



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:00 AM UTC

PDB ID : 2P1I / pdb_00002p1i
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

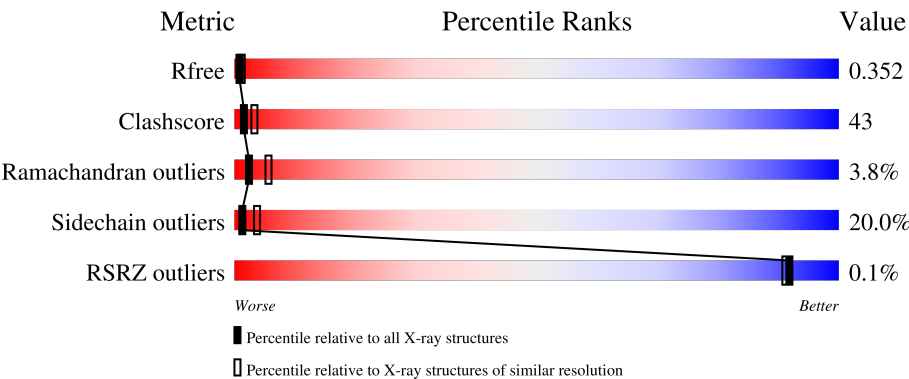
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	349	29%32%12%•26%
1	B	349	26%32%11%•28%
1	C	349	23%33%16%•27%
1	D	349	30%30%12%•26%
1	E	349	24%37%12%•26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	349	31%34%8%•26%
1	G	349	25%32%13%•28%
1	H	349	28%32%13%•26%

2 Entry composition [i](#)

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 (CCD ID: FE) (formula: Fe).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Fe 1	0	0
2	H	1	Total 1	Fe 1	0	0

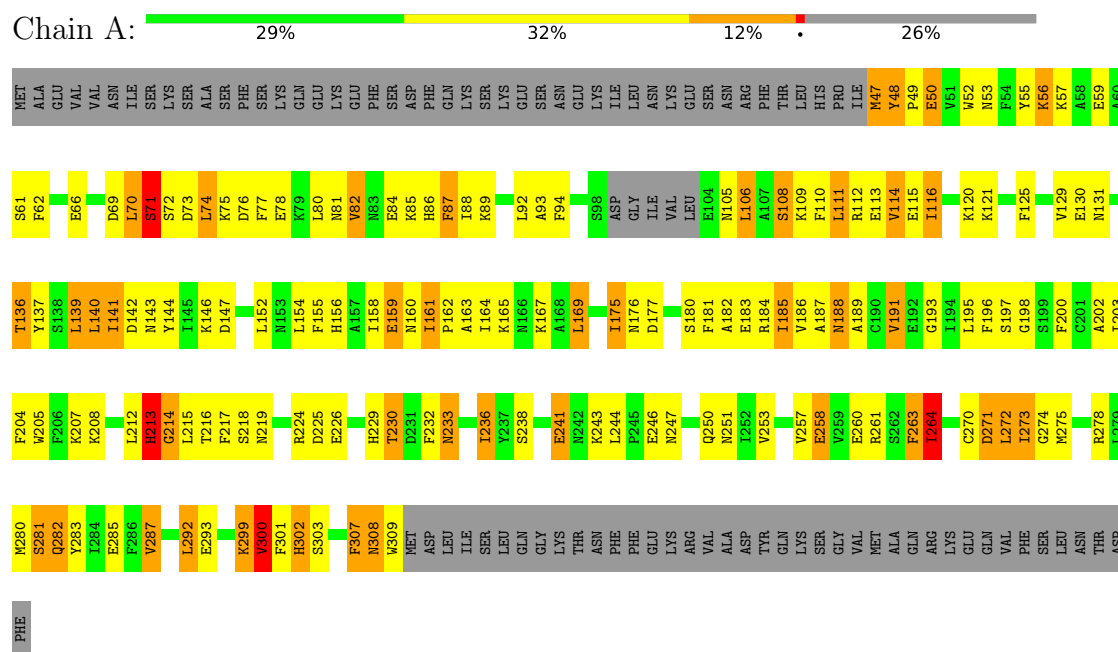
- Molecule 3 is water.

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

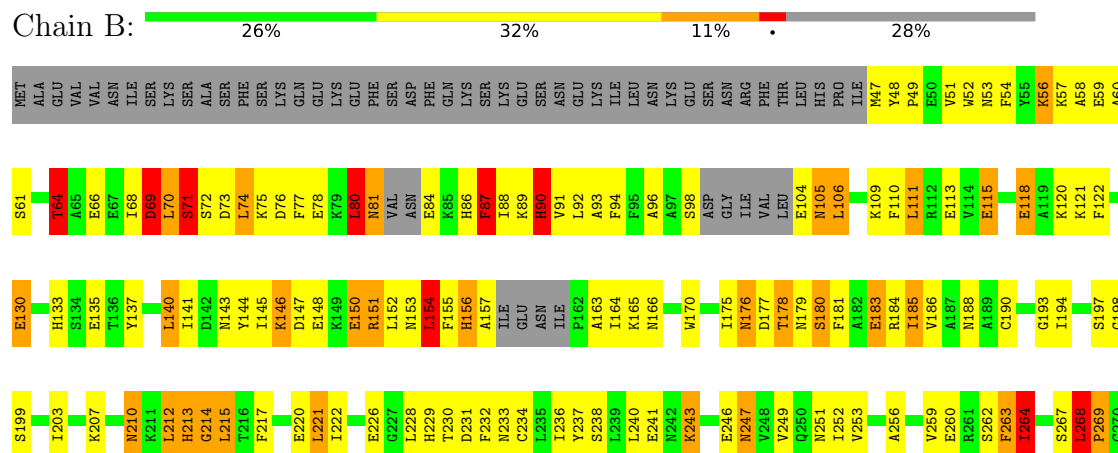
3 Residue-property plots

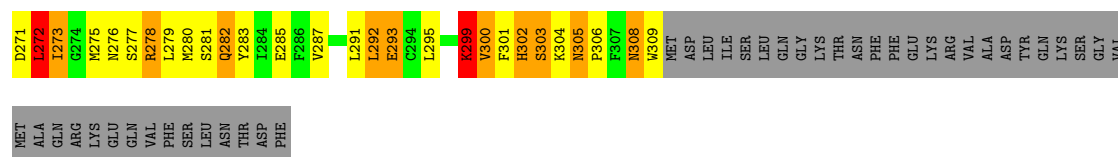
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Ribonucleotide reductase, small chain



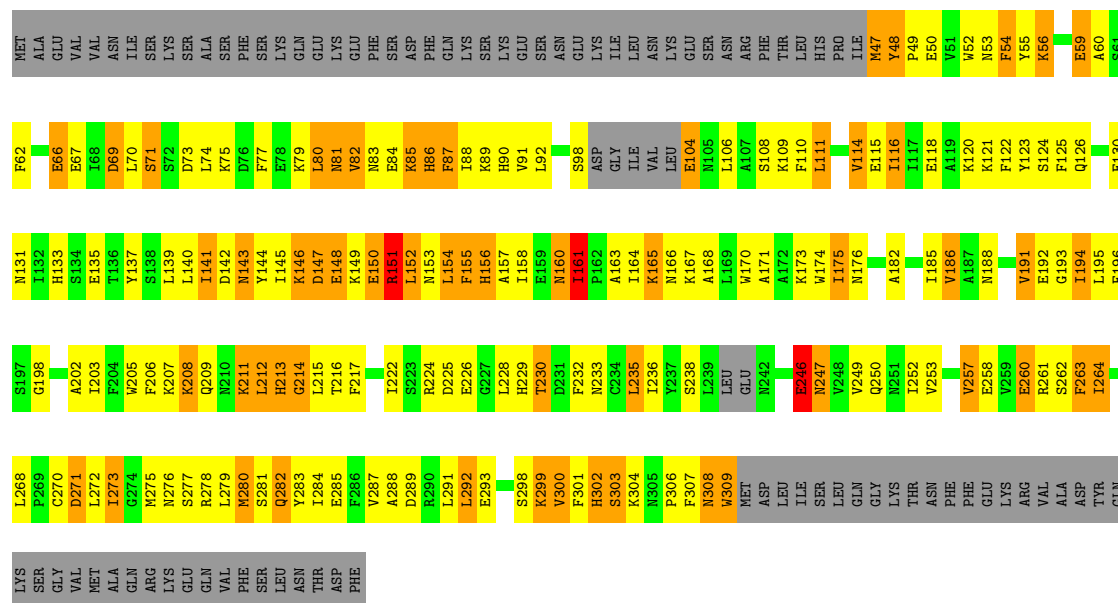
- Molecule 1: Ribonucleotide reductase, small chain





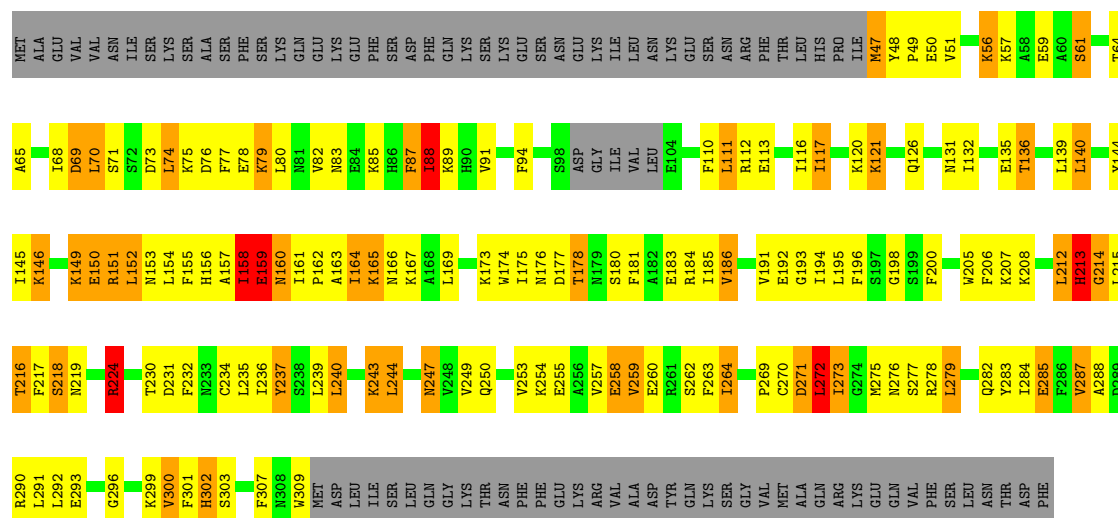
- Molecule 1: Ribonucleotide reductase, small chain

Chain C: 23% 33% 16% 27%



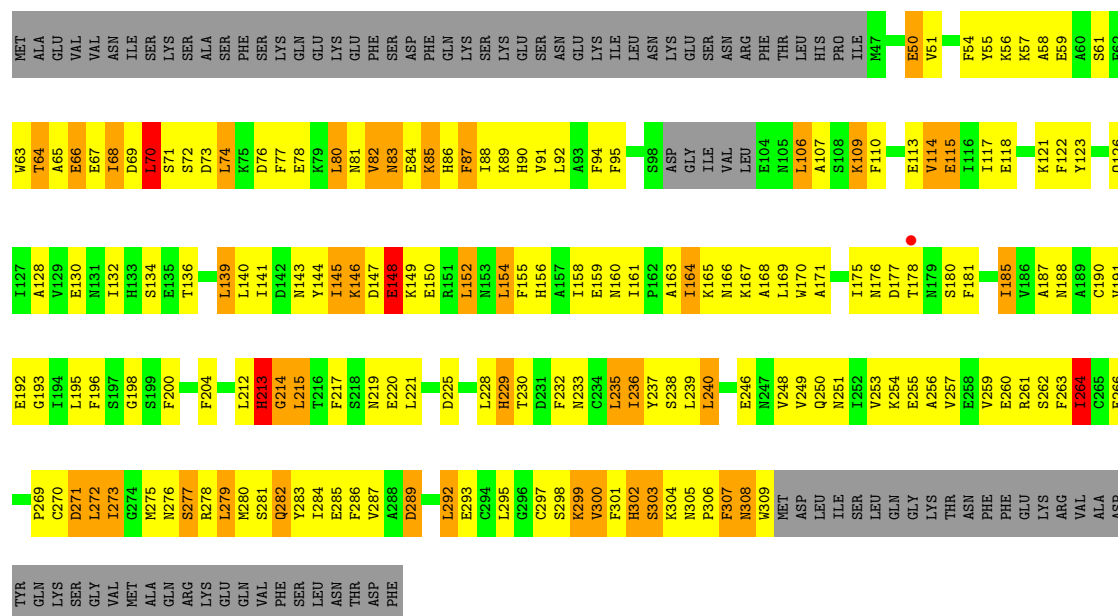
- Molecule 1: Ribonucleotide reductase, small chain

Chain D: 30% 30% 12% 26%

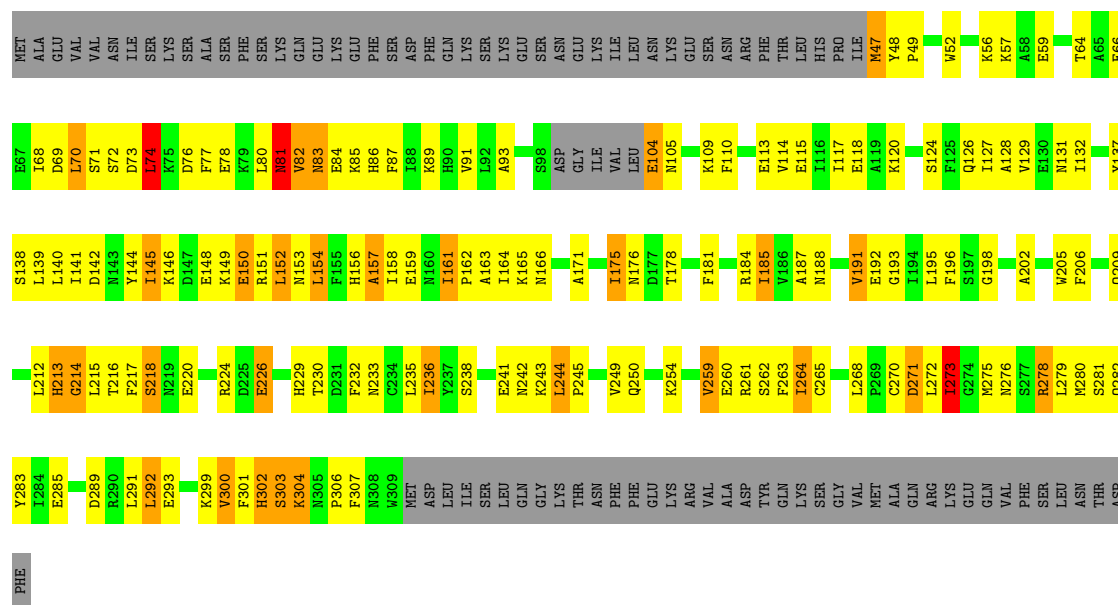


- Molecule 1: Ribonucleotide reductase, small chain

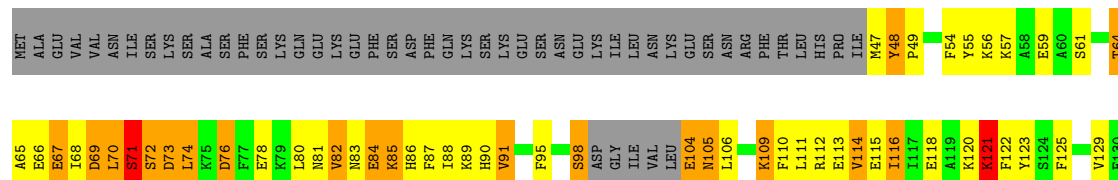
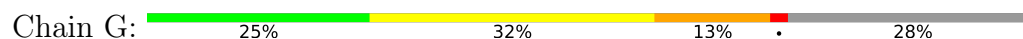
Chain E: 24% 37% 12% 26%

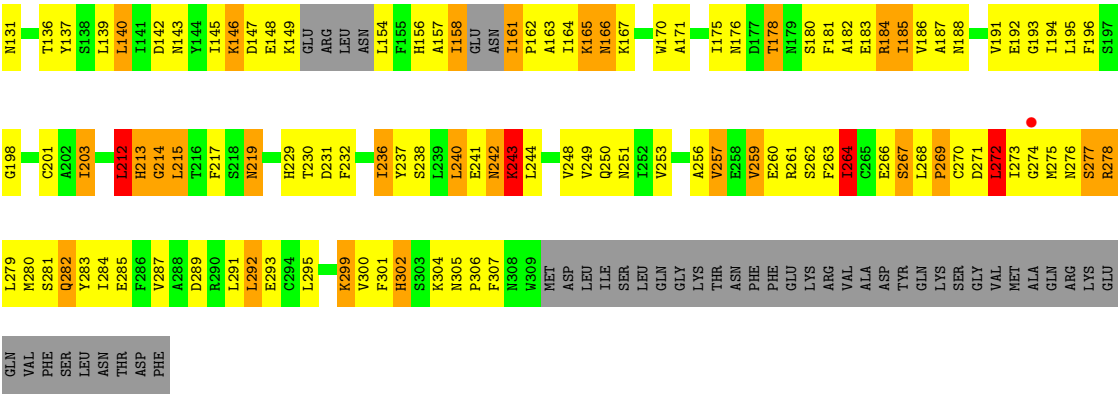


• Molecule 1: Ribonucleotide reductase, small chain

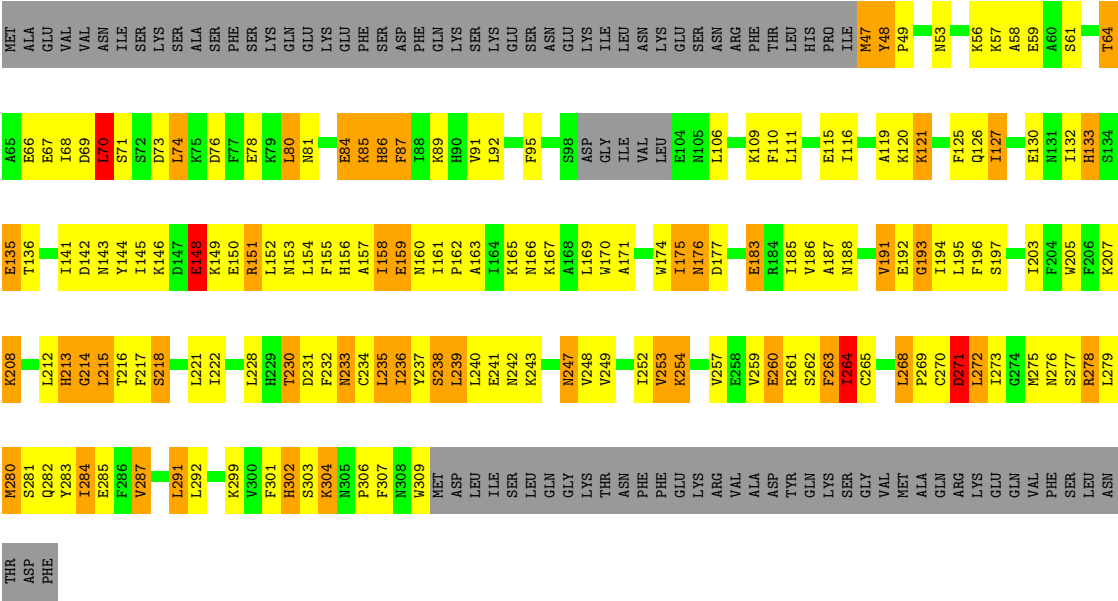
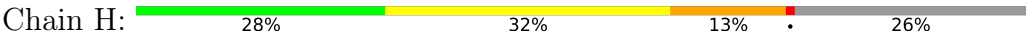


• Molecule 1: Ribonucleotide reductase, small chain





● Molecule 1: Ribonucleotide reductase, small chain



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 , 76.1	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	0.93	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	1.40	8/2154 (0.4%)	1.40	17/2911 (0.6%)
1	B	1.16	4/2104 (0.2%)	1.32	16/2837 (0.6%)
1	C	1.10	1/2148 (0.0%)	1.29	13/2898 (0.4%)
1	D	1.44	10/2166 (0.5%)	1.46	20/2924 (0.7%)
1	E	1.14	2/2159 (0.1%)	1.36	16/2913 (0.5%)
1	F	1.13	4/2166 (0.2%)	1.32	7/2924 (0.2%)
1	G	1.18	12/2107 (0.6%)	1.34	12/2841 (0.4%)
1	H	0.97	3/2166 (0.1%)	1.22	13/2924 (0.4%)
All	All	1.20	44/17170 (0.3%)	1.34	114/23172 (0.5%)

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 (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ILE	CA-CB	9.32	1.67	1.54
1	G	76	ASP	CG-OD2	9.20	1.42	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	ALA	CA-CB	-8.22	1.40	1.53
1	D	116	ILE	CA-CB	7.93	1.64	1.54
1	E	128	ALA	CA-CB	-7.80	1.41	1.53
1	G	241	GLU	CD-OE2	7.44	1.39	1.25
1	D	216	THR	CA-CB	-7.37	1.42	1.53
1	A	175	ILE	C-N	7.37	1.44	1.33
1	D	88	ILE	CA-CB	7.23	1.62	1.54
1	G	76	ASP	CG-OD1	7.11	1.38	1.25
1	A	129	VAL	CA-CB	7.05	1.63	1.54
1	G	91	VAL	CA-CB	-6.83	1.45	1.54
1	G	257	VAL	CA-CB	6.59	1.62	1.54
1	G	243	LYS	CE-NZ	6.47	1.68	1.49
1	B	146	LYS	CE-NZ	6.45	1.68	1.49
1	D	287	VAL	CA-CB	6.35	1.61	1.54
1	A	136	THR	CA-CB	6.14	1.63	1.53
1	G	242	ASN	CG-ND2	6.14	1.46	1.33
1	G	121	LYS	CE-NZ	6.12	1.67	1.49
1	D	87	PHE	N-CA	-6.03	1.39	1.46
1	F	146	LYS	CE-NZ	5.97	1.67	1.49
1	C	230	THR	CA-CB	5.89	1.62	1.53
1	F	83	ASN	N-CA	5.89	1.53	1.46
1	B	299	LYS	CE-NZ	5.86	1.67	1.49
1	A	287	VAL	CA-CB	5.84	1.60	1.54
1	G	242	ASN	CG-OD1	5.80	1.34	1.23
1	H	287	VAL	CA-CB	5.74	1.61	1.54
1	G	287	VAL	CA-CB	5.73	1.61	1.54
1	G	269	PRO	CA-C	-5.70	1.47	1.52
1	D	79	LYS	N-CA	5.69	1.53	1.46
1	G	186	VAL	CA-CB	5.63	1.60	1.54
1	F	117	ILE	CA-CB	5.57	1.61	1.54
1	A	243	LYS	CE-NZ	5.57	1.66	1.49
1	H	127	ILE	CA-CB	5.45	1.61	1.54
1	B	147	ASP	CG-OD1	5.41	1.35	1.25
1	D	186	VAL	CA-CB	5.41	1.60	1.54
1	E	287	VAL	CA-CB	5.39	1.60	1.54
1	B	147	ASP	CG-OD2	5.23	1.35	1.25
1	D	205	TRP	CE2-CZ2	5.18	1.50	1.39
1	A	203	ILE	CA-CB	5.11	1.61	1.54
1	A	300	VAL	CA-CB	5.09	1.61	1.54
1	F	191	VAL	CA-CB	-5.03	1.48	1.54
1	D	68	ILE	CA-CB	5.02	1.60	1.55
1	H	203	ILE	CA-CB	5.01	1.61	1.54

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	269	PRO	CB-CA-C	-14.19	98.49	111.40
1	F	151	ARG	N-CA-C	-12.24	97.94	111.28
1	C	74	LEU	N-CA-C	-10.17	100.99	113.50
1	D	151	ARG	N-CA-C	-9.37	99.86	111.11
1	D	218	SER	N-CA-C	-9.19	100.19	111.40
1	B	87	PHE	N-CA-C	-9.11	101.30	111.14
1	A	74	LEU	N-CA-C	-9.02	102.00	113.72
1	F	74	LEU	N-CA-C	-8.92	102.53	113.50
1	D	273	ILE	N-CA-C	-8.60	104.64	112.90
1	F	273	ILE	CB-CA-C	8.54	119.15	110.70
1	D	74	LEU	N-CA-C	-8.18	103.09	113.72
1	H	215	LEU	N-CA-C	-8.04	102.59	111.36
1	C	87	PHE	N-CA-C	-8.04	102.46	111.14
1	E	215	LEU	N-CA-C	-8.00	102.56	111.28
1	A	82	VAL	N-CA-C	7.95	123.34	111.89
1	A	264	ILE	N-CA-C	7.95	120.99	111.05
1	C	48	TYR	CA-C-N	7.92	127.59	119.19
1	C	48	TYR	C-N-CA	7.92	127.59	119.19
1	B	74	LEU	N-CA-C	-7.82	103.55	113.72
1	F	157	ALA	N-CA-C	-7.28	104.92	114.31
1	A	191	VAL	N-CA-C	-7.26	103.38	110.72
1	E	74	LEU	N-CA-C	-7.21	104.51	113.38
1	D	213	HIS	CA-C-N	-7.20	109.03	122.05
1	D	213	HIS	C-N-CA	-7.20	109.03	122.05
1	A	281	SER	CA-CB-OG	-7.12	96.85	111.10
1	H	74	LEU	N-CA-C	-7.10	104.65	113.38
1	E	87	PHE	N-CA-C	-7.03	103.55	111.14
1	G	74	LEU	N-CA-C	-6.99	104.78	113.38
1	A	218	SER	N-CA-C	-6.94	103.33	111.03
1	E	83	ASN	N-CA-C	-6.92	104.47	113.12
1	F	87	PHE	N-CA-C	-6.91	103.68	111.14
1	B	268	LEU	CA-C-N	6.80	127.87	119.98
1	B	268	LEU	C-N-CA	6.80	127.87	119.98
1	G	273	ILE	N-CA-C	-6.80	103.76	113.07
1	A	48	TYR	CA-C-N	6.78	126.48	119.56
1	A	48	TYR	C-N-CA	6.78	126.48	119.56
1	E	159	GLU	N-CA-C	-6.73	103.97	111.71
1	H	268	LEU	CA-C-N	6.66	127.71	119.98
1	H	268	LEU	C-N-CA	6.66	127.71	119.98
1	A	82	VAL	CB-CA-C	-6.62	99.14	111.79
1	C	273	ILE	N-CA-C	-6.52	106.88	113.47
1	D	87	PHE	N-CA-C	-6.51	103.80	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	LYS	N-CA-C	-6.50	105.98	114.04
1	B	241	GLU	N-CA-C	-6.47	101.01	111.04
1	B	273	ILE	N-CA-C	-6.46	105.28	113.22
1	A	264	ILE	CB-CA-C	-6.43	102.20	112.16
1	A	213	HIS	CA-C-N	-6.40	112.03	122.20
1	A	213	HIS	C-N-CA	-6.40	112.03	122.20
1	G	48	TYR	CA-C-N	6.37	126.06	119.56
1	G	48	TYR	C-N-CA	6.37	126.06	119.56
1	F	273	ILE	N-CA-C	-6.24	107.21	113.20
1	A	50	GLU	N-CA-C	-6.24	103.78	112.45
1	E	82	VAL	N-CA-C	6.21	122.26	109.34
1	B	90	HIS	N-CA-CB	6.17	120.07	110.44
1	A	87	PHE	N-CA-C	-6.16	104.49	111.14
1	B	215	LEU	N-CA-C	-6.12	104.69	111.36
1	E	139	LEU	CA-CB-CG	-6.11	94.93	116.30
1	D	165	LYS	N-CA-C	-6.05	104.69	111.28
1	G	84	GLU	N-CA-C	-6.00	105.79	113.23
1	G	212	LEU	N-CA-C	5.98	119.64	111.39
1	D	244	LEU	CA-C-N	-5.96	113.55	119.99
1	D	244	LEU	C-N-CA	-5.96	113.55	119.99
1	E	289	ASP	N-CA-C	5.93	117.41	111.07
1	E	88	ILE	CB-CA-C	-5.92	104.30	111.88
1	E	64	THR	N-CA-C	5.82	118.26	109.41
1	H	284	ILE	N-CA-CB	5.74	117.27	110.55
1	C	246	GLU	CB-CG-CD	-5.74	102.85	112.60
1	B	51	VAL	N-CA-C	5.71	117.13	110.62
1	D	224	ARG	N-CA-C	-5.70	105.07	111.28
1	E	50	GLU	N-CA-C	-5.67	104.71	111.69
1	G	215	LEU	N-CA-C	-5.66	105.19	111.36
1	D	185	ILE	CB-CA-C	-5.65	104.51	112.14
1	H	264	ILE	CA-C-N	-5.64	113.75	122.49
1	H	264	ILE	C-N-CA	-5.64	113.75	122.49
1	E	264	ILE	N-CA-C	5.63	118.09	111.05
1	D	156	HIS	N-CA-C	-5.63	106.77	113.97
1	D	284	ILE	N-CA-CB	5.58	116.48	110.62
1	H	157	ALA	N-CA-C	-5.58	105.97	112.89
1	C	161	ILE	N-CA-C	5.56	113.95	107.89
1	A	273	ILE	CB-CA-C	-5.55	104.83	110.93
1	E	152	LEU	N-CA-C	5.50	118.20	111.82
1	H	148	GLU	N-CA-C	5.49	122.48	110.80
1	B	147	ASP	CB-CA-C	5.48	118.79	109.80
1	A	139	LEU	N-CA-C	5.46	117.23	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	87	PHE	N-CA-C	-5.45	105.03	110.97
1	H	133	HIS	CB-CA-C	-5.44	102.34	110.88
1	D	237	TYR	N-CA-C	-5.43	105.44	111.36
1	B	264	ILE	N-CA-C	5.42	117.87	111.09
1	D	200	PHE	N-CA-C	-5.41	105.47	111.36
1	A	188	ASN	N-CA-C	5.38	116.83	111.07
1	B	71	SER	CA-C-N	-5.37	114.17	122.49
1	B	71	SER	C-N-CA	-5.37	114.17	122.49
1	C	155	PHE	N-CA-C	-5.37	105.47	112.23
1	F	226	GLU	OE1-CD-OE2	5.34	135.72	122.90
1	C	191	VAL	CB-CA-C	-5.30	104.99	112.14
1	B	269	PRO	CB-CA-C	-5.27	104.86	111.71
1	E	160	ASN	N-CA-C	5.26	119.23	109.56
1	H	218	SER	N-CA-C	-5.23	105.50	111.14
1	G	85	LYS	N-CA-C	5.18	117.01	111.36
1	G	67	GLU	CA-C-N	-5.16	117.87	123.08
1	G	67	GLU	C-N-CA	-5.16	117.87	123.08
1	C	156	HIS	N-CA-C	-5.15	106.84	113.02
1	D	61	SER	N-CA-C	-5.14	105.70	112.94
1	H	253	VAL	CB-CA-C	5.13	118.74	112.02
1	D	296	GLY	N-CA-C	-5.11	105.21	114.46
1	E	155	PHE	N-CA-C	-5.11	107.00	113.18
1	D	212	LEU	N-CA-C	5.11	118.43	111.39
1	G	264	ILE	N-CA-C	5.11	119.19	112.04
1	B	64	THR	N-CA-C	5.08	117.39	109.52
1	C	186	VAL	CB-CA-C	-5.05	105.50	111.97
1	C	60	ALA	N-CA-C	-5.04	107.10	113.20
1	B	140	LEU	CA-CB-CG	5.01	133.84	116.30
1	D	158	ILE	N-CA-C	5.01	119.76	109.34
1	E	213	HIS	CB-CA-C	-5.01	100.46	110.42

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	166	0
1	B	2056	0	1992	198	7
1	C	2099	0	2056	195	0
1	D	2116	0	2074	156	0
1	E	2109	0	2061	196	2
1	F	2116	0	2074	161	0
1	G	2059	0	2019	177	3
1	H	2116	0	2074	178	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	13	0	0	6	0
3	D	18	0	0	4	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	1411	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 43.

All (1411) 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:NZ	1:G:243:LYS:CE	1.68	1.55
1:B:146:LYS:CE	1:B:146:LYS:NZ	1.68	1.54
1:G:121:LYS:CE	1:G:121:LYS:NZ	1.67	1.52
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:B:93:ALA:CB	1:B:154:LEU:HD11	1.86	1.04
1:E:292:LEU:CD1	1:E:297:CYS:HB2	1.87	1.04
1:B:163:ALA:HB1	1:B:263:PHE:HD2	0.89	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:150:GLU:HA	1:C:150:GLU:OE2	1.54	1.02
1:D:163:ALA:HB1	1:D:263:PHE:CD2	1.95	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:E:148:GLU:HG3	1:E:148:GLU:O	1.20	0.99
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: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:H	1:E:70:LEU:HD22	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:O	1:H:301:PHE:CD1	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:F:81:ASN:C	1:F:83:ASN:H	1.74	0.94
1:E:148:GLU:O	1:E:148:GLU:CG	2.12	0.94
1:F:81:ASN:HB3	1:F:84:GLU:H	1.30	0.94
1:F:175:ILE:HD12	1:F:175:ILE:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:ASP:HB2	1:H:213:HIS:ND1	1.84	0.91
1:H:115:GLU:HA	1:H:120:LYS:HZ1	1.34	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:H	1:H:247:ASN:HD22	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:B:80:LEU:HD23	1:B:84:GLU:HB3	1.54	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
1:F:285:GLU:HG3	1:F:301:PHE:CE1	2.08	0.89
1:B:301:PHE:HD1	1:B:303:SER:HG	1.18	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:SD	1:C:47:MET:N	2.45	0.88
1:E:282:GLN:NE2	1:E:306:PRO:CG	2.37	0.88
1:D:213:HIS:CD2	1:D:213:HIS:O	2.26	0.88
1:H:247:ASN:H	1:H:247:ASN:ND2	1.62	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:HG3	1:C:148:GLU:O	1.75	0.86
1:H:213:HIS:O	1:H:213:HIS:CD2	2.28	0.86
1:G:115:GLU:HA	1:G:120:LYS:HZ1	1.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:115:GLU:HA	1:A:120:LYS:HZ1	1.40	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:A:113:GLU:CD	1:A:184:ARG:HH21	1.85	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:A:152:LEU:C	1:A:154:LEU:H	1.82	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:O	1:B:301:PHE:CD1	2.31	0.83
1:E:279:LEU:HD13	1:E:307:PHE:HE1	0.74	0.83
1:C:98:SER:CB	1:C:167:LYS:NZ	2.41	0.83
1:C:304:LYS:O	1:C:306:PRO:HD3	1.79	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:H:301:PHE:O	1:H:301:PHE:HD1	1.59	0.82
1:E:301:PHE:O	1:E:302:HIS:C	2.20	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: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:207:LYS:HE3	1:B:220:GLU:OE1	1.81	0.81
1:B:106:LEU:HD11	3:B:361:HOH:O	1.81	0.81
1:H:115:GLU:HA	1:H:120:LYS:HZ3	1.43	0.81
1:A:308:ASN:H	1:A:308:ASN:HD22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:HB2	1:A:213:HIS:HB3	1.63	0.80
1:A:175:ILE:HG22	1:A:176:ASN:N	1.97	0.80
1:H:74:LEU:O	1:H:78:GLU:HG2	1.81	0.80
1:H:170:TRP:HZ3	1:H:175:ILE:HD11	1.46	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: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:D:301:PHE:O	1:D:302:HIS:C	2.23	0.78
1:G:213:HIS:O	1:G:213:HIS:CD2	2.36	0.78
1:H:270:CYS:C	1:H:272:LEU:H	1.91	0.78
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:70:LEU:CD1	1:D:140:LEU:HD12	2.13	0.78
1:D:214:GLY:HA2	1:D:217:PHE:HB3	1.65	0.78
1:H:247:ASN:HD22	1:H:247:ASN:N	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:115:GLU:CA	1:H:120:LYS:HZ1	1.99	0.75
1:D:213:HIS:O	1:D:213:HIS:HD2	1.70	0.75
1:E:270:CYS:C	1:E:272:LEU:H	1.93	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:81:ASN:C	1:F:83:ASN:N	2.41	0.74
1:A:73:ASP:CG	1:A:76:ASP:OD2	2.31	0.74
1:F:224:ARG:HG2	3:F:352:HOH:O	1.88	0.74
1:B:141:ILE:HG23	1:B:145:ILE:HD12	1.69	0.74
1:B:280:MET:HE3	1:B:280:MET:HA	1.68	0.74
1:C:301:PHE:HD1	1:C:303:SER:HG	1.36	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: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:E:70:LEU:HD22	1:E:70:LEU:N	2.02	0.73
1:E:282:GLN:NE2	1:E:306:PRO:HD3	2.02	0.73
1:G:106:LEU:CD2	1:G:188:ASN:HD21	2.01	0.73
1:H:49:PRO:O	1:H:53:ASN:ND2	2.22	0.73
1:H:299:LYS:HD2	1:H:302:HIS:CD2	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:PHE:O	1:B:302:HIS:C	2.30	0.73
1:A:270:CYS:C	1:A:272:LEU:H	1.97	0.72
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:F:301:PHE:O	1:F:302:HIS:C	2.30	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:H	1:H:264:ILE:CD1	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: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
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:C:150:GLU:O	1:C:151:ARG:C	2.34	0.70
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:C:301:PHE:O	1:C:302:HIS:C	2.32	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:163:ALA:CB	1:D:263:PHE:CD2	2.71	0.70
1:D:237:TYR:O	1:D:240:LEU:HB2	1.90	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:B:81:ASN:CG	1:B:81:ASN:O	2.34	0.70
1:C:154:LEU:O	1:C:154:LEU:HD12	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PHE:HB2	1:D:184:ARG:NH2	2.07	0.70
1:E:118:GLU:CD	1:E:118:GLU:H	1.99	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: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:71:SER:HB2	3:E:365:HOH:O	1.91	0.69
1:E:213:HIS:O	1:E:213:HIS:CG	2.41	0.69
1:C:90:HIS:HB3	1:C:268:LEU:HD22	1.74	0.69
1:C:175:ILE:O	1:C:176:ASN:C	2.32	0.69
1:C:299:LYS:HZ2	1:C:302:HIS:HD2	0.70	0.69
1:G:81:ASN:OD1	1:G:82:VAL:N	2.25	0.69
1:G:271:ASP:OD1	1:G:275:MET:O	2.11	0.69
1:A:113:GLU:CD	1:A:184:ARG:NH2	2.51	0.69
1:A:301:PHE:O	1:A:302:HIS:C	2.35	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:D:150:GLU:O	1:D:151:ARG:C	2.32	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:G:192:GLU:O	1:G:230:THR:OG1	2.11	0.68
1:G:285:GLU:CD	1:G:301:PHE:HD1	2.00	0.68
1:B:143:ASN:HA	1:B:146:LYS:HG3	1.75	0.68
1:C:106:LEU:HD22	3:C:352:HOH:O	1.93	0.68
1:F:73:ASP:HB3	1:F:76:ASP:CG	2.19	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:TRP:CZ3	1:G:175:ILE:HD11	2.29	0.67
1:A:73:ASP:O	1:A:213:HIS:CE1	2.48	0.67
1:A:226:GLU:OE1	1:A:226:GLU:HA	1.94	0.67
1:B:92:LEU:HD21	1:B:215:LEU:HD11	1.76	0.67
1:C:247:ASN:N	1:C:247:ASN:HD22	1.89	0.67
1:G:180:SER:HB2	1:G:183:GLU:CD	2.20	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:HD3	1:A:278:ARG:N	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: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: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:D:77:PHE:CD2	1:D:144:TYR:CD2	2.83	0.66
1:A:115:GLU:HA	1:A:120:LYS:HZ2	1.58	0.66
1:B:150:GLU:C	1:B:152:LEU:N	2.51	0.66
1:D:117:ILE:HD12	1:D:117:ILE:H	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:A:258:GLU:OE2	1:A:258:GLU:HA	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:C	1:A:154:LEU:N	2.51	0.65
1:A:158:ILE:O	1:A:159:GLU:C	2.40	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:H:309:TRP:O	1:H:309:TRP:CE3	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:G:165:LYS:HG2	1:G:166:ASN:N	2.12	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: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:G:301:PHE:O	1:G:302:HIS:C	2.40	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
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: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:57:LYS:O	1:E:61:SER:HB2	1.98	0.64
1:E:175:ILE:HG22	1:E:176:ASN:N	2.12	0.64
1:F:47:MET:SD	1:F:47:MET:N	2.71	0.64
1:G:249:VAL:O	1:G:253:VAL:HG23	1.98	0.64
1:D:175:ILE:O	1:D:176:ASN:C	2.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:281:SER:O	1:G:285:GLU:HG2	1.98	0.63
1:C:88:ILE:HD11	1:C:206:PHE:CE1	2.34	0.63
1:C:122:PHE:CZ	1:C:228:LEU:CD2	2.82	0.63
1:G:91:VAL:CG2	1:G:268:LEU:HD23	2.28	0.63
1:G:215:LEU:O	1:G:219:ASN:HB3	1.98	0.63
1:H:269:PRO:O	1:H:272:LEU:HB2	1.99	0.63
1:E:72:SER:OG	1:E:73:ASP:OD2	2.12	0.63
1:E:301:PHE:HD1	1:E:303:SER:HG	1.46	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:HD12	1:C:175:ILE:N	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:73:ASP:HB2	1:A:213:HIS:CB	2.29	0.62
1:A:270:CYS:O	1:A:272:LEU:N	2.31	0.62
1:B:89:LYS:HA	1:B:145:ILE:HD11	1.80	0.62
1:B:150:GLU:O	1:B:151:ARG:C	2.39	0.62
1:B:212:LEU:C	1:B:213:HIS:HD2	2.07	0.62
1:B:285:GLU:HB3	1:B:301:PHE:CD1	2.34	0.62
1:C:90:HIS:HB3	1:C:268:LEU:CD2	2.29	0.62
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: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:E:213:HIS:CD2	1:E:213:HIS:C	2.77	0.62
1:F:70:LEU:O	1:F:213:HIS:HE1	1.81	0.62
1:F:236:ILE:HD12	1:F:236:ILE:H	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:A:69:ASP:C	1:A:71:SER:H	2.07	0.62
1:F:47:MET:O	1:F:49:PRO:HD3	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:HIS:CG	1:C:213:HIS:O	2.52	0.62
1:B:87:PHE:CZ	1:B:91:VAL:HG21	2.35	0.62
1:F:81:ASN:CB	1:F:84:GLU:N	2.55	0.62
1:F:124:SER:HA	1:F:127:ILE:HD12	1.81	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:N	1:H:264:ILE:CD1	2.54	0.61
1:E:217:PHE:CE1	1:E:221:LEU:HD21	2.35	0.61
1:G:55:TYR:CD1	1:G:56:LYS:HD3	2.33	0.61
1:G:185:ILE:CD1	1:G:236:ILE:CG2	2.78	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:E:280:MET:HE1	1:E:283:TYR:HD2	1.65	0.61
1:F:175:ILE:O	1:F:176:ASN:C	2.41	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:ND2	1:H:247:ASN:N	2.39	0.61
1:H:301:PHE:O	1:H:302:HIS:C	2.42	0.61
1:B:264:ILE:HD12	1:B:264:ILE:H	1.65	0.61
1:D:150:GLU:OE1	1:D:153:ASN:HB3	2.00	0.61
1:F:285:GLU:CD	1:F:301:PHE:CE2	2.79	0.61
1:G:78:GLU:OE2	1:G:78:GLU:HA	2.00	0.61
1:B:81:ASN:O	1:B:81:ASN:OD1	2.19	0.61
1:E:280:MET:HE3	1:E:283:TYR:HB3	1.82	0.61
1:G:146:LYS:CD	1:G:146:LYS:H	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:HD12	1:B:264:ILE:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:PHE:CE2	1:F:185:ILE:HD11	2.36	0.60
1:F:270:CYS:C	1:F:272:LEU:H	2.08	0.60
1:G:64:THR:OG1	1:G:65:ALA:N	2.32	0.60
1:G:198:GLY:HA3	1:G:264:ILE:HG12	1.83	0.60
1:H:213:HIS:O	1:H:213:HIS:CG	2.49	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:D:247:ASN:HD22	1:D:247:ASN:N	2.00	0.60
1:E:121:LYS:HZ3	1:F:131:ASN:HB3	1.66	0.60
1:E:170:TRP:CZ2	1:E:256:ALA:HB2	2.36	0.60
1:G:146:LYS:H	1:G:146:LYS:HD3	1.67	0.60
1:B:74:LEU:HD12	1:B:77:PHE:HB3	1.82	0.60
1:C:69:ASP:C	1:C:71:SER:H	2.09	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:47:MET:SD	1:H:47:MET:N	2.75	0.60
1:H:214:GLY:HA2	1:H:217:PHE:H	1.65	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:OD1	1:B:305:ASN:N	2.33	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:G:285:GLU:CD	1:G:301:PHE:CD1	2.79	0.60
1:B:148:GLU:C	1:B:150:GLU:H	2.10	0.60
1:C:214:GLY:HA2	1:C:217:PHE:H	1.65	0.60
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: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:A:280:MET:HE3	1:A:283:TYR:HB3	1.83	0.59
1:E:117:ILE:H	1:E:117:ILE:CD1	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:B:72:SER:C	1:B:73:ASP:OD2	2.46	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:81:ASN:CG	1:F:84:GLU:OE1	2.46	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:299:LYS:HZ3	1:D:302:HIS:HD2	1.49	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:54:PHE:O	1:B:122:PHE:HE2	1.85	0.59
1:B:146:LYS:NZ	1:B:146:LYS:CD	2.61	0.59
1:E:80:LEU:HD23	1:E:84:GLU:HB3	1.85	0.59
1:E:140:LEU:HD22	1:E:215:LEU:HD13	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:81:ASN:OD1	1:E:81:ASN:C	2.45	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:A:121:LYS:HZ3	1:D:131:ASN:HB3	1.67	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:81:ASN:CG	1:A:84:GLU:HG3	2.28	0.58
1:A:137:TYR:O	1:A:141:ILE:HD12	2.03	0.58
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:291:LEU:HD13	1:G:291:LEU:C	2.28	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: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:N	1:D:48:TYR:CD1	2.72	0.57
1:F:226:GLU:OE1	1:F:226:GLU:HA	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:50:GLU:HA	1:A:53:ASN:ND2	2.19	0.57
1:A:113:GLU:OE2	1:A:184:ARG:NH2	2.37	0.57
1:C:85:LYS:O	1:C:89:LYS:HG3	2.04	0.57
1:H:150:GLU:O	1:H:151:ARG:C	2.47	0.57
1:B:282:GLN:C	1:B:282:GLN:HE21	2.13	0.57
1:E:282:GLN:C	1:E:282:GLN:HE21	2.11	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: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:B:308:ASN:OD1	1:B:308:ASN:C	2.47	0.57
1:C:195:LEU:HA	1:C:260:GLU:CG	2.35	0.57
1:B:73:ASP:CG	1:B:213:HIS:HB3	2.28	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:50:GLU:HG2	1:E:235:LEU:HD22	1.85	0.57
1:E:113:GLU:O	1:E:115:GLU:HG2	2.05	0.57
1:F:144:TYR:CE1	1:F:215:LEU:HD22	2.39	0.57
1:H:261:ARG:NH2	1:H:285:GLU:CD	2.63	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
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:D:207:LYS:HB2	1:D:216:THR:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:LEU:O	1:F:142:ASP:HB3	2.04	0.56
1:H:66:GLU:OE2	1:H:66:GLU:HA	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:D:258:GLU:OE2	1:D:258:GLU:HA	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: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:E:270:CYS:C	1:E:272:LEU:N	2.64	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:N	1:C:247:ASN:ND2	2.51	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:O	1:A:77:PHE:CD1	2.59	0.56
1:C:123:TYR:OH	1:C:236:ILE:HD12	2.05	0.56
1:H:145:ILE:HG22	1:H:145:ILE:O	2.04	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:E:177:ASP:CG	1:E:178:THR:H	2.14	0.56
1:A:94:PHE:CD1	1:A:196:PHE:HE1	2.24	0.56
1:A:202:ALA:HB1	1:A:273:ILE:CD1	2.36	0.56
1:C:224:ARG:NH2	1:C:225:ASP:OD1	2.39	0.56
1:D:218:SER:O	1:D:219:ASN:C	2.47	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
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:48:TYR:N	1:C:48:TYR:CD1	2.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:77:PHE:CD2	1:E:144:TYR:CD2	2.94	0.55
1:E:181:PHE:CZ	1:E:185:ILE:HD11	2.41	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:D:213:HIS:CD2	1:D:213:HIS:C	2.83	0.55
1:H:87:PHE:HA	1:H:268:LEU:HD21	1.89	0.55
1:H:150:GLU:O	1:H:152:LEU:N	2.38	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: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:G:213:HIS:CD2	1:G:213:HIS:C	2.85	0.55
1:A:52:TRP:HZ2	1:D:135:GLU:OE2	1.90	0.55
1:A:155:PHE:O	1:A:159:GLU:HG2	2.06	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:A:77:PHE:CD1	1:A:77:PHE:C	2.83	0.54
1:B:150:GLU:O	1:B:154:LEU:HB2	2.07	0.54
1:C:147:ASP:O	1:C:147:ASP:OD2	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

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	0.54
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:A:81:ASN:OD1	1:A:84:GLU:HG3	2.07	0.54
1:A:158:ILE:O	1:A:160:ASN:N	2.41	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:A:70:LEU:HD21	1:A:140:LEU:HD11	1.90	0.54
1:E:80:LEU:HD23	1:E:84:GLU:CB	2.37	0.54
1:E:141:ILE:HA	1:E:145:ILE:HD12	1.88	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:A:280:MET:HE1	1:A:283:TYR:CD2	2.43	0.54
1:A:87:PHE:CD2	1:A:273:ILE:HG21	2.42	0.54
1:C:87:PHE:CD1	1:C:268:LEU:HG	2.43	0.54
1:C:152:LEU:O	1:C:154:LEU:N	2.41	0.54
1:E:109:LYS:NZ	1:E:176:ASN:HA	2.17	0.54
1:G:115:GLU:HA	1:G:120:LYS:HZ2	1.66	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: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:E:147:ASP:C	1:E:147:ASP:OD1	2.50	0.53
1:H:86:HIS:CA	1:H:89:LYS:HD3	2.25	0.53
1:B:69:ASP:C	1:B:71:SER:H	2.15	0.53
1:E:92:LEU:HD11	1:E:144:TYR:CD1	2.41	0.53
1:B:76:ASP:HB2	1:B:212:LEU:HD23	1.91	0.53
1:B:96:ALA:O	1:B:155:PHE:CE2	2.62	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
1:H:115:GLU:C	1:H:120:LYS:NZ	2.67	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:81:ASN:C	1:G:83:ASN:H	2.16	0.52
1:H:253:VAL:O	1:H:257:VAL:HG23	2.09	0.52
1:C:235:LEU:O	1:C:238:SER:HB3	2.09	0.52
1:H:205:TRP:CE3	1:H:275:MET:HE3	2.44	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:B:232:PHE:CE2	1:B:236:ILE:CD1	2.93	0.52
1:C:111:LEU:HD21	1:C:124:SER:N	2.25	0.52
1:E:63:TRP:N	1:E:63:TRP:CD1	2.77	0.52
1:E:164:ILE:HD12	1:E:164:ILE:H	1.74	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:73:ASP:H	1:F:213:HIS:CE1	2.27	0.52
1:G:74:LEU:HG	1:G:74:LEU:O	2.10	0.52
1:G:278:ARG:H	1:G:278:ARG:CD	2.14	0.52
1:H:193:GLY:O	1:H:197:SER:OG	2.27	0.52
1:A:57:LYS:O	1:A:61:SER:HB3	2.10	0.52
1:C:152:LEU:C	1:C:154:LEU:H	2.18	0.52
1:D:195:LEU:O	1:D:196:PHE:HB2	2.10	0.52
1:E:74:LEU:HD11	1:E:144:TYR:HA	1.92	0.52
1:E:170:TRP:HH2	1:E:190:CYS:HB2	1.75	0.52
1:F:270:CYS:C	1:F:272:LEU:N	2.68	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:121:LYS:CE	1:C:131:ASN:HB3	2.40	0.51
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: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:69:ASP:C	1:G:71:SER:H	2.19	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
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:B:177:ASP:CG	1:B:178:THR:H	2.18	0.51
1:D:158:ILE:C	1:D:160:ASN:H	2.19	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:B:212:LEU:C	1:B:213:HIS:CD2	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:MET:O	1:D:49:PRO:CD	2.59	0.51
1:D:149:LYS:HD3	1:D:149:LYS:C	2.36	0.51
1:D:214:GLY:HA2	1:D:217:PHE:CB	2.40	0.51
1:E:177:ASP:CG	1:E:178:THR:N	2.69	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: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: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:D:253:VAL:O	1:D:254:LYS:C	2.54	0.51
1:G:121:LYS:NZ	1:H:135:GLU:OE1	2.44	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: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:81:ASN:OD1	1:B:81:ASN:C	2.54	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: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: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:64:THR:HG23	1:B:66:GLU:H	1.77	0.50
1:B:212:LEU:HA	1:B:213:HIS:HD2	1.76	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
1:B:118:GLU:H	1:B:118:GLU:CD	2.20	0.50
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:198:GLY:HA2	1:G:280:MET:CE	2.42	0.50
1:A:175:ILE:O	1:A:176:ASN:C	2.54	0.50
1:C:81:ASN:CG	1:C:84:GLU:HG2	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:270:CYS:C	1:H:272:LEU:N	2.63	0.50
1:H:271:ASP:HA	1:H:275:MET:O	2.12	0.50
1:D:270:CYS:C	1:D:272:LEU:H	2.20	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:O	1:D:217:PHE:CD1	2.65	0.49
1:D:237:TYR:HH	1:D:244:LEU:HB2	1.75	0.49
1:F:233:ASN:C	1:F:236:ILE:HD12	2.37	0.49
1:H:81:ASN:OD1	1:H:84:GLU:HG2	2.12	0.49
1:H:151:ARG:O	1:H:155:PHE:HD1	1.95	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:HE3	1:H:208:LYS:HA	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:174:TRP:CD1	1:C:252:ILE:HG23	2.48	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: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:B:144:TYR:C	1:B:145:ILE:HG13	2.37	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
1:E:73:ASP:CG	1:E:213:HIS:HB3	2.37	0.49
1:H:187:ALA:O	1:H:191:VAL:HG23	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:55:TYR:CE2	1:E:121:LYS:HG2	2.47	0.49
1:E:77:PHE:CE2	1:E:144:TYR:HB3	2.47	0.49
1:E:106:LEU:CD2	1:E:188:ASN:HD21	2.25	0.49
1:G:198:GLY:HA2	1:G:280:MET:HE2	1.94	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:F:152:LEU:C	1:F:154:LEU:H	2.20	0.49
1:H:69:ASP:C	1:H:71:SER:H	2.21	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:HG12	1:F:273:ILE:O	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:HD22	1:D:247:ASN:H	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:HA	1:F:285:GLU:OE1	2.13	0.48
1:H:271:ASP:CG	1:H:277:SER:H	2.20	0.48
1:A:69:ASP:O	1:A:71:SER:N	2.46	0.48
1:A:299:LYS:HD2	1:A:302:HIS:CD2	2.49	0.48
1:B:148:GLU:C	1:B:150:GLU:N	2.71	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:G:280:MET:HE1	1:G:283:TYR:HD2	1.78	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:214:GLY:HA2	1:H:217:PHE:N	2.29	0.48
1:H:217:PHE:CZ	1:H:221:LEU:HD11	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CG	1:F:213:HIS:O	2.61	0.48
1:A:59:GLU:C	1:A:61:SER:H	2.21	0.48
1:B:194:ILE:HD11	1:B:253:VAL:HG13	1.94	0.48
1:G:73:ASP:HB3	1:G:76:ASP:HB2	1.95	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: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:73:ASP:CB	1:H:76:ASP:OD2	2.61	0.48
1:H:110:PHE:CD1	1:H:110:PHE:N	2.81	0.48
1:A:114:VAL:HG12	1:A:116:ILE:HG13	1.94	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:D:208:LYS:O	1:D:208:LYS:HG3	2.14	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: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:73:ASP:CG	1:H:76:ASP:OD2	2.57	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:E:73:ASP:OD2	1:E:213:HIS:HB3	2.14	0.47
1:A:280:MET:HE3	1:A:280:MET:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:48:TYR:CD1	1:H:48:TYR:N	2.83	0.47
1:H:195:LEU:O	1:H:196:PHE:HB2	2.13	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:OE1	1:F:150:GLU:HA	2.14	0.47
1:A:253:VAL:O	1:A:257:VAL:HG23	2.15	0.47
1:B:58:ALA:HB2	1:B:228:LEU:HD21	1.96	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:F:299:LYS:HZ2	1:F:302:HIS:CD2	2.32	0.47
1:H:233:ASN:HA	1:H:236:ILE:HD11	1.84	0.47
1:H:276:ASN:HB3	1:H:279:LEU:HB2	1.96	0.47
1:A:87:PHE:CD2	1:A:273:ILE:CG2	2.97	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: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:D:145:ILE:HG22	1:D:145:ILE:O	2.15	0.47
1:E:280:MET:HE2	1:E:284:ILE:HD11	1.96	0.47
1:G:48:TYR:CD1	1:G:48:TYR:N	2.82	0.47
1:G:257:VAL:O	1:G:261:ARG:HG3	2.15	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
1:B:54:PHE:C	1:B:122:PHE:HE2	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:CD2	1:B:89:LYS:HD2	2.51	0.46
1:C:250:GLN:CD	1:C:300:VAL:HG21	2.40	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: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:D:213:HIS:O	1:D:213:HIS:CG	2.52	0.46
1:F:69:ASP:C	1:F:71:SER:H	2.22	0.46
1:F:285:GLU:CG	1:F:301:PHE:CE1	2.92	0.46
1:B:47:MET:C	1:B:48:TYR:CD1	2.93	0.46
1:B:194:ILE:CD1	1:B:253:VAL:HG13	2.46	0.46
1:B:247:ASN:N	1:B:247:ASN:ND2	2.58	0.46
1:C:175:ILE:HG22	1:C:176:ASN:H	1.79	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:H:240:LEU:HG	1:H:242:ASN:C	2.40	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:54:PHE:HD2	1:C:54:PHE:HA	1.66	0.46
1:C:203:ILE:CG2	1:C:216:THR:HG22	2.46	0.46
1:C:214:GLY:HA2	1:C:217:PHE:N	2.30	0.46
1:D:70:LEU:HD21	1:D:140:LEU:HD11	1.97	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: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:H:192:GLU:O	1:H:230:THR:OG1	2.31	0.46
1:B:163:ALA:CB	1:B:263:PHE:CD2	2.54	0.46
1:E:50:GLU:HG2	1:E:235:LEU:CD2	2.45	0.46
1:F:81:ASN:HB3	1:F:83:ASN:N	2.29	0.46
1:F:270:CYS:O	1:F:272:LEU:N	2.48	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:150:GLU:C	1:B:152:LEU:H	2.23	0.46
1:B:280:MET:O	1:B:283:TYR:HB3	2.16	0.46
1:D:144:TYR:HH	1:D:213:HIS:CE1	2.33	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:C:104:GLU:C	3:C:352:HOH:O	2.59	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:F:285:GLU:CD	1:F:301:PHE:CD2	2.94	0.45
1:G:185:ILE:HD12	1:G:236:ILE:HG23	1.98	0.45
1:B:87:PHE:CD2	1:B:273:ILE:HG21	2.51	0.45
1:B:247:ASN:H	1:B:247:ASN:ND2	2.07	0.45
1:B:273:ILE:HG13	1:B:275:MET:HG3	1.98	0.45
1:B:52:TRP:NE1	3:B:360:HOH:O	2.48	0.45
1:C:90:HIS:HB2	1:C:268:LEU:HD21	1.97	0.45
1:C:122:PHE:CE2	1:C:228:LEU:CD2	3.00	0.45
1:H:261:ARG:HH12	1:H:281:SER:HB3	1.81	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:E:308:ASN:OD1	1:E:308:ASN:C	2.59	0.45
1:F:48:TYR:CD1	1:F:48:TYR:N	2.85	0.45
1:G:87:PHE:CZ	1:G:91:VAL:HG21	2.49	0.45
1:H:307:PHE:CD1	1:H:309:TRP:CZ2	3.04	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:64:THR:HG23	1:H:66:GLU:H	1.80	0.45
1:H:240:LEU:HD23	1:H:243:LYS:HG2	1.98	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:C:56:LYS:NZ	1:C:59:GLU:OE2	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:PHE:CD2	1:D:181:PHE:HE1	2.34	0.45
1:E:64:THR:HG23	1:E:66:GLU:HG2	1.99	0.45
1:E:269:PRO:O	1:E:272:LEU:HB2	2.16	0.45
1:F:195:LEU:O	1:F:196:PHE:HB2	2.16	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:CD2	1:G:263:PHE:N	2.81	0.45
1:B:156:HIS:O	1:B:157:ALA:CB	2.64	0.45
1:F:154:LEU:HD12	1:F:154:LEU:HA	1.70	0.45
1:A:56:LYS:NZ	1:A:59:GLU:OE1	2.50	0.45
1:A:301:PHE:HD1	1:A:303:SER:OG	2.00	0.45
1:B:104:GLU:OE1	1:B:106:LEU:HD12	2.17	0.45
1:C:86:HIS:ND1	1:C:86:HIS:C	2.75	0.45
1:C:130:GLU:O	1:C:133:HIS:HB2	2.17	0.45
1:C:152:LEU:C	1:C:154:LEU:N	2.73	0.45
1:E:144:TYR:OH	1:E:213:HIS:NE2	2.45	0.45
1:E:282:GLN:CD	1:E:306:PRO:HG3	2.42	0.45
1:A:264:ILE:H	1:A:264:ILE:HG13	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: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:A:213:HIS:CD2	1:A:213:HIS:C	2.95	0.44
1:B:73:ASP:OD2	1:B:213:HIS:HB3	2.17	0.44
1:C:283:TYR:O	1:C:287:VAL:HG23	2.17	0.44
1:G:277:SER:C	1:G:278:ARG:HD3	2.32	0.44
1:B:213:HIS:CG	1:B:213:HIS:O	2.68	0.44
1:C:213:HIS:O	1:C:213:HIS:CD2	2.70	0.44
1:D:131:ASN:HD22	1:D:131:ASN:HA	1.53	0.44
1:D:277:SER:HB3	1:D:278:ARG:HH11	1.82	0.44
1:D:57:LYS:O	1:D:61:SER:CB	2.63	0.44
1:D:232:PHE:CZ	1:D:236:ILE:HD11	2.52	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:N	1:A:278:ARG:CD	2.80	0.44
1:B:301:PHE:O	1:B:302:HIS:O	2.35	0.44
1:C:143:ASN:ND2	1:C:143:ASN:N	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:F:159:GLU:C	1:F:159:GLU:CD	2.86	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: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:73:ASP:HB3	1:H:76:ASP:CG	2.43	0.44
1:B:90:HIS:CE1	1:B:93:ALA:HB3	2.51	0.44
1:B:277:SER:OG	1:B:278:ARG:NH1	2.50	0.44
1:C:141:ILE:HA	1:C:145:ILE:HD13	1.99	0.44
1:D:152:LEU:C	1:D:154:LEU:H	2.26	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:C:270:CYS:C	1:C:272:LEU:H	2.26	0.43
1:H:279:LEU:HD13	1:H:307:PHE:CZ	2.52	0.43
1:A:270:CYS:C	1:A:272:LEU:N	2.63	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:C:198:GLY:HA2	1:C:280:MET:HE1	2.00	0.43
1:E:94:PHE:HE2	1:E:164:ILE:HD11	1.84	0.43
1:F:152:LEU:C	1:F:154:LEU:N	2.77	0.43
1:F:280:MET:HE3	1:F:283:TYR:HB3	2.00	0.43
1:A:142:ASP:O	1:A:142:ASP:OD2	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:E:309:TRP:H	1:E:309:TRP:CD1	2.36	0.43
1:G:47:MET:C	1:G:49:PRO:HD3	2.43	0.43
1:G:305:ASN:HD22	1:G:305:ASN:C	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:CZ2	1:D:135:GLU:OE2	2.70	0.43
1:C:160:ASN:O	1:C:160:ASN:CG	2.62	0.43
1:E:77:PHE:CZ	1:E:89:LYS:HE2	2.54	0.43
1:A:280:MET:HE1	1:A:283:TYR:HD2	1.82	0.43
1:B:77:PHE:CD2	1:B:144:TYR:CE2	3.05	0.43
1:B:207:LYS:HE3	1:B:220:GLU:CD	2.44	0.43
1:G:167:LYS:NZ	1:G:195:LEU:HD13	2.33	0.43
1:B:77:PHE:CE2	1:B:144:TYR:CD2	3.05	0.43
1:D:51:VAL:HG13	1:D:232:PHE:CE1	2.53	0.43
1:D:69:ASP:C	1:D:71:SER:H	2.27	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:F:192:GLU:O	1:F:230:THR:OG1	2.29	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: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:87:PHE:CD2	1:D:273:ILE:HG21	2.53	0.43
1:D:307:PHE:HB3	1:D:309:TRP:NE1	2.34	0.43
1:E:285:GLU:HG2	1:E:285:GLU:H	1.54	0.43
1:F:259:VAL:O	1:F:262:SER:OG	2.33	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:H:284:ILE:O	1:H:285:GLU:C	2.62	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: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:C:152:LEU:O	1:C:153:ASN:C	2.61	0.43
1:E:164:ILE:H	1:E:164:ILE:CD1	2.32	0.43
1:F:115:GLU:HA	1:F:120:LYS:HZ1	1.84	0.43
1:G:86:HIS:HA	1:G:89:LYS:HG3	2.01	0.43
1:H:150:GLU:C	1:H:152:LEU:N	2.77	0.43
1:H:253:VAL:O	1:H:254:LYS:C	2.62	0.43
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.98	0.42
1:B:54:PHE:C	1:B:122:PHE:CE2	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LYS:HE3	1:C:174:TRP:CZ2	2.54	0.42
1:E:66:GLU:OE2	1:F:56:LYS:NZ	2.49	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:F:271:ASP:C	1:F:272:LEU:HD12	2.44	0.42
1:H:213:HIS:O	1:H:213:HIS:HD2	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:56:LYS:NZ	1:C:66:GLU:OE2	2.50	0.42
1:B:73:ASP:O	1:B:213:HIS:NE2	2.52	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:121:LYS:HZ1	1:D:131:ASN:C	2.25	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:94:PHE:CD1	1:D:196:PHE:HE1	2.37	0.42
1:D:275:MET:CE	1:D:309:TRP:HH2	2.33	0.42
1:E:214:GLY:HA2	1:E:217:PHE:N	2.33	0.42
1:F:153:ASN:O	1:F:153:ASN:CG	2.62	0.42
1:G:57:LYS:O	1:G:61:SER:HB2	2.19	0.42
1:G:214:GLY:HA2	1:G:217:PHE:N	2.32	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: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:109:LYS:NZ	1:F:176:ASN:HA	2.34	0.42
1:F:129:VAL:HA	1:F:132:ILE:HD12	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:C	1:C:152:LEU:N	2.76	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:HE	1:D:224:ARG:HB3	1.70	0.42
1:F:264:ILE:HD12	1:F:265:CYS:SG	2.60	0.42
1:G:271:ASP:CG	1:G:276:ASN:HA	2.45	0.42
1:A:62:PHE:HD2	1:A:125:PHE:CZ	2.38	0.42
1:A:161:ILE:O	1:A:163:ALA:N	2.52	0.42
1:A:161:ILE:HD13	1:A:161:ILE:HA	1.80	0.42
1:A:182:ALA:HB1	1:A:244:LEU:HG	2.01	0.42
1:C:148:GLU:O	1:C:148:GLU:CG	2.57	0.42
1:E:237:TYR:HE1	1:E:295:LEU:O	2.01	0.42
1:B:105:ASN:ND2	1:B:105:ASN:C	2.77	0.42
1:B:166:ASN:HB3	1:B:259:VAL:HG22	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: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:G:213:HIS:O	1:G:213:HIS:HD2	1.94	0.42
1:A:263:PHE:CD2	1:A:263:PHE:N	2.86	0.42
1:B:47:MET:HG2	3:B:354:HOH:O	2.19	0.42
1:C:163:ALA:CB	1:C:263:PHE:CD2	3.03	0.42
1:C:214:GLY:CA	1:C:217:PHE:H	2.33	0.42
1:D:275:MET:HE3	1:D:309:TRP:HH2	1.85	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:G:81:ASN:C	1:G:83:ASN:N	2.78	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: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:H:110:PHE:N	1:H:110:PHE:HD1	2.18	0.41
1:B:291:LEU:O	1:B:292:LEU:C	2.63	0.41
1:C:144:TYR:HB2	1:C:145:ILE:HD12	2.02	0.41
1:D:150:GLU:C	1:D:152:LEU:N	2.73	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

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:HZ3	2.13	0.41
1:E:87:PHE:CD2	1:E:273:ILE:HG21	2.55	0.41
1:E:246:GLU:O	1:E:250:GLN:HG3	2.20	0.41
1:E:301:PHE:CD1	1:E:301:PHE:O	2.74	0.41
1:G:59:GLU:HA	1:G:125:PHE:HE2	1.85	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:74:LEU:O	1:F:78:GLU:HG2	2.20	0.41
1:F:152:LEU:O	1:F:154:LEU:N	2.53	0.41
1:F:263:PHE:CD2	1:F:263:PHE:N	2.88	0.41
1:H:261:ARG:NH1	1:H:281:SER:HB3	2.35	0.41
1:H:309:TRP:O	1:H:309:TRP:HE3	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:50:GLU:HB3	1:C:235:LEU:HD11	2.03	0.41
1:C:168:ALA:O	1:C:171:ALA:HB3	2.20	0.41
1:A:47:MET:C	1:A:48:TYR:CD1	2.98	0.41
1:B:285:GLU:OE1	1:B:285:GLU:HA	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:78:GLU:OE2	1:G:78:GLU:CA	2.67	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: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:C:212:LEU:C	1:C:213:HIS:HD2	2.28	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:110:PHE:CE1	1:A:181:PHE:HE1	2.38	0.41
1:A:136:THR:O	1:A:140:LEU:HD22	2.21	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:B:309:TRP:CD1	1:B:309:TRP:H	2.38	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:D:309:TRP:CD1	1:D:309:TRP:H	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:G:243:LYS:CD	2.70	0.41
1:H:291:LEU:HD23	1:H:291:LEU:HA	1.87	0.41
1:A:69:ASP:C	1:A:71:SER:N	2.75	0.41
1:A:108:SER:HA	1:A:111:LEU:HB2	2.03	0.41
1:B:56:LYS:O	1:B:60:ALA:CB	2.69	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
1:B:276:ASN:ND2	1:B:279:LEU:H	2.19	0.41
1:C:55:TYR:CD1	1:C:55:TYR:C	2.99	0.41
1:C:118:GLU:CD	1:C:118:GLU:H	2.28	0.41
1:C:202:ALA:O	1:C:205:TRP:HB3	2.21	0.41
1:D:73:ASP:CG	1:D:76:ASP:OD2	2.64	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:81:ASN:CB	1:F:83:ASN:H	2.33	0.41
1:F:198:GLY:C	1:F:264:ILE:HG21	2.45	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: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:95:PHE:CE1	1:H:196:PHE:CD1	3.08	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:180:SER:O	1:A:184:ARG:HG3	2.21	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: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:C:270:CYS:C	1:C:272:LEU:N	2.79	0.40
1:E:59:GLU:CD	1:F:64:THR:OG1	2.63	0.40
1:E:163:ALA:O	1:E:167:LYS:HB2	2.21	0.40
1:F:195:LEU:HA	1:F:260:GLU:OE1	2.21	0.40
1:G:47:MET:C	1:G:48:TYR:CD1	2.99	0.40
1:H:57:LYS:O	1:H:61:SER:HB3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HA	1:A:162:PRO:HD3	1.93	0.40
1:B:151:ARG:O	1:B:151:ARG:HG3	2.15	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:O	1:G:148:GLU:CG	2.69	0.40
1:H:70:LEU:H	1:H:70:LEU:HG	1.44	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:A:55:TYR:O	1:A:59:GLU:HB2	2.22	0.40
1:B:68:ILE:CG2	1:B:70:LEU:CD2	2.99	0.40
1:B:263:PHE:HA	1:B:267:SER:HB2	2.01	0.40
1:C:59:GLU:O	1:C:62:PHE:HB2	2.21	0.40
1:C:143:ASN:N	1:C:143:ASN:HD22	2.19	0.40
1:C:276:ASN:OD1	1:C:278:ARG:CG	2.68	0.40
1:D:75:LYS:H	1:D:75:LYS:HG3	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:131:ASN:HB3	1:D:121:LYS:HZ3	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
1:B:285:GLU:HG3	1:B:301:PHE:CE1	2.57	0.40
1:C:98:SER:HB2	1:C:167:LYS:CE	2.49	0.40
1:C:145:ILE:O	1:C:145:ILE:CG2	2.64	0.40
1:D:270:CYS:C	1:D:272:LEU:N	2.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/349 (73%)	219 (86%)	25 (10%)	10 (4%)	2	5
1	B	244/349 (70%)	208 (85%)	26 (11%)	10 (4%)	2	5
1	C	250/349 (72%)	206 (82%)	35 (14%)	9 (4%)	2	6
1	D	254/349 (73%)	215 (85%)	27 (11%)	12 (5%)	2	3
1	E	254/349 (73%)	219 (86%)	25 (10%)	10 (4%)	2	5
1	F	254/349 (73%)	220 (87%)	26 (10%)	8 (3%)	3	8
1	G	244/349 (70%)	209 (86%)	27 (11%)	8 (3%)	3	7
1	H	254/349 (73%)	220 (87%)	24 (9%)	10 (4%)	2	5
All	All	2008/2792 (72%)	1716 (86%)	215 (11%)	77 (4%)	2	5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	190 (83%)	39 (17%)	2 6
1	B	223/316 (71%)	170 (76%)	53 (24%)	1 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	230/316 (73%)	172 (75%)	58 (25%)	0	2
1	D	232/316 (73%)	194 (84%)	38 (16%)	2	6
1	E	230/316 (73%)	182 (79%)	48 (21%)	1	3
1	F	232/316 (73%)	191 (82%)	41 (18%)	2	5
1	G	225/316 (71%)	182 (81%)	43 (19%)	1	4
1	H	232/316 (73%)	186 (80%)	46 (20%)	1	4
All	All	1833/2528 (72%)	1467 (80%)	366 (20%)	1	4

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	MET
1	A	56	LYS
1	A	66	GLU
1	A	71	SER
1	A	80	LEU
1	A	82	VAL
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
1	A	140	LEU
1	A	141	ILE
1	A	143	ASN
1	A	146	LYS
1	A	147	ASP
1	A	161	ILE
1	A	169	LEU
1	A	177	ASP
1	A	185	ILE
1	A	197	SER
1	A	208	LYS
1	A	230	THR
1	A	233	ASN
1	A	238	SER
1	A	241	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	258	GLU
1	A	263	PHE
1	A	264	ILE
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	56	LYS
1	B	59	GLU
1	B	64	THR
1	B	69	ASP
1	B	70	LEU
1	B	71	SER
1	B	75	LYS
1	B	78	GLU
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	118	GLU
1	B	130	GLU
1	B	135	GLU
1	B	140	LEU
1	B	150	GLU
1	B	151	ARG
1	B	154	LEU
1	B	156	HIS
1	B	164	ILE
1	B	165	LYS
1	B	178	THR
1	B	180	SER
1	B	183	GLU
1	B	185	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	199	SER
1	B	203	ILE
1	B	210	ASN
1	B	221	LEU
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	295	LEU
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	56	LYS
1	C	59	GLU
1	C	66	GLU
1	C	67	GLU
1	C	75	LYS
1	C	79	LYS
1	C	80	LEU
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	111	LEU
1	C	114	VAL
1	C	116	ILE
1	C	126	GLN
1	C	135	GLU
1	C	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	141	ILE
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	154	LEU
1	C	156	HIS
1	C	160	ASN
1	C	161	ILE
1	C	164	ILE
1	C	165	LYS
1	C	175	ILE
1	C	185	ILE
1	C	188	ASN
1	C	194	ILE
1	C	208	LYS
1	C	211	LYS
1	C	235	LEU
1	C	246	GLU
1	C	247	ASN
1	C	257	VAL
1	C	260	GLU
1	C	263	PHE
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	299	LYS
1	C	300	VAL
1	C	303	SER
1	C	307	PHE
1	C	308	ASN
1	C	309	TRP
1	D	47	MET
1	D	50	GLU
1	D	56	LYS
1	D	74	LEU
1	D	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	79	LYS
1	D	85	LYS
1	D	88	ILE
1	D	91	VAL
1	D	111	LEU
1	D	117	ILE
1	D	121	LYS
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	224	ARG
1	D	239	LEU
1	D	240	LEU
1	D	243	LYS
1	D	247	ASN
1	D	258	GLU
1	D	259	VAL
1	D	264	ILE
1	D	279	LEU
1	D	285	GLU
1	D	290	ARG
1	D	291	LEU
1	D	292	LEU
1	D	303	SER
1	E	56	LYS
1	E	66	GLU
1	E	67	GLU
1	E	68	ILE
1	E	69	ASP
1	E	70	LEU
1	E	85	LYS
1	E	91	VAL
1	E	106	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	109	LYS
1	E	114	VAL
1	E	115	GLU
1	E	126	GLN
1	E	130	GLU
1	E	132	ILE
1	E	134	SER
1	E	136	THR
1	E	145	ILE
1	E	146	LYS
1	E	148	GLU
1	E	149	LYS
1	E	152	LEU
1	E	154	LEU
1	E	156	HIS
1	E	158	ILE
1	E	161	ILE
1	E	164	ILE
1	E	180	SER
1	E	185	ILE
1	E	229	HIS
1	E	235	LEU
1	E	236	ILE
1	E	239	LEU
1	E	240	LEU
1	E	254	LYS
1	E	261	ARG
1	E	264	ILE
1	E	272	LEU
1	E	273	ILE
1	E	277	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	68	ILE
1	F	74	LEU
1	F	80	LEU
1	F	81	ASN
1	F	82	VAL
1	F	91	VAL
1	F	104	GLU
1	F	138	SER
1	F	140	LEU
1	F	145	ILE
1	F	148	GLU
1	F	149	LYS
1	F	150	GLU
1	F	152	LEU
1	F	154	LEU
1	F	156	HIS
1	F	161	ILE
1	F	164	ILE
1	F	175	ILE
1	F	178	THR
1	F	185	ILE
1	F	188	ASN
1	F	218	SER
1	F	236	ILE
1	F	242	ASN
1	F	243	LYS
1	F	244	LEU
1	F	249	VAL
1	F	254	LYS
1	F	259	VAL
1	F	264	ILE
1	F	273	ILE
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	67	GLU
1	G	71	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	72	SER
1	G	73	ASP
1	G	80	LEU
1	G	98	SER
1	G	104	GLU
1	G	105	ASN
1	G	109	LYS
1	G	111	LEU
1	G	112	ARG
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	165	LYS
1	G	166	ASN
1	G	178	THR
1	G	184	ARG
1	G	185	ILE
1	G	194	ILE
1	G	201	CYS
1	G	203	ILE
1	G	219	ASN
1	G	236	ILE
1	G	238	SER
1	G	240	LEU
1	G	243	LYS
1	G	259	VAL
1	G	264	ILE
1	G	267	SER
1	G	277	SER
1	G	278	ARG
1	G	282	GLN
1	G	292	LEU
1	G	293	GLU
1	G	295	LEU
1	G	299	LYS
1	H	47	MET
1	H	56	LYS
1	H	64	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	67	GLU
1	H	70	LEU
1	H	84	GLU
1	H	85	LYS
1	H	86	HIS
1	H	91	VAL
1	H	111	LEU
1	H	121	LYS
1	H	127	ILE
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	161	ILE
1	H	175	ILE
1	H	183	GLU
1	H	185	ILE
1	H	191	VAL
1	H	208	LYS
1	H	230	THR
1	H	233	ASN
1	H	235	LEU
1	H	236	ILE
1	H	238	SER
1	H	239	LEU
1	H	241	GLU
1	H	247	ASN
1	H	254	LYS
1	H	260	GLU
1	H	263	PHE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) 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	282	GLN
1	A	308	ASN
1	B	53	ASN
1	B	105	ASN
1	B	153	ASN
1	B	188	ASN
1	B	247	ASN
1	B	276	ASN
1	B	282	GLN
1	B	302	HIS
1	C	81	ASN
1	C	83	ASN
1	C	105	ASN
1	C	126	GLN
1	C	131	ASN
1	C	133	HIS
1	C	153	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	131	ASN
1	D	153	ASN
1	D	166	ASN
1	D	179	ASN
1	D	188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	219	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	219	ASN
1	E	250	GLN
1	E	282	GLN
1	F	81	ASN
1	F	86	HIS
1	F	126	GLN
1	F	213	HIS
1	F	250	GLN
1	F	282	GLN
1	F	302	HIS
1	G	90	HIS
1	G	166	ASN
1	G	176	ASN
1	G	188	ASN
1	G	219	ASN
1	G	242	ASN
1	G	282	GLN
1	G	305	ASN
1	H	126	GLN
1	H	131	ASN
1	H	156	HIS
1	H	160	ASN
1	H	166	ASN
1	H	176	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	258/349 (73%)	-1.07	0	100	100	24, 42, 49, 55	0
1	B	252/349 (72%)	-1.05	0	100	100	27, 42, 48, 52	0
1	C	256/349 (73%)	-1.07	0	100	100	27, 42, 47, 53	0
1	D	258/349 (73%)	-1.10	0	100	100	32, 42, 49, 54	0
1	E	258/349 (73%)	-1.05	1 (0%)	88	87	26, 42, 48, 51	0
1	F	258/349 (73%)	-1.11	0	100	100	30, 42, 47, 54	0
1	G	252/349 (72%)	-1.06	1 (0%)	88	87	31, 42, 48, 56	0
1	H	258/349 (73%)	-1.10	0	100	100	34, 42, 48, 53	0
All	All	2050/2792 (73%)	-1.08	2 (0%)	92	91	24, 42, 48, 56	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	THR	3.4
1	G	274	GLY	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	0.97	0.18	65,65,65,65	1
2	FE	A	350	1/1	0.99	0.08	47,47,47,47	1
2	FE	C	350	1/1	0.99	0.02	61,61,61,61	1
2	FE	D	350	1/1	0.99	0.06	49,49,49,49	1
2	FE	E	350	1/1	0.99	0.03	63,63,63,63	1
2	FE	F	350	1/1	0.99	0.03	54,54,54,54	1
2	FE	G	350	1/1	0.99	0.03	58,58,58,58	1
2	FE	H	350	1/1	0.99	0.03	53,53,53,53	1

6.5 Other polymers [i](#)

There are no such residues in this entry.