	6.29	125.51	118.97
1	A	184	SER	C-N-CA	6.29	125.51	118.97
1	A	181	MET	CA-C-N	6.28	127.69	119.84
1	A	181	MET	C-N-CA	6.28	127.69	119.84
1	A	115	THR	N-CA-C	6.28	121.08	112.04
1	A	321	MET	N-CA-C	-6.22	103.43	111.02
1	B	37	ILE	CA-C-N	6.22	127.62	119.84
1	B	37	ILE	C-N-CA	6.22	127.62	119.84
1	A	70	GLY	N-CA-C	6.19	117.83	111.95
1	B	412	VAL	N-CA-C	6.15	117.70	111.00
1	A	232	LYS	N-CA-C	6.13	120.02	112.54
1	A	37	ILE	CA-C-N	6.10	127.47	119.84
1	A	37	ILE	C-N-CA	6.10	127.47	119.84
1	A	247	ALA	N-CA-C	6.07	118.86	111.82
1	A	133	GLY	N-CA-C	-6.03	105.29	113.37
1	B	419	ILE	N-CA-C	6.01	120.86	112.50
1	A	266	PHE	N-CA-C	6.00	118.61	111.71
1	B	34	HIS	N-CA-C	6.00	118.58	111.33
1	A	126	THR	N-CA-C	-5.90	106.13	113.15
1	A	214	LEU	N-CA-C	-5.88	104.87	111.28
1	A	174	LEU	N-CA-C	-5.86	104.89	111.28
1	A	314	MET	CB-CG-SD	5.85	130.25	112.70
1	B	254	GLY	N-CA-C	5.80	119.80	110.87
1	A	157	ILE	N-CA-C	5.78	115.97	110.42
1	B	60	GLY	N-CA-C	-5.75	105.83	112.50
1	A	116	VAL	N-CA-CB	5.73	114.11	110.50
1	B	161	ARG	N-CA-C	-5.68	105.17	111.36
1	A	262	SER	CA-C-N	-5.67	111.69	120.31
1	A	262	SER	C-N-CA	-5.67	111.69	120.31
1	A	203	ILE	N-CA-C	5.67	115.86	110.42
1	B	271	LEU	N-CA-C	5.67	117.54	110.91
1	A	296	PHE	N-CA-C	5.59	118.57	111.69
1	B	100	ILE	N-CA-C	5.52	115.72	110.42
1	B	408	ALA	N-CA-C	-5.45	105.36	112.23
1	B	44	GLU	N-CA-C	-5.37	105.09	111.69
1	B	339	VAL	N-CA-C	5.36	115.57	110.42
1	A	342	SER	N-CA-C	-5.34	104.86	111.33
1	A	295	ILE	CB-CA-C	-5.33	105.06	111.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	ARG	N-CA-C	5.32	117.55	110.53
1	B	226	SER	N-CA-C	5.31	117.88	111.40
1	A	231	ILE	N-CA-C	5.30	120.37	109.34
1	B	298	VAL	N-CA-C	-5.26	105.58	110.53
1	A	161	ARG	N-CA-C	-5.25	105.24	111.69
1	B	252	PHE	CA-C-N	-5.24	115.83	122.43
1	B	252	PHE	C-N-CA	-5.24	115.83	122.43
1	A	116	VAL	N-CA-C	5.23	120.20	112.61
1	B	180	PHE	N-CA-C	5.23	119.81	113.38
1	A	211	ASP	N-CA-C	-5.22	105.23	111.03
1	A	56	ILE	N-CA-C	5.22	115.33	110.42
1	B	351	SER	N-CA-C	5.16	121.78	110.80
1	A	250	GLN	N-CA-C	5.15	118.02	111.69
1	A	110	GLY	N-CA-C	-5.11	106.60	112.73
1	B	206	ASP	N-CA-C	5.10	121.66	110.80
1	B	164	LEU	N-CA-C	-5.10	105.80	111.36
1	B	229	THR	N-CA-C	5.04	117.50	111.71
1	B	207	ASP	N-CA-C	5.03	121.52	110.80
1	B	400	THR	N-CA-C	5.03	116.95	109.25

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PRO	Peptide
1	A	400	THR	Peptide
1	B	206	ASP	Peptide
1	B	233	SER	Peptide
1	B	234	PRO	Peptide
1	B	399	SER	Peptide
1	B	423	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3194	0	3399	319	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3194	0	3399	268	0
All	All	6388	0	6798	582	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 44.

All (582) 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:186:ARG:HG2	1:B:217:MET:HG2	1.32	1.04
1:B:92:SER:HA	1:B:97:LEU:HD11	1.38	1.01
1:A:330:ILE:HA	1:A:333:SER:HB3	1.49	0.94
1:B:351:SER:HG	1:B:352:TRP:HD1	1.15	0.94
1:A:324:LEU:HD11	1:A:336:ILE:HB	1.52	0.90
1:A:283:ILE:HD11	1:A:342:SER:HA	1.53	0.89
1:A:163:MET:HA	1:A:166:LEU:HB2	1.54	0.88
1:A:318:LEU:HD23	1:A:404:PHE:HB3	1.55	0.86
1:A:18:LEU:HD11	1:A:171:SER:HA	1.54	0.86
1:B:253:ILE:HG13	1:B:410:ILE:HG22	1.57	0.84
1:B:315:ILE:HG23	1:B:408:ALA:HB1	1.61	0.82
1:A:185:PRO:HA	1:A:188:LEU:HD12	1.62	0.81
1:A:323:ILE:HG21	1:B:415:MET:HE3	1.63	0.80
1:B:351:SER:HG	1:B:352:TRP:CD1	1.98	0.80
1:B:172:VAL:HA	1:B:175:LEU:HB2	1.61	0.80
1:B:334:ALA:HA	1:B:337:ILE:HB	1.61	0.80
1:A:82:PHE:HB3	1:A:171:SER:HB2	1.64	0.80
1:A:25:VAL:HG13	1:A:160:TRP:HH2	1.47	0.79
1:A:83:ILE:HA	1:A:168:VAL:HG22	1.65	0.79
1:A:351:SER:HB2	1:A:352:TRP:CD1	2.19	0.78
1:B:411:GLY:O	1:B:415:MET:HB2	1.83	0.78
1:A:130:GLY:O	1:A:133:GLY:N	2.16	0.77
1:A:409:PHE:HA	1:A:412:VAL:HB	1.66	0.77
1:B:35:LYS:HB3	1:B:157:ILE:HD11	1.66	0.77
1:A:76:MET:SD	1:A:178:ILE:HB	2.25	0.76
1:B:186:ARG:HG3	1:B:189:LEU:HD12	1.69	0.75
1:B:234:PRO:HB2	1:B:238:ARG:HH21	1.50	0.75
1:A:388:SER:OG	1:A:389:LEU:N	2.15	0.75
1:A:276:SER:O	1:A:280:SER:OG	2.03	0.74
1:A:284:GLY:O	1:A:287:ASN:ND2	2.20	0.74
1:B:409:PHE:HA	1:B:412:VAL:HB	1.68	0.74
1:A:30:LEU:HG	1:A:264:SER:HB2	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:HA	1:B:244:CYS:HB2	1.70	0.74
1:A:19:TYR:OH	1:A:113:MET:HE3	1.88	0.74
1:B:318:LEU:HD23	1:B:404:PHE:HD1	1.53	0.73
1:A:406:ILE:O	1:A:409:PHE:N	2.22	0.73
1:A:25:VAL:HG22	1:A:160:TRP:HZ3	1.54	0.72
1:A:246:PHE:CE2	1:A:356:LEU:HG	2.23	0.72
1:A:387:VAL:HG13	1:A:391:PHE:HD2	1.54	0.72
1:A:87:LEU:HG	1:A:168:VAL:HG21	1.69	0.72
1:A:312:ILE:HG12	1:B:320:ILE:HG12	1.72	0.72
1:A:131:SER:O	1:A:134:SER:OG	2.07	0.72
1:A:387:VAL:HG13	1:A:391:PHE:CD2	2.25	0.71
1:A:266:PHE:CE1	1:A:338:ILE:HA	2.25	0.71
1:B:227:THR:HG21	1:B:367:ARG:HH11	1.55	0.71
1:B:398:LEU:HD12	1:B:400:THR:HB	1.73	0.71
1:A:51:MET:HE2	1:A:102:ARG:HH21	1.56	0.71
1:A:315:ILE:HA	1:A:318:LEU:HB2	1.71	0.71
1:B:265:ILE:HD13	1:B:337:ILE:HD13	1.72	0.70
1:A:253:ILE:HD11	1:A:410:ILE:HG22	1.74	0.70
1:A:311:ASN:CG	1:A:314:MET:HE3	2.17	0.70
1:A:346:VAL:O	1:A:350:ILE:HG12	1.92	0.70
1:A:32:PHE:HB3	1:A:157:ILE:HD11	1.73	0.69
1:A:25:VAL:HG13	1:A:160:TRP:CH2	2.27	0.69
1:A:217:MET:HA	1:A:220:ILE:HG12	1.75	0.69
1:B:175:LEU:HG	1:B:179:TYR:HE1	1.58	0.68
1:A:351:SER:HB2	1:A:352:TRP:HD1	1.57	0.68
1:B:87:LEU:HG	1:B:168:VAL:HG21	1.76	0.68
1:A:246:PHE:CZ	1:A:360:LEU:HG	2.29	0.67
1:A:273:GLU:O	1:A:276:SER:N	2.27	0.67
1:A:207:ASP:HA	1:A:210:ILE:HG12	1.75	0.67
1:B:158:GLU:HG2	1:B:161:ARG:HH21	1.59	0.67
1:A:89:LEU:HB3	1:A:164:LEU:HD12	1.77	0.67
1:B:395:SER:HA	1:B:400:THR:HG21	1.76	0.67
1:B:324:LEU:HB3	1:B:333:SER:HB2	1.77	0.66
1:B:394:LEU:HD13	1:B:398:LEU:HD11	1.77	0.66
1:A:265:ILE:O	1:A:269:ALA:HB3	1.95	0.66
1:B:141:THR:HG22	1:B:288:VAL:HG22	1.78	0.66
1:A:244:CYS:HB3	1:A:379:VAL:HG11	1.78	0.65
1:A:283:ILE:HA	1:A:286:ILE:HD12	1.78	0.65
1:B:171:SER:O	1:B:175:LEU:N	2.30	0.65
1:B:407:PHE:HA	1:B:410:ILE:HB	1.79	0.65
1:A:145:LEU:HD23	1:A:284:GLY:HA3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:HA	1:B:260:PHE:HA	1.79	0.65
1:A:322:ALA:HB1	1:A:401:GLU:HG2	1.78	0.65
1:B:253:ILE:HG23	1:B:407:PHE:HB3	1.79	0.65
1:B:308:VAL:HG22	1:B:418:VAL:HG11	1.79	0.64
1:B:122:GLU:HG2	1:B:186:ARG:HB2	1.79	0.64
1:A:266:PHE:HB3	1:A:275:ALA:O	1.98	0.64
1:A:257:ALA:HB2	1:A:387:VAL:HG12	1.79	0.64
1:A:47:VAL:O	1:A:50:SER:OG	2.16	0.64
1:B:334:ALA:C	1:B:337:ILE:H	2.05	0.64
1:A:146:ALA:HA	1:A:149:LEU:HD13	1.80	0.64
1:B:44:GLU:HA	1:B:47:VAL:HB	1.79	0.64
1:A:89:LEU:HD13	1:A:101:GLY:HA3	1.79	0.63
1:A:317:SER:HA	1:A:320:ILE:HG22	1.80	0.63
1:A:41:SER:HA	1:A:44:GLU:CD	2.24	0.63
1:B:303:ARG:HB3	1:B:359:MET:HE2	1.79	0.63
1:B:21:TYR:HA	1:B:147:ALA:HB2	1.81	0.63
1:A:84:ILE:HG22	1:A:104:ILE:HG21	1.79	0.62
1:B:176:VAL:HA	1:B:179:TYR:HB2	1.81	0.62
1:B:335:TRP:O	1:B:338:ILE:HB	1.99	0.62
1:A:80:ILE:HA	1:A:83:ILE:HG22	1.81	0.62
1:A:92:SER:HA	1:A:97:LEU:HD21	1.81	0.62
1:B:26:ILE:HG13	1:B:29:ALA:HB3	1.82	0.62
1:A:151:ASN:HA	1:A:163:MET:SD	2.40	0.62
1:A:273:GLU:C	1:A:276:SER:H	2.08	0.62
1:B:200:VAL:HA	1:B:203:ILE:HB	1.82	0.62
1:B:315:ILE:HD13	1:B:412:VAL:HG23	1.82	0.62
1:A:152:TYR:CZ	1:A:273:GLU:HB2	2.34	0.62
1:A:75:VAL:HG21	1:A:119:TYR:CG	2.35	0.62
1:A:403:VAL:O	1:A:406:ILE:N	2.33	0.62
1:A:72:ARG:NH2	1:A:181:MET:O	2.33	0.62
1:A:189:LEU:HD11	1:A:214:LEU:HD22	1.82	0.62
1:A:312:ILE:HG23	1:B:320:ILE:HD11	1.80	0.62
1:A:323:ILE:HG21	1:B:415:MET:CE	2.28	0.61
1:A:159:GLY:O	1:A:162:TRP:HB3	1.99	0.61
1:B:400:THR:O	1:B:400:THR:OG1	2.17	0.61
1:A:100:ILE:HA	1:A:103:LEU:HD12	1.81	0.61
1:A:257:ALA:HB2	1:A:387:VAL:CG1	2.32	0.60
1:B:45:GLY:O	1:B:49:SER:OG	2.09	0.60
1:B:255:ILE:HA	1:B:258:VAL:HB	1.83	0.60
1:A:51:MET:HA	1:A:102:ARG:O	2.01	0.60
1:A:306:LEU:O	1:A:351:SER:OG	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ALA:HB2	1:B:178:ILE:HD12	1.83	0.60
1:B:325:ILE:HG21	1:B:400:THR:O	2.02	0.60
1:A:275:ALA:O	1:A:279:GLY:HA3	2.02	0.60
1:A:334:ALA:HA	1:A:337:ILE:HB	1.82	0.60
1:A:144:ILE:O	1:A:147:ALA:HB3	2.01	0.60
1:A:249:PHE:HD2	1:A:414:ALA:HB2	1.67	0.60
1:B:158:GLU:HA	1:B:161:ARG:NE	2.17	0.59
1:A:45:GLY:O	1:A:49:SER:OG	2.14	0.59
1:A:79:ALA:O	1:A:82:PHE:HB2	2.02	0.59
1:B:315:ILE:HG12	1:B:408:ALA:O	2.03	0.59
1:A:118:VAL:HA	1:A:121:SER:HB3	1.84	0.59
1:B:46:ILE:HA	1:B:49:SER:HB2	1.85	0.59
1:B:42:THR:HA	1:B:393:ILE:HG22	1.85	0.59
1:A:42:THR:HG22	1:A:393:ILE:HB	1.83	0.59
1:A:175:LEU:HG	1:A:179:TYR:CE1	2.38	0.59
1:B:170:PRO:HA	1:B:173:ILE:HG12	1.85	0.59
1:A:20:GLY:O	1:A:144:ILE:HG13	2.03	0.59
1:A:256:ASN:O	1:A:260:PHE:HE1	1.84	0.59
1:B:253:ILE:HG21	1:B:314:MET:HE3	1.85	0.59
1:A:318:LEU:HD13	1:A:408:ALA:HA	1.85	0.58
1:B:26:ILE:HD11	1:B:48:VAL:HG22	1.84	0.58
1:A:352:TRP:HE3	1:A:356:LEU:HD22	1.68	0.58
1:A:310:GLY:O	1:A:347:PHE:HB3	2.03	0.58
1:B:214:LEU:O	1:B:218:LYS:HB2	2.03	0.58
1:A:266:PHE:O	1:A:270:GLY:HA3	2.03	0.58
1:A:253:ILE:CD1	1:A:410:ILE:HG22	2.33	0.58
1:A:173:ILE:O	1:A:177:GLY:N	2.35	0.58
1:A:409:PHE:CA	1:A:412:VAL:HB	2.34	0.58
1:A:51:MET:HB2	1:A:102:ARG:HE	1.68	0.58
1:B:313:GLY:HA3	1:B:347:PHE:CD2	2.38	0.58
1:B:318:LEU:HB3	1:B:404:PHE:HB3	1.85	0.57
1:B:383:GLY:O	1:B:387:VAL:HG23	2.04	0.57
1:A:315:ILE:HD11	1:A:411:GLY:O	2.04	0.57
1:B:233:SER:HB3	1:B:234:PRO:HD3	1.86	0.57
1:A:28:GLY:O	1:A:31:LEU:HB3	2.04	0.57
1:A:79:ALA:HA	1:A:82:PHE:HD2	1.69	0.57
1:B:253:ILE:CG1	1:B:410:ILE:HG22	2.32	0.57
1:B:306:LEU:HD22	1:B:351:SER:HB3	1.87	0.57
1:A:336:ILE:O	1:A:339:VAL:HB	2.03	0.57
1:A:9:PHE:CE1	1:A:120:LEU:HG	2.40	0.57
1:A:313:GLY:O	1:A:316:ALA:HB3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:PHE:C	1:A:412:VAL:HB	2.30	0.57
1:B:144:ILE:HG23	1:B:148:TYR:CE2	2.40	0.57
1:B:185:PRO:HA	1:B:188:LEU:HD12	1.86	0.57
1:A:28:GLY:HA3	1:A:151:ASN:CG	2.30	0.57
1:B:252:PHE:CZ	1:B:383:GLY:HA2	2.40	0.57
1:B:311:ASN:HB3	1:B:415:MET:SD	2.45	0.57
1:B:407:PHE:HD1	1:B:410:ILE:HD12	1.70	0.57
1:B:284:GLY:O	1:B:288:VAL:HG23	2.05	0.56
1:A:247:ALA:O	1:A:380:LEU:HD12	2.05	0.56
1:A:258:VAL:O	1:A:262:SER:OG	2.21	0.56
1:A:352:TRP:CE3	1:A:356:LEU:HD22	2.40	0.56
1:B:359:MET:O	1:B:363:LEU:HG	2.05	0.56
1:B:174:LEU:HD13	1:B:177:GLY:HA3	1.87	0.56
1:B:51:MET:HB2	1:B:102:ARG:HD3	1.87	0.56
1:A:315:ILE:HG23	1:A:408:ALA:HB1	1.88	0.56
1:A:128:TYR:HB3	1:A:132:LEU:HD11	1.88	0.56
1:A:24:GLY:O	1:A:27:SER:HB3	2.05	0.56
1:A:300:LYS:O	1:A:426:ARG:NH1	2.39	0.56
1:B:315:ILE:HD11	1:B:411:GLY:C	2.31	0.56
1:A:261:TYR:OH	1:A:403:VAL:HG21	2.05	0.56
1:A:307:LEU:HD11	1:A:356:LEU:HD13	1.86	0.56
1:B:387:VAL:HA	1:B:391:PHE:CD2	2.41	0.56
1:B:417:PHE:HA	1:B:421:PHE:HD2	1.71	0.56
1:A:389:LEU:O	1:A:393:ILE:HG23	2.06	0.55
1:B:413:LEU:HD23	1:B:416:ILE:HG21	1.87	0.55
1:B:125:PRO:HA	1:B:186:ARG:HH22	1.72	0.55
1:A:27:SER:HA	1:A:260:PHE:HA	1.87	0.55
1:A:85:GLY:O	1:A:89:LEU:HB2	2.07	0.55
1:A:176:VAL:HA	1:A:179:TYR:CG	2.42	0.55
1:B:112:SER:OG	1:B:113:MET:N	2.40	0.55
1:A:246:PHE:CE2	1:A:360:LEU:HG	2.42	0.55
1:B:57:VAL:O	1:B:61:SER:OG	2.16	0.55
1:A:311:ASN:OD1	1:A:314:MET:HE3	2.07	0.55
1:B:86:ALA:O	1:B:164:LEU:HB3	2.07	0.55
1:B:141:THR:HG21	1:B:288:VAL:HA	1.89	0.55
1:B:374:GLY:O	1:B:377:ALA:HB3	2.06	0.55
1:B:419:ILE:O	1:B:423:PRO:HG3	2.07	0.55
1:A:29:ALA:O	1:A:32:PHE:N	2.41	0.54
1:B:242:VAL:O	1:B:245:ILE:HG22	2.07	0.54
1:B:257:ALA:HA	1:B:260:PHE:CD2	2.43	0.54
1:A:77:LEU:O	1:A:81:VAL:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TRP:HA	1:A:163:MET:HG2	1.89	0.54
1:B:287:ASN:HA	1:B:290:VAL:HG12	1.88	0.54
1:B:43:THR:HA	1:B:46:ILE:HB	1.89	0.54
1:B:125:PRO:HA	1:B:186:ARG:NH2	2.23	0.54
1:B:246:PHE:HD1	1:B:417:PHE:CE1	2.26	0.54
1:A:352:TRP:CD1	1:A:352:TRP:N	2.76	0.54
1:A:390:PHE:HB3	1:A:391:PHE:CD1	2.42	0.54
1:A:343:LEU:O	1:A:346:VAL:N	2.40	0.54
1:B:71:ARG:O	1:B:75:VAL:HG23	2.08	0.54
1:B:308:VAL:HG22	1:B:418:VAL:CG1	2.37	0.54
1:A:122:GLU:HG2	1:A:186:ARG:HB3	1.90	0.54
1:B:170:PRO:O	1:B:174:LEU:N	2.41	0.54
1:A:321:MET:SD	1:A:337:ILE:HG12	2.47	0.53
1:B:137:GLN:O	1:B:140:ILE:HB	2.08	0.53
1:A:175:LEU:HA	1:A:178:ILE:HD12	1.90	0.53
1:B:234:PRO:O	1:B:236:LEU:N	2.41	0.53
1:B:307:LEU:HA	1:B:351:SER:OG	2.08	0.53
1:A:336:ILE:C	1:A:339:VAL:HB	2.32	0.53
1:B:378:LEU:O	1:B:382:ILE:HG13	2.08	0.53
1:B:122:GLU:O	1:B:201:MET:HE1	2.08	0.53
1:A:26:ILE:HG12	1:A:48:VAL:CG2	2.38	0.53
1:A:315:ILE:HG22	1:A:319:LEU:HD12	1.89	0.53
1:A:405:LEU:O	1:A:408:ALA:HB3	2.09	0.53
1:B:80:ILE:HG13	1:B:175:LEU:HD11	1.89	0.53
1:B:249:PHE:CZ	1:B:413:LEU:HD22	2.44	0.53
1:B:233:SER:HB3	1:B:234:PRO:CD	2.39	0.53
1:B:357:TRP:O	1:B:360:LEU:N	2.41	0.53
1:A:19:TYR:CE1	1:A:109:VAL:HG13	2.44	0.53
1:A:252:PHE:HB3	1:A:410:ILE:HG21	1.91	0.53
1:A:143:GLY:O	1:A:147:ALA:HB2	2.09	0.52
1:A:308:VAL:HG22	1:A:415:MET:HE1	1.91	0.52
1:B:259:ILE:HA	1:B:262:SER:HB3	1.91	0.52
1:B:125:PRO:HB3	1:B:213:GLU:CD	2.34	0.52
1:B:130:GLY:O	1:B:133:GLY:N	2.42	0.52
1:B:313:GLY:HA3	1:B:347:PHE:CE2	2.45	0.52
1:A:190:GLU:HG3	1:A:221:ASN:CG	2.35	0.52
1:A:211:ASP:O	1:A:215:LYS:HB2	2.09	0.52
1:B:187:TRP:HE3	1:B:188:LEU:HG	1.75	0.52
1:B:324:LEU:HD11	1:B:336:ILE:HD12	1.92	0.52
1:A:22:ASP:OD2	1:A:105:ILE:HG23	2.09	0.52
1:A:318:LEU:CD2	1:A:404:PHE:HB3	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:VAL:O	1:A:342:SER:N	2.43	0.52
1:B:152:TYR:HE1	1:B:273:GLU:HB2	1.75	0.52
1:A:46:ILE:O	1:A:49:SER:HB2	2.09	0.51
1:A:261:TYR:O	1:A:264:SER:HB3	2.10	0.51
1:A:341:LEU:O	1:A:344:PHE:N	2.43	0.51
1:B:26:ILE:HA	1:B:29:ALA:HB3	1.92	0.51
1:A:54:GLY:HA3	1:A:103:LEU:O	2.10	0.51
1:B:21:TYR:HE1	1:B:167:ALA:HB2	1.75	0.51
1:B:99:ILE:O	1:B:103:LEU:HG	2.10	0.51
1:A:246:PHE:CD2	1:A:356:LEU:HG	2.46	0.51
1:A:47:VAL:HG21	1:A:98:LEU:HD13	1.91	0.51
1:B:148:TYR:OH	1:B:284:GLY:HA3	2.11	0.51
1:B:189:LEU:HD22	1:B:218:LYS:HZ2	1.75	0.51
1:B:287:ASN:O	1:B:291:THR:HG23	2.11	0.51
1:A:339:VAL:O	1:A:343:LEU:HD22	2.10	0.51
1:B:196:ALA:HA	1:B:199:GLN:HB2	1.93	0.51
1:B:326:TRP:O	1:B:328:ILE:N	2.44	0.51
1:A:318:LEU:HB3	1:A:408:ALA:HB2	1.91	0.51
1:A:320:ILE:O	1:A:324:LEU:HB2	2.10	0.51
1:A:390:PHE:O	1:A:393:ILE:HG12	2.10	0.51
1:B:75:VAL:HB	1:B:178:ILE:HG21	1.93	0.51
1:A:266:PHE:HZ	1:A:341:LEU:HD23	1.75	0.51
1:B:141:THR:O	1:B:144:ILE:HG22	2.11	0.51
1:B:326:TRP:C	1:B:328:ILE:H	2.18	0.51
1:A:33:ILE:HD12	1:A:34:HIS:H	1.75	0.51
1:A:125:PRO:C	1:A:127:GLU:H	2.17	0.51
1:A:404:PHE:CD1	1:A:404:PHE:N	2.77	0.51
1:A:417:PHE:CD1	1:A:417:PHE:C	2.89	0.51
1:B:173:ILE:HA	1:B:176:VAL:HB	1.93	0.51
1:B:296:PHE:CE1	1:B:300:LYS:HD2	2.45	0.51
1:B:310:GLY:HA2	1:B:347:PHE:CD1	2.46	0.51
1:B:414:ALA:O	1:B:418:VAL:HG23	2.10	0.51
1:A:148:TYR:HE1	1:A:280:SER:C	2.19	0.50
1:A:266:PHE:CZ	1:A:341:LEU:HD23	2.46	0.50
1:B:123:MET:HE1	1:B:182:PRO:HD2	1.93	0.50
1:B:132:LEU:O	1:B:135:LEU:HB3	2.12	0.50
1:A:10:ILE:O	1:A:14:LEU:HG	2.12	0.50
1:B:248:ILE:HG23	1:B:252:PHE:CD2	2.46	0.50
1:B:335:TRP:O	1:B:339:VAL:HG23	2.11	0.50
1:B:74:LEU:O	1:B:78:ILE:HG13	2.12	0.50
1:B:93:THR:H	1:B:97:LEU:HG	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLU:O	1:B:276:SER:N	2.36	0.50
1:A:30:LEU:HD12	1:A:33:ILE:HG12	1.94	0.50
1:A:261:TYR:HA	1:A:264:SER:HB3	1.94	0.50
1:A:404:PHE:HA	1:A:407:PHE:HB2	1.94	0.50
1:B:131:SER:O	1:B:134:SER:OG	2.25	0.50
1:B:360:LEU:HB3	1:B:361:PRO:HD3	1.93	0.50
1:A:400:THR:C	1:A:402:TRP:N	2.66	0.49
1:A:190:GLU:HG3	1:A:221:ASN:HB3	1.94	0.49
1:A:308:VAL:O	1:A:312:ILE:HB	2.11	0.49
1:B:145:LEU:HD23	1:B:288:VAL:HG21	1.95	0.49
1:B:357:TRP:O	1:B:361:PRO:HD2	2.13	0.49
1:A:25:VAL:HG22	1:A:160:TRP:CZ3	2.41	0.49
1:A:172:VAL:O	1:A:175:LEU:HB3	2.11	0.49
1:A:325:ILE:HG12	1:A:333:SER:OG	2.12	0.49
1:B:86:ALA:HA	1:B:164:LEU:HD12	1.92	0.49
1:B:90:ALA:O	1:B:161:ARG:HB3	2.11	0.49
1:A:236:LEU:HD12	1:A:236:LEU:H	1.77	0.49
1:B:44:GLU:O	1:B:48:VAL:HG23	2.12	0.49
1:B:76:MET:SD	1:B:178:ILE:HB	2.52	0.49
1:B:234:PRO:HB2	1:B:238:ARG:NH2	2.22	0.49
1:B:315:ILE:HA	1:B:318:LEU:HD12	1.93	0.49
1:B:303:ARG:HG2	1:B:359:MET:HG2	1.94	0.49
1:B:193:ASN:O	1:B:195:GLU:N	2.46	0.48
1:B:232:LYS:HD2	1:B:233:SER:HB2	1.95	0.48
1:A:263:SER:OG	1:A:280:SER:OG	2.31	0.48
1:B:26:ILE:HG23	1:B:260:PHE:CE1	2.48	0.48
1:B:26:ILE:HA	1:B:29:ALA:CB	2.44	0.48
1:B:87:LEU:CG	1:B:168:VAL:HG21	2.43	0.48
1:B:187:TRP:CE3	1:B:188:LEU:HG	2.48	0.48
1:A:34:HIS:HA	1:A:38:PRO:HG2	1.95	0.48
1:A:410:ILE:C	1:A:412:VAL:H	2.20	0.48
1:A:357:TRP:HZ2	1:A:380:LEU:HD22	1.77	0.48
1:B:27:SER:HB2	1:B:259:ILE:HD12	1.94	0.48
1:B:174:LEU:HD13	1:B:174:LEU:HA	1.66	0.48
1:B:253:ILE:HD13	1:B:314:MET:HE1	1.94	0.48
1:B:321:MET:HE2	1:B:337:ILE:HG12	1.95	0.48
1:A:186:ARG:HA	1:A:189:LEU:HB2	1.96	0.48
1:A:188:LEU:HD13	1:A:196:ALA:HB3	1.96	0.48
1:B:26:ILE:HG21	1:B:51:MET:SD	2.54	0.48
1:A:26:ILE:HD13	1:A:102:ARG:NH1	2.29	0.48
1:A:41:SER:O	1:A:44:GLU:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HA	1:A:415:MET:SD	2.53	0.48
1:B:152:TYR:CE1	1:B:273:GLU:HB2	2.49	0.48
1:B:37:ILE:HG22	1:B:39:LEU:HD12	1.96	0.48
1:A:86:ALA:HB3	1:A:168:VAL:HG23	1.96	0.47
1:B:185:PRO:O	1:B:197:ALA:HB2	2.14	0.47
1:A:409:PHE:HD1	1:A:412:VAL:HG21	1.79	0.47
1:B:13:ALA:O	1:B:139:MET:HG2	2.13	0.47
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.70	0.47
1:A:258:VAL:O	1:A:262:SER:CB	2.62	0.47
1:A:290:VAL:HG11	1:A:349:GLY:HA3	1.96	0.47
1:A:305:LYS:HA	1:A:308:VAL:HB	1.96	0.47
1:A:409:PHE:HA	1:A:412:VAL:CB	2.38	0.47
1:B:326:TRP:C	1:B:328:ILE:N	2.72	0.47
1:B:334:ALA:O	1:B:337:ILE:N	2.47	0.47
1:A:26:ILE:HG23	1:A:260:PHE:CG	2.50	0.47
1:A:52:LEU:HA	1:A:55:ALA:HB3	1.96	0.47
1:A:251:GLN:NE2	1:A:256:ASN:HB2	2.29	0.47
1:A:416:ILE:O	1:A:420:LYS:HB2	2.15	0.47
1:B:249:PHE:HD2	1:B:417:PHE:CD2	2.33	0.47
1:A:27:SER:HB3	1:A:148:TYR:HB3	1.96	0.47
1:A:164:LEU:O	1:A:167:ALA:HB3	2.14	0.47
1:B:122:GLU:HB3	1:B:186:ARG:H	1.80	0.47
1:A:264:SER:O	1:A:268:LYS:HB2	2.15	0.47
1:B:189:LEU:HD22	1:B:218:LYS:NZ	2.29	0.47
1:B:379:VAL:HA	1:B:382:ILE:HD12	1.97	0.47
1:A:407:PHE:HA	1:A:410:ILE:HG13	1.96	0.47
1:B:290:VAL:CG1	1:B:349:GLY:HA3	2.45	0.47
1:A:76:MET:HE1	1:A:179:TYR:HD1	1.79	0.47
1:A:265:ILE:O	1:A:270:GLY:N	2.41	0.47
1:A:359:MET:HE3	1:A:359:MET:HB3	1.77	0.46
1:A:400:THR:HB	1:A:402:TRP:HB2	1.97	0.46
1:A:318:LEU:HD13	1:A:407:PHE:C	2.40	0.46
1:B:26:ILE:HD12	1:B:102:ARG:HH11	1.81	0.46
1:B:415:MET:HA	1:B:418:VAL:HB	1.96	0.46
1:A:69:LEU:HD22	1:A:73:ARG:HH21	1.80	0.46
1:B:26:ILE:HG21	1:B:51:MET:HE1	1.98	0.46
1:B:235:TRP:H	1:B:238:ARG:HH21	1.62	0.46
1:B:336:ILE:HA	1:B:339:VAL:HG23	1.97	0.46
1:B:379:VAL:O	1:B:382:ILE:HB	2.15	0.46
1:A:38:PRO:C	1:A:39:LEU:HD13	2.39	0.46
1:A:199:GLN:O	1:A:202:LYS:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HD13	1:B:356:LEU:HD11	1.97	0.46
1:A:26:ILE:HG23	1:A:260:PHE:HB3	1.97	0.46
1:A:84:ILE:O	1:A:88:ILE:HB	2.16	0.46
1:A:174:LEU:O	1:A:178:ILE:HG13	2.15	0.46
1:A:318:LEU:HD13	1:A:407:PHE:O	2.15	0.46
1:B:173:ILE:O	1:B:177:GLY:N	2.48	0.46
1:B:261:TYR:HA	1:B:264:SER:HB3	1.97	0.46
1:B:322:ALA:O	1:B:325:ILE:HB	2.15	0.46
1:A:26:ILE:HG23	1:A:260:PHE:CB	2.46	0.46
1:A:181:MET:HA	1:A:182:PRO:HD3	1.66	0.46
1:B:297:VAL:HA	1:B:300:LYS:HB3	1.98	0.46
1:B:307:LEU:HD12	1:B:418:VAL:HG22	1.98	0.46
1:B:326:TRP:O	1:B:328:ILE:HD12	2.16	0.46
1:A:198:ARG:O	1:A:201:MET:HB2	2.16	0.46
1:B:86:ALA:N	1:B:105:ILE:HD11	2.31	0.46
1:B:148:TYR:HE1	1:B:281:VAL:HG13	1.80	0.46
1:B:312:ILE:HG22	1:B:313:GLY:N	2.30	0.46
1:B:97:LEU:C	1:B:97:LEU:HD12	2.40	0.46
1:A:26:ILE:HG12	1:A:48:VAL:HG21	1.97	0.45
1:A:89:LEU:HD21	1:A:102:ARG:HG2	1.97	0.45
1:A:89:LEU:HB3	1:A:164:LEU:CD1	2.46	0.45
1:A:321:MET:HG2	1:A:404:PHE:CD1	2.52	0.45
1:B:43:THR:O	1:B:47:VAL:HG23	2.15	0.45
1:B:175:LEU:O	1:B:179:TYR:HD1	2.00	0.45
1:A:236:LEU:O	1:A:239:ILE:HG22	2.16	0.45
1:B:64:PRO:HA	1:B:67:ASP:HB2	1.97	0.45
1:B:188:LEU:HD13	1:B:197:ALA:N	2.31	0.45
1:B:415:MET:O	1:B:418:VAL:HB	2.17	0.45
1:A:26:ILE:HA	1:A:29:ALA:HB3	1.99	0.45
1:B:265:ILE:HG22	1:B:268:LYS:HB3	1.99	0.45
1:A:133:GLY:O	1:A:136:ASN:HB3	2.16	0.45
1:A:279:GLY:O	1:A:283:ILE:HB	2.17	0.45
1:A:21:TYR:HA	1:A:147:ALA:HB2	1.98	0.45
1:A:94:ASN:N	1:A:94:ASN:OD1	2.50	0.45
1:A:402:TRP:O	1:A:406:ILE:HG12	2.16	0.45
1:B:160:TRP:O	1:B:163:MET:HG2	2.17	0.45
1:A:160:TRP:CA	1:A:163:MET:HG2	2.47	0.45
1:A:248:ILE:HD11	1:A:382:ILE:HG22	1.98	0.45
1:A:307:LEU:HD13	1:A:352:TRP:CH2	2.52	0.45
1:B:118:VAL:O	1:B:122:GLU:HG3	2.17	0.45
1:B:144:ILE:HG23	1:B:148:TYR:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TRP:CH2	1:B:236:LEU:HD11	2.52	0.45
1:A:144:ILE:HG22	1:A:145:LEU:N	2.31	0.45
1:A:324:LEU:HD12	1:A:340:CYS:SG	2.57	0.45
1:B:29:ALA:O	1:B:33:ILE:HG23	2.17	0.45
1:B:138:LEU:HA	1:B:141:THR:OG1	2.17	0.45
1:A:31:LEU:HD11	1:A:152:TYR:CG	2.52	0.44
1:A:21:TYR:OH	1:A:167:ALA:HB2	2.17	0.44
1:A:176:VAL:HA	1:A:179:TYR:CD2	2.52	0.44
1:A:259:ILE:HG23	1:A:260:PHE:H	1.81	0.44
1:A:325:ILE:O	1:A:328:ILE:N	2.44	0.44
1:B:347:PHE:CE1	1:B:350:ILE:HD11	2.51	0.44
1:B:21:TYR:CZ	1:B:25:VAL:HG21	2.53	0.44
1:B:75:VAL:HG12	1:B:178:ILE:HD13	1.99	0.44
1:B:77:LEU:O	1:B:81:VAL:HG23	2.16	0.44
1:B:184:SER:HA	1:B:185:PRO:HD3	1.81	0.44
1:B:304:LYS:HE3	1:B:305:LYS:HE3	1.99	0.44
1:A:24:GLY:O	1:A:148:TYR:HB3	2.16	0.44
1:A:37:ILE:N	1:A:38:PRO:HD3	2.31	0.44
1:A:351:SER:CB	1:A:352:TRP:CD1	2.97	0.44
1:A:138:LEU:HD11	1:A:295:ILE:HD11	2.00	0.44
1:B:117:PRO:HA	1:B:120:LEU:HB3	1.99	0.44
1:A:100:ILE:O	1:A:103:LEU:HB2	2.18	0.44
1:A:164:LEU:HD22	1:A:164:LEU:HA	1.64	0.44
1:B:51:MET:SD	1:B:102:ARG:NH1	2.91	0.44
1:B:246:PHE:HB2	1:B:417:PHE:CZ	2.53	0.44
1:B:307:LEU:C	1:B:352:TRP:HE1	2.23	0.44
1:A:189:LEU:HD21	1:A:214:LEU:CD1	2.48	0.44
1:A:334:ALA:O	1:A:337:ILE:N	2.49	0.44
1:B:246:PHE:O	1:B:250:GLN:HB3	2.18	0.44
1:B:122:GLU:HB3	1:B:185:PRO:HD2	1.99	0.44
1:B:246:PHE:HB2	1:B:417:PHE:HZ	1.83	0.44
1:B:321:MET:HB2	1:B:340:CYS:HB3	1.99	0.44
1:B:403:VAL:HG13	1:B:407:PHE:CE2	2.53	0.44
1:A:87:LEU:CG	1:A:168:VAL:HG21	2.44	0.43
1:A:164:LEU:HD22	1:A:167:ALA:HB2	1.99	0.43
1:A:188:LEU:HB2	1:A:197:ALA:HB2	2.00	0.43
1:A:320:ILE:O	1:A:321:MET:C	2.61	0.43
1:A:386:ILE:O	1:A:390:PHE:HB2	2.18	0.43
1:A:194:GLU:O	1:A:197:ALA:HB3	2.18	0.43
1:B:21:TYR:CD2	1:B:147:ALA:HA	2.53	0.43
1:B:89:LEU:HD12	1:B:89:LEU:HA	1.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TRP:HE3	1:A:231:ILE:HG13	1.82	0.43
1:A:267:ALA:HB2	1:A:273:GLU:HA	2.00	0.43
1:A:336:ILE:O	1:A:340:CYS:SG	2.64	0.43
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.69	0.43
1:A:400:THR:C	1:A:402:TRP:H	2.27	0.43
1:A:104:ILE:HA	1:A:107:LEU:HD12	2.00	0.43
1:A:230:VAL:O	1:A:236:LEU:HD13	2.19	0.43
1:A:334:ALA:C	1:A:337:ILE:H	2.27	0.43
1:B:27:SER:OG	1:B:28:GLY:N	2.51	0.43
1:B:194:GLU:O	1:B:197:ALA:HB3	2.18	0.43
1:A:52:LEU:HB2	1:A:385:LEU:HG	2.00	0.43
1:A:83:ILE:HG13	1:A:168:VAL:HG13	2.01	0.43
1:B:249:PHE:HD2	1:B:417:PHE:HD2	1.67	0.43
1:B:79:ALA:HB2	1:B:178:ILE:CD1	2.47	0.43
1:B:163:MET:HA	1:B:166:LEU:HB2	2.01	0.43
1:A:26:ILE:HG12	1:A:48:VAL:HG22	2.01	0.43
1:A:186:ARG:NH1	1:A:201:MET:SD	2.89	0.43
1:A:280:SER:O	1:A:283:ILE:HG22	2.18	0.43
1:B:318:LEU:HD22	1:B:404:PHE:HA	2.01	0.43
1:A:79:ALA:HB3	1:A:175:LEU:HD13	2.01	0.43
1:A:189:LEU:HA	1:A:194:GLU:HB2	2.01	0.43
1:B:145:LEU:HA	1:B:148:TYR:CE1	2.54	0.43
1:A:70:GLY:O	1:A:74:LEU:HB2	2.19	0.43
1:A:222:ALA:O	1:A:225:GLU:HB2	2.19	0.43
1:A:252:PHE:HE1	1:A:383:GLY:HA2	1.84	0.43
1:A:315:ILE:HG23	1:A:408:ALA:CB	2.48	0.43
1:B:315:ILE:O	1:B:319:LEU:HD12	2.19	0.43
1:B:417:PHE:HA	1:B:421:PHE:CD2	2.53	0.43
1:A:234:PRO:O	1:A:236:LEU:N	2.52	0.42
1:A:278:LEU:HD13	1:A:278:LEU:HA	1.81	0.42
1:A:287:ASN:O	1:A:291:THR:HG23	2.19	0.42
1:B:247:ALA:HA	1:B:250:GLN:OE1	2.19	0.42
1:B:257:ALA:HB1	1:B:261:TYR:CE2	2.54	0.42
1:B:394:LEU:HB2	1:B:398:LEU:HD21	2.00	0.42
1:A:92:SER:HA	1:A:97:LEU:HD11	2.01	0.42
1:A:168:VAL:HA	1:A:171:SER:HB3	2.00	0.42
1:A:350:ILE:HG12	1:A:350:ILE:H	1.66	0.42
1:B:125:PRO:HB2	1:B:128:TYR:HD2	1.84	0.42
1:B:248:ILE:HG23	1:B:252:PHE:CE2	2.54	0.42
1:A:87:LEU:HG	1:A:168:VAL:CG2	2.44	0.42
1:A:321:MET:SD	1:A:337:ILE:HD11	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HD13	1:B:88:ILE:HA	1.93	0.42
1:B:296:PHE:CD1	1:B:300:LYS:HD2	2.55	0.42
1:A:72:ARG:HG3	1:A:182:PRO:O	2.19	0.42
1:A:145:LEU:O	1:A:149:LEU:HB2	2.18	0.42
1:A:253:ILE:HD12	1:A:253:ILE:N	2.35	0.42
1:A:343:LEU:HD22	1:A:343:LEU:H	1.84	0.42
1:B:307:LEU:HB2	1:B:352:TRP:NE1	2.34	0.42
1:B:413:LEU:HA	1:B:416:ILE:HB	2.01	0.42
1:B:415:MET:O	1:B:419:ILE:HG13	2.20	0.42
1:A:146:ALA:O	1:A:149:LEU:HB3	2.20	0.42
1:A:307:LEU:HD22	1:A:352:TRP:CD2	2.55	0.42
1:A:315:ILE:HG23	1:A:408:ALA:CA	2.49	0.42
1:A:341:LEU:O	1:A:342:SER:C	2.62	0.42
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.58	0.42
1:B:71:ARG:HB3	1:B:119:TYR:CD2	2.54	0.42
1:A:125:PRO:C	1:A:127:GLU:N	2.77	0.42
1:A:400:THR:HB	1:A:402:TRP:N	2.35	0.42
1:B:359:MET:O	1:B:363:LEU:N	2.53	0.42
1:A:259:ILE:HG23	1:A:260:PHE:N	2.34	0.42
1:A:417:PHE:O	1:A:421:PHE:HD1	2.03	0.42
1:B:152:TYR:HD2	1:B:277:ILE:HD12	1.85	0.42
1:B:243:GLY:C	1:B:246:PHE:HB3	2.44	0.42
1:B:345:ILE:HD13	1:B:345:ILE:HA	1.82	0.42
1:B:290:VAL:O	1:B:293:VAL:HG12	2.19	0.42
1:A:42:THR:HA	1:A:393:ILE:HG22	2.02	0.42
1:A:217:MET:SD	1:A:220:ILE:HD11	2.60	0.42
1:B:75:VAL:HG12	1:B:178:ILE:CD1	2.50	0.42
1:B:275:ALA:O	1:B:279:GLY:HA3	2.20	0.42
1:A:152:TYR:CG	1:A:152:TYR:O	2.72	0.41
1:A:189:LEU:HD21	1:A:214:LEU:HD13	2.01	0.41
1:A:388:SER:O	1:A:392:PRO:HD2	2.20	0.41
1:B:46:ILE:HA	1:B:49:SER:CB	2.48	0.41
1:A:152:TYR:CE2	1:A:273:GLU:O	2.73	0.41
1:A:361:PRO:O	1:A:369:ARG:NH2	2.53	0.41
1:B:148:TYR:CD1	1:B:281:VAL:HG22	2.55	0.41
1:B:235:TRP:N	1:B:238:ARG:HH21	2.18	0.41
1:B:261:TYR:CE2	1:B:392:PRO:HG3	2.55	0.41
1:B:390:PHE:O	1:B:393:ILE:HG23	2.20	0.41
1:A:26:ILE:O	1:A:260:PHE:HB2	2.21	0.41
1:A:52:LEU:O	1:A:56:ILE:HG13	2.21	0.41
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HG	1:B:179:TYR:CE1	2.47	0.41
1:B:376:SER:O	1:B:380:LEU:HB2	2.20	0.41
1:A:160:TRP:CZ3	1:A:164:LEU:HD23	2.54	0.41
1:A:233:SER:CB	1:A:234:PRO:HD2	2.50	0.41
1:A:251:GLN:CD	1:A:256:ASN:HB2	2.45	0.41
1:A:315:ILE:HG12	1:A:408:ALA:O	2.20	0.41
1:A:385:LEU:HA	1:A:388:SER:HB3	2.03	0.41
1:B:13:ALA:HB1	1:B:139:MET:HE3	2.03	0.41
1:B:83:ILE:HA	1:B:168:VAL:HG22	2.02	0.41
1:A:19:TYR:HE1	1:A:109:VAL:HG13	1.82	0.41
1:A:36:ASP:OD1	1:A:157:ILE:HG13	2.20	0.41
1:A:246:PHE:CD1	1:A:246:PHE:C	2.98	0.41
1:A:282:GLY:O	1:A:286:ILE:HG13	2.21	0.41
1:A:363:LEU:HD13	1:A:364:PHE:CE1	2.55	0.41
1:B:148:TYR:CE1	1:B:281:VAL:HA	2.55	0.41
1:B:217:MET:O	1:B:217:MET:HG3	2.18	0.41
1:B:261:TYR:CD2	1:B:392:PRO:HG3	2.55	0.41
1:A:251:GLN:OE1	1:A:384:THR:HG22	2.21	0.41
1:B:83:ILE:N	1:B:171:SER:OG	2.53	0.41
1:B:93:THR:H	1:B:97:LEU:CG	2.34	0.41
1:B:243:GLY:HA2	1:B:246:PHE:HB3	2.03	0.41
1:B:342:SER:O	1:B:346:VAL:HG23	2.20	0.41
1:A:164:LEU:C	1:A:167:ALA:H	2.29	0.41
1:B:38:PRO:C	1:B:39:LEU:HD13	2.45	0.41
1:B:133:GLY:O	1:B:136:ASN:HB3	2.21	0.41
1:B:161:ARG:O	1:B:164:LEU:HB2	2.20	0.41
1:A:293:VAL:O	1:A:297:VAL:HG22	2.21	0.41
1:A:307:LEU:HB3	1:A:352:TRP:CZ2	2.56	0.41
1:A:340:CYS:HA	1:A:343:LEU:HD23	2.03	0.41
1:B:298:VAL:HG23	1:B:299:ASP:OD1	2.21	0.41
1:A:32:PHE:HD1	1:A:32:PHE:HA	1.68	0.41
1:A:90:ALA:C	1:A:161:ARG:HG2	2.46	0.41
1:B:75:VAL:O	1:B:178:ILE:HD13	2.21	0.41
1:A:148:TYR:OH	1:A:280:SER:O	2.28	0.40
1:A:255:ILE:HA	1:A:258:VAL:HB	2.03	0.40
1:A:400:THR:HB	1:A:402:TRP:CA	2.51	0.40
1:A:416:ILE:HG23	1:B:327:THR:HG22	2.02	0.40
1:B:30:LEU:HD22	1:B:260:PHE:HB3	2.01	0.40
1:B:45:GLY:HA2	1:B:388:SER:O	2.20	0.40
1:A:170:PRO:O	1:A:173:ILE:HG12	2.21	0.40
1:A:251:GLN:HG2	1:A:384:THR:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:OE2	1:A:405:LEU:HD12	2.21	0.40
1:A:411:GLY:HA2	1:A:414:ALA:HB3	2.03	0.40
1:B:116:VAL:HB	1:B:117:PRO:HD3	2.02	0.40
1:B:123:MET:HE1	1:B:200:VAL:HG11	2.03	0.40
1:B:165:GLY:O	1:B:168:VAL:HB	2.21	0.40
1:A:128:TYR:O	1:A:132:LEU:HG	2.21	0.40
1:A:130:GLY:O	1:A:132:LEU:N	2.55	0.40
1:A:190:GLU:HG3	1:A:221:ASN:CB	2.52	0.40
1:A:304:LYS:O	1:A:307:LEU:HB2	2.22	0.40
1:B:394:LEU:O	1:B:398:LEU:HG	2.20	0.40
1:A:175:LEU:O	1:A:179:TYR:N	2.55	0.40
1:A:385:LEU:O	1:A:385:LEU:HD23	2.22	0.40
1:B:318:LEU:HB3	1:B:404:PHE:O	2.21	0.40
1:A:313:GLY:HA2	1:A:316:ALA:CB	2.52	0.40
1:A:318:LEU:HD13	1:A:408:ALA:CA	2.51	0.40
1:B:238:ARG:O	1:B:242:VAL:HG23	2.22	0.40
1:B:311:ASN:O	1:B:315:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/446 (94%)	350 (84%)	58 (14%)	11 (3%)	4	26
1	B	419/446 (94%)	355 (85%)	58 (14%)	6 (1%)	9	39
All	All	838/892 (94%)	705 (84%)	116 (14%)	17 (2%)	6	31

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	TRP
1	B	234	PRO
1	B	328	ILE
1	B	194	GLU
1	B	235	TRP
1	A	129	ARG
1	A	131	SER
1	B	233	SER
1	A	403	VAL
1	A	233	SER
1	A	38	PRO
1	A	354	PRO
1	A	328	ILE
1	A	339	VAL
1	B	423	PRO
1	A	308	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	341/363 (94%)	238 (70%)	103 (30%)	0	1
1	B	341/363 (94%)	261 (76%)	80 (24%)	1	4
All	All	682/726 (94%)	499 (73%)	183 (27%)	0	2

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	22	ASP
1	A	25	VAL
1	A	30	LEU
1	A	33	ILE
1	A	37	ILE
1	A	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	ASN
1	A	46	ILE
1	A	47	VAL
1	A	51	MET
1	A	53	ILE
1	A	71	ARG
1	A	74	LEU
1	A	80	ILE
1	A	84	ILE
1	A	88	ILE
1	A	94	ASN
1	A	99	ILE
1	A	105	ILE
1	A	109	VAL
1	A	116	VAL
1	A	120	LEU
1	A	127	GLU
1	A	136	ASN
1	A	137	GLN
1	A	140	ILE
1	A	142	ILE
1	A	144	ILE
1	A	145	LEU
1	A	156	ASP
1	A	160	TRP
1	A	163	MET
1	A	164	LEU
1	A	168	VAL
1	A	171	SER
1	A	178	ILE
1	A	179	TYR
1	A	189	LEU
1	A	190	GLU
1	A	194	GLU
1	A	195	GLU
1	A	200	VAL
1	A	203	ILE
1	A	210	ILE
1	A	211	ASP
1	A	214	LEU
1	A	215	LYS
1	A	217	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	ILE
1	A	230	VAL
1	A	233	SER
1	A	245	ILE
1	A	246	PHE
1	A	248	ILE
1	A	250	GLN
1	A	251	GLN
1	A	255	ILE
1	A	259	ILE
1	A	261	TYR
1	A	265	ILE
1	A	268	LYS
1	A	273	GLU
1	A	277	ILE
1	A	278	LEU
1	A	281	VAL
1	A	283	ILE
1	A	287	ASN
1	A	292	ILE
1	A	298	VAL
1	A	306	LEU
1	A	307	LEU
1	A	312	ILE
1	A	315	ILE
1	A	320	ILE
1	A	321	MET
1	A	323	ILE
1	A	324	LEU
1	A	325	ILE
1	A	328	ILE
1	A	330	ILE
1	A	336	ILE
1	A	337	ILE
1	A	343	LEU
1	A	345	ILE
1	A	346	VAL
1	A	350	ILE
1	A	352	TRP
1	A	360	LEU
1	A	363	LEU
1	A	373	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	382	ILE
1	A	388	SER
1	A	390	PHE
1	A	393	ILE
1	A	394	LEU
1	A	398	LEU
1	A	404	PHE
1	A	405	LEU
1	A	412	VAL
1	A	417	PHE
1	A	422	LEU
1	A	425	THR
1	B	7	LEU
1	B	8	ILE
1	B	11	LEU
1	B	31	LEU
1	B	33	ILE
1	B	37	ILE
1	B	39	LEU
1	B	46	ILE
1	B	47	VAL
1	B	50	SER
1	B	67	ASP
1	B	74	LEU
1	B	80	ILE
1	B	82	PHE
1	B	83	ILE
1	B	97	LEU
1	B	98	LEU
1	B	113	MET
1	B	120	LEU
1	B	127	GLU
1	B	132	LEU
1	B	137	GLN
1	B	144	ILE
1	B	145	LEU
1	B	161	ARG
1	B	162	TRP
1	B	166	LEU
1	B	174	LEU
1	B	178	ILE
1	B	186	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	192	ARG
1	B	199	GLN
1	B	201	MET
1	B	203	ILE
1	B	204	THR
1	B	210	ILE
1	B	217	MET
1	B	220	ILE
1	B	227	THR
1	B	230	VAL
1	B	231	ILE
1	B	233	SER
1	B	236	LEU
1	B	239	ILE
1	B	244	CYS
1	B	245	ILE
1	B	253	ILE
1	B	258	VAL
1	B	259	ILE
1	B	261	TYR
1	B	262	SER
1	B	273	GLU
1	B	277	ILE
1	B	283	ILE
1	B	285	THR
1	B	290	VAL
1	B	306	LEU
1	B	307	LEU
1	B	312	ILE
1	B	317	SER
1	B	319	LEU
1	B	321	MET
1	B	328	ILE
1	B	337	ILE
1	B	339	VAL
1	B	341	LEU
1	B	360	LEU
1	B	379	VAL
1	B	390	PHE
1	B	393	ILE
1	B	398	LEU
1	B	400	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	405	LEU
1	B	413	LEU
1	B	415	MET
1	B	416	ILE
1	B	419	ILE
1	B	422	LEU
1	B	423	PRO
1	B	425	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	136	ASN
1	B	34	HIS
1	B	221	ASN
1	B	311	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	421/446 (94%)	3.04	262 (62%)  	10, 149, 347, 447	0
1	B	421/446 (94%)	3.04	264 (62%)  	10, 224, 394, 532	0
All	All	842/892 (94%)	3.04	526 (62%)  	10, 185, 372, 532	0

All (526) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	GLY	14.4
1	A	427	GLY	13.2
1	A	371	ALA	13.0
1	A	185	PRO	12.7
1	B	67	ASP	12.5
1	B	371	ALA	12.2
1	B	331	ALA	10.2
1	B	152	TYR	9.9
1	B	372	ALA	9.9
1	B	64	PRO	9.8
1	B	355	VAL	9.5
1	A	306	LEU	9.3
1	A	256	ASN	9.2
1	A	326	TRP	9.2
1	B	267	ALA	9.2
1	A	228	TRP	9.1
1	B	209	GLU	9.1
1	A	56	ILE	8.9
1	A	156	ASP	8.7
1	B	261	TYR	8.6
1	A	188	LEU	8.4
1	B	207	ASP	8.3
1	A	59	ALA	8.3
1	B	208	SER	8.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	93	THR	8.1
1	A	128	TYR	8.1
1	B	332	SER	8.1
1	B	142	ILE	8.0
1	A	18	LEU	7.8
1	A	207	ASP	7.8
1	A	311	ASN	7.8
1	A	187	TRP	7.7
1	A	399	SER	7.7
1	B	210	ILE	7.7
1	B	32	PHE	7.6
1	A	220	ILE	7.6
1	B	181	MET	7.6
1	A	183	GLU	7.5
1	B	250	GLN	7.5
1	B	348	PHE	7.5
1	A	165	GLY	7.3
1	A	348	PHE	7.3
1	A	357	TRP	7.3
1	B	370	GLY	7.2
1	B	26	ILE	7.2
1	B	238	ARG	7.1
1	A	372	ALA	7.1
1	B	50	SER	7.1
1	B	264	SER	7.0
1	A	354	PRO	7.0
1	B	419	ILE	7.0
1	A	167	ALA	6.9
1	B	80	ILE	6.8
1	A	90	ALA	6.7
1	B	301	ILE	6.7
1	B	266	PHE	6.6
1	B	350	ILE	6.5
1	A	215	LYS	6.5
1	B	155	ALA	6.4
1	A	166	LEU	6.4
1	A	211	ASP	6.4
1	A	424	GLU	6.3
1	B	148	TYR	6.3
1	A	278	LEU	6.3
1	A	35	LYS	6.3
1	A	26	ILE	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	157	ILE	6.3
1	B	44	GLU	6.3
1	A	123	MET	6.3
1	B	18	LEU	6.2
1	A	20	GLY	6.2
1	B	269	ALA	6.2
1	A	135	LEU	6.2
1	A	322	ALA	6.1
1	A	182	PRO	6.1
1	A	158	GLU	6.0
1	B	92	SER	6.0
1	B	33	ILE	6.0
1	B	134	SER	6.0
1	B	333	SER	6.0
1	B	326	TRP	6.0
1	B	137	GLN	6.0
1	A	219	GLU	6.0
1	A	226	SER	6.0
1	B	395	SER	6.0
1	A	225	GLU	5.9
1	B	31	LEU	5.9
1	B	218	LYS	5.9
1	B	323	ILE	5.9
1	B	28	GLY	5.9
1	B	375	ILE	5.8
1	A	356	LEU	5.8
1	A	28	GLY	5.7
1	A	239	ILE	5.7
1	A	121	SER	5.7
1	A	57	VAL	5.7
1	A	240	LEU	5.7
1	A	210	ILE	5.6
1	A	191	ASN	5.6
1	A	67	ASP	5.6
1	A	152	TYR	5.6
1	A	55	ALA	5.6
1	B	304	LYS	5.6
1	B	230	VAL	5.5
1	B	236	LEU	5.5
1	B	265	ILE	5.5
1	A	369	ARG	5.5
1	A	85	GLY	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	69	LEU	5.4
1	A	335	TRP	5.4
1	B	356	LEU	5.4
1	B	156	ASP	5.4
1	A	401	GLU	5.3
1	A	262	SER	5.3
1	B	234	PRO	5.3
1	B	65	LEU	5.3
1	B	19	TYR	5.3
1	B	11	LEU	5.3
1	B	129	ARG	5.3
1	A	395	SER	5.2
1	B	274	ALA	5.2
1	B	252	PHE	5.2
1	B	422	LEU	5.2
1	B	237	GLY	5.2
1	B	418	VAL	5.2
1	A	246	PHE	5.2
1	B	262	SER	5.2
1	B	49	SER	5.2
1	B	157	ILE	5.1
1	A	31	LEU	5.1
1	A	272	GLY	5.1
1	A	405	LEU	5.1
1	B	9	PHE	5.1
1	A	105	ILE	5.1
1	A	200	VAL	5.1
1	B	199	GLN	5.0
1	A	299	ASP	5.0
1	B	231	ILE	5.0
1	B	228	TRP	5.0
1	B	386	ILE	5.0
1	A	334	ALA	5.0
1	A	109	VAL	5.0
1	A	193	ASN	5.0
1	A	328	ILE	4.9
1	A	307	LEU	4.9
1	A	25	VAL	4.9
1	A	384	THR	4.9
1	B	338	ILE	4.9
1	B	87	LEU	4.9
1	B	138	LEU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	24	GLY	4.9
1	A	82	PHE	4.8
1	B	240	LEU	4.8
1	A	95	LEU	4.8
1	B	283	ILE	4.8
1	A	178	ILE	4.8
1	A	44	GLU	4.8
1	B	227	THR	4.8
1	A	355	VAL	4.8
1	B	127	GLU	4.7
1	A	127	GLU	4.7
1	B	105	ILE	4.7
1	B	354	PRO	4.7
1	B	302	ASP	4.7
1	B	154	PHE	4.7
1	B	53	ILE	4.6
1	B	314	MET	4.6
1	B	253	ILE	4.6
1	A	78	ILE	4.6
1	B	198	ARG	4.6
1	A	93	THR	4.6
1	B	79	ALA	4.6
1	A	227	THR	4.6
1	B	59	ALA	4.6
1	A	104	ILE	4.6
1	B	52	LEU	4.6
1	A	115	THR	4.6
1	B	180	PHE	4.6
1	B	366	MET	4.6
1	B	21	TYR	4.5
1	B	369	ARG	4.5
1	A	350	ILE	4.5
1	B	263	SER	4.5
1	A	45	GLY	4.5
1	A	169	VAL	4.5
1	A	91	ALA	4.5
1	A	231	ILE	4.5
1	B	23	ASN	4.5
1	B	220	ILE	4.5
1	A	217	MET	4.5
1	B	315	ILE	4.5
1	B	325	ILE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	174	LEU	4.5
1	A	160	TRP	4.4
1	A	402	TRP	4.4
1	B	310	GLY	4.4
1	A	205	TYR	4.4
1	A	73	ARG	4.4
1	B	15	GLY	4.4
1	A	129	ARG	4.4
1	A	75	VAL	4.4
1	A	378	LEU	4.4
1	B	357	TRP	4.4
1	A	11	LEU	4.4
1	A	277	ILE	4.4
1	B	56	ILE	4.4
1	A	214	LEU	4.3
1	B	255	ILE	4.3
1	A	358	VAL	4.3
1	B	361	PRO	4.3
1	A	29	ALA	4.3
1	B	86	ALA	4.3
1	B	226	SER	4.3
1	B	42	THR	4.3
1	B	279	GLY	4.3
1	B	217	MET	4.2
1	A	419	ILE	4.2
1	A	216	GLU	4.2
1	A	330	ILE	4.2
1	A	254	GLY	4.2
1	B	351	SER	4.2
1	A	74	LEU	4.2
1	B	17	LEU	4.2
1	B	295	ILE	4.2
1	A	229	THR	4.2
1	A	333	SER	4.2
1	A	159	GLY	4.2
1	A	186	ARG	4.2
1	A	30	LEU	4.1
1	B	311	ASN	4.1
1	A	112	SER	4.1
1	B	160	TRP	4.1
1	B	257	ALA	4.1
1	B	290	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	305	LYS	4.1
1	A	89	LEU	4.0
1	B	221	ASN	4.0
1	A	261	TYR	4.0
1	A	46	ILE	4.0
1	B	330	ILE	4.0
1	A	426	ARG	4.0
1	A	58	GLY	4.0
1	B	35	LYS	4.0
1	B	123	MET	4.0
1	B	344	PHE	4.0
1	B	118	VAL	4.0
1	A	221	ASN	4.0
1	B	131	SER	4.0
1	B	270	GLY	3.9
1	A	265	ILE	3.9
1	A	304	LYS	3.9
1	A	173	ILE	3.9
1	B	214	LEU	3.9
1	A	12	GLY	3.9
1	A	141	THR	3.9
1	B	170	PRO	3.9
1	B	46	ILE	3.9
1	A	196	ALA	3.9
1	A	77	LEU	3.9
1	A	19	TYR	3.8
1	A	51	MET	3.8
1	B	277	ILE	3.8
1	A	376	SER	3.8
1	B	36	ASP	3.8
1	B	173	ILE	3.8
1	B	183	GLU	3.8
1	B	282	GLY	3.8
1	A	271	LEU	3.8
1	A	136	ASN	3.7
1	A	398	LEU	3.7
1	A	8	ILE	3.7
1	B	113	MET	3.7
1	A	301	ILE	3.7
1	A	184	SER	3.7
1	A	303	ARG	3.7
1	A	245	ILE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	177	GLY	3.7
1	B	349	GLY	3.7
1	B	362	GLU	3.7
1	B	401	GLU	3.7
1	A	360	LEU	3.7
1	B	130	GLY	3.7
1	B	25	VAL	3.6
1	B	109	VAL	3.6
1	B	358	VAL	3.6
1	A	134	SER	3.6
1	A	286	ILE	3.6
1	A	151	ASN	3.6
1	A	410	ILE	3.6
1	B	390	PHE	3.6
1	A	235	TRP	3.6
1	B	55	ALA	3.5
1	B	423	PRO	3.5
1	A	416	ILE	3.5
1	A	309	GLY	3.5
1	B	319	LEU	3.5
1	B	12	GLY	3.5
1	A	119	TYR	3.5
1	B	115	THR	3.5
1	A	194	GLU	3.5
1	B	305	LYS	3.5
1	A	224	SER	3.5
1	B	103	LEU	3.5
1	B	196	ALA	3.5
1	B	38	PRO	3.5
1	A	204	THR	3.4
1	A	377	ALA	3.4
1	A	118	VAL	3.4
1	A	339	VAL	3.4
1	B	78	ILE	3.4
1	A	168	VAL	3.4
1	A	70	GLY	3.4
1	B	415	MET	3.4
1	A	53	ILE	3.4
1	B	178	ILE	3.4
1	A	174	LEU	3.4
1	B	189	LEU	3.4
1	B	246	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	86	ALA	3.3
1	B	85	GLY	3.3
1	A	71	ARG	3.3
1	B	352	TRP	3.3
1	A	172	VAL	3.3
1	B	136	ASN	3.3
1	B	402	TRP	3.3
1	A	345	ILE	3.3
1	B	24	GLY	3.3
1	B	70	GLY	3.3
1	A	131	SER	3.2
1	B	413	LEU	3.2
1	A	154	PHE	3.2
1	B	245	ILE	3.2
1	B	63	GLY	3.2
1	A	190	GLU	3.2
1	B	101	GLY	3.2
1	B	190	GLU	3.2
1	B	30	LEU	3.2
1	A	297	VAL	3.2
1	B	41	SER	3.2
1	A	177	GLY	3.2
1	A	250	GLN	3.2
1	B	114	SER	3.2
1	A	126	THR	3.2
1	A	331	ALA	3.2
1	A	116	VAL	3.2
1	A	361	PRO	3.2
1	A	52	LEU	3.1
1	A	107	LEU	3.1
1	B	404	PHE	3.1
1	B	367	ARG	3.1
1	A	146	ALA	3.1
1	B	396	ASP	3.1
1	A	391	PHE	3.1
1	B	205	TYR	3.1
1	B	289	LEU	3.1
1	B	306	LEU	3.1
1	A	201	MET	3.1
1	B	393	ILE	3.1
1	A	199	GLN	3.1
1	A	353	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	92	SER	3.1
1	B	235	TRP	3.1
1	A	139	MET	3.1
1	B	29	ALA	3.0
1	B	363	LEU	3.0
1	B	45	GLY	3.0
1	A	293	VAL	3.0
1	A	332	SER	3.0
1	B	388	SER	3.0
1	A	163	MET	3.0
1	A	197	ALA	3.0
1	B	329	GLY	3.0
1	A	170	PRO	3.0
1	A	181	MET	3.0
1	B	102	ARG	3.0
1	B	259	ILE	3.0
1	B	162	TRP	3.0
1	A	171	SER	3.0
1	A	37	ILE	3.0
1	B	248	ILE	3.0
1	B	166	LEU	2.9
1	A	298	VAL	2.9
1	A	138	LEU	2.9
1	B	16	GLY	2.9
1	B	22	ASP	2.9
1	A	76	MET	2.9
1	A	352	TRP	2.9
1	B	258	VAL	2.9
1	B	112	SER	2.9
1	B	328	ILE	2.9
1	B	347	PHE	2.9
1	A	387	VAL	2.9
1	A	133	GLY	2.9
1	B	48	VAL	2.8
1	B	151	ASN	2.8
1	A	80	ILE	2.8
1	B	251	GLN	2.8
1	B	150	VAL	2.8
1	A	33	ILE	2.8
1	A	149	LEU	2.8
1	B	14	LEU	2.8
1	B	82	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	324	LEU	2.8
1	A	22	ASP	2.8
1	B	213	GLU	2.8
1	A	164	LEU	2.8
1	B	389	LEU	2.8
1	A	368	ALA	2.8
1	B	182	PRO	2.8
1	A	161	ARG	2.8
1	A	65	LEU	2.8
1	B	335	TRP	2.7
1	A	362	GLU	2.7
1	A	344	PHE	2.7
1	B	91	ALA	2.7
1	B	307	LEU	2.7
1	B	76	MET	2.7
1	B	169	VAL	2.7
1	B	292	ILE	2.6
1	B	8	ILE	2.6
1	B	425	THR	2.6
1	B	116	VAL	2.6
1	A	34	HIS	2.6
1	B	104	ILE	2.6
1	B	140	ILE	2.6
1	B	120	LEU	2.6
1	A	13	ALA	2.6
1	B	211	ASP	2.6
1	A	94	ASN	2.6
1	B	346	VAL	2.6
1	A	137	GLN	2.6
1	A	14	LEU	2.5
1	B	225	GLU	2.5
1	A	317	SER	2.5
1	A	213	GLU	2.5
1	A	323	ILE	2.5
1	B	185	PRO	2.5
1	A	367	ARG	2.5
1	B	268	LYS	2.5
1	B	84	ILE	2.5
1	B	13	ALA	2.5
1	A	209	GLU	2.5
1	A	69	LEU	2.5
1	A	394	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	383	GLY	2.5
1	A	281	VAL	2.5
1	A	10	ILE	2.4
1	A	198	ARG	2.4
1	B	398	LEU	2.4
1	A	88	ILE	2.4
1	B	405	LEU	2.4
1	A	313	GLY	2.4
1	B	119	TYR	2.4
1	B	368	ALA	2.4
1	A	97	LEU	2.4
1	A	382	ILE	2.4
1	A	202	LYS	2.4
1	A	132	LEU	2.4
1	A	236	LEU	2.4
1	B	394	LEU	2.4
1	A	142	ILE	2.4
1	B	275	ALA	2.4
1	B	318	LEU	2.4
1	A	9	PHE	2.3
1	A	337	ILE	2.3
1	B	99	ILE	2.3
1	A	189	LEU	2.3
1	A	218	LYS	2.3
1	B	232	LYS	2.3
1	B	186	ARG	2.3
1	B	229	THR	2.3
1	B	294	ALA	2.3
1	B	71	ARG	2.3
1	A	253	ILE	2.3
1	A	179	TYR	2.3
1	B	249	PHE	2.3
1	A	102	ARG	2.3
1	A	418	VAL	2.3
1	A	294	ALA	2.3
1	B	426	ARG	2.3
1	A	308	VAL	2.3
1	B	308	VAL	2.3
1	B	392	PRO	2.2
1	A	341	LEU	2.2
1	B	391	PHE	2.2
1	A	103	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	139	MET	2.2
1	B	98	LEU	2.2
1	A	340	CYS	2.2
1	A	252	PHE	2.2
1	B	260	PHE	2.2
1	A	42	THR	2.2
1	B	187	TRP	2.2
1	A	230	VAL	2.1
1	B	81	VAL	2.1
1	A	325	ILE	2.1
1	B	107	LEU	2.1
1	A	110	GLY	2.1
1	A	287	ASN	2.1
1	B	133	GLY	2.1
1	B	399	SER	2.1
1	A	244	CYS	2.1
1	B	200	VAL	2.1
1	A	98	LEU	2.1
1	A	397	ALA	2.1
1	B	364	PHE	2.1
1	A	393	ILE	2.1
1	B	10	ILE	2.1
1	B	159	GLY	2.1
1	B	254	GLY	2.1
1	A	346	VAL	2.1
1	B	75	VAL	2.1
1	B	256	ASN	2.1
1	B	204	THR	2.1
1	B	400	THR	2.1
1	A	96	ALA	2.1
1	A	147	ALA	2.1
1	B	143	GLY	2.1
1	A	36	ASP	2.0
1	B	126	THR	2.0
1	B	47	VAL	2.0
1	B	72	ARG	2.0
1	A	241	ILE	2.0
1	A	148	TYR	2.0
1	A	195	GLU	2.0
1	A	292	ILE	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.