



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:53 am BST

PDB ID : 2P1I
Title : Plasmodium yoelii Ribonucleotide Reductase Subunit R2 (PY03671)
Authors : Wernimont, A.K.; Dong, A.; Choe, J.; Gao, M.; Walker, J.; Lew, J.; Alam, Z.; Zhao, Y.; Nordlund, P.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Sundstrom, M.; Bochkarev, A.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on : 2007-03-05
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

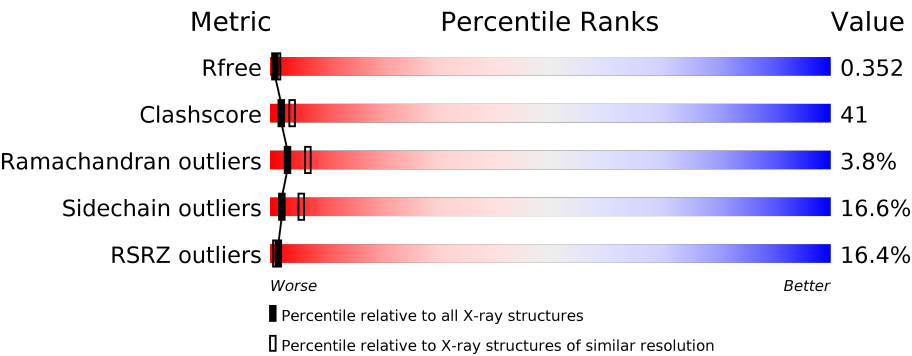
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	349	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>30%</div><div>35%</div><div>8%</div><div>•</div><div>26%</div></div>
1	B	349	<div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>28%</div><div>32%</div><div>10%</div><div>•</div><div>28%</div></div>
1	C	349	<div><div>16%</div><div><div></div><div></div><div></div><div></div></div><div>24%</div><div>38%</div><div>10%</div><div>•</div><div>27%</div></div>
1	D	349	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>31%</div><div>34%</div><div>8%</div><div>•</div><div>26%</div></div>
1	E	349	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>27%</div><div>37%</div><div>8%</div><div>•</div><div>26%</div></div>
1	F	349	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>33%</div><div>33%</div><div>7%</div><div>•</div><div>26%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	349	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>15%27%34%9%28%</div></div>
1	H	349	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%28%34%10%26%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16904 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 Ribonucleotide reductase, small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2104	1364	343	387	10			
1	B	252	Total	C	N	O	S	0	0	0
			2056	1332	335	379	10			
1	C	256	Total	C	N	O	S	0	0	0
			2099	1361	343	385	10			
1	D	258	Total	C	N	O	S	0	0	0
			2116	1372	345	389	10			
1	E	258	Total	C	N	O	S	0	0	0
			2109	1367	344	388	10			
1	F	258	Total	C	N	O	S	0	0	0
			2116	1372	345	389	10			
1	G	252	Total	C	N	O	S	0	0	0
			2059	1340	333	376	10			
1	H	258	Total	C	N	O	S	0	0	0
			2116	1372	345	389	10			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	H	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0
2	F	1	Total 1	Fe 1	0	0

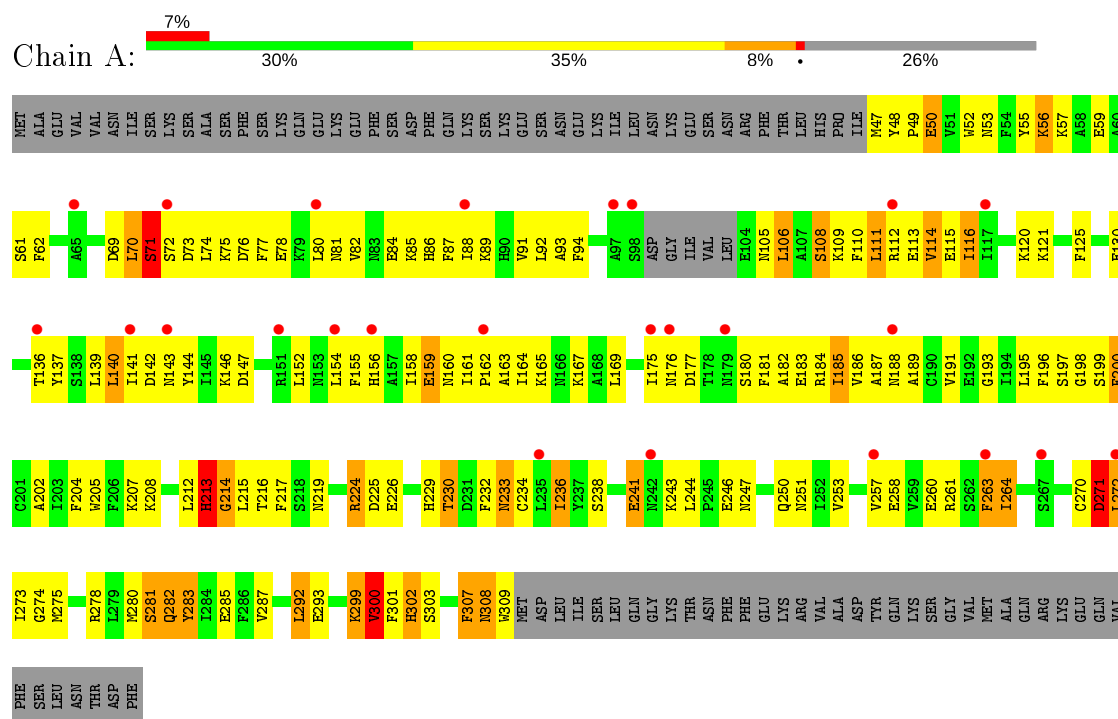
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	11	Total 11	O 11	0	0
3	C	13	Total 13	O 13	0	0
3	D	18	Total 18	O 18	0	0
3	E	15	Total 15	O 15	0	0
3	F	15	Total 15	O 15	0	0
3	G	19	Total 19	O 19	0	0
3	H	11	Total 11	O 11	0	0

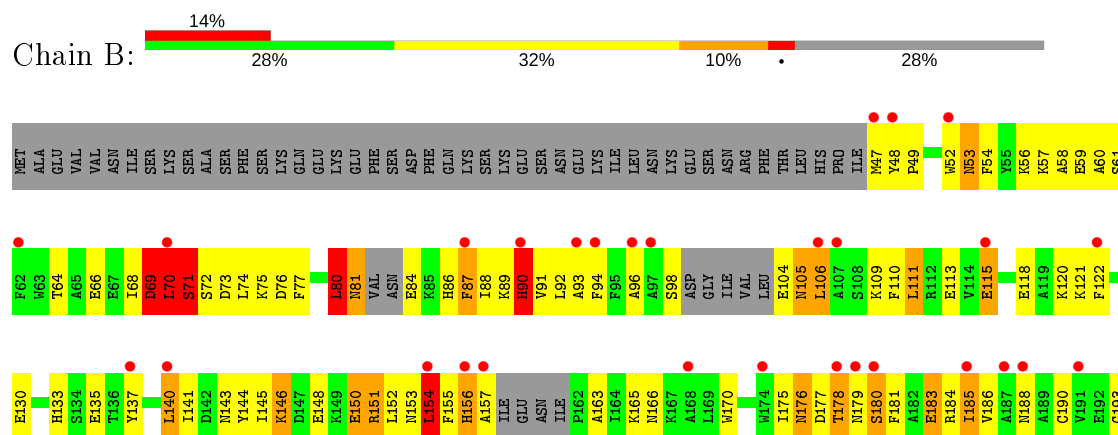
3 Residue-property plots

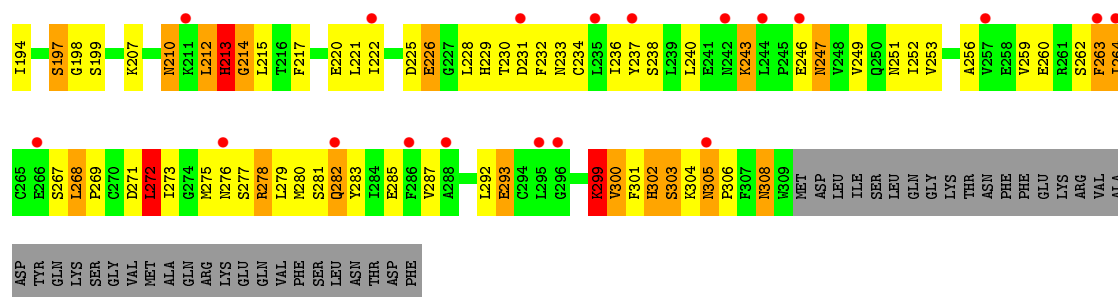
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

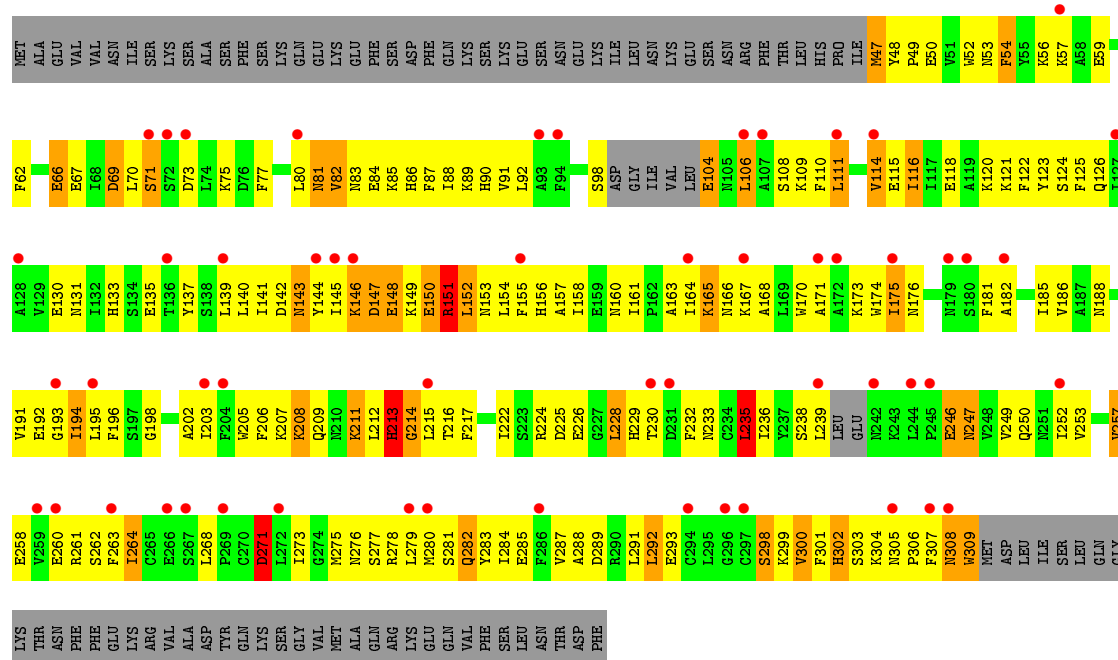
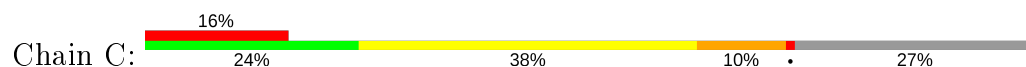


• Molecule 1: Ribonucleotide reductase, small chain

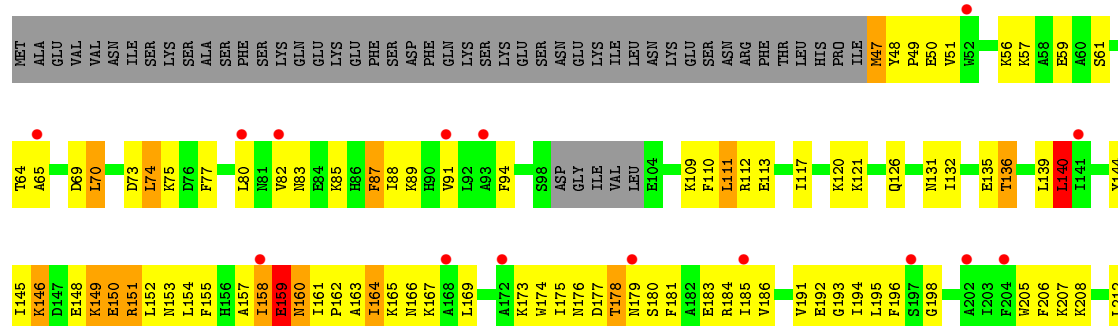


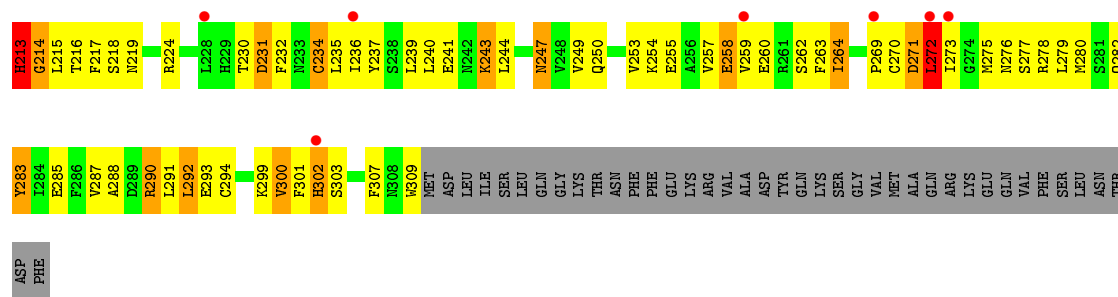


- Molecule 1: Ribonucleotide reductase, small chain

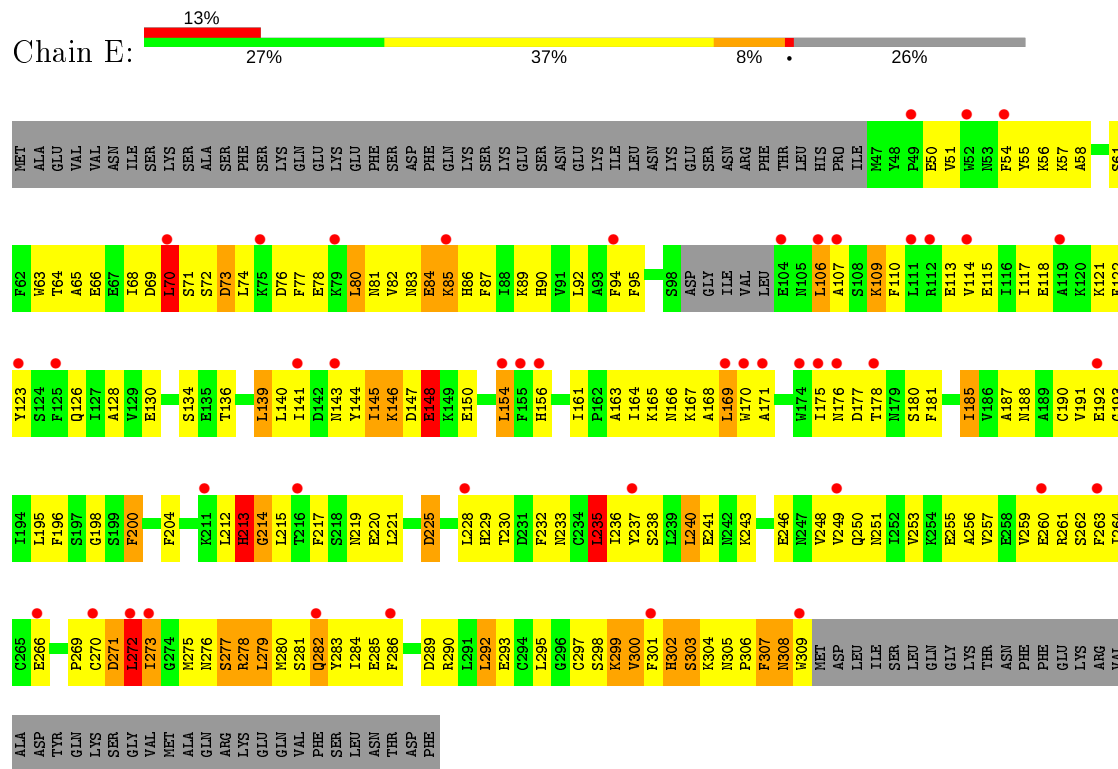


- Molecule 1: Ribonucleotide reductase, small chain

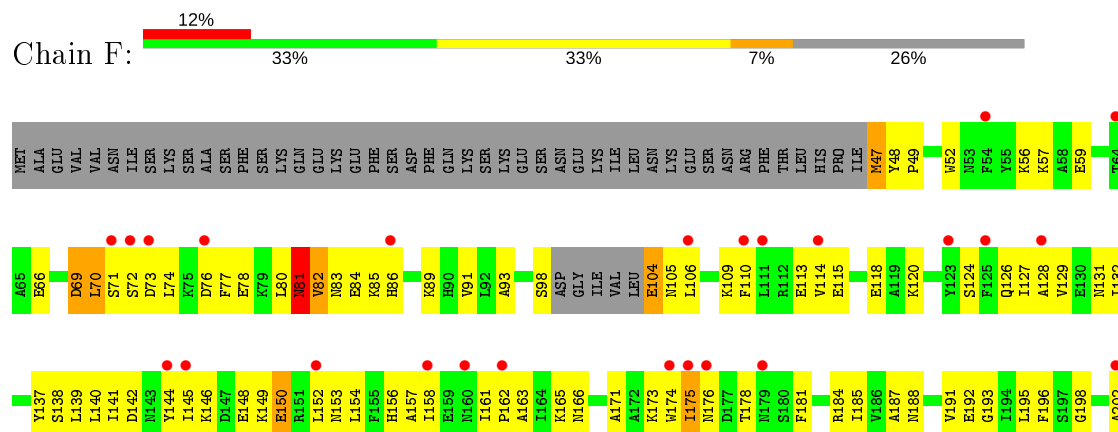


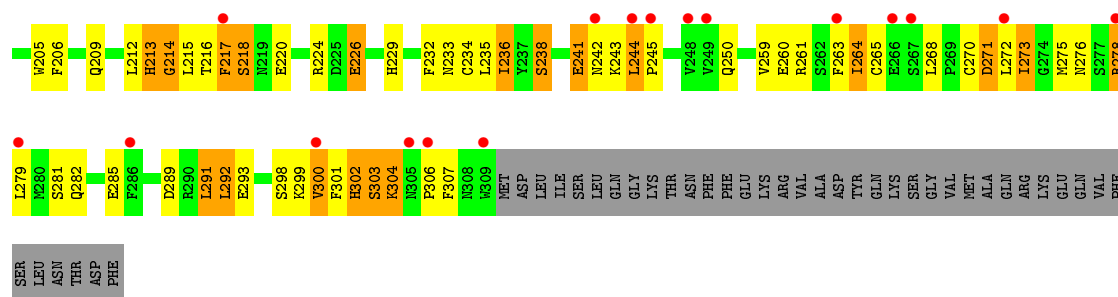


- Molecule 1: Ribonucleotide reductase, small chain

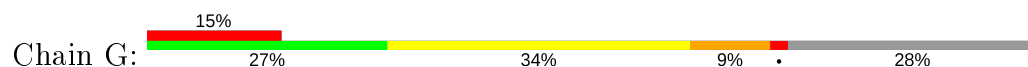


- Molecule 1: Ribonucleotide reductase, small chain

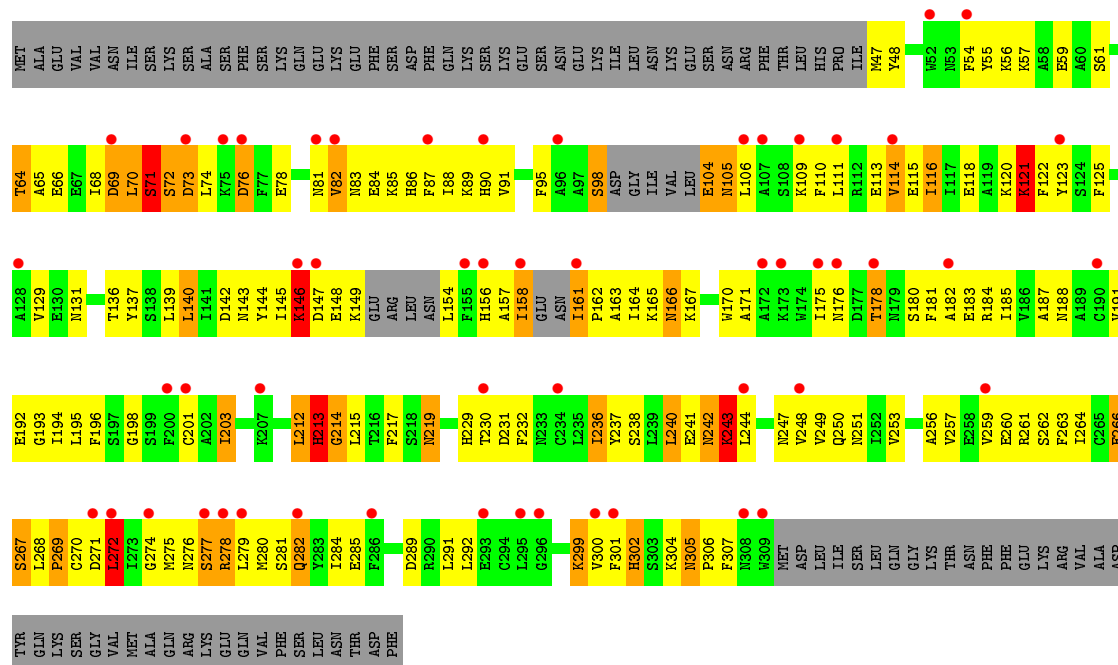




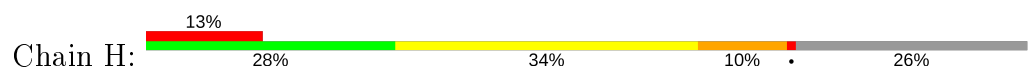
- Molecule 1: Ribonucleotide reductase, small chain



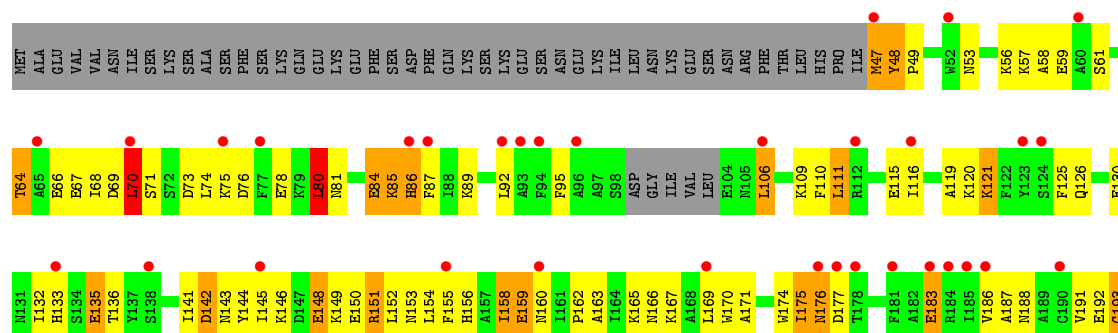
Chain G:



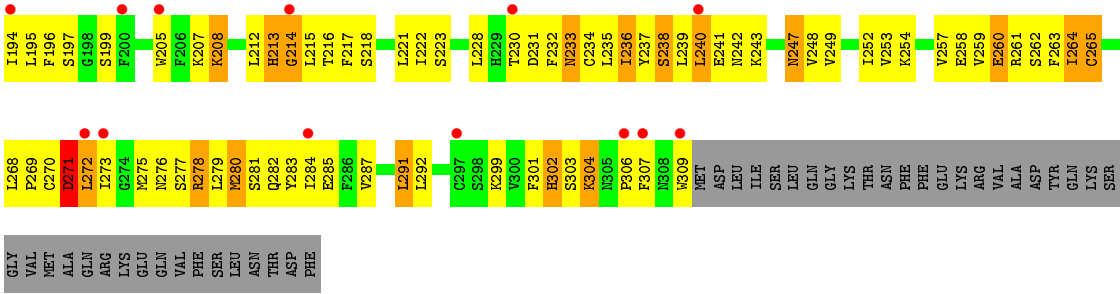
- Molecule 1: Ribonucleotide reductase, small chain



Chain H:



Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.04Å 153.46Å 143.36Å 90.00° 132.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.70) 87.6 (19.99-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.304 , 0.368 0.297 , 0.352	Depositor DCC
R_{free} test set	3552 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.180 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16904	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9897e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.22	10/2154 (0.5%)	1.06	5/2911 (0.2%)
1	B	1.03	3/2104 (0.1%)	0.98	6/2837 (0.2%)
1	C	0.99	3/2148 (0.1%)	0.95	6/2898 (0.2%)
1	D	1.26	11/2166 (0.5%)	1.11	10/2924 (0.3%)
1	E	1.02	4/2159 (0.2%)	1.04	10/2913 (0.3%)
1	F	1.03	8/2166 (0.4%)	0.97	3/2924 (0.1%)
1	G	1.08	9/2107 (0.4%)	0.95	1/2841 (0.0%)
1	H	0.83	1/2166 (0.0%)	0.88	5/2924 (0.2%)
All	All	1.06	49/17170 (0.3%)	1.00	46/23172 (0.2%)

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	3
1	B	0	4
1	C	0	3
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	4
1	H	0	1
All	All	0	22

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	241	GLU	CD-OE2	12.58	1.39	1.25
1	G	243	LYS	CE-NZ	7.88	1.68	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	LYS	CE-NZ	7.86	1.68	1.49
1	G	76	ASP	CG-OD2	7.60	1.42	1.25
1	G	241	GLU	CD-OE1	7.58	1.33	1.25
1	G	121	LYS	CE-NZ	7.46	1.67	1.49
1	G	266	GLU	CG-CD	7.35	1.62	1.51
1	F	146	LYS	CE-NZ	7.28	1.67	1.49
1	F	241	GLU	CB-CG	7.26	1.66	1.52
1	A	241	GLU	CB-CG	7.25	1.66	1.52
1	B	299	LYS	CE-NZ	7.15	1.67	1.49
1	A	243	LYS	CE-NZ	6.80	1.66	1.49
1	A	91	VAL	CB-CG2	-6.58	1.39	1.52
1	D	205	TRP	CE2-CZ2	6.46	1.50	1.39
1	B	226	GLU	CB-CG	6.42	1.64	1.52
1	D	294	CYS	CB-SG	-6.26	1.71	1.82
1	E	84	GLU	CB-CG	6.19	1.64	1.52
1	D	148	GLU	CD-OE2	6.17	1.32	1.25
1	C	298	SER	CB-OG	6.16	1.50	1.42
1	F	173	LYS	CD-CE	6.08	1.66	1.51
1	H	265	CYS	CB-SG	-6.05	1.72	1.82
1	E	241	GLU	CD-OE1	5.92	1.32	1.25
1	A	283	TYR	CG-CD2	5.89	1.46	1.39
1	G	76	ASP	CG-OD1	5.87	1.38	1.25
1	A	50	GLU	CG-CD	5.78	1.60	1.51
1	D	241	GLU	CB-CG	5.70	1.62	1.52
1	D	288	ALA	CA-CB	-5.70	1.40	1.52
1	D	205	TRP	CD1-NE1	5.65	1.47	1.38
1	A	241	GLU	CG-CD	5.58	1.60	1.51
1	G	146	LYS	CE-NZ	5.57	1.62	1.49
1	D	205	TRP	CE3-CZ3	5.51	1.47	1.38
1	D	234	CYS	CB-SG	5.50	1.91	1.82
1	D	283	TYR	CD2-CE2	5.49	1.47	1.39
1	A	236	ILE	CA-CB	5.45	1.67	1.54
1	A	234	CYS	CB-SG	-5.40	1.73	1.81
1	E	128	ALA	CA-CB	-5.36	1.41	1.52
1	C	246	GLU	CB-CG	5.35	1.62	1.52
1	G	242	ASN	CG-ND2	5.32	1.46	1.32
1	F	241	GLU	CG-CD	5.29	1.59	1.51
1	F	234	CYS	CB-SG	5.21	1.91	1.82
1	D	283	TYR	CE2-CZ	5.10	1.45	1.38
1	F	241	GLU	CD-OE2	5.08	1.31	1.25
1	E	200	PHE	CE1-CZ	5.06	1.47	1.37
1	F	174	TRP	CB-CG	5.06	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	87	PHE	CE1-CZ	5.05	1.47	1.37
1	A	283	TYR	CE2-CZ	5.04	1.45	1.38
1	C	305	ASN	CB-CG	5.04	1.62	1.51
1	A	200	PHE	CB-CG	-5.03	1.42	1.51
1	F	298	SER	CB-OG	5.02	1.48	1.42

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	226	GLU	OE1-CD-OE2	10.35	135.72	123.30
1	E	139	LEU	CA-CB-CG	-8.86	94.93	115.30
1	B	140	LEU	CA-CB-CG	8.06	133.84	115.30
1	E	272	LEU	CB-CG-CD1	7.17	123.20	111.00
1	A	224	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	F	106	LEU	CA-CB-CG	7.00	131.39	115.30
1	E	225	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	151	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	H	106	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	82	VAL	CB-CA-C	-6.45	99.14	111.40
1	E	272	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	213	HIS	C-N-CA	-6.32	109.03	122.30
1	A	243	LYS	CD-CE-NZ	-6.29	97.22	111.70
1	B	140	LEU	CB-CG-CD1	6.24	121.61	111.00
1	C	106	LEU	CA-CB-CG	6.24	129.65	115.30
1	C	235	LEU	CA-CB-CG	6.17	129.50	115.30
1	D	290	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	E	106	LEU	CA-CB-CG	6.00	129.10	115.30
1	E	290	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	239	LEU	CA-CB-CG	5.80	128.65	115.30
1	D	140	LEU	CA-CB-CG	5.80	128.63	115.30
1	E	73	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	231	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	74	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	225	ASP	CB-CG-OD1	5.70	123.43	118.30
1	E	235	LEU	CA-CB-CG	5.48	127.91	115.30
1	D	292	LEU	CA-CB-CG	5.48	127.90	115.30
1	G	269	PRO	CB-CA-C	-5.41	98.49	112.00
1	E	225	ASP	CB-CG-OD1	5.38	123.15	118.30
1	B	70	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	281	SER	CA-CB-OG	-5.31	96.85	111.20
1	D	151	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	E	169	LEU	CA-CB-CG	5.26	127.41	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	142	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	90	HIS	N-CA-CB	5.26	120.07	110.60
1	A	236	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	B	154	LEU	CA-CB-CG	5.19	127.25	115.30
1	D	185	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	F	291	LEU	CA-CB-CG	5.16	127.17	115.30
1	H	111	LEU	CA-CB-CG	5.12	127.07	115.30
1	H	80	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	C	57	LYS	CD-CE-NZ	5.07	123.36	111.70
1	H	240	LEU	CA-CB-CG	5.06	126.94	115.30
1	C	111	LEU	CA-CB-CG	5.05	126.93	115.30
1	D	294	CYS	CA-CB-SG	-5.05	104.91	114.00
1	C	271	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	LEU	Peptide
1	A	214	GLY	Peptide
1	A	71	SER	Peptide
1	B	212	LEU	Peptide
1	B	214	GLY	Peptide
1	B	272	LEU	Peptide
1	B	71	SER	Peptide
1	C	212	LEU	Peptide
1	C	214	GLY	Peptide
1	C	71	SER	Peptide
1	D	212	LEU	Peptide
1	D	214	GLY	Peptide
1	D	272	LEU	Peptide
1	E	212	LEU	Peptide
1	E	214	GLY	Peptide
1	F	214	GLY	Peptide
1	F	81	ASN	Peptide
1	G	212	LEU	Peptide
1	G	214	GLY	Peptide
1	G	272	LEU	Peptide
1	G	71	SER	Peptide
1	H	214	GLY	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	2104	0	2048	160	0
1	B	2056	0	1992	194	7
1	C	2099	0	2056	185	0
1	D	2116	0	2074	150	0
1	E	2109	0	2061	193	2
1	F	2116	0	2074	151	0
1	G	2059	0	2019	170	3
1	H	2116	0	2074	172	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	19	0	0	5	0
3	B	11	0	0	5	0
3	C	13	0	0	6	0
3	D	18	0	0	5	0
3	E	15	0	0	5	0
3	F	15	0	0	4	0
3	G	19	0	0	5	0
3	H	11	0	0	7	0
All	All	16904	0	16398	1363	10

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 41.

All (1363) 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:G:243:LYS:CE	1:G:243:LYS:NZ	1.68	1.55
1:B:146:LYS:NZ	1:B:146:LYS:CE	1.68	1.54
1:G:121:LYS:CE	1:G:121:LYS:NZ	1.67	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ALA:HB1	1:B:263:PHE:CD2	1.65	1.30
1:E:279:LEU:HD13	1:E:307:PHE:CE1	1.66	1.28
1:C:299:LYS:NZ	1:C:302:HIS:HD2	1.35	1.25
1:G:278:ARG:HD3	1:G:278:ARG:N	1.57	1.18
1:H:233:ASN:HA	1:H:236:ILE:CD1	1.73	1.18
1:C:299:LYS:HZ2	1:C:302:HIS:CD2	1.62	1.16
1:H:257:VAL:O	1:H:261:ARG:HG3	1.48	1.14
1:H:264:ILE:HD12	1:H:264:ILE:H	1.12	1.11
1:H:257:VAL:HG12	1:H:261:ARG:HE	1.10	1.10
1:B:282:GLN:HE22	1:B:306:PRO:HD3	1.10	1.10
1:B:163:ALA:CB	1:B:263:PHE:HD2	1.65	1.09
1:E:279:LEU:CD1	1:E:307:PHE:HE1	1.67	1.07
1:H:115:GLU:HA	1:H:120:LYS:NZ	1.69	1.07
1:E:292:LEU:CD1	1:E:297:CYS:CB	2.32	1.07
1:C:82:VAL:HG22	3:C:360:HOH:O	1.55	1.06
1:B:93:ALA:CB	1:B:154:LEU:CD1	2.33	1.05
1:D:180:SER:HB3	1:D:183:GLU:HG3	1.35	1.05
1:D:70:LEU:HD11	1:D:140:LEU:HD12	1.37	1.05
1:E:86:HIS:CE1	1:E:89:LYS:HD2	1.90	1.05
1:B:73:ASP:HB2	1:B:213:HIS:CG	1.91	1.05
3:A:366:HOH:O	1:E:147:ASP:HB2	1.55	1.04
1:E:292:LEU:CD1	1:E:297:CYS:HB2	1.87	1.04
1:B:93:ALA:CB	1:B:154:LEU:HD11	1.86	1.04
1:B:163:ALA:HB1	1:B:263:PHE:HD2	0.89	1.04
1:B:276:ASN:HD22	1:B:279:LEU:HG	1.16	1.04
1:G:163:ALA:HB1	1:G:263:PHE:CD2	1.90	1.03
1:A:86:HIS:CE1	1:A:89:LYS:HD2	1.92	1.03
1:D:73:ASP:HB2	1:D:213:HIS:ND1	1.72	1.03
1:F:81:ASN:CB	1:F:84:GLU:H	1.72	1.03
1:F:233:ASN:HA	1:F:236:ILE:CD1	1.86	1.03
1:H:280:MET:HA	3:H:357:HOH:O	1.58	1.03
1:D:163:ALA:HB1	1:D:263:PHE:CD2	1.95	1.02
1:C:150:GLU:OE2	1:C:150:GLU:HA	1.54	1.02
1:D:175:ILE:HG22	1:D:176:ASN:H	1.25	1.02
1:H:233:ASN:HA	1:H:236:ILE:HD12	1.02	1.02
1:A:282:GLN:NE2	1:A:303:SER:HB2	1.75	1.01
1:H:86:HIS:HA	1:H:89:LYS:HD3	1.41	0.99
1:H:233:ASN:CA	1:H:236:ILE:HD12	1.93	0.99
1:A:115:GLU:HA	1:A:120:LYS:NZ	1.78	0.99
1:B:301:PHE:HD1	1:B:303:SER:HG	1.01	0.99
1:E:148:GLU:HG3	1:E:148:GLU:O	1.20	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:ASN:HB2	1:G:259:VAL:HG22	1.43	0.99
1:G:81:ASN:HB3	1:G:84:GLU:HB2	1.44	0.98
1:E:282:GLN:HE22	1:E:306:PRO:HD3	1.29	0.97
1:H:115:GLU:HA	1:H:120:LYS:HZ1	1.24	0.97
1:G:87:PHE:CE2	1:G:91:VAL:HG21	1.99	0.97
1:C:299:LYS:NZ	1:C:302:HIS:CD2	2.23	0.97
1:E:307:PHE:HB3	1:E:309:TRP:NE1	1.80	0.97
1:C:98:SER:HB2	1:C:167:LYS:NZ	1.81	0.96
1:C:104:GLU:HB3	3:C:352:HOH:O	1.61	0.96
1:G:242:ASN:HA	3:G:367:HOH:O	1.63	0.96
1:E:70:LEU:HD22	1:E:70:LEU:H	1.31	0.96
1:G:47:MET:HB2	1:G:118:GLU:OE1	1.64	0.96
1:E:285:GLU:HB3	1:E:301:PHE:CD1	2.01	0.96
1:H:264:ILE:HD12	1:H:264:ILE:N	1.80	0.95
1:H:301:PHE:CD1	1:H:301:PHE:O	2.20	0.95
1:C:214:GLY:HA2	1:C:217:PHE:HB3	1.49	0.94
1:H:167:LYS:HD2	1:H:263:PHE:CZ	2.02	0.94
1:E:148:GLU:CG	1:E:148:GLU:O	2.12	0.94
1:F:81:ASN:HB3	1:F:84:GLU:H	1.30	0.94
1:F:175:ILE:H	1:F:175:ILE:HD12	1.32	0.94
1:G:115:GLU:HA	1:G:120:LYS:NZ	1.82	0.94
1:H:167:LYS:HD2	1:H:263:PHE:HZ	1.31	0.93
1:G:269:PRO:HG2	1:G:269:PRO:O	1.63	0.93
1:D:263:PHE:HB3	3:D:356:HOH:O	1.66	0.93
1:G:162:PRO:O	1:G:165:LYS:HB3	1.69	0.92
1:H:73:ASP:HB2	1:H:213:HIS:ND1	1.84	0.91
1:A:49:PRO:O	1:A:53:ASN:ND2	2.03	0.91
1:C:308:ASN:H	1:C:308:ASN:HD22	1.17	0.91
1:H:247:ASN:HD22	1:H:247:ASN:H	0.91	0.91
1:E:292:LEU:CD1	1:E:297:CYS:HB3	1.99	0.90
1:G:278:ARG:HD3	1:G:278:ARG:H	1.35	0.90
1:F:171:ALA:HA	1:F:175:ILE:HD13	1.51	0.90
1:H:148:GLU:OE1	1:H:151:ARG:HD3	1.72	0.90
1:H:247:ASN:ND2	1:H:247:ASN:H	1.62	0.90
1:A:115:GLU:HA	1:A:120:LYS:HZ2	1.33	0.89
1:B:80:LEU:HD23	1:B:84:GLU:HB3	1.54	0.89
1:F:81:ASN:C	1:F:83:ASN:H	1.74	0.89
1:E:292:LEU:HD11	1:E:297:CYS:HB3	1.50	0.89
1:B:282:GLN:HE22	1:B:306:PRO:CD	1.85	0.89
1:E:144:TYR:OH	1:E:215:LEU:HB2	1.71	0.89
1:E:292:LEU:HD12	1:E:297:CYS:CB	2.01	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:GLU:HG3	1:F:301:PHE:CE1	2.08	0.89
1:H:73:ASP:O	1:H:213:HIS:CE1	2.26	0.89
1:H:80:LEU:HG	1:H:84:GLU:HB2	1.54	0.89
1:G:166:ASN:ND2	1:G:262:SER:OG	2.06	0.89
1:B:93:ALA:HB2	1:B:154:LEU:HD11	1.51	0.88
1:E:165:LYS:O	1:E:169:LEU:HG	1.73	0.88
1:E:282:GLN:NE2	1:E:306:PRO:HG3	1.89	0.88
1:C:47:MET:N	1:C:47:MET:SD	2.45	0.88
1:E:282:GLN:NE2	1:E:306:PRO:CG	2.37	0.88
1:D:213:HIS:O	1:D:213:HIS:CD2	2.26	0.88
1:B:93:ALA:CB	1:B:154:LEU:HD12	2.04	0.87
1:E:109:LYS:HZ1	1:E:176:ASN:HA	1.38	0.87
1:H:257:VAL:CG1	1:H:261:ARG:HE	1.86	0.87
1:E:219:ASN:HA	3:E:360:HOH:O	1.74	0.87
1:G:86:HIS:O	1:G:90:HIS:HD2	1.58	0.87
1:C:148:GLU:O	1:C:148:GLU:HG3	1.75	0.86
1:H:213:HIS:CD2	1:H:213:HIS:O	2.28	0.86
1:H:78:GLU:HB2	3:H:361:HOH:O	1.74	0.86
1:B:282:GLN:NE2	1:B:306:PRO:HD3	1.89	0.86
1:A:154:LEU:HB2	3:A:364:HOH:O	1.74	0.86
1:A:282:GLN:HE21	1:A:303:SER:HB2	1.37	0.85
1:F:214:GLY:O	1:F:218:SER:OG	1.94	0.85
1:C:98:SER:HB2	1:C:167:LYS:HZ3	1.37	0.85
1:H:214:GLY:HA2	1:H:217:PHE:HB3	1.59	0.85
1:C:49:PRO:O	1:C:53:ASN:ND2	2.10	0.85
1:E:117:ILE:HD12	1:E:117:ILE:H	1.40	0.85
1:B:73:ASP:HB2	1:B:213:HIS:CD2	2.10	0.85
1:B:49:PRO:O	1:B:53:ASN:ND2	2.09	0.85
1:C:116:ILE:HG22	1:C:118:GLU:OE2	1.76	0.84
1:H:257:VAL:HG12	1:H:261:ARG:NE	1.91	0.84
1:E:70:LEU:H	1:E:70:LEU:CD2	1.90	0.84
1:B:90:HIS:ND1	1:B:93:ALA:HB3	1.92	0.84
1:H:87:PHE:HE1	1:H:270:CYS:HA	1.43	0.84
1:B:276:ASN:ND2	1:B:279:LEU:HG	1.92	0.84
1:B:301:PHE:HD1	1:B:303:SER:OG	1.60	0.84
1:G:181:PHE:HA	1:G:184:ARG:NH1	1.92	0.83
1:B:214:GLY:HA2	1:B:217:PHE:HB3	1.58	0.83
1:F:175:ILE:HD12	1:F:175:ILE:N	1.92	0.83
1:B:301:PHE:CD1	1:B:301:PHE:O	2.31	0.83
1:E:279:LEU:HD13	1:E:307:PHE:HE1	0.74	0.83
1:C:304:LYS:O	1:C:306:PRO:HD3	1.79	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:SER:CB	1:C:167:LYS:NZ	2.41	0.83
1:B:77:PHE:CD2	1:B:144:TYR:CD2	2.67	0.82
1:E:304:LYS:O	1:E:306:PRO:HD3	1.79	0.82
1:A:187:ALA:O	1:A:191:VAL:HG23	1.78	0.82
1:C:192:GLU:O	1:C:230:THR:OG1	1.98	0.82
1:F:163:ALA:HB1	1:F:263:PHE:CD2	2.15	0.82
1:F:282:GLN:NE2	1:F:303:SER:HB2	1.93	0.82
1:A:152:LEU:C	1:A:154:LEU:H	1.82	0.82
1:H:301:PHE:O	1:H:301:PHE:HD1	1.59	0.82
1:E:118:GLU:OE1	3:E:363:HOH:O	1.97	0.82
1:E:279:LEU:CD2	1:E:306:PRO:HB3	2.10	0.81
1:B:207:LYS:HE3	1:B:220:GLU:OE1	1.81	0.81
1:B:84:GLU:O	1:B:88:ILE:HG13	1.81	0.81
1:B:93:ALA:HB1	1:B:154:LEU:HD12	1.60	0.81
1:B:106:LEU:HD11	3:B:361:HOH:O	1.81	0.81
1:A:308:ASN:HD22	1:A:308:ASN:H	1.27	0.81
1:A:144:TYR:OH	1:A:213:HIS:NE2	2.07	0.81
1:B:237:TYR:O	1:B:243:LYS:HD2	1.80	0.81
1:G:180:SER:HB2	1:G:183:GLU:OE1	1.79	0.80
1:F:250:GLN:NE2	1:F:300:VAL:HG11	1.95	0.80
1:A:175:ILE:HG22	1:A:176:ASN:N	1.97	0.80
1:A:73:ASP:HB2	1:A:213:HIS:HB3	1.63	0.80
1:H:170:TRP:HZ3	1:H:175:ILE:HD11	1.46	0.80
1:H:74:LEU:O	1:H:78:GLU:HG2	1.81	0.80
1:H:156:HIS:HA	1:H:159:GLU:HB2	1.64	0.80
1:F:187:ALA:O	1:F:191:VAL:HG23	1.82	0.80
1:E:214:GLY:HA2	1:E:217:PHE:HB3	1.65	0.79
1:G:185:ILE:HD13	1:G:236:ILE:CG2	2.12	0.79
1:A:214:GLY:HA2	1:A:217:PHE:HB3	1.63	0.79
1:G:55:TYR:HD1	1:G:56:LYS:HD3	1.46	0.79
1:H:271:ASP:OD1	1:H:276:ASN:HA	1.83	0.79
1:D:175:ILE:HG22	1:D:176:ASN:N	1.97	0.79
1:A:113:GLU:CD	1:A:184:ARG:HH21	1.85	0.79
1:B:276:ASN:HB3	1:B:279:LEU:HD12	1.63	0.79
1:D:89:LYS:HD3	1:D:145:ILE:HG12	1.63	0.79
1:G:106:LEU:HD21	1:G:188:ASN:ND2	1.97	0.79
1:C:141:ILE:HD13	1:C:155:PHE:HZ	1.46	0.78
1:F:250:GLN:HE21	1:F:300:VAL:HG11	1.49	0.78
1:H:237:TYR:CE1	1:H:243:LYS:HD3	2.17	0.78
1:E:198:GLY:HA3	1:E:264:ILE:HG12	1.65	0.78
1:G:213:HIS:CD2	1:G:213:HIS:O	2.36	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:PHE:CE2	1:C:236:ILE:HD11	2.19	0.78
1:E:229:HIS:O	1:E:233:ASN:ND2	2.17	0.78
1:C:226:GLU:OE1	1:C:229:HIS:ND1	2.14	0.78
1:B:80:LEU:CD2	1:B:84:GLU:HB3	2.13	0.78
1:B:93:ALA:HB2	1:B:154:LEU:CD1	2.09	0.78
1:D:214:GLY:HA2	1:D:217:PHE:HB3	1.65	0.78
1:D:70:LEU:CD1	1:D:140:LEU:HD12	2.13	0.78
1:H:247:ASN:N	1:H:247:ASN:HD22	1.77	0.77
1:A:50:GLU:HA	1:A:53:ASN:HD22	1.50	0.77
1:G:70:LEU:HD21	1:G:140:LEU:HD12	1.65	0.77
1:G:269:PRO:O	1:G:269:PRO:CG	2.29	0.77
1:G:154:LEU:HG	1:G:158:ILE:HG13	1.65	0.77
1:C:98:SER:CB	1:C:167:LYS:HZ1	1.97	0.77
1:E:301:PHE:O	1:E:302:HIS:C	2.20	0.77
1:B:301:PHE:CD1	1:B:303:SER:OG	2.36	0.77
1:B:130:GLU:HA	1:B:133:HIS:HD2	1.50	0.77
1:G:163:ALA:HB1	1:G:263:PHE:CE2	2.20	0.77
1:G:143:ASN:O	1:G:146:LYS:HG3	1.84	0.77
1:B:247:ASN:HD22	1:B:247:ASN:H	1.33	0.76
1:G:73:ASP:OD2	1:G:213:HIS:HB3	1.85	0.76
1:G:115:GLU:HA	1:G:120:LYS:HZ1	1.46	0.76
1:C:175:ILE:H	1:C:175:ILE:HD12	1.50	0.76
1:D:250:GLN:HE21	1:D:300:VAL:HG22	1.51	0.76
1:H:188:ASN:HA	1:H:191:VAL:HG23	1.66	0.76
1:C:191:VAL:HA	1:C:195:LEU:HD12	1.68	0.76
1:D:237:TYR:OH	1:D:244:LEU:HB2	1.86	0.76
1:C:77:PHE:CD2	1:C:144:TYR:CD2	2.73	0.76
1:B:77:PHE:CD2	1:B:144:TYR:HD2	2.01	0.76
1:A:77:PHE:HE1	3:A:363:HOH:O	1.68	0.75
1:G:131:ASN:HB3	1:H:121:LYS:HE2	1.66	0.75
1:D:213:HIS:O	1:D:213:HIS:HD2	1.70	0.75
1:C:301:PHE:HD1	1:C:303:SER:HG	1.35	0.75
1:E:292:LEU:HD13	1:E:297:CYS:HB2	1.68	0.75
1:D:163:ALA:HB1	1:D:263:PHE:CE2	2.22	0.75
1:H:115:GLU:CA	1:H:120:LYS:NZ	2.49	0.75
1:F:191:VAL:HA	1:F:195:LEU:HD12	1.68	0.75
1:C:77:PHE:CE2	1:C:144:TYR:HD2	2.03	0.75
1:D:192:GLU:O	1:D:230:THR:OG1	2.04	0.75
1:C:122:PHE:HZ	1:C:228:LEU:HD23	1.51	0.74
1:F:81:ASN:HB2	1:F:84:GLU:H	1.50	0.74
1:F:224:ARG:HG2	3:F:352:HOH:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ILE:HG23	1:B:145:ILE:HD12	1.69	0.74
1:H:270:CYS:C	1:H:272:LEU:H	1.91	0.74
1:D:73:ASP:O	1:D:213:HIS:CE1	2.41	0.74
1:F:141:ILE:HG23	1:F:145:ILE:HD12	1.68	0.74
1:H:87:PHE:CE1	1:H:270:CYS:HA	2.23	0.74
1:B:93:ALA:HB3	1:B:154:LEU:HD11	1.69	0.74
1:G:86:HIS:O	1:G:90:HIS:CD2	2.40	0.74
1:D:301:PHE:O	1:D:302:HIS:C	2.23	0.73
1:B:121:LYS:HE2	1:C:131:ASN:HB3	1.71	0.73
1:B:276:ASN:HD22	1:B:279:LEU:CG	1.98	0.73
1:F:81:ASN:HB3	1:F:84:GLU:N	2.02	0.73
1:H:115:GLU:HA	1:H:120:LYS:HZ2	1.53	0.73
1:E:282:GLN:NE2	1:E:306:PRO:HD3	2.02	0.73
1:E:70:LEU:HD22	1:E:70:LEU:N	2.02	0.73
1:G:106:LEU:CD2	1:G:188:ASN:HD21	2.01	0.73
1:H:299:LYS:HD2	1:H:302:HIS:CD2	2.23	0.73
1:H:49:PRO:O	1:H:53:ASN:ND2	2.22	0.73
1:E:282:GLN:HA	1:E:285:GLU:HG3	1.69	0.73
1:F:154:LEU:O	1:F:158:ILE:HG13	1.89	0.73
1:E:282:GLN:HE22	1:E:306:PRO:CD	2.00	0.72
1:E:164:ILE:N	1:E:164:ILE:HD12	2.05	0.72
1:E:237:TYR:CE1	1:E:295:LEU:O	2.42	0.72
1:E:307:PHE:HB3	1:E:309:TRP:CE2	2.22	0.72
1:D:165:LYS:O	1:D:169:LEU:HG	1.90	0.72
1:F:261:ARG:NH2	1:F:285:GLU:OE2	2.19	0.72
1:H:264:ILE:CD1	1:H:264:ILE:H	1.90	0.72
1:B:247:ASN:HD22	1:B:247:ASN:N	1.87	0.72
1:D:51:VAL:HG22	1:D:235:LEU:CD2	2.20	0.72
1:G:115:GLU:HA	1:G:120:LYS:HZ2	1.54	0.72
1:F:89:LYS:HD3	1:F:145:ILE:HG12	1.70	0.72
1:F:293:GLU:OE2	1:F:299:LYS:HG3	1.90	0.72
1:C:52:TRP:CZ3	1:C:121:LYS:HG2	2.25	0.72
1:C:115:GLU:HA	1:C:120:LYS:NZ	2.04	0.71
1:C:50:GLU:HG2	1:C:235:LEU:HD21	1.73	0.71
1:G:163:ALA:CB	1:G:263:PHE:CD2	2.71	0.71
1:E:282:GLN:NE2	1:E:306:PRO:CD	2.53	0.71
1:H:73:ASP:O	1:H:213:HIS:HE1	1.72	0.71
1:E:279:LEU:HD22	1:E:306:PRO:HB3	1.71	0.71
1:A:224:ARG:NH2	1:A:225:ASP:OD1	2.23	0.71
1:B:57:LYS:O	1:B:61:SER:HB2	1.90	0.71
1:D:163:ALA:HB1	1:D:263:PHE:HD2	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:SER:O	1:E:285:GLU:HG2	1.89	0.71
1:C:165:LYS:HG2	1:C:166:ASN:N	2.06	0.71
1:F:104:GLU:HG2	1:F:105:ASN:N	2.05	0.70
1:C:229:HIS:O	1:C:233:ASN:ND2	2.24	0.70
1:E:270:CYS:C	1:E:272:LEU:H	1.93	0.70
1:G:278:ARG:N	1:G:278:ARG:CD	2.40	0.70
1:A:162:PRO:O	1:A:165:LYS:HG2	1.92	0.70
1:A:165:LYS:O	1:A:169:LEU:HD12	1.91	0.70
1:A:175:ILE:HG22	1:A:176:ASN:H	1.57	0.70
1:C:145:ILE:HG22	1:C:145:ILE:O	1.92	0.70
1:D:237:TYR:O	1:D:240:LEU:HB2	1.90	0.70
1:D:163:ALA:CB	1:D:263:PHE:CD2	2.71	0.70
1:F:73:ASP:HB2	1:F:213:HIS:CD2	2.26	0.70
1:A:163:ALA:HB1	1:A:263:PHE:CD2	2.25	0.70
1:C:154:LEU:O	1:C:154:LEU:HD12	1.92	0.70
1:D:181:PHE:HB2	1:D:184:ARG:NH2	2.07	0.70
1:B:229:HIS:O	1:B:233:ASN:ND2	2.25	0.70
1:B:271:ASP:HA	1:B:275:MET:O	1.92	0.70
1:G:91:VAL:HG22	1:G:268:LEU:HD23	1.73	0.70
1:A:73:ASP:CG	1:A:76:ASP:OD2	2.31	0.69
1:F:144:TYR:HE1	1:F:215:LEU:HD22	1.57	0.69
1:C:139:LEU:O	1:C:143:ASN:ND2	2.25	0.69
1:E:213:HIS:O	1:E:213:HIS:CD2	2.46	0.69
1:B:52:TRP:CD1	3:B:360:HOH:O	2.44	0.69
1:D:293:GLU:OE2	1:D:299:LYS:HG2	1.93	0.69
1:F:233:ASN:HA	1:F:236:ILE:HD11	1.73	0.69
1:E:213:HIS:O	1:E:213:HIS:CG	2.41	0.69
1:E:71:SER:HB2	3:E:365:HOH:O	1.91	0.69
1:C:90:HIS:HB3	1:C:268:LEU:HD22	1.74	0.69
1:C:299:LYS:HZ2	1:C:302:HIS:HD2	0.70	0.69
1:G:271:ASP:OD1	1:G:275:MET:O	2.11	0.69
1:G:81:ASN:OD1	1:G:82:VAL:N	2.25	0.69
1:C:153:ASN:O	1:C:157:ALA:HB2	1.92	0.69
1:C:257:VAL:HG22	1:C:284:ILE:HG22	1.73	0.69
1:D:111:LEU:HD23	1:D:120:LYS:HB3	1.74	0.69
1:G:185:ILE:HD13	1:G:236:ILE:HG21	1.74	0.69
1:D:163:ALA:CB	1:D:263:PHE:HD2	2.05	0.69
1:B:154:LEU:O	1:B:157:ALA:HB3	1.92	0.68
1:F:282:GLN:HE21	1:F:303:SER:HB2	1.59	0.68
1:D:180:SER:HB3	1:D:183:GLU:CG	2.18	0.68
1:B:143:ASN:HA	1:B:146:LYS:HG3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:ASN:C	1:F:83:ASN:N	2.41	0.68
1:C:106:LEU:HD22	3:C:352:HOH:O	1.93	0.68
1:B:301:PHE:O	1:B:302:HIS:C	2.30	0.68
1:C:282:GLN:NE2	1:C:303:SER:HB2	2.08	0.68
1:D:51:VAL:HG22	1:D:235:LEU:HD21	1.75	0.68
1:F:301:PHE:O	1:F:302:HIS:C	2.30	0.68
1:A:74:LEU:O	1:A:78:GLU:HG2	1.94	0.68
1:C:115:GLU:HA	1:C:120:LYS:HZ3	1.59	0.68
1:E:76:ASP:O	1:E:80:LEU:HD13	1.94	0.68
1:H:143:ASN:O	1:H:146:LYS:HG3	1.93	0.67
1:G:113:GLU:O	1:G:115:GLU:HG2	1.94	0.67
1:G:170:TRP:CZ3	1:G:175:ILE:HD11	2.29	0.67
1:A:226:GLU:HA	1:A:226:GLU:OE1	1.94	0.67
1:A:73:ASP:O	1:A:213:HIS:CE1	2.48	0.67
1:B:92:LEU:HD21	1:B:215:LEU:HD11	1.76	0.67
1:C:247:ASN:HD22	1:C:247:ASN:N	1.89	0.67
1:E:292:LEU:HD12	1:E:297:CYS:HB2	1.64	0.67
1:H:109:LYS:NZ	1:H:176:ASN:HA	2.09	0.67
1:A:278:ARG:N	1:A:278:ARG:HD3	2.09	0.67
1:F:52:TRP:CZ2	1:F:56:LYS:HD3	2.30	0.67
1:A:158:ILE:O	1:A:161:ILE:HB	1.94	0.67
1:C:281:SER:O	1:C:285:GLU:HG2	1.93	0.67
1:A:270:CYS:C	1:A:272:LEU:H	1.97	0.67
1:E:94:PHE:HD1	3:E:351:HOH:O	1.77	0.67
1:C:73:ASP:HB2	1:C:213:HIS:CG	2.29	0.67
1:E:280:MET:HE3	1:E:283:TYR:HB3	1.77	0.67
1:H:166:ASN:HB3	1:H:259:VAL:HG22	1.77	0.67
1:A:73:ASP:HB2	1:A:213:HIS:CG	2.29	0.66
1:B:232:PHE:CE2	1:B:236:ILE:HD11	2.29	0.66
1:G:214:GLY:HA2	1:G:217:PHE:HB3	1.76	0.66
1:H:162:PRO:O	1:H:165:LYS:HB3	1.95	0.66
1:D:178:THR:OG1	3:D:359:HOH:O	2.13	0.66
1:E:166:ASN:HB3	1:E:259:VAL:HG22	1.76	0.66
1:B:281:SER:O	1:B:285:GLU:HG2	1.96	0.66
1:G:106:LEU:CD2	1:G:188:ASN:ND2	2.58	0.66
1:A:253:VAL:HG11	1:A:292:LEU:HD21	1.77	0.66
1:C:52:TRP:HZ3	1:C:121:LYS:HG2	1.60	0.66
1:B:263:PHE:HB3	1:B:268:LEU:HD21	1.75	0.66
1:B:177:ASP:OD2	1:B:178:THR:N	2.28	0.66
1:D:73:ASP:CB	1:D:213:HIS:ND1	2.55	0.66
1:C:150:GLU:O	1:C:151:ARG:C	2.34	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:PHE:O	1:C:302:HIS:C	2.32	0.66
1:D:77:PHE:CD2	1:D:144:TYR:CD2	2.83	0.66
1:D:117:ILE:H	1:D:117:ILE:HD12	1.61	0.66
1:B:175:ILE:CG2	1:B:176:ASN:N	2.59	0.66
1:C:82:VAL:HG23	1:C:83:ASN:ND2	2.11	0.66
1:D:94:PHE:HE2	1:D:164:ILE:CD1	2.08	0.66
1:E:286:PHE:HD1	1:E:303:SER:O	1.78	0.65
1:F:70:LEU:O	1:F:213:HIS:CE1	2.49	0.65
1:G:91:VAL:CG2	1:G:268:LEU:CD2	2.74	0.65
1:F:81:ASN:HB3	1:F:83:ASN:H	1.61	0.65
1:C:137:TYR:O	1:C:141:ILE:HG13	1.96	0.65
1:B:81:ASN:O	1:B:81:ASN:CG	2.34	0.65
1:E:118:GLU:CD	1:E:118:GLU:H	1.99	0.65
1:G:192:GLU:O	1:G:230:THR:OG1	2.11	0.65
1:A:258:GLU:OE2	1:A:258:GLU:HA	1.96	0.65
1:A:285:GLU:HB3	1:A:301:PHE:CD1	2.32	0.65
1:C:214:GLY:CA	1:C:217:PHE:HB3	2.23	0.65
1:D:144:TYR:OH	1:D:213:HIS:NE2	2.28	0.65
1:G:165:LYS:HG2	1:G:166:ASN:N	2.12	0.65
1:H:309:TRP:CE3	1:H:309:TRP:O	2.49	0.65
1:B:214:GLY:HA2	1:B:217:PHE:H	1.61	0.65
1:C:198:GLY:HA3	1:C:264:ILE:HG12	1.77	0.65
1:E:289:ASP:HB3	1:E:299:LYS:HG2	1.77	0.65
1:H:73:ASP:HB3	1:H:76:ASP:OD2	1.97	0.65
1:A:152:LEU:O	1:A:154:LEU:N	2.30	0.65
1:A:232:PHE:CZ	1:A:236:ILE:HD11	2.32	0.65
1:F:233:ASN:CA	1:F:236:ILE:CD1	2.70	0.65
1:C:77:PHE:CD2	1:C:144:TYR:HD2	2.15	0.64
1:H:194:ILE:HD11	1:H:253:VAL:HG13	1.78	0.64
1:B:155:PHE:HB2	3:B:356:HOH:O	1.97	0.64
1:C:175:ILE:O	1:C:176:ASN:C	2.32	0.64
1:E:232:PHE:CE2	1:E:236:ILE:HD11	2.32	0.64
1:E:192:GLU:O	1:E:230:THR:OG1	2.10	0.64
1:A:113:GLU:CD	1:A:184:ARG:NH2	2.51	0.64
1:A:301:PHE:O	1:A:302:HIS:C	2.35	0.64
1:C:299:LYS:HZ3	1:C:302:HIS:CD2	2.15	0.64
1:D:283:TYR:O	1:D:287:VAL:HG23	1.97	0.64
1:E:167:LYS:HD2	1:E:263:PHE:CZ	2.33	0.64
1:A:105:ASN:HD21	1:A:108:SER:CB	2.11	0.64
1:D:132:ILE:O	1:D:136:THR:OG1	2.15	0.64
1:D:146:LYS:HE2	3:D:360:HOH:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:O	1:D:61:SER:HB2	1.97	0.64
1:C:301:PHE:O	1:C:301:PHE:CD1	2.51	0.64
1:E:92:LEU:HD11	1:E:144:TYR:HD1	1.63	0.64
1:F:157:ALA:O	1:F:161:ILE:HG12	1.97	0.64
1:G:185:ILE:CD1	1:G:236:ILE:HG23	2.27	0.64
1:D:150:GLU:O	1:D:151:ARG:C	2.32	0.64
1:B:68:ILE:HG22	1:B:70:LEU:HD23	1.78	0.64
1:D:237:TYR:HA	1:D:240:LEU:HD22	1.80	0.64
1:E:175:ILE:HG22	1:E:176:ASN:N	2.12	0.64
1:E:57:LYS:O	1:E:61:SER:HB2	1.98	0.64
1:F:47:MET:N	1:F:47:MET:SD	2.71	0.64
1:G:249:VAL:O	1:G:253:VAL:HG23	1.98	0.64
1:G:285:GLU:CD	1:G:301:PHE:HD1	2.00	0.64
1:A:86:HIS:ND1	1:A:89:LYS:HD2	2.13	0.63
1:F:233:ASN:HA	1:F:236:ILE:HD13	1.80	0.63
1:G:121:LYS:NZ	1:G:121:LYS:CD	2.59	0.63
1:D:174:TRP:NE1	1:D:255:GLU:OE2	2.31	0.63
1:E:236:ILE:HD13	1:E:236:ILE:N	2.14	0.63
1:A:175:ILE:CG2	1:A:176:ASN:H	2.11	0.63
1:D:166:ASN:HB3	1:D:259:VAL:HG22	1.80	0.63
1:F:73:ASP:HB3	1:F:76:ASP:CG	2.19	0.63
1:G:281:SER:O	1:G:285:GLU:HG2	1.98	0.63
1:C:122:PHE:CZ	1:C:228:LEU:CD2	2.82	0.63
1:C:88:ILE:HD11	1:C:206:PHE:CE1	2.34	0.63
1:G:215:LEU:O	1:G:219:ASN:HB3	1.98	0.63
1:G:91:VAL:CG2	1:G:268:LEU:HD23	2.28	0.63
1:H:269:PRO:O	1:H:272:LEU:HB2	1.99	0.63
1:E:301:PHE:HD1	1:E:303:SER:HG	1.46	0.63
1:A:152:LEU:C	1:A:154:LEU:N	2.51	0.63
1:A:175:ILE:CG2	1:A:176:ASN:N	2.61	0.63
1:F:285:GLU:OE2	1:F:301:PHE:CE2	2.52	0.63
1:A:112:ARG:NH2	1:D:112:ARG:HH12	1.97	0.63
1:C:195:LEU:O	1:C:196:PHE:HB2	1.99	0.63
1:C:175:ILE:N	1:C:175:ILE:HD12	2.14	0.63
1:A:247:ASN:O	1:A:251:ASN:OD1	2.17	0.63
1:C:271:ASP:HA	1:C:275:MET:O	1.99	0.63
1:A:270:CYS:O	1:A:272:LEU:N	2.31	0.62
1:A:73:ASP:HB2	1:A:213:HIS:CB	2.29	0.62
1:B:285:GLU:HB3	1:B:301:PHE:CD1	2.34	0.62
1:B:89:LYS:HA	1:B:145:ILE:HD11	1.80	0.62
1:C:90:HIS:HB3	1:C:268:LEU:CD2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:CE2	1:A:185:ILE:HD11	2.33	0.62
1:B:260:GLU:HA	1:B:263:PHE:CE1	2.35	0.62
1:C:257:VAL:HG22	1:C:284:ILE:CG2	2.29	0.62
1:F:81:ASN:O	1:F:83:ASN:N	2.32	0.62
1:G:180:SER:HB2	1:G:183:GLU:CD	2.20	0.62
1:A:198:GLY:HA3	1:A:264:ILE:HG12	1.82	0.62
1:C:293:GLU:OE2	1:C:299:LYS:HG3	2.00	0.62
1:D:232:PHE:CE2	1:D:236:ILE:HD11	2.34	0.62
1:F:70:LEU:O	1:F:213:HIS:HE1	1.81	0.62
1:F:236:ILE:H	1:F:236:ILE:HD12	1.65	0.62
1:G:260:GLU:HG2	1:G:284:ILE:HD12	1.80	0.62
1:H:240:LEU:CD2	1:H:243:LYS:HA	2.29	0.62
1:B:186:VAL:HG12	1:B:252:ILE:HG21	1.81	0.62
1:E:72:SER:OG	1:E:73:ASP:OD2	2.12	0.62
1:F:47:MET:O	1:F:49:PRO:HD3	2.00	0.62
1:C:213:HIS:CG	1:C:213:HIS:O	2.52	0.62
1:A:115:GLU:HA	1:A:120:LYS:HZ1	1.65	0.62
1:B:87:PHE:CZ	1:B:91:VAL:HG21	2.35	0.62
1:F:124:SER:HA	1:F:127:ILE:HD12	1.81	0.62
1:F:81:ASN:CB	1:F:84:GLU:N	2.55	0.62
1:C:195:LEU:HA	1:C:260:GLU:HG2	1.80	0.61
1:E:293:GLU:OE1	1:E:299:LYS:HE3	2.00	0.61
1:G:95:PHE:CD2	1:G:137:TYR:CE1	2.88	0.61
1:H:264:ILE:CD1	1:H:264:ILE:N	2.54	0.61
1:E:217:PHE:CE1	1:E:221:LEU:HD21	2.35	0.61
1:G:185:ILE:CD1	1:G:236:ILE:CG2	2.78	0.61
1:G:55:TYR:CD1	1:G:56:LYS:HD3	2.33	0.61
1:A:70:LEU:HD21	1:A:140:LEU:CD1	2.30	0.61
1:A:167:LYS:NZ	1:A:195:LEU:HD13	2.14	0.61
1:F:285:GLU:HB3	1:F:301:PHE:CD1	2.35	0.61
1:G:91:VAL:HG12	1:G:95:PHE:CE2	2.35	0.61
1:E:150:GLU:OE1	1:E:154:LEU:HD23	2.00	0.61
1:A:271:ASP:HA	1:A:275:MET:O	2.00	0.61
1:B:93:ALA:HB3	1:B:154:LEU:CD1	2.26	0.61
1:F:175:ILE:H	1:F:175:ILE:CD1	2.10	0.61
1:H:247:ASN:N	1:H:247:ASN:ND2	2.39	0.61
1:B:264:ILE:H	1:B:264:ILE:HD12	1.65	0.61
1:D:150:GLU:OE1	1:D:153:ASN:HB3	2.00	0.61
1:G:78:GLU:OE2	1:G:78:GLU:HA	2.00	0.61
1:B:150:GLU:C	1:B:152:LEU:N	2.51	0.61
1:B:81:ASN:OD1	1:B:81:ASN:O	2.19	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:LYS:H	1:G:146:LYS:CD	2.13	0.61
1:G:181:PHE:HD1	1:G:184:ARG:HH12	1.47	0.61
1:H:277:SER:OG	1:H:278:ARG:CZ	2.49	0.61
1:A:229:HIS:O	1:A:233:ASN:ND2	2.34	0.61
1:A:301:PHE:O	1:A:301:PHE:CD1	2.53	0.61
1:E:279:LEU:HD22	1:E:306:PRO:CB	2.31	0.61
1:F:81:ASN:HB2	1:F:84:GLU:CB	2.31	0.61
1:A:261:ARG:HA	1:A:264:ILE:CD1	2.31	0.61
1:B:264:ILE:N	1:B:264:ILE:HD12	2.16	0.61
1:H:166:ASN:ND2	3:H:353:HOH:O	2.29	0.61
1:D:61:SER:OG	1:D:224:ARG:NH2	2.34	0.61
1:C:293:GLU:OE2	1:C:299:LYS:CG	2.49	0.60
1:A:121:LYS:HZ3	1:D:131:ASN:HB3	1.65	0.60
1:F:181:PHE:CE2	1:F:185:ILE:HD11	2.36	0.60
1:G:198:GLY:HA3	1:G:264:ILE:HG12	1.83	0.60
1:G:64:THR:OG1	1:G:65:ALA:N	2.32	0.60
1:H:213:HIS:CG	1:H:213:HIS:O	2.49	0.60
1:E:121:LYS:HZ3	1:F:131:ASN:HB3	1.66	0.60
1:G:70:LEU:HD21	1:G:140:LEU:CD1	2.30	0.60
1:D:299:LYS:NZ	1:D:302:HIS:HD2	1.99	0.60
1:E:80:LEU:HG	1:E:84:GLU:HG3	1.82	0.60
1:F:271:ASP:HA	1:F:275:MET:O	2.01	0.60
1:A:158:ILE:O	1:A:159:GLU:C	2.40	0.60
1:D:247:ASN:HD22	1:D:247:ASN:N	2.00	0.60
1:E:170:TRP:CZ2	1:E:256:ALA:HB2	2.36	0.60
1:G:146:LYS:HD3	1:G:146:LYS:H	1.67	0.60
1:B:74:LEU:HD12	1:B:77:PHE:HB3	1.82	0.60
1:C:122:PHE:HZ	1:C:228:LEU:CD2	2.14	0.60
1:C:289:ASP:O	1:C:292:LEU:HB2	2.02	0.60
1:H:214:GLY:HA2	1:H:217:PHE:H	1.65	0.60
1:H:47:MET:N	1:H:47:MET:SD	2.75	0.60
1:E:292:LEU:HG	1:E:298:SER:O	2.02	0.60
1:F:85:LYS:HE2	3:F:363:HOH:O	2.00	0.60
1:G:106:LEU:O	1:G:109:LYS:HB3	2.01	0.60
1:H:240:LEU:HD23	1:H:243:LYS:HA	1.83	0.60
1:B:276:ASN:HD21	1:B:278:ARG:HB2	1.65	0.60
1:B:305:ASN:N	1:B:305:ASN:OD1	2.33	0.60
1:H:115:GLU:CA	1:H:120:LYS:HZ2	2.13	0.60
1:A:293:GLU:OE2	1:A:299:LYS:HE2	2.01	0.60
1:B:130:GLU:HA	1:B:133:HIS:CD2	2.36	0.60
1:C:214:GLY:HA2	1:C:217:PHE:H	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:276:ASN:HB3	1:G:279:LEU:HD12	1.83	0.60
1:E:237:TYR:O	1:E:240:LEU:HB2	2.02	0.59
1:G:170:TRP:HZ3	1:G:175:ILE:HD11	1.67	0.59
1:G:301:PHE:O	1:G:302:HIS:C	2.40	0.59
1:A:250:GLN:NE2	1:A:300:VAL:HG23	2.17	0.59
1:A:105:ASN:HD21	1:A:108:SER:HB3	1.66	0.59
1:E:117:ILE:CD1	1:E:117:ILE:H	2.14	0.59
1:H:307:PHE:HE2	3:H:357:HOH:O	1.86	0.59
1:A:73:ASP:HB2	1:A:213:HIS:ND1	2.16	0.59
1:C:282:GLN:HA	1:C:285:GLU:HG3	1.84	0.59
1:D:173:LYS:HE2	1:D:174:TRP:CZ2	2.38	0.59
1:E:260:GLU:O	1:E:263:PHE:HB2	2.03	0.59
1:H:170:TRP:HZ3	1:H:175:ILE:CD1	2.16	0.59
1:F:226:GLU:OE1	1:F:229:HIS:ND1	2.28	0.59
1:G:91:VAL:HG22	1:G:268:LEU:CD2	2.32	0.59
1:H:235:LEU:HA	1:H:238:SER:HB3	1.82	0.59
1:C:308:ASN:H	1:C:308:ASN:ND2	1.93	0.59
1:D:175:ILE:O	1:D:176:ASN:C	2.41	0.59
1:F:56:LYS:NZ	1:F:59:GLU:OE1	2.28	0.59
1:A:112:ARG:HH22	1:D:112:ARG:HH12	1.50	0.59
1:B:146:LYS:NZ	1:B:146:LYS:CD	2.61	0.59
1:B:54:PHE:O	1:B:122:PHE:HE2	1.85	0.59
1:E:140:LEU:HD22	1:E:215:LEU:HD13	1.85	0.59
1:E:80:LEU:HD23	1:E:84:GLU:HB3	1.85	0.59
1:B:89:LYS:HG2	1:B:145:ILE:HG12	1.84	0.59
1:B:237:TYR:CE2	1:B:243:LYS:HG3	2.38	0.59
1:C:163:ALA:HB1	1:C:263:PHE:CD2	2.38	0.59
1:E:301:PHE:HD1	1:E:303:SER:OG	1.85	0.59
1:G:184:ARG:HH11	1:G:184:ARG:HB2	1.68	0.59
1:C:122:PHE:CZ	1:C:228:LEU:HD23	2.37	0.58
1:H:47:MET:O	1:H:49:PRO:HD3	2.03	0.58
1:B:90:HIS:HD1	1:B:93:ALA:HB3	1.65	0.58
1:C:111:LEU:HD23	1:C:123:TYR:HB2	1.85	0.58
1:C:249:VAL:O	1:C:253:VAL:HG23	2.03	0.58
1:E:285:GLU:CB	1:E:301:PHE:CD1	2.82	0.58
1:F:285:GLU:HG3	1:F:301:PHE:CZ	2.38	0.58
1:H:299:LYS:HD2	1:H:302:HIS:HD2	1.64	0.58
1:B:283:TYR:CE2	1:B:287:VAL:HG21	2.38	0.58
1:C:122:PHE:CE2	1:C:228:LEU:HD21	2.39	0.58
1:G:161:ILE:HG13	1:G:164:ILE:HD12	1.85	0.58
1:A:137:TYR:O	1:A:141:ILE:HD12	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:PHE:HE2	1:C:236:ILE:HD11	1.64	0.58
1:H:167:LYS:NZ	1:H:196:PHE:CE2	2.71	0.58
1:D:167:LYS:NZ	1:D:195:LEU:HD13	2.18	0.58
1:F:86:HIS:HD2	1:F:89:LYS:HG3	1.68	0.58
1:G:260:GLU:CG	1:G:284:ILE:HD12	2.34	0.58
1:C:142:ASP:OD2	1:C:151:ARG:NH1	2.36	0.58
1:C:150:GLU:OE2	1:C:153:ASN:HB3	2.03	0.58
1:D:198:GLY:HA3	1:D:264:ILE:HG12	1.84	0.58
1:E:150:GLU:OE1	1:E:154:LEU:CD2	2.52	0.58
1:B:150:GLU:O	1:B:151:ARG:C	2.39	0.58
1:B:212:LEU:C	1:B:213:HIS:HD2	2.07	0.58
1:E:271:ASP:HA	1:E:275:MET:O	2.04	0.58
1:F:206:PHE:CE1	1:F:273:ILE:HG13	2.39	0.58
1:H:145:ILE:HG22	1:H:145:ILE:O	2.04	0.58
1:B:214:GLY:CA	1:B:217:PHE:HB3	2.31	0.58
1:C:88:ILE:O	1:C:92:LEU:HG	2.04	0.58
1:D:307:PHE:HB3	1:D:309:TRP:CE2	2.39	0.58
1:D:48:TYR:CD1	1:D:48:TYR:N	2.72	0.57
1:F:226:GLU:HA	1:F:226:GLU:OE1	2.03	0.57
1:C:88:ILE:HD11	1:C:206:PHE:CZ	2.39	0.57
1:F:129:VAL:HG22	3:F:357:HOH:O	2.04	0.57
1:A:113:GLU:OE2	1:A:184:ARG:NH2	2.37	0.57
1:A:50:GLU:HA	1:A:53:ASN:ND2	2.19	0.57
1:C:85:LYS:O	1:C:89:LYS:HG3	2.04	0.57
1:E:213:HIS:C	1:E:213:HIS:CD2	2.77	0.57
1:H:183:GLU:OE1	1:H:248:VAL:HG11	2.03	0.57
1:A:226:GLU:O	1:A:230:THR:OG1	2.22	0.57
1:A:69:ASP:C	1:A:71:SER:H	2.07	0.57
1:B:54:PHE:HB3	1:B:122:PHE:CE2	2.38	0.57
1:B:133:HIS:ND1	1:B:222:ILE:HG23	2.18	0.57
1:D:82:VAL:HG23	1:D:83:ASN:N	2.19	0.57
1:E:74:LEU:O	1:E:78:GLU:HG2	2.04	0.57
1:C:195:LEU:HA	1:C:260:GLU:CG	2.35	0.57
1:B:110:PHE:CE1	1:B:188:ASN:ND2	2.73	0.57
1:C:214:GLY:HA2	1:C:217:PHE:CB	2.31	0.57
1:D:94:PHE:CE2	1:D:164:ILE:CD1	2.88	0.57
1:E:113:GLU:O	1:E:115:GLU:HG2	2.05	0.57
1:E:50:GLU:HG2	1:E:235:LEU:HD22	1.85	0.57
1:F:144:TYR:CE1	1:F:215:LEU:HD22	2.39	0.57
1:A:106:LEU:HD11	1:A:188:ASN:OD1	2.04	0.57
1:F:271:ASP:O	1:F:272:LEU:HG	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ASN:OD1	1:C:278:ARG:HG2	2.04	0.56
1:E:200:PHE:O	1:E:204:PHE:HD1	1.88	0.56
1:E:217:PHE:O	1:E:220:GLU:HB3	2.05	0.56
1:F:175:ILE:O	1:F:176:ASN:C	2.41	0.56
1:D:207:LYS:HB2	1:D:216:THR:HB	1.87	0.56
1:F:139:LEU:O	1:F:142:ASP:HB3	2.04	0.56
1:H:301:PHE:O	1:H:302:HIS:C	2.42	0.56
1:H:66:GLU:HA	1:H:66:GLU:OE2	2.06	0.56
1:H:80:LEU:CG	1:H:84:GLU:HB2	2.31	0.56
1:C:141:ILE:HD13	1:C:155:PHE:CZ	2.35	0.56
1:F:285:GLU:CD	1:F:301:PHE:CE2	2.79	0.56
1:G:85:LYS:O	1:G:89:LYS:HG3	2.06	0.56
1:H:214:GLY:CA	1:H:217:PHE:HB3	2.35	0.56
1:D:258:GLU:HA	1:D:258:GLU:OE2	2.06	0.56
1:E:81:ASN:O	1:E:83:ASN:N	2.39	0.56
1:F:175:ILE:HG13	1:F:187:ALA:HB1	1.88	0.56
1:F:212:LEU:HD13	1:F:215:LEU:HD23	1.85	0.56
1:F:205:TRP:O	1:F:209:GLN:HG3	2.06	0.56
1:H:194:ILE:CD1	1:H:253:VAL:HG13	2.35	0.56
1:C:282:GLN:O	1:C:285:GLU:HB2	2.05	0.56
1:D:175:ILE:CG2	1:D:176:ASN:H	2.09	0.56
1:H:156:HIS:CD2	1:H:159:GLU:OE1	2.59	0.56
1:H:271:ASP:OD1	1:H:275:MET:O	2.23	0.56
1:C:247:ASN:ND2	1:C:247:ASN:N	2.51	0.56
1:F:270:CYS:C	1:F:272:LEU:H	2.08	0.56
1:G:68:ILE:HG12	1:G:217:PHE:CE2	2.40	0.56
1:D:73:ASP:O	1:D:213:HIS:HE1	1.87	0.56
1:F:217:PHE:O	1:F:220:GLU:HB3	2.06	0.56
1:A:72:SER:O	1:A:75:LYS:HE2	2.05	0.56
1:A:77:PHE:CD1	1:A:77:PHE:O	2.59	0.56
1:C:123:TYR:OH	1:C:236:ILE:HD12	2.05	0.56
1:H:212:LEU:HB3	1:H:215:LEU:HD23	1.88	0.56
1:A:156:HIS:CD2	1:B:304:LYS:HG3	2.41	0.56
1:A:202:ALA:HB1	1:A:273:ILE:CD1	2.36	0.56
1:A:94:PHE:CD1	1:A:196:PHE:HE1	2.24	0.56
1:C:224:ARG:NH2	1:C:225:ASP:OD1	2.39	0.56
1:C:69:ASP:C	1:C:71:SER:H	2.09	0.56
1:A:281:SER:O	1:A:285:GLU:HG2	2.07	0.55
1:D:166:ASN:ND2	1:D:262:SER:CB	2.69	0.55
1:H:126:GLN:OE1	1:H:192:GLU:OE2	2.24	0.55
1:B:247:ASN:O	1:B:251:ASN:OD1	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:HIS:N	1:E:229:HIS:CD2	2.72	0.55
1:F:198:GLY:HA3	1:F:264:ILE:HG12	1.88	0.55
1:C:59:GLU:HA	1:C:125:PHE:CZ	2.41	0.55
1:C:209:GLN:HB3	1:C:211:LYS:NZ	2.22	0.55
1:C:48:TYR:N	1:C:48:TYR:CD1	2.73	0.55
1:E:58:ALA:HB2	1:E:228:LEU:HD21	1.89	0.55
1:F:244:LEU:HD13	1:F:245:PRO:HD2	1.88	0.55
1:G:181:PHE:HA	1:G:184:ARG:CZ	2.35	0.55
1:G:214:GLY:HA2	1:G:217:PHE:H	1.72	0.55
1:G:304:LYS:O	1:G:306:PRO:HD3	2.05	0.55
1:A:202:ALA:HB1	1:A:273:ILE:HD13	1.87	0.55
1:A:308:ASN:ND2	1:A:308:ASN:H	2.02	0.55
1:E:181:PHE:CZ	1:E:185:ILE:HD11	2.41	0.55
1:E:77:PHE:CD2	1:E:144:TYR:CD2	2.94	0.55
1:F:48:TYR:CD1	1:F:118:GLU:OE2	2.60	0.55
1:F:81:ASN:HB2	1:F:84:GLU:CG	2.37	0.55
1:G:180:SER:CB	1:G:183:GLU:OE1	2.51	0.55
1:H:116:ILE:HD11	1:H:119:ALA:HB2	1.88	0.55
1:B:163:ALA:HB1	1:B:263:PHE:CE2	2.36	0.55
1:B:175:ILE:HG22	1:B:176:ASN:N	2.22	0.55
1:C:123:TYR:OH	1:C:236:ILE:CD1	2.54	0.55
1:C:170:TRP:CZ3	1:C:175:ILE:HD11	2.41	0.55
1:H:150:GLU:O	1:H:152:LEU:N	2.38	0.55
1:H:87:PHE:HA	1:H:268:LEU:HD21	1.89	0.55
1:B:137:TYR:O	1:B:141:ILE:HG13	2.06	0.55
1:F:86:HIS:CD2	1:F:89:LYS:HG3	2.42	0.55
1:B:148:GLU:C	1:B:150:GLU:H	2.10	0.55
1:B:301:PHE:HD1	1:B:301:PHE:O	1.88	0.55
1:C:133:HIS:CD2	1:C:222:ILE:HG12	2.42	0.55
1:G:54:PHE:HE2	1:G:231:ASP:HB2	1.72	0.55
1:C:203:ILE:O	1:C:203:ILE:HG22	2.07	0.55
1:D:254:LYS:O	1:D:257:VAL:HB	2.06	0.55
1:F:150:GLU:OE1	1:F:153:ASN:HB3	2.06	0.55
1:A:155:PHE:O	1:A:159:GLU:HG2	2.06	0.55
1:A:52:TRP:HZ2	1:D:135:GLU:OE2	1.90	0.55
1:D:293:GLU:OE2	1:D:299:LYS:CG	2.54	0.55
1:F:212:LEU:HA	1:F:213:HIS:HD2	1.71	0.55
1:C:208:LYS:HB2	3:C:356:HOH:O	2.07	0.55
1:E:163:ALA:HB1	1:E:263:PHE:CD2	2.42	0.55
1:B:150:GLU:O	1:B:154:LEU:HB2	2.07	0.54
1:B:72:SER:C	1:B:73:ASP:OD2	2.46	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASP:OD2	1:C:147:ASP:O	2.24	0.54
1:G:187:ALA:O	1:G:191:VAL:HG23	2.06	0.54
1:B:180:SER:HB2	1:B:183:GLU:OE1	2.07	0.54
1:B:190:CYS:SG	1:B:194:ILE:HD12	2.47	0.54
1:E:63:TRP:HZ3	1:E:68:ILE:HD11	1.73	0.54
1:F:81:ASN:CG	1:F:84:GLU:OE1	2.46	0.54
1:H:85:LYS:HG3	1:H:89:LYS:HD2	1.88	0.54
1:D:51:VAL:HG22	1:D:235:LEU:HD23	1.89	0.54
1:E:280:MET:HE1	1:E:283:TYR:HD2	1.72	0.54
1:A:158:ILE:O	1:A:160:ASN:N	2.41	0.54
1:A:81:ASN:OD1	1:A:84:GLU:HG3	2.07	0.54
1:C:195:LEU:HD23	1:C:260:GLU:HG2	1.89	0.54
1:G:54:PHE:HB3	1:G:122:PHE:CE2	2.42	0.54
1:E:214:GLY:HA2	1:E:217:PHE:H	1.73	0.54
1:E:81:ASN:C	1:E:81:ASN:OD1	2.45	0.54
1:A:70:LEU:HD21	1:A:140:LEU:HD11	1.90	0.54
1:E:141:ILE:HA	1:E:145:ILE:HD12	1.88	0.54
1:E:80:LEU:HD23	1:E:84:GLU:CB	2.37	0.54
1:F:171:ALA:HA	1:F:175:ILE:CD1	2.33	0.54
1:H:165:LYS:O	1:H:169:LEU:HD12	2.08	0.54
1:H:171:ALA:HA	1:H:175:ILE:HG13	1.89	0.54
1:D:213:HIS:O	1:D:213:HIS:CG	2.52	0.54
1:A:87:PHE:CD2	1:A:273:ILE:HG21	2.42	0.54
1:C:152:LEU:O	1:C:154:LEU:N	2.41	0.54
1:C:87:PHE:CD1	1:C:268:LEU:HG	2.43	0.54
1:E:109:LYS:NZ	1:E:176:ASN:HA	2.17	0.54
1:G:144:TYR:HH	1:G:213:HIS:HE2	1.54	0.54
1:A:81:ASN:CG	1:A:84:GLU:HG3	2.28	0.54
1:E:70:LEU:HB2	1:E:143:ASN:OD1	2.07	0.54
1:G:248:VAL:O	1:G:251:ASN:HB2	2.08	0.54
1:G:285:GLU:CD	1:G:301:PHE:CD1	2.79	0.54
1:A:57:LYS:O	1:A:61:SER:CB	2.56	0.53
1:E:279:LEU:CD1	1:E:307:PHE:CE1	2.59	0.53
1:F:212:LEU:O	1:F:216:THR:HG23	2.08	0.53
1:D:271:ASP:O	1:D:272:LEU:HB2	2.08	0.53
1:H:86:HIS:CA	1:H:89:LYS:HD3	2.25	0.53
1:E:92:LEU:HD11	1:E:144:TYR:CD1	2.41	0.53
1:B:96:ALA:O	1:B:155:PHE:CE2	2.62	0.53
1:B:76:ASP:HB2	1:B:212:LEU:HD23	1.91	0.53
1:D:113:GLU:OE2	1:D:184:ARG:NH2	2.40	0.53
1:E:271:ASP:OD1	1:E:275:MET:O	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:LEU:C	1:G:291:LEU:HD13	2.28	0.53
1:G:203:ILE:HG22	1:G:219:ASN:ND2	2.23	0.53
1:A:61:SER:OG	1:A:224:ARG:NH2	2.41	0.53
1:B:293:GLU:OE2	1:B:299:LYS:HE3	2.09	0.53
1:D:253:VAL:O	1:D:257:VAL:HG23	2.09	0.53
1:H:163:ALA:HB1	1:H:263:PHE:CD2	2.43	0.53
1:C:262:SER:O	1:C:262:SER:OG	2.25	0.53
1:D:260:GLU:HA	1:D:263:PHE:CE1	2.44	0.53
1:A:180:SER:HB2	1:A:183:GLU:OE2	2.09	0.53
1:B:143:ASN:O	1:B:146:LYS:HD2	2.08	0.53
1:E:73:ASP:HB2	1:E:213:HIS:CG	2.44	0.53
1:H:304:LYS:O	1:H:306:PRO:HD3	2.08	0.53
1:C:301:PHE:HD1	1:C:303:SER:OG	1.92	0.53
1:D:270:CYS:O	1:D:272:LEU:N	2.42	0.53
1:G:91:VAL:HG23	1:G:268:LEU:CD2	2.39	0.53
1:H:150:GLU:O	1:H:151:ARG:C	2.47	0.53
1:C:150:GLU:OE2	1:C:150:GLU:CA	2.37	0.53
1:E:147:ASP:OD1	1:E:148:GLU:N	2.42	0.53
1:E:282:GLN:HE21	1:E:282:GLN:C	2.11	0.53
1:G:157:ALA:HB3	3:G:365:HOH:O	2.09	0.53
1:A:94:PHE:CE1	1:A:196:PHE:CE1	2.97	0.52
1:D:144:TYR:OH	1:D:215:LEU:HB2	2.09	0.52
1:H:253:VAL:O	1:H:257:VAL:HG23	2.09	0.52
1:B:282:GLN:C	1:B:282:GLN:HE21	2.13	0.52
1:B:308:ASN:OD1	1:B:308:ASN:C	2.47	0.52
1:B:73:ASP:CG	1:B:213:HIS:HB3	2.28	0.52
1:C:235:LEU:O	1:C:238:SER:HB3	2.09	0.52
1:B:111:LEU:HD23	1:B:120:LYS:HG2	1.91	0.52
1:C:194:ILE:O	1:C:260:GLU:HG3	2.09	0.52
1:C:258:GLU:OE2	1:C:261:ARG:HD2	2.09	0.52
1:E:250:GLN:NE2	1:E:300:VAL:HG13	2.24	0.52
1:F:73:ASP:O	1:F:213:HIS:NE2	2.42	0.52
1:G:175:ILE:HG22	1:G:176:ASN:N	2.24	0.52
1:B:175:ILE:HG23	1:B:176:ASN:H	1.75	0.52
1:D:77:PHE:CD2	1:D:144:TYR:HD2	2.28	0.52
1:D:194:ILE:CD1	1:D:253:VAL:HG13	2.39	0.52
1:E:167:LYS:HD2	1:E:263:PHE:HZ	1.71	0.52
1:G:277:SER:CB	1:G:278:ARG:NH1	2.73	0.52
1:H:214:GLY:HA2	1:H:217:PHE:CB	2.36	0.52
1:H:261:ARG:NH2	1:H:285:GLU:CD	2.63	0.52
1:B:232:PHE:CE2	1:B:236:ILE:CD1	2.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD21	1:C:124:SER:N	2.25	0.52
1:E:164:ILE:HD12	1:E:164:ILE:H	1.74	0.52
1:E:63:TRP:CD1	1:E:63:TRP:N	2.77	0.52
1:H:170:TRP:CZ3	1:H:175:ILE:HD11	2.37	0.52
1:A:93:ALA:HB2	1:A:154:LEU:HD21	1.91	0.52
1:A:270:CYS:C	1:A:272:LEU:N	2.63	0.52
1:B:214:GLY:HA2	1:B:217:PHE:CB	2.36	0.52
1:B:282:GLN:O	1:B:285:GLU:HB2	2.09	0.52
1:C:111:LEU:HD23	1:C:123:TYR:CB	2.39	0.52
1:G:57:LYS:O	1:G:61:SER:CB	2.58	0.52
1:H:183:GLU:OE1	1:H:248:VAL:CG1	2.58	0.52
1:B:73:ASP:HB3	1:B:76:ASP:OD2	2.09	0.52
1:G:156:HIS:HB3	3:G:365:HOH:O	2.10	0.52
1:H:166:ASN:HD22	1:H:262:SER:HB3	1.74	0.52
1:C:182:ALA:O	1:C:186:VAL:HG23	2.10	0.52
1:D:181:PHE:HA	1:D:184:ARG:CZ	2.40	0.52
1:D:195:LEU:O	1:D:196:PHE:HB2	2.10	0.52
1:F:73:ASP:H	1:F:213:HIS:CE1	2.27	0.52
1:G:278:ARG:H	1:G:278:ARG:CD	2.14	0.52
1:G:74:LEU:O	1:G:74:LEU:HG	2.10	0.52
1:H:193:GLY:O	1:H:197:SER:OG	2.27	0.52
1:A:280:MET:HE1	1:A:283:TYR:HD2	1.75	0.52
1:A:57:LYS:O	1:A:61:SER:HB3	2.10	0.52
1:E:170:TRP:HH2	1:E:190:CYS:HB2	1.75	0.52
1:E:74:LEU:HD11	1:E:144:TYR:HA	1.92	0.52
1:G:175:ILE:HG22	1:G:176:ASN:H	1.73	0.52
1:H:133:HIS:O	1:H:136:THR:HB	2.10	0.52
1:B:210:ASN:OD1	1:B:210:ASN:N	2.43	0.51
1:C:106:LEU:O	1:C:109:LYS:HB2	2.10	0.51
1:B:121:LYS:CE	1:C:131:ASN:HB3	2.40	0.51
1:E:270:CYS:C	1:E:272:LEU:N	2.64	0.51
1:G:289:ASP:HB3	1:G:299:LYS:HG2	1.91	0.51
1:E:225:ASP:O	1:E:229:HIS:CD2	2.63	0.51
1:F:205:TRP:CD1	1:F:273:ILE:HG12	2.45	0.51
1:G:171:ALA:HA	1:G:175:ILE:HD12	1.91	0.51
1:H:235:LEU:O	1:H:239:LEU:HG	2.10	0.51
1:C:141:ILE:HG23	1:C:145:ILE:HD13	1.91	0.51
1:D:264:ILE:H	1:D:264:ILE:HD12	1.74	0.51
1:E:64:THR:OG1	1:E:65:ALA:N	2.36	0.51
1:G:157:ALA:CB	3:G:365:HOH:O	2.58	0.51
1:H:285:GLU:HA	1:H:285:GLU:OE1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLU:OE2	1:B:301:PHE:CE2	2.64	0.51
1:C:271:ASP:HB2	1:C:277:SER:HB2	1.93	0.51
1:F:233:ASN:HA	1:F:236:ILE:HD12	1.85	0.51
1:D:264:ILE:HD12	1:D:264:ILE:N	2.25	0.51
1:E:123:TYR:OH	1:E:233:ASN:OD1	2.27	0.51
1:G:277:SER:HB3	1:G:278:ARG:HH11	1.76	0.51
1:H:270:CYS:SG	1:H:280:MET:SD	3.09	0.51
1:A:139:LEU:O	1:A:142:ASP:HB3	2.09	0.51
1:D:214:GLY:HA2	1:D:217:PHE:CB	2.40	0.51
1:D:47:MET:O	1:D:49:PRO:CD	2.59	0.51
1:E:270:CYS:O	1:E:272:LEU:N	2.40	0.51
1:F:142:ASP:O	1:F:142:ASP:OD2	2.29	0.51
1:H:154:LEU:O	1:H:158:ILE:HB	2.09	0.51
1:D:218:SER:O	1:D:219:ASN:C	2.47	0.51
1:G:196:PHE:N	1:G:260:GLU:OE1	2.43	0.51
1:D:82:VAL:CG2	1:D:83:ASN:N	2.73	0.51
1:G:250:GLN:HG2	1:G:300:VAL:CG2	2.41	0.51
1:E:177:ASP:CG	1:E:178:THR:H	2.14	0.51
1:G:213:HIS:O	1:G:213:HIS:CG	2.52	0.51
1:C:77:PHE:HA	1:C:80:LEU:HD22	1.92	0.51
1:H:231:ASP:O	1:H:234:CYS:HB2	2.10	0.51
1:B:214:GLY:HA2	1:B:217:PHE:N	2.24	0.50
1:E:147:ASP:C	1:E:147:ASP:OD1	2.50	0.50
1:F:137:TYR:O	1:F:141:ILE:HD12	2.10	0.50
1:H:279:LEU:HB3	1:H:307:PHE:CZ	2.45	0.50
1:B:229:HIS:N	1:B:229:HIS:CD2	2.78	0.50
1:F:81:ASN:HB2	1:F:84:GLU:N	2.22	0.50
1:G:91:VAL:HG23	1:G:268:LEU:HD21	1.93	0.50
1:A:213:HIS:HD2	1:A:215:LEU:H	1.59	0.50
1:B:212:LEU:CA	1:B:213:HIS:HD2	2.24	0.50
1:D:213:HIS:CD2	1:D:213:HIS:C	2.83	0.50
1:E:237:TYR:HA	1:E:240:LEU:HD22	1.93	0.50
1:G:271:ASP:OD1	1:G:276:ASN:HA	2.11	0.50
1:A:185:ILE:HG22	1:A:233:ASN:HB3	1.93	0.50
1:B:247:ASN:ND2	1:B:247:ASN:N	2.58	0.50
1:E:175:ILE:CG2	1:E:176:ASN:N	2.74	0.50
1:G:154:LEU:HG	1:G:158:ILE:CG1	2.40	0.50
1:B:212:LEU:HA	1:B:213:HIS:HD2	1.76	0.50
1:B:64:THR:HG23	1:B:66:GLU:H	1.77	0.50
1:G:163:ALA:CB	1:G:263:PHE:HD2	2.24	0.50
1:H:81:ASN:OD1	1:H:84:GLU:CG	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:PHE:HE1	1:E:188:ASN:ND2	2.09	0.50
1:E:145:ILE:CG2	1:E:150:GLU:HB3	2.42	0.50
1:E:164:ILE:N	1:E:164:ILE:CD1	2.73	0.50
1:G:110:PHE:HA	1:G:113:GLU:OE1	2.11	0.50
1:G:213:HIS:CD2	1:G:213:HIS:C	2.85	0.50
1:G:198:GLY:HA2	1:G:280:MET:CE	2.42	0.50
1:A:77:PHE:CD1	1:A:77:PHE:C	2.83	0.50
1:A:214:GLY:HA2	1:A:217:PHE:H	1.76	0.50
1:B:212:LEU:HA	1:B:213:HIS:CD2	2.47	0.50
1:B:221:LEU:HD23	1:B:221:LEU:N	2.27	0.50
1:D:64:THR:OG1	1:D:65:ALA:N	2.44	0.50
1:E:54:PHE:HB3	1:E:122:PHE:CE2	2.47	0.50
1:F:250:GLN:NE2	1:F:300:VAL:CG1	2.71	0.50
1:H:59:GLU:HA	1:H:125:PHE:CZ	2.47	0.50
1:H:271:ASP:HA	1:H:275:MET:O	2.12	0.50
1:F:113:GLU:OE2	1:F:181:PHE:HD1	1.95	0.50
1:H:106:LEU:HG	1:H:188:ASN:HD21	1.77	0.50
1:A:253:VAL:HG11	1:A:292:LEU:CD2	2.41	0.49
1:B:153:ASN:OD1	1:B:153:ASN:O	2.29	0.49
1:D:191:VAL:HA	1:D:195:LEU:HD12	1.94	0.49
1:D:217:PHE:CD1	1:D:217:PHE:O	2.65	0.49
1:H:151:ARG:O	1:H:155:PHE:HD1	1.95	0.49
1:H:81:ASN:OD1	1:H:84:GLU:HG2	2.12	0.49
1:A:261:ARG:HA	1:A:264:ILE:HD12	1.94	0.49
1:F:301:PHE:HD1	1:F:303:SER:OG	1.94	0.49
1:G:73:ASP:O	1:G:213:HIS:CE1	2.65	0.49
1:H:208:LYS:HA	1:H:208:LYS:HE3	1.94	0.49
1:H:265:CYS:HB2	1:H:277:SER:HB2	1.93	0.49
1:A:308:ASN:HD22	1:A:308:ASN:N	2.04	0.49
1:B:175:ILE:CG2	1:B:176:ASN:H	2.23	0.49
1:C:203:ILE:HG22	1:C:216:THR:HG22	1.94	0.49
1:C:247:ASN:ND2	1:C:247:ASN:H	2.10	0.49
1:C:174:TRP:CD1	1:C:252:ILE:HG23	2.48	0.49
1:G:87:PHE:CD1	1:G:268:LEU:HG	2.47	0.49
1:H:174:TRP:HE3	1:H:183:GLU:HG2	1.77	0.49
1:C:90:HIS:CB	1:C:268:LEU:HD21	2.42	0.49
1:E:86:HIS:O	1:E:90:HIS:HD2	1.95	0.49
1:F:232:PHE:CD2	1:F:236:ILE:HD11	2.47	0.49
1:A:301:PHE:CE1	1:A:303:SER:HB3	2.48	0.49
1:C:84:GLU:HB3	1:C:273:ILE:HA	1.93	0.49
1:D:73:ASP:HB2	1:D:213:HIS:CG	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:LEU:HD12	1:E:297:CYS:C	2.33	0.49
1:H:187:ALA:O	1:H:191:VAL:HG23	2.13	0.49
1:G:57:LYS:O	1:G:61:SER:HB3	2.13	0.49
1:C:285:GLU:HB3	1:C:301:PHE:CD1	2.47	0.49
1:E:106:LEU:CD2	1:E:188:ASN:HD21	2.25	0.49
1:E:77:PHE:CE2	1:E:144:TYR:HB3	2.47	0.49
1:E:55:TYR:CE2	1:E:121:LYS:HG2	2.47	0.49
1:B:299:LYS:HB2	1:B:302:HIS:CD2	2.48	0.49
1:G:81:ASN:O	1:G:85:LYS:HD3	2.13	0.49
1:A:77:PHE:HZ	1:A:89:LYS:HE2	1.78	0.49
1:B:105:ASN:ND2	1:B:109:LYS:HG2	2.28	0.49
1:E:168:ALA:O	1:E:171:ALA:HB3	2.12	0.49
1:F:81:ASN:HB2	1:F:84:GLU:HB2	1.94	0.49
1:B:69:ASP:C	1:B:71:SER:H	2.15	0.49
1:C:309:TRP:O	3:C:351:HOH:O	2.20	0.49
1:F:235:LEU:HA	1:F:238:SER:HB3	1.94	0.49
1:A:72:SER:HB2	3:A:365:HOH:O	2.11	0.48
1:B:76:ASP:CB	1:B:212:LEU:HD23	2.43	0.48
1:F:273:ILE:O	1:F:273:ILE:HG12	2.13	0.48
1:G:106:LEU:HD21	1:G:188:ASN:HD22	1.77	0.48
1:C:150:GLU:O	1:C:152:LEU:N	2.46	0.48
1:D:247:ASN:H	1:D:247:ASN:HD22	1.58	0.48
1:E:141:ILE:HA	1:E:145:ILE:CD1	2.43	0.48
1:F:166:ASN:HB3	1:F:259:VAL:HG22	1.94	0.48
1:F:285:GLU:OE1	1:F:285:GLU:HA	2.13	0.48
1:H:115:GLU:C	1:H:120:LYS:NZ	2.67	0.48
1:A:299:LYS:HD2	1:A:302:HIS:CD2	2.49	0.48
1:A:69:ASP:O	1:A:71:SER:N	2.46	0.48
1:H:270:CYS:O	1:H:272:LEU:N	2.46	0.48
1:C:282:GLN:HA	1:C:285:GLU:CG	2.44	0.48
1:F:145:ILE:HG23	3:F:365:HOH:O	2.12	0.48
1:F:233:ASN:CA	1:F:236:ILE:HD12	2.40	0.48
1:D:146:LYS:CE	3:D:360:HOH:O	2.59	0.48
1:H:130:GLU:HA	1:H:133:HIS:ND1	2.28	0.48
1:H:217:PHE:CZ	1:H:221:LEU:HD11	2.48	0.48
1:H:214:GLY:HA2	1:H:217:PHE:N	2.29	0.48
1:A:70:LEU:CD2	1:A:140:LEU:CD1	2.91	0.48
1:A:144:TYR:HH	1:A:213:HIS:CE1	2.26	0.48
1:A:236:ILE:HD12	1:A:236:ILE:N	2.28	0.48
1:B:86:HIS:HA	1:B:89:LYS:HB2	1.95	0.48
1:C:166:ASN:ND2	1:C:262:SER:CB	2.76	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ALA:CB	1:F:158:ILE:HD12	2.44	0.48
1:G:212:LEU:CD1	1:G:215:LEU:HD23	2.43	0.48
1:H:205:TRP:HZ3	1:H:309:TRP:HZ2	1.61	0.48
1:H:232:PHE:CD2	1:H:236:ILE:HD11	2.49	0.48
1:A:94:PHE:CE2	1:A:164:ILE:HD11	2.48	0.48
1:C:141:ILE:O	1:C:145:ILE:HB	2.14	0.48
1:E:107:ALA:HB1	1:E:123:TYR:HD1	1.78	0.48
1:E:139:LEU:HA	1:E:139:LEU:HD12	1.22	0.48
1:F:213:HIS:O	1:F:213:HIS:CG	2.61	0.48
1:B:194:ILE:HD11	1:B:253:VAL:HG13	1.94	0.48
1:G:161:ILE:HB	1:G:162:PRO:HD2	1.96	0.48
1:G:262:SER:HA	1:G:266:GLU:HB2	1.95	0.48
1:G:277:SER:HB3	1:G:278:ARG:NH1	2.29	0.48
1:G:73:ASP:HB3	1:G:76:ASP:HB2	1.95	0.48
1:A:200:PHE:O	1:A:204:PHE:HD1	1.97	0.48
1:A:307:PHE:HB3	1:A:309:TRP:CE2	2.48	0.48
1:E:276:ASN:OD1	1:E:278:ARG:N	2.46	0.48
1:G:277:SER:HB2	1:G:278:ARG:NH1	2.29	0.48
1:H:110:PHE:N	1:H:110:PHE:CD1	2.81	0.48
1:H:73:ASP:CB	1:H:76:ASP:OD2	2.61	0.48
1:A:114:VAL:HG12	1:A:116:ILE:HG13	1.94	0.48
1:D:208:LYS:O	1:D:208:LYS:HG3	2.14	0.48
1:D:282:GLN:HA	1:D:285:GLU:HG3	1.96	0.48
1:E:282:GLN:NE2	1:E:282:GLN:O	2.47	0.48
1:F:289:ASP:HB3	1:F:299:LYS:CD	2.44	0.48
1:G:123:TYR:CZ	1:G:232:PHE:HE2	2.32	0.48
1:A:86:HIS:HE1	1:A:89:LYS:HD2	1.69	0.47
1:A:94:PHE:CE1	1:A:196:PHE:HE1	2.32	0.47
1:E:249:VAL:O	1:E:253:VAL:HG23	2.13	0.47
1:E:276:ASN:HB3	1:E:279:LEU:HB2	1.96	0.47
1:F:270:CYS:C	1:F:272:LEU:N	2.68	0.47
1:G:249:VAL:HG12	1:G:292:LEU:HD11	1.95	0.47
1:G:305:ASN:ND2	1:G:307:PHE:O	2.47	0.47
1:F:285:GLU:HB3	1:F:301:PHE:CG	2.49	0.47
1:H:109:LYS:HZ1	1:H:176:ASN:HA	1.78	0.47
1:H:207:LYS:HB2	1:H:216:THR:HB	1.96	0.47
1:B:280:MET:HA	1:B:280:MET:HE3	1.97	0.47
1:E:73:ASP:OD2	1:E:213:HIS:HB3	2.14	0.47
1:B:214:GLY:CA	1:B:217:PHE:H	2.27	0.47
1:C:98:SER:HB3	1:C:167:LYS:HZ1	1.77	0.47
1:D:144:TYR:HH	1:D:213:HIS:CE1	2.31	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:LEU:HD12	1:E:297:CYS:CA	2.44	0.47
1:F:175:ILE:HG13	1:F:187:ALA:CB	2.44	0.47
1:G:81:ASN:C	1:G:83:ASN:H	2.16	0.47
1:A:282:GLN:HA	1:A:285:GLU:HG3	1.95	0.47
1:D:276:ASN:OD1	1:D:279:LEU:N	2.35	0.47
1:G:68:ILE:HG12	1:G:217:PHE:HE2	1.79	0.47
1:H:195:LEU:O	1:H:196:PHE:HB2	2.13	0.47
1:H:48:TYR:N	1:H:48:TYR:CD1	2.83	0.47
1:B:282:GLN:NE2	1:B:306:PRO:CD	2.64	0.47
1:C:276:ASN:HB3	1:C:279:LEU:HB2	1.95	0.47
1:E:143:ASN:O	1:E:146:LYS:HG3	2.14	0.47
1:E:187:ALA:O	1:E:191:VAL:HG23	2.14	0.47
1:F:150:GLU:HA	1:F:150:GLU:OE1	2.14	0.47
1:A:253:VAL:O	1:A:257:VAL:HG23	2.15	0.47
1:B:231:ASP:O	1:B:234:CYS:HB2	2.15	0.47
1:B:237:TYR:CZ	1:B:243:LYS:HG3	2.50	0.47
1:E:63:TRP:CZ3	1:E:221:LEU:HD12	2.49	0.47
1:H:276:ASN:HB3	1:H:279:LEU:HB2	1.96	0.47
1:B:58:ALA:HB2	1:B:228:LEU:HD21	1.96	0.47
1:C:152:LEU:C	1:C:154:LEU:H	2.18	0.47
1:E:280:MET:HE2	1:E:284:ILE:HD11	1.95	0.47
1:H:233:ASN:HA	1:H:236:ILE:HD11	1.84	0.47
1:A:87:PHE:CD2	1:A:273:ILE:CG2	2.97	0.47
1:B:212:LEU:C	1:B:213:HIS:CD2	2.88	0.47
1:F:93:ALA:HB1	1:F:158:ILE:HD12	1.96	0.47
1:B:181:PHE:CE1	1:B:185:ILE:HD11	2.50	0.47
1:C:122:PHE:HE2	1:C:228:LEU:HD21	1.77	0.47
1:E:110:PHE:CE1	1:E:188:ASN:ND2	2.83	0.47
1:E:253:VAL:O	1:E:257:VAL:HG23	2.15	0.47
1:E:271:ASP:HB2	1:E:277:SER:HB2	1.97	0.47
1:F:163:ALA:CB	1:F:263:PHE:CD2	2.92	0.47
1:A:213:HIS:HB2	3:A:365:HOH:O	2.14	0.47
1:D:145:ILE:O	1:D:145:ILE:HG22	2.15	0.47
1:D:47:MET:O	1:D:49:PRO:HD3	2.15	0.47
1:D:94:PHE:HE2	1:D:164:ILE:HD13	1.76	0.47
1:G:257:VAL:O	1:G:261:ARG:HG3	2.15	0.47
1:G:48:TYR:CD1	1:G:48:TYR:N	2.82	0.47
1:G:69:ASP:C	1:G:71:SER:H	2.19	0.47
1:H:170:TRP:CH2	1:H:187:ALA:HB1	2.50	0.47
1:H:260:GLU:HG3	1:H:284:ILE:HD12	1.97	0.47
1:H:126:GLN:NE2	3:H:358:HOH:O	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ASP:CG	1:B:178:THR:H	2.18	0.46
1:B:86:HIS:CD2	1:B:89:LYS:HD2	2.51	0.46
1:D:158:ILE:C	1:D:160:ASN:H	2.19	0.46
1:D:73:ASP:OD2	1:D:213:HIS:HB3	2.15	0.46
1:E:191:VAL:HA	1:E:195:LEU:HD12	1.97	0.46
1:E:251:ASN:O	1:E:255:GLU:HG3	2.16	0.46
1:H:270:CYS:C	1:H:272:LEU:N	2.63	0.46
1:B:194:ILE:O	1:B:197:SER:HB2	2.15	0.46
1:C:207:LYS:HB2	1:C:216:THR:HB	1.96	0.46
1:C:257:VAL:HG21	1:C:288:ALA:HB2	1.96	0.46
1:D:51:VAL:HG13	1:D:232:PHE:HE1	1.80	0.46
1:E:177:ASP:CG	1:E:178:THR:N	2.69	0.46
1:F:285:GLU:CG	1:F:301:PHE:CE1	2.92	0.46
1:B:194:ILE:CD1	1:B:253:VAL:HG13	2.46	0.46
1:C:175:ILE:HG22	1:C:176:ASN:H	1.79	0.46
1:D:149:LYS:HD3	1:D:149:LYS:C	2.36	0.46
1:F:163:ALA:HB1	1:F:263:PHE:CE2	2.51	0.46
1:B:113:GLU:O	1:B:115:GLU:HG2	2.15	0.46
1:B:151:ARG:HG3	1:B:151:ARG:O	2.15	0.46
1:C:90:HIS:CB	1:C:268:LEU:CD2	2.94	0.46
1:D:240:LEU:HA	1:D:240:LEU:HD12	1.50	0.46
1:D:264:ILE:O	1:D:269:PRO:HA	2.15	0.46
1:E:170:TRP:HE1	1:E:255:GLU:HB2	1.80	0.46
1:B:249:VAL:HA	1:B:252:ILE:HD12	1.97	0.46
1:C:214:GLY:HA2	1:C:217:PHE:N	2.30	0.46
1:C:203:ILE:CG2	1:C:216:THR:HG22	2.46	0.46
1:C:54:PHE:HA	1:C:54:PHE:HD2	1.66	0.46
1:D:111:LEU:CD2	1:D:120:LYS:HB3	2.43	0.46
1:D:167:LYS:HZ2	1:D:195:LEU:HD13	1.79	0.46
1:D:70:LEU:HD21	1:D:140:LEU:HD11	1.97	0.46
1:E:71:SER:CB	3:E:365:HOH:O	2.57	0.46
1:F:293:GLU:OE1	1:F:299:LYS:HE3	2.15	0.46
1:G:139:LEU:O	1:G:142:ASP:HB3	2.16	0.46
1:G:147:ASP:OD2	1:G:149:LYS:HB2	2.15	0.46
1:B:163:ALA:CB	1:B:263:PHE:CD2	2.54	0.46
1:D:253:VAL:O	1:D:254:LYS:C	2.54	0.46
1:E:50:GLU:HG2	1:E:235:LEU:CD2	2.45	0.46
1:F:270:CYS:O	1:F:272:LEU:N	2.48	0.46
1:F:81:ASN:HB3	1:F:83:ASN:N	2.29	0.46
1:H:249:VAL:HA	1:H:252:ILE:HD12	1.96	0.46
1:A:213:HIS:CD2	1:A:213:HIS:O	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:MET:O	1:B:283:TYR:HB3	2.16	0.46
1:B:81:ASN:OD1	1:B:81:ASN:C	2.54	0.46
1:D:155:PHE:O	1:D:159:GLU:HB2	2.15	0.46
1:E:262:SER:HA	1:E:266:GLU:HB2	1.97	0.46
1:G:237:TYR:O	1:G:240:LEU:HB2	2.15	0.46
1:B:93:ALA:O	1:B:155:PHE:CE2	2.69	0.45
1:D:158:ILE:O	1:D:160:ASN:N	2.49	0.45
1:E:63:TRP:CZ3	1:E:68:ILE:HD11	2.51	0.45
1:G:185:ILE:HD12	1:G:236:ILE:HG23	1.98	0.45
1:B:247:ASN:ND2	1:B:247:ASN:H	2.07	0.45
1:B:273:ILE:HG13	1:B:275:MET:HG3	1.98	0.45
1:B:87:PHE:CD2	1:B:273:ILE:HG21	2.51	0.45
1:B:52:TRP:NE1	3:B:360:HOH:O	2.48	0.45
1:C:122:PHE:CE2	1:C:228:LEU:CD2	3.00	0.45
1:C:90:HIS:HB2	1:C:268:LEU:HD21	1.97	0.45
1:H:261:ARG:HH12	1:H:281:SER:HB3	1.81	0.45
1:B:118:GLU:CD	1:B:118:GLU:H	2.20	0.45
1:C:81:ASN:CG	1:C:84:GLU:HG2	2.37	0.45
1:D:186:VAL:HG11	1:D:249:VAL:HG13	1.97	0.45
1:E:171:ALA:HA	1:E:175:ILE:HD12	1.98	0.45
1:F:48:TYR:N	1:F:48:TYR:CD1	2.85	0.45
1:G:87:PHE:CZ	1:G:91:VAL:HG21	2.49	0.45
1:G:121:LYS:NZ	1:H:135:GLU:OE1	2.44	0.45
1:H:307:PHE:CD1	1:H:309:TRP:CZ2	3.04	0.45
1:A:175:ILE:O	1:A:176:ASN:C	2.54	0.45
1:B:166:ASN:HD22	1:B:262:SER:CB	2.29	0.45
1:C:153:ASN:O	1:C:153:ASN:ND2	2.49	0.45
1:D:126:GLN:NE2	1:D:192:GLU:OE2	2.50	0.45
1:E:282:GLN:HE21	1:E:306:PRO:CG	2.28	0.45
1:H:240:LEU:HD23	1:H:243:LYS:HG2	1.98	0.45
1:H:64:THR:HG23	1:H:66:GLU:H	1.80	0.45
1:B:240:LEU:HB3	1:B:243:LYS:HD3	1.98	0.45
1:B:282:GLN:NE2	1:B:306:PRO:HB3	2.31	0.45
1:D:94:PHE:CE2	1:D:164:ILE:HD11	2.51	0.45
1:D:166:ASN:ND2	1:D:262:SER:HB2	2.31	0.45
1:E:167:LYS:CD	1:E:263:PHE:HZ	2.29	0.45
1:F:276:ASN:OD1	1:F:278:ARG:N	2.49	0.45
1:G:178:THR:O	1:G:178:THR:OG1	2.33	0.45
1:H:109:LYS:HZ3	1:H:176:ASN:HA	1.79	0.45
1:C:246:GLU:O	1:C:250:GLN:HB2	2.17	0.45
1:D:110:PHE:CD2	1:D:181:PHE:HE1	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:PRO:O	1:E:272:LEU:HB2	2.16	0.45
1:E:64:THR:HG23	1:E:66:GLU:HG2	1.99	0.45
1:F:195:LEU:O	1:F:196:PHE:HB2	2.16	0.45
1:F:233:ASN:C	1:F:236:ILE:HD12	2.37	0.45
1:G:87:PHE:CE2	1:G:91:VAL:CG2	2.87	0.45
1:H:141:ILE:HA	1:H:145:ILE:HD12	1.99	0.45
1:H:212:LEU:CB	1:H:215:LEU:HD23	2.47	0.45
1:C:110:PHE:O	1:C:114:VAL:HG23	2.17	0.45
1:G:154:LEU:HA	1:G:158:ILE:HB	1.99	0.45
1:G:263:PHE:N	1:G:263:PHE:CD2	2.81	0.45
1:B:156:HIS:O	1:B:157:ALA:CB	2.64	0.45
1:B:73:ASP:OD2	1:B:213:HIS:HB3	2.17	0.45
1:D:149:LYS:NZ	3:D:354:HOH:O	2.45	0.45
1:D:270:CYS:C	1:D:272:LEU:H	2.20	0.45
1:F:154:LEU:HA	1:F:154:LEU:HD12	1.70	0.45
1:A:301:PHE:HD1	1:A:303:SER:OG	2.00	0.45
1:A:56:LYS:NZ	1:A:59:GLU:OE1	2.50	0.45
1:B:104:GLU:OE1	1:B:106:LEU:HD12	2.17	0.45
1:C:130:GLU:O	1:C:133:HIS:HB2	2.17	0.45
1:E:144:TYR:OH	1:E:213:HIS:NE2	2.45	0.45
1:A:115:GLU:CA	1:A:120:LYS:HZ2	2.17	0.44
1:A:264:ILE:HG13	1:A:264:ILE:H	1.38	0.44
1:A:299:LYS:HB2	1:A:302:HIS:NE2	2.33	0.44
1:D:56:LYS:NZ	1:D:59:GLU:OE1	2.50	0.44
1:E:73:ASP:CG	1:E:213:HIS:HB3	2.37	0.44
1:F:152:LEU:C	1:F:154:LEU:H	2.20	0.44
1:G:271:ASP:HA	1:G:275:MET:O	2.17	0.44
1:H:280:MET:CA	3:H:357:HOH:O	2.39	0.44
1:A:200:PHE:O	1:A:204:PHE:CD1	2.70	0.44
1:C:283:TYR:O	1:C:287:VAL:HG23	2.17	0.44
1:B:213:HIS:O	1:B:213:HIS:CG	2.68	0.44
1:C:213:HIS:CD2	1:C:213:HIS:O	2.70	0.44
1:D:131:ASN:HA	1:D:131:ASN:HD22	1.53	0.44
1:D:277:SER:HB3	1:D:278:ARG:HH11	1.82	0.44
1:D:232:PHE:CZ	1:D:236:ILE:HD11	2.52	0.44
1:D:57:LYS:O	1:D:61:SER:CB	2.63	0.44
1:E:86:HIS:NE2	1:E:89:LYS:HD2	2.25	0.44
1:F:285:GLU:CB	1:F:301:PHE:CD1	3.01	0.44
1:G:181:PHE:CE2	1:G:185:ILE:HD11	2.52	0.44
1:H:279:LEU:HB3	1:H:307:PHE:HZ	1.82	0.44
1:A:205:TRP:HE1	1:A:274:GLY:HA3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:CD	1:A:278:ARG:N	2.80	0.44
1:B:301:PHE:O	1:B:302:HIS:O	2.35	0.44
1:C:143:ASN:N	1:C:143:ASN:ND2	2.66	0.44
1:D:88:ILE:HD11	1:D:206:PHE:CZ	2.53	0.44
1:E:118:GLU:OE2	1:E:118:GLU:N	2.38	0.44
1:E:273:ILE:HD13	1:E:273:ILE:HG21	1.60	0.44
1:H:69:ASP:C	1:H:71:SER:H	2.21	0.44
1:C:109:LYS:HB3	1:C:109:LYS:HE2	1.75	0.44
1:F:113:GLU:OE2	1:F:181:PHE:CD1	2.70	0.44
1:F:299:LYS:HB2	1:F:299:LYS:HZ2	1.83	0.44
1:A:283:TYR:O	1:A:287:VAL:HG23	2.18	0.44
1:D:163:ALA:HB2	1:D:263:PHE:HD2	1.83	0.44
1:G:264:ILE:HA	1:G:268:LEU:O	2.17	0.44
1:G:270:CYS:O	1:G:272:LEU:N	2.49	0.44
1:H:271:ASP:CG	1:H:277:SER:H	2.20	0.44
1:B:277:SER:OG	1:B:278:ARG:NH1	2.50	0.44
1:B:90:HIS:CE1	1:B:93:ALA:HB3	2.51	0.44
1:C:141:ILE:HA	1:C:145:ILE:HD13	1.99	0.44
1:E:86:HIS:NE2	1:E:89:LYS:CE	2.80	0.44
1:H:58:ALA:HB2	1:H:228:LEU:HD21	1.99	0.44
1:H:92:LEU:HD11	1:H:144:TYR:HD1	1.83	0.44
1:A:57:LYS:O	1:A:61:SER:HB2	2.18	0.43
1:C:258:GLU:OE2	1:C:261:ARG:NH1	2.48	0.43
1:H:279:LEU:HD13	1:H:307:PHE:CZ	2.52	0.43
1:B:130:GLU:OE1	1:B:226:GLU:OE2	2.36	0.43
1:C:146:LYS:HG3	1:C:147:ASP:H	1.83	0.43
1:E:94:PHE:HE2	1:E:164:ILE:HD11	1.84	0.43
1:A:142:ASP:OD2	1:A:142:ASP:O	2.36	0.43
1:A:207:LYS:HB2	1:A:216:THR:HB	1.99	0.43
1:B:133:HIS:ND1	1:B:222:ILE:HG12	2.34	0.43
1:C:154:LEU:HA	1:C:157:ALA:HB3	2.00	0.43
1:D:231:ASP:O	1:D:234:CYS:HB2	2.19	0.43
1:E:279:LEU:HD23	1:E:306:PRO:HB3	1.95	0.43
1:A:52:TRP:CZ2	1:D:135:GLU:OE2	2.70	0.43
1:E:77:PHE:CZ	1:E:89:LYS:HE2	2.54	0.43
1:B:77:PHE:CD2	1:B:144:TYR:CE2	3.05	0.43
1:D:299:LYS:HZ3	1:D:302:HIS:HD2	1.65	0.43
1:G:167:LYS:NZ	1:G:195:LEU:HD13	2.33	0.43
1:B:144:TYR:C	1:B:145:ILE:HG13	2.37	0.43
1:B:77:PHE:CE2	1:B:144:TYR:CD2	3.05	0.43
1:C:56:LYS:NZ	1:C:59:GLU:OE2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG13	1:D:232:PHE:CE1	2.53	0.43
1:E:86:HIS:CE1	1:E:89:LYS:CD	2.82	0.43
1:F:128:ALA:O	1:F:131:ASN:HB2	2.18	0.43
1:G:114:VAL:HG12	1:G:116:ILE:HG13	2.00	0.43
1:G:182:ALA:HB1	1:G:244:LEU:HG	2.01	0.43
1:A:59:GLU:C	1:A:61:SER:H	2.21	0.43
1:F:292:LEU:HD21	1:F:300:VAL:HG22	2.01	0.43
1:G:81:ASN:HB3	1:G:84:GLU:CB	2.32	0.43
1:H:212:LEU:HB3	1:H:215:LEU:HB3	1.99	0.43
1:A:94:PHE:HE2	1:A:164:ILE:CD1	2.32	0.43
1:C:77:PHE:CD2	1:C:144:TYR:CE2	3.06	0.43
1:D:307:PHE:HB3	1:D:309:TRP:NE1	2.34	0.43
1:D:87:PHE:CD2	1:D:273:ILE:HG21	2.53	0.43
1:E:285:GLU:H	1:E:285:GLU:HG2	1.54	0.43
1:G:68:ILE:CG1	1:G:217:PHE:HE2	2.32	0.43
1:G:89:LYS:HA	1:G:145:ILE:HD11	2.01	0.43
1:H:273:ILE:HG13	1:H:275:MET:HG3	2.01	0.43
1:B:232:PHE:CD2	1:B:236:ILE:HD13	2.54	0.43
1:C:263:PHE:CD2	1:C:263:PHE:N	2.85	0.43
1:F:73:ASP:HB2	1:F:213:HIS:CG	2.54	0.43
1:H:73:ASP:CG	1:H:76:ASP:OD2	2.57	0.43
1:A:93:ALA:CB	1:A:158:ILE:HD11	2.49	0.43
1:A:182:ALA:O	1:A:186:VAL:HG23	2.18	0.43
1:E:164:ILE:CD1	1:E:164:ILE:H	2.32	0.43
1:G:86:HIS:HA	1:G:89:LYS:HG3	2.01	0.43
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.98	0.42
1:C:173:LYS:HE3	1:C:174:TRP:CZ2	2.54	0.42
1:E:114:VAL:O	1:E:114:VAL:HG12	2.19	0.42
1:E:141:ILE:HG23	1:E:145:ILE:HD13	2.01	0.42
1:E:248:VAL:O	1:E:251:ASN:HB2	2.18	0.42
1:H:213:HIS:HD2	1:H:213:HIS:O	1.96	0.42
1:A:175:ILE:CD1	1:A:191:VAL:HG21	2.49	0.42
1:C:195:LEU:O	1:C:196:PHE:CB	2.66	0.42
1:D:240:LEU:HB3	1:D:243:LYS:HG3	2.00	0.42
1:E:235:LEU:HA	1:E:238:SER:HB2	2.01	0.42
1:E:299:LYS:HB2	1:E:302:HIS:CE1	2.53	0.42
1:G:229:HIS:N	1:G:229:HIS:CD2	2.86	0.42
1:G:253:VAL:HG11	1:G:292:LEU:CD2	2.49	0.42
1:H:150:GLU:O	1:H:153:ASN:N	2.52	0.42
1:H:186:VAL:HG12	1:H:252:ILE:HG21	2.02	0.42
1:B:150:GLU:C	1:B:152:LEU:H	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ASP:O	1:B:213:HIS:NE2	2.52	0.42
1:B:56:LYS:NZ	1:C:66:GLU:OE2	2.50	0.42
1:D:300:VAL:O	1:D:300:VAL:HG12	2.19	0.42
1:E:95:PHE:CE1	1:E:196:PHE:CD1	3.07	0.42
1:F:279:LEU:HD23	1:F:279:LEU:HA	1.80	0.42
1:G:104:GLU:OE1	1:G:105:ASN:N	2.51	0.42
1:G:146:LYS:HD3	1:G:146:LYS:N	2.34	0.42
1:A:216:THR:O	1:A:219:ASN:HB3	2.19	0.42
1:A:280:MET:CE	1:A:283:TYR:HD2	2.32	0.42
1:D:275:MET:CE	1:D:309:TRP:HH2	2.33	0.42
1:D:94:PHE:CD1	1:D:196:PHE:HE1	2.37	0.42
1:E:214:GLY:HA2	1:E:217:PHE:N	2.33	0.42
1:G:214:GLY:HA2	1:G:217:PHE:N	2.32	0.42
1:G:57:LYS:O	1:G:61:SER:HB2	2.19	0.42
1:H:86:HIS:HB3	3:H:351:HOH:O	2.20	0.42
1:A:144:TYR:HE1	1:A:215:LEU:HD22	1.84	0.42
1:C:148:GLU:CG	1:C:148:GLU:O	2.57	0.42
1:D:175:ILE:CG2	1:D:176:ASN:N	2.70	0.42
1:E:281:SER:O	1:E:285:GLU:CG	2.63	0.42
1:F:129:VAL:HA	1:F:132:ILE:HD12	2.00	0.42
1:F:109:LYS:NZ	1:F:176:ASN:HA	2.34	0.42
1:F:202:ALA:O	1:F:205:TRP:HB3	2.19	0.42
1:G:282:GLN:HA	1:G:285:GLU:HG3	2.02	0.42
1:B:237:TYR:CZ	1:B:243:LYS:CG	3.03	0.42
1:F:110:PHE:HZ	1:F:184:ARG:HB3	1.85	0.42
1:B:264:ILE:HA	1:B:268:LEU:O	2.19	0.42
1:C:81:ASN:O	1:C:85:LYS:HB2	2.20	0.42
1:D:150:GLU:O	1:D:154:LEU:HB2	2.19	0.42
1:D:224:ARG:HB3	1:D:224:ARG:HE	1.70	0.42
1:F:264:ILE:HD12	1:F:265:CYS:SG	2.60	0.42
1:A:62:PHE:HD2	1:A:125:PHE:CZ	2.38	0.42
1:A:161:ILE:HA	1:A:161:ILE:HD13	1.80	0.42
1:A:161:ILE:O	1:A:163:ALA:N	2.52	0.42
1:A:182:ALA:HB1	1:A:244:LEU:HG	2.01	0.42
1:E:237:TYR:HE1	1:E:295:LEU:O	2.01	0.42
1:B:179:ASN:H	1:B:184:ARG:HH12	1.68	0.42
1:B:198:GLY:HA3	1:B:264:ILE:HG12	2.01	0.42
1:B:166:ASN:HB3	1:B:259:VAL:HG22	2.01	0.42
1:D:77:PHE:HD2	1:D:144:TYR:CD2	2.33	0.42
1:E:107:ALA:HB1	1:E:123:TYR:CD1	2.55	0.42
1:F:69:ASP:C	1:F:71:SER:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:HIS:O	1:G:213:HIS:HD2	1.94	0.42
1:A:263:PHE:N	1:A:263:PHE:CD2	2.86	0.42
1:B:54:PHE:C	1:B:122:PHE:HE2	2.23	0.42
1:B:47:MET:HG2	3:B:354:HOH:O	2.19	0.42
1:C:214:GLY:CA	1:C:217:PHE:H	2.33	0.42
1:C:250:GLN:CD	1:C:300:VAL:HG21	2.40	0.42
1:C:163:ALA:CB	1:C:263:PHE:CD2	3.03	0.42
1:F:48:TYR:HD1	1:F:118:GLU:OE2	2.03	0.42
1:F:72:SER:O	1:F:73:ASP:OD1	2.37	0.42
1:F:77:PHE:HZ	1:F:89:LYS:HE3	1.85	0.42
1:A:92:LEU:O	1:A:141:ILE:HD11	2.20	0.41
1:B:271:ASP:OD2	1:B:276:ASN:HA	2.18	0.41
1:B:276:ASN:OD1	1:B:278:ARG:HG2	2.20	0.41
1:B:47:MET:C	1:B:48:TYR:CD1	2.93	0.41
1:D:166:ASN:HD22	1:D:262:SER:CB	2.33	0.41
1:E:301:PHE:CD1	1:E:303:SER:OG	2.69	0.41
1:F:115:GLU:HA	1:F:120:LYS:HZ1	1.85	0.41
1:H:110:PHE:N	1:H:110:PHE:HD1	2.18	0.41
1:C:144:TYR:HB2	1:C:145:ILE:HD12	2.02	0.41
1:D:214:GLY:HA2	1:D:217:PHE:H	1.85	0.41
1:G:72:SER:HB2	1:G:73:ASP:OD2	2.20	0.41
1:C:98:SER:CB	1:C:167:LYS:HZ3	2.13	0.41
1:E:144:TYR:HH	1:E:213:HIS:HE2	1.62	0.41
1:E:246:GLU:O	1:E:250:GLN:HG3	2.20	0.41
1:E:87:PHE:CD2	1:E:273:ILE:HG21	2.55	0.41
1:E:301:PHE:O	1:E:301:PHE:CD1	2.74	0.41
1:G:59:GLU:HA	1:G:125:PHE:HE2	1.85	0.41
1:H:240:LEU:HG	1:H:242:ASN:C	2.40	0.41
1:C:152:LEU:C	1:C:154:LEU:N	2.73	0.41
1:C:203:ILE:O	1:C:203:ILE:CG2	2.67	0.41
1:E:307:PHE:CB	1:E:309:TRP:CE2	3.00	0.41
1:F:152:LEU:O	1:F:154:LEU:N	2.53	0.41
1:F:263:PHE:N	1:F:263:PHE:CD2	2.88	0.41
1:F:285:GLU:CD	1:F:301:PHE:CD2	2.94	0.41
1:F:74:LEU:O	1:F:78:GLU:HG2	2.20	0.41
1:H:261:ARG:NH1	1:H:281:SER:HB3	2.35	0.41
1:H:309:TRP:HE3	1:H:309:TRP:O	1.99	0.41
1:A:48:TYR:CD1	1:A:48:TYR:N	2.88	0.41
1:B:240:LEU:HD23	1:B:243:LYS:HA	2.02	0.41
1:C:168:ALA:O	1:C:171:ALA:HB3	2.20	0.41
1:C:50:GLU:HB3	1:C:235:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLU:HA	1:B:285:GLU:OE1	2.20	0.41
1:E:264:ILE:O	1:E:269:PRO:HA	2.20	0.41
1:F:126:GLN:NE2	1:F:192:GLU:OE2	2.53	0.41
1:F:281:SER:O	1:F:285:GLU:HG2	2.21	0.41
1:G:136:THR:O	1:G:140:LEU:HD13	2.20	0.41
1:G:272:LEU:HA	1:G:274:GLY:H	1.86	0.41
1:G:78:GLU:OE2	1:G:78:GLU:CA	2.67	0.41
1:H:150:GLU:O	1:H:154:LEU:HB2	2.21	0.41
1:A:113:GLU:OE1	1:A:181:PHE:CD1	2.73	0.41
1:B:181:PHE:CD1	1:B:181:PHE:O	2.74	0.41
1:C:92:LEU:HD21	1:C:215:LEU:HD11	2.02	0.41
1:D:299:LYS:HZ2	1:D:302:HIS:HD2	1.65	0.41
1:D:94:PHE:HD1	1:D:196:PHE:HE1	1.68	0.41
1:E:51:VAL:HG13	1:E:232:PHE:CZ	2.55	0.41
1:G:98:SER:CA	3:G:351:HOH:O	2.69	0.41
1:H:151:ARG:O	1:H:155:PHE:CD1	2.74	0.41
1:A:136:THR:O	1:A:140:LEU:HD22	2.21	0.41
1:A:110:PHE:CE1	1:A:181:PHE:HE1	2.38	0.41
1:A:260:GLU:OE1	1:A:263:PHE:CE1	2.74	0.41
1:B:73:ASP:CB	1:B:213:HIS:CG	2.83	0.41
1:C:56:LYS:HA	1:C:56:LYS:HD2	1.86	0.41
1:D:162:PRO:O	1:D:165:LYS:HG2	2.21	0.41
1:F:162:PRO:O	1:F:165:LYS:HB3	2.20	0.41
1:F:268:LEU:HD12	1:F:268:LEU:HA	1.90	0.41
1:G:243:LYS:CD	1:G:243:LYS:NZ	2.70	0.41
1:H:291:LEU:HA	1:H:291:LEU:HD23	1.87	0.41
1:B:56:LYS:O	1:B:60:ALA:CB	2.69	0.41
1:C:104:GLU:C	3:C:352:HOH:O	2.59	0.41
1:C:202:ALA:O	1:C:205:TRP:HB3	2.21	0.41
1:D:175:ILE:O	1:D:177:ASP:HB2	2.21	0.41
1:D:259:VAL:O	1:D:262:SER:OG	2.27	0.41
1:F:264:ILE:H	1:F:264:ILE:HG13	1.38	0.41
1:F:304:LYS:O	1:F:306:PRO:HD3	2.21	0.41
1:F:81:ASN:CB	1:F:83:ASN:H	2.33	0.41
1:G:170:TRP:CZ2	1:G:256:ALA:HB2	2.56	0.41
1:G:271:ASP:O	1:G:272:LEU:CB	2.69	0.41
1:H:270:CYS:SG	1:H:277:SER:HA	2.61	0.41
1:H:283:TYR:O	1:H:287:VAL:HG23	2.21	0.41
1:A:108:SER:HA	1:A:111:LEU:HB2	2.03	0.41
1:B:105:ASN:HD22	1:B:106:LEU:N	2.18	0.41
1:B:143:ASN:CA	1:B:146:LYS:HG3	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASN:ND2	1:B:279:LEU:H	2.19	0.41
1:H:95:PHE:CE1	1:H:196:PHE:CD1	3.08	0.41
1:A:180:SER:O	1:A:184:ARG:HG3	2.21	0.41
1:B:148:GLU:C	1:B:150:GLU:N	2.71	0.41
1:C:158:ILE:HA	1:C:161:ILE:HG12	2.03	0.41
1:C:165:LYS:HG2	1:C:166:ASN:OD1	2.21	0.41
1:D:299:LYS:HZ2	1:D:302:HIS:CD2	2.39	0.41
1:E:175:ILE:HG22	1:E:176:ASN:H	1.85	0.41
1:F:114:VAL:O	1:F:120:LYS:NZ	2.54	0.41
1:A:163:ALA:HB1	1:A:263:PHE:HD2	1.81	0.40
1:A:189:ALA:HB2	1:A:233:ASN:HB2	2.03	0.40
1:B:54:PHE:O	1:B:122:PHE:CE2	2.70	0.40
1:E:163:ALA:O	1:E:167:LYS:HB2	2.21	0.40
1:E:308:ASN:C	1:E:308:ASN:OD1	2.59	0.40
1:F:195:LEU:HA	1:F:260:GLU:OE1	2.21	0.40
1:H:299:LYS:HB2	1:H:302:HIS:CD2	2.55	0.40
1:H:299:LYS:HB2	1:H:302:HIS:NE2	2.36	0.40
1:H:57:LYS:O	1:H:61:SER:HB3	2.21	0.40
1:A:161:ILE:HA	1:A:162:PRO:HD3	1.93	0.40
1:B:170:TRP:CZ2	1:B:256:ALA:HB2	2.55	0.40
1:C:299:LYS:HB2	1:C:302:HIS:NE2	2.36	0.40
1:F:158:ILE:HA	1:F:161:ILE:CG1	2.52	0.40
1:F:278:ARG:H	1:F:278:ARG:HG2	1.64	0.40
1:G:148:GLU:CG	1:G:148:GLU:O	2.69	0.40
1:H:175:ILE:O	1:H:177:ASP:HB2	2.21	0.40
1:H:218:SER:O	1:H:222:ILE:HG13	2.22	0.40
1:H:70:LEU:HG	1:H:70:LEU:H	1.44	0.40
1:A:55:TYR:O	1:A:59:GLU:HB2	2.22	0.40
1:B:150:GLU:O	1:B:152:LEU:N	2.53	0.40
1:B:263:PHE:HA	1:B:267:SER:HB2	2.01	0.40
1:B:68:ILE:CG2	1:B:70:LEU:CD2	2.99	0.40
1:C:143:ASN:HD22	1:C:143:ASN:N	2.19	0.40
1:C:276:ASN:OD1	1:C:278:ARG:CG	2.68	0.40
1:C:59:GLU:O	1:C:62:PHE:HB2	2.21	0.40
1:D:280:MET:HE3	1:D:283:TYR:HB3	2.02	0.40
1:D:75:LYS:HG3	1:D:75:LYS:H	1.64	0.40
1:F:109:LYS:O	1:F:113:GLU:HG3	2.22	0.40
1:G:106:LEU:HD23	1:G:188:ASN:HD21	1.79	0.40
1:H:68:ILE:HD13	1:H:217:PHE:HE2	1.87	0.40
1:A:167:LYS:HZ3	1:A:195:LEU:HD13	1.86	0.40
1:A:307:PHE:HB3	1:A:309:TRP:NE1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLU:HG3	1:B:301:PHE:CE1	2.57	0.40
1:C:145:ILE:CG2	1:C:145:ILE:O	2.64	0.40
1:C:98:SER:HB2	1:C:167:LYS:CE	2.49	0.40
1:G:88:ILE:H	1:G:88:ILE:HG12	1.68	0.40
1:D:301:PHE:O	1:D:301:PHE:CD1	2.75	0.40
1:F:109:LYS:NZ	1:F:176:ASN:OD1	2.54	0.40
1:H:130:GLU:HA	1:H:133:HIS:CE1	2.56	0.40

All (10) 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)
1:E:302:HIS:ND1	1:G:71:SER:O[3_444]	1.31	0.89
1:G:267:SER:O	1:G:267:SER:O[2_657]	1.60	0.60
1:B:267:SER:O	1:B:272:LEU:O[2_555]	1.87	0.33
1:B:267:SER:C	1:B:272:LEU:O[2_555]	2.06	0.14
1:B:276:ASN:OD1	1:B:278:ARG:NE[2_555]	2.11	0.09
1:B:271:ASP:OD1	1:B:277:SER:CB[2_555]	2.15	0.05
1:B:271:ASP:OD1	1:B:278:ARG:NH2[2_555]	2.16	0.04
1:E:279:LEU:CG	1:G:147:ASP:OD1[3_444]	2.16	0.04
1:B:269:PRO:CB	1:B:272:LEU:N[2_555]	2.17	0.03
1:B:271:ASP:CB	1:B:271:ASP:CB[2_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/349 (73%)	219 (86%)	25 (10%)	10 (4%)	3	6
1	B	244/349 (70%)	208 (85%)	26 (11%)	10 (4%)	3	6
1	C	250/349 (72%)	206 (82%)	35 (14%)	9 (4%)	3	7
1	D	254/349 (73%)	215 (85%)	27 (11%)	12 (5%)	2	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	254/349 (73%)	219 (86%)	25 (10%)	10 (4%)	3	6
1	F	254/349 (73%)	220 (87%)	26 (10%)	8 (3%)	4	9
1	G	244/349 (70%)	209 (86%)	27 (11%)	8 (3%)	4	8
1	H	254/349 (73%)	220 (87%)	24 (9%)	10 (4%)	3	6
All	All	2008/2792 (72%)	1716 (86%)	215 (11%)	77 (4%)	3	7

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLU
1	A	302	HIS
1	B	176	ASN
1	B	272	LEU
1	E	80	LEU
1	E	82	VAL
1	E	302	HIS
1	F	82	VAL
1	F	213	HIS
1	G	272	LEU
1	H	80	LEU
1	H	213	HIS
1	A	70	LEU
1	A	193	GLY
1	A	271	ASP
1	B	80	LEU
1	B	213	HIS
1	B	302	HIS
1	C	146	LYS
1	C	193	GLY
1	C	213	HIS
1	C	302	HIS
1	D	69	ASP
1	D	158	ILE
1	D	159	GLU
1	D	213	HIS
1	D	271	ASP
1	D	302	HIS
1	E	213	HIS
1	F	302	HIS
1	G	70	LEU
1	G	82	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	302	HIS
1	H	70	LEU
1	H	151	ARG
1	H	302	HIS
1	A	246	GLU
1	B	193	GLY
1	C	69	ASP
1	C	148	GLU
1	C	151	ARG
1	D	272	LEU
1	E	148	GLU
1	E	193	GLY
1	G	69	ASP
1	G	213	HIS
1	H	148	GLU
1	H	193	GLY
1	H	271	ASP
1	A	241	GLU
1	B	69	ASP
1	B	154	LEU
1	D	80	LEU
1	D	193	GLY
1	E	70	LEU
1	E	85	LYS
1	E	271	ASP
1	F	70	LEU
1	F	193	GLY
1	F	241	GLU
1	G	193	GLY
1	H	176	ASN
1	A	213	HIS
1	B	299	LYS
1	C	70	LEU
1	C	271	ASP
1	D	70	LEU
1	F	271	ASP
1	D	157	ALA
1	D	300	VAL
1	G	114	VAL
1	A	114	VAL
1	A	300	VAL
1	B	300	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	305	ASN
1	F	300	VAL
1	H	48	TYR

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	229/316 (72%)	194 (85%)	35 (15%)	2	7
1	B	223/316 (71%)	176 (79%)	47 (21%)	1	3
1	C	230/316 (73%)	182 (79%)	48 (21%)	1	3
1	D	232/316 (73%)	202 (87%)	30 (13%)	4	10
1	E	230/316 (73%)	196 (85%)	34 (15%)	3	7
1	F	232/316 (73%)	198 (85%)	34 (15%)	3	7
1	G	225/316 (71%)	191 (85%)	34 (15%)	3	7
1	H	232/316 (73%)	190 (82%)	42 (18%)	1	4
All	All	1833/2528 (72%)	1529 (83%)	304 (17%)	2	5

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	MET
1	A	56	LYS
1	A	71	SER
1	A	80	LEU
1	A	85	LYS
1	A	88	ILE
1	A	106	LEU
1	A	108	SER
1	A	109	LYS
1	A	111	LEU
1	A	116	ILE
1	A	130	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140	LEU
1	A	143	ASN
1	A	146	LYS
1	A	147	ASP
1	A	177	ASP
1	A	185	ILE
1	A	197	SER
1	A	199	SER
1	A	208	LYS
1	A	213	HIS
1	A	230	THR
1	A	233	ASN
1	A	238	SER
1	A	263	PHE
1	A	264	ILE
1	A	271	ASP
1	A	272	LEU
1	A	282	GLN
1	A	292	LEU
1	A	299	LYS
1	A	300	VAL
1	A	307	PHE
1	A	308	ASN
1	B	53	ASN
1	B	59	GLU
1	B	69	ASP
1	B	70	LEU
1	B	71	SER
1	B	75	LYS
1	B	80	LEU
1	B	81	ASN
1	B	87	PHE
1	B	90	HIS
1	B	94	PHE
1	B	98	SER
1	B	105	ASN
1	B	106	LEU
1	B	111	LEU
1	B	115	GLU
1	B	135	GLU
1	B	140	LEU
1	B	150	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	ARG
1	B	154	LEU
1	B	156	HIS
1	B	165	LYS
1	B	178	THR
1	B	180	SER
1	B	183	GLU
1	B	185	ILE
1	B	197	SER
1	B	199	SER
1	B	210	ASN
1	B	213	HIS
1	B	230	THR
1	B	238	SER
1	B	243	LYS
1	B	246	GLU
1	B	247	ASN
1	B	263	PHE
1	B	264	ILE
1	B	268	LEU
1	B	278	ARG
1	B	282	GLN
1	B	292	LEU
1	B	293	GLU
1	B	300	VAL
1	B	303	SER
1	B	305	ASN
1	B	308	ASN
1	C	47	MET
1	C	54	PHE
1	C	66	GLU
1	C	67	GLU
1	C	75	LYS
1	C	81	ASN
1	C	82	VAL
1	C	86	HIS
1	C	91	VAL
1	C	104	GLU
1	C	108	SER
1	C	114	VAL
1	C	116	ILE
1	C	126	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	135	GLU
1	C	140	LEU
1	C	143	ASN
1	C	147	ASP
1	C	149	LYS
1	C	150	GLU
1	C	151	ARG
1	C	152	LEU
1	C	156	HIS
1	C	160	ASN
1	C	164	ILE
1	C	165	LYS
1	C	175	ILE
1	C	181	PHE
1	C	185	ILE
1	C	188	ASN
1	C	194	ILE
1	C	208	LYS
1	C	211	LYS
1	C	213	HIS
1	C	228	LEU
1	C	235	LEU
1	C	247	ASN
1	C	257	VAL
1	C	264	ILE
1	C	280	MET
1	C	282	GLN
1	C	291	LEU
1	C	292	LEU
1	C	298	SER
1	C	300	VAL
1	C	307	PHE
1	C	308	ASN
1	C	309	TRP
1	D	47	MET
1	D	50	GLU
1	D	74	LEU
1	D	85	LYS
1	D	91	VAL
1	D	109	LYS
1	D	111	LEU
1	D	121	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	136	THR
1	D	139	LEU
1	D	140	LEU
1	D	146	LYS
1	D	149	LYS
1	D	150	GLU
1	D	152	LEU
1	D	159	GLU
1	D	160	ASN
1	D	161	ILE
1	D	164	ILE
1	D	178	THR
1	D	179	ASN
1	D	239	LEU
1	D	243	LYS
1	D	247	ASN
1	D	258	GLU
1	D	264	ILE
1	D	290	ARG
1	D	291	LEU
1	D	292	LEU
1	D	303	SER
1	E	56	LYS
1	E	69	ASP
1	E	70	LEU
1	E	85	LYS
1	E	109	LYS
1	E	126	GLN
1	E	130	GLU
1	E	134	SER
1	E	136	THR
1	E	145	ILE
1	E	146	LYS
1	E	148	GLU
1	E	154	LEU
1	E	156	HIS
1	E	161	ILE
1	E	180	SER
1	E	185	ILE
1	E	213	HIS
1	E	235	LEU
1	E	240	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	243	LYS
1	E	261	ARG
1	E	272	LEU
1	E	273	ILE
1	E	277	SER
1	E	278	ARG
1	E	279	LEU
1	E	282	GLN
1	E	292	LEU
1	E	299	LYS
1	E	300	VAL
1	E	303	SER
1	E	307	PHE
1	E	308	ASN
1	F	47	MET
1	F	57	LYS
1	F	66	GLU
1	F	69	ASP
1	F	80	LEU
1	F	81	ASN
1	F	82	VAL
1	F	91	VAL
1	F	98	SER
1	F	104	GLU
1	F	138	SER
1	F	140	LEU
1	F	148	GLU
1	F	149	LYS
1	F	150	GLU
1	F	156	HIS
1	F	175	ILE
1	F	178	THR
1	F	188	ASN
1	F	217	PHE
1	F	218	SER
1	F	236	ILE
1	F	238	SER
1	F	242	ASN
1	F	243	LYS
1	F	244	LEU
1	F	264	ILE
1	F	273	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	278	ARG
1	F	291	LEU
1	F	292	LEU
1	F	303	SER
1	F	304	LYS
1	F	307	PHE
1	G	64	THR
1	G	66	GLU
1	G	71	SER
1	G	72	SER
1	G	73	ASP
1	G	98	SER
1	G	104	GLU
1	G	105	ASN
1	G	111	LEU
1	G	116	ILE
1	G	121	LYS
1	G	129	VAL
1	G	140	LEU
1	G	146	LYS
1	G	158	ILE
1	G	161	ILE
1	G	166	ASN
1	G	178	THR
1	G	194	ILE
1	G	201	CYS
1	G	203	ILE
1	G	213	HIS
1	G	219	ASN
1	G	236	ILE
1	G	238	SER
1	G	240	LEU
1	G	243	LYS
1	G	247	ASN
1	G	267	SER
1	G	277	SER
1	G	278	ARG
1	G	282	GLN
1	G	299	LYS
1	G	305	ASN
1	H	47	MET
1	H	56	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	64	THR
1	H	67	GLU
1	H	70	LEU
1	H	75	LYS
1	H	84	GLU
1	H	85	LYS
1	H	86	HIS
1	H	111	LEU
1	H	121	LYS
1	H	132	ILE
1	H	135	GLU
1	H	142	ASP
1	H	149	LYS
1	H	158	ILE
1	H	159	GLU
1	H	160	ASN
1	H	175	ILE
1	H	183	GLU
1	H	199	SER
1	H	208	LYS
1	H	223	SER
1	H	230	THR
1	H	233	ASN
1	H	236	ILE
1	H	238	SER
1	H	241	GLU
1	H	247	ASN
1	H	254	LYS
1	H	258	GLU
1	H	260	GLU
1	H	264	ILE
1	H	271	ASP
1	H	272	LEU
1	H	278	ARG
1	H	280	MET
1	H	282	GLN
1	H	291	LEU
1	H	292	LEU
1	H	303	SER
1	H	304	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	90	HIS
1	A	105	ASN
1	A	131	ASN
1	A	179	ASN
1	A	233	ASN
1	A	251	ASN
1	A	282	GLN
1	A	308	ASN
1	B	53	ASN
1	B	105	ASN
1	B	153	ASN
1	B	188	ASN
1	B	233	ASN
1	B	247	ASN
1	B	276	ASN
1	B	282	GLN
1	C	53	ASN
1	C	81	ASN
1	C	83	ASN
1	C	105	ASN
1	C	126	GLN
1	C	153	ASN
1	C	160	ASN
1	C	166	ASN
1	C	233	ASN
1	C	247	ASN
1	C	282	GLN
1	C	302	HIS
1	C	305	ASN
1	C	308	ASN
1	D	53	ASN
1	D	86	HIS
1	D	153	ASN
1	D	179	ASN
1	D	233	ASN
1	D	247	ASN
1	D	250	GLN
1	D	302	HIS
1	E	90	HIS
1	E	105	ASN
1	E	188	ASN
1	E	250	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	282	GLN
1	F	81	ASN
1	F	86	HIS
1	F	213	HIS
1	F	250	GLN
1	F	302	HIS
1	G	90	HIS
1	G	166	ASN
1	G	188	ASN
1	G	219	ASN
1	G	242	ASN
1	G	282	GLN
1	G	305	ASN
1	H	105	ASN
1	H	126	GLN
1	H	131	ASN
1	H	156	HIS
1	H	160	ASN
1	H	166	ASN
1	H	213	HIS
1	H	247	ASN
1	H	251	ASN
1	H	282	GLN
1	H	302	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/349 (73%)	0.99	25 (9%) 7 6	24, 42, 49, 55	0
1	B	252/349 (72%)	1.05	48 (19%) 1 0	27, 42, 48, 52	0
1	C	256/349 (73%)	1.13	55 (21%) 0 0	27, 42, 47, 53	0
1	D	258/349 (73%)	1.00	22 (8%) 10 9	32, 42, 49, 54	0
1	E	258/349 (73%)	1.05	45 (17%) 1 1	26, 42, 48, 51	0
1	F	258/349 (73%)	0.95	42 (16%) 1 1	30, 42, 47, 54	0
1	G	252/349 (72%)	1.16	54 (21%) 0 0	31, 42, 48, 56	0
1	H	258/349 (73%)	0.97	46 (17%) 1 1	34, 42, 48, 53	0
All	All	2050/2792 (73%)	1.04	337 (16%) 1 1	24, 42, 48, 56	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	274	GLY	9.6
1	E	178	THR	8.5
1	G	175	ILE	8.3
1	E	111	LEU	7.9
1	G	146	LYS	7.8
1	C	297	CYS	7.1
1	B	107	ALA	7.1
1	H	145	ILE	7.0
1	F	266	GLU	6.7
1	E	175	ILE	6.7
1	C	244	LEU	6.5
1	E	263	PHE	6.5
1	E	249	VAL	6.4
1	G	309	TRP	5.6
1	F	106	LEU	5.6
1	C	286	PHE	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	111	LEU	5.3
1	C	239	LEU	5.2
1	E	270	CYS	5.2
1	G	279	LEU	5.1
1	E	49	PRO	4.9
1	C	180	SER	4.9
1	C	139	LEU	4.8
1	F	202	ALA	4.8
1	F	309	TRP	4.8
1	G	147	ASP	4.7
1	H	177	ASP	4.7
1	H	93	ALA	4.7
1	G	54	PHE	4.6
1	F	244	LEU	4.6
1	B	90	HIS	4.6
1	C	175	ILE	4.6
1	F	111	LEU	4.5
1	E	273	ILE	4.5
1	H	106	LEU	4.5
1	B	174	TRP	4.5
1	F	279	LEU	4.5
1	C	267	SER	4.4
1	H	190	CYS	4.4
1	E	143	ASN	4.4
1	H	92	LEU	4.4
1	F	176	ASN	4.4
1	G	52	TRP	4.4
1	F	300	VAL	4.3
1	F	249	VAL	4.3
1	G	301	PHE	4.3
1	F	272	LEU	4.3
1	G	230	THR	4.3
1	G	156	HIS	4.2
1	C	263	PHE	4.2
1	E	237	TYR	4.2
1	E	174	TRP	4.2
1	D	179	ASN	4.2
1	G	111	LEU	4.2
1	E	211	LYS	4.2
1	A	98	SER	4.1
1	B	154	LEU	4.1
1	A	176	ASN	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	72	SER	4.0
1	G	158	ILE	4.0
1	G	201	CYS	4.0
1	C	145	ILE	3.9
1	E	176	ASN	3.9
1	B	48	TYR	3.9
1	B	122	PHE	3.9
1	B	211	LYS	3.8
1	C	307	PHE	3.8
1	G	123	TYR	3.8
1	B	257	VAL	3.8
1	E	107	ALA	3.8
1	D	204	PHE	3.8
1	C	106	LEU	3.8
1	A	151	ARG	3.8
1	G	69	ASP	3.7
1	E	272	LEU	3.7
1	F	174	TRP	3.7
1	G	96	ALA	3.7
1	H	52	TRP	3.7
1	C	144	TYR	3.7
1	F	123	TYR	3.7
1	F	125	PHE	3.6
1	G	182	ALA	3.6
1	G	308	ASN	3.6
1	H	96	ALA	3.6
1	C	305	ASN	3.6
1	D	302	HIS	3.6
1	E	266	GLU	3.6
1	H	75	LYS	3.5
1	H	169	LEU	3.5
1	F	114	VAL	3.5
1	B	188	ASN	3.4
1	H	178	THR	3.4
1	A	72	SER	3.4
1	B	237	TYR	3.4
1	F	305	ASN	3.4
1	E	228	LEU	3.4
1	E	170	TRP	3.4
1	H	309	TRP	3.4
1	H	230	THR	3.4
1	H	176	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	136	THR	3.3
1	F	248	VAL	3.4
1	B	178	THR	3.3
1	B	305	ASN	3.3
1	B	179	ASN	3.2
1	G	87	PHE	3.2
1	E	216	THR	3.2
1	F	144	TYR	3.2
1	D	52	TRP	3.2
1	F	267	SER	3.2
1	G	271	ASP	3.2
1	E	301	PHE	3.2
1	A	112	ARG	3.2
1	F	286	PHE	3.1
1	B	106	LEU	3.1
1	G	178	THR	3.1
1	G	81	ASN	3.1
1	B	231	ASP	3.1
1	B	47	MET	3.1
1	E	75	LYS	3.1
1	G	73	ASP	3.1
1	E	94	PHE	3.1
1	G	155	PHE	3.1
1	H	307	PHE	3.1
1	G	293	GLU	3.1
1	G	106	LEU	3.0
1	C	260	GLU	3.0
1	H	272	LEU	3.0
1	H	116	ILE	3.0
1	E	155	PHE	3.0
1	E	260	GLU	3.0
1	A	154	LEU	3.0
1	F	278	ARG	3.0
1	D	202	ALA	3.0
1	G	295	LEU	3.0
1	B	93	ALA	3.0
1	C	179	ASN	3.0
1	G	286	PHE	3.0
1	B	140	LEU	3.0
1	B	295	LEU	3.0
1	C	171	ALA	3.0
1	A	175	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	123	TYR	2.9
1	B	180	SER	2.9
1	G	207	LYS	2.9
1	A	179	ASN	2.9
1	D	259	VAL	2.9
1	F	158	ILE	2.9
1	C	294	CYS	2.9
1	H	185	ILE	2.9
1	E	125	PHE	2.9
1	C	80	LEU	2.9
1	H	194	ILE	2.9
1	B	263	PHE	2.9
1	G	200	PHE	2.9
1	B	242	ASN	2.9
1	A	242	ASN	2.9
1	H	205	TRP	2.8
1	E	70	LEU	2.8
1	E	171	ALA	2.8
1	C	231	ASP	2.8
1	B	288	ALA	2.8
1	G	109	LYS	2.8
1	H	186	VAL	2.8
1	F	71	SER	2.8
1	C	242	ASN	2.8
1	G	296	GLY	2.8
1	C	245	PRO	2.8
1	C	155	PHE	2.8
1	C	230	THR	2.8
1	B	191	VAL	2.8
1	G	107	ALA	2.8
1	C	280	MET	2.8
1	A	117	ILE	2.8
1	H	94	PHE	2.8
1	G	173	LYS	2.8
1	G	278	ARG	2.7
1	H	183	GLU	2.7
1	E	286	PHE	2.7
1	F	64	THR	2.7
1	A	257	VAL	2.7
1	D	65	ALA	2.7
1	D	236	ILE	2.7
1	C	172	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	286	PHE	2.7
1	C	127	ILE	2.7
1	C	259	VAL	2.7
1	H	77	PHE	2.7
1	C	269	PRO	2.7
1	G	172	ALA	2.7
1	G	176	ASN	2.7
1	F	263	PHE	2.7
1	F	175	ILE	2.7
1	E	106	LEU	2.6
1	G	272	LEU	2.6
1	B	96	ALA	2.6
1	D	82	VAL	2.6
1	H	155	PHE	2.6
1	G	90	HIS	2.6
1	B	235	LEU	2.6
1	E	192	GLU	2.6
1	B	244	LEU	2.6
1	E	52	TRP	2.6
1	F	145	ILE	2.6
1	G	114	VAL	2.6
1	F	162	PRO	2.6
1	D	185	ILE	2.5
1	E	114	VAL	2.5
1	F	54	PHE	2.5
1	F	217	PHE	2.5
1	H	124	SER	2.5
1	F	242	ASN	2.5
1	B	168	ALA	2.5
1	D	168	ALA	2.5
1	A	80	LEU	2.5
1	A	272	LEU	2.5
1	D	228	LEU	2.5
1	H	47	MET	2.5
1	G	190	CYS	2.5
1	G	282	GLN	2.5
1	H	70	LEU	2.5
1	H	184	ARG	2.5
1	A	65	ALA	2.5
1	G	300	VAL	2.5
1	B	246	GLU	2.4
1	C	128	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	222	ILE	2.4
1	H	181	PHE	2.4
1	A	162	PRO	2.4
1	E	154	LEU	2.4
1	F	160	ASN	2.4
1	H	133	HIS	2.4
1	E	141	ILE	2.4
1	B	266	GLU	2.4
1	A	235	LEU	2.4
1	E	309	TRP	2.4
1	C	93	ALA	2.4
1	C	146	LYS	2.4
1	E	79	LYS	2.4
1	A	143	ASN	2.4
1	C	296	GLY	2.4
1	D	91	VAL	2.4
1	E	156	HIS	2.4
1	C	73	ASP	2.4
1	D	141	ILE	2.4
1	F	73	ASP	2.4
1	A	141	ILE	2.4
1	C	308	ASN	2.4
1	E	112	ARG	2.3
1	B	94	PHE	2.3
1	G	75	LYS	2.3
1	B	70	LEU	2.3
1	H	160	ASN	2.3
1	E	54	PHE	2.3
1	H	200	PHE	2.3
1	A	267	SER	2.3
1	C	193	GLY	2.3
1	F	152	LEU	2.3
1	C	114	VAL	2.3
1	D	197	SER	2.3
1	B	187	ALA	2.3
1	H	60	ALA	2.3
1	C	94	PHE	2.3
1	D	273	ILE	2.3
1	G	82	VAL	2.3
1	F	86	HIS	2.3
1	G	128	ALA	2.3
1	G	248	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	71	SER	2.3
1	F	245	PRO	2.3
1	E	169	LEU	2.3
1	H	240	LEU	2.3
1	D	272	LEU	2.3
1	B	157	ALA	2.3
1	D	172	ALA	2.3
1	D	158	ILE	2.3
1	H	87	PHE	2.3
1	H	297	CYS	2.2
1	B	52	TRP	2.2
1	G	76	ASP	2.2
1	F	72	SER	2.2
1	G	277	SER	2.2
1	B	156	HIS	2.2
1	B	97	ALA	2.2
1	B	115	GLU	2.2
1	F	110	PHE	2.2
1	B	185	ILE	2.2
1	H	284	ILE	2.2
1	C	195	LEU	2.2
1	F	306	PRO	2.2
1	H	65	ALA	2.2
1	B	62	PHE	2.2
1	B	264	ILE	2.2
1	C	203	ILE	2.2
1	G	244	LEU	2.2
1	C	266	GLU	2.2
1	F	128	ALA	2.2
1	E	119	ALA	2.2
1	A	88	ILE	2.1
1	C	252	ILE	2.1
1	D	80	LEU	2.1
1	H	86	HIS	2.1
1	C	107	ALA	2.1
1	C	136	THR	2.1
1	C	164	ILE	2.1
1	A	156	HIS	2.1
1	C	272	LEU	2.1
1	H	112	ARG	2.1
1	G	234	CYS	2.1
1	H	138	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	161	ILE	2.1
1	H	273	ILE	2.1
1	B	137	TYR	2.1
1	B	282	GLN	2.1
1	B	276	ASN	2.1
1	A	263	PHE	2.1
1	B	87	PHE	2.1
1	C	57	LYS	2.1
1	H	214	GLY	2.1
1	E	282	GLN	2.1
1	B	296	GLY	2.1
1	F	76	ASP	2.1
1	C	279	LEU	2.1
1	H	306	PRO	2.1
1	E	104	GLU	2.1
1	C	215	LEU	2.1
1	A	97	ALA	2.1
1	A	188	ASN	2.1
1	F	179	ASN	2.1
1	D	269	PRO	2.0
1	D	93	ALA	2.0
1	C	182	ALA	2.0
1	E	85	LYS	2.0
1	C	204	PHE	2.0
1	H	123	TYR	2.0
1	C	167	LYS	2.0
1	G	259	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	B	350	1/1	0.82	0.44	65,65,65,65	1
2	FE	D	350	1/1	0.86	0.13	49,49,49,49	1
2	FE	G	350	1/1	0.92	0.06	58,58,58,58	1
2	FE	C	350	1/1	0.92	0.09	61,61,61,61	1
2	FE	E	350	1/1	0.94	0.06	63,63,63,63	1
2	FE	F	350	1/1	0.96	0.09	54,54,54,54	1
2	FE	A	350	1/1	0.96	0.26	47,47,47,47	1
2	FE	H	350	1/1	0.97	0.06	53,53,53,53	1

6.5 Other polymers ⓘ

There are no such residues in this entry.