



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2021 – 12:14 PM JST

PDB ID : 7EI1
Title : Structure of Pyrococcus furiosus Cas1Cas2 complex
Authors : Yu, Y.; Chen, Q.
Deposited on : 2021-03-30
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

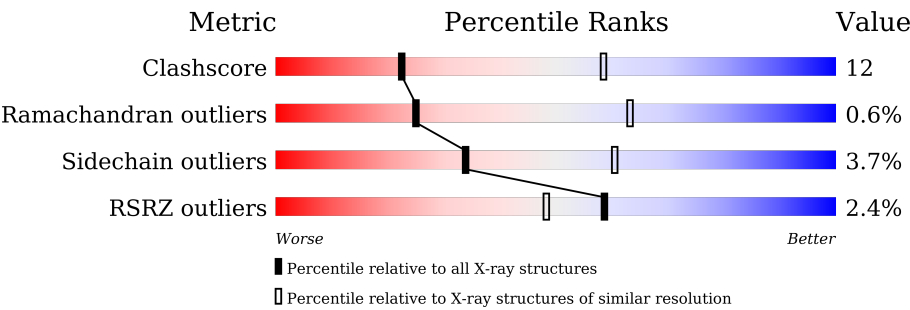
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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))
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	322	<div><div>4%</div><div><div></div><div>73%</div><div>21%</div><div>..</div></div></div>
1	B	322	<div><div>%</div><div><div></div><div>65%</div><div>30%</div><div>..</div></div></div>
1	C	322	<div><div>3%</div><div><div></div><div>63%</div><div>31%</div><div>..</div></div></div>
1	D	322	<div><div></div><div><div></div><div>63%</div><div>29%</div><div>...</div></div></div>
1	E	322	<div><div>2%</div><div><div></div><div>69%</div><div>26%</div><div>..</div></div></div>
1	F	322	<div><div>3%</div><div><div></div><div>70%</div><div>25%</div><div>..</div></div></div>
1	G	322	<div><div>2%</div><div><div></div><div>70%</div><div>25%</div><div>..</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	322	
1	I	322	
1	J	322	
1	K	322	
1	L	322	
1	M	322	
1	N	322	
1	O	322	
1	P	322	
2	Q	85	
2	R	85	
2	S	85	
2	T	85	
2	U	85	
2	V	85	
2	W	85	
2	X	85	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 90949 atoms, of which 44675 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 CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total 5002	C 1647	H 2443	N 449	O 458	S 5	0	0	0
1	B	308	Total 4941	C 1633	H 2409	N 439	O 455	S 5	0	0	0
1	C	312	Total 5020	C 1656	H 2450	N 450	O 459	S 5	0	0	0
1	D	308	Total 4937	C 1633	H 2405	N 439	O 455	S 5	0	0	0
1	E	312	Total 5003	C 1656	H 2433	N 450	O 459	S 5	0	0	0
1	F	308	Total 4950	C 1633	H 2418	N 439	O 455	S 5	0	0	0
1	G	312	Total 5016	C 1656	H 2446	N 450	O 459	S 5	0	0	0
1	H	306	Total 4926	C 1624	H 2408	N 437	O 452	S 5	0	0	0
1	K	310	Total 5012	C 1636	H 2467	N 447	O 457	S 5	0	0	0
1	L	308	Total 4958	C 1633	H 2426	N 439	O 455	S 5	0	0	0
1	M	314	Total 5070	C 1668	H 2481	N 455	O 461	S 5	0	0	0
1	N	305	Total 4905	C 1619	H 2396	N 436	O 449	S 5	0	0	0
1	I	312	Total 5037	C 1656	H 2467	N 450	O 459	S 5	0	0	0
1	J	307	Total 4924	C 1629	H 2399	N 438	O 453	S 5	0	0	0
1	O	311	Total 5024	C 1647	H 2465	N 449	O 458	S 5	0	0	0
1	P	306	Total 4937	C 1624	H 2419	N 437	O 452	S 5	0	0	0

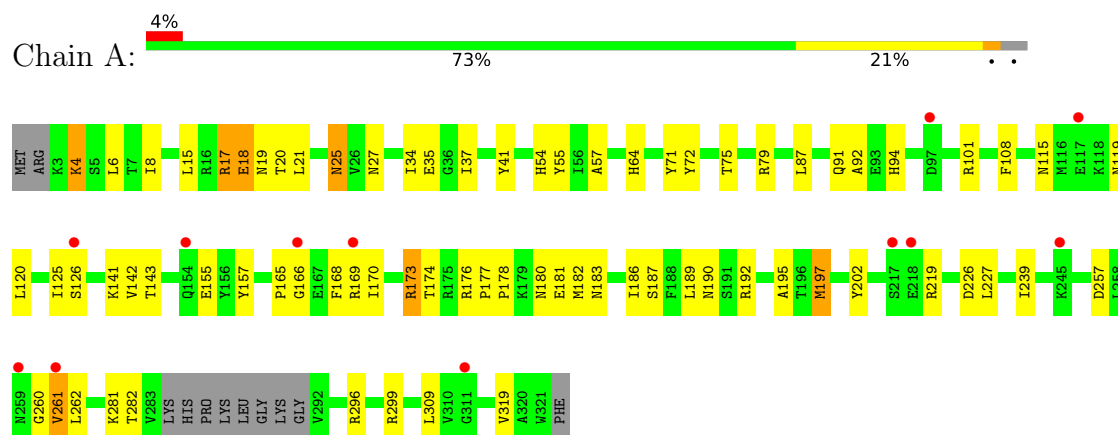
- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Q	84	Total	C	H	N	O	S	0	0	0
			1401	447	708	116	127	3			
2	R	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	S	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	T	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	U	84	Total	C	H	N	O	S	0	0	0
			1412	447	719	116	127	3			
2	V	84	Total	C	H	N	O	S	0	0	0
			1411	447	718	116	127	3			
2	W	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	X	84	Total	C	H	N	O	S	0	0	0
			1411	447	718	116	127	3			

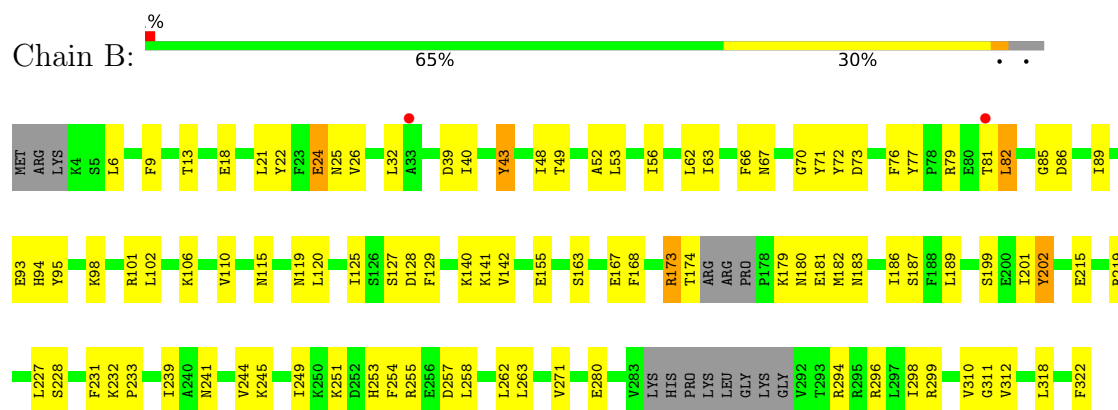
3 Residue-property plots

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.

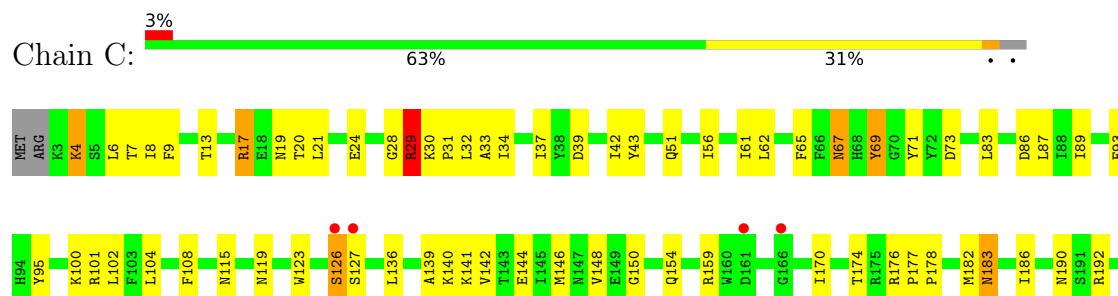
• Molecule 1: CRISPR-associated endonuclease Cas1

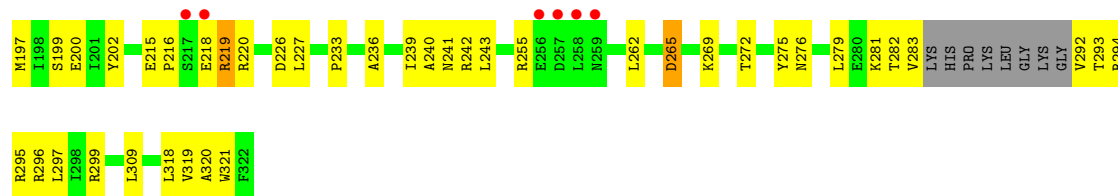


• Molecule 1: CRISPR-associated endonuclease Cas1



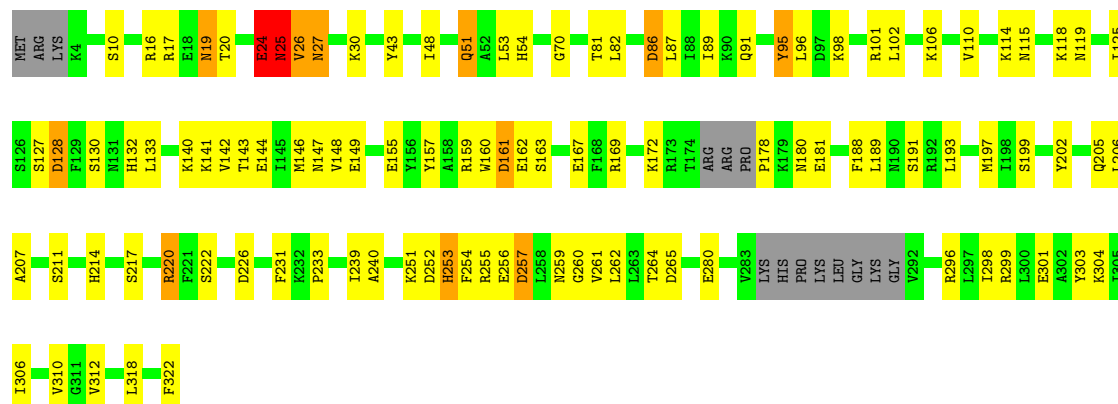
• Molecule 1: CRISPR-associated endonuclease Cas1





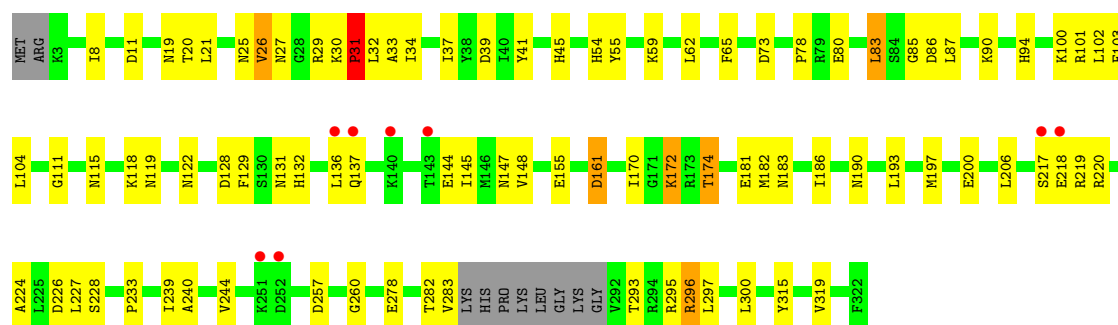
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain D: 63% 29%



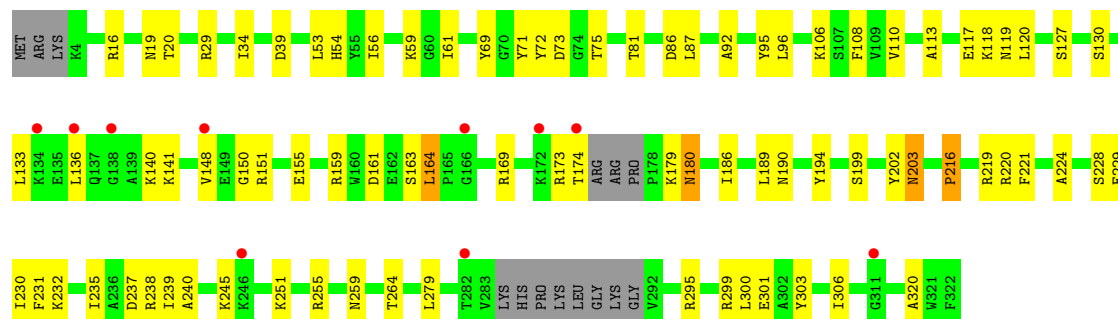
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain E: 2% 69% 26%

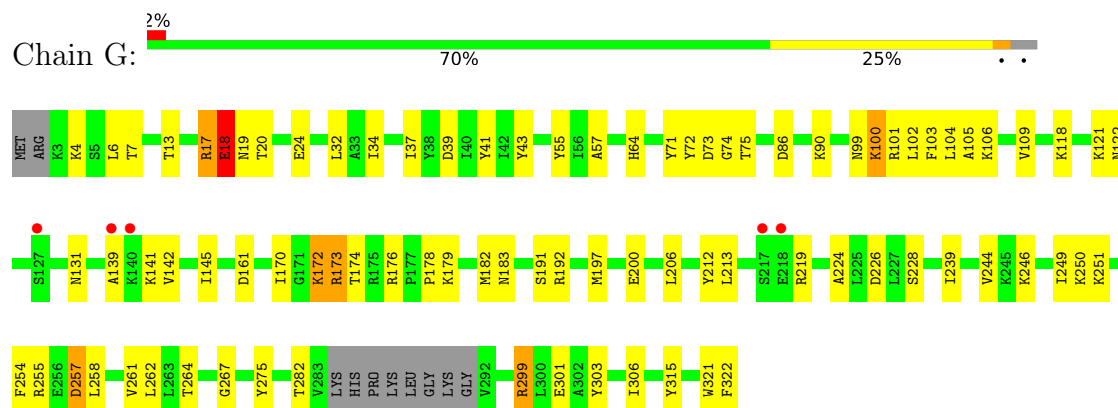


• Molecule 1: CRISPR-associated endonuclease Cas1

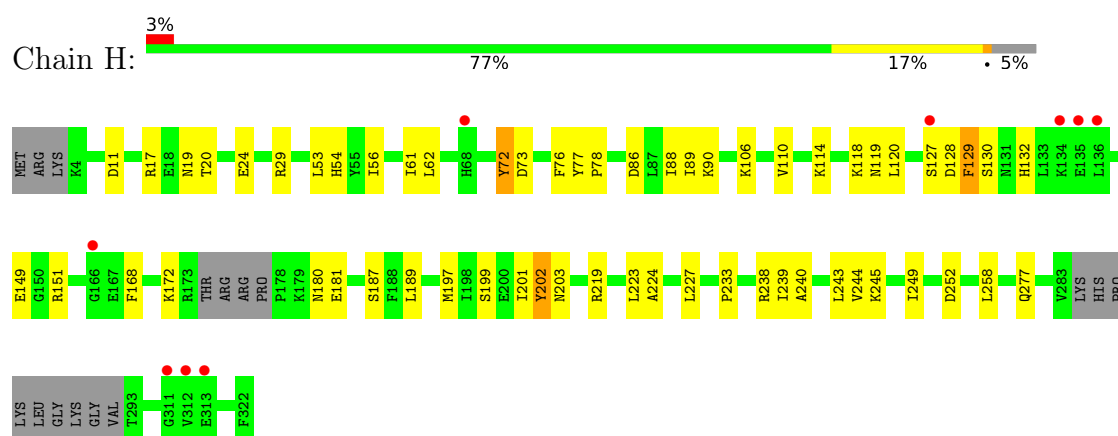
Chain F: 3% 70% 25%



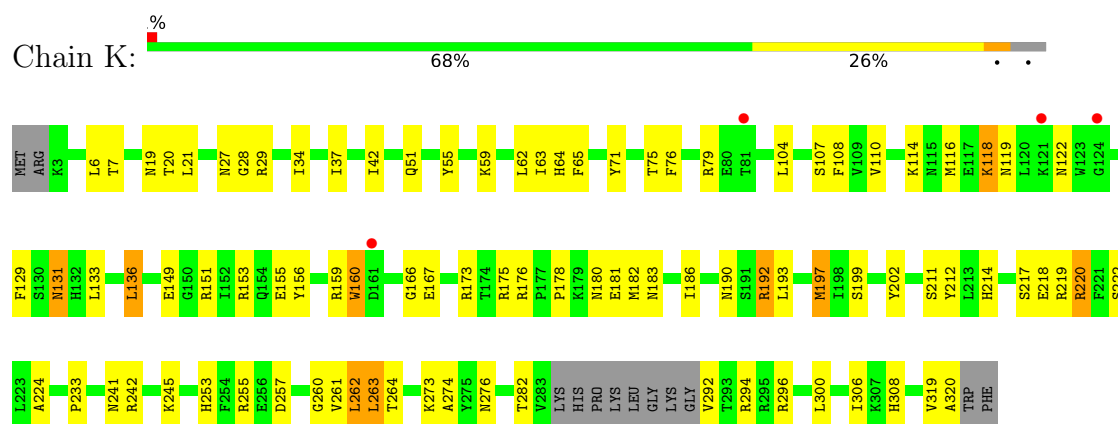
• Molecule 1: CRISPR-associated endonuclease Cas1



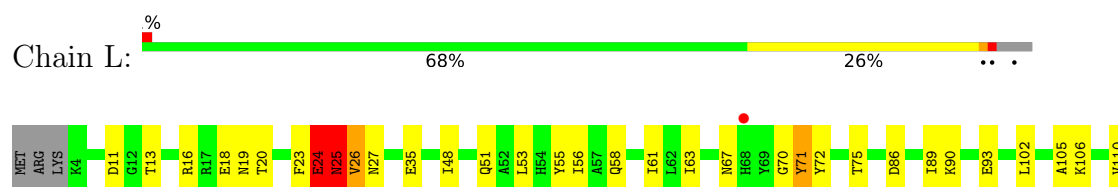
• Molecule 1: CRISPR-associated endonuclease Cas1

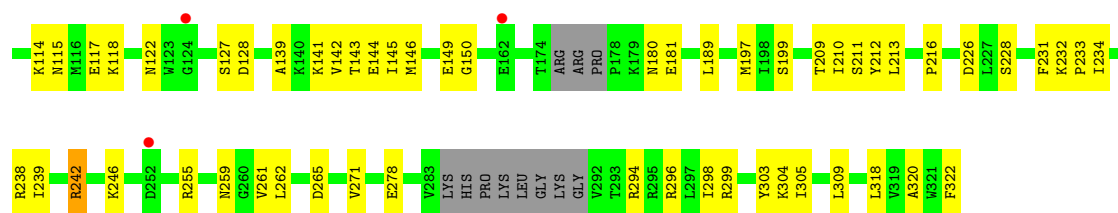


• Molecule 1: CRISPR-associated endonuclease Cas1

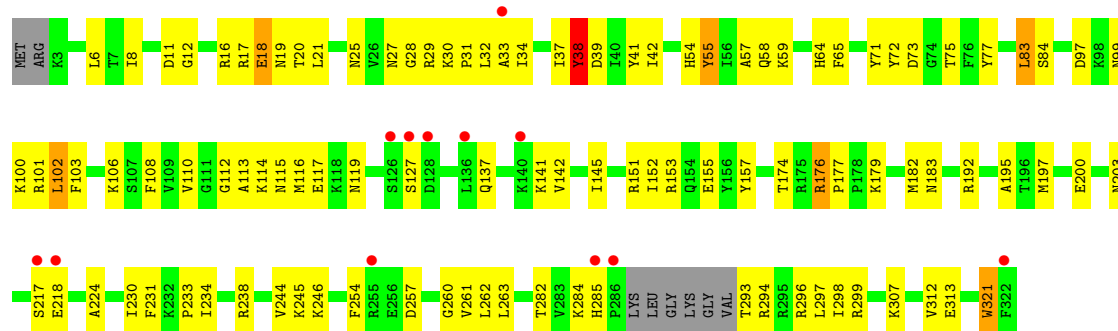


• Molecule 1: CRISPR-associated endonuclease Cas1

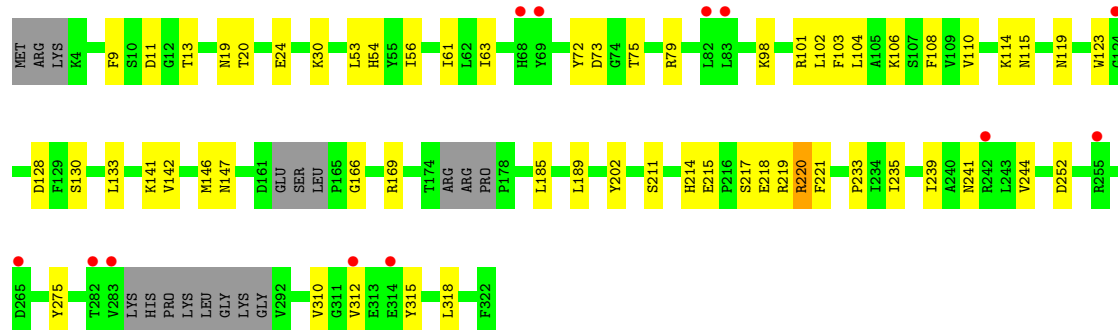
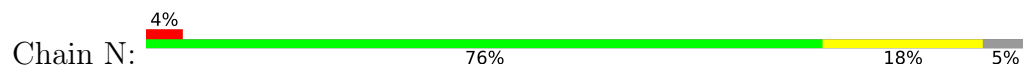




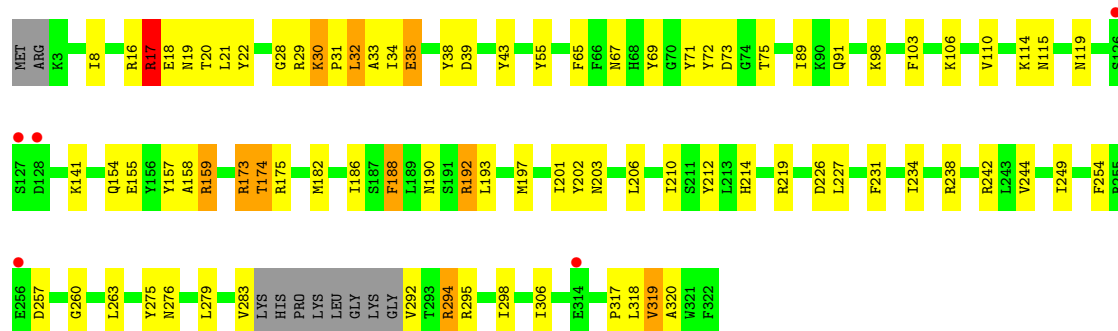
• Molecule 1: CRISPR-associated endonuclease Cas1



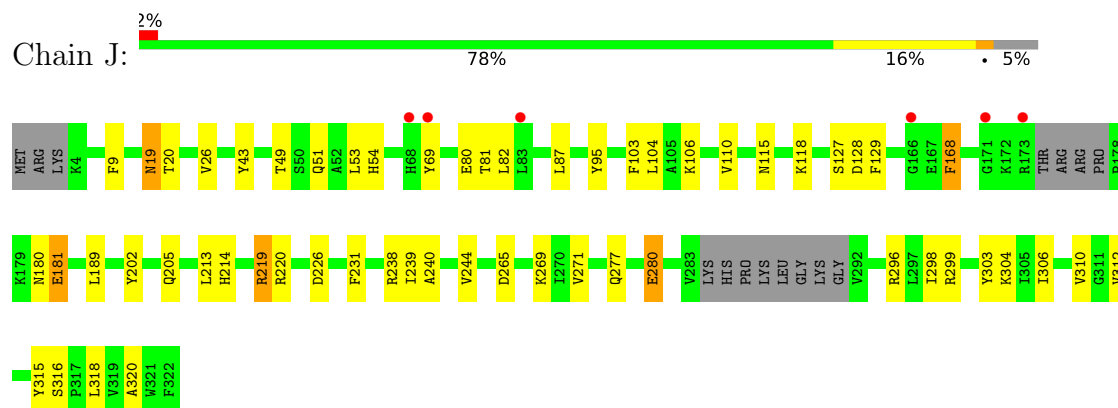
• Molecule 1: CRISPR-associated endonuclease Cas1



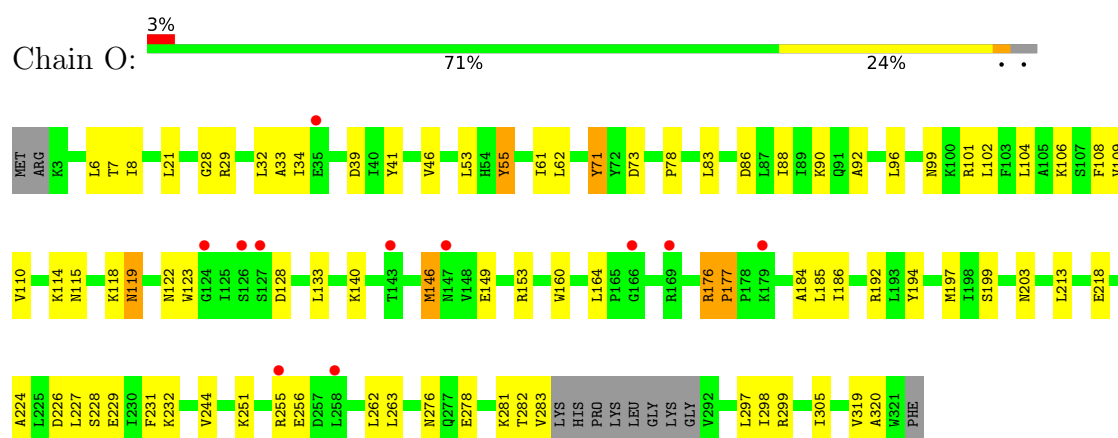
• Molecule 1: CRISPR-associated endonuclease Cas1



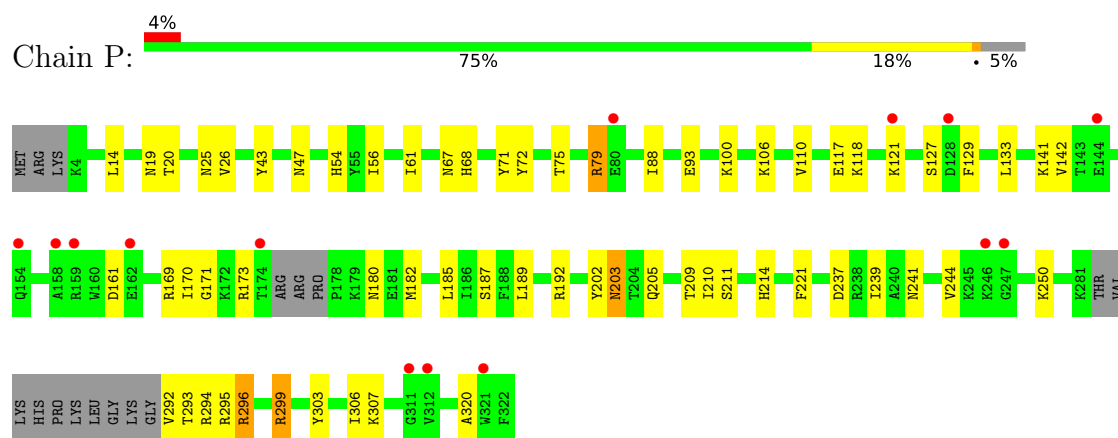
- Molecule 1: CRISPR-associated endonuclease Cas1



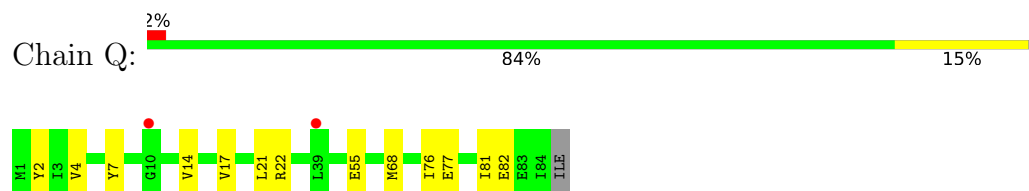
- Molecule 1: CRISPR-associated endonuclease Cas1



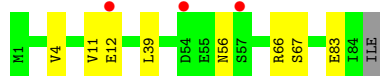
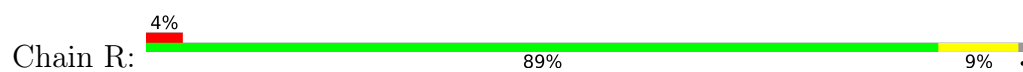
- Molecule 1: CRISPR-associated endonuclease Cas1



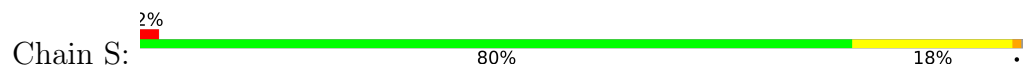
- Molecule 2: CRISPR-associated endonuclease Cas2



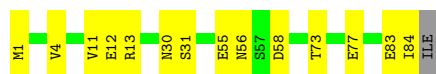
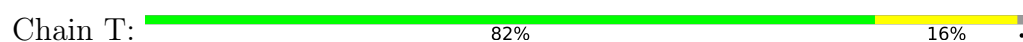
- Molecule 2: CRISPR-associated endonuclease Cas2



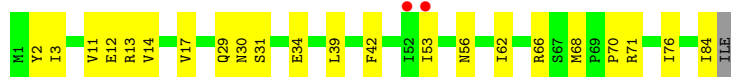
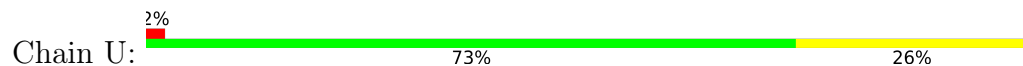
- Molecule 2: CRISPR-associated endoribonuclease Cas2



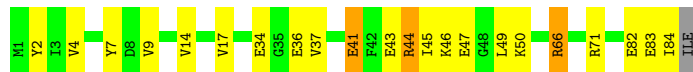
- Molecule 2: CRISPR-associated endoribonuclease Cas2



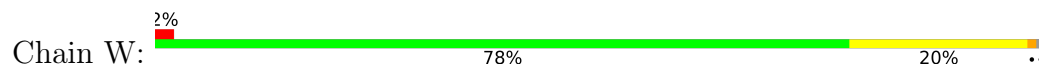
- Molecule 2: CRISPR-associated endoribonuclease Cas2



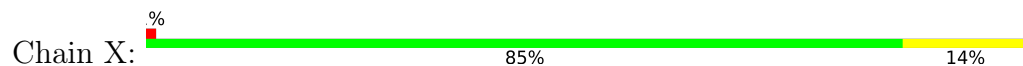
- Molecule 2: CRISPR-associated endoribonuclease Cas2



- Molecule 2: CRISPR-associated endoribonuclease Cas2



- Molecule 2: CRISPR-associated endoribonuclease Cas2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.76Å 180.47Å 338.85Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	36.53 – 3.90 37.58 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (36.53-3.90) 93.7 (37.58-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 3.87Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.281 , 0.328 0.281 , (Not available)	Depositor DCC
R_{free} test set	971 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	90949	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.56 % 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 7.8394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/2612	0.54	1/3517 (0.0%)
1	B	0.26	0/2584	0.51	0/3478
1	C	0.28	0/2624	0.50	0/3533
1	D	0.27	0/2584	0.52	1/3478 (0.0%)
1	E	0.28	0/2624	0.52	2/3533 (0.1%)
1	F	0.26	0/2584	0.48	0/3478
1	G	0.27	0/2624	0.50	0/3533
1	H	0.27	0/2570	0.47	0/3458
1	I	0.30	0/2624	0.54	0/3533
1	J	0.25	0/2577	0.45	0/3468
1	K	0.28	0/2596	0.53	0/3494
1	L	0.26	0/2584	0.51	0/3478
1	M	0.36	1/2645 (0.0%)	0.53	0/3561
1	N	0.25	0/2560	0.46	0/3443
1	O	0.27	0/2612	0.49	0/3517
1	P	0.25	0/2570	0.45	0/3458
2	Q	0.26	0/704	0.45	0/947
2	R	0.26	0/704	0.44	0/947
2	S	0.27	0/704	0.46	0/947
2	T	0.29	0/704	0.50	1/947 (0.1%)
2	U	0.26	0/704	0.48	0/947
2	V	0.27	0/704	0.48	0/947
2	W	0.26	0/704	0.46	0/947
2	X	0.26	0/704	0.45	0/947
All	All	0.27	1/47206 (0.0%)	0.50	5/63536 (0.0%)

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	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	3
1	E	0	3
1	F	0	1
1	G	0	4
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	2
1	O	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	38	TYR	CD2-CE2	-7.43	1.28	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	VAL	CG1-CB-CG2	8.11	123.88	110.90
1	A	261	VAL	CG1-CB-CG2	7.42	122.78	110.90
2	T	4	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	E	26	VAL	CA-CB-CG2	5.14	118.61	110.90
1	E	31	PRO	N-CA-C	5.02	125.14	112.10

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	ARG	Peptide
1	C	17	ARG	Peptide
1	D	149	GLU	Peptide
1	D	24	GLU	Peptide
1	D	25	ASN	Peptide
1	E	111	GLY	Peptide
1	E	174	THR	Peptide
1	E	31	PRO	Peptide
1	F	216	PRO	Peptide
1	G	17	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	G	172	LYS	Peptide
1	G	18	GLU	Mainchain
1	G	257	ASP	Peptide
1	I	17	ARG	Peptide
1	I	174	THR	Peptide
1	J	219	ARG	Peptide
1	K	176	ARG	Peptide
1	L	24	GLU	Peptide
1	M	16	ARG	Peptide
1	M	176	ARG	Peptide
1	O	176	ARG	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	2559	2443	2609	69	0
1	B	2532	2409	2572	73	1
1	C	2570	2450	2618	101	0
1	D	2532	2405	2572	72	1
1	E	2570	2433	2618	83	0
1	F	2532	2418	2572	63	1
1	G	2570	2446	2618	63	0
1	H	2518	2408	2556	42	1
1	I	2570	2467	2618	78	0
1	J	2525	2399	2565	38	1
1	K	2545	2467	2599	71	0
1	L	2532	2426	2572	67	1
1	M	2589	2481	2636	94	0
1	N	2509	2396	2550	42	1
1	O	2559	2465	2609	80	0
1	P	2518	2419	2556	47	1
2	Q	693	708	721	9	0
2	R	693	720	721	7	0
2	S	693	720	721	11	0
2	T	693	720	721	9	0
2	U	693	719	721	15	0
2	V	693	718	721	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	693	720	721	14	0
2	X	693	718	721	9	0
All	All	46274	44675	47208	1085	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1085) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:NZ	2:Q:77:GLU:OE2	1.74	1.21
1:K:133:LEU:O	1:K:136:LEU:CD2	1.99	1.10
1:L:278:GLU:OE2	1:L:294:ARG:NH1	1.85	1.09
1:K:133:LEU:O	1:K:136:LEU:HD22	1.55	1.06
1:M:38:TYR:OH	1:M:299:ARG:NH1	1.88	1.06
1:K:6:LEU:HD12	1:K:37:ILE:HD13	1.40	1.01
1:K:6:LEU:CD1	1:K:37:ILE:HD13	1.92	0.99
1:C:28:GLY:C	1:C:29:ARG:HD3	1.87	0.95
1:M:38:TYR:OH	1:M:299:ARG:CZ	2.16	0.94
1:B:163:SER:O	1:B:245:LYS:NZ	2.01	0.93
1:O:71:TYR:HE2	1:P:79:ARG:NH1	1.66	0.93
1:L:189:LEU:HD22	1:L:239:ILE:HD11	1.51	0.92
1:M:72:TYR:OH	1:M:75:THR:OG1	1.87	0.91
1:C:115:ASN:ND2	1:C:319:VAL:O	2.03	0.90
2:X:83:GLU:OE2	1:O:276:ASN:ND2	2.04	0.90
1:L:16:ARG:NH1	1:L:18:GLU:O	2.04	0.89
1:L:25:ASN:O	1:L:27:ASN:N	2.04	0.89
1:K:133:LEU:O	1:K:136:LEU:HD23	1.73	0.88
1:M:203:ASN:CG	1:M:299:ARG:NH1	2.25	0.88
1:A:17:ARG:O	1:A:18:GLU:O	1.92	0.87
1:H:189:LEU:HD22	1:H:239:ILE:HD11	1.57	0.87
1:M:284:LYS:O	1:M:285:HIS:ND1	2.08	0.86
1:O:153:ARG:NH2	1:O:229:GLU:OE1	2.08	0.86
1:H:189:LEU:CD2	1:H:239:ILE:HD11	2.05	0.86
1:I:72:TYR:HH	1:I:75:THR:HG1	1.11	0.86
1:A:115:ASN:ND2	1:A:319:VAL:O	2.09	0.85
1:M:54:HIS:ND1	1:N:73:ASP:OD1	2.08	0.84
1:H:219:ARG:HG3	1:H:219:ARG:HH11	1.39	0.84
1:M:17:ARG:O	1:M:18:GLU:O	1.96	0.83
1:O:115:ASN:ND2	1:O:319:VAL:O	2.10	0.83
1:H:239:ILE:HD12	1:H:240:ALA:N	1.93	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:ASN:OD1	1:F:232:LYS:NZ	2.10	0.83
1:A:87:LEU:HD21	1:A:309:LEU:HD23	1.59	0.83
1:B:163:SER:OG	1:B:245:LYS:NZ	2.11	0.83
1:E:39:ASP:OD2	1:E:41:TYR:OH	1.96	0.83
1:K:28:GLY:O	1:K:29:ARG:HG3	1.77	0.83
1:O:73:ASP:OD2	1:P:54:HIS:ND1	2.11	0.83
2:X:34:GLU:OE2	2:X:71:ARG:NH2	2.11	0.83
1:M:102:LEU:HD12	1:M:103:PHE:N	1.94	0.82
1:H:128:ASP:O	1:H:130:SER:N	2.13	0.81
1:N:72:TYR:OH	1:N:75:THR:OG1	1.98	0.81
1:A:120:LEU:CD2	1:A:125:ILE:HB	2.11	0.81
1:E:219:ARG:HB3	1:F:81:THR:HG21	1.60	0.81
1:G:17:ARG:O	1:G:18:GLU:O	1.97	0.81
1:C:176:ARG:HB2	1:G:258:LEU:HD21	1.61	0.81
1:M:102:LEU:HD12	1:M:103:PHE:H	1.45	0.81
1:B:119:ASN:ND2	1:B:233:PRO:O	2.15	0.80
1:G:257:ASP:O	1:G:258:LEU:HD12	1.82	0.80
1:C:219:ARG:HB3	1:D:81:THR:HG21	1.65	0.79
1:D:189:LEU:HD13	1:D:239:ILE:HD11	1.64	0.79
2:W:13:ARG:NH2	2:W:58:ASP:OD2	2.16	0.79
1:L:72:TYR:OH	1:L:75:THR:OG1	2.00	0.79
1:P:118:LYS:HE3	1:P:320:ALA:O	1.83	0.79
1:O:6:LEU:HD23	1:O:7:THR:N	1.97	0.78
1:O:71:TYR:CE2	1:P:79:ARG:NH1	2.52	0.78
1:O:118:LYS:O	1:O:122:ASN:ND2	2.17	0.78
1:I:234:ILE:O	1:I:238:ARG:NE	2.16	0.77
1:E:34:ILE:HD11	1:E:55:TYR:CE2	2.20	0.77
1:F:161:ASP:O	1:F:169:ARG:NH1	2.17	0.77
1:N:106:LYS:O	1:N:110:VAL:HG23	1.84	0.77
1:O:28:GLY:C	1:O:29:ARG:HD3	2.05	0.77
1:L:19:ASN:O	1:L:20:THR:OG1	2.02	0.77
1:A:178:PRO:O	1:A:261:VAL:HG22	1.86	0.75
1:B:189:LEU:HD13	1:B:239:ILE:HD11	1.68	0.75
1:B:219:ARG:HG3	1:B:219:ARG:HH11	1.51	0.75
1:M:38:TYR:CE2	1:M:299:ARG:NH2	2.54	0.75
1:M:174:THR:O	1:M:183:ASN:ND2	2.18	0.75
1:A:186:ILE:O	1:A:190:ASN:ND2	2.20	0.75
2:T:83:GLU:OE1	1:K:276:ASN:ND2	2.19	0.75
1:I:73:ASP:OD2	1:J:54:HIS:ND1	2.20	0.75
1:F:72:TYR:HH	1:F:75:THR:HG1	1.30	0.75
1:H:86:ASP:O	1:H:90:LYS:HG2	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ASP:HA	1:F:164:LEU:HD21	1.68	0.74
1:K:257:ASP:OD1	1:K:260:GLY:N	2.20	0.74
1:M:203:ASN:CG	1:M:299:ARG:HH12	1.91	0.74
1:N:19:ASN:O	1:N:20:THR:OG1	2.06	0.74
1:A:219:ARG:HB2	1:B:81:THR:OG1	1.89	0.73
1:C:126:SER:O	1:C:159:ARG:NE	2.22	0.73
1:C:67:ASN:OD1	1:C:176:ARG:NH2	2.20	0.73
1:C:119:ASN:ND2	1:C:233:PRO:O	2.22	0.73
1:E:115:ASN:ND2	1:E:319:VAL:O	2.21	0.73
1:M:21:LEU:HB3	1:M:32:LEU:HD22	1.71	0.73
1:D:119:ASN:ND2	1:D:233:PRO:O	2.21	0.73
1:I:28:GLY:O	1:I:29:ARG:HG3	1.88	0.73
1:I:19:ASN:O	1:I:20:THR:HG23	1.89	0.72
1:A:170:ILE:O	1:A:170:ILE:HD12	1.89	0.72
1:D:211:SER:OG	1:D:214:HIS:O	2.07	0.72
1:G:224:ALA:O	1:G:228:SER:OG	2.05	0.72
1:A:25:ASN:OD1	1:A:25:ASN:N	2.22	0.72
1:M:200:GLU:HB3	1:M:299:ARG:HG2	1.71	0.72
1:H:114:LYS:O	1:H:118:LYS:HG2	1.90	0.72
1:E:32:LEU:HD21	1:E:37:ILE:HD11	1.70	0.71
1:F:174:THR:OG1	1:F:179:LYS:O	2.08	0.71
1:C:19:ASN:O	1:C:20:THR:OG1	2.06	0.71
1:N:110:VAL:HG12	1:N:114:LYS:HD2	1.70	0.71
1:J:213:LEU:N	1:J:226:ASP:OD2	2.23	0.71
1:B:70:GLY:O	1:B:199:SER:OG	2.07	0.71
1:F:163:SER:OG	1:F:245:LYS:NZ	2.24	0.71
1:J:189:LEU:HD22	1:J:239:ILE:HD11	1.72	0.71
1:P:43:TYR:OH	1:P:299:ARG:NH2	2.24	0.71
1:P:141:LYS:NZ	1:P:142:VAL:HG12	2.06	0.70
1:C:28:GLY:O	1:C:29:ARG:HD3	1.92	0.70
1:J:115:ASN:ND2	1:J:318:LEU:O	2.24	0.70
1:C:6:LEU:CD1	1:C:37:ILE:HG12	2.22	0.70
1:C:6:LEU:HD12	1:C:37:ILE:HG12	1.72	0.70
1:L:141:LYS:HG2	1:L:142:VAL:H	1.57	0.69
1:P:293:THR:O	1:P:296:ARG:N	2.21	0.69
2:Q:82:GLU:OE1	2:Q:82:GLU:N	2.25	0.69
1:L:35:GLU:N	1:L:35:GLU:OE1	2.24	0.69
1:G:174:THR:N	1:G:183:ASN:OD1	2.26	0.69
1:C:6:LEU:HD12	1:C:37:ILE:CG1	2.22	0.68
1:D:180:ASN:OD1	1:D:181:GLU:N	2.26	0.68
1:J:189:LEU:HD21	1:J:271:VAL:CG1	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:13:ARG:NH2	2:S:58:ASP:OD2	2.26	0.68
1:K:21:LEU:CD1	1:K:34:ILE:HD12	2.24	0.68
1:D:162:GLU:N	1:D:162:GLU:OE2	2.27	0.67
1:D:301:GLU:OE1	1:D:304:LYS:NZ	2.27	0.67
1:I:318:LEU:O	1:I:320:ALA:N	2.26	0.67
2:R:66:ARG:O	1:I:29:ARG:NH1	2.27	0.67
1:E:161:ASP:OD2	1:E:170:ILE:N	2.28	0.67
1:D:19:ASN:O	1:D:20:THR:OG1	2.12	0.66
1:P:72:TYR:OH	1:P:75:THR:OG1	2.13	0.66
1:D:189:LEU:CD1	1:D:239:ILE:HD11	2.24	0.66
1:P:19:ASN:O	1:P:20:THR:OG1	2.12	0.66
1:I:91:GLN:NE2	1:I:210:ILE:O	2.29	0.66
1:E:119:ASN:ND2	1:E:233:PRO:O	2.27	0.66
1:J:127:SER:OG	1:J:128:ASP:N	2.29	0.66
1:J:106:LYS:O	1:J:110:VAL:HG22	1.95	0.66
1:L:238:ARG:HH11	1:L:278:GLU:HG3	1.60	0.66
1:P:72:TYR:HH	1:P:75:THR:HG1	1.44	0.66
1:B:115:ASN:ND2	1:B:318:LEU:O	2.29	0.65
1:D:132:HIS:NE2	1:D:155:GLU:OE2	2.29	0.65
1:H:219:ARG:HH11	1:H:219:ARG:CG	2.08	0.65
1:K:211:SER:OG	1:K:214:HIS:O	2.09	0.65
1:L:239:ILE:HA	1:L:242:ARG:HD2	1.77	0.65
1:M:203:ASN:ND2	1:M:299:ARG:HH12	1.94	0.65
1:B:311:GLY:O	1:E:147:ASN:ND2	2.28	0.65
1:F:92:ALA:O	1:F:95:TYR:N	2.28	0.65
1:M:203:ASN:CB	1:M:299:ARG:HH11	2.10	0.65
1:F:194:TYR:OH	1:F:220:ARG:O	2.14	0.65
1:I:214:HIS:ND1	1:I:226:ASP:OD1	2.30	0.65
1:H:199:SER:O	1:H:203:ASN:N	2.30	0.65
1:A:18:GLU:HG2	1:A:19:ASN:N	2.12	0.64
1:C:215:GLU:O	1:C:220:ARG:NH1	2.29	0.64
1:D:114:LYS:O	1:D:118:LYS:HG2	1.97	0.64
1:A:170:ILE:O	1:A:170:ILE:CD1	2.45	0.64
1:F:118:LYS:HG2	1:F:320:ALA:O	1.97	0.64
1:P:292:VAL:HG11	1:P:296:ARG:NH2	2.12	0.64
1:F:299:ARG:O	1:F:303:TYR:N	2.29	0.64
1:A:18:GLU:O	1:A:20:THR:N	2.29	0.64
2:U:34:GLU:OE2	2:U:71:ARG:NH1	2.30	0.64
1:P:106:LYS:O	1:P:110:VAL:HG23	1.96	0.64
1:C:176:ARG:CB	1:G:258:LEU:HD21	2.26	0.64
1:O:110:VAL:HG22	1:O:133:LEU:HD11	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:LEU:HD21	1:F:221:PHE:CE1	2.33	0.63
1:L:26:VAL:O	1:L:27:ASN:OD1	2.17	0.63
2:V:43:GLU:O	2:V:47:GLU:N	2.28	0.63
1:M:115:ASN:HB3	1:M:233:PRO:HB2	1.79	0.63
1:B:102:LEU:HD21	1:B:140:LYS:O	1.99	0.63
1:M:83:LEU:HD21	1:N:221:PHE:CE1	2.33	0.63
1:M:200:GLU:OE1	1:M:299:ARG:NE	2.31	0.63
1:B:173:ARG:O	1:B:174:THR:OG1	2.15	0.63
1:F:186:ILE:O	1:F:190:ASN:ND2	2.31	0.63
1:H:239:ILE:HD12	1:H:239:ILE:C	2.19	0.63
1:N:13:THR:N	1:N:24:GLU:O	2.31	0.63
1:A:178:PRO:HD2	1:A:261:VAL:HG21	1.81	0.62
1:K:217:SER:OG	1:K:220:ARG:NH1	2.32	0.62
1:A:19:ASN:O	1:A:20:THR:HG23	1.99	0.62
1:B:98:LYS:O	1:B:102:LEU:HD13	2.00	0.62
1:M:38:TYR:HE2	1:M:299:ARG:NH2	1.97	0.62
1:L:189:LEU:HD21	1:L:271:VAL:CG1	2.30	0.62
1:H:189:LEU:HD21	1:H:239:ILE:HD11	1.82	0.62
1:C:218:GLU:OE2	1:D:205:GLN:HG2	1.99	0.62
1:G:257:ASP:O	1:G:258:LEU:CD1	2.48	0.61
1:F:120:LEU:HD13	1:F:127:SER:HB3	1.82	0.61
1:A:87:LEU:CD2	1:A:309:LEU:HD23	2.29	0.61
1:K:6:LEU:HD13	1:K:37:ILE:HD13	1.80	0.61
1:C:139:ALA:HB1	1:C:144:GLU:HB3	1.81	0.61
1:C:219:ARG:HB2	1:D:81:THR:OG1	1.99	0.61
1:H:219:ARG:HG3	1:H:219:ARG:NH1	2.14	0.61
1:L:118:LYS:HG2	1:L:320:ALA:O	2.01	0.61
1:N:130:SER:O	1:N:133:LEU:N	2.29	0.61
2:T:83:GLU:OE1	1:K:276:ASN:CG	2.39	0.61
1:E:131:ASN:OD1	1:E:132:HIS:N	2.34	0.60
1:M:203:ASN:CB	1:M:299:ARG:NH1	2.63	0.60
1:D:169:ARG:O	1:D:180:ASN:ND2	2.35	0.60
1:B:219:ARG:HG3	1:B:219:ARG:NH1	2.14	0.60
1:B:249:ILE:HG12	1:B:253:HIS:HD2	1.65	0.60
1:G:301:GLU:OE2	1:G:315:TYR:OH	2.09	0.60
1:P:67:ASN:OD1	1:P:68:HIS:N	2.33	0.60
1:B:43:TYR:HB3	1:B:66:PHE:HB2	1.83	0.60
1:P:117:GLU:HG2	1:P:127:SER:HB2	1.83	0.60
1:B:189:LEU:CD1	1:B:239:ILE:HD11	2.31	0.60
1:M:115:ASN:O	1:M:119:ASN:N	2.34	0.60
1:E:118:LYS:HG3	1:E:122:ASN:ND2	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:ASN:OD1	1:J:181:GLU:N	2.30	0.59
1:H:132:HIS:CE1	1:H:151:ARG:HG2	2.37	0.59
1:M:19:ASN:O	1:M:20:THR:OG1	2.19	0.59
1:G:174:THR:HG21	1:G:179:LYS:H	1.66	0.59
1:H:219:ARG:CG	1:H:219:ARG:NH1	2.62	0.59
1:F:19:ASN:O	1:F:20:THR:OG1	2.16	0.59
1:H:180:ASN:OD1	1:H:181:GLU:N	2.33	0.59
1:K:180:ASN:OD1	1:K:181:GLU:N	2.34	0.59
1:I:283:VAL:CG1	1:I:292:VAL:HG12	2.33	0.59
2:V:34:GLU:OE1	2:V:71:ARG:NH2	2.36	0.59
1:C:197:MET:HE3	1:C:227:LEU:HB3	1.84	0.59
1:M:285:HIS:HB2	1:M:321:TRP:CZ2	2.38	0.59
1:O:86:ASP:O	1:O:90:LYS:HG2	2.03	0.59
1:B:201:ILE:HD11	1:B:227:LEU:CD1	2.33	0.58
1:N:103:PHE:O	1:N:104:LEU:HB2	2.03	0.58
1:A:197:MET:HE2	1:A:227:LEU:HB3	1.86	0.58
1:K:156:TYR:O	1:K:160:TRP:N	2.37	0.58
1:H:17:ARG:NH1	1:H:29:ARG:HH12	2.01	0.58
1:I:283:VAL:HG11	1:I:292:VAL:HG12	1.85	0.58
1:C:6:LEU:CD1	1:C:37:ILE:CD1	2.82	0.58
1:H:106:LYS:O	1:H:110:VAL:HG23	2.02	0.58
1:M:39:ASP:OD2	1:M:41:TYR:OH	2.10	0.58
1:K:197:MET:HB3	1:K:224:ALA:HB1	1.84	0.58
1:O:92:ALA:O	1:O:96:LEU:HD12	2.04	0.58
1:M:28:GLY:O	1:M:29:ARG:HG3	2.04	0.58
1:M:203:ASN:HB3	1:M:299:ARG:HH11	1.69	0.58
1:E:33:ALA:HB2	2:U:70:PRO:HB3	1.86	0.58
1:K:34:ILE:HD11	1:K:59:LYS:HG3	1.86	0.58
1:B:6:LEU:HD21	1:B:40:ILE:HG12	1.85	0.57
1:M:55:TYR:O	1:M:58:GLN:N	2.37	0.57
1:M:257:ASP:OD1	1:M:260:GLY:N	2.37	0.57
1:J:19:ASN:O	1:J:20:THR:OG1	2.20	0.57
1:C:6:LEU:CD1	1:C:37:ILE:HD11	2.35	0.57
2:R:39:LEU:O	2:R:39:LEU:HD23	2.04	0.57
2:S:13:ARG:NH1	2:S:58:ASP:OD2	2.37	0.57
1:K:19:ASN:O	1:K:20:THR:HG23	2.05	0.57
1:O:283:VAL:HG21	1:O:297:LEU:HD11	1.87	0.57
1:A:101:ARG:NH2	1:A:142:VAL:HG21	2.18	0.57
1:L:122:ASN:ND2	1:L:322:PHE:O	2.38	0.57
1:O:71:TYR:HE2	1:P:79:ARG:HH12	1.52	0.57
1:C:87:LEU:HD23	1:C:87:LEU:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:PHE:O	1:J:104:LEU:HB2	2.04	0.57
1:C:29:ARG:HH11	1:C:29:ARG:HG2	1.69	0.57
1:L:232:LYS:HG2	1:L:233:PRO:HD3	1.87	0.57
1:N:141:LYS:HG2	1:N:142:VAL:H	1.68	0.57
1:C:7:THR:HG21	1:C:192:ARG:NH2	2.20	0.57
1:G:19:ASN:O	1:G:20:THR:HG23	2.05	0.57
1:K:118:LYS:O	1:K:122:ASN:ND2	2.35	0.57
1:N:185:LEU:O	1:N:189:LEU:HD12	2.04	0.57
1:F:72:TYR:OH	1:F:75:THR:OG1	2.06	0.56
1:A:157:TYR:HB3	1:A:170:ILE:HD13	1.86	0.56
1:C:28:GLY:O	1:C:29:ARG:NH1	2.37	0.56
1:E:54:HIS:ND1	1:F:73:ASP:OD2	2.37	0.56
1:K:218:GLU:HB2	1:L:86:ASP:HA	1.87	0.56
1:F:140:LYS:HD2	1:F:141:LYS:CE	2.36	0.56
1:O:115:ASN:O	1:O:119:ASN:N	2.37	0.56
1:D:10:SER:HB3	1:D:26:VAL:HG21	1.86	0.56
1:K:104:LEU:HD13	1:K:212:TYR:CE1	2.41	0.56
1:G:7:THR:HG21	1:G:192:ARG:NH2	2.21	0.56
1:G:74:GLY:HA3	1:H:78:PRO:HA	1.87	0.56
2:R:67:SER:HB3	1:I:29:ARG:HD3	1.87	0.56
2:V:37:VAL:HB	2:V:41:GLU:OE1	2.06	0.56
2:V:66:ARG:O	1:M:29:ARG:NH1	2.39	0.56
1:L:189:LEU:HD21	1:L:271:VAL:HG13	1.87	0.56
1:B:296:ARG:O	1:B:299:ARG:N	2.39	0.56
1:A:34:ILE:HG13	1:A:35:GLU:H	1.69	0.56
1:M:38:TYR:CZ	1:M:299:ARG:NH2	2.73	0.56
1:M:203:ASN:OD1	1:M:299:ARG:NH1	2.38	0.56
1:E:83:LEU:HD21	1:F:221:PHE:HE1	1.70	0.55
1:I:155:GLU:O	1:I:159:ARG:HG2	2.06	0.55
1:O:6:LEU:HD22	1:O:8:ILE:HG23	1.88	0.55
1:L:117:GLU:HG3	1:L:127:SER:HB2	1.87	0.55
1:L:146:MET:O	1:L:149:GLU:N	2.39	0.55
1:E:186:ILE:O	1:E:190:ASN:ND2	2.40	0.55
1:H:120:LEU:HD13	1:H:127:SER:HB3	1.88	0.55
1:M:38:TYR:OH	1:M:299:ARG:NH2	2.39	0.55
1:M:293:THR:HG22	1:M:294:ARG:H	1.71	0.55
1:E:39:ASP:OD1	1:E:39:ASP:N	2.39	0.55
1:C:100:LYS:O	1:C:104:LEU:HD12	2.06	0.55
1:I:279:LEU:O	1:I:279:LEU:HD23	2.07	0.55
1:O:34:ILE:HD11	1:O:61:ILE:HD12	1.89	0.55
1:C:281:LYS:O	1:C:294:ARG:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:TYR:CE2	1:E:59:LYS:HG3	2.41	0.55
1:K:79:ARG:O	1:K:202:TYR:OH	2.22	0.55
1:C:159:ARG:HG2	1:C:159:ARG:O	2.07	0.55
1:G:39:ASP:N	1:G:39:ASP:OD1	2.40	0.55
1:G:86:ASP:O	1:G:90:LYS:HG2	2.07	0.55
1:H:128:ASP:OD1	1:H:129:PHE:N	2.40	0.55
1:M:113:ALA:HB2	1:M:152:ILE:HG21	1.89	0.55
1:E:239:ILE:HD11	1:E:278:GLU:HB2	1.89	0.54
1:M:203:ASN:CG	1:M:299:ARG:HH11	2.09	0.54
1:C:127:SER:OG	1:C:159:ARG:HD3	2.07	0.54
1:C:186:ILE:O	1:C:190:ASN:ND2	2.41	0.54
1:K:42:ILE:HD11	1:K:63:ILE:HD11	1.89	0.54
1:F:140:LYS:HG2	1:F:141:LYS:HD3	1.90	0.54
2:R:83:GLU:OE1	1:I:276:ASN:ND2	2.39	0.54
2:X:30:ASN:O	2:X:31:SER:OG	2.21	0.54
1:I:158:ALA:O	1:I:159:ARG:NE	2.40	0.54
1:I:158:ALA:C	1:I:159:ARG:HE	2.10	0.54
1:E:11:ASP:O	1:E:26:VAL:CG1	2.56	0.54
1:F:279:LEU:HB3	1:F:295:ARG:HB2	1.89	0.54
1:E:296:ARG:C	1:E:296:ARG:HD3	2.28	0.54
1:A:91:GLN:CG	1:A:309:LEU:HD21	2.38	0.54
1:C:292:VAL:N	2:T:56:ASN:OD1	2.40	0.54
1:K:261:VAL:O	1:K:262:LEU:O	2.25	0.54
1:K:292:VAL:HG13	1:K:292:VAL:O	2.08	0.54
1:O:197:MET:HE2	1:O:227:LEU:HB3	1.89	0.54
1:K:63:ILE:HG22	1:K:76:PHE:HB3	1.89	0.54
1:P:110:VAL:HG22	1:P:133:LEU:HD11	1.89	0.54
1:D:161:ASP:OD2	1:D:169:ARG:HG3	2.07	0.54
1:L:180:ASN:OD1	1:L:181:GLU:N	2.41	0.54
1:L:213:LEU:N	1:L:226:ASP:OD2	2.38	0.54
1:O:176:ARG:HG2	1:O:177:PRO:HD3	1.90	0.54
1:E:32:LEU:CD2	1:E:37:ILE:HD11	2.38	0.53
1:E:80:GLU:O	1:E:83:LEU:HD23	2.08	0.53
1:K:211:SER:HB3	1:K:222:SER:O	2.08	0.53
1:M:97:ASP:O	1:M:99:ASN:N	2.41	0.53
1:N:115:ASN:ND2	1:N:318:LEU:O	2.39	0.53
1:I:158:ALA:O	1:I:159:ARG:NH2	2.41	0.53
1:P:189:LEU:HD11	1:P:239:ILE:CG1	2.38	0.53
1:D:220:ARG:NH1	1:D:222:SER:OG	2.36	0.53
1:L:11:ASP:N	1:L:11:ASP:OD1	2.41	0.53
1:J:118:LYS:HG2	1:J:320:ALA:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ILE:HG23	1:F:61:ILE:HB	1.88	0.53
1:I:173:ARG:O	1:I:174:THR:OG1	2.21	0.53
2:W:81:ILE:O	2:W:81:ILE:HG22	2.08	0.53
1:C:6:LEU:HD12	1:C:37:ILE:CD1	2.39	0.53
1:D:98:LYS:HZ3	1:D:141:LYS:HZ2	1.57	0.53
1:E:296:ARG:NE	1:E:300:LEU:HD21	2.24	0.53
1:P:169:ARG:O	1:P:180:ASN:ND2	2.41	0.53
1:D:102:LEU:HD11	1:D:140:LYS:O	2.09	0.53
1:E:296:ARG:HE	1:E:300:LEU:HD21	1.72	0.53
1:O:96:LEU:HD21	1:P:93:GLU:HB2	1.91	0.53
1:A:115:ASN:O	1:A:119:ASN:N	2.40	0.52
1:L:26:VAL:O	1:L:27:ASN:CG	2.47	0.52
1:I:32:LEU:HD23	1:I:33:ALA:O	2.08	0.52
1:B:95:TYR:CD2	1:B:95:TYR:O	2.62	0.52
2:W:28:VAL:HG22	2:W:81:ILE:HG13	1.91	0.52
1:L:70:GLY:O	1:L:199:SER:OG	2.21	0.52
1:M:21:LEU:CB	1:M:32:LEU:HD22	2.39	0.52
1:P:170:ILE:HG22	1:P:171:GLY:H	1.73	0.52
1:C:218:GLU:HG3	1:C:219:ARG:HD2	1.92	0.52
1:C:279:LEU:CD2	1:C:295:ARG:HB2	2.40	0.52
1:F:106:LYS:O	1:F:110:VAL:HG23	2.10	0.52
1:M:27:ASN:OD1	1:M:27:ASN:N	2.42	0.52
1:O:6:LEU:CD1	1:O:32:LEU:HD11	2.40	0.52
1:C:174:THR:N	1:C:183:ASN:OD1	2.39	0.52
1:I:38:TYR:OH	1:I:295:ARG:NH1	2.42	0.52
1:J:303:TYR:O	1:J:306:ILE:N	2.42	0.52
1:C:87:LEU:HD21	1:C:309:LEU:HD13	1.91	0.52
2:V:66:ARG:CD	2:V:66:ARG:H	2.22	0.52
1:L:139:ALA:HB1	1:L:144:GLU:HB3	1.91	0.52
1:M:176:ARG:HG3	1:M:177:PRO:HD3	1.90	0.52
1:O:213:LEU:HB3	1:O:226:ASP:OD2	2.08	0.52
1:L:238:ARG:NH1	1:L:239:ILE:HG22	2.24	0.52
1:C:19:ASN:C	1:C:20:THR:HG1	2.10	0.52
1:B:189:LEU:HD21	1:B:271:VAL:CG1	2.40	0.52
1:B:257:ASP:OD1	1:B:258:LEU:N	2.40	0.52
1:C:21:LEU:HD13	1:C:34:ILE:HD12	1.92	0.52
1:E:54:HIS:HD1	1:F:73:ASP:CG	2.13	0.52
1:B:101:ARG:NH2	1:B:215:GLU:OE2	2.40	0.52
1:H:132:HIS:CE1	1:H:151:ARG:HD3	2.45	0.52
1:O:109:VAL:HG22	1:O:213:LEU:HD11	1.91	0.52
1:P:211:SER:OG	1:P:214:HIS:O	2.12	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:LYS:NZ	1:L:142:VAL:HG12	2.25	0.51
1:J:168:PHE:CD1	1:J:244:VAL:HG13	2.45	0.51
1:P:127:SER:O	1:P:129:PHE:HD2	1.92	0.51
1:A:91:GLN:HG2	1:A:309:LEU:HD21	1.92	0.51
1:D:48:ILE:HG21	1:D:53:LEU:HD11	1.92	0.51
2:V:66:ARG:H	2:V:66:ARG:HD3	1.74	0.51
1:K:160:TRP:HZ2	1:K:241:ASN:HB2	1.74	0.51
1:D:26:VAL:O	1:D:27:ASN:HB2	2.11	0.51
1:L:238:ARG:NH1	1:L:278:GLU:HG3	2.24	0.51
1:M:39:ASP:OD1	1:M:39:ASP:N	2.43	0.51
1:B:127:SER:O	1:B:129:PHE:CD1	2.63	0.51
1:E:11:ASP:O	1:E:26:VAL:HG13	2.10	0.51
2:V:41:GLU:HA	2:V:44:ARG:CD	2.39	0.51
1:O:39:ASP:OD1	1:O:39:ASP:N	2.43	0.51
1:P:141:LYS:HZ3	1:P:142:VAL:HG12	1.75	0.51
1:P:293:THR:O	1:P:295:ARG:N	2.42	0.51
1:E:240:ALA:O	1:E:244:VAL:HG23	2.10	0.51
1:G:105:ALA:O	1:G:109:VAL:HG23	2.11	0.51
2:T:13:ARG:NH1	2:T:58:ASP:OD2	2.44	0.51
1:C:176:ARG:HB2	1:G:258:LEU:CD2	2.38	0.51
1:I:197:MET:HE1	1:I:227:LEU:HB3	1.93	0.51
1:D:51:GLN:HA	1:D:54:HIS:HD2	1.75	0.51
1:E:296:ARG:HE	1:E:300:LEU:CD2	2.23	0.51
1:F:136:LEU:HB3	1:F:148:VAL:HG11	1.92	0.51
1:N:101:ARG:O	1:N:102:LEU:HB2	2.11	0.51
1:O:262:LEU:HD12	1:O:263:LEU:O	2.11	0.51
1:C:239:ILE:O	1:C:240:ALA:HB3	2.11	0.51
1:M:73:ASP:O	1:N:79:ARG:N	2.43	0.51
1:M:73:ASP:OD2	1:N:54:HIS:ND1	2.44	0.51
1:P:141:LYS:HZ2	1:P:142:VAL:HG12	1.76	0.51
1:A:261:VAL:O	1:A:262:LEU:HB2	2.11	0.51
1:D:253:HIS:O	1:D:264:THR:HG22	2.11	0.51
1:L:56:ILE:HG21	1:L:63:ILE:HD11	1.92	0.51
1:P:121:LYS:HG3	1:P:127:SER:HB3	1.91	0.50
1:C:150:GLY:O	1:C:154:GLN:NE2	2.43	0.50
1:K:62:LEU:HD12	1:K:62:LEU:O	2.10	0.50
1:A:21:LEU:HB2	1:A:34:ILE:CG2	2.41	0.50
1:C:192:ARG:HH22	1:C:272:THR:HG23	1.76	0.50
1:E:80:GLU:HG3	1:E:83:LEU:HD23	1.93	0.50
1:K:253:HIS:O	1:K:264:THR:HG22	2.11	0.50
1:L:56:ILE:HG23	1:L:61:ILE:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:LYS:HG2	1:L:142:VAL:N	2.27	0.50
1:L:303:TYR:O	1:L:304:LYS:HB2	2.12	0.50
1:O:255:ARG:HG2	1:O:256:GLU:H	1.76	0.50
1:B:106:LYS:O	1:B:110:VAL:HG23	2.10	0.50
1:C:6:LEU:HD12	1:C:37:ILE:HD11	1.92	0.50
1:C:13:THR:N	1:C:24:GLU:O	2.36	0.50
1:I:257:ASP:OD1	1:I:260:GLY:N	2.43	0.50
1:A:87:LEU:O	1:A:87:LEU:HD23	2.12	0.50
1:D:16:ARG:HB3	1:D:51:GLN:OE1	2.11	0.50
1:F:179:LYS:O	1:F:180:ASN:HB2	2.11	0.50
1:O:62:LEU:HD23	1:O:78:PRO:HD2	1.93	0.50
1:K:7:THR:CG2	1:K:192:ARG:HH12	2.23	0.50
1:A:125:ILE:HG22	1:A:126:SER:N	2.26	0.50
1:K:167:GLU:O	1:K:167:GLU:HG2	2.12	0.50
1:K:263:LEU:H	1:K:263:LEU:HD23	1.76	0.50
1:M:245:LYS:O	1:M:246:LYS:HB2	2.12	0.50
1:D:141:LYS:HG3	1:D:143:THR:H	1.75	0.50
1:D:239:ILE:C	1:D:239:ILE:HD12	2.31	0.50
1:G:192:ARG:HH11	1:G:192:ARG:HB3	1.77	0.50
1:O:228:SER:HB2	1:O:232:LYS:HE3	1.94	0.50
1:A:197:MET:CE	1:A:227:LEU:HB3	2.40	0.49
1:C:87:LEU:HD21	1:C:309:LEU:CD1	2.42	0.49
1:C:219:ARG:HH22	1:D:82:LEU:HD11	1.77	0.49
1:D:98:LYS:NZ	1:D:141:LYS:NZ	2.60	0.49
1:F:92:ALA:O	1:F:96:LEU:HD12	2.12	0.49
1:K:218:GLU:OE1	1:K:219:ARG:NH1	2.45	0.49
1:L:105:ALA:O	1:L:106:LYS:HB2	2.12	0.49
1:A:15:LEU:CD1	1:A:17:ARG:H	2.25	0.49
1:C:102:LEU:HD11	1:C:140:LYS:HA	1.94	0.49
1:C:176:ARG:HA	1:C:178:PRO:HD3	1.94	0.49
1:D:24:GLU:O	1:D:25:ASN:O	2.30	0.49
1:B:6:LEU:CD2	1:B:40:ILE:HG12	2.42	0.49
2:T:73:THR:OG1	2:T:77:GLU:OE2	2.30	0.49
1:N:211:SER:OG	1:N:214:HIS:O	2.19	0.49
1:O:21:LEU:HD13	1:O:55:TYR:CE2	2.48	0.49
1:C:6:LEU:HD11	1:C:37:ILE:CD1	2.42	0.49
1:E:73:ASP:OD2	1:F:54:HIS:HB2	2.12	0.49
2:V:83:GLU:O	2:V:84:ILE:HG13	2.13	0.49
1:M:106:LYS:HD3	1:M:137:GLN:HG2	1.95	0.49
1:M:113:ALA:CB	1:M:152:ILE:HG21	2.41	0.49
1:P:303:TYR:HA	1:P:306:ILE:HG12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:CD1	1:C:37:ILE:CG1	2.85	0.49
1:C:176:ARG:O	1:G:258:LEU:HD11	2.11	0.49
1:C:218:GLU:HG3	1:C:219:ARG:CD	2.43	0.49
1:C:318:LEU:HD13	1:C:319:VAL:N	2.27	0.49
2:U:62:ILE:HG23	2:U:62:ILE:O	2.13	0.49
1:M:57:ALA:HB1	1:N:73:ASP:O	2.12	0.49
1:I:115:ASN:CG	1:I:319:VAL:HG13	2.32	0.49
1:E:118:LYS:HE3	1:E:122:ASN:HD21	1.78	0.49
1:G:299:ARG:O	1:G:303:TYR:N	2.44	0.49
1:K:71:TYR:OH	1:K:178:PRO:HG3	2.12	0.49
1:J:127:SER:O	1:J:129:PHE:CD2	2.66	0.49
1:A:183:ASN:HA	1:A:186:ILE:HG22	1.95	0.49
1:D:98:LYS:HZ1	1:D:141:LYS:HZ1	1.61	0.49
1:D:157:TYR:O	1:D:160:TRP:N	2.29	0.49
1:F:303:TYR:O	1:F:306:ILE:HG22	2.13	0.49
1:I:106:LYS:O	1:I:110:VAL:HG12	2.12	0.49
1:J:189:LEU:HD21	1:J:271:VAL:HG13	1.93	0.49
1:C:95:TYR:CE1	1:C:101:ARG:NH1	2.81	0.49
1:C:182:MET:HE1	1:C:240:ALA:HB1	1.94	0.49
1:G:17:ARG:C	1:G:18:GLU:O	2.50	0.49
1:I:72:TYR:OH	1:I:75:THR:OG1	1.96	0.49
1:D:101:ARG:NH2	1:D:142:VAL:HG21	2.28	0.48
1:F:194:TYR:OH	1:F:220:ARG:HG3	2.12	0.48
1:A:71:TYR:HE1	1:A:187:SER:HG	1.61	0.48
1:B:52:ALA:O	1:B:56:ILE:HD13	2.12	0.48
1:C:29:ARG:HG2	1:C:29:ARG:NH1	2.28	0.48
1:C:32:LEU:HD23	1:C:33:ALA:N	2.28	0.48
1:H:24:GLU:HG3	1:H:29:ARG:CG	2.43	0.48
1:L:231:PHE:CE2	1:L:298:ILE:HA	2.48	0.48
1:I:91:GLN:NE2	1:I:210:ILE:HG23	2.28	0.48
1:B:49:THR:HG23	1:B:52:ALA:H	1.78	0.48
1:B:167:GLU:OE2	1:B:251:LYS:HG3	2.13	0.48
1:E:161:ASP:OD2	1:E:170:ILE:O	2.31	0.48
1:G:13:THR:N	1:G:24:GLU:O	2.46	0.48
2:S:73:THR:HG23	2:S:77:GLU:OE2	2.13	0.48
2:U:14:VAL:O	2:U:17:VAL:HG22	2.13	0.48
1:M:31:PRO:O	1:M:32:LEU:HB2	2.14	0.48
1:O:110:VAL:HG22	1:O:133:LEU:CD1	2.43	0.48
1:C:255:ARG:HA	1:C:255:ARG:NE	2.28	0.48
1:D:26:VAL:O	1:D:26:VAL:HG12	2.13	0.48
1:D:82:LEU:HB3	1:G:172:LYS:NZ	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ASP:OD1	1:D:253:HIS:ND1	2.46	0.48
1:E:174:THR:HG22	1:E:183:ASN:HB3	1.95	0.48
1:E:197:MET:CG	1:E:227:LEU:HD11	2.43	0.48
1:E:296:ARG:HD3	1:E:297:LEU:N	2.28	0.48
1:O:6:LEU:CD2	1:O:8:ILE:HG23	2.43	0.48
1:G:174:THR:OG1	1:G:178:PRO:HA	2.13	0.48
2:Q:81:ILE:HG22	2:Q:81:ILE:O	2.13	0.48
1:I:318:LEU:C	1:I:318:LEU:HD12	2.34	0.48
1:F:279:LEU:O	1:F:295:ARG:HB2	2.13	0.48
1:O:28:GLY:O	1:O:29:ARG:HD3	2.12	0.48
1:A:189:LEU:HD21	1:A:239:ILE:HB	1.94	0.48
1:G:34:ILE:HG12	1:G:55:TYR:CE1	2.48	0.48
1:G:212:TYR:O	1:G:226:ASP:OD2	2.31	0.48
1:J:49:THR:HB	1:J:51:GLN:OE1	2.14	0.48
1:D:231:PHE:CE2	1:D:298:ILE:HA	2.49	0.48
1:E:136:LEU:CD1	1:E:148:VAL:HG21	2.44	0.48
1:I:159:ARG:NE	1:I:159:ARG:HA	2.29	0.48
1:O:118:LYS:O	1:O:118:LYS:HD2	2.14	0.48
1:E:87:LEU:HD21	1:E:206:LEU:HD23	1.95	0.48
1:K:131:ASN:C	1:K:131:ASN:HD22	2.10	0.48
1:L:110:VAL:HG12	1:L:114:LYS:HD3	1.95	0.48
1:M:119:ASN:OD1	1:M:238:ARG:NH2	2.47	0.48
1:M:200:GLU:OE1	1:M:299:ARG:CD	2.62	0.48
1:C:200:GLU:HG3	1:C:299:ARG:HG3	1.96	0.47
1:L:142:VAL:HG13	1:L:143:THR:N	2.29	0.47
1:M:192:ARG:O	1:M:195:ALA:O	2.31	0.47
1:I:39:ASP:N	1:I:39:ASP:OD1	2.46	0.47
1:I:279:LEU:CD2	1:I:295:ARG:HB3	2.43	0.47
1:A:219:ARG:HE	1:B:62:LEU:HB2	1.79	0.47
2:X:70:PRO:HB3	1:O:33:ALA:CB	2.44	0.47
1:I:28:GLY:O	1:I:29:ARG:CG	2.62	0.47
1:A:296:ARG:O	1:A:299:ARG:N	2.47	0.47
1:B:180:ASN:OD1	1:B:181:GLU:N	2.47	0.47
1:N:104:LEU:O	1:N:108:PHE:CD2	2.66	0.47
1:J:80:GLU:O	1:J:81:THR:OG1	2.31	0.47
1:B:89:ILE:O	1:B:93:GLU:N	2.42	0.47
1:C:8:ILE:HD11	1:C:42:ILE:HG12	1.97	0.47
1:I:279:LEU:O	1:I:294:ARG:HB2	2.14	0.47
1:D:91:GLN:NE2	1:D:207:ALA:O	2.46	0.47
2:Q:7:TYR:HE2	2:Q:21:LEU:HD12	1.79	0.47
1:I:98:LYS:NZ	1:I:141:LYS:HG3	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLY:O	1:C:29:ARG:CD	2.61	0.47
1:F:117:GLU:OE2	1:F:130:SER:N	2.48	0.47
1:H:88:ILE:HG23	1:H:89:ILE:HD12	1.97	0.47
1:O:231:PHE:HE1	1:O:298:ILE:HA	1.78	0.47
1:A:34:ILE:HG13	1:A:35:GLU:N	2.29	0.47
1:B:72:TYR:CD1	1:B:202:TYR:HB3	2.50	0.47
1:C:170:ILE:O	1:C:170:ILE:HG13	2.15	0.47
1:F:194:TYR:HE1	1:F:224:ALA:HB3	1.80	0.47
1:G:174:THR:HG21	1:G:179:LYS:N	2.27	0.47
1:K:119:ASN:ND2	1:K:233:PRO:O	2.44	0.47
1:L:211:SER:H	1:L:216:PRO:HB3	1.80	0.47
1:L:255:ARG:CZ	1:L:262:LEU:HD11	2.44	0.47
1:M:102:LEU:CD1	1:M:103:PHE:N	2.73	0.47
1:I:157:TYR:O	1:I:158:ALA:HB3	2.15	0.47
1:D:127:SER:O	1:D:128:ASP:HB3	2.15	0.47
1:D:255:ARG:HE	1:D:262:LEU:HD11	1.80	0.47
2:S:53:ILE:HD13	2:S:60:VAL:HG21	1.97	0.47
1:K:116:MET:HG2	1:K:233:PRO:HB3	1.97	0.47
1:L:90:LYS:O	1:L:93:GLU:N	2.48	0.47
1:O:88:ILE:HG21	1:P:88:ILE:HD11	1.96	0.47
1:D:239:ILE:HD12	1:D:240:ALA:N	2.30	0.47
1:G:178:PRO:HG2	1:G:261:VAL:O	2.15	0.47
1:E:136:LEU:HD12	1:E:148:VAL:HG21	1.96	0.46
1:H:201:ILE:HD11	1:H:227:LEU:HD22	1.96	0.46
1:K:262:LEU:C	1:K:262:LEU:HD12	2.35	0.46
1:L:106:LYS:O	1:L:110:VAL:HG23	2.15	0.46
1:L:305:ILE:O	1:L:309:LEU:HG	2.16	0.46
1:I:21:LEU:HD11	1:I:55:TYR:CD1	2.50	0.46
1:E:21:LEU:HB3	1:E:32:LEU:HD22	1.96	0.46
1:P:14:LEU:N	1:P:47:ASN:O	2.48	0.46
1:A:8:ILE:HG13	1:A:8:ILE:O	2.15	0.46
1:C:29:ARG:O	1:C:31:PRO:CD	2.63	0.46
1:E:87:LEU:O	1:E:90:LYS:N	2.49	0.46
1:E:172:LYS:HD2	1:E:172:LYS:O	2.16	0.46
1:G:118:LYS:HG2	1:G:122:ASN:OD1	2.16	0.46
1:G:219:ARG:HD3	1:H:62:LEU:HD11	1.98	0.46
2:V:41:GLU:HA	2:V:44:ARG:HD2	1.98	0.46
1:L:86:ASP:HB3	1:L:89:ILE:HD12	1.96	0.46
1:A:25:ASN:HB2	1:A:27:ASN:OD1	2.16	0.46
1:B:168:PHE:CD1	1:B:244:VAL:HG22	2.50	0.46
1:E:94:HIS:O	1:E:101:ARG:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:53:LEU:HD23	1:O:53:LEU:C	2.36	0.46
1:P:189:LEU:HD11	1:P:239:ILE:HG12	1.97	0.46
1:A:72:TYR:CD2	1:B:79:ARG:HB2	2.50	0.46
1:B:63:ILE:HG12	1:B:76:PHE:HB3	1.97	0.46
1:G:57:ALA:HB1	1:H:73:ASP:O	2.16	0.46
1:N:310:VAL:HG23	1:N:312:VAL:HG23	1.98	0.46
1:A:157:TYR:CE2	1:A:173:ARG:HD3	2.51	0.46
1:B:21:LEU:HD22	1:B:32:LEU:HB2	1.98	0.46
1:C:174:THR:HG23	1:C:174:THR:O	2.15	0.46
1:F:231:PHE:HE2	1:F:301:GLU:HG2	1.81	0.46
1:G:182:MET:CE	1:G:244:VAL:HG21	2.45	0.46
2:S:56:ASN:OD1	1:K:282:THR:OG1	2.33	0.46
1:K:155:GLU:O	1:K:159:ARG:N	2.47	0.46
1:I:158:ALA:O	1:I:159:ARG:CZ	2.63	0.46
1:B:6:LEU:HD21	1:B:40:ILE:HG23	1.97	0.46
1:C:43:TYR:OH	1:C:192:ARG:NH1	2.48	0.46
1:C:141:LYS:HG2	1:C:142:VAL:H	1.80	0.46
1:D:106:LYS:O	1:D:110:VAL:HG23	2.16	0.46
1:K:242:ARG:HH22	1:K:274:ALA:HB1	1.81	0.46
1:O:176:ARG:HG2	1:O:177:PRO:CD	2.45	0.46
1:O:228:SER:CB	1:O:232:LYS:HE3	2.46	0.46
1:C:275:TYR:CZ	1:C:279:LEU:HD12	2.51	0.46
1:E:25:ASN:ND2	1:E:27:ASN:OD1	2.45	0.46
1:F:29:ARG:HG2	1:F:29:ARG:O	2.14	0.46
1:G:206:LEU:HG	1:G:306:ILE:HD11	1.98	0.46
1:K:319:VAL:HG12	1:K:320:ALA:N	2.30	0.46
1:M:102:LEU:O	1:M:106:LYS:HB2	2.16	0.46
1:J:231:PHE:CE2	1:J:298:ILE:HA	2.51	0.46
1:O:184:ALA:O	1:O:185:LEU:HB3	2.15	0.46
1:O:184:ALA:C	1:O:186:ILE:H	2.19	0.46
1:C:192:ARG:HG3	1:C:275:TYR:CZ	2.51	0.46
1:F:189:LEU:HD11	1:F:240:ALA:HB2	1.98	0.46
2:S:55:GLU:OE1	2:S:55:GLU:N	2.46	0.46
1:L:238:ARG:HH11	1:L:239:ILE:HG22	1.80	0.46
1:M:261:VAL:HG12	1:M:262:LEU:N	2.31	0.46
1:I:21:LEU:CD1	1:I:55:TYR:CD1	2.99	0.46
1:A:120:LEU:HD22	1:A:125:ILE:HB	1.96	0.46
1:B:254:PHE:CE2	1:B:263:LEU:HD22	2.50	0.46
1:L:211:SER:N	1:L:216:PRO:HB3	2.31	0.46
1:N:241:ASN:HA	1:N:244:VAL:HG22	1.98	0.46
1:H:72:TYR:CD2	1:H:202:TYR:HB3	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:56:ASN:CG	1:M:282:THR:HG1	2.19	0.45
2:W:28:VAL:HG21	2:W:34:GLU:HG2	1.97	0.45
2:X:70:PRO:HB3	1:O:33:ALA:HB2	1.98	0.45
1:M:34:ILE:HD13	1:M:55:TYR:CZ	2.51	0.45
1:M:254:PHE:CE1	1:M:263:LEU:HD22	2.51	0.45
1:O:231:PHE:CE1	1:O:298:ILE:HA	2.51	0.45
1:B:81:THR:HG22	1:B:82:LEU:O	2.16	0.45
1:B:101:ARG:CZ	1:B:142:VAL:HG11	2.46	0.45
1:D:43:TYR:OH	1:D:299:ARG:NH2	2.50	0.45
1:D:181:GLU:HB3	1:D:254:PHE:CD1	2.52	0.45
1:H:132:HIS:CE1	1:H:151:ARG:CD	3.00	0.45
1:M:37:ILE:HG22	1:M:38:TYR:N	2.32	0.45
1:N:119:ASN:ND2	1:N:233:PRO:O	2.42	0.45
1:I:206:LEU:HG	1:I:306:ILE:HD11	1.97	0.45
1:J:296:ARG:O	1:J:299:ARG:N	2.49	0.45
1:O:146:MET:O	1:O:149:GLU:N	2.50	0.45
1:A:34:ILE:HD13	1:A:55:TYR:CE2	2.50	0.45
1:C:89:ILE:HG12	1:D:95:TYR:CD1	2.51	0.45
1:D:296:ARG:O	1:D:299:ARG:N	2.49	0.45
1:F:87:LEU:HD21	1:F:306:ILE:HG13	1.99	0.45
2:T:84:ILE:HB	1:K:7:THR:O	2.16	0.45
1:O:197:MET:HB3	1:O:224:ALA:HB1	1.98	0.45
1:O:319:VAL:O	1:O:320:ALA:HB2	2.16	0.45
1:A:54:HIS:NE2	1:B:67:ASN:OD1	2.50	0.45
1:B:241:ASN:OD1	1:B:245:LYS:HD2	2.16	0.45
1:D:146:MET:O	1:D:147:ASN:HB3	2.17	0.45
1:F:150:GLY:O	1:F:151:ARG:HB3	2.16	0.45
1:G:34:ILE:HG12	1:G:55:TYR:HE1	1.81	0.45
2:S:13:ARG:CZ	2:S:58:ASP:OD2	2.64	0.45
1:M:141:LYS:HG2	1:M:142:VAL:N	2.32	0.45
1:O:102:LEU:HD11	1:O:140:LYS:HA	1.97	0.45
1:O:123:TRP:CZ3	1:O:160:TRP:NE1	2.85	0.45
2:U:62:ILE:O	2:U:62:ILE:CG2	2.65	0.45
2:V:82:GLU:OE2	2:V:82:GLU:N	2.41	0.45
1:M:106:LYS:O	1:M:110:VAL:HG12	2.16	0.45
1:A:64:HIS:ND1	1:A:195:ALA:HB1	2.31	0.45
1:G:264:THR:O	1:G:267:GLY:N	2.49	0.45
2:T:55:GLU:OE1	2:T:55:GLU:N	2.49	0.45
2:W:82:GLU:O	2:W:83:GLU:HB3	2.16	0.45
1:L:115:ASN:OD1	1:L:320:ALA:HB2	2.17	0.45
1:O:227:LEU:HD21	1:O:305:ILE:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ARG:CZ	1:B:262:LEU:HD11	2.47	0.45
1:E:219:ARG:HB3	1:F:81:THR:CG2	2.40	0.45
2:V:14:VAL:O	2:V:17:VAL:HG22	2.16	0.45
1:K:21:LEU:HD11	1:K:34:ILE:HD12	1.99	0.45
1:M:12:GLY:HA3	1:M:25:ASN:HA	1.97	0.45
1:O:99:ASN:C	1:O:101:ARG:H	2.20	0.45
1:O:118:LYS:HG2	1:O:320:ALA:HB3	1.99	0.45
1:P:292:VAL:HG11	1:P:296:ARG:HH22	1.81	0.45
1:B:43:TYR:HB3	1:B:66:PHE:CB	2.46	0.45
1:D:256:GLU:O	1:D:257:ASP:HB2	2.16	0.45
1:E:34:ILE:HD11	1:E:55:TYR:CZ	2.51	0.45
1:H:19:ASN:O	1:H:20:THR:HG23	2.17	0.45
1:H:132:HIS:HE1	1:H:151:ARG:HD3	1.81	0.45
1:K:273:LYS:O	1:K:274:ALA:HB3	2.17	0.45
1:M:108:PHE:O	1:M:112:GLY:N	2.46	0.45
1:J:189:LEU:HD21	1:J:271:VAL:HG12	1.99	0.45
1:J:310:VAL:HG23	1:J:312:VAL:HG23	1.98	0.45
1:B:94:HIS:O	1:B:95:TYR:HB3	2.16	0.45
1:C:37:ILE:HD12	1:C:37:ILE:HA	1.82	0.45
1:C:279:LEU:HD23	1:C:279:LEU:O	2.17	0.45
1:D:125:ILE:HG21	1:D:159:ARG:O	2.16	0.45
2:Q:55:GLU:OE1	2:Q:55:GLU:N	2.48	0.45
2:W:5:VAL:HG12	2:W:62:ILE:HG12	1.99	0.45
1:K:149:GLU:O	1:K:153:ARG:HG2	2.17	0.45
1:I:34:ILE:CD1	1:I:35:GLU:OE2	2.65	0.45
1:J:26:VAL:HG23	1:J:26:VAL:O	2.17	0.45
1:O:203:ASN:OD1	1:O:299:ARG:NH1	2.44	0.45
1:P:56:ILE:HG23	1:P:61:ILE:HB	1.98	0.45
1:F:113:ALA:HB3	1:F:133:LEU:HD21	1.98	0.45
1:L:67:ASN:HB2	1:L:71:TYR:HB3	1.99	0.45
1:M:73:ASP:HA	1:N:79:ARG:HD3	1.99	0.45
1:O:102:LEU:O	1:O:106:LYS:HG3	2.17	0.45
1:D:178:PRO:O	1:D:260:GLY:HA3	2.17	0.44
1:E:282:THR:O	1:E:283:VAL:HG23	2.18	0.44
2:X:29:GLN:HG2	2:X:30:ASN:N	2.32	0.44
1:K:255:ARG:O	1:K:261:VAL:O	2.35	0.44
1:M:73:ASP:O	1:N:79:ARG:HB3	2.17	0.44
1:M:84:SER:HA	1:N:218:GLU:O	2.16	0.44
1:M:153:ARG:NH2	1:M:157:TYR:OH	2.51	0.44
1:I:231:PHE:CE2	1:I:298:ILE:HA	2.52	0.44
1:O:197:MET:HE2	1:O:227:LEU:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:43:TYR:OH	1:P:203:ASN:OD1	2.33	0.44
1:C:141:LYS:HG2	1:C:142:VAL:N	2.31	0.44
1:B:127:SER:O	1:B:129:PHE:N	2.50	0.44
1:E:197:MET:HB3	1:E:224:ALA:HB1	2.00	0.44
1:H:245:LYS:HE2	1:H:245:LYS:HA	1.99	0.44
1:M:6:LEU:HD21	1:M:37:ILE:HD13	1.98	0.44
1:N:146:MET:O	1:N:147:ASN:HB2	2.18	0.44
1:J:104:LEU:HD23	1:J:315:TYR:CD2	2.51	0.44
1:J:168:PHE:HD1	1:J:244:VAL:HG13	1.80	0.44
1:B:86:ASP:HB2	1:B:89:ILE:HG22	1.99	0.44
1:C:62:LEU:CD1	1:C:199:SER:HA	2.47	0.44
1:C:65:PHE:CE1	1:D:53:LEU:HD12	2.53	0.44
1:E:197:MET:SD	1:E:227:LEU:HD11	2.57	0.44
1:G:250:LYS:HG3	1:G:251:LYS:H	1.83	0.44
1:J:87:LEU:HD12	1:J:205:GLN:HB3	2.00	0.44
1:O:34:ILE:HD13	1:O:55:TYR:HE2	1.82	0.44
1:D:87:LEU:HD22	1:D:206:LEU:HD23	1.99	0.44
1:E:118:LYS:HG3	1:E:122:ASN:HD21	1.82	0.44
1:E:218:GLU:N	1:F:86:ASP:OD1	2.51	0.44
1:M:231:PHE:CE1	1:M:298:ILE:HA	2.53	0.44
1:I:219:ARG:HB3	1:J:81:THR:HB	1.99	0.44
1:B:254:PHE:CD2	1:B:263:LEU:HD22	2.52	0.44
1:C:86:ASP:HB2	1:D:217:SER:CB	2.48	0.44
1:D:167:GLU:OE2	1:D:251:LYS:HG3	2.18	0.44
1:G:141:LYS:HG2	1:G:142:VAL:N	2.33	0.44
1:K:193:LEU:O	1:K:197:MET:HB2	2.18	0.44
1:N:104:LEU:HD23	1:N:315:TYR:CD2	2.51	0.44
1:I:98:LYS:HZ3	1:I:141:LYS:HG3	1.82	0.44
1:I:275:TYR:CE1	1:I:279:LEU:HD12	2.52	0.44
1:J:168:PHE:HD2	1:J:181:GLU:HG2	1.83	0.44
1:J:219:ARG:O	1:J:220:ARG:HG2	2.18	0.44
1:O:34:ILE:HD13	1:O:55:TYR:CE2	2.53	0.44
1:P:203:ASN:OD1	1:P:299:ARG:NH2	2.50	0.44
1:C:56:ILE:HG23	1:C:61:ILE:HB	1.99	0.44
1:G:6:LEU:HD22	1:G:32:LEU:HD22	1.98	0.44
1:G:32:LEU:HB3	1:G:37:ILE:HD11	1.99	0.44
1:H:243:LEU:HB3	1:H:249:ILE:CD1	2.48	0.44
2:V:46:LYS:O	2:V:50:LYS:HG3	2.17	0.44
1:K:7:THR:HG22	1:K:192:ARG:HH12	1.83	0.44
1:M:112:GLY:HA2	1:M:230:ILE:HA	2.00	0.44
1:N:239:ILE:CD1	1:N:275:TYR:HA	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLU:CG	1:A:19:ASN:N	2.79	0.44
1:D:188:PHE:O	1:D:191:SER:OG	2.32	0.44
1:F:224:ALA:O	1:F:228:SER:OG	2.20	0.44
1:E:128:ASP:O	1:E:131:ASN:ND2	2.51	0.44
2:V:45:ILE:O	2:V:49:LEU:HB2	2.18	0.44
1:K:133:LEU:C	1:K:136:LEU:HD22	2.31	0.44
1:L:16:ARG:HE	1:L:51:GLN:HB3	1.82	0.44
1:M:18:GLU:O	1:M:20:THR:N	2.49	0.44
1:A:141:LYS:HD2	1:A:142:VAL:H	1.83	0.43
2:Q:14:VAL:O	2:Q:17:VAL:HG22	2.17	0.43
1:K:241:ASN:O	1:K:245:LYS:HG2	2.18	0.43
1:L:212:TYR:CD1	1:L:212:TYR:N	2.85	0.43
1:I:30:LYS:N	1:I:30:LYS:CD	2.81	0.43
1:C:89:ILE:O	1:C:93:GLU:N	2.42	0.43
1:G:172:LYS:O	1:G:173:ARG:NE	2.51	0.43
1:K:166:GLY:O	1:K:167:GLU:HB3	2.18	0.43
1:J:127:SER:O	1:J:129:PHE:HD2	2.01	0.43
1:P:303:TYR:O	1:P:307:LYS:HG2	2.17	0.43
2:Q:76:ILE:CG2	2:R:56:ASN:HA	2.48	0.43
1:K:21:LEU:HD12	1:K:34:ILE:HD12	1.98	0.43
1:L:232:LYS:CG	1:L:233:PRO:HD3	2.47	0.43
1:M:32:LEU:HD21	1:M:37:ILE:CD1	2.48	0.43
1:N:101:ARG:C	1:N:103:PHE:H	2.20	0.43
1:N:219:ARG:O	1:N:220:ARG:HG2	2.18	0.43
1:I:89:ILE:HD12	1:J:95:TYR:CD2	2.53	0.43
1:I:182:MET:SD	1:I:244:VAL:HG21	2.58	0.43
1:B:13:THR:O	1:B:24:GLU:HB2	2.19	0.43
1:E:83:LEU:CD2	1:F:221:PHE:HE1	2.31	0.43
2:X:38:THR:HG23	2:X:41:GLU:H	1.84	0.43
1:M:200:GLU:OE1	1:M:299:ARG:CZ	2.66	0.43
1:I:91:GLN:HG2	1:I:212:TYR:OH	2.19	0.43
1:H:197:MET:HG3	1:H:224:ALA:HB1	1.99	0.43
1:I:22:TYR:HB3	1:I:30:LYS:HB2	2.00	0.43
1:P:25:ASN:O	1:P:26:VAL:C	2.56	0.43
1:B:310:VAL:HG23	1:B:312:VAL:HG23	2.01	0.43
1:F:155:GLU:HG2	1:F:159:ARG:NH1	2.34	0.43
1:G:261:VAL:HG12	1:G:262:LEU:H	1.84	0.43
2:W:21:LEU:HD12	2:W:33:PHE:CD1	2.54	0.43
1:K:242:ARG:NH2	1:K:274:ALA:HB1	2.33	0.43
1:M:217:SER:O	1:M:218:GLU:CG	2.66	0.43
1:I:159:ARG:NE	1:I:159:ARG:CA	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LYS:HZ3	2:S:73:THR:CG2	2.31	0.43
1:C:216:PRO:HB2	1:D:86:ASP:OD1	2.19	0.43
1:E:19:ASN:O	1:E:20:THR:HG23	2.18	0.43
1:E:217:SER:HB3	1:E:220:ARG:HB3	2.01	0.43
1:F:300:LEU:HA	1:F:303:TYR:HB2	2.00	0.43
2:R:11:VAL:O	2:R:12:GLU:HB2	2.18	0.43
2:V:2:TYR:HD1	2:V:36:GLU:HG2	1.84	0.43
1:N:166:GLY:O	1:N:169:ARG:HG3	2.18	0.43
1:C:282:THR:HG1	1:C:292:VAL:N	2.15	0.43
1:G:172:LYS:O	1:G:173:ARG:HB3	2.18	0.43
1:K:110:VAL:O	1:K:114:LYS:HB2	2.19	0.43
1:L:242:ARG:O	1:L:246:LYS:HB2	2.19	0.43
1:I:193:LEU:O	1:I:197:MET:HG2	2.19	0.43
1:A:181:GLU:O	1:A:182:MET:HB3	2.18	0.43
1:B:56:ILE:HD12	1:B:56:ILE:H	1.83	0.43
1:C:42:ILE:HD12	1:C:65:PHE:CE1	2.54	0.43
1:F:120:LEU:HD13	1:F:127:SER:CB	2.47	0.43
1:G:43:TYR:OH	1:G:192:ARG:NE	2.52	0.43
1:G:100:LYS:O	1:G:104:LEU:HD12	2.19	0.43
1:K:63:ILE:HG23	1:K:63:ILE:O	2.19	0.43
1:L:106:LYS:HG3	1:L:145:ILE:HD12	2.00	0.43
1:I:115:ASN:OD1	1:I:234:ILE:HD11	2.19	0.43
1:I:283:VAL:HG12	1:I:292:VAL:O	2.18	0.43
1:A:186:ILE:HG23	1:A:187:SER:N	2.34	0.43
1:C:126:SER:HB3	1:C:159:ARG:HH21	1.83	0.43
1:E:293:THR:O	1:E:296:ARG:HG3	2.19	0.43
1:G:257:ASP:CG	1:G:258:LEU:H	2.22	0.43
1:I:110:VAL:O	1:I:114:LYS:HB2	2.19	0.43
1:J:304:LYS:NZ	1:J:316:SER:O	2.45	0.43
1:O:7:THR:HG22	1:O:41:TYR:HB2	2.01	0.43
1:O:8:ILE:CD1	1:O:46:VAL:HG21	2.49	0.43
1:C:108:PHE:CE2	1:C:226:ASP:HB3	2.54	0.42
1:E:32:LEU:HD21	1:E:37:ILE:CD1	2.43	0.42
2:W:2:TYR:HD1	2:W:3:ILE:N	2.17	0.42
1:K:27:ASN:OD1	1:K:27:ASN:N	2.52	0.42
1:K:186:ILE:O	1:K:190:ASN:ND2	2.49	0.42
1:J:239:ILE:HG13	1:J:240:ALA:N	2.34	0.42
1:A:92:ALA:HB1	1:B:89:ILE:HD12	2.00	0.42
1:B:174:THR:HG21	1:B:179:LYS:H	1.84	0.42
1:E:257:ASP:N	1:E:260:GLY:O	2.51	0.42
1:K:107:SER:O	1:K:108:PHE:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:THR:OG1	1:L:24:GLU:HB3	2.19	0.42
1:M:231:PHE:HE1	1:M:298:ILE:HA	1.84	0.42
1:O:128:ASP:OD1	1:O:128:ASP:O	2.37	0.42
1:C:136:LEU:HD23	1:C:148:VAL:HG11	2.00	0.42
1:D:86:ASP:HB2	1:D:89:ILE:HD12	2.02	0.42
1:D:98:LYS:NZ	1:D:141:LYS:HZ1	2.17	0.42
1:E:11:ASP:CG	1:E:45:HIS:H	2.22	0.42
1:E:182:MET:HE1	1:E:240:ALA:HB1	2.01	0.42
1:G:64:HIS:CD2	1:G:75:THR:HG23	2.54	0.42
1:G:212:TYR:O	1:G:213:LEU:HB3	2.19	0.42
1:L:261:VAL:HG12	1:L:262:LEU:N	2.33	0.42
1:M:8:ILE:HD11	1:M:42:ILE:CD1	2.49	0.42
1:M:141:LYS:HG2	1:M:142:VAL:H	1.84	0.42
1:I:16:ARG:O	1:I:17:ARG:O	2.37	0.42
1:O:228:SER:OG	1:O:232:LYS:HE3	2.19	0.42
1:P:182:MET:HE1	1:P:244:VAL:HG21	2.01	0.42
1:A:257:ASP:OD1	1:A:260:GLY:N	2.51	0.42
1:C:87:LEU:CD2	1:C:309:LEU:HD13	2.49	0.42
1:D:130:SER:O	1:D:133:LEU:N	2.52	0.42
1:H:258:LEU:HD23	1:H:258:LEU:O	2.19	0.42
1:I:43:TYR:OH	1:I:192:ARG:HD2	2.19	0.42
1:I:115:ASN:O	1:I:119:ASN:N	2.45	0.42
1:O:160:TRP:O	1:O:160:TRP:CD1	2.72	0.42
1:O:164:LEU:HD23	1:O:244:VAL:HG11	2.02	0.42
1:P:161:ASP:OD2	1:P:170:ILE:O	2.36	0.42
1:B:9:PHE:HE1	1:B:43:TYR:HH	1.66	0.42
1:B:189:LEU:HD22	1:B:239:ILE:HD11	2.01	0.42
1:C:101:ARG:HH21	1:C:142:VAL:HG11	1.84	0.42
1:E:282:THR:CG2	2:U:76:ILE:HG21	2.50	0.42
1:F:239:ILE:HG13	1:F:240:ALA:N	2.35	0.42
1:G:161:ASP:CG	1:G:170:ILE:O	2.58	0.42
2:U:30:ASN:O	2:U:31:SER:OG	2.30	0.42
1:L:189:LEU:CD2	1:L:239:ILE:HD11	2.35	0.42
1:M:32:LEU:HD23	1:M:33:ALA:N	2.33	0.42
1:M:77:TYR:N	1:N:75:THR:O	2.43	0.42
1:M:294:ARG:O	1:M:297:LEU:HB3	2.19	0.42
1:I:8:ILE:O	1:I:8:ILE:HG13	2.18	0.42
1:O:6:LEU:HD12	1:O:32:LEU:HD11	2.01	0.42
1:O:8:ILE:O	1:O:8:ILE:HG13	2.20	0.42
1:O:55:TYR:CD2	1:O:55:TYR:C	2.93	0.42
1:B:48:ILE:HG22	1:B:49:THR:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:CD	1:C:219:ARG:N	2.83	0.42
1:C:219:ARG:NH2	1:D:82:LEU:HD11	2.35	0.42
1:E:193:LEU:HD11	1:E:197:MET:HE1	2.00	0.42
1:E:200:GLU:OE2	1:E:295:ARG:NH1	2.52	0.42
1:F:140:LYS:HD3	1:F:141:LYS:NZ	2.35	0.42
1:G:102:LEU:O	1:G:106:LYS:HB2	2.20	0.42
1:H:239:ILE:CD1	1:H:240:ALA:N	2.75	0.42
1:K:65:PHE:CZ	1:L:53:LEU:HD23	2.54	0.42
1:M:197:MET:HB3	1:M:224:ALA:HB1	2.01	0.42
1:N:141:LYS:HG2	1:N:142:VAL:N	2.32	0.42
1:I:188:PHE:CD2	1:I:263:LEU:HD12	2.54	0.42
1:I:249:ILE:HG21	1:I:254:PHE:CE2	2.55	0.42
1:A:176:ARG:HA	1:A:177:PRO:HA	1.92	0.42
1:A:178:PRO:HD2	1:A:261:VAL:CG2	2.47	0.42
1:B:95:TYR:HD2	1:B:101:ARG:HD2	1.85	0.42
1:B:186:ILE:HG13	1:B:187:SER:N	2.35	0.42
1:C:69:TYR:CD2	1:C:262:LEU:CD2	3.02	0.42
1:C:240:ALA:HA	1:C:243:LEU:HB3	2.00	0.42
1:D:70:GLY:O	1:D:199:SER:OG	2.29	0.42
1:D:214:HIS:N	1:D:226:ASP:OD1	2.49	0.42
1:E:86:ASP:O	1:E:90:LYS:HG2	2.19	0.42
1:G:200:GLU:OE1	1:G:299:ARG:NE	2.50	0.42
1:L:231:PHE:HE1	1:L:318:LEU:HD22	1.83	0.42
1:N:215:GLU:O	1:N:217:SER:N	2.52	0.42
1:I:21:LEU:HD11	1:I:55:TYR:HD1	1.84	0.42
1:I:159:ARG:HE	1:I:159:ARG:N	2.17	0.42
1:O:6:LEU:HD11	1:O:32:LEU:HD11	2.02	0.42
1:C:283:VAL:HG22	1:C:293:THR:OG1	2.19	0.42
1:E:296:ARG:NH2	1:E:300:LEU:HD21	2.35	0.42
1:F:140:LYS:HB3	1:F:140:LYS:HE3	1.86	0.42
2:U:29:GLN:HG2	2:U:30:ASN:N	2.35	0.42
1:K:104:LEU:HD11	1:K:308:HIS:CD2	2.54	0.42
1:M:73:ASP:OD2	1:N:54:HIS:CE1	2.72	0.42
1:M:142:VAL:O	1:M:145:ILE:HG22	2.20	0.42
1:N:235:ILE:O	1:N:239:ILE:HG22	2.19	0.42
1:I:186:ILE:O	1:I:190:ASN:ND2	2.47	0.42
1:I:254:PHE:CE2	1:I:263:LEU:CD2	3.03	0.42
1:O:6:LEU:CD2	1:O:7:THR:N	2.76	0.42
1:A:15:LEU:HD12	1:A:17:ARG:H	1.85	0.42
1:A:281:LYS:O	1:A:282:THR:HB	2.19	0.42
1:D:25:ASN:C	1:D:27:ASN:H	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:MET:HE3	1:E:228:SER:HA	2.02	0.42
1:G:72:TYR:HB2	1:G:191:SER:HB3	2.02	0.42
2:S:20:PHE:HE2	2:S:49:LEU:N	2.18	0.42
1:L:242:ARG:HD3	1:L:242:ARG:C	2.39	0.42
1:N:56:ILE:HG23	1:N:61:ILE:HB	2.00	0.42
1:N:56:ILE:HG21	1:N:63:ILE:HD11	2.01	0.42
1:I:67:ASN:N	1:I:71:TYR:O	2.51	0.42
1:I:174:THR:O	1:I:175:ARG:C	2.57	0.42
1:J:277:GLN:O	1:J:280:GLU:HG3	2.19	0.42
1:O:7:THR:HG21	1:O:192:ARG:NH1	2.35	0.42
1:O:228:SER:O	1:O:232:LYS:HD3	2.19	0.42
1:P:292:VAL:CG1	1:P:296:ARG:NH2	2.82	0.42
1:A:6:LEU:HD13	1:A:37:ILE:HG21	2.02	0.42
1:E:8:ILE:O	1:E:8:ILE:HG13	2.20	0.42
1:G:4:LYS:H	1:G:4:LYS:HG2	1.71	0.42
1:G:41:TYR:HD2	1:G:192:ARG:HH22	1.68	0.42
1:G:41:TYR:HE1	1:G:64:HIS:HD1	1.67	0.42
2:V:7:TYR:CD1	2:V:9:VAL:HG23	2.55	0.42
2:W:48:GLY:O	2:W:52:ILE:HG13	2.19	0.42
1:K:306:ILE:N	1:K:306:ILE:HD12	2.35	0.42
1:L:141:LYS:HZ2	1:L:142:VAL:HG12	1.85	0.42
1:M:65:PHE:CZ	1:N:53:LEU:HD23	2.55	0.42
1:I:318:LEU:O	1:I:318:LEU:HD12	2.20	0.42
1:J:81:THR:O	1:J:82:LEU:C	2.58	0.42
1:A:18:GLU:HG2	1:A:19:ASN:H	1.84	0.41
1:A:108:PHE:CE2	1:A:226:ASP:HB3	2.54	0.41
1:C:29:ARG:O	1:C:31:PRO:HD2	2.20	0.41
1:E:8:ILE:HG22	2:U:84:ILE:HG23	2.02	0.41
1:E:182:MET:CE	1:E:240:ALA:HB1	2.50	0.41
1:F:174:THR:HG21	1:F:179:LYS:HB2	2.00	0.41
1:G:73:ASP:OD2	1:H:54:HIS:HB2	2.20	0.41
2:U:39:LEU:O	2:U:42:PHE:N	2.52	0.41
1:K:64:HIS:CE1	1:K:75:THR:HG23	2.55	0.41
1:E:172:LYS:HD2	1:E:172:LYS:C	2.41	0.41
1:F:235:ILE:HG21	1:F:279:LEU:HD21	2.02	0.41
2:W:2:TYR:CD2	2:W:68:MET:HA	2.54	0.41
1:M:55:TYR:HE2	1:M:59:LYS:CG	2.32	0.41
1:M:231:PHE:HD2	1:M:234:ILE:HD12	1.85	0.41
1:A:94:HIS:O	1:A:101:ARG:HB2	2.20	0.41
1:B:53:LEU:HD11	1:B:76:PHE:CD2	2.55	0.41
1:B:141:LYS:HG2	1:B:142:VAL:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HB2	1:B:233:PRO:HD3	2.02	0.41
1:C:293:THR:O	1:C:297:LEU:HG	2.21	0.41
1:E:37:ILE:H	1:E:37:ILE:HD12	1.85	0.41
1:G:75:THR:O	1:H:77:TYR:N	2.48	0.41
1:H:168:PHE:CD1	1:H:244:VAL:HG23	2.56	0.41
2:V:4:VAL:O	2:V:4:VAL:HG23	2.20	0.41
2:W:2:TYR:HE1	2:W:34:GLU:HB2	1.85	0.41
1:K:151:ARG:O	1:K:155:GLU:HB2	2.19	0.41
1:L:48:ILE:HG21	1:L:53:LEU:HD22	2.02	0.41
1:P:209:THR:HG23	1:P:210:ILE:HD12	2.02	0.41
1:A:75:THR:O	1:B:77:TYR:N	2.53	0.41
1:E:104:LEU:HD23	1:E:315:TYR:HD2	1.84	0.41
1:E:174:THR:HG22	1:E:183:ASN:CB	2.50	0.41
1:H:56:ILE:HG23	1:H:61:ILE:HB	2.03	0.41
2:S:27:TRP:HD1	2:S:33:PHE:CZ	2.39	0.41
1:K:62:LEU:HD21	1:K:199:SER:HA	2.02	0.41
1:K:175:ARG:CZ	1:K:175:ARG:HB2	2.50	0.41
1:L:146:MET:O	1:L:150:GLY:N	2.50	0.41
1:O:104:LEU:HD23	1:O:104:LEU:HA	1.89	0.41
1:A:41:TYR:CD1	1:A:64:HIS:HB2	2.55	0.41
1:A:72:TYR:O	1:B:79:ARG:HD2	2.20	0.41
1:C:123:TRP:NE1	1:C:241:ASN:OD1	2.53	0.41
1:D:51:GLN:O	1:D:54:HIS:CD2	2.74	0.41
1:G:239:ILE:HD13	1:G:275:TYR:HD2	1.86	0.41
2:T:11:VAL:HG12	2:T:12:GLU:N	2.35	0.41
1:N:98:LYS:O	1:N:101:ARG:O	2.39	0.41
1:O:218:GLU:OE2	1:P:205:GLN:HG3	2.19	0.41
1:A:141:LYS:HG3	1:A:143:THR:H	1.86	0.41
1:C:182:MET:HG3	1:C:182:MET:O	2.21	0.41
1:C:236:ALA:O	1:C:239:ILE:O	2.38	0.41
1:G:139:ALA:HB1	1:G:145:ILE:HG13	2.01	0.41
1:H:119:ASN:ND2	1:H:233:PRO:O	2.40	0.41
1:H:223:LEU:HD23	1:H:227:LEU:HD13	2.02	0.41
2:U:3:ILE:HD12	2:U:62:ILE:HD11	2.02	0.41
1:I:317:PRO:HB2	1:I:319:VAL:HG23	2.02	0.41
1:A:180:ASN:OD1	1:A:183:ASN:HB2	2.20	0.41
1:B:168:PHE:CD1	1:B:244:VAL:HG13	2.56	0.41
1:B:231:PHE:CD2	1:B:298:ILE:HD13	2.56	0.41
1:C:265:ASP:O	1:C:269:LYS:HD3	2.21	0.41
1:D:82:LEU:HB2	1:G:172:LYS:HE2	2.01	0.41
1:E:129:PHE:CE1	1:E:155:GLU:OE2	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:5:VAL:HG21	2:W:21:LEU:HD13	2.02	0.41
1:L:197:MET:CE	1:L:228:SER:HA	2.51	0.41
1:M:99:ASN:C	1:M:100:LYS:HG3	2.41	0.41
1:I:306:ILE:N	1:I:306:ILE:HD12	2.35	0.41
1:O:194:TYR:HE1	1:O:224:ALA:HB3	1.84	0.41
1:P:67:ASN:CG	1:P:68:HIS:N	2.73	0.41
1:P:237:ASP:O	1:P:241:ASN:N	2.53	0.41
1:A:34:ILE:O	1:A:37:ILE:HG12	2.20	0.41
1:C:8:ILE:HG13	1:C:8:ILE:O	2.21	0.41
1:E:181:GLU:O	1:E:182:MET:HB3	2.20	0.41
1:K:104:LEU:HD11	1:K:308:HIS:HD2	1.84	0.41
1:L:115:ASN:OD1	1:L:234:ILE:HD11	2.21	0.41
1:L:127:SER:O	1:L:128:ASP:OD1	2.37	0.41
1:L:303:TYR:C	1:L:305:ILE:H	2.23	0.41
1:M:151:ARG:O	1:M:155:GLU:HB2	2.21	0.41
1:A:57:ALA:HB1	1:B:73:ASP:O	2.21	0.41
1:B:21:LEU:HD23	1:B:22:TYR:N	2.35	0.41
1:B:66:PHE:CD1	1:B:72:TYR:HA	2.56	0.41
1:B:120:LEU:HD22	1:B:125:ILE:HB	2.03	0.41
1:C:176:ARG:HA	1:C:177:PRO:HA	1.90	0.41
1:E:129:PHE:CZ	1:E:155:GLU:OE2	2.74	0.41
1:E:136:LEU:HD22	1:E:144:GLU:CD	2.42	0.41
1:F:34:ILE:HD12	1:F:59:LYS:HD3	2.03	0.41
1:F:108:PHE:HD1	1:F:230:ILE:HD11	1.85	0.41
1:F:119:ASN:OD1	1:F:238:ARG:NH2	2.54	0.41
1:F:150:GLY:O	1:F:151:ARG:CB	2.68	0.41
1:G:249:ILE:HD12	1:G:254:PHE:CE2	2.56	0.41
1:H:53:LEU:HD11	1:H:76:PHE:CD1	2.56	0.41
2:Q:4:VAL:O	2:Q:4:VAL:HG23	2.20	0.41
2:W:38:THR:HG23	2:W:41:GLU:H	1.86	0.41
1:K:296:ARG:HG2	1:K:300:LEU:HG	2.02	0.41
1:L:102:LEU:O	1:L:105:ALA:O	2.39	0.41
1:M:99:ASN:C	1:M:101:ARG:H	2.23	0.41
1:N:123:TRP:N	1:N:123:TRP:CD1	2.89	0.41
1:N:128:ASP:O	1:N:128:ASP:OD2	2.38	0.41
1:J:43:TYR:OH	1:J:299:ARG:NH2	2.53	0.41
1:O:62:LEU:CD1	1:O:199:SER:HA	2.51	0.41
1:B:228:SER:O	1:B:232:LYS:HG3	2.21	0.41
1:C:73:ASP:OD2	1:D:54:HIS:HB2	2.21	0.41
1:F:255:ARG:CG	1:F:264:THR:HG22	2.51	0.41
1:F:303:TYR:HA	1:F:306:ILE:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ASN:C	1:G:101:ARG:H	2.24	0.41
1:G:109:VAL:HG21	1:G:145:ILE:CG2	2.51	0.41
1:M:117:GLU:HG3	1:M:127:SER:HB2	2.02	0.41
1:I:21:LEU:HB3	1:I:32:LEU:HD22	2.02	0.41
1:I:65:PHE:CZ	1:J:53:LEU:HD23	2.57	0.41
1:I:188:PHE:C	1:I:188:PHE:CD1	2.93	0.41
1:O:62:LEU:HD23	1:O:78:PRO:CD	2.50	0.41
1:A:165:PRO:HG2	1:A:168:PHE:HD2	1.86	0.40
1:A:166:GLY:O	1:A:169:ARG:HG2	2.20	0.40
1:D:146:MET:C	1:D:148:VAL:H	2.24	0.40
1:D:310:VAL:HG23	1:D:312:VAL:HG23	2.03	0.40
1:E:62:LEU:HD23	1:E:78:PRO:CD	2.51	0.40
1:E:102:LEU:CD2	1:E:145:ILE:HD11	2.51	0.40
1:F:199:SER:O	1:F:203:ASN:N	2.54	0.40
1:G:282:THR:OG1	2:X:56:ASN:OD1	2.33	0.40
2:T:30:ASN:O	2:T:31:SER:OG	2.28	0.40
1:L:296:ARG:O	1:L:299:ARG:N	2.54	0.40
1:M:110:VAL:O	1:M:114:LYS:HB2	2.21	0.40
1:M:182:MET:CE	1:M:244:VAL:HG21	2.51	0.40
1:B:168:PHE:HB3	1:B:182:MET:HB2	2.04	0.40
1:D:115:ASN:ND2	1:D:318:LEU:O	2.52	0.40
1:D:181:GLU:HB3	1:D:254:PHE:CE1	2.56	0.40
1:E:65:PHE:CZ	1:F:53:LEU:HD23	2.57	0.40
2:Q:2:TYR:CD2	2:Q:68:MET:HA	2.57	0.40
2:R:4:VAL:O	2:R:4:VAL:HG23	2.21	0.40
2:V:83:GLU:HG2	2:V:84:ILE:HG23	2.03	0.40
2:W:28:VAL:HG12	2:X:61:ILE:CD1	2.51	0.40
1:K:64:HIS:ND1	1:K:75:THR:HG23	2.36	0.40
1:L:209:THR:HG23	1:L:210:ILE:HD12	2.02	0.40
1:I:43:TYR:OH	1:I:188:PHE:HE1	2.04	0.40
1:O:108:PHE:CD2	1:O:226:ASP:OD2	2.74	0.40
1:A:34:ILE:HD13	1:A:55:TYR:HE2	1.87	0.40
1:A:157:TYR:O	1:A:170:ILE:HD11	2.21	0.40
1:A:174:THR:CG2	1:A:178:PRO:HA	2.51	0.40
1:B:25:ASN:OD1	1:B:26:VAL:N	2.54	0.40
1:E:85:GLY:HA3	1:F:216:PRO:HB2	2.03	0.40
1:F:140:LYS:HD2	1:F:141:LYS:HD3	2.03	0.40
1:M:313:GLU:O	1:M:313:GLU:HG2	2.22	0.40
1:J:214:HIS:N	1:J:226:ASP:OD1	2.52	0.40
1:J:219:ARG:O	1:J:220:ARG:CG	2.69	0.40
1:O:83:LEU:HD21	1:P:221:PHE:CE1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:281:LYS:HG2	1:O:282:THR:H	1.86	0.40
1:C:29:ARG:O	1:C:31:PRO:HD3	2.21	0.40
1:D:125:ILE:HD11	1:D:163:SER:HB2	2.02	0.40
1:E:26:VAL:O	1:E:26:VAL:HG23	2.21	0.40
1:E:31:PRO:CB	2:U:68:MET:HB2	2.51	0.40
1:F:219:ARG:CG	1:F:219:ARG:O	2.69	0.40
1:G:239:ILE:CD1	1:G:275:TYR:HD2	2.34	0.40
1:M:307:LYS:O	1:M:312:VAL:N	2.48	0.40
1:O:83:LEU:HD21	1:P:221:PHE:HE1	1.86	0.40
1:O:114:LYS:HE2	1:O:319:VAL:HG22	2.03	0.40
1:P:182:MET:CE	1:P:244:VAL:HG21	2.51	0.40
1:C:29:ARG:HG2	1:C:29:ARG:O	2.22	0.40
1:D:193:LEU:O	1:D:197:MET:HG2	2.21	0.40
1:D:303:TYR:O	1:D:306:ILE:N	2.54	0.40
1:E:100:LYS:HA	1:E:103:PHE:HB3	2.03	0.40
1:F:140:LYS:CD	1:F:141:LYS:NZ	2.85	0.40
2:S:7:TYR:CD1	2:S:9:VAL:HG23	2.57	0.40
2:U:11:VAL:HG12	2:U:12:GLU:N	2.36	0.40
2:U:17:VAL:HG11	2:U:53:ILE:HG12	2.04	0.40
1:K:71:TYR:CE1	1:K:178:PRO:HG3	2.57	0.40
1:M:25:ASN:OD1	1:M:27:ASN:O	2.39	0.40
1:N:123:TRP:CH2	1:N:241:ASN:HB2	2.57	0.40
1:I:69:TYR:CD1	1:I:69:TYR:N	2.88	0.40
1:I:154:GLN:O	1:I:157:TYR:O	2.39	0.40
1:I:197:MET:O	1:I:201:ILE:HG12	2.21	0.40
1:I:275:TYR:O	1:I:279:LEU:N	2.53	0.40
1:I:279:LEU:HD22	1:I:295:ARG:HB3	2.02	0.40
1:O:29:ARG:HD3	1:O:29:ARG:N	2.36	0.40
1:P:185:LEU:O	1:P:189:LEU:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:252:ASP:O	1:J:219:ARG:NH1[1_455]	1.86	0.34
1:B:187:SER:OG	1:F:259:ASN:ND2[1_655]	2.06	0.14
1:D:259:ASN:HD21	1:H:187:SER:O[1_455]	1.57	0.03
1:L:259:ASN:HD21	1:P:187:SER:O[1_455]	1.58	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/322 (95%)	285 (93%)	21 (7%)	1 (0%)	41	75
1	B	302/322 (94%)	275 (91%)	25 (8%)	2 (1%)	22	60
1	C	308/322 (96%)	278 (90%)	26 (8%)	4 (1%)	12	48
1	D	302/322 (94%)	274 (91%)	21 (7%)	7 (2%)	6	38
1	E	308/322 (96%)	288 (94%)	19 (6%)	1 (0%)	41	75
1	F	302/322 (94%)	273 (90%)	28 (9%)	1 (0%)	41	75
1	G	308/322 (96%)	279 (91%)	27 (9%)	2 (1%)	25	63
1	H	300/322 (93%)	287 (96%)	12 (4%)	1 (0%)	41	75
1	I	308/322 (96%)	282 (92%)	21 (7%)	5 (2%)	9	44
1	J	301/322 (94%)	279 (93%)	22 (7%)	0	100	100
1	K	306/322 (95%)	279 (91%)	26 (8%)	1 (0%)	41	75
1	L	302/322 (94%)	267 (88%)	32 (11%)	3 (1%)	15	52
1	M	310/322 (96%)	275 (89%)	34 (11%)	1 (0%)	41	75
1	N	297/322 (92%)	273 (92%)	24 (8%)	0	100	100
1	O	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	41	75
1	P	300/322 (93%)	283 (94%)	16 (5%)	1 (0%)	41	75
2	Q	82/85 (96%)	76 (93%)	6 (7%)	0	100	100
2	R	82/85 (96%)	74 (90%)	8 (10%)	0	100	100
2	S	82/85 (96%)	75 (92%)	7 (8%)	0	100	100
2	T	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
2	U	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
2	V	82/85 (96%)	76 (93%)	6 (7%)	0	100	100
2	W	82/85 (96%)	71 (87%)	11 (13%)	0	100	100
2	X	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
All	All	5524/5832 (95%)	5066 (92%)	427 (8%)	31 (1%)	25	63

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	B	128	ASP
1	D	25	ASN
1	D	26	VAL
1	D	257	ASP
1	G	18	GLU
1	G	173	ARG
1	H	129	PHE
1	K	262	LEU
1	L	25	ASN
1	L	26	VAL
1	M	18	GLU
1	I	18	GLU
1	I	319	VAL
1	C	321	TRP
1	D	27	ASN
1	D	128	ASP
1	F	180	ASN
1	I	17	ARG
1	P	294	ARG
1	C	29	ARG
1	D	24	GLU
1	E	31	PRO
1	L	24	GLU
1	I	32	LEU
1	C	320	ALA
1	D	19	ASN
1	I	31	PRO
1	B	85	GLY
1	C	30	LYS
1	O	177	PRO

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	275/284 (97%)	267 (97%)	8 (3%)	42	65
1	B	272/284 (96%)	259 (95%)	13 (5%)	25	54
1	C	276/284 (97%)	257 (93%)	19 (7%)	15	45
1	D	272/284 (96%)	257 (94%)	15 (6%)	21	51
1	E	276/284 (97%)	268 (97%)	8 (3%)	42	65
1	F	272/284 (96%)	261 (96%)	11 (4%)	31	58
1	G	276/284 (97%)	264 (96%)	12 (4%)	29	57
1	H	270/284 (95%)	262 (97%)	8 (3%)	41	64
1	I	276/284 (97%)	265 (96%)	11 (4%)	31	58
1	J	271/284 (95%)	261 (96%)	10 (4%)	34	60
1	K	274/284 (96%)	259 (94%)	15 (6%)	21	51
1	L	272/284 (96%)	265 (97%)	7 (3%)	46	68
1	M	278/284 (98%)	266 (96%)	12 (4%)	29	57
1	N	269/284 (95%)	264 (98%)	5 (2%)	57	75
1	O	275/284 (97%)	269 (98%)	6 (2%)	52	71
1	P	270/284 (95%)	260 (96%)	10 (4%)	34	60
2	Q	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	R	79/80 (99%)	79 (100%)	0	100	100
2	S	79/80 (99%)	76 (96%)	3 (4%)	33	59
2	T	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	U	79/80 (99%)	76 (96%)	3 (4%)	33	59
2	V	79/80 (99%)	76 (96%)	3 (4%)	33	59
2	W	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	X	79/80 (99%)	78 (99%)	1 (1%)	69	82
All	All	5006/5184 (97%)	4823 (96%)	183 (4%)	34	60

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

Mol	Chain	Res	Type
1	A	4	LYS
1	A	25	ASN
1	A	79	ARG
1	A	155	GLU
1	A	173	ARG
1	A	192	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	MET
1	A	202	TYR
1	B	18	GLU
1	B	24	GLU
1	B	39	ASP
1	B	43	TYR
1	B	71	TYR
1	B	82	LEU
1	B	155	GLU
1	B	173	ARG
1	B	183	ASN
1	B	202	TYR
1	B	280	GLU
1	B	294	ARG
1	B	322	PHE
1	C	4	LYS
1	C	9	PHE
1	C	17	ARG
1	C	29	ARG
1	C	39	ASP
1	C	51	GLN
1	C	67	ASN
1	C	69	TYR
1	C	71	TYR
1	C	83	LEU
1	C	126	SER
1	C	146	MET
1	C	183	ASN
1	C	202	TYR
1	C	219	ARG
1	C	242	ARG
1	C	265	ASP
1	C	276	ASN
1	C	296	ARG
1	D	17	ARG
1	D	30	LYS
1	D	51	GLN
1	D	86	ASP
1	D	95	TYR
1	D	96	LEU
1	D	144	GLU
1	D	161	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	172	LYS
1	D	202	TYR
1	D	220	ARG
1	D	253	HIS
1	D	265	ASP
1	D	280	GLU
1	D	322	PHE
1	E	29	ARG
1	E	30	LYS
1	E	83	LEU
1	E	137	GLN
1	E	161	ASP
1	E	172	LYS
1	E	226	ASP
1	E	296	ARG
1	F	16	ARG
1	F	39	ASP
1	F	69	TYR
1	F	71	TYR
1	F	164	LEU
1	F	173	ARG
1	F	202	TYR
1	F	203	ASN
1	F	229	GLU
1	F	237	ASP
1	F	251	LYS
1	G	71	TYR
1	G	100	LYS
1	G	103	PHE
1	G	121	LYS
1	G	131	ASN
1	G	176	ARG
1	G	197	MET
1	G	246	LYS
1	G	255	ARG
1	G	299	ARG
1	G	321	TRP
1	G	322	PHE
1	H	11	ASP
1	H	72	TYR
1	H	149	GLU
1	H	172	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	202	TYR
1	H	238	ARG
1	H	252	ASP
1	H	277	GLN
2	Q	22	ARG
2	S	13	ARG
2	S	19	LYS
2	S	71	ARG
2	T	1	MET
2	U	2	TYR
2	U	13	ARG
2	U	66	ARG
2	V	41	GLU
2	V	44	ARG
2	V	66	ARG
2	W	2	TYR
2	X	66	ARG
1	K	51	GLN
1	K	55	TYR
1	K	118	LYS
1	K	129	PHE
1	K	131	ASN
1	K	136	LEU
1	K	160	TRP
1	K	173	ARG
1	K	182	MET
1	K	183	ASN
1	K	192	ARG
1	K	197	MET
1	K	220	ARG
1	K	263	LEU
1	K	294	ARG
1	L	23	PHE
1	L	25	ASN
1	L	55	TYR
1	L	58	GLN
1	L	71	TYR
1	L	242	ARG
1	L	265	ASP
1	M	11	ASP
1	M	30	LYS
1	M	38	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	55	TYR
1	M	64	HIS
1	M	71	TYR
1	M	83	LEU
1	M	102	LEU
1	M	116	MET
1	M	179	LYS
1	M	296	ARG
1	M	321	TRP
1	N	9	PHE
1	N	11	ASP
1	N	30	LYS
1	N	202	TYR
1	N	220	ARG
1	I	30	LYS
1	I	35	GLU
1	I	103	PHE
1	I	159	ARG
1	I	173	ARG
1	I	188	PHE
1	I	192	ARG
1	I	202	TYR
1	I	203	ASN
1	I	242	ARG
1	I	294	ARG
1	J	9	PHE
1	J	19	ASN
1	J	69	TYR
1	J	168	PHE
1	J	181	GLU
1	J	202	TYR
1	J	238	ARG
1	J	265	ASP
1	J	269	LYS
1	J	280	GLU
1	O	55	TYR
1	O	71	TYR
1	O	119	ASN
1	O	146	MET
1	O	251	LYS
1	O	278	GLU
1	P	71	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	79	ARG
1	P	100	LYS
1	P	173	ARG
1	P	192	ARG
1	P	202	TYR
1	P	203	ASN
1	P	250	LYS
1	P	296	ARG
1	P	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	HIS
1	B	253	HIS
1	B	308	HIS
1	C	190	ASN
1	C	214	HIS
1	D	54	HIS
1	D	308	HIS
1	E	68	HIS
1	E	122	ASN
1	E	132	HIS
1	G	214	HIS
1	H	132	HIS
2	Q	24	HIS
1	K	68	HIS
1	K	308	HIS
1	L	94	HIS
1	L	308	HIS
1	M	115	ASN
1	M	203	ASN
1	M	214	HIS
1	N	308	HIS
1	I	91	GLN
1	I	132	HIS
1	I	308	HIS
1	J	308	HIS
1	O	45	HIS
1	O	276	ASN
1	P	308	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/322 (96%)	0.16	12 (3%) 39 30	15, 49, 99, 125	0
1	B	308/322 (95%)	-0.09	2 (0%) 89 84	16, 43, 75, 116	0
1	C	312/322 (96%)	0.08	10 (3%) 47 37	10, 45, 94, 114	0
1	D	308/322 (95%)	-0.17	0 100 100	15, 38, 73, 105	0
1	E	312/322 (96%)	0.06	8 (2%) 56 45	11, 47, 87, 126	0
1	F	308/322 (95%)	0.12	10 (3%) 47 37	16, 60, 95, 109	0
1	G	312/322 (96%)	0.01	5 (1%) 72 62	8, 41, 88, 122	0
1	H	306/322 (95%)	0.07	9 (2%) 51 40	13, 54, 93, 106	0
1	I	312/322 (96%)	0.06	5 (1%) 72 62	12, 47, 81, 100	0
1	J	307/322 (95%)	0.11	6 (1%) 65 55	21, 58, 87, 107	0
1	K	310/322 (96%)	0.01	4 (1%) 77 68	11, 41, 79, 112	0
1	L	308/322 (95%)	0.11	4 (1%) 77 68	14, 52, 85, 103	0
1	M	314/322 (97%)	0.10	12 (3%) 40 31	13, 53, 91, 132	0
1	N	305/322 (94%)	0.35	12 (3%) 39 30	30, 70, 102, 117	0
1	O	311/322 (96%)	0.07	11 (3%) 44 34	9, 46, 89, 116	0
1	P	306/322 (95%)	0.26	14 (4%) 32 26	22, 67, 96, 120	0
2	Q	84/85 (98%)	0.15	2 (2%) 59 48	17, 49, 83, 88	0
2	R	84/85 (98%)	0.12	3 (3%) 42 33	12, 44, 71, 103	0
2	S	84/85 (98%)	0.06	2 (2%) 59 48	11, 44, 77, 102	0
2	T	84/85 (98%)	0.03	0 100 100	9, 40, 68, 94	0
2	U	84/85 (98%)	0.06	2 (2%) 59 48	15, 45, 92, 103	0
2	V	84/85 (98%)	-0.04	0 100 100	14, 47, 71, 81	0
2	W	84/85 (98%)	-0.03	2 (2%) 59 48	15, 40, 78, 102	0
2	X	84/85 (98%)	-0.01	1 (1%) 79 70	11, 42, 67, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5622/5832 (96%)	0.08	136 (2%)	59	48	8, 50, 91, 132	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	LEU	4.5
1	P	311	GLY	4.5
1	N	68	HIS	4.0
1	H	68	HIS	3.8
1	O	143	THR	3.8
1	E	218	GLU	3.7
1	G	217	SER	3.6
1	N	83	LEU	3.6
1	P	158	ALA	3.6
1	N	283	VAL	3.6
1	N	69	TYR	3.6
1	P	159	ARG	3.6
1	P	162	GLU	3.6
1	M	217	SER	3.5
1	G	218	GLU	3.5
1	M	127	SER	3.4
1	E	217	SER	3.3
1	G	140	LYS	3.3
1	N	314	GLU	3.2
1	M	286	PRO	3.2
1	A	311	GLY	3.2
1	A	217	SER	3.2
1	P	128	ASP	3.2
1	N	282	THR	3.1
2	U	52	ILE	3.1
1	M	285	HIS	3.0
1	O	147	ASN	3.0
1	C	126	SER	2.9
1	F	166	GLY	2.8
2	Q	10	GLY	2.8
1	N	82	LEU	2.8
1	H	134	LYS	2.8
2	S	56	ASN	2.7
1	F	282	THR	2.7
1	H	166	GLY	2.7
1	O	166	GLY	2.7
2	R	54	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	314	GLU	2.7
1	C	259	ASN	2.7
1	C	166	GLY	2.7
1	F	148	VAL	2.6
1	O	35	GLU	2.6
1	H	311	GLY	2.6
1	O	124	GLY	2.6
1	N	265	ASP	2.6
2	S	12	GLU	2.6
1	O	255	ARG	2.6
1	P	246	LYS	2.6
1	N	312	VAL	2.6
1	A	97	ASP	2.5
1	I	127	SER	2.5
1	P	144	GLU	2.5
2	W	12	GLU	2.5
1	C	217	SER	2.5
1	J	68	HIS	2.5
1	C	218	GLU	2.5
1	P	321	TRP	2.5
1	C	257	ASP	2.5
1	I	128	ASP	2.5
1	P	174	THR	2.5
1	M	128	ASP	2.5
1	N	124	GLY	2.5
1	H	136	LEU	2.5
1	H	312	VAL	2.5
1	G	127	SER	2.5
1	M	33	ALA	2.4
1	M	255	ARG	2.4
1	M	136	LEU	2.4
1	A	218	GLU	2.4
1	A	259	ASN	2.4
1	M	126	SER	2.4
1	N	242	ARG	2.4
1	P	247	GLY	2.4
1	M	140	LYS	2.4
2	U	53	ILE	2.3
2	X	12	GLU	2.3
1	A	117	GLU	2.3
1	J	173	ARG	2.3
1	C	256	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	12	GLU	2.3
1	N	255	ARG	2.3
1	A	245	LYS	2.3
1	P	312	VAL	2.3
1	K	124	GLY	2.3
1	F	172	LYS	2.3
2	Q	39	LEU	2.3
1	O	127	SER	2.3
1	L	124	GLY	2.2
1	O	258	LEU	2.2
1	A	154	GLN	2.2
1	F	174	THR	2.2
1	J	83	LEU	2.2
1	H	127	SER	2.2
1	L	68	HIS	2.2
1	E	140	LYS	2.2
1	E	143	THR	2.2
1	F	134	LYS	2.2
1	C	127	SER	2.2
1	B	33	ALA	2.2
1	K	121	LYS	2.2
1	A	261	VAL	2.2
1	C	161	ASP	2.2
1	I	126	SER	2.2
1	F	311	GLY	2.1
1	L	162	GLU	2.2
1	O	126	SER	2.1
2	W	57	SER	2.1
1	O	179	LYS	2.1
1	B	81	THR	2.1
1	P	80	GLU	2.1
1	J	166	GLY	2.1
2	R	57	SER	2.1
1	A	126	SER	2.1
1	A	169	ARG	2.1
1	M	322	PHE	2.1
1	M	218	GLU	2.1
1	K	81	THR	2.1
1	G	139	ALA	2.1
1	A	166	GLY	2.1
1	I	256	GLU	2.1
1	L	252	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	69	TYR	2.1
1	J	171	GLY	2.1
1	F	138	GLY	2.1
1	H	313	GLU	2.1
1	F	136	LEU	2.0
1	E	137	GLN	2.0
1	P	154	GLN	2.0
1	F	246	LYS	2.0
1	E	252	ASP	2.0
1	K	161	ASP	2.0
1	O	169	ARG	2.0
1	E	136	LEU	2.0
1	E	251	LYS	2.0
1	P	121	LYS	2.0
1	H	135	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.