



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 4FHN / pdb_00004fhn
Title : Nup37-Nup120 full-length complex from Schizosaccharomyces pombe
Authors : Bilokapic, S.; Schwartz, T.U.
Deposited on : 2012-06-06
Resolution : 6.99 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

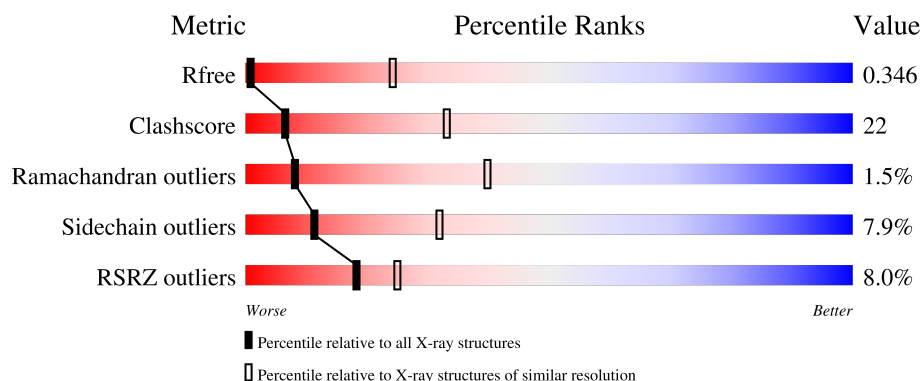
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.99 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	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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	394	9% 54% 28% • • 13%
1	C	394	13% 56% 29% • • 13%
2	B	1139	5% 42% 41% 7% 10%
2	D	1139	9% 42% 38% 5% 14%
3	X	450	3% 56% 39% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24772 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NUCLEOPORIN NUP37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2638	1676	447	500	15			
1	C	344	Total	C	N	O	S	0	0	0
			2646	1680	449	502	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP O36030
A	-1	GLY	-	expression tag	UNP O36030
A	0	SER	-	expression tag	UNP O36030
C	-2	PRO	-	expression tag	UNP O36030
C	-1	GLY	-	expression tag	UNP O36030
C	0	SER	-	expression tag	UNP O36030

- Molecule 2 is a protein called Nucleoporin nup120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1022	Total	C	N	O	S	0	0	0
			8251	5335	1322	1563	31			
2	D	977	Total	C	N	O	S	0	0	0
			7871	5094	1258	1488	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	expression tag	UNP O43044
B	-1	GLY	-	expression tag	UNP O43044
B	0	SER	-	expression tag	UNP O43044
D	-2	PRO	-	expression tag	UNP O43044
D	-1	GLY	-	expression tag	UNP O43044
D	0	SER	-	expression tag	UNP O43044

- Molecule 3 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			

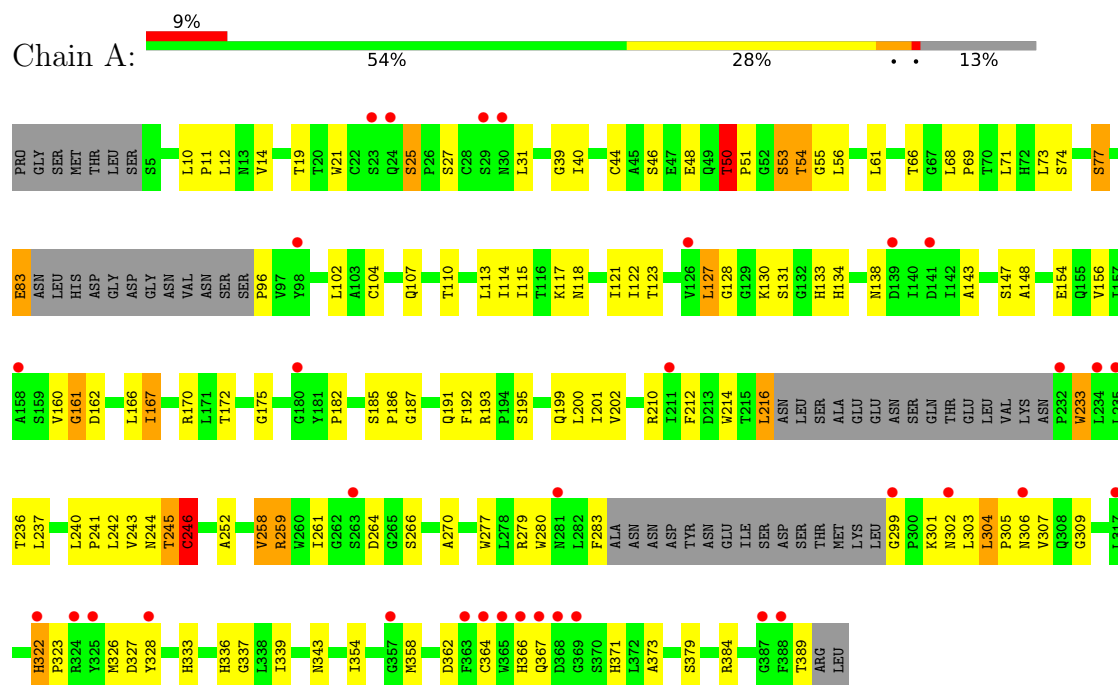
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	PRO	-	expression tag	UNP Q8XDW9
X	-1	GLY	-	expression tag	UNP Q8XDW9
X	0	SER	-	expression tag	UNP Q8XDW9

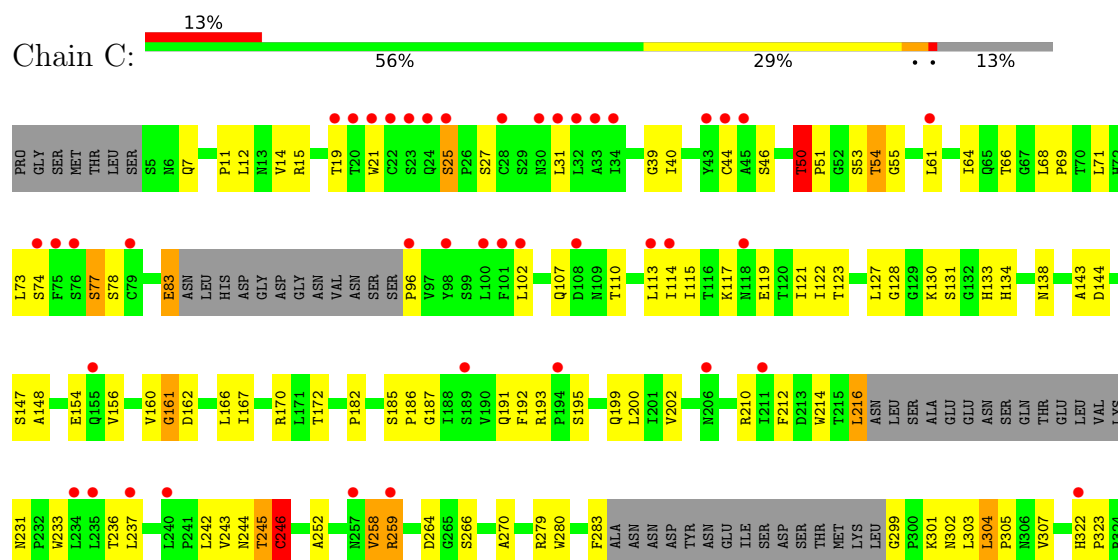
3 Residue-property plots

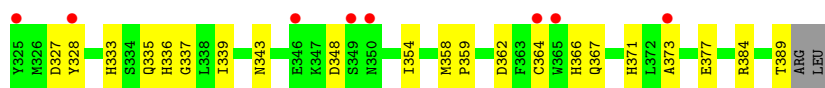
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: NUCLEOPORIN NUP37

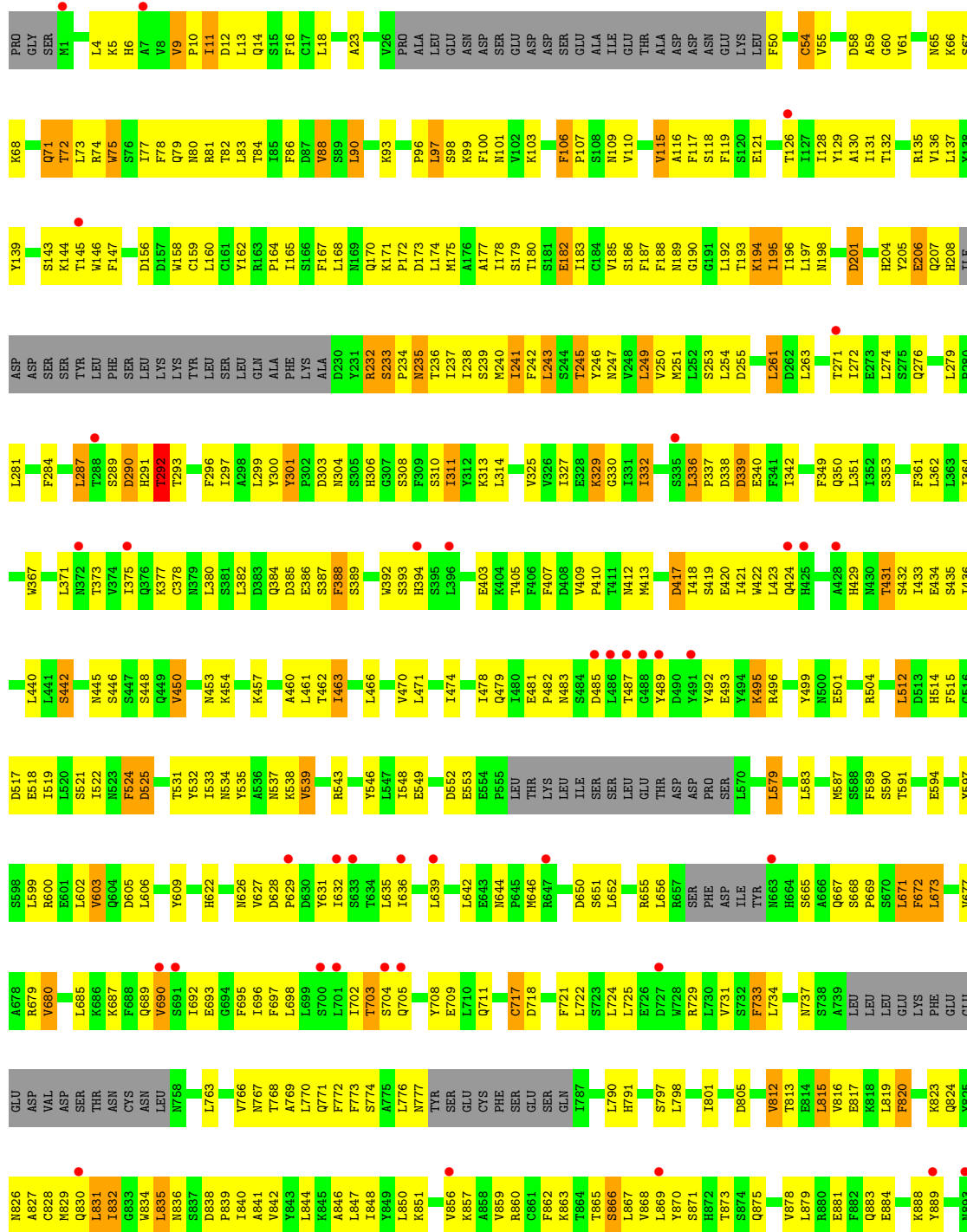


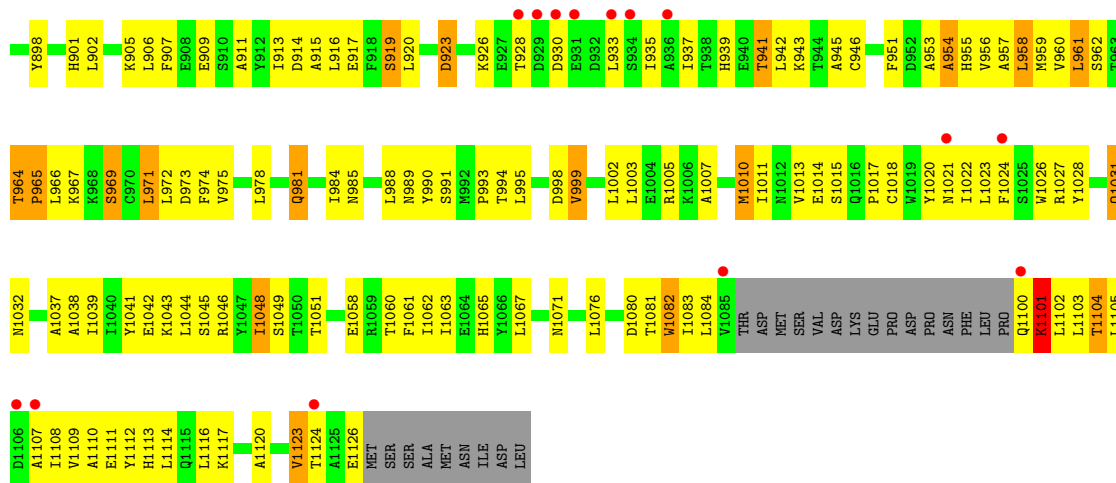
• Molecule 1: NUCLEOPORIN NUP37



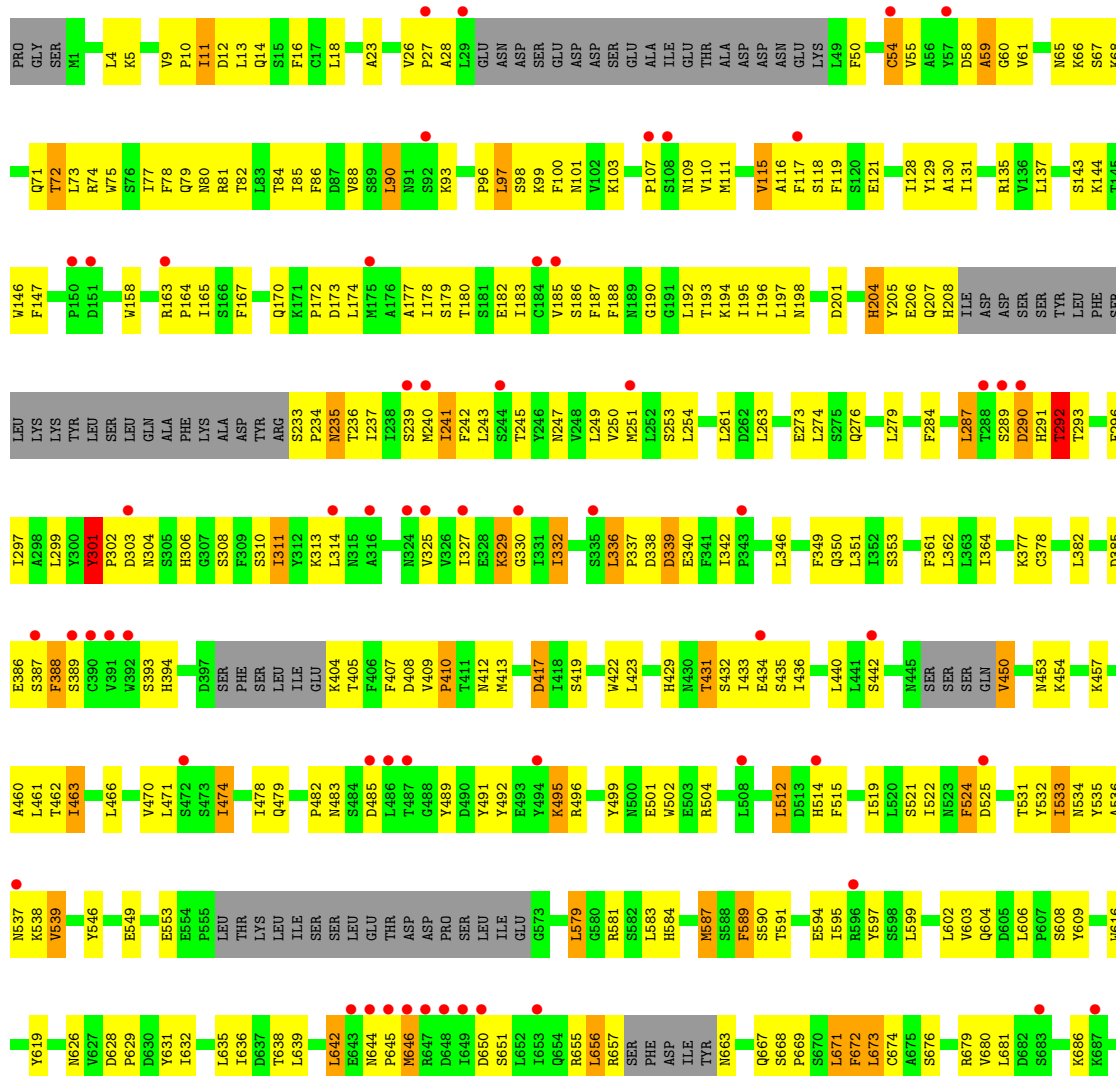


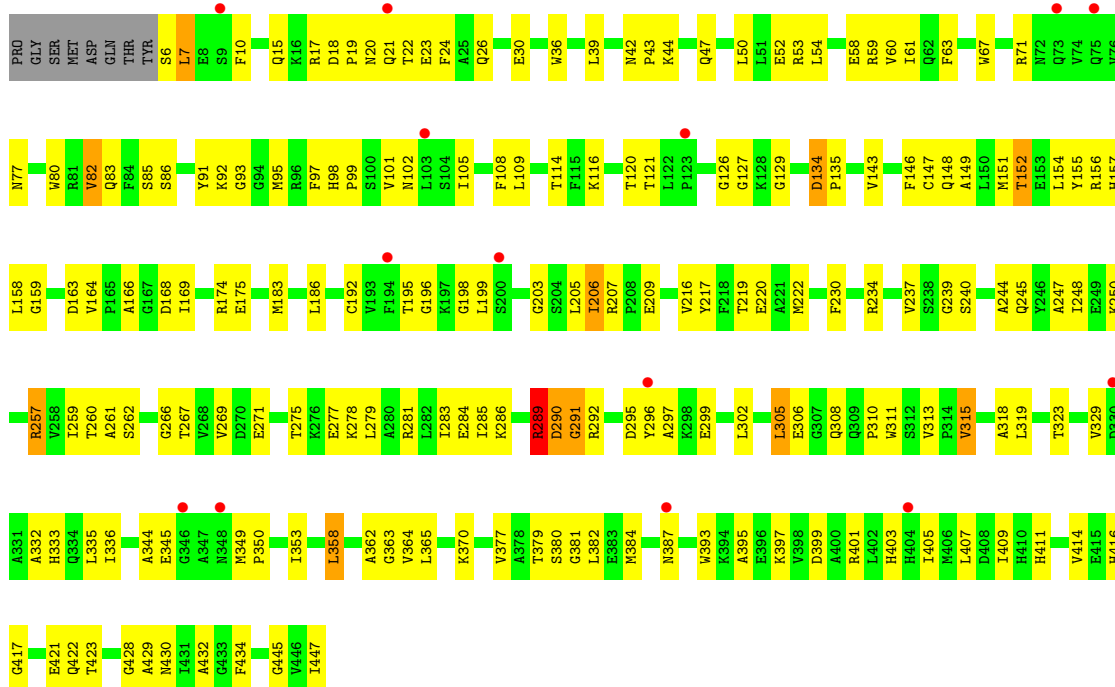
• Molecule 2: Nucleoporin nup120





• Molecule 2: Nucleoporin nup120





4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	330.00Å 330.00Å 350.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.12 – 6.99 95.12 – 6.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (95.12-6.99) 99.4 (95.12-6.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 6.73Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.285 , 0.346 0.279 , 0.346	Depositor DCC
R_{free} test set	939 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	456.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 930.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	24772	wwPDB-VP
Average B, all atoms (Å ²)	672.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/2702	1.01	13/3689 (0.4%)
1	C	0.39	0/2710	0.87	4/3701 (0.1%)
2	B	0.49	0/8433	1.11	57/11445 (0.5%)
2	D	0.41	0/8039	0.92	30/10903 (0.3%)
3	X	0.58	0/3431	0.98	9/4630 (0.2%)
All	All	0.47	0/25315	1.00	113/34368 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	THR	N-CA-C	-18.05	91.68	113.88
2	B	72	THR	N-CA-C	11.62	127.44	110.59
2	D	245	THR	N-CA-C	-11.48	97.87	112.90
2	B	957	ALA	N-CA-C	-10.98	98.52	112.90
2	B	117	PHE	N-CA-C	9.86	124.59	108.52
2	B	958	LEU	N-CA-C	-8.26	101.32	111.40
2	B	964	THR	CA-C-N	-8.16	109.64	119.84
2	B	964	THR	C-N-CA	-8.16	109.64	119.84
2	B	868	VAL	N-CA-C	-8.11	105.24	113.10
2	B	292	THR	N-CA-C	8.10	120.84	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	HIS	N-CA-C	-8.09	102.44	112.88
2	D	292	THR	N-CA-C	8.04	120.73	108.52
1	A	246	CYS	N-CA-C	-7.70	102.89	111.28
2	B	159	CYS	N-CA-C	7.46	120.79	109.23
3	X	42	ASN	CA-C-N	7.38	128.03	119.47
3	X	42	ASN	C-N-CA	7.38	128.03	119.47
2	D	644	ASN	CA-C-N	7.27	126.80	119.24
2	D	644	ASN	C-N-CA	7.27	126.80	119.24
2	B	463	ILE	N-CA-C	7.15	118.80	111.00
2	B	168	LEU	N-CA-C	-7.09	103.48	111.07
2	B	690	VAL	N-CA-C	7.01	118.62	110.62
2	D	117	PHE	N-CA-C	6.91	120.00	108.73
2	D	514	HIS	N-CA-C	-6.83	104.07	112.88
2	D	409	VAL	N-CA-C	6.74	114.81	107.60
2	B	981	GLN	N-CA-C	-6.71	103.89	111.14
1	C	50	THR	CA-C-N	-6.42	111.82	119.84
1	C	50	THR	C-N-CA	-6.42	111.82	119.84
2	B	1048	ILE	CB-CA-C	-6.41	103.67	111.88
2	B	409	VAL	N-CA-C	6.37	114.42	107.60
2	D	72	THR	N-CA-C	6.32	119.72	110.17
2	D	26	VAL	CA-C-N	6.30	127.72	119.84
2	D	26	VAL	C-N-CA	6.30	127.72	119.84
2	B	733	PHE	N-CA-C	-6.18	104.55	111.28
2	B	603	VAL	N-CA-C	6.17	116.22	110.42
2	B	195	ILE	N-CA-C	6.12	116.94	108.12
1	A	50	THR	CA-C-N	-6.09	112.23	119.84
1	A	50	THR	C-N-CA	-6.09	112.23	119.84
2	B	255	ASP	N-CA-C	-6.08	105.13	112.54
2	B	171	LYS	CA-C-N	-6.03	114.40	120.31
2	B	171	LYS	C-N-CA	-6.03	114.40	120.31
2	B	386	GLU	N-CA-C	-5.97	105.96	113.18
2	D	914	ASP	N-CA-C	-5.96	104.90	111.82
1	C	246	CYS	N-CA-C	-5.94	104.81	111.28
2	B	525	ASP	CA-C-N	5.89	125.27	118.85
2	B	525	ASP	C-N-CA	5.89	125.27	118.85
2	B	644	ASN	CA-C-N	5.89	127.20	119.84
2	B	644	ASN	C-N-CA	5.89	127.20	119.84
2	B	766	VAL	N-CA-C	5.88	116.06	110.53
1	A	175	GLY	CA-C-N	5.87	125.63	119.76
1	A	175	GLY	C-N-CA	5.87	125.63	119.76
3	X	152	THR	N-CA-C	-5.87	105.01	111.82
3	X	134	ASP	CA-C-N	5.82	125.44	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	134	ASP	C-N-CA	5.82	125.44	119.56
1	A	306	ASN	N-CA-C	5.81	118.40	111.71
2	B	194	LYS	N-CA-C	-5.75	100.42	109.50
2	D	912	TYR	N-CA-C	5.74	121.03	112.94
2	B	106	PHE	CA-C-N	5.72	125.85	119.32
2	B	106	PHE	C-N-CA	5.72	125.85	119.32
3	X	82	VAL	CB-CA-C	-5.71	105.06	111.23
2	B	336	LEU	CA-C-N	-5.71	112.71	119.84
2	B	336	LEU	C-N-CA	-5.71	112.71	119.84
2	D	833	GLY	N-CA-C	-5.69	107.28	114.16
2	D	762	ALA	N-CA-C	-5.67	105.24	111.82
1	C	161	GLY	N-CA-C	5.63	119.51	111.12
2	B	145	THR	N-CA-C	-5.62	105.16	111.28
2	D	1016	GLN	CA-C-N	-5.59	115.13	120.83
2	D	1016	GLN	C-N-CA	-5.59	115.13	120.83
2	B	201	ASP	N-CA-C	5.56	117.56	108.55
1	A	322	HIS	CA-C-N	5.56	125.17	119.56
1	A	322	HIS	C-N-CA	5.56	125.17	119.56
2	B	300	TYR	N-CA-C	5.54	117.52	108.76
2	D	233	SER	CA-C-N	5.52	126.74	119.84
2	D	233	SER	C-N-CA	5.52	126.74	119.84
2	B	1082	TRP	N-CA-C	5.51	118.44	108.69
2	B	301	TYR	CA-C-N	5.50	125.86	119.47
2	B	301	TYR	C-N-CA	5.50	125.86	119.47
1	A	118	ASN	CB-CA-C	-5.50	110.22	116.54
1	A	161	GLY	N-CA-C	5.47	119.28	111.12
2	B	75	TRP	N-CA-C	5.47	118.40	109.59
2	D	386	GLU	N-CA-C	-5.42	106.63	113.18
2	B	9	VAL	CA-C-N	5.42	125.72	119.93
2	B	9	VAL	C-N-CA	5.42	125.72	119.93
1	A	104	CYS	N-CA-C	5.40	117.01	108.96
2	B	243	LEU	CA-C-N	-5.40	114.84	122.94
2	B	243	LEU	C-N-CA	-5.40	114.84	122.94
2	B	126	THR	N-CA-C	5.34	117.22	108.52
1	A	167	ILE	N-CA-C	5.32	115.52	107.80
2	D	525	ASP	CA-C-N	5.32	124.65	118.85
2	D	525	ASP	C-N-CA	5.32	124.65	118.85
2	D	336	LEU	CA-C-N	-5.31	113.20	119.84
2	D	336	LEU	C-N-CA	-5.31	113.20	119.84
2	D	204	HIS	N-CA-C	5.31	117.25	109.24
2	B	261	LEU	N-CA-C	5.28	118.01	109.40
2	B	173	ASP	N-CA-C	-5.28	108.10	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	GLU	N-CA-C	-5.27	101.57	109.79
2	D	463	ILE	N-CA-C	5.23	116.70	111.00
2	B	156	ASP	N-CA-C	5.22	116.22	108.86
3	X	313	VAL	N-CA-C	5.15	112.96	107.76
2	D	301	TYR	CA-C-N	5.13	125.42	119.47
2	D	301	TYR	C-N-CA	5.13	125.42	119.47
2	B	830	GLN	N-CA-C	-5.12	105.89	111.82
2	D	304	ASN	N-CA-C	5.11	115.56	108.00
2	B	304	ASN	N-CA-C	5.08	115.52	108.00
2	B	776	LEU	N-CA-C	5.08	116.50	109.54
2	B	71	GLN	N-CA-C	5.08	121.61	110.80
2	D	163	ARG	CA-C-N	5.07	126.18	119.84
2	D	163	ARG	C-N-CA	5.07	126.18	119.84
2	B	233	SER	CA-C-N	5.07	126.18	119.84
2	B	233	SER	C-N-CA	5.07	126.18	119.84
2	B	292	THR	CB-CA-C	-5.05	101.87	109.99
2	B	442	SER	N-CA-C	-5.05	107.25	113.41
3	X	114	THR	N-CA-C	-5.03	105.80	111.28
3	X	311	TRP	N-CA-C	5.00	118.64	112.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	TRP	Peptide
1	A	50	THR	Peptide
1	A	53	SER	Peptide
2	B	206	GLU	Peptide
2	D	206	GLU	Peptide

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	2638	0	2588	99	0
1	C	2646	0	2593	95	0
2	B	8251	0	8211	435	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	7871	0	7847	377	2
3	X	3366	0	3324	127	2
All	All	24772	0	24563	1073	4

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 22.

All (1073) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:828:CYS:HA	2:B:831:LEU:HB2	1.40	1.01
2:B:174:LEU:HD11	2:B:240:MET:H	1.31	0.95
2:D:744:LYS:H	2:D:823:LYS:HD3	1.32	0.95
1:A:252:ALA:HB2	2:B:826:ASN:HD22	1.39	0.88
2:B:942:LEU:HD11	2:B:961:LEU:HG	1.56	0.86
2:D:174:LEU:HD11	2:D:240:MET:H	1.40	0.84
1:C:133:HIS:CD2	1:C:167:ILE:HD12	2.13	0.83
2:D:1015:SER:HB2	2:D:1018:CYS:HB2	1.62	0.82
2:D:93:LYS:H	2:D:96:PRO:HG3	1.45	0.82
2:B:93:LYS:H	2:B:96:PRO:HG3	1.46	0.81
2:B:1116:LEU:HB3	2:D:1067:LEU:HB3	1.60	0.81
2:B:1080:ASP:HB2	2:B:1101:LYS:HE3	1.62	0.81
3:X:60:VAL:HG22	3:X:82:VAL:HG13	1.62	0.81
2:D:10:PRO:HG3	2:D:431:THR:HA	1.62	0.80
3:X:349:MET:HE2	3:X:370:LYS:HE2	1.63	0.80
2:B:599:LEU:HD23	2:B:602:LEU:HD12	1.63	0.79
2:B:86:PHE:HB3	2:B:101:ASN:HD22	1.47	0.78
2:D:66:LYS:HG3	2:D:119:PHE:HB2	1.65	0.77
2:B:10:PRO:HG3	2:B:431:THR:HA	1.64	0.77
2:B:174:LEU:HB3	2:B:186:SER:HB3	1.65	0.77
2:D:86:PHE:HB3	2:D:101:ASN:HD22	1.48	0.77
3:X:59:ARG:NH1	3:X:83:GLN:OE1	2.17	0.77
2:B:66:LYS:HG3	2:B:119:PHE:HB2	1.66	0.76
2:B:1124:THR:O	2:D:1027:ARG:NE	2.17	0.76
2:D:174:LEU:HB3	2:D:186:SER:HB3	1.68	0.76
2:B:165:ILE:HD13	2:B:187:PHE:HE2	1.51	0.76
2:B:1116:LEU:HD13	2:D:1067:LEU:HD22	1.67	0.76
2:D:646:MET:HE2	2:D:717:CYS:HB3	1.67	0.75
2:B:1027:ARG:NH2	2:D:1126:GLU:O	2.17	0.75
2:D:10:PRO:HB3	2:D:433:ILE:HD11	1.66	0.75
2:D:165:ILE:HD13	2:D:187:PHE:HE2	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1102:LEU:HA	2:D:1105:LEU:HD12	1.67	0.75
2:D:740:LEU:HD13	2:D:827:ALA:HB1	1.69	0.74
2:B:1126:GLU:O	2:D:1027:ARG:NH2	2.18	0.74
2:D:1000:ASP:OD1	2:D:1028:TYR:OH	2.04	0.73
2:D:1026:TRP:CD1	2:D:1037:ALA:HB1	2.24	0.73
2:B:10:PRO:HB3	2:B:433:ILE:HD11	1.71	0.73
2:B:915:ALA:O	2:B:919:SER:OG	2.06	0.73
2:D:673:LEU:HD13	2:D:770:LEU:HD13	1.68	0.72
1:C:15:ARG:NH1	2:D:917:GLU:OE1	2.22	0.72
2:B:602:LEU:HD22	2:B:606:LEU:HD13	1.70	0.72
2:B:866:SER:OG	2:B:867:LEU:N	2.21	0.72
2:B:946:CYS:SG	2:B:974:PHE:HB3	2.29	0.71
3:X:60:VAL:HG13	3:X:82:VAL:HG22	1.70	0.71
2:B:839:PRO:HB2	2:B:869:LEU:HD11	1.71	0.71
2:B:942:LEU:HD22	2:B:958:LEU:HD23	1.73	0.71
1:A:193:ARG:NH1	1:A:199:GLN:OE1	2.21	0.70
1:A:154:GLU:HG2	1:A:172:THR:HG22	1.73	0.70
1:C:55:GLY:H	1:C:384:ARG:HH11	1.38	0.70
2:B:1082:TRP:CD1	3:X:308:GLN:HE22	2.08	0.70
1:C:193:ARG:NH1	1:C:199:GLN:OE1	2.22	0.70
2:B:232:ARG:HG2	2:B:254:LEU:HD21	1.74	0.70
2:B:1067:LEU:HD22	2:D:1116:LEU:HD13	1.74	0.69
2:B:501:GLU:OE1	2:B:504:ARG:NH2	2.25	0.69
2:B:412:ASN:ND2	2:B:594:GLU:OE2	2.25	0.69
2:B:975:VAL:HA	2:B:978:LEU:HD12	1.74	0.69
2:B:926:LYS:HZ3	2:B:933:LEU:HD23	1.58	0.69
2:B:190:GLY:HA2	2:B:236:THR:HA	1.74	0.69
2:B:247:ASN:HB3	2:B:263:LEU:HD12	1.75	0.69
2:B:953:ALA:C	2:B:955:HIS:H	2.00	0.69
2:B:118:SER:HB3	2:B:129:TYR:HB2	1.73	0.69
2:D:1020:TYR:HA	2:D:1023:LEU:HD12	1.74	0.69
2:B:665:SER:HB3	2:B:777:ASN:HB3	1.75	0.69
2:D:708:TYR:HA	2:D:711:GLN:HG3	1.75	0.69
1:A:303:LEU:HD21	2:B:479:GLN:HA	1.75	0.68
2:D:190:GLY:HA2	2:D:236:THR:HA	1.73	0.68
2:B:90:LEU:HA	2:B:669:PRO:HG3	1.74	0.68
2:B:174:LEU:HD11	2:B:240:MET:N	2.08	0.68
2:B:67:SER:HB2	2:B:73:LEU:HG	1.76	0.68
2:B:1022:ILE:HD13	2:B:1044:LEU:HD22	1.74	0.68
3:X:67:TRP:NE1	3:X:77:ASN:OD1	2.26	0.68
2:D:501:GLU:OE1	2:D:504:ARG:NH2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ALA:O	2:B:130:ALA:HA	1.94	0.67
3:X:417:GLY:HA3	3:X:423:THR:HG23	1.76	0.67
1:C:133:HIS:HD2	1:C:167:ILE:HD12	1.59	0.67
1:C:335:GLN:NE2	2:D:910:SER:OG	2.28	0.67
2:D:100:PHE:HE1	2:D:147:PHE:HA	1.59	0.67
2:B:100:PHE:HE1	2:B:147:PHE:HA	1.59	0.67
2:B:419:SER:HB2	2:B:471:LEU:HD21	1.76	0.66
2:B:838:ASP:H	2:B:841:ALA:HB3	1.60	0.66
2:B:192:LEU:HD11	2:B:251:MET:SD	2.35	0.66
1:C:339:ILE:HB	1:C:354:ILE:HB	1.77	0.66
2:D:192:LEU:HD11	2:D:251:MET:SD	2.34	0.66
2:D:67:SER:HB2	2:D:73:LEU:HG	1.78	0.66
2:D:174:LEU:HD11	2:D:240:MET:N	2.09	0.66
2:D:412:ASN:ND2	2:D:594:GLU:OE2	2.29	0.66
1:C:154:GLU:HG2	1:C:172:THR:HG22	1.76	0.65
3:X:53:ARG:NH2	3:X:445:GLY:O	2.28	0.65
1:A:21:TRP:CD1	1:A:364:CYS:HG	2.15	0.65
1:A:301:LYS:HD3	2:B:479:GLN:HB3	1.77	0.65
2:B:337:PRO:HG3	2:B:394:HIS:HE1	1.61	0.65
2:D:116:ALA:O	2:D:130:ALA:HA	1.95	0.65
2:D:236:THR:O	2:D:254:LEU:N	2.27	0.65
1:A:117:LYS:HG2	1:A:122:ILE:HD13	1.78	0.65
1:A:339:ILE:HB	1:A:354:ILE:HB	1.79	0.65
2:B:239:SER:HB3	2:B:289:SER:HB2	1.79	0.65
1:A:110:THR:HG22	1:A:128:GLY:HA3	1.79	0.65
2:B:237:ILE:HA	2:B:253:SER:HA	1.78	0.65
2:D:419:SER:HB2	2:D:471:LEU:HD21	1.78	0.65
2:D:971:LEU:HA	2:D:974:PHE:HD2	1.63	0.65
2:B:236:THR:O	2:B:254:LEU:N	2.29	0.64
2:B:955:HIS:CE1	2:B:978:LEU:HD13	2.32	0.64
2:B:1007:ALA:HA	2:B:1010:MET:HE2	1.79	0.64
2:B:364:ILE:HG23	2:B:522:ILE:HD12	1.79	0.64
2:B:72:THR:OG1	2:B:73:LEU:N	2.30	0.64
1:C:21:TRP:CD1	1:C:364:CYS:HG	2.16	0.64
2:B:310:SER:OG	2:B:311:ILE:N	2.29	0.64
1:C:359:PRO:HD3	2:D:912:TYR:CZ	2.32	0.64
2:B:164:PRO:HB3	2:B:204:HIS:CD2	2.33	0.64
2:D:435:SER:HB2	2:D:512:LEU:HB3	1.78	0.64
2:D:72:THR:OG1	2:D:73:LEU:N	2.29	0.64
3:X:17:ARG:NH2	3:X:52:GLU:OE2	2.31	0.64
3:X:149:ALA:O	3:X:152:THR:OG1	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:PRO:HG3	2:D:394:HIS:HE1	1.62	0.63
3:X:333:HIS:HA	3:X:336:ILE:HD12	1.80	0.63
1:A:53:SER:OG	1:A:54:THR:N	2.29	0.63
2:D:249:LEU:HD23	2:D:261:LEU:HD23	1.81	0.63
2:D:237:ILE:HA	2:D:253:SER:HA	1.81	0.63
2:B:1003:LEU:HD12	2:B:1028:TYR:CG	2.34	0.63
1:C:117:LYS:HG2	1:C:122:ILE:HD13	1.80	0.63
2:D:311:ILE:HB	2:D:332:ILE:HG13	1.81	0.63
2:D:639:LEU:HA	2:D:642:LEU:HD22	1.79	0.63
1:A:200:LEU:HD11	1:A:212:PHE:HD2	1.63	0.63
2:D:79:GLN:HB3	2:D:82:THR:HB	1.80	0.63
2:D:975:VAL:HA	2:D:978:LEU:HD12	1.81	0.62
3:X:291:GLY:O	3:X:292:ARG:NH1	2.31	0.62
2:B:718:ASP:O	2:B:721:PHE:HB3	2.00	0.62
2:D:247:ASN:HB3	2:D:263:LEU:HD12	1.81	0.62
2:D:454:LYS:HD2	2:D:457:LYS:HD2	1.81	0.62
2:B:959:MET:HE2	2:B:995:LEU:H	1.65	0.62
2:B:602:LEU:HB3	2:B:606:LEU:HD22	1.81	0.62
1:A:371:HIS:CE1	1:A:384:ARG:HD2	2.35	0.62
2:B:763:LEU:HD22	2:B:771:GLN:HG2	1.82	0.62
2:B:1043:LYS:HA	2:B:1046:ARG:HD2	1.80	0.62
2:D:118:SER:HB3	2:D:129:TYR:HB2	1.80	0.62
2:B:74:ARG:HH22	2:B:144:LYS:HG2	1.63	0.62
1:C:110:THR:HG22	1:C:128:GLY:HA3	1.81	0.62
2:D:12:ASP:HB2	2:D:433:ILE:HG23	1.82	0.62
2:B:1082:TRP:CZ3	2:B:1100:GLN:HA	2.34	0.62
2:D:945:ALA:O	2:D:949:GLY:N	2.28	0.62
2:D:90:LEU:HA	2:D:669:PRO:HG3	1.81	0.61
1:A:55:GLY:H	1:A:384:ARG:HH11	1.46	0.61
2:B:1080:ASP:HB2	2:B:1101:LYS:CE	2.30	0.61
2:D:310:SER:OG	2:D:311:ILE:N	2.31	0.61
2:D:349:PHE:HA	2:D:522:ILE:HD11	1.82	0.61
2:B:772:PHE:HD1	2:B:815:LEU:HD21	1.64	0.61
2:B:174:LEU:HD22	2:B:240:MET:HE3	1.82	0.61
2:B:249:LEU:HD23	2:B:261:LEU:HD23	1.80	0.61
2:B:435:SER:HB2	2:B:512:LEU:HB3	1.82	0.61
2:B:958:LEU:HB3	2:B:971:LEU:HD13	1.82	0.61
2:D:619:TYR:CD2	2:D:700:SER:HA	2.36	0.61
3:X:155:TYR:HA	3:X:183:MET:HE1	1.81	0.61
1:C:7:GLN:OE1	2:D:950:LYS:NZ	2.34	0.61
1:C:371:HIS:CE1	1:C:384:ARG:HD2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:ILE:HG23	2:D:522:ILE:HD12	1.83	0.61
2:D:239:SER:HB3	2:D:289:SER:HB2	1.83	0.61
2:B:695:PHE:CZ	2:B:724:LEU:HB3	2.36	0.60
2:D:767:ASN:HB3	2:D:770:LEU:HD11	1.82	0.60
2:D:310:SER:HA	2:D:332:ILE:H	1.65	0.60
1:A:130:LYS:HD3	2:B:609:TYR:HE1	1.66	0.60
2:B:79:GLN:HB3	2:B:82:THR:HB	1.83	0.60
2:B:543:ARG:HB3	2:B:679:ARG:HH12	1.66	0.60
2:D:174:LEU:HD22	2:D:240:MET:HE3	1.83	0.60
2:B:68:LYS:HG3	2:B:121:GLU:HG2	1.81	0.60
2:B:1103:LEU:HD22	3:X:271:GLU:HB2	1.83	0.60
2:B:1026:TRP:HD1	2:B:1037:ALA:HB1	1.67	0.60
1:C:335:GLN:HE22	2:D:910:SER:C	2.10	0.60
2:B:310:SER:HA	2:B:332:ILE:H	1.66	0.59
2:B:603:VAL:HG13	2:B:729:ARG:HD2	1.84	0.59
2:B:1058:GLU:HA	2:B:1061:PHE:HD2	1.67	0.59
2:B:1113:HIS:HA	2:B:1116:LEU:HG	1.84	0.59
1:C:301:LYS:HD3	2:D:479:GLN:HB3	1.84	0.59
2:D:913:ILE:HA	2:D:916:LEU:HB2	1.82	0.59
2:B:587:MET:HG2	2:B:591:THR:HG21	1.85	0.59
2:B:311:ILE:HB	2:B:332:ILE:HG13	1.83	0.59
2:D:976:ASN:OD1	2:D:1006:LYS:NZ	2.29	0.59
1:A:160:VAL:HB	1:A:187:GLY:HA3	1.83	0.59
3:X:168:ASP:OD1	3:X:169:ILE:N	2.33	0.59
1:A:210:ARG:HH12	2:B:417:ASP:H	1.51	0.59
2:B:293:THR:HG23	2:B:353:SER:H	1.68	0.59
2:B:668:SER:HB2	2:B:672:PHE:HD2	1.67	0.59
2:B:906:LEU:HD22	2:B:914:ASP:HB2	1.83	0.59
3:X:15:GLN:HG2	3:X:19:PRO:HA	1.83	0.59
2:B:835:LEU:HD21	2:B:841:ALA:HB1	1.83	0.59
2:D:61:VAL:HG22	2:D:78:PHE:HB3	1.83	0.59
2:D:1059:ARG:O	2:D:1063:ILE:HG13	2.02	0.59
3:X:98:HIS:HB3	3:X:101:VAL:HG23	1.85	0.59
3:X:216:VAL:HG21	3:X:250:LYS:HB3	1.84	0.59
2:D:587:MET:HG2	2:D:591:THR:HG21	1.85	0.59
2:D:693:GLU:HB3	2:D:697:PHE:CZ	2.38	0.59
2:D:798:LEU:HD23	2:D:801:ILE:HD12	1.83	0.59
2:D:1112:TYR:CE2	2:D:1116:LEU:HD11	2.38	0.59
2:B:164:PRO:HG2	2:B:195:ILE:HD13	1.83	0.59
2:B:838:ASP:O	2:B:842:VAL:N	2.36	0.59
2:B:349:PHE:HA	2:B:522:ILE:HD11	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1082:TRP:HZ2	3:X:305:LEU:HD22	1.68	0.58
1:C:304:LEU:HD22	1:C:305:PRO:HD2	1.85	0.58
2:D:74:ARG:HH22	2:D:144:LYS:HG2	1.67	0.58
2:D:247:ASN:HB3	2:D:263:LEU:HB2	1.85	0.58
1:C:200:LEU:HD11	1:C:212:PHE:HD2	1.67	0.58
2:B:453:ASN:O	2:B:457:LYS:HG3	2.03	0.58
2:D:776:LEU:HD13	2:D:797:SER:HA	1.85	0.58
2:B:71:GLN:HB3	2:B:93:LYS:HE2	1.85	0.58
2:D:830:GLN:HG3	2:D:831:LEU:HD23	1.85	0.58
2:D:835:LEU:HD21	2:D:841:ALA:HB1	1.85	0.58
2:B:628:ASP:HB3	2:B:631:TYR:HD2	1.67	0.58
2:D:1112:TYR:CE1	2:D:1116:LEU:HD21	2.38	0.58
1:A:44:CYS:HB2	1:A:61:LEU:HD11	1.85	0.58
2:B:482:PRO:HA	2:B:489:TYR:HA	1.85	0.58
2:B:548:ILE:HD13	2:B:687:LYS:HD2	1.86	0.58
2:D:71:GLN:HB3	2:D:93:LYS:HE2	1.86	0.58
2:B:1103:LEU:HD13	3:X:271:GLU:H	1.68	0.58
2:B:668:SER:HB2	2:B:672:PHE:CD2	2.38	0.58
2:B:693:GLU:HB3	2:B:697:PHE:CZ	2.39	0.58
2:B:812:VAL:HG21	2:B:835:LEU:HB2	1.86	0.58
2:B:985:ASN:O	2:B:989:ASN:ND2	2.37	0.58
2:D:842:VAL:HG11	2:D:865:THR:HG21	1.85	0.58
2:B:708:TYR:HA	2:B:711:GLN:HG3	1.84	0.58
2:B:989:ASN:O	2:B:993:PRO:HD3	2.04	0.58
2:D:164:PRO:HB3	2:D:204:HIS:CD2	2.39	0.58
2:D:599:LEU:HD23	2:D:602:LEU:HD12	1.86	0.58
3:X:18:ASP:HB3	3:X:21:GLN:HB2	1.85	0.58
2:D:650:ASP:OD1	2:D:651:SER:N	2.37	0.57
2:D:734:LEU:HA	2:D:737:ASN:HB2	1.86	0.57
1:A:384:ARG:HH21	1:A:389:THR:HG21	1.67	0.57
2:B:61:VAL:HG22	2:B:78:PHE:HB3	1.87	0.57
2:B:167:PHE:HD2	2:B:172:PRO:HD3	1.69	0.57
1:C:44:CYS:HB2	1:C:61:LEU:HD11	1.86	0.57
1:C:160:VAL:HB	1:C:187:GLY:HA3	1.85	0.57
2:D:535:TYR:HB2	2:D:538:LYS:O	2.05	0.57
2:D:68:LYS:HG3	2:D:121:GLU:HG2	1.85	0.57
2:D:314:LEU:HG	2:D:327:ILE:HG12	1.87	0.57
2:D:810:ASP:O	2:D:813:THR:OG1	2.21	0.57
3:X:259:ILE:HG13	3:X:260:THR:HG23	1.86	0.57
1:A:304:LEU:HD22	1:A:305:PRO:HD2	1.85	0.57
2:D:313:LYS:HB3	2:D:329:LYS:HD3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:741:LEU:HA	2:D:768:THR:HB	1.86	0.57
2:B:337:PRO:HG3	2:B:394:HIS:CE1	2.40	0.57
2:D:847:LEU:HD23	2:D:850:LEU:HD12	1.86	0.57
3:X:175:GLU:CD	3:X:175:GLU:H	2.13	0.57
2:B:445:ASN:HB2	2:B:448:SER:HB2	1.87	0.57
1:A:182:PRO:O	2:B:413:MET:HB2	2.04	0.57
1:C:166:LEU:HD22	1:C:202:VAL:HG21	1.86	0.57
2:D:453:ASN:O	2:D:457:LYS:HG3	2.04	0.57
2:D:482:PRO:HA	2:D:489:TYR:HA	1.86	0.57
1:A:166:LEU:HD22	1:A:202:VAL:HG21	1.87	0.57
2:B:65:ASN:HD21	2:B:73:LEU:HD21	1.70	0.57
2:D:639:LEU:HD13	2:D:701:LEU:HB3	1.87	0.57
2:B:917:GLU:O	2:B:920:LEU:HB2	2.04	0.56
2:D:996:ARG:HH11	2:D:1031:GLN:HG3	1.70	0.56
2:B:1026:TRP:CD1	2:B:1037:ALA:HB1	2.40	0.56
2:D:674:CYS:SG	2:D:767:ASN:ND2	2.77	0.56
2:D:862:PHE:CZ	2:D:902:LEU:HD21	2.40	0.56
2:D:1026:TRP:HE1	2:D:1072:THR:HG22	1.71	0.56
3:X:219:THR:HB	3:X:230:PHE:CZ	2.41	0.56
1:A:333:HIS:HD2	1:A:336:HIS:H	1.52	0.56
3:X:54:LEU:HD22	3:X:434:PHE:HE1	1.71	0.56
2:D:619:TYR:HD2	2:D:700:SER:HA	1.68	0.56
2:B:770:LEU:O	2:B:773:PHE:N	2.39	0.56
2:D:1080:ASP:N	2:D:1101:LYS:HG2	2.21	0.56
2:B:956:VAL:O	2:B:960:VAL:HG23	2.04	0.56
1:A:21:TRP:CZ3	1:A:366:HIS:HD2	2.24	0.56
2:D:912:TYR:CE2	2:D:947:ALA:HB1	2.41	0.56
1:A:242:LEU:HD13	1:A:305:PRO:HG3	1.88	0.55
2:B:237:ILE:HD13	2:B:251:MET:SD	2.46	0.55
2:B:734:LEU:HA	2:B:737:ASN:HB2	1.87	0.55
1:C:71:LEU:HD11	2:D:860:ARG:CZ	2.36	0.55
1:C:242:LEU:HD13	1:C:305:PRO:HG3	1.87	0.55
2:D:549:GLU:O	2:D:553:GLU:HG2	2.07	0.55
2:D:1121:VAL:HA	2:D:1124:THR:HG22	1.88	0.55
3:X:159:GLY:O	3:X:163:ASP:N	2.38	0.55
3:X:209:GLU:N	3:X:209:GLU:OE1	2.38	0.55
2:B:118:SER:OG	2:B:177:ALA:HB2	2.06	0.55
2:B:549:GLU:O	2:B:553:GLU:HG2	2.05	0.55
2:D:337:PRO:HG3	2:D:394:HIS:CE1	2.41	0.55
2:B:12:ASP:H	2:B:433:ILE:HG13	1.71	0.55
2:B:54:CYS:SG	2:B:55:VAL:N	2.79	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:TYR:HB2	2:B:538:LYS:O	2.07	0.55
3:X:289:ARG:HH11	3:X:289:ARG:HG2	1.71	0.55
3:X:379:THR:HA	3:X:382:LEU:HG	1.88	0.55
1:C:107:GLN:HA	2:D:860:ARG:CZ	2.36	0.55
3:X:148:GLN:O	3:X:152:THR:HG23	2.06	0.55
2:B:433:ILE:HG22	2:B:434:GLU:HG3	1.89	0.55
2:D:177:ALA:HA	2:D:183:ILE:HG13	1.87	0.55
2:D:982:GLY:HA3	2:D:987:LEU:HD11	1.89	0.55
2:B:984:ILE:HG13	2:B:1024:PHE:CE2	2.41	0.55
2:B:194:LYS:HB3	2:B:205:TYR:HB2	1.89	0.55
2:B:12:ASP:HB2	2:B:433:ILE:HG23	1.88	0.54
2:B:247:ASN:HB3	2:B:263:LEU:HB2	1.89	0.54
2:B:450:VAL:O	2:B:454:LYS:N	2.38	0.54
2:B:651:SER:O	2:B:655:ARG:HG3	2.07	0.54
1:C:21:TRP:CZ3	1:C:366:HIS:HD2	2.26	0.54
2:B:177:ALA:HA	2:B:183:ILE:HG13	1.89	0.54
1:C:384:ARG:HE	1:C:389:THR:HG21	1.71	0.54
2:D:729:ARG:HH12	2:D:812:VAL:HG11	1.72	0.54
3:X:260:THR:HG22	3:X:269:VAL:HG22	1.88	0.54
2:B:313:LYS:HD2	2:B:351:LEU:HD21	1.88	0.54
2:B:669:PRO:HD2	2:B:672:PHE:CD2	2.43	0.54
1:C:384:ARG:HH21	1:C:389:THR:HG21	1.72	0.54
2:D:350:GLN:HG2	2:D:524:PHE:HB2	1.89	0.54
2:D:54:CYS:SG	2:D:55:VAL:N	2.80	0.54
1:C:55:GLY:H	1:C:384:ARG:NH1	2.06	0.54
2:D:1003:LEU:HD12	2:D:1028:TYR:CZ	2.43	0.54
3:X:219:THR:HB	3:X:230:PHE:CE2	2.42	0.54
2:B:79:GLN:HG3	2:B:80:ASN:N	2.23	0.54
2:B:241:ILE:HG22	2:B:250:VAL:HB	1.89	0.54
2:B:926:LYS:HZ1	2:B:930:ASP:HB2	1.73	0.54
2:D:579:LEU:O	2:D:583:LEU:HG	2.08	0.54
3:X:86:SER:HB3	3:X:91:TYR:CZ	2.42	0.54
2:B:165:ILE:HD13	2:B:187:PHE:CE2	2.38	0.54
2:D:933:LEU:O	2:D:937:ILE:HG13	2.07	0.54
1:A:107:GLN:HA	2:B:860:ARG:NH2	2.22	0.54
2:B:314:LEU:HG	2:B:327:ILE:HG12	1.89	0.54
2:D:695:PHE:CE1	2:D:724:LEU:HB3	2.42	0.54
2:B:332:ILE:HG12	2:B:388:PHE:CE2	2.43	0.53
2:B:689:GLN:O	2:B:693:GLU:HG3	2.08	0.53
2:D:4:LEU:HG	2:D:393:SER:OG	2.08	0.53
2:D:167:PHE:HD2	2:D:172:PRO:HD3	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:6:SER:HB3	3:X:36:TRP:HE1	1.72	0.53
2:B:972:LEU:HD11	2:B:1005:ARG:HH11	1.73	0.53
2:D:306:HIS:ND1	2:D:308:SER:HB3	2.23	0.53
1:C:83:GLU:HA	1:C:96:PRO:HA	1.89	0.53
2:D:799:SER:O	2:D:803:ILE:HG12	2.08	0.53
2:D:65:ASN:HD21	2:D:73:LEU:HD21	1.73	0.53
2:D:587:MET:HE1	2:D:696:ILE:HG21	1.90	0.53
3:X:275:THR:H	3:X:278:LYS:HB2	1.74	0.53
2:D:1080:ASP:H	2:D:1101:LYS:HG2	1.73	0.53
3:X:411:HIS:O	3:X:414:VAL:HG22	2.09	0.53
2:B:1083:ILE:HD13	2:B:1100:GLN:N	2.24	0.53
3:X:278:LYS:HB3	3:X:296:TYR:OH	2.08	0.53
2:B:185:VAL:HB	2:B:193:THR:HG22	1.91	0.53
2:B:840:ILE:HG23	2:B:875:GLN:HE21	1.72	0.53
2:D:815:LEU:HD22	2:D:819:LEU:HD11	1.91	0.53
3:X:267:THR:O	3:X:305:LEU:HG	2.08	0.53
1:A:11:PRO:HB2	1:A:14:VAL:HG23	1.90	0.53
2:D:12:ASP:H	2:D:433:ILE:HG13	1.73	0.53
2:B:842:VAL:HG11	2:B:865:THR:OG1	2.08	0.53
2:D:293:THR:HG23	2:D:353:SER:H	1.73	0.53
2:B:972:LEU:HD21	2:B:1005:ARG:HD3	1.91	0.52
2:D:460:ALA:O	2:D:462:THR:N	2.41	0.52
2:D:1109:VAL:O	2:D:1112:TYR:HB3	2.09	0.52
2:B:13:LEU:HA	2:B:16:PHE:HD2	1.75	0.52
1:C:279:ARG:HB3	1:C:307:VAL:HG12	1.92	0.52
2:D:164:PRO:HG2	2:D:195:ILE:HD13	1.90	0.52
1:A:138:ASN:HD22	1:A:161:GLY:HA2	1.74	0.52
1:A:237:LEU:HD13	1:A:280:TRP:CE2	2.44	0.52
2:B:771:GLN:HB3	2:B:819:LEU:HD22	1.91	0.52
2:B:847:LEU:O	2:B:851:LYS:HG2	2.10	0.52
2:D:1066:TYR:CE1	2:D:1108:ILE:HB	2.44	0.52
3:X:23:GLU:N	3:X:23:GLU:OE1	2.43	0.52
2:B:1067:LEU:O	2:B:1071:ASN:ND2	2.40	0.52
3:X:143:VAL:HG21	3:X:174:ARG:NH2	2.24	0.52
2:B:462:THR:O	2:B:466:LEU:HG	2.09	0.52
2:D:332:ILE:HG12	2:D:388:PHE:CE2	2.44	0.52
2:D:912:TYR:CZ	2:D:947:ALA:HB1	2.44	0.52
2:B:306:HIS:ND1	2:B:308:SER:HB3	2.25	0.52
2:B:454:LYS:HD2	2:B:457:LYS:HD2	1.92	0.52
2:B:590:SER:O	2:B:594:GLU:HG2	2.10	0.52
1:C:237:LEU:HD13	1:C:280:TRP:CE2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:ARG:H	2:D:109:ASN:HB3	1.75	0.52
2:D:165:ILE:HD13	2:D:187:PHE:CE2	2.39	0.52
2:B:81:ARG:H	2:B:109:ASN:HB3	1.74	0.52
2:B:1102:LEU:HA	2:B:1105:LEU:HD12	1.91	0.52
2:D:632:ILE:O	2:D:636:ILE:HG12	2.09	0.52
2:D:635:LEU:O	2:D:639:LEU:HG	2.09	0.52
2:D:237:ILE:HD13	2:D:251:MET:SD	2.49	0.52
2:D:1029:LYS:HB2	2:D:1037:ALA:HB2	1.92	0.52
1:A:83:GLU:HA	1:A:96:PRO:HA	1.92	0.52
2:B:926:LYS:NZ	2:B:930:ASP:H	2.08	0.52
2:B:953:ALA:O	2:B:955:HIS:N	2.43	0.52
1:C:333:HIS:HD2	1:C:336:HIS:H	1.55	0.52
3:X:399:ASP:O	3:X:403:HIS:HB2	2.09	0.52
2:B:4:LEU:HG	2:B:393:SER:OG	2.10	0.52
2:B:955:HIS:O	2:B:958:LEU:HB2	2.10	0.52
2:D:118:SER:OG	2:D:177:ALA:HB2	2.11	0.51
1:A:143:ALA:CB	1:A:192:PHE:HD2	2.23	0.51
2:D:478:ILE:HD11	2:D:501:GLU:HG2	1.91	0.51
3:X:196:GLY:O	3:X:207:ARG:NH2	2.43	0.51
2:B:164:PRO:HB3	2:B:204:HIS:NE2	2.26	0.51
2:B:650:ASP:OD1	2:B:651:SER:N	2.44	0.51
2:D:485:ASP:OD1	2:D:485:ASP:N	2.43	0.51
2:D:816:VAL:HG11	2:D:832:ILE:HD13	1.92	0.51
2:D:1060:THR:O	2:D:1063:ILE:HB	2.10	0.51
2:D:194:LYS:HB3	2:D:205:TYR:HB2	1.91	0.51
3:X:319:LEU:HD22	3:X:344:ALA:HB3	1.92	0.51
1:A:130:LYS:O	1:A:134:HIS:NE2	2.41	0.51
1:A:264:ASP:OD1	1:A:264:ASP:N	2.40	0.51
2:B:377:LYS:HG2	2:B:393:SER:HB3	1.92	0.51
2:B:478:ILE:HD11	2:B:501:GLU:HG2	1.92	0.51
2:B:767:ASN:HB3	2:B:770:LEU:HD11	1.92	0.51
2:B:971:LEU:HD12	2:B:1002:LEU:HD11	1.91	0.51
2:D:663:ASN:OD1	2:D:796:SER:OG	2.22	0.51
1:A:337:GLY:HA3	1:A:358:MET:O	2.11	0.51
2:B:1082:TRP:CG	3:X:308:GLN:HE22	2.29	0.51
1:C:264:ASP:OD1	1:C:264:ASP:N	2.42	0.51
2:D:13:LEU:HA	2:D:16:PHE:HD2	1.76	0.51
3:X:147:CYS:O	3:X:151:MET:HG2	2.11	0.51
1:A:240:LEU:HB3	1:A:241:PRO:HD3	1.92	0.51
2:B:965:PRO:HG3	2:B:967:LYS:NZ	2.25	0.51
1:C:279:ARG:NH1	1:C:327:ASP:OD1	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:PHE:CE1	2:D:147:PHE:HA	2.44	0.51
2:D:690:VAL:O	2:D:693:GLU:HB2	2.10	0.51
2:D:1060:THR:HA	2:D:1063:ILE:HD12	1.93	0.51
1:A:55:GLY:H	1:A:384:ARG:NH1	2.09	0.51
2:B:1113:HIS:O	2:B:1117:LYS:HG3	2.10	0.51
2:D:313:LYS:HD2	2:D:351:LEU:HD21	1.93	0.51
2:D:998:ASP:O	2:D:1002:LEU:HG	2.11	0.51
2:B:524:PHE:CE1	2:B:531:THR:HA	2.45	0.51
1:C:7:GLN:NE2	2:D:983:LYS:HD2	2.26	0.51
2:D:65:ASN:HB2	2:D:75:TRP:CD1	2.46	0.51
2:D:828:CYS:HA	2:D:831:LEU:HB2	1.92	0.51
1:A:212:PHE:HE1	1:A:233:TRP:CE3	2.29	0.51
2:B:935:ILE:HG23	2:B:967:LYS:HZ3	1.74	0.51
2:B:969:SER:O	2:B:972:LEU:HB2	2.11	0.51
2:D:462:THR:O	2:D:466:LEU:HG	2.11	0.51
3:X:166:ALA:HB2	3:X:195:THR:HG1	1.75	0.51
1:A:102:LEU:O	1:A:113:LEU:HD12	2.10	0.50
1:A:283:PHE:C	2:B:487:THR:HB	2.35	0.50
2:B:695:PHE:CE1	2:B:724:LEU:HB3	2.45	0.50
2:B:923:ASP:OD1	2:B:941:THR:OG1	2.18	0.50
1:C:162:ASP:HA	1:C:186:PRO:HB3	1.93	0.50
2:D:492:TYR:OH	2:D:496:ARG:NH2	2.45	0.50
3:X:54:LEU:HD22	3:X:434:PHE:CE1	2.46	0.50
3:X:416:HIS:CE1	3:X:432:ALA:HA	2.46	0.50
1:A:114:ILE:HG23	1:A:121:ILE:HG23	1.93	0.50
1:A:130:LYS:HD3	2:B:609:TYR:CE1	2.45	0.50
1:A:133:HIS:CD2	1:A:167:ILE:HD12	2.46	0.50
1:A:258:VAL:HG13	1:A:270:ALA:HB2	1.93	0.50
2:B:237:ILE:HG21	2:B:251:MET:SD	2.51	0.50
2:B:939:HIS:O	2:B:942:LEU:HB2	2.12	0.50
2:B:990:TYR:O	2:B:994:THR:HG23	2.12	0.50
2:D:815:LEU:O	2:D:819:LEU:HG	2.11	0.50
2:B:546:TYR:HE1	2:B:791:HIS:CE1	2.29	0.50
2:B:859:VAL:HG12	2:B:863:LYS:HE3	1.93	0.50
1:C:40:ILE:HG23	1:C:73:LEU:HD11	1.93	0.50
2:D:642:LEU:HB3	2:D:645:PRO:HD3	1.92	0.50
2:D:723:SER:O	2:D:726:GLU:HB3	2.11	0.50
2:D:812:VAL:HG21	2:D:835:LEU:HB2	1.93	0.50
2:B:350:GLN:HG2	2:B:524:PHE:HB2	1.94	0.50
2:B:937:ILE:O	2:B:941:THR:OG1	2.29	0.50
2:B:1060:THR:O	2:B:1063:ILE:HB	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:TRP:CZ2	2:D:499:TYR:HA	2.46	0.50
2:D:636:ILE:HA	2:D:639:LEU:HD12	1.92	0.50
1:A:384:ARG:HE	1:A:389:THR:CG2	2.24	0.50
2:B:170:GLN:OE1	2:B:208:HIS:NE2	2.44	0.50
2:D:985:ASN:HA	2:D:988:LEU:HD12	1.93	0.50
1:C:258:VAL:HG13	1:C:270:ALA:HB2	1.93	0.50
2:D:676:SER:HB2	2:D:773:PHE:CE1	2.47	0.50
2:D:768:THR:C	2:D:770:LEU:H	2.19	0.50
2:B:943:LYS:HG3	2:B:974:PHE:CZ	2.47	0.50
2:B:965:PRO:HG3	2:B:967:LYS:HZ2	1.75	0.50
1:C:283:PHE:HB2	1:C:299:GLY:N	2.27	0.50
2:D:977:GLN:O	2:D:981:GLN:HG3	2.11	0.50
2:B:131:ILE:HG12	2:B:137:LEU:HD23	1.93	0.49
2:B:313:LYS:HB3	2:B:329:LYS:HD3	1.94	0.49
2:B:332:ILE:HG12	2:B:388:PHE:HE2	1.76	0.49
2:B:881:GLU:CB	2:B:901:HIS:HE1	2.25	0.49
1:C:252:ALA:HB2	2:D:826:ASN:HD22	1.77	0.49
2:B:646:MET:HE2	2:B:717:CYS:HB3	1.93	0.49
2:D:742:LEU:HD22	2:D:826:ASN:HD21	1.77	0.49
2:D:767:ASN:OD1	2:D:768:THR:N	2.44	0.49
2:D:1047:TYR:O	2:D:1050:THR:OG1	2.31	0.49
2:D:1119:VAL:O	2:D:1123:VAL:HG23	2.13	0.49
2:B:50:PHE:CZ	2:B:442:SER:HA	2.48	0.49
2:B:86:PHE:HB3	2:B:101:ASN:ND2	2.21	0.49
2:B:873:THR:HG22	2:B:883:GLN:HE22	1.77	0.49
1:C:51:PRO:C	1:C:53:SER:H	2.18	0.49
1:C:231:ASN:ND2	2:D:491:TYR:OH	2.45	0.49
2:D:1073:LEU:HD11	2:D:1105:LEU:HD13	1.94	0.49
3:X:92:LYS:HD2	3:X:164:VAL:O	2.12	0.49
3:X:381:GLY:O	3:X:384:MET:HB2	2.11	0.49
1:A:192:PHE:HE1	1:A:200:LEU:HD22	1.77	0.49
3:X:95:MET:HA	3:X:129:GLY:O	2.13	0.49
3:X:237:VAL:H	3:X:260:THR:HG1	1.54	0.49
2:B:1042:GLU:O	2:B:1045:SER:OG	2.24	0.49
2:D:546:TYR:HE1	2:D:791:HIS:NE2	2.10	0.49
3:X:83:GLN:HB3	3:X:91:TYR:CZ	2.48	0.49
1:A:283:PHE:HB2	1:A:299:GLY:N	2.27	0.49
2:B:129:TYR:OH	2:B:180:THR:O	2.31	0.49
2:D:9:VAL:HB	2:D:539:VAL:HG23	1.95	0.49
3:X:363:GLY:O	3:X:422:GLN:NE2	2.35	0.49
1:A:280:TRP:CD1	1:A:305:PRO:HA	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:919:SER:HB2	2:B:941:THR:HG23	1.93	0.49
1:C:130:LYS:HE2	2:D:608:SER:HB3	1.95	0.49
2:D:629:PRO:HA	2:D:632:ILE:HD12	1.95	0.49
2:B:172:PRO:HA	2:B:187:PHE:HD1	1.78	0.49
2:D:332:ILE:HG12	2:D:388:PHE:HE2	1.77	0.49
2:D:1063:ILE:HG12	2:D:1112:TYR:HE1	1.78	0.49
3:X:289:ARG:HG2	3:X:289:ARG:NH1	2.24	0.49
1:A:51:PRO:C	1:A:53:SER:H	2.18	0.49
2:B:178:ILE:HD11	2:B:182:GLU:HB2	1.95	0.49
2:B:905:LYS:O	2:B:909:GLU:HG3	2.12	0.49
2:D:939:HIS:O	2:D:942:LEU:HB2	2.12	0.49
2:D:982:GLY:O	2:D:984:ILE:N	2.46	0.49
1:A:162:ASP:HA	1:A:186:PRO:HB3	1.94	0.48
2:B:118:SER:HB2	2:B:175:MET:HE3	1.95	0.48
2:B:422:TRP:CZ2	2:B:499:TYR:HA	2.48	0.48
2:B:1063:ILE:HG12	2:B:1112:TYR:HE1	1.78	0.48
2:B:1120:ALA:HA	2:B:1123:VAL:HG23	1.94	0.48
2:D:524:PHE:CE1	2:D:531:THR:HA	2.47	0.48
2:B:9:VAL:HB	2:B:539:VAL:HG23	1.94	0.48
2:B:188:PHE:O	2:B:236:THR:OG1	2.25	0.48
2:B:492:TYR:OH	2:B:496:ARG:NH2	2.46	0.48
2:B:817:GLU:HA	2:B:844:LEU:HD11	1.95	0.48
2:B:884:GLU:O	2:B:888:LYS:HG3	2.13	0.48
1:C:12:LEU:HD22	2:D:951:PHE:HB3	1.96	0.48
2:D:590:SER:O	2:D:594:GLU:HG2	2.12	0.48
2:B:1062:ILE:HA	2:B:1065:HIS:CD2	2.48	0.48
1:C:170:ARG:HD3	1:C:214:TRP:CZ3	2.48	0.48
2:D:86:PHE:HB3	2:D:101:ASN:ND2	2.22	0.48
2:D:170:GLN:OE1	2:D:208:HIS:NE2	2.46	0.48
2:D:903:SER:OG	2:D:940:GLU:OE1	2.26	0.48
3:X:205:LEU:C	3:X:207:ARG:H	2.21	0.48
3:X:222:MET:SD	3:X:365:LEU:HB3	2.53	0.48
1:A:71:LEU:HD11	2:B:860:ARG:NH2	2.29	0.48
2:B:733:PHE:CZ	2:B:812:VAL:HG23	2.49	0.48
2:B:959:MET:SD	2:B:994:THR:HB	2.54	0.48
2:D:284:PHE:CD2	2:D:287:LEU:HD13	2.48	0.48
2:D:945:ALA:HB1	2:D:954:ALA:CB	2.43	0.48
3:X:332:ALA:HA	3:X:335:LEU:HD12	1.94	0.48
2:B:460:ALA:O	2:B:462:THR:N	2.42	0.48
2:B:824:GLN:HG2	2:B:827:ALA:HB3	1.95	0.48
2:D:185:VAL:HB	2:D:193:THR:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:492:TYR:O	2:D:495:LYS:HB3	2.14	0.48
2:B:60:GLY:HA2	2:B:78:PHE:O	2.13	0.48
2:B:65:ASN:HB2	2:B:75:TRP:CD1	2.49	0.48
2:B:840:ILE:HG23	2:B:875:GLN:NE2	2.29	0.48
2:B:879:LEU:HD23	2:B:879:LEU:HA	1.68	0.48
2:B:913:ILE:O	2:B:916:LEU:HB2	2.13	0.48
2:B:1045:SER:HA	2:B:1048:ILE:HD12	1.96	0.48
2:B:1105:LEU:HA	2:B:1108:ILE:HG12	1.94	0.48
1:C:192:PHE:HE1	1:C:200:LEU:HD22	1.78	0.48
2:D:768:THR:O	2:D:770:LEU:N	2.47	0.48
3:X:43:PRO:O	3:X:47:GLN:NE2	2.38	0.48
2:B:600:ARG:HG3	2:B:834:TRP:NE1	2.28	0.48
2:B:1010:MET:O	2:B:1013:VAL:HG12	2.13	0.48
1:C:182:PRO:HB3	2:D:597:TYR:CZ	2.49	0.48
1:C:233:TRP:HD1	2:D:413:MET:SD	2.37	0.48
2:D:433:ILE:HG22	2:D:434:GLU:HG3	1.96	0.48
2:D:703:THR:HG23	2:D:704:SER:H	1.79	0.48
2:D:742:LEU:HB2	2:D:824:GLN:HG3	1.96	0.48
3:X:405:ILE:O	3:X:409:ILE:HG13	2.14	0.48
1:C:78:SER:OG	1:C:144:ASP:OD2	2.30	0.48
1:C:130:LYS:O	1:C:134:HIS:NE2	2.40	0.48
2:D:1066:TYR:CD2	2:D:1112:TYR:HB2	2.48	0.48
1:A:280:TRP:CE2	1:A:305:PRO:HB3	2.49	0.48
2:B:768:THR:C	2:B:770:LEU:H	2.21	0.48
2:D:60:GLY:HA2	2:D:78:PHE:O	2.13	0.48
2:D:935:ILE:CG2	2:D:967:LYS:HZ3	2.27	0.48
2:D:1040:ILE:HG22	2:D:1044:LEU:HD11	1.94	0.48
3:X:166:ALA:HB2	3:X:195:THR:OG1	2.12	0.48
2:B:98:SER:O	2:B:99:LYS:HD3	2.13	0.48
2:B:115:VAL:O	2:B:116:ALA:HB3	2.12	0.48
2:B:241:ILE:CG2	2:B:250:VAL:HB	2.44	0.48
2:B:492:TYR:O	2:B:495:LYS:HB3	2.14	0.48
1:C:138:ASN:HD22	1:C:161:GLY:HA2	1.79	0.48
2:D:290:ASP:OD1	2:D:290:ASP:N	2.47	0.48
2:D:814:GLU:O	2:D:817:GLU:HB3	2.14	0.48
2:B:763:LEU:HD21	2:B:774:SER:OG	2.14	0.47
2:D:975:VAL:HA	2:D:978:LEU:HB2	1.96	0.47
3:X:277:GLU:CD	3:X:277:GLU:H	2.21	0.47
3:X:306:GLU:O	3:X:308:GLN:HG3	2.14	0.47
2:B:485:ASP:OD1	2:B:485:ASP:N	2.42	0.47
2:D:353:SER:HB2	2:D:361:PHE:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:673:LEU:HB2	2:D:770:LEU:HD22	1.95	0.47
3:X:333:HIS:CE1	3:X:358:LEU:HD11	2.49	0.47
1:A:40:ILE:HG23	1:A:73:LEU:HD11	1.96	0.47
2:B:816:VAL:O	2:B:820:PHE:HB3	2.14	0.47
2:B:1015:SER:HB3	2:B:1018:CYS:HB2	1.95	0.47
2:D:906:LEU:HD22	2:D:914:ASP:HB2	1.95	0.47
2:B:207:GLN:O	2:B:207:GLN:HG3	2.14	0.47
2:B:419:SER:O	2:B:423:LEU:HD12	2.14	0.47
2:B:958:LEU:HD13	2:B:975:VAL:HG22	1.96	0.47
2:B:1067:LEU:HD13	2:D:1116:LEU:HD22	1.95	0.47
1:C:337:GLY:HA3	1:C:358:MET:O	2.13	0.47
2:D:11:ILE:HA	2:D:14:GLN:CD	2.40	0.47
2:B:293:THR:CG2	2:B:353:SER:H	2.27	0.47
2:B:548:ILE:CD1	2:B:687:LYS:HD2	2.44	0.47
2:B:1109:VAL:O	2:B:1112:TYR:HB3	2.14	0.47
1:C:156:VAL:HG21	1:C:214:TRP:CH2	2.50	0.47
2:D:419:SER:O	2:D:423:LEU:HD12	2.14	0.47
2:D:636:ILE:HD13	2:D:639:LEU:HD12	1.95	0.47
2:D:968:LYS:HA	2:D:971:LEU:HD12	1.96	0.47
2:D:1063:ILE:HG12	2:D:1112:TYR:CE1	2.50	0.47
1:A:39:GLY:HA2	1:A:66:THR:OG1	2.15	0.47
1:A:210:ARG:HH12	2:B:417:ASP:N	2.12	0.47
2:B:284:PHE:HD2	2:B:287:LEU:HD13	1.80	0.47
2:B:632:ILE:O	2:B:636:ILE:HG12	2.14	0.47
2:B:945:ALA:HB1	2:B:954:ALA:HB1	1.96	0.47
2:B:1101:LYS:O	2:B:1105:LEU:HG	2.14	0.47
2:D:13:LEU:HB3	2:D:674:CYS:SG	2.54	0.47
2:D:129:TYR:OH	2:D:180:THR:O	2.32	0.47
2:D:182:GLU:HG2	2:D:196:ILE:HG13	1.96	0.47
2:D:241:ILE:HG22	2:D:250:VAL:HB	1.95	0.47
2:D:339:ASP:O	2:D:342:ILE:HB	2.13	0.47
2:D:826:ASN:OD1	2:D:826:ASN:N	2.43	0.47
2:D:859:VAL:HG13	2:D:918:PHE:HZ	1.79	0.47
1:A:182:PRO:HB3	2:B:597:TYR:CE2	2.49	0.47
1:A:244:ASN:HB3	1:A:246:CYS:SG	2.55	0.47
1:A:252:ALA:HB2	2:B:826:ASN:ND2	2.18	0.47
1:A:279:ARG:HB3	1:A:307:VAL:HG12	1.96	0.47
2:B:673:LEU:O	2:B:677:VAL:HG23	2.15	0.47
2:D:196:ILE:HD13	2:D:205:TYR:HE2	1.80	0.47
2:D:405:THR:HB	2:D:589:PHE:CZ	2.50	0.47
2:D:955:HIS:HA	2:D:958:LEU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:HB2	1:A:264:ASP:HA	1.96	0.47
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.78	0.47
2:B:131:ILE:HG12	2:B:137:LEU:CD2	2.45	0.47
2:B:339:ASP:O	2:B:342:ILE:HB	2.15	0.47
2:B:705:GLN:O	2:B:709:GLU:HG3	2.15	0.47
2:B:965:PRO:HG2	2:B:967:LYS:HG3	1.95	0.47
2:D:81:ARG:H	2:D:109:ASN:CB	2.28	0.47
2:D:293:THR:CG2	2:D:353:SER:H	2.28	0.47
3:X:199:LEU:HD23	3:X:203:GLY:O	2.15	0.47
2:B:978:LEU:O	2:B:981:GLN:HB3	2.15	0.47
2:D:314:LEU:HD21	2:D:325:VAL:HG13	1.97	0.47
3:X:318:ALA:O	3:X:319:LEU:HD23	2.15	0.47
2:B:271:THR:C	2:B:272:ILE:HD12	2.40	0.46
2:B:284:PHE:CD2	2:B:287:LEU:HD13	2.50	0.46
2:B:466:LEU:O	2:B:470:VAL:HG23	2.14	0.46
2:B:652:LEU:HD23	2:B:655:ARG:NE	2.30	0.46
1:C:114:ILE:HG23	1:C:121:ILE:HG23	1.97	0.46
2:D:18:LEU:HD13	2:D:101:ASN:HB2	1.97	0.46
2:D:638:THR:O	2:D:642:LEU:HD13	2.15	0.46
1:A:143:ALA:HB2	1:A:192:PHE:HD2	1.80	0.46
2:B:521:SER:O	2:B:534:ASN:HB2	2.15	0.46
2:D:237:ILE:HG21	2:D:251:MET:SD	2.55	0.46
2:D:584:HIS:HB3	2:D:693:GLU:HG2	1.96	0.46
3:X:292:ARG:HB2	3:X:295:ASP:CG	2.40	0.46
2:B:718:ASP:O	2:B:722:LEU:HG	2.15	0.46
2:B:828:CYS:O	2:B:832:ILE:HB	2.15	0.46
1:C:147:SER:OG	1:C:148:ALA:N	2.48	0.46
3:X:393:TRP:CG	3:X:397:LYS:HD3	2.50	0.46
2:B:139:TYR:HB3	2:B:160:LEU:O	2.16	0.46
2:B:178:ILE:HG21	2:B:263:LEU:HD21	1.97	0.46
2:B:629:PRO:HA	2:B:632:ILE:HD12	1.98	0.46
2:B:815:LEU:HD22	2:B:819:LEU:HD11	1.97	0.46
2:B:995:LEU:O	2:B:999:VAL:HG23	2.15	0.46
2:B:1063:ILE:O	2:B:1067:LEU:HG	2.14	0.46
2:B:1101:LYS:O	2:B:1104:THR:HG23	2.16	0.46
1:C:53:SER:OG	1:C:54:THR:N	2.27	0.46
1:C:192:PHE:CE1	1:C:200:LEU:HD22	2.50	0.46
2:D:289:SER:O	2:D:299:LEU:HB2	2.14	0.46
2:D:1062:ILE:HG22	2:D:1066:TYR:CE2	2.50	0.46
3:X:377:VAL:O	3:X:380:SER:OG	2.22	0.46
1:A:147:SER:OG	1:A:148:ALA:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:OE1	1:A:259:ARG:HD2	2.16	0.46
2:B:672:PHE:HE1	2:B:790:LEU:HD23	1.81	0.46
2:B:984:ILE:HG21	2:B:1024:PHE:CG	2.51	0.46
2:D:584:HIS:HA	2:D:587:MET:HE3	1.97	0.46
2:B:243:LEU:HD21	2:B:292:THR:HG21	1.97	0.46
1:C:143:ALA:CB	1:C:192:PHE:HD2	2.29	0.46
1:C:191:GLN:OE1	1:C:259:ARG:HD2	2.16	0.46
2:D:172:PRO:HA	2:D:187:PHE:HD1	1.80	0.46
2:D:241:ILE:CG2	2:D:250:VAL:HB	2.46	0.46
1:A:12:LEU:HD13	2:B:951:PHE:HD1	1.81	0.46
1:A:170:ARG:HD3	1:A:214:TRP:CZ3	2.51	0.46
2:B:18:LEU:HD13	2:B:101:ASN:HB2	1.98	0.46
2:B:826:ASN:O	2:B:829:MET:HB2	2.16	0.46
2:B:1017:PRO:HA	2:B:1020:TYR:HD2	1.81	0.46
2:B:1116:LEU:HD22	2:D:1067:LEU:HD13	1.97	0.46
2:B:353:SER:HB2	2:B:361:PHE:CD2	2.51	0.46
2:B:690:VAL:O	2:B:693:GLU:HB2	2.16	0.46
1:C:11:PRO:HB2	1:C:14:VAL:HG23	1.98	0.46
1:C:130:LYS:HD3	2:D:609:TYR:CE1	2.51	0.46
1:C:384:ARG:HE	1:C:389:THR:CG2	2.29	0.46
2:D:340:GLU:HB3	2:D:342:ILE:HD13	1.98	0.46
2:D:742:LEU:HD12	2:D:827:ALA:HB2	1.98	0.46
1:A:134:HIS:HB3	2:B:605:ASP:OD1	2.16	0.46
2:B:162:TYR:HE2	2:B:204:HIS:CE1	2.34	0.46
2:B:198:ASN:HB3	2:B:201:ASP:HB3	1.96	0.46
2:B:875:GLN:HB2	2:B:879:LEU:HG	1.98	0.46
2:D:450:VAL:O	2:D:454:LYS:N	2.37	0.46
2:D:466:LEU:O	2:D:470:VAL:HG23	2.15	0.46
2:D:697:PHE:O	2:D:701:LEU:HG	2.16	0.46
2:D:828:CYS:O	2:D:832:ILE:HB	2.16	0.46
2:D:948:ALA:O	2:D:950:LYS:HG2	2.16	0.46
2:D:1019:TRP:CZ2	2:D:1048:ILE:HD11	2.51	0.46
2:D:1112:TYR:O	2:D:1116:LEU:HG	2.15	0.46
2:D:50:PHE:CZ	2:D:442:SER:HA	2.50	0.46
2:D:178:ILE:HG21	2:D:263:LEU:HD21	1.97	0.46
2:D:512:LEU:HD22	2:D:512:LEU:HA	1.86	0.46
2:D:671:LEU:HD12	2:D:672:PHE:H	1.81	0.46
2:D:708:TYR:OH	2:D:713:LYS:HD2	2.15	0.46
2:D:1025:SER:O	2:D:1029:LYS:HG2	2.15	0.46
2:D:1034:ARG:HH21	2:D:1076:LEU:HD22	1.81	0.46
2:B:832:ILE:HG13	2:B:835:LEU:HD22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:HIS:HA	1:C:323:PRO:HD3	1.84	0.45
2:D:198:ASN:HB3	2:D:201:ASP:HB3	1.97	0.45
2:D:639:LEU:HD22	2:D:701:LEU:HD13	1.98	0.45
2:D:695:PHE:CZ	2:D:724:LEU:HB3	2.51	0.45
2:D:919:SER:HB2	2:D:941:THR:OG1	2.16	0.45
3:X:333:HIS:NE2	3:X:358:LEU:HD11	2.30	0.45
1:C:243:VAL:O	1:C:245:THR:OG1	2.33	0.45
2:D:284:PHE:HD2	2:D:287:LEU:HD13	1.81	0.45
2:D:329:LYS:HB3	2:D:329:LYS:HZ2	1.82	0.45
2:D:959:MET:SD	2:D:994:THR:OG1	2.60	0.45
1:A:156:VAL:HG21	1:A:214:TRP:CH2	2.51	0.45
2:B:5:LYS:HE2	2:B:549:GLU:HG3	1.97	0.45
2:B:543:ARG:CB	2:B:679:ARG:HH12	2.30	0.45
2:B:680:VAL:HG11	2:B:773:PHE:HZ	1.81	0.45
2:B:815:LEU:O	2:B:819:LEU:HG	2.16	0.45
2:B:953:ALA:C	2:B:955:HIS:N	2.64	0.45
1:C:102:LEU:O	1:C:113:LEU:HD12	2.16	0.45
2:D:1104:THR:O	2:D:1108:ILE:HG23	2.17	0.45
3:X:85:SER:O	3:X:126:GLY:N	2.48	0.45
2:B:729:ARG:HH12	2:B:812:VAL:HG11	1.81	0.45
2:B:812:VAL:CG2	2:B:835:LEU:HB2	2.47	0.45
2:B:1028:TYR:O	2:B:1031:GLN:HB3	2.15	0.45
2:D:377:LYS:HG2	2:D:393:SER:HB3	1.97	0.45
2:D:803:ILE:HG21	2:D:807:THR:HG23	1.99	0.45
3:X:83:GLN:HB3	3:X:91:TYR:CE1	2.51	0.45
3:X:199:LEU:HD23	3:X:203:GLY:C	2.41	0.45
3:X:281:ARG:O	3:X:284:GLU:HB2	2.16	0.45
3:X:353:ILE:HD12	3:X:353:ILE:H	1.82	0.45
1:A:11:PRO:HB2	1:A:14:VAL:CG2	2.47	0.45
2:B:81:ARG:H	2:B:109:ASN:CB	2.29	0.45
2:B:97:LEU:O	2:B:99:LYS:HG2	2.17	0.45
2:B:1044:LEU:O	2:B:1048:ILE:HG13	2.17	0.45
1:A:277:TRP:CZ2	1:A:309:GLY:HA3	2.51	0.45
1:C:343:ASN:H	1:C:348:ASP:HB2	1.82	0.45
2:D:639:LEU:O	2:D:642:LEU:HB2	2.17	0.45
2:D:738:SER:O	2:D:738:SER:OG	2.26	0.45
2:D:1105:LEU:O	2:D:1108:ILE:HG12	2.17	0.45
3:X:239:GLY:N	3:X:262:SER:OG	2.37	0.45
2:B:1010:MET:SD	2:B:1021:ASN:HB3	2.57	0.45
1:C:130:LYS:HD3	2:D:609:TYR:HE1	1.81	0.45
1:C:160:VAL:HG11	1:C:202:VAL:HG13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ILE:HG12	2:D:137:LEU:HD23	1.98	0.45
2:D:276:GLN:HB3	2:D:279:LEU:HD23	1.99	0.45
3:X:279:LEU:O	3:X:283:ILE:HG13	2.17	0.45
1:A:243:VAL:O	1:A:245:THR:OG1	2.35	0.45
2:B:81:ARG:HA	2:B:109:ASN:HA	1.98	0.45
2:D:158:TRP:H	2:D:158:TRP:HE3	1.64	0.45
2:D:668:SER:HB2	2:D:672:PHE:HD2	1.82	0.45
1:A:107:GLN:HE22	2:B:860:ARG:HG2	1.80	0.45
2:B:417:ASP:HB2	2:B:418:ILE:H	1.52	0.45
2:B:916:LEU:CD2	2:B:945:ALA:HA	2.47	0.45
2:B:995:LEU:C	2:B:999:VAL:HG23	2.42	0.45
2:D:1019:TRP:CH2	2:D:1048:ILE:HD11	2.51	0.45
2:B:955:HIS:HA	2:B:958:LEU:HD12	1.99	0.45
2:B:75:TRP:CE3	2:B:539:VAL:HG13	2.51	0.44
2:B:881:GLU:HB3	2:B:901:HIS:HE1	1.82	0.44
2:B:1103:LEU:CD1	3:X:271:GLU:H	2.29	0.44
1:C:107:GLN:HA	2:D:860:ARG:NH2	2.32	0.44
2:D:587:MET:SD	2:D:696:ILE:HD13	2.57	0.44
2:D:1058:GLU:O	2:D:1062:ILE:HG13	2.17	0.44
3:X:206:ILE:HD11	3:X:395:ALA:HB1	1.99	0.44
1:A:21:TRP:CZ2	1:A:373:ALA:HB2	2.52	0.44
1:A:53:SER:O	1:A:384:ARG:HD3	2.17	0.44
2:B:340:GLU:HB3	2:B:342:ILE:HD13	2.00	0.44
2:B:1100:GLN:O	2:B:1101:LYS:NZ	2.50	0.44
1:C:212:PHE:HE1	1:C:233:TRP:CE3	2.34	0.44
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.81	0.44
2:D:12:ASP:HB2	2:D:433:ILE:CG2	2.45	0.44
2:D:28:ALA:HB1	2:D:107:PRO:HB3	1.98	0.44
2:D:436:ILE:O	2:D:440:LEU:HG	2.18	0.44
2:D:474:ILE:HG12	2:D:502:TRP:CZ2	2.52	0.44
2:D:595:ILE:HD13	2:D:696:ILE:HD11	1.98	0.44
2:B:382:LEU:HD21	2:B:389:SER:H	1.82	0.44
2:B:1023:LEU:O	2:B:1026:TRP:HB3	2.18	0.44
2:D:602:LEU:HD22	2:D:606:LEU:HD13	1.99	0.44
2:D:907:PHE:HE2	2:D:943:LYS:HD3	1.83	0.44
2:B:579:LEU:O	2:B:583:LEU:HG	2.17	0.44
2:B:1082:TRP:CH2	2:B:1100:GLN:HG3	2.52	0.44
1:C:195:SER:HB2	1:C:264:ASP:HA	1.99	0.44
2:D:23:ALA:HA	2:D:103:LYS:O	2.18	0.44
2:D:77:ILE:HB	2:D:84:THR:OG1	2.18	0.44
2:D:97:LEU:HD21	2:D:762:ALA:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:ILE:HD13	2:D:205:TYR:CE2	2.52	0.44
2:D:940:GLU:O	2:D:944:THR:HG23	2.17	0.44
1:A:210:ARG:NH1	2:B:417:ASP:OD1	2.50	0.44
2:B:622:HIS:O	2:B:627:VAL:HG21	2.16	0.44
2:B:1060:THR:HG22	2:B:1063:ILE:HD12	2.00	0.44
1:C:236:THR:HG21	2:D:417:ASP:OD1	2.18	0.44
1:C:280:TRP:CE2	1:C:305:PRO:HB3	2.53	0.44
2:D:533:ILE:HD12	2:D:535:TYR:HE1	1.83	0.44
2:D:616:TRP:NE1	2:D:706:GLN:HE21	2.16	0.44
2:D:838:ASP:O	2:D:842:VAL:N	2.43	0.44
3:X:175:GLU:CD	3:X:175:GLU:N	2.76	0.44
1:A:302:ASN:O	1:A:303:LEU:HD23	2.17	0.44
2:B:77:ILE:HB	2:B:84:THR:OG1	2.18	0.44
2:B:436:ILE:O	2:B:440:LEU:HG	2.17	0.44
2:B:600:ARG:HG3	2:B:834:TRP:HE1	1.82	0.44
2:B:1058:GLU:O	2:B:1062:ILE:HG13	2.17	0.44
2:D:382:LEU:HD21	2:D:389:SER:H	1.83	0.44
2:B:844:LEU:HD23	2:B:844:LEU:HA	1.63	0.44
2:B:1039:ILE:HG23	2:B:1083:ILE:HG13	2.00	0.44
2:D:1115:GLN:O	2:D:1119:VAL:HG23	2.17	0.44
2:B:88:VAL:HB	2:B:671:LEU:HD23	1.99	0.44
2:B:385:ASP:HB3	2:B:387:SER:HB3	2.00	0.44
2:B:1013:VAL:HG13	2:B:1015:SER:H	1.83	0.44
1:C:280:TRP:CD1	1:C:305:PRO:HA	2.53	0.44
2:D:207:GLN:O	2:D:207:GLN:HG3	2.18	0.44
2:D:243:LEU:HD21	2:D:292:THR:HG21	2.00	0.44
2:D:914:ASP:O	2:D:918:PHE:HD1	2.01	0.44
3:X:245:GLN:O	3:X:248:ILE:HB	2.17	0.44
3:X:261:ALA:O	3:X:267:THR:HG23	2.18	0.44
2:B:66:LYS:CG	2:B:119:PHE:HB2	2.43	0.43
2:B:543:ARG:HB3	2:B:679:ARG:HH22	1.82	0.43
2:B:703:THR:HG23	2:B:704:SER:H	1.83	0.43
2:B:798:LEU:HA	2:B:801:ILE:HD12	2.00	0.43
2:B:871:SER:H	2:B:883:GLN:HG2	1.83	0.43
2:B:1010:MET:HE2	2:B:1010:MET:HB2	1.85	0.43
1:C:25:SER:HB2	1:C:77:SER:HA	2.00	0.43
2:D:249:LEU:HB2	2:D:261:LEU:HB3	2.00	0.43
3:X:36:TRP:HA	3:X:39:LEU:HD12	2.00	0.43
3:X:289:ARG:HH11	3:X:289:ARG:CG	2.30	0.43
3:X:379:THR:HA	3:X:382:LEU:CG	2.48	0.43
2:B:4:LEU:HD23	2:B:4:LEU:HA	1.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:61:ILE:HG22	3:X:63:PHE:HD1	1.81	0.43
3:X:151:MET:SD	3:X:154:LEU:HD23	2.58	0.43
1:A:192:PHE:CE1	1:A:200:LEU:HD22	2.52	0.43
1:A:279:ARG:NH1	1:A:327:ASP:OD1	2.43	0.43
1:C:252:ALA:HB2	2:D:826:ASN:HB3	2.00	0.43
1:C:377:GLU:CD	2:D:913:ILE:HB	2.44	0.43
2:D:301:TYR:HA	2:D:302:PRO:HD3	1.88	0.43
2:D:417:ASP:OD1	2:D:417:ASP:N	2.50	0.43
1:A:138:ASN:OD1	2:B:857:LYS:NZ	2.49	0.43
2:B:463:ILE:HA	2:B:466:LEU:HG	1.98	0.43
2:B:933:LEU:O	2:B:937:ILE:HG13	2.17	0.43
2:B:945:ALA:HB1	2:B:954:ALA:CB	2.48	0.43
2:B:955:HIS:HE1	2:B:978:LEU:HD13	1.81	0.43
2:D:131:ILE:HG12	2:D:137:LEU:CD2	2.47	0.43
2:D:651:SER:O	2:D:655:ARG:HG3	2.18	0.43
1:A:10:LEU:HG	1:A:379:SER:HA	2.01	0.43
1:A:115:ILE:HB	1:A:123:THR:HB	2.01	0.43
2:B:158:TRP:H	2:B:158:TRP:HE3	1.64	0.43
2:B:178:ILE:HG13	2:B:179:SER:N	2.33	0.43
2:B:279:LEU:HD21	2:B:303:ASP:HA	2.00	0.43
2:B:290:ASP:OD1	2:B:290:ASP:N	2.51	0.43
2:B:587:MET:HE1	2:B:696:ILE:HD13	2.00	0.43
2:B:889:TYR:CG	2:B:933:LEU:HD13	2.53	0.43
2:D:362:LEU:HD12	2:D:378:CYS:O	2.18	0.43
2:D:1030:HIS:HA	2:D:1034:ARG:CG	2.48	0.43
3:X:266:GLY:HA3	3:X:305:LEU:O	2.19	0.43
1:A:25:SER:HB2	1:A:77:SER:HA	2.01	0.43
2:D:173:ASP:HB2	2:D:188:PHE:CE1	2.53	0.43
2:D:978:LEU:O	2:D:982:GLY:N	2.50	0.43
2:D:1111:GLU:HA	2:D:1114:LEU:HD12	1.99	0.43
1:A:322:HIS:HA	1:A:323:PRO:HD3	1.84	0.43
2:B:11:ILE:HA	2:B:14:GLN:CD	2.43	0.43
2:B:445:ASN:OD1	2:B:446:SER:N	2.51	0.43
2:B:988:LEU:O	2:B:991:SER:OG	2.26	0.43
1:C:39:GLY:HA2	1:C:66:THR:OG1	2.19	0.43
1:C:69:PRO:HD2	1:C:107:GLN:HB2	2.01	0.43
2:D:812:VAL:CG2	2:D:835:LEU:HB2	2.48	0.43
3:X:109:LEU:HD23	3:X:109:LEU:HA	1.88	0.43
2:B:991:SER:O	2:B:994:THR:OG1	2.37	0.43
2:D:198:ASN:HB3	2:D:201:ASP:CB	2.49	0.43
2:D:287:LEU:HD12	2:D:346:LEU:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:LYS:HB3	2:D:329:LYS:NZ	2.33	0.43
2:D:733:PHE:HA	2:D:834:TRP:CZ3	2.54	0.43
2:D:742:LEU:HD13	2:D:826:ASN:CG	2.43	0.43
3:X:345:GLU:CD	3:X:350:PRO:HD2	2.44	0.43
2:B:245:THR:HG23	2:B:246:TYR:HD1	1.84	0.43
2:B:417:ASP:N	2:B:417:ASP:OD1	2.52	0.43
2:B:909:GLU:C	2:B:911:ALA:H	2.27	0.43
2:D:75:TRP:CE3	2:D:539:VAL:HG13	2.53	0.43
2:D:1076:LEU:HA	2:D:1077:PRO:HD3	1.84	0.43
3:X:58:GLU:CD	3:X:86:SER:H	2.27	0.43
3:X:157:HIS:O	3:X:158:LEU:HD23	2.18	0.43
2:B:12:ASP:HB2	2:B:433:ILE:CG2	2.48	0.43
2:B:23:ALA:HA	2:B:103:LYS:O	2.18	0.43
2:D:407:PHE:CG	2:D:422:TRP:CH2	3.07	0.43
2:D:1073:LEU:HD21	2:D:1105:LEU:HD13	2.00	0.43
3:X:116:LYS:HD3	3:X:377:VAL:HG21	2.00	0.43
3:X:234:ARG:C	3:X:315:VAL:HG22	2.44	0.43
1:A:19:THR:HG22	1:A:362:ASP:HB3	2.01	0.42
2:B:182:GLU:HG2	2:B:196:ILE:HG13	2.00	0.42
2:B:289:SER:O	2:B:299:LEU:HB2	2.18	0.42
1:C:115:ILE:HB	1:C:123:THR:HB	2.00	0.42
3:X:198:GLY:O	3:X:203:GLY:N	2.52	0.42
1:A:69:PRO:HD2	1:A:107:GLN:HB2	2.00	0.42
1:A:328:TYR:CE1	1:A:343:ASN:HB2	2.54	0.42
2:B:238:ILE:HG23	2:B:239:SER:H	1.84	0.42
2:B:242:PHE:HD1	2:B:249:LEU:HD13	1.84	0.42
2:B:380:LEU:HD23	2:B:389:SER:O	2.19	0.42
2:B:635:LEU:O	2:B:639:LEU:HG	2.19	0.42
2:B:1038:ALA:O	2:B:1041:TYR:HB2	2.18	0.42
2:D:767:ASN:HB3	2:D:770:LEU:HD21	2.01	0.42
3:X:61:ILE:O	3:X:80:TRP:HA	2.19	0.42
2:B:196:ILE:HD13	2:B:205:TYR:CE2	2.54	0.42
2:B:471:LEU:HD23	2:B:471:LEU:HA	1.78	0.42
2:B:923:ASP:OD1	2:B:937:ILE:HG22	2.20	0.42
1:C:19:THR:HG22	1:C:362:ASP:HB3	2.01	0.42
1:C:302:ASN:O	1:C:303:LEU:HD23	2.20	0.42
2:D:75:TRP:O	2:D:85:ILE:HG13	2.20	0.42
2:D:79:GLN:HG3	2:D:80:ASN:N	2.35	0.42
2:D:235:ASN:O	2:D:235:ASN:ND2	2.47	0.42
2:D:340:GLU:O	2:D:340:GLU:HG3	2.20	0.42
2:D:603:VAL:HG13	2:D:729:ARG:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:SER:O	2:D:99:LYS:HD3	2.19	0.42
3:X:44:LYS:HA	3:X:47:GLN:HG2	2.00	0.42
3:X:120:THR:O	3:X:121:THR:OG1	2.21	0.42
3:X:237:VAL:N	3:X:260:THR:OG1	2.32	0.42
1:A:182:PRO:HB3	2:B:597:TYR:CZ	2.55	0.42
2:B:276:GLN:HB3	2:B:279:LEU:HD23	2.00	0.42
2:B:421:ILE:H	2:B:421:ILE:HG13	1.67	0.42
2:B:729:ARG:NH1	2:B:836:ASN:HB2	2.34	0.42
2:B:994:THR:OG1	2:B:999:VAL:HG22	2.20	0.42
2:B:1014:GLU:HG3	2:B:1014:GLU:O	2.18	0.42
2:D:59:ALA:O	2:D:536:ALA:HB1	2.20	0.42
3:X:93:GLY:HA3	3:X:127:GLY:O	2.18	0.42
3:X:429:ALA:O	3:X:432:ALA:N	2.52	0.42
2:B:162:TYR:HE2	2:B:204:HIS:HE1	1.66	0.42
2:B:797:SER:OG	2:B:798:LEU:N	2.52	0.42
2:B:906:LEU:HD13	2:B:914:ASP:C	2.44	0.42
2:B:1113:HIS:HA	2:B:1116:LEU:CD1	2.50	0.42
2:D:81:ARG:HA	2:D:109:ASN:HA	2.01	0.42
2:D:1068:ILE:O	2:D:1072:THR:HG23	2.19	0.42
2:B:432:SER:O	2:B:433:ILE:HD13	2.20	0.42
2:B:823:LYS:HB3	2:B:824:GLN:H	1.62	0.42
2:B:848:ILE:C	2:B:850:LEU:N	2.78	0.42
1:C:21:TRP:CZ2	1:C:373:ALA:HB2	2.54	0.42
2:D:178:ILE:HD11	2:D:182:GLU:HB2	2.01	0.42
3:X:134:ASP:HA	3:X:135:PRO:HD3	1.88	0.42
3:X:217:TYR:O	3:X:220:GLU:HB3	2.19	0.42
2:B:6:HIS:CE1	2:B:375:ILE:HD12	2.55	0.42
2:B:233:SER:O	2:B:235:ASN:N	2.51	0.42
2:B:698:LEU:HD23	2:B:698:LEU:HA	1.91	0.42
2:B:959:MET:HE1	2:B:998:ASP:HB2	2.02	0.42
2:D:143:SER:O	2:D:146:TRP:HB3	2.20	0.42
2:D:956:VAL:O	2:D:960:VAL:HG23	2.19	0.42
2:D:1069:VAL:O	2:D:1073:LEU:HG	2.19	0.42
2:B:198:ASN:HB3	2:B:201:ASP:CB	2.50	0.42
2:B:731:VAL:O	2:B:734:LEU:HB2	2.19	0.42
2:B:1017:PRO:HA	2:B:1020:TYR:CD2	2.55	0.42
2:D:423:LEU:HD11	2:D:471:LEU:HG	2.01	0.42
2:D:681:LEU:HD12	2:D:738:SER:OG	2.20	0.42
2:D:1056:LYS:HE2	2:D:1122:GLN:OE1	2.19	0.42
3:X:281:ARG:NE	3:X:299:GLU:OE2	2.53	0.42
1:A:200:LEU:HD12	1:A:200:LEU:C	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:798:LEU:HD23	2:B:801:ILE:HD12	2.01	0.42
2:B:984:ILE:HG21	2:B:1024:PHE:CD1	2.55	0.42
1:C:328:TYR:CE1	1:C:343:ASN:HB2	2.55	0.42
2:D:279:LEU:HD11	2:D:303:ASP:H	1.83	0.42
2:D:1066:TYR:CE2	2:D:1112:TYR:HB2	2.54	0.42
2:D:1105:LEU:O	2:D:1109:VAL:HG23	2.20	0.42
3:X:192:CYS:HB2	3:X:387:ASN:OD1	2.20	0.42
3:X:297:ALA:HA	3:X:302:LEU:HB2	2.02	0.42
1:A:107:GLN:HA	2:B:860:ARG:CZ	2.50	0.41
2:B:100:PHE:CE1	2:B:147:PHE:HA	2.45	0.41
2:B:367:TRP:O	2:B:373:THR:HG23	2.20	0.41
2:B:420:GLU:O	2:B:424:GLN:HG3	2.20	0.41
1:C:237:LEU:HD13	1:C:280:TRP:CD2	2.55	0.41
2:D:432:SER:O	2:D:433:ILE:HD13	2.20	0.41
2:D:521:SER:O	2:D:534:ASN:HB2	2.20	0.41
2:D:990:TYR:C	2:D:993:PRO:HD2	2.44	0.41
2:D:1062:ILE:HA	2:D:1065:HIS:ND1	2.35	0.41
2:B:106:PHE:HB3	2:B:107:PRO:HD2	2.02	0.41
2:B:990:TYR:O	2:B:993:PRO:HD2	2.20	0.41
2:B:1107:ALA:O	2:B:1110:ALA:HB3	2.20	0.41
2:B:1111:GLU:HA	2:B:1114:LEU:HD12	2.02	0.41
2:B:1112:TYR:O	2:B:1116:LEU:HG	2.20	0.41
1:C:143:ALA:HB3	1:C:192:PHE:HD2	1.85	0.41
2:D:581:ARG:HG3	2:D:693:GLU:OE2	2.19	0.41
2:D:706:GLN:HA	2:D:709:GLU:CD	2.46	0.41
3:X:20:ASN:O	3:X:22:THR:N	2.50	0.41
3:X:21:GLN:HB3	3:X:24:PHE:HB3	2.01	0.41
3:X:50:LEU:O	3:X:53:ARG:HB2	2.19	0.41
3:X:97:PHE:CE2	3:X:146:PHE:HE2	2.38	0.41
1:A:160:VAL:HG11	1:A:202:VAL:HG13	2.01	0.41
2:B:898:TYR:CD1	2:B:898:TYR:C	2.98	0.41
2:B:961:LEU:HD22	2:B:961:LEU:HA	1.85	0.41
2:B:1082:TRP:CZ2	3:X:305:LEU:HD22	2.50	0.41
2:B:1100:GLN:HB3	2:B:1104:THR:CG2	2.50	0.41
2:B:1112:TYR:CZ	2:B:1116:LEU:HD21	2.56	0.41
1:C:53:SER:O	1:C:384:ARG:HD3	2.19	0.41
2:D:1064:GLU:HA	2:D:1067:LEU:HG	2.01	0.41
3:X:260:THR:HG21	3:X:310:PRO:HB3	2.02	0.41
2:B:73:LEU:HD11	2:B:525:ASP:OD2	2.21	0.41
2:B:481:GLU:HB3	2:B:493:GLU:OE1	2.20	0.41
2:B:870:TYR:O	2:B:871:SER:OG	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1081:THR:O	2:B:1101:LYS:NZ	2.54	0.41
1:C:170:ARG:HD3	1:C:214:TRP:HZ3	1.85	0.41
2:D:656:LEU:HD13	2:D:657:ARG:HG2	2.02	0.41
2:D:794:VAL:O	2:D:797:SER:OG	2.37	0.41
2:D:1042:GLU:O	2:D:1045:SER:OG	2.21	0.41
3:X:362:ALA:HB3	3:X:364:VAL:HG23	2.03	0.41
2:B:196:ILE:HD13	2:B:205:TYR:HE2	1.84	0.41
2:B:329:LYS:NZ	2:B:329:LYS:HB3	2.35	0.41
2:B:847:LEU:O	2:B:850:LEU:HB2	2.20	0.41
2:B:1081:THR:C	2:B:1082:TRP:CD1	2.99	0.41
2:D:5:LYS:HE2	2:D:549:GLU:HG3	2.01	0.41
2:D:602:LEU:HD22	2:D:606:LEU:HD22	2.03	0.41
2:D:772:PHE:HD1	2:D:815:LEU:HD21	1.86	0.41
2:B:143:SER:O	2:B:146:TRP:HB3	2.20	0.41
2:B:951:PHE:CE2	2:B:953:ALA:HB2	2.56	0.41
2:D:385:ASP:HB3	2:D:387:SER:HB3	2.03	0.41
3:X:286:LYS:HD2	3:X:286:LYS:HA	1.72	0.41
1:A:191:GLN:O	1:A:201:ILE:HG22	2.21	0.41
1:A:236:THR:HG21	2:B:417:ASP:OD1	2.20	0.41
2:B:279:LEU:HD11	2:B:303:ASP:H	1.84	0.41
2:B:378:CYS:HB2	2:B:392:TRP:CZ3	2.55	0.41
2:B:405:THR:HB	2:B:589:PHE:CZ	2.55	0.41
2:B:423:LEU:HD11	2:B:471:LEU:HG	2.02	0.41
2:B:445:ASN:O	2:B:448:SER:OG	2.29	0.41
2:B:708:TYR:HA	2:B:711:GLN:CG	2.50	0.41
2:B:768:THR:OG1	2:B:769:ALA:N	2.53	0.41
2:B:1063:ILE:HG12	2:B:1112:TYR:CE1	2.56	0.41
1:C:64:ILE:HG12	1:C:119:GLU:HA	2.02	0.41
1:C:210:ARG:HH12	2:D:417:ASP:H	1.68	0.41
1:C:244:ASN:HB3	1:C:246:CYS:SG	2.61	0.41
2:D:549:GLU:OE1	2:D:686:LYS:NZ	2.30	0.41
3:X:379:THR:O	3:X:382:LEU:HB2	2.21	0.41
1:A:170:ARG:HD3	1:A:214:TRP:HZ3	1.85	0.41
2:B:132:THR:OG1	2:B:136:VAL:HG22	2.21	0.41
2:B:407:PHE:CG	2:B:422:TRP:CH2	3.09	0.41
2:D:4:LEU:HD23	2:D:4:LEU:HA	1.91	0.41
2:D:242:PHE:HD1	2:D:249:LEU:HD13	1.85	0.41
3:X:98:HIS:CG	3:X:99:PRO:HD2	2.55	0.41
3:X:216:VAL:O	3:X:230:PHE:HE2	2.03	0.41
2:B:1080:ASP:OD1	2:B:1082:TRP:NE1	2.49	0.41
2:D:115:VAL:O	2:D:116:ALA:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:471:LEU:HA	2:D:471:LEU:HD23	1.75	0.41
2:D:718:ASP:O	2:D:722:LEU:HG	2.21	0.41
2:D:815:LEU:HD23	2:D:815:LEU:HA	1.83	0.41
2:D:847:LEU:HD23	2:D:847:LEU:HA	1.89	0.41
1:A:384:ARG:HE	1:A:389:THR:HG21	1.86	0.41
2:B:83:LEU:HG	2:B:84:THR:N	2.36	0.41
2:B:314:LEU:HD21	2:B:325:VAL:HG13	2.01	0.41
2:B:846:ALA:HB1	2:B:862:PHE:CZ	2.56	0.41
2:B:926:LYS:HZ2	2:B:928:THR:HB	1.86	0.41
2:D:84:THR:HG22	2:D:103:LYS:HG3	2.02	0.41
2:D:408:ASP:O	2:D:410:PRO:HD3	2.21	0.41
2:D:628:ASP:HB3	2:D:631:TYR:HD2	1.86	0.41
3:X:245:GLN:H	3:X:245:GLN:HG3	1.62	0.41
1:A:51:PRO:O	1:A:53:SER:N	2.45	0.40
1:A:143:ALA:HB3	1:A:192:PHE:CD2	2.57	0.40
2:B:329:LYS:HB3	2:B:329:LYS:HZ2	1.86	0.40
2:B:875:GLN:OE1	2:B:879:LEU:HG	2.21	0.40
2:B:1112:TYR:CE2	2:B:1116:LEU:HD11	2.57	0.40
1:C:182:PRO:O	2:D:413:MET:HB2	2.22	0.40
2:D:243:LEU:HD23	2:D:243:LEU:HA	1.89	0.40
3:X:244:ALA:O	3:X:247:ALA:HB3	2.21	0.40
3:X:429:ALA:O	3:X:430:ASN:C	2.64	0.40
2:B:362:LEU:HD12	2:B:378:CYS:O	2.21	0.40
2:B:1112:TYR:CE1	2:B:1116:LEU:HD21	2.56	0.40
2:D:165:ILE:HG21	2:D:187:PHE:HZ	1.85	0.40
2:D:724:LEU:O	2:D:727:ASP:HB2	2.21	0.40
2:D:849:TYR:HB3	2:D:858:ALA:HB2	2.03	0.40
2:D:906:LEU:HD13	2:D:914:ASP:C	2.46	0.40
3:X:333:HIS:O	3:X:336:ILE:HB	2.20	0.40
3:X:416:HIS:HB2	3:X:428:GLY:HA2	2.02	0.40
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.97	0.40
2:B:193:THR:HA	2:B:206:GLU:HA	2.04	0.40
2:B:913:ILE:HG13	2:B:916:LEU:HD12	2.03	0.40
1:C:182:PRO:HB3	2:D:597:TYR:CE2	2.57	0.40
1:C:200:LEU:HD23	1:C:214:TRP:CD1	2.57	0.40
2:D:982:GLY:C	2:D:984:ILE:H	2.29	0.40
2:D:1066:TYR:HE1	2:D:1108:ILE:HB	1.86	0.40
2:D:1113:HIS:HA	2:D:1116:LEU:HG	2.02	0.40
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.94	0.40
1:A:261:ILE:HG13	1:A:326:MET:HE3	2.04	0.40
2:B:548:ILE:O	2:B:552:ASP:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:PHE:HA	2:B:834:TRP:CZ3	2.56	0.40
2:B:962:SER:HB3	2:B:971:LEU:HD11	2.03	0.40
2:B:995:LEU:HD23	2:B:995:LEU:HA	1.87	0.40
2:D:178:ILE:HG13	2:D:179:SER:N	2.36	0.40
2:D:362:LEU:HD11	2:D:377:LYS:HB2	2.03	0.40
2:D:463:ILE:HA	2:D:466:LEU:HG	2.04	0.40
3:X:7:LEU:O	3:X:10:PHE:HB3	2.22	0.40
3:X:26:GLN:O	3:X:30:GLU:HG3	2.20	0.40
3:X:257:ARG:O	3:X:257:ARG:HG3	2.20	0.40
1:A:56:LEU:HB2	1:A:371:HIS:NE2	2.37	0.40
1:A:212:PHE:CE1	1:A:233:TRP:CE3	3.08	0.40
2:B:673:LEU:HD13	2:B:770:LEU:HD13	2.04	0.40
2:B:767:ASN:HB3	2:B:770:LEU:HD21	2.03	0.40
2:B:1105:LEU:O	2:B:1108:ILE:HG12	2.22	0.40
2:D:959:MET:HE2	2:D:995:LEU:HG	2.03	0.40
3:X:102:ASN:OD1	3:X:105:ILE:N	2.30	0.40
3:X:289:ARG:HB3	3:X:290:ASP:H	1.51	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ASN:O	2:D:404:LYS:NZ[8_555]	2.07	0.13
3:X:156:ARG:NH1	3:X:186:LEU:O[12_544]	2.13	0.07
3:X:155:TYR:OH	3:X:186:LEU:O[12_544]	2.16	0.04
2:B:384:GLN:NE2	2:D:273:GLU:OE1[6_554]	2.17	0.03

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	335/394 (85%)	315 (94%)	19 (6%)	1 (0%)	36 72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	336/394 (85%)	319 (95%)	16 (5%)	1 (0%)	36	72
2	B	1006/1139 (88%)	869 (86%)	117 (12%)	20 (2%)	6	31
2	D	951/1139 (84%)	821 (86%)	108 (11%)	22 (2%)	5	28
3	X	440/450 (98%)	420 (96%)	17 (4%)	3 (1%)	18	56
All	All	3068/3516 (87%)	2744 (89%)	277 (9%)	47 (2%)	8	40

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	965	PRO
2	D	951	PHE
3	X	206	ILE
3	X	289	ARG
1	A	50	THR
2	B	115	VAL
2	B	410	PRO
2	B	856	VAL
2	B	1101	LYS
1	C	50	THR
2	D	27	PRO
2	D	115	VAL
2	D	626	ASN
2	D	952	ASP
3	X	291	GLY
2	B	59	ALA
2	B	234	PRO
2	B	287	LEU
2	B	403	GLU
2	B	495	LYS
2	B	626	ASN
2	D	59	ALA
2	D	287	LEU
2	D	410	PRO
2	D	461	LEU
2	D	495	LYS
2	D	698	LEU
2	D	950	LYS
2	D	983	LYS
2	B	110	VAL
2	B	135	ARG
2	B	815	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	954	ALA
2	B	1051	THR
2	D	234	PRO
2	D	769	ALA
2	D	1032	ASN
2	B	1032	ASN
2	D	110	VAL
2	D	135	ARG
2	D	1078	LYS
2	B	461	LEU
2	B	517	ASP
2	D	111	MET
2	D	984	ILE
2	B	330	GLY
2	D	330	GLY

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	299/345 (87%)	278 (93%)	21 (7%)	14	35
1	C	300/345 (87%)	279 (93%)	21 (7%)	14	35
2	B	940/1050 (90%)	852 (91%)	88 (9%)	8	25
2	D	897/1050 (85%)	824 (92%)	73 (8%)	11	31
3	X	347/354 (98%)	330 (95%)	17 (5%)	22	43
All	All	2783/3144 (88%)	2563 (92%)	220 (8%)	11	32

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	27	SER
1	A	31	LEU
1	A	46	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	50	THR
1	A	54	THR
1	A	68	LEU
1	A	74	SER
1	A	77	SER
1	A	83	GLU
1	A	127	LEU
1	A	131	SER
1	A	185	SER
1	A	216	LEU
1	A	245	THR
1	A	246	CYS
1	A	258	VAL
1	A	259	ARG
1	A	266	SER
1	A	304	LEU
1	A	367	GLN
2	B	11	ILE
2	B	54	CYS
2	B	58	ASP
2	B	88	VAL
2	B	90	LEU
2	B	97	LEU
2	B	128	ILE
2	B	182	GLU
2	B	197	LEU
2	B	232	ARG
2	B	235	ASN
2	B	241	ILE
2	B	249	LEU
2	B	274	LEU
2	B	281	LEU
2	B	290	ASP
2	B	291	HIS
2	B	292	THR
2	B	296	PHE
2	B	297	ILE
2	B	301	TYR
2	B	311	ILE
2	B	329	LYS
2	B	332	ILE
2	B	336	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	338	ASP
2	B	339	ASP
2	B	371	LEU
2	B	388	PHE
2	B	417	ASP
2	B	429	HIS
2	B	431	THR
2	B	450	VAL
2	B	474	ILE
2	B	483	ASN
2	B	512	LEU
2	B	515	PHE
2	B	518	GLU
2	B	519	ILE
2	B	524	PHE
2	B	532	TYR
2	B	533	ILE
2	B	537	ASN
2	B	539	VAL
2	B	579	LEU
2	B	642	LEU
2	B	656	LEU
2	B	667	GLN
2	B	671	LEU
2	B	672	PHE
2	B	673	LEU
2	B	680	VAL
2	B	685	LEU
2	B	692	ILE
2	B	702	ILE
2	B	703	THR
2	B	717	CYS
2	B	725	LEU
2	B	805	ASP
2	B	812	VAL
2	B	813	THR
2	B	820	PHE
2	B	831	LEU
2	B	832	ILE
2	B	835	LEU
2	B	866	SER
2	B	878	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	902	LEU
2	B	907	PHE
2	B	919	SER
2	B	923	ASP
2	B	941	THR
2	B	961	LEU
2	B	964	THR
2	B	966	LEU
2	B	969	SER
2	B	971	LEU
2	B	973	ASP
2	B	999	VAL
2	B	1010	MET
2	B	1011	ILE
2	B	1031	GLN
2	B	1049	SER
2	B	1076	LEU
2	B	1084	LEU
2	B	1101	LYS
2	B	1104	THR
2	B	1123	VAL
1	C	25	SER
1	C	27	SER
1	C	31	LEU
1	C	46	SER
1	C	50	THR
1	C	54	THR
1	C	68	LEU
1	C	74	SER
1	C	77	SER
1	C	83	GLU
1	C	127	LEU
1	C	131	SER
1	C	185	SER
1	C	216	LEU
1	C	245	THR
1	C	246	CYS
1	C	258	VAL
1	C	259	ARG
1	C	266	SER
1	C	304	LEU
1	C	367	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	11	ILE
2	D	54	CYS
2	D	58	ASP
2	D	88	VAL
2	D	90	LEU
2	D	97	LEU
2	D	128	ILE
2	D	197	LEU
2	D	235	ASN
2	D	241	ILE
2	D	274	LEU
2	D	290	ASP
2	D	291	HIS
2	D	292	THR
2	D	296	PHE
2	D	297	ILE
2	D	301	TYR
2	D	311	ILE
2	D	329	LYS
2	D	332	ILE
2	D	336	LEU
2	D	338	ASP
2	D	339	ASP
2	D	388	PHE
2	D	417	ASP
2	D	429	HIS
2	D	431	THR
2	D	450	VAL
2	D	474	ILE
2	D	483	ASN
2	D	512	LEU
2	D	515	PHE
2	D	519	ILE
2	D	524	PHE
2	D	532	TYR
2	D	533	ILE
2	D	537	ASN
2	D	539	VAL
2	D	579	LEU
2	D	587	MET
2	D	589	PHE
2	D	604	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	642	LEU
2	D	646	MET
2	D	656	LEU
2	D	667	GLN
2	D	671	LEU
2	D	672	PHE
2	D	673	LEU
2	D	679	ARG
2	D	680	VAL
2	D	692	ILE
2	D	700	SER
2	D	702	ILE
2	D	703	THR
2	D	725	LEU
2	D	741	LEU
2	D	743	GLU
2	D	766	VAL
2	D	795	ILE
2	D	807	THR
2	D	812	VAL
2	D	820	PHE
2	D	826	ASN
2	D	835	LEU
2	D	902	LEU
2	D	907	PHE
2	D	913	ILE
2	D	916	LEU
2	D	937	ILE
2	D	981	GLN
2	D	1031	GLN
2	D	1101	LYS
3	X	7	LEU
3	X	71	ARG
3	X	108	PHE
3	X	240	SER
3	X	257	ARG
3	X	285	ILE
3	X	289	ARG
3	X	290	ASP
3	X	305	LEU
3	X	315	VAL
3	X	323	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	329	VAL
3	X	358	LEU
3	X	401	ARG
3	X	407	LEU
3	X	421	GLU
3	X	447	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	GLN
1	A	24	GLN
1	A	150	ASN
1	A	350	ASN
2	B	65	ASN
2	B	101	ASN
2	B	198	ASN
2	B	204	HIS
2	B	394	HIS
2	B	791	HIS
2	B	955	HIS
2	B	989	ASN
2	B	1100	GLN
1	C	6	ASN
1	C	24	GLN
1	C	150	ASN
1	C	231	ASN
1	C	335	GLN
1	C	350	ASN
2	D	80	ASN
2	D	101	ASN
2	D	198	ASN
2	D	204	HIS
2	D	394	HIS
2	D	758	ASN
2	D	986	GLN
2	D	1030	HIS
3	X	42	ASN
3	X	73	GLN
3	X	113	GLN
3	X	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	416	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	343/394 (87%)	0.61	34 (9%)	13 20	358, 705, 903, 929	0
1	C	344/394 (87%)	0.77	50 (14%)	6 14	422, 848, 1029, 1070	0
2	B	1022/1139 (89%)	0.33	53 (5%)	33 35	273, 650, 901, 955	0
2	D	977/1139 (85%)	0.59	100 (10%)	12 20	298, 714, 927, 984	0
3	X	442/450 (98%)	0.08	14 (3%)	50 45	219, 451, 760, 881	0
All	All	3128/3516 (88%)	0.46	251 (8%)	18 25	219, 672, 935, 1070	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	646	MET	11.7
2	D	717	CYS	9.5
2	D	716	GLY	8.7
2	D	645	PRO	7.9
2	D	327	ILE	7.2
2	D	715	ALA	6.7
1	C	32	LEU	6.6
2	D	649	ILE	5.7
1	C	33	ALA	5.5
2	D	653	ILE	5.2
1	C	114	ILE	4.8
1	A	367	GLN	4.7
1	C	20	THR	4.6
2	B	335	SER	4.6
2	B	705	GLN	4.6
2	D	1042	GLU	4.5
2	D	244	SER	4.5
1	A	368	ASP	4.5
1	C	102	LEU	4.4
1	C	21	TRP	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	324	ASN	4.3
2	D	185	VAL	4.3
2	D	486	LEU	4.3
1	A	23	SER	4.3
1	A	299	GLY	4.2
2	D	718	ASP	4.2
2	D	644	ASN	4.2
1	A	328	TYR	4.2
2	D	316	ALA	4.2
2	D	964	THR	4.2
2	B	629	PRO	4.1
2	D	648	ASP	4.1
1	C	96	PRO	4.1
2	D	650	ASP	4.1
1	A	365	TRP	4.1
2	B	889	TYR	4.1
2	D	721	PHE	4.1
1	A	24	GLN	4.0
2	B	933	LEU	4.0
1	A	302	ASN	3.9
2	D	239	SER	3.9
1	C	19	THR	3.8
2	D	288	THR	3.8
1	A	322	HIS	3.8
2	B	704	SER	3.8
1	C	24	GLN	3.8
2	D	691	SER	3.7
1	A	324	ARG	3.7
1	C	118	ASN	3.7
1	C	206	ASN	3.7
2	D	643	GLU	3.7
2	B	633	SER	3.7
2	D	537	ASN	3.7
2	B	700	SER	3.6
1	C	79	CYS	3.6
1	A	30	ASN	3.6
3	X	348	ASN	3.6
1	A	325	TYR	3.5
1	C	113	LEU	3.5
3	X	75	GLN	3.5
2	B	930	ASP	3.5
1	C	240	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	720	LEU	3.4
1	A	369	GLY	3.4
2	D	1038	ALA	3.4
2	B	1024	PHE	3.4
2	D	1019	TRP	3.4
2	D	799	SER	3.4
2	D	690	VAL	3.3
2	D	1041	TYR	3.3
1	A	366	HIS	3.3
2	D	687	LYS	3.3
1	C	364	CYS	3.3
2	D	107	PRO	3.3
2	D	759	THR	3.3
2	D	708	TYR	3.3
2	D	150	PRO	3.2
2	D	963	THR	3.2
2	D	931	GLU	3.2
2	D	712	SER	3.2
2	D	1073	LEU	3.2
2	D	289	SER	3.2
2	B	424	GLN	3.2
1	A	388	PHE	3.2
2	D	709	GLU	3.1
2	D	714	PHE	3.1
2	D	700	SER	3.1
1	A	357	GLY	3.1
1	C	22	CYS	3.1
2	B	928	THR	3.1
2	D	494	TYR	3.1
2	D	722	LEU	3.1
2	B	691	SER	3.0
1	C	44	CYS	3.0
2	B	1107	ALA	3.0
1	C	76	SER	3.0
2	D	325	VAL	3.0
2	B	271	THR	3.0
2	D	724	LEU	3.0
1	A	232	PRO	3.0
2	D	647	ARG	3.0
2	B	1124	THR	3.0
2	D	175	MET	2.9
3	X	296	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	61	LEU	2.9
2	B	639	LEU	2.9
2	D	1044	LEU	2.9
1	C	365	TRP	2.9
1	C	235	LEU	2.9
2	B	931	GLU	2.9
2	B	701	LEU	2.9
2	D	57	TYR	2.8
2	D	151	ASP	2.8
1	C	98	TYR	2.8
2	B	425	HIS	2.8
2	D	508	LEU	2.8
2	D	1040	ILE	2.8
2	D	314	LEU	2.8
2	B	929	ASP	2.8
2	D	1026	TRP	2.8
1	C	43	TYR	2.8
1	A	234	LEU	2.8
1	C	45	ALA	2.7
1	C	322	HIS	2.7
1	C	100	LEU	2.7
3	X	200	SER	2.7
2	B	488	GLY	2.7
1	C	257	ASN	2.7
1	A	29	SER	2.7
1	C	349	SER	2.7
1	C	75	PHE	2.7
2	B	487	THR	2.6
2	B	936	ALA	2.6
2	D	698	LEU	2.6
2	B	632	ILE	2.6
2	B	1085	VAL	2.6
2	D	487	THR	2.6
2	D	525	ASP	2.6
2	D	727	ASP	2.6
2	B	491	TYR	2.6
3	X	346	GLY	2.6
2	D	596	ARG	2.6
1	C	194	PRO	2.6
1	A	387	GLY	2.5
2	B	1106	ASP	2.5
1	C	234	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1045	SER	2.5
2	D	29	LEU	2.5
2	D	387	SER	2.5
2	D	442	SER	2.5
1	C	346	GLU	2.5
1	A	317	LEU	2.5
1	C	211	ILE	2.5
3	X	21	GLN	2.5
2	D	390	CYS	2.5
1	C	23	SER	2.5
2	B	489	TYR	2.5
1	A	306	ASN	2.5
2	D	391	VAL	2.4
2	D	251	MET	2.4
1	A	281	ASN	2.4
2	B	375	ILE	2.4
2	D	117	PHE	2.4
2	D	92	SER	2.4
2	B	1021	ASN	2.4
3	X	404	HIS	2.4
1	A	180	GLY	2.4
1	A	364	CYS	2.4
1	C	101	PHE	2.4
2	D	335	SER	2.4
2	B	647	ARG	2.4
3	X	103	LEU	2.4
2	B	830	GLN	2.3
1	A	126	VAL	2.3
2	D	27	PRO	2.3
3	X	9	SER	2.3
1	A	98	TYR	2.3
1	C	373	ALA	2.3
2	B	428	ALA	2.3
1	C	34	ILE	2.3
2	B	636	ILE	2.3
2	D	434	GLU	2.3
2	D	303	ASP	2.3
2	D	711	GLN	2.3
2	D	330	GLY	2.3
1	A	139	ASP	2.3
2	D	485	ASP	2.3
3	X	73	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	328	TYR	2.2
2	D	1072	THR	2.2
1	A	263	SER	2.2
3	X	330	ASP	2.2
2	B	1	MET	2.2
1	A	141	ASP	2.2
1	C	237	LEU	2.2
2	D	1037	ALA	2.2
1	C	189	SER	2.2
2	D	108	SER	2.2
2	B	394	HIS	2.2
2	B	396	LEU	2.2
2	D	769	ALA	2.2
2	D	970	CYS	2.2
1	C	108	ASP	2.2
1	C	325	TYR	2.2
2	B	485	ASP	2.2
2	D	163	ARG	2.2
3	X	123	PRO	2.2
2	D	514	HIS	2.2
1	C	28	CYS	2.2
2	D	54	CYS	2.2
2	D	184	CYS	2.2
1	A	235	LEU	2.1
1	C	31	LEU	2.1
1	C	350	ASN	2.1
2	B	869	LEU	2.1
1	C	155	GLN	2.1
2	B	663	ASN	2.1
2	B	1100	GLN	2.1
2	D	343	PRO	2.1
2	D	290	ASP	2.1
1	C	30	ASN	2.1
2	B	372	ASN	2.1
3	X	387	ASN	2.1
2	B	288	THR	2.1
2	D	683	SER	2.1
2	D	713	LYS	2.1
2	D	1009	GLN	2.1
2	D	802	PHE	2.1
2	B	145	THR	2.1
2	D	936	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	240	MET	2.1
2	B	727	ASP	2.1
1	A	158	ALA	2.1
1	A	211	ILE	2.1
1	C	25	SER	2.1
1	C	74	SER	2.1
2	B	934	SER	2.1
2	D	389	SER	2.1
3	X	194	PHE	2.0
2	D	392	TRP	2.0
2	D	472	SER	2.0
2	B	486	LEU	2.0
2	D	798	LEU	2.0
2	B	7	ALA	2.0
2	B	126	THR	2.0
2	B	893	ASN	2.0
2	D	731	VAL	2.0
2	B	690	VAL	2.0
2	B	856	VAL	2.0
1	C	259	ARG	2.0
1	A	363	PHE	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.