



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2016 – 06:11 PM EST

PDB ID : 5IKN
Title : Crystal Structure of the T7 Replisome in the Absence of DNA
Authors : Wallen, J.R.; Ellenberger, T.
Deposited on : 2016-03-03
Resolution : 4.80 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

<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

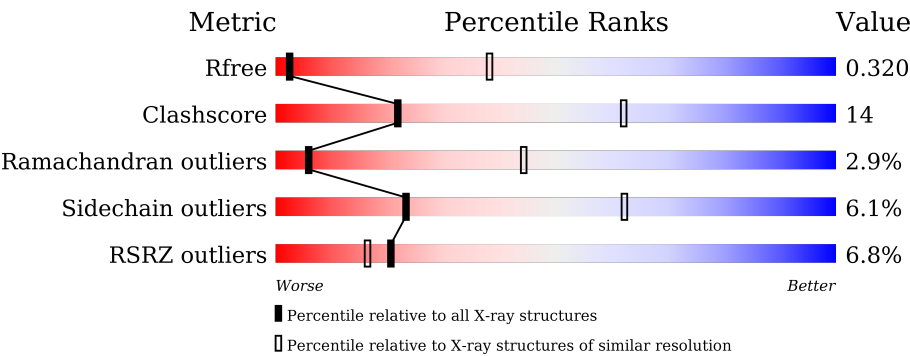
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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}	91344	1117 (6.00-3.60)
Clashscore	102246	1017 (5.96-3.64)
Ramachandran outliers	100387	1156 (6.00-3.60)
Sidechain outliers	100360	1134 (6.00-3.60)
RSRZ outliers	91569	1120 (6.00-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	704	<div><div>4%</div><div><div></div><div>65%</div><div>22%</div><div>•</div><div>9%</div></div></div>
1	B	704	<div><div>2%</div><div><div></div><div>65%</div><div>23%</div><div>•</div><div>10%</div></div></div>
1	C	704	<div><div>5%</div><div><div></div><div>65%</div><div>23%</div><div>•</div><div>10%</div></div></div>
2	D	486	<div><div>10%</div><div><div></div><div>66%</div><div>30%</div><div>•</div></div></div>
2	E	486	<div><div>4%</div><div><div></div><div>64%</div><div>32%</div><div>•</div></div></div>
2	F	486	<div><div>8%</div><div><div></div><div>61%</div><div>34%</div><div>5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	486	<div><div></div><div>10%63%31%<div><div></div><div></div><div></div></div></div></div>
2	H	486	<div><div></div><div>6%67%29%<div><div></div><div></div><div></div></div></div></div>
2	I	486	<div><div></div><div>8%55%34%7%<div><div></div><div></div><div></div></div></div></div>
2	J	486	<div><div></div><div>5%64%31%<div><div></div><div></div><div></div></div></div></div>
3	K	105	<div><div></div><div>22%79%18%<div><div></div><div></div><div></div></div></div></div>
3	L	105	<div><div></div><div>3%67%30%<div><div></div><div></div><div></div></div></div></div>
3	M	105	<div><div></div><div>26%85%14%<div><div></div><div></div><div></div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43846 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 DNA-directed DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5092	3236	888	947	21			
1	B	636	Total	C	N	O	S	0	0	0
			5073	3226	884	942	21			
1	C	633	Total	C	N	O	S	0	0	0
			5041	3201	880	939	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	ASP	engineered mutation	UNP P00581
A	7	ALA	GLU	engineered mutation	UNP P00581
B	5	ALA	ASP	engineered mutation	UNP P00581
B	7	ALA	GLU	engineered mutation	UNP P00581
C	5	ALA	ASP	engineered mutation	UNP P00581
C	7	ALA	GLU	engineered mutation	UNP P00581

- Molecule 2 is a protein called DNA primase/helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	485	Total	C	N	O	S	0	0	0
			3763	2353	660	725	25			
2	E	485	Total	C	N	O	S	0	0	0
			3763	2353	660	725	25			
2	F	486	Total	C	N	O	S	0	0	0
			3768	2355	661	727	25			
2	G	484	Total	C	N	O	S	0	0	0
			3757	2350	659	723	25			
2	H	486	Total	C	N	O	S	0	0	0
			3768	2355	661	727	25			
2	I	472	Total	C	N	O	S	0	0	0
			3670	2295	647	703	25			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	483	Total	C	N	O	S	0	0	0
			3745	2341	658	721	25			

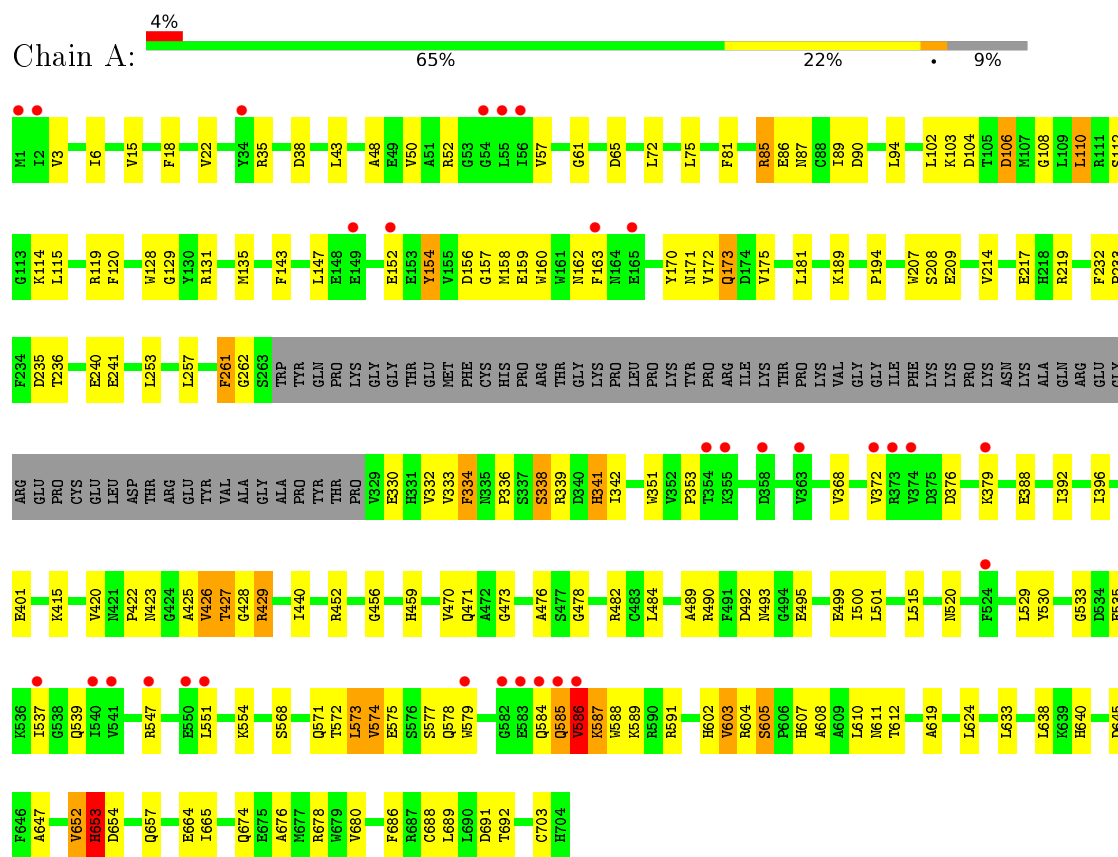
- Molecule 3 is a protein called Thioredoxin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			
3	L	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			
3	M	105	Total	C	N	O	S	0	0	0
			802	518	129	152	3			

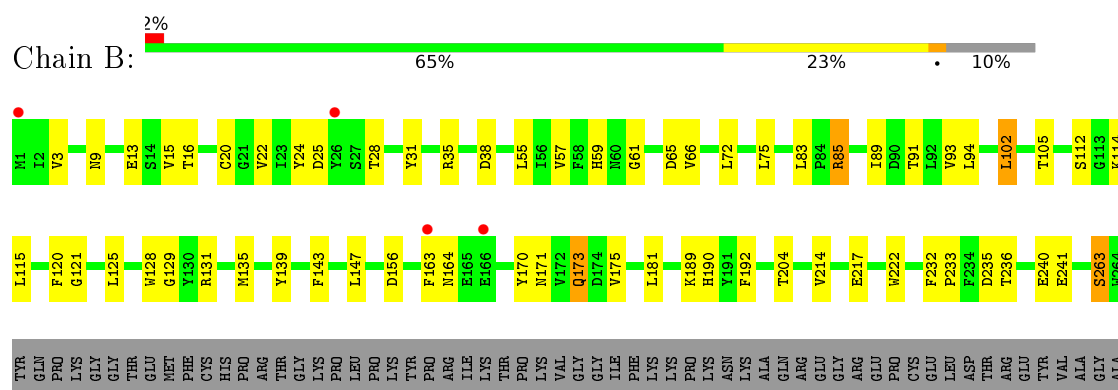
3 Residue-property plots

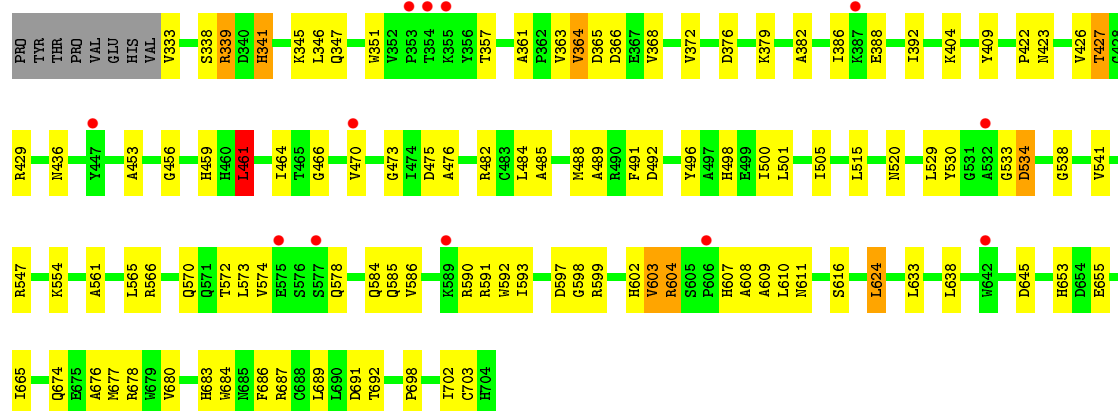
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA-directed DNA polymerase



- Molecule 1: DNA-directed DNA polymerase

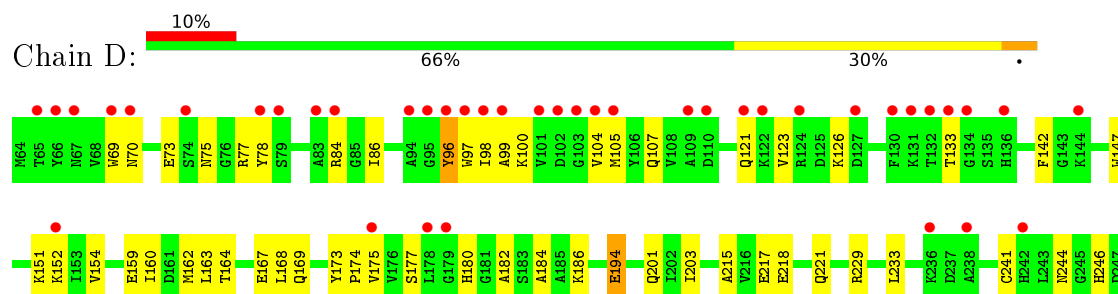


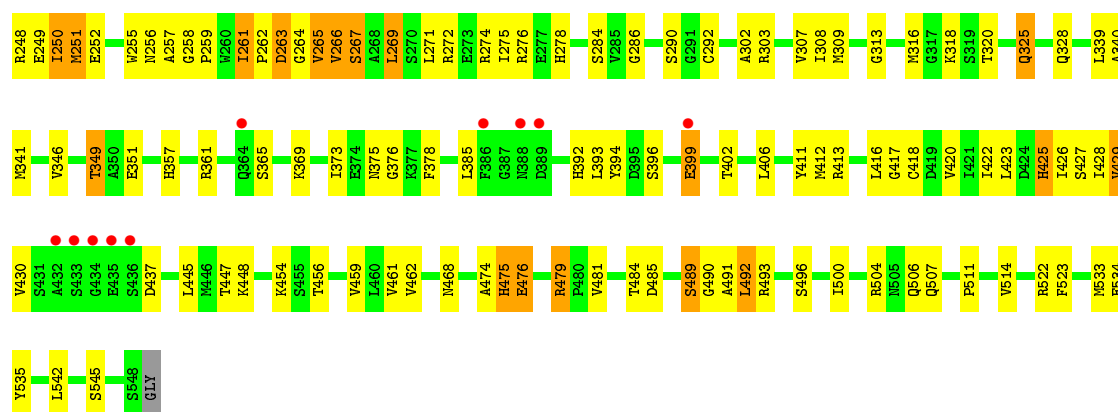


• Molecule 1: DNA-directed DNA polymerase

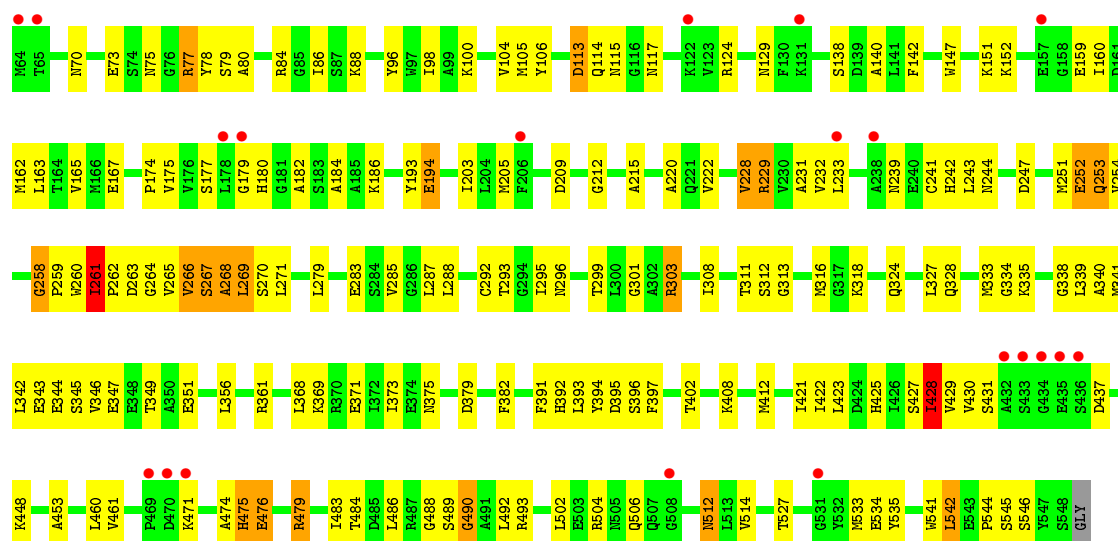


• Molecule 2: DNA primase/helicase

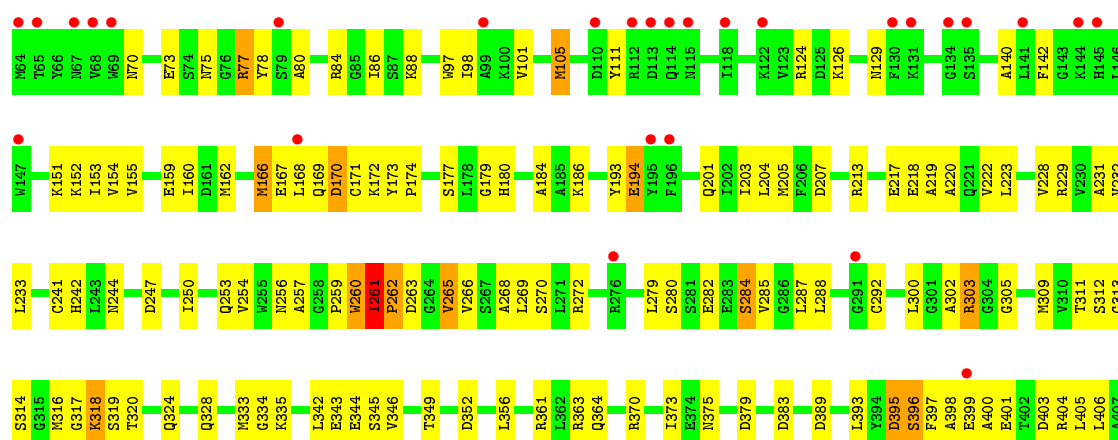


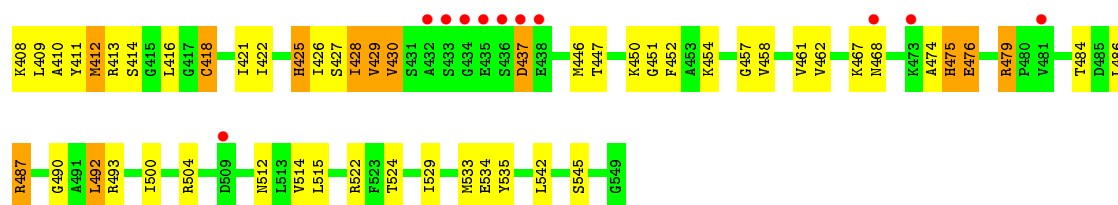


• Molecule 2: DNA primase/helicase

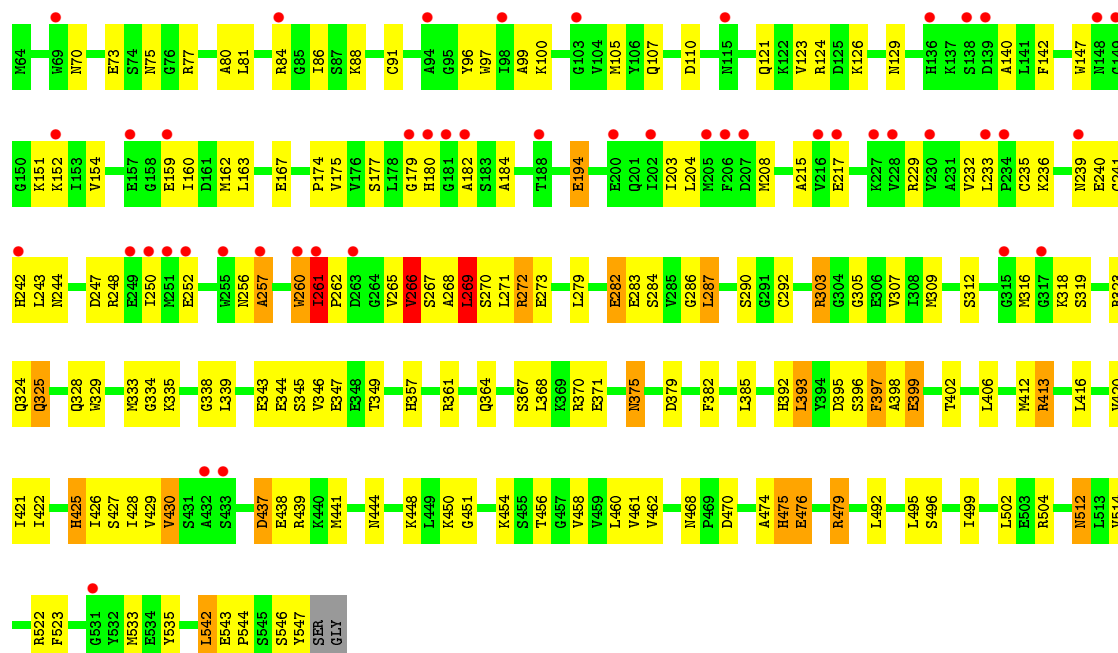


• Molecule 2: DNA primase/helicase

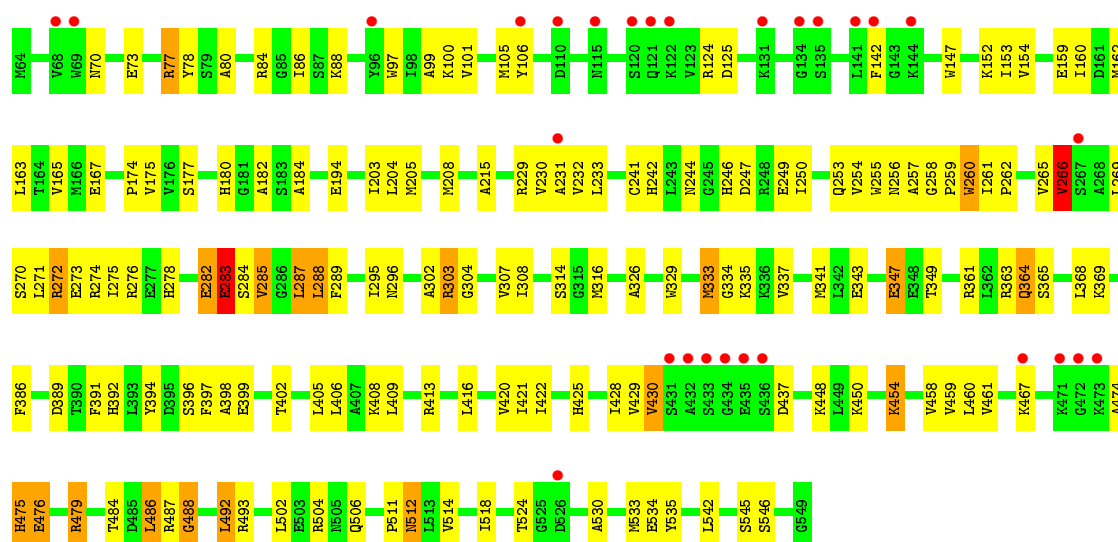




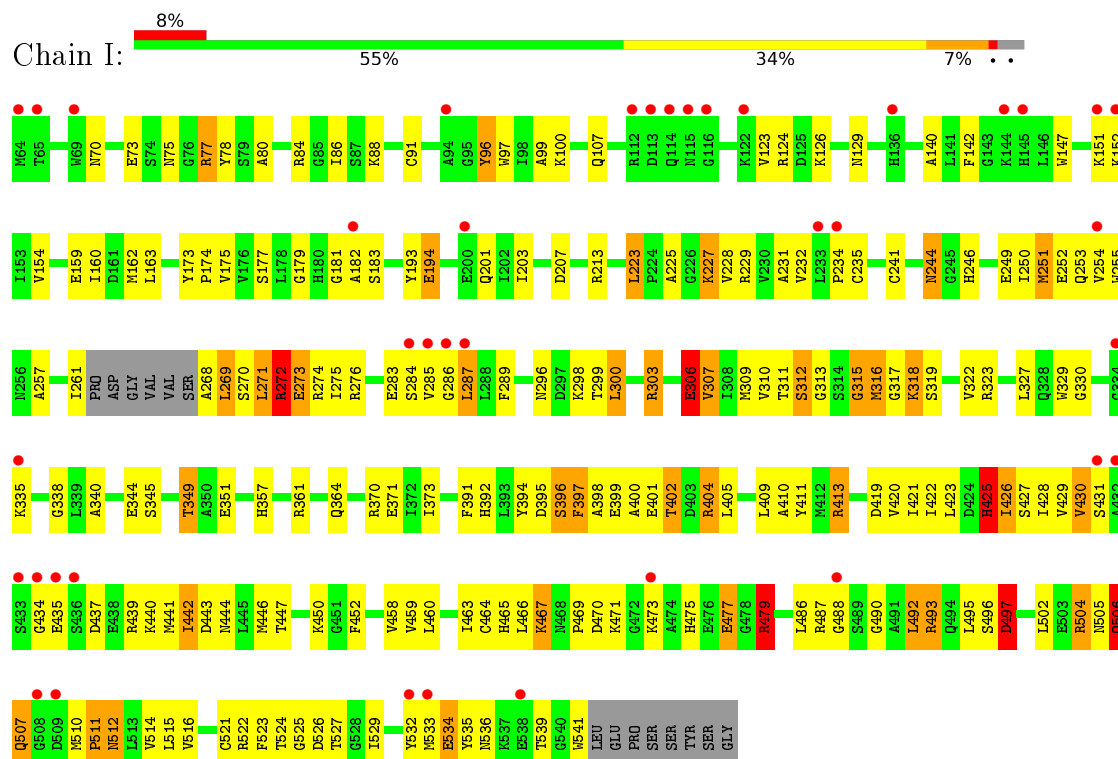
• Molecule 2: DNA primase/helicase



• Molecule 2: DNA primase/helicase



- Molecule 2: DNA primase/helicase




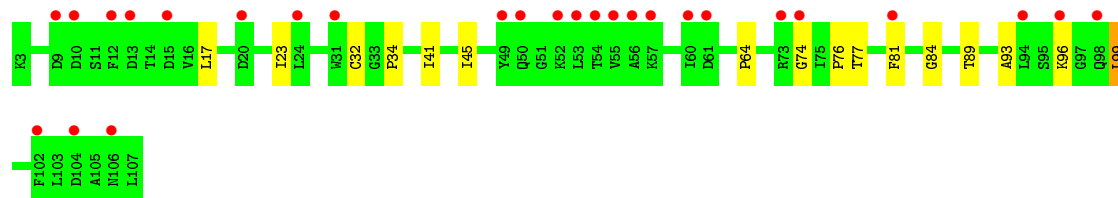
- Molecule 3: Thioredoxin-1

Chain L:  3% 67% 30% .



- Molecule 3: Thioredoxin-1

Chain M:  26% 85% 14% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.87Å 238.09Å 243.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 4.80 49.20 – 4.80	Depositor EDS
% Data completeness (in resolution range)	82.2 (29.98-4.80) 82.4 (49.20-4.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 4.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.275 , 0.318 0.278 , 0.320	Depositor DCC
R_{free} test set	2100 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	177.0	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 201.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	43846	wwPDB-VP
Average B, all atoms (Å ²)	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/5211	0.42	0/7045
1	B	0.26	0/5193	0.41	0/7021
1	C	0.25	0/5158	0.40	0/6972
2	D	0.26	0/3826	0.44	0/5152
2	E	0.28	0/3826	0.48	0/5152
2	F	0.28	0/3831	0.49	0/5157
2	G	0.26	0/3820	0.45	0/5144
2	H	0.27	0/3831	0.48	0/5157
2	I	0.35	2/3729 (0.1%)	0.55	4/5016 (0.1%)
2	J	0.26	0/3807	0.46	0/5126
3	K	0.25	0/817	0.43	0/1108
3	L	0.27	0/817	0.46	0/1108
3	M	0.25	0/817	0.43	0/1108
All	All	0.27	2/44683 (0.0%)	0.46	4/60266 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	312	SER	CA-CB	7.75	1.64	1.52
2	I	318	LYS	CD-CE	5.98	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	318	LYS	CD-CE-NZ	13.48	142.71	111.70
2	I	312	SER	N-CA-CB	7.40	121.60	110.50
2	I	318	LYS	CA-CB-CG	-5.66	100.96	113.40
2	I	312	SER	CB-CA-C	-5.31	100.02	110.10

There are no chirality outliers.

There are no planarity outliers.

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	5092	0	4986	118	0
1	B	5073	0	4965	102	0
1	C	5041	0	4937	100	0
2	D	3763	0	3724	123	0
2	E	3763	0	3724	125	0
2	F	3768	0	3727	147	1
2	G	3757	0	3719	134	0
2	H	3768	0	3727	131	0
2	I	3670	0	3638	184	0
2	J	3745	0	3710	123	0
3	K	802	0	816	15	0
3	L	802	0	816	21	1
3	M	802	0	816	10	0
All	All	43846	0	43305	1221	1

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 14.

All (1221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:318:LYS:NZ	2:I:502:LEU:H	1.20	1.34
2:I:318:LYS:HZ1	2:I:502:LEU:N	1.34	1.25
2:I:318:LYS:HE3	2:I:502:LEU:HB2	1.47	0.95
2:I:312:SER:HB3	2:I:318:LYS:CE	1.97	0.94
2:I:318:LYS:NZ	2:I:502:LEU:N	2.03	0.93
2:I:311:THR:O	2:I:318:LYS:NZ	2.06	0.86
1:B:263:SER:HG	1:B:333:VAL:N	1.76	0.84
2:E:252:GLU:H	2:E:252:GLU:CD	1.79	0.84
2:E:261:ILE:HB	2:E:262:PRO:HD3	1.58	0.83
2:G:105:MET:HB2	2:G:126:LYS:HD3	1.60	0.81
3:L:74:GLY:O	3:L:77:THR:OG1	1.99	0.80
1:A:495:GLU:HA	2:E:544:PRO:HG2	1.64	0.79
2:I:312:SER:N	2:I:318:LYS:HD2	1.97	0.79
2:J:283:GLU:HB3	2:J:286:GLY:HA3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:425:HIS:H	2:I:463:ILE:HB	1.47	0.79
2:I:318:LYS:HE2	2:I:502:LEU:HD13	1.65	0.78
2:E:220:ALA:HB1	2:E:260:TRP:CD1	2.18	0.78
2:G:283:GLU:HB3	2:G:286:GLY:HA2	1.66	0.78
2:F:344:GLU:HA	2:G:454:LYS:HE2	1.66	0.78
2:J:223:LEU:HD13	2:J:228:VAL:HG21	1.66	0.78
2:E:344:GLU:HA	2:F:454:LYS:HE2	1.66	0.77
1:C:501:LEU:HD11	2:G:370:ARG:HD3	1.65	0.76
2:E:220:ALA:HB1	2:E:260:TRP:HD1	1.49	0.76
2:G:271:LEU:O	2:G:273:GLU:N	2.19	0.76
1:A:603:VAL:HG22	1:A:604:ARG:H	1.52	0.75
2:G:261:ILE:HG23	2:G:262:PRO:HD3	1.69	0.74
2:E:342:LEU:HB2	2:E:428:ILE:HD12	1.68	0.74
1:C:212:GLU:OE2	1:C:683:HIS:NE2	2.20	0.74
2:H:77:ARG:HH12	2:H:100:LYS:HD2	1.51	0.74
2:H:534:GLU:HG3	2:H:545:SER:HB2	1.70	0.74
2:G:379:ASP:OD1	2:H:276:ARG:NH2	2.21	0.73
2:F:124:ARG:HH22	2:F:159:GLU:HB2	1.53	0.73
1:B:22:VAL:HB	1:B:175:VAL:HG21	1.71	0.73
2:E:324:GLN:HE22	2:E:542:LEU:HB2	1.54	0.73
1:C:55:LEU:HD13	1:C:89:ILE:HD11	1.72	0.72
2:E:259:PRO:HA	2:E:260:TRP:HB3	1.72	0.72
1:A:604:ARG:HG3	1:A:605:SER:H	1.55	0.72
3:L:77:THR:HG23	3:L:91:VAL:HG22	1.72	0.71
2:J:98:ILE:HG13	2:J:107:GLN:HG2	1.71	0.71
2:I:492:LEU:HD12	2:I:492:LEU:H	1.55	0.71
2:D:201:GLN:OE1	2:D:229:ARG:NH1	2.20	0.71
2:H:142:PHE:HB3	2:H:177:SER:HB3	1.72	0.71
2:G:346:VAL:HB	2:G:393:LEU:HD13	1.72	0.71
1:A:484:LEU:HD22	1:A:529:LEU:HD21	1.73	0.71
2:I:486:LEU:O	2:I:493:ARG:NH1	2.23	0.71
1:B:22:VAL:HG23	1:B:171:ASN:HD22	1.57	0.70
2:G:437:ASP:HB3	2:G:439:ARG:HG2	1.73	0.70
2:J:223:LEU:O	2:J:225:ALA:N	2.23	0.70
2:H:232:VAL:N	2:H:253:GLN:OE1	2.24	0.70
2:D:75:ASN:ND2	2:D:100:LYS:O	2.24	0.70
2:I:515:LEU:HD21	2:I:529:ILE:HD12	1.72	0.70
2:E:408:LYS:HD3	2:F:263:ASP:HB3	1.73	0.70
1:A:114:LYS:HG3	1:A:115:LEU:HG	1.74	0.69
3:L:26:ASP:HB3	3:L:57:LYS:HD2	1.73	0.69
3:L:38:ILE:HA	3:L:41:ILE:HD13	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:364:GLN:HG3	2:I:300:LEU:HD11	1.74	0.69
2:D:523:PHE:O	2:J:364:GLN:NE2	2.26	0.69
1:C:568:SER:O	1:C:572:THR:OG1	2.07	0.69
2:D:251:MET:SD	2:D:252:GLU:N	2.65	0.69
1:A:572:THR:N	1:A:573:LEU:HA	2.08	0.69
1:A:633:LEU:HD22	1:A:638:LEU:HD12	1.74	0.69
2:H:152:LYS:HD2	2:H:255:TRP:HD1	1.56	0.69
2:H:347:GLU:HB3	2:I:275:ILE:HG12	1.73	0.69
2:I:318:LYS:CE	2:I:502:LEU:HD13	2.23	0.69
2:E:471:LYS:O	2:E:479:ARG:NH2	2.25	0.69
1:C:674:GLN:HE21	1:C:678:ARG:HH22	1.38	0.68
2:H:361:ARG:NH1	2:H:535:TYR:OH	2.25	0.68
2:I:86:ILE:HG12	2:I:163:LEU:HB3	1.75	0.68
2:E:84:ARG:HE	2:E:160:ILE:HG21	1.59	0.68
2:F:395:ASP:HB3	2:G:266:VAL:HG21	1.75	0.68
1:B:376:ASP:HB3	1:B:379:LYS:HB2	1.75	0.68
1:C:1:MET:HB3	1:C:199:THR:HG23	1.75	0.68
2:H:307:VAL:HG22	2:H:460:LEU:HB3	1.74	0.68
2:I:312:SER:H	2:I:466:LEU:HD21	1.59	0.68
2:I:272:ARG:HD2	2:I:273:GLU:H	1.58	0.68
2:I:318:LYS:HZ2	2:I:502:LEU:H	1.38	0.68
2:J:361:ARG:NH1	2:J:535:TYR:OH	2.26	0.68
2:G:84:ARG:HE	2:G:160:ILE:HG21	1.59	0.68
2:I:318:LYS:HZ1	2:I:502:LEU:H	0.68	0.68
2:G:204:LEU:N	2:G:229:ARG:O	2.26	0.68
2:J:152:LYS:HG3	2:J:201:GLN:HG3	1.74	0.68
3:M:45:ILE:HG13	3:M:99:LEU:HD13	1.76	0.68
2:D:261:ILE:HG13	2:J:396:SER:HA	1.75	0.68
2:G:70:ASN:HB3	2:G:73:GLU:HB2	1.75	0.68
2:I:322:VAL:HG21	2:I:463:ILE:HD11	1.76	0.67
2:F:287:LEU:HD11	2:F:303:ARG:HD3	1.75	0.67
2:H:204:LEU:N	2:H:229:ARG:O	2.22	0.67
2:J:152:LYS:HD3	2:J:203:ILE:HD11	1.77	0.67
2:I:318:LYS:HE2	2:I:502:LEU:CD1	2.24	0.67
2:F:364:GLN:NE2	2:G:523:PHE:O	2.28	0.67
2:G:124:ARG:HH22	2:G:159:GLU:HB2	1.60	0.67
2:F:219:ALA:HA	2:F:223:LEU:HD13	1.77	0.67
2:F:287:LEU:HA	2:F:302:ALA:H	1.58	0.67
2:G:361:ARG:NH1	2:G:535:TYR:OH	2.27	0.66
2:I:307:VAL:HG22	2:I:460:LEU:HD23	1.75	0.66
2:J:180:HIS:HB2	2:J:184:ALA:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLN:NE2	1:A:657:GLN:OE1	2.26	0.66
2:I:312:SER:HB3	2:I:318:LYS:HE3	1.78	0.66
2:J:402:THR:HG23	2:J:445:LEU:HD13	1.75	0.66
1:B:345:LYS:O	1:B:347:GLN:N	2.24	0.66
2:H:287:LEU:HD21	2:H:302:ALA:HB3	1.78	0.66
2:I:234:PRO:HG3	2:I:249:GLU:HG2	1.78	0.66
2:G:252:GLU:O	2:G:257:ALA:N	2.28	0.66
2:G:154:VAL:HA	2:G:203:ILE:HB	1.77	0.66
2:I:246:HIS:HB3	2:I:249:GLU:HB2	1.78	0.66
2:I:400:ALA:HB1	2:I:404:ARG:HD2	1.77	0.66
1:B:427:THR:HG22	1:B:429:ARG:H	1.61	0.66
2:G:393:LEU:HD21	2:H:271:LEU:HD11	1.78	0.66
2:I:272:ARG:HD2	2:I:273:GLU:N	2.10	0.66
2:J:263:ASP:O	2:J:265:VAL:N	2.29	0.66
1:A:61:GLY:N	1:A:90:ASP:OD1	2.28	0.65
1:C:574:VAL:HG13	1:C:586:VAL:HG13	1.78	0.65
2:G:345:SER:HA	2:H:454:LYS:HE3	1.77	0.65
1:A:575:GLU:HB2	1:A:589:LYS:HG3	1.78	0.65
2:D:186:LYS:HB2	2:D:218:GLU:HB3	1.79	0.65
3:L:45:ILE:HG12	3:L:99:LEU:HD23	1.76	0.65
2:E:313:GLY:O	2:E:318:LYS:NZ	2.30	0.65
2:E:475:HIS:H	2:E:479:ARG:HD2	1.62	0.65
2:F:162:MET:HB2	2:F:177:SER:HB2	1.79	0.65
2:F:422:ILE:HD13	2:F:461:VAL:HB	1.78	0.65
1:B:9:ASN:ND2	1:B:16:THR:OG1	2.29	0.64
1:C:15:VAL:HG22	1:C:72:LEU:HD21	1.79	0.64
2:D:454:LYS:HE2	2:J:344:GLU:HA	1.78	0.64
2:E:422:ILE:HD13	2:E:461:VAL:HB	1.79	0.64
1:A:112:SER:HB2	1:A:114:LYS:HG2	1.79	0.64
2:H:506:GLN:NE2	2:I:529:ILE:O	2.31	0.64
2:F:228:VAL:HB	2:F:260:TRP:CD1	2.31	0.64
2:G:397:PHE:HB2	2:H:454:LYS:HD2	1.77	0.64
2:G:425:HIS:CE1	2:G:427:SER:HB2	2.33	0.64
2:J:330:GLY:HA2	2:J:335:LYS:H	1.61	0.64
2:H:288:LEU:HD21	2:H:333:MET:HG2	1.79	0.64
2:I:318:LYS:CE	2:I:502:LEU:HB2	2.25	0.64
2:J:107:GLN:OE1	2:J:124:ARG:NH1	2.30	0.64
2:F:324:GLN:HG3	2:F:356:LEU:HD21	1.80	0.64
2:J:287:LEU:HD21	2:J:335:LYS:HG3	1.80	0.64
2:I:467:LYS:HA	2:I:487:ARG:HG3	1.79	0.64
2:H:486:LEU:HD12	2:H:487:ARG:H	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:LEU:HD12	2:F:428:ILE:HD13	1.80	0.63
2:H:266:VAL:HG11	2:H:271:LEU:HD13	1.79	0.63
3:M:23:ILE:HB	3:M:81:PHE:HB2	1.81	0.63
1:A:22:VAL:HG21	1:A:172:VAL:HG22	1.79	0.63
2:D:229:ARG:HH21	2:D:257:ALA:H	1.47	0.63
2:G:450:LYS:HG2	2:G:495:LEU:HD12	1.80	0.63
1:C:94:LEU:HD21	1:C:214:VAL:HG13	1.79	0.63
2:D:447:THR:HB	2:J:430:VAL:HG22	1.80	0.63
2:D:316:MET:HE3	2:D:504:ARG:HG2	1.78	0.63
2:J:429:VAL:O	2:J:431:SER:N	2.31	0.63
1:A:103:LYS:N	1:A:104:ASP:HB2	2.14	0.63
1:A:577:SER:HA	1:A:587:LYS:HE2	1.81	0.63
2:J:186:LYS:HD3	2:J:218:GLU:HG3	1.81	0.63
2:E:394:TYR:HA	2:F:265:VAL:HG21	1.79	0.63
3:K:41:ILE:HD12	3:K:96:LYS:HB2	1.80	0.63
1:C:476:ALA:HB3	1:C:654:ASP:HB2	1.80	0.63
1:C:339:ARG:NH1	1:C:364:VAL:O	2.31	0.63
2:F:268:ALA:O	2:F:270:SER:N	2.30	0.63
2:I:521:CYS:O	2:I:525:GLY:N	2.24	0.63
2:F:409:LEU:HA	2:F:412:MET:HE2	1.81	0.62
2:D:84:ARG:HE	2:D:160:ILE:HG21	1.63	0.62
1:C:602:HIS:CG	1:C:603:VAL:H	2.18	0.62
2:E:260:TRP:CD1	2:E:261:ILE:HG12	2.33	0.62
2:E:484:THR:HA	2:E:493:ARG:HH22	1.65	0.62
2:E:267:SER:O	2:E:269:LEU:N	2.30	0.62
1:B:501:LEU:HD21	1:B:689:LEU:HB3	1.81	0.62
2:G:316:MET:HE3	2:G:504:ARG:HG2	1.81	0.62
2:I:284:SER:HA	2:I:523:PHE:HZ	1.65	0.62
1:B:94:LEU:HD21	1:B:214:VAL:HG13	1.82	0.61
1:B:645:ASP:HB3	1:B:665:ILE:HD13	1.82	0.61
2:E:340:ALA:HB3	2:E:423:LEU:HA	1.83	0.61
2:I:311:THR:O	2:I:311:THR:HG23	1.99	0.61
1:B:530:TYR:HA	1:B:611:ASN:HB2	1.83	0.61
1:C:49:GLU:OE1	1:C:52:ARG:NH2	2.26	0.61
2:E:299:THR:O	2:E:303:ARG:NH1	2.33	0.61
2:H:242:HIS:ND1	2:H:247:ASP:OD1	2.30	0.61
2:H:316:MET:HE3	2:H:504:ARG:HG2	1.81	0.61
2:E:209:ASP:OD1	2:E:212:GLY:N	2.31	0.61
2:I:490:GLY:HA2	2:I:493:ARG:HE	1.66	0.61
1:B:15:VAL:HG22	1:B:72:LEU:HD21	1.83	0.61
1:C:217:GLU:OE2	1:C:623:LYS:NZ	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:LEU:HD22	1:C:638:LEU:HD12	1.81	0.61
2:F:242:HIS:ND1	2:F:247:ASP:OD1	2.26	0.61
1:A:3:VAL:HA	1:A:57:VAL:HB	1.83	0.61
2:D:142:PHE:HB3	2:D:177:SER:HB3	1.82	0.61
2:E:341:MET:HB3	2:E:344:GLU:HG2	1.81	0.61
2:E:474:ALA:O	2:E:476:GLU:N	2.34	0.61
1:A:573:LEU:HD23	1:A:574:VAL:H	1.67	0.60
1:B:61:GLY:HA2	1:B:65:ASP:HB2	1.82	0.60
2:E:261:ILE:HB	2:E:262:PRO:CD	2.30	0.60
2:G:282:GLU:HG3	2:G:284:SER:H	1.65	0.60
1:C:404:LYS:HA	1:C:409:TYR:HE2	1.66	0.60
2:D:402:THR:HG23	2:D:445:LEU:HD13	1.82	0.60
2:J:506:GLN:HA	2:J:511:PRO:HB3	1.81	0.60
2:D:276:ARG:HD3	2:J:373:ILE:HG12	1.82	0.60
1:A:571:GLN:HA	1:A:573:LEU:HG	1.83	0.60
2:I:316:MET:N	2:I:316:MET:SD	2.72	0.60
2:I:395:ASP:H	2:J:265:VAL:HG11	1.66	0.60
1:B:128:TRP:CE3	1:B:131:ARG:HD2	2.37	0.60
2:F:260:TRP:HA	2:F:261:ILE:HB	1.82	0.60
2:F:305:GLY:HA2	2:F:454:LYS:HA	1.84	0.60
2:I:351:GLU:OE1	2:J:278:HIS:ND1	2.34	0.60
2:G:422:ILE:HD13	2:G:461:VAL:HB	1.84	0.60
2:D:105:MET:HB2	2:D:126:LYS:HE3	1.83	0.60
2:D:265:VAL:HG13	2:D:266:VAL:H	1.65	0.60
2:G:86:ILE:HG12	2:G:163:LEU:HB3	1.82	0.60
1:A:429:ARG:HH12	1:A:652:VAL:HG12	1.67	0.59
2:E:86:ILE:HG12	2:E:163:LEU:HB3	1.83	0.59
1:A:129:GLY:HA3	1:A:135:MET:HG2	1.83	0.59
1:A:476:ALA:HB3	1:A:654:ASP:HB2	1.83	0.59
2:G:180:HIS:HB2	2:G:184:ALA:HB3	1.85	0.59
1:A:341:HIS:CG	1:A:342:ILE:H	2.21	0.59
2:D:276:ARG:NH2	2:J:379:ASP:OD2	2.34	0.59
2:F:260:TRP:CD2	2:F:261:ILE:HG22	2.38	0.59
2:H:394:TYR:CZ	2:H:396:SER:HB2	2.37	0.59
2:I:312:SER:HB3	2:I:318:LYS:CD	2.32	0.59
2:D:250:ILE:HD12	2:D:251:MET:H	1.67	0.59
2:H:474:ALA:O	2:H:476:GLU:N	2.35	0.59
2:I:312:SER:O	2:I:466:LEU:HG	2.03	0.59
2:E:345:SER:H	2:F:454:LYS:HE3	1.67	0.59
2:H:258:GLY:N	2:H:259:PRO:HD3	2.18	0.59
3:M:23:ILE:O	3:M:81:PHE:N	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:426:ILE:HD12	2:D:462:VAL:HG11	1.84	0.59
1:A:18:PHE:HB2	1:A:72:LEU:HD13	1.85	0.59
1:B:363:VAL:HG22	1:B:364:VAL:H	1.68	0.59
2:G:346:VAL:HG11	2:G:395:ASP:HB2	1.84	0.59
1:C:590:ARG:HD2	1:C:592:TRP:O	2.02	0.58
2:D:506:GLN:HA	2:D:511:PRO:HB3	1.84	0.58
2:I:505:ASN:O	2:I:507:GLN:N	2.36	0.58
2:H:154:VAL:HA	2:H:203:ILE:HB	1.84	0.58
2:I:207:ASP:O	2:I:213:ARG:NH2	2.32	0.58
2:J:514:VAL:HG13	2:J:533:MET:HB2	1.85	0.58
1:A:515:LEU:HD12	1:A:520:ASN:HB3	1.84	0.58
1:B:633:LEU:HD22	1:B:638:LEU:HD12	1.85	0.58
2:F:352:ASP:OD2	2:F:363:ARG:NH2	2.37	0.58
2:H:271:LEU:HD12	2:H:275:ILE:HD11	1.84	0.58
2:F:166:MET:SD	2:F:167:GLU:N	2.76	0.58
1:A:233:PRO:HA	1:A:415:LYS:HG2	1.85	0.58
1:A:425:ALA:O	1:A:427:THR:N	2.36	0.58
2:D:86:ILE:HG12	2:D:163:LEU:HB3	1.84	0.58
2:I:521:CYS:SG	2:I:524:THR:OG1	2.58	0.58
1:A:61:GLY:HA2	1:A:65:ASP:HB2	1.85	0.58
2:H:256:ASN:O	2:H:258:GLY:N	2.36	0.58
2:H:287:LEU:HD11	2:H:302:ALA:H	1.69	0.58
2:J:201:GLN:HB2	2:J:229:ARG:HD2	1.86	0.58
2:J:84:ARG:NH1	2:J:239:ASN:OD1	2.36	0.58
1:A:376:ASP:HB3	1:A:379:LYS:HB2	1.86	0.58
1:A:473:GLY:HA3	1:A:703:CYS:HB3	1.84	0.58
1:A:585:GLN:O	1:A:587:LYS:HD3	2.04	0.58
2:D:373:ILE:HA	2:D:378:PHE:HB2	1.86	0.58
2:D:399:GLU:HB3	2:D:430:VAL:HG11	1.85	0.58
2:E:100:LYS:HG3	2:E:105:MET:SD	2.44	0.58
2:G:248:ARG:O	2:G:252:GLU:HG3	2.04	0.58
2:G:474:ALA:O	2:G:476:GLU:N	2.37	0.58
1:A:501:LEU:HD21	1:A:689:LEU:HB3	1.85	0.58
2:I:396:SER:O	2:I:398:ALA:N	2.37	0.58
2:J:313:GLY:O	2:J:318:LYS:NZ	2.37	0.58
2:I:312:SER:OG	2:I:315:GLY:O	2.22	0.58
1:B:590:ARG:NH1	1:B:592:TRP:O	2.37	0.57
2:E:142:PHE:HB3	2:E:177:SER:HB3	1.86	0.57
2:I:162:MET:HB2	2:I:177:SER:HB2	1.85	0.57
2:D:393:LEU:O	2:E:265:VAL:HB	2.03	0.57
2:F:186:LYS:HG3	2:F:222:VAL:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:399:GLU:HB2	2:G:430:VAL:HG11	1.85	0.57
2:H:154:VAL:HG11	2:H:165:VAL:HG11	1.86	0.57
2:I:251:MET:SD	2:I:252:GLU:N	2.77	0.57
1:C:263:SER:HB2	3:M:64:PRO:HB2	1.86	0.57
2:G:397:PHE:CD2	2:H:454:LYS:HB3	2.39	0.57
2:H:506:GLN:HA	2:H:511:PRO:HB3	1.86	0.57
2:H:162:MET:HG2	2:H:175:VAL:HG12	1.85	0.57
2:J:422:ILE:HD13	2:J:461:VAL:HB	1.85	0.57
2:J:118:ILE:HD13	2:J:118:ILE:H	1.67	0.57
1:A:645:ASP:HB3	1:A:665:ILE:HD13	1.85	0.57
2:D:493:ARG:NH2	2:J:468:ASN:OD1	2.38	0.57
2:H:422:ILE:HD13	2:H:461:VAL:HB	1.86	0.57
2:H:475:HIS:H	2:H:479:ARG:HD2	1.69	0.57
2:I:241:CYS:HB3	2:I:246:HIS:HB2	1.87	0.57
2:J:228:VAL:O	2:J:259:PRO:HA	2.04	0.57
1:B:404:LYS:HA	1:B:409:TYR:HE2	1.70	0.57
2:E:361:ARG:NH1	2:E:535:TYR:OH	2.38	0.57
2:F:474:ALA:O	2:F:476:GLU:N	2.38	0.57
2:F:70:ASN:HB3	2:F:73:GLU:HB2	1.86	0.57
2:F:416:LEU:HG	2:G:262:PRO:HG2	1.85	0.57
2:I:147:TRP:CE2	2:I:174:PRO:HA	2.39	0.57
1:B:473:GLY:HA3	1:B:703:CYS:HB3	1.87	0.57
2:D:425:HIS:CE1	2:D:427:SER:HB2	2.40	0.57
1:C:26:TYR:CG	1:C:199:THR:HG21	2.40	0.56
2:H:389:ASP:HA	2:I:268:ALA:HB2	1.85	0.56
3:L:82:LYS:NZ	3:L:106:ASN:O	2.38	0.56
2:I:405:LEU:O	2:I:409:LEU:HD12	2.06	0.56
2:G:252:GLU:HG2	2:G:256:ASN:HB3	1.86	0.56
2:J:229:ARG:HH21	2:J:259:PRO:HD3	1.71	0.56
1:B:482:ARG:HG2	1:B:500:ILE:HG21	1.86	0.56
2:E:488:GLY:O	2:E:490:GLY:N	2.39	0.56
2:H:282:GLU:HG2	2:H:283:GLU:HG2	1.87	0.56
2:H:283:GLU:OE1	2:H:304:GLY:N	2.33	0.56
2:H:484:THR:HA	2:H:493:ARG:HH22	1.70	0.56
2:I:306:GLU:N	2:I:497:ASP:HB2	2.20	0.56
1:B:674:GLN:HG2	1:B:692:THR:OG1	2.05	0.56
2:F:426:ILE:HD12	2:F:462:VAL:HG11	1.86	0.56
2:J:234:PRO:HG2	2:J:249:GLU:HG2	1.86	0.56
2:D:229:ARG:HE	2:D:257:ALA:HB3	1.70	0.56
2:D:365:SER:O	2:D:369:LYS:HG3	2.06	0.56
2:D:475:HIS:H	2:D:479:ARG:HB3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:338:GLY:O	2:E:422:ILE:N	2.38	0.56
2:D:476:GLU:HG3	2:E:483:ILE:HD12	1.88	0.56
2:F:413:ARG:HD3	2:F:458:VAL:HB	1.87	0.56
2:G:96:TYR:OH	2:G:107:GLN:NE2	2.34	0.56
2:I:327:LEU:HD21	2:I:357:HIS:CD2	2.41	0.56
2:J:239:ASN:HA	2:J:242:HIS:CD2	2.41	0.56
3:K:74:GLY:O	3:K:77:THR:OG1	2.24	0.56
1:B:603:VAL:HG13	1:B:604:ARG:H	1.70	0.56
2:F:400:ALA:HB1	2:F:405:LEU:HD22	1.87	0.56
1:A:674:GLN:HG2	1:A:692:THR:OG1	2.06	0.55
2:F:410:ALA:HA	2:F:452:PHE:CE1	2.41	0.55
1:A:170:TYR:HA	1:A:173:GLN:HB2	1.89	0.55
2:D:489:SER:O	2:D:491:ALA:N	2.40	0.55
2:E:316:MET:HE3	2:E:504:ARG:HG2	1.88	0.55
2:F:166:MET:HG2	2:F:171:CYS:HA	1.89	0.55
2:H:283:GLU:HA	2:H:285:VAL:HG12	1.88	0.55
2:I:229:ARG:HA	2:I:257:ALA:HA	1.88	0.55
2:J:278:HIS:CE1	2:J:282:GLU:HG3	2.41	0.55
2:D:484:THR:HG21	2:J:474:ALA:HB3	1.89	0.55
2:F:425:HIS:CE1	2:F:427:SER:HB2	2.41	0.55
1:B:591:ARG:O	1:B:602:HIS:ND1	2.39	0.55
2:D:221:GLN:O	2:D:274:ARG:NH2	2.39	0.55
2:F:180:HIS:HB2	2:F:184:ALA:HB3	1.89	0.55
3:L:45:ILE:HD11	3:L:96:LYS:HG3	1.89	0.55
1:C:61:GLY:HA2	1:C:65:ASP:HB2	1.88	0.55
2:D:261:ILE:HD13	2:D:261:ILE:H	1.72	0.55
2:D:70:ASN:HB3	2:D:73:GLU:HB2	1.88	0.55
2:H:386:PHE:HB3	2:I:268:ALA:N	2.22	0.55
1:A:189:LYS:HG2	1:A:194:PRO:HG3	1.89	0.55
1:B:129:GLY:HA3	1:B:135:MET:HG2	1.89	0.55
2:F:142:PHE:HB3	2:F:177:SER:HB3	1.89	0.55
2:F:412:MET:O	2:F:414:SER:N	2.34	0.55
1:B:20:CYS:HB3	1:B:163:PHE:HE1	1.71	0.55
2:D:180:HIS:HB2	2:D:184:ALA:HB3	1.88	0.55
2:F:203:ILE:HA	2:F:229:ARG:HB2	1.88	0.55
2:H:408:LYS:HE2	2:I:261:ILE:HD12	1.89	0.55
2:D:339:LEU:N	2:D:392:HIS:O	2.36	0.55
3:M:74:GLY:O	3:M:77:THR:OG1	2.24	0.55
1:A:106:ASP:O	1:A:110:LEU:N	2.36	0.54
1:B:170:TYR:HA	1:B:173:GLN:HB2	1.89	0.54
2:E:162:MET:HG2	2:E:175:VAL:HG12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:272:ARG:HB3	2:I:275:ILE:HD12	1.89	0.54
2:I:467:LYS:HG3	2:I:487:ARG:HA	1.87	0.54
1:A:591:ARG:HG2	1:A:602:HIS:O	2.07	0.54
2:E:205:MET:HA	2:E:231:ALA:HB3	1.87	0.54
2:H:271:LEU:HB3	2:H:275:ILE:HD12	1.88	0.54
3:K:23:ILE:HB	3:K:81:PHE:HB2	1.88	0.54
3:K:45:ILE:HG13	3:K:99:LEU:HD13	1.88	0.54
2:H:289:PHE:HB2	2:H:296:ASN:OD1	2.07	0.54
2:I:446:MET:HG3	2:I:492:LEU:HG	1.89	0.54
1:A:22:VAL:HB	1:A:175:VAL:HG21	1.89	0.54
2:E:180:HIS:HB2	2:E:184:ALA:HB3	1.90	0.54
2:F:343:GLU:OE1	2:G:522:ARG:NH2	2.41	0.54
1:C:501:LEU:HD21	1:C:689:LEU:HB3	1.89	0.54
2:D:276:ARG:HH21	2:J:378:PHE:HD2	1.54	0.54
2:G:343:GLU:HA	2:G:397:PHE:HE1	1.73	0.54
2:H:397:PHE:O	2:H:399:GLU:N	2.39	0.54
2:J:242:HIS:HB2	2:J:247:ASP:OD1	2.07	0.54
2:D:392:HIS:CD2	2:D:416:LEU:HD13	2.43	0.54
2:F:425:HIS:HE1	2:F:427:SER:HB2	1.73	0.54
2:G:208:MET:HE3	2:G:233:LEU:HB2	1.90	0.54
2:H:314:SER:HG	2:I:527:THR:HG1	1.55	0.54
2:J:340:ALA:HA	2:J:394:TYR:HB3	1.89	0.54
1:C:9:ASN:ND2	1:C:16:THR:OG1	2.41	0.54
2:E:514:VAL:HG13	2:E:533:MET:HB2	1.90	0.54
2:G:100:LYS:HG3	2:G:105:MET:SD	2.48	0.54
2:G:81:LEU:HD21	2:G:96:TYR:HE2	1.72	0.54
2:H:333:MET:SD	2:H:333:MET:N	2.81	0.54
2:I:232:VAL:HG21	2:I:270:SER:HB3	1.89	0.54
1:A:102:LEU:HD11	1:A:131:ARG:NH2	2.23	0.54
1:C:461:LEU:HD22	1:C:468:PRO:HA	1.90	0.54
2:F:151:LYS:HD2	2:F:152:LYS:HG3	1.89	0.54
2:F:383:ASP:OD1	2:G:272:ARG:NH2	2.40	0.54
2:D:290:SER:N	2:D:325:GLN:OE1	2.41	0.54
2:G:339:LEU:HB2	2:G:393:LEU:HB3	1.89	0.54
2:J:261:ILE:O	2:J:263:ASP:N	2.40	0.54
1:B:204:THR:O	2:F:375:ASN:ND2	2.42	0.53
1:B:683:HIS:CE1	2:F:370:ARG:HH12	2.26	0.53
2:F:232:VAL:N	2:F:253:GLN:OE1	2.23	0.53
2:H:86:ILE:HG12	2:H:163:LEU:HB3	1.90	0.53
2:J:74:SER:O	2:J:76:GLY:N	2.35	0.53
2:E:70:ASN:HB3	2:E:73:GLU:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:259:PRO:HA	2:F:260:TRP:HB3	1.90	0.53
3:L:90:LYS:HD3	3:L:91:VAL:N	2.23	0.53
2:G:268:ALA:O	2:G:270:SER:N	2.39	0.53
2:I:401:GLU:H	2:I:431:SER:HB3	1.74	0.53
1:A:86:GLU:O	1:A:207:TRP:NE1	2.35	0.53
1:B:102:LEU:HD23	1:B:105:THR:HB	1.90	0.53
2:H:272:ARG:HH21	2:H:276:ARG:HB3	1.73	0.53
2:I:318:LYS:CE	2:I:502:LEU:CD1	2.85	0.53
1:C:22:VAL:HB	1:C:175:VAL:HG21	1.90	0.53
1:C:423:ASN:HB2	1:C:623:LYS:NZ	2.24	0.53
2:I:477:GLU:HG3	2:I:507:GLN:HE22	1.73	0.53
2:I:442:ILE:HD12	2:I:492:LEU:HD11	1.91	0.53
2:J:162:MET:HB2	2:J:177:SER:HB2	1.91	0.53
2:D:272:ARG:HB2	2:J:382:PHE:CZ	2.44	0.53
1:A:493:ASN:ND2	2:E:292:CYS:SG	2.82	0.53
2:I:124:ARG:HH22	2:I:159:GLU:HB2	1.73	0.53
2:I:70:ASN:HB3	2:I:73:GLU:HB2	1.90	0.53
2:J:110:ASP:OD1	2:J:121:GLN:NE2	2.39	0.53
1:C:573:LEU:HD11	1:C:593:ILE:HG12	1.91	0.53
2:I:201:GLN:HA	2:I:227:LYS:HG2	1.91	0.53
2:H:399:GLU:HB3	2:H:430:VAL:HG11	1.91	0.53
2:F:395:ASP:HB3	2:G:266:VAL:CG2	2.39	0.53
2:G:438:GLU:HA	2:G:441:MET:HG2	1.91	0.53
2:I:231:ALA:HA	2:I:253:GLN:HB3	1.91	0.53
1:C:482:ARG:NH1	1:C:689:LEU:O	2.43	0.52
2:E:397:PHE:CE2	2:F:450:LYS:HG3	2.44	0.52
2:E:79:SER:HB3	2:E:98:ILE:HD13	1.91	0.52
2:F:261:ILE:HG23	2:F:262:PRO:HD3	1.91	0.52
2:J:162:MET:HG2	2:J:175:VAL:HG12	1.90	0.52
1:B:235:ASP:HB2	1:B:459:HIS:CG	2.44	0.52
2:J:166:MET:O	2:J:171:CYS:N	2.36	0.52
1:A:233:PRO:HG3	1:A:415:LYS:HE3	1.91	0.52
2:E:371:GLU:O	2:E:375:ASN:ND2	2.39	0.52
1:A:575:GLU:CB	1:A:589:LYS:HG3	2.40	0.52
1:B:492:ASP:HB3	1:B:561:ALA:HB2	1.90	0.52
2:D:422:ILE:HD13	2:D:461:VAL:HB	1.91	0.52
2:E:316:MET:HA	2:E:504:ARG:HH11	1.75	0.52
2:F:220:ALA:HB2	2:F:261:ILE:HG21	1.90	0.52
2:J:141:LEU:HD23	2:J:192:ASN:HD22	1.74	0.52
2:J:429:VAL:HG13	2:J:430:VAL:H	1.74	0.52
1:B:541:VAL:HG21	1:B:547:ARG:HD3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ILE:HD12	2:D:251:MET:N	2.24	0.52
2:F:312:SER:N	2:F:318:LYS:HD3	2.23	0.52
2:F:317:GLY:O	2:F:319:SER:N	2.40	0.52
2:H:333:MET:O	2:H:335:LYS:HG2	2.09	0.52
2:D:351:GLU:HG3	2:E:279:LEU:HD21	1.91	0.52
2:G:392:HIS:CD2	2:G:416:LEU:HD13	2.45	0.52
2:H:502:LEU:HD23	2:H:514:VAL:HG21	1.92	0.52
2:I:373:ILE:HD12	2:J:276:ARG:HD3	1.91	0.52
1:C:423:ASN:HB2	1:C:623:LYS:HZ1	1.74	0.52
2:E:333:MET:O	2:E:335:LYS:N	2.42	0.52
2:G:241:CYS:HB2	2:G:250:ILE:HD11	1.90	0.52
2:G:364:GLN:HE21	2:H:524:THR:HA	1.73	0.52
2:I:84:ARG:HE	2:I:160:ILE:HG21	1.75	0.52
2:I:287:LEU:HD11	2:I:335:LYS:HE2	1.91	0.52
2:I:404:ARG:HB3	2:I:404:ARG:HH21	1.74	0.52
2:I:505:ASN:HB2	2:I:510:MET:HB2	1.91	0.52
2:E:343:GLU:OE1	2:F:522:ARG:NH2	2.42	0.52
2:E:340:ALA:N	2:E:422:ILE:O	2.42	0.52
2:I:533:MET:SD	2:I:534:GLU:N	2.83	0.52
1:C:22:VAL:HG21	1:C:172:VAL:HG22	1.92	0.52
2:F:389:ASP:HA	2:G:269:LEU:HD13	1.91	0.52
2:I:420:VAL:HG22	2:I:459:VAL:HB	1.92	0.52
2:D:269:LEU:HD13	2:J:382:PHE:HE1	1.74	0.52
1:A:608:ALA:O	1:A:610:LEU:N	2.38	0.52
1:C:212:GLU:CD	1:C:683:HIS:HE2	2.12	0.52
2:D:246:HIS:HB3	2:D:249:GLU:HB2	1.92	0.52
2:E:232:VAL:HB	2:E:253:GLN:HE22	1.75	0.52
2:E:339:LEU:HB2	2:E:393:LEU:HA	1.92	0.52
2:E:512:ASN:OD1	2:E:512:ASN:N	2.43	0.52
2:F:284:SER:HB3	2:F:303:ARG:HG3	1.92	0.52
1:B:55:LEU:HD13	1:B:89:ILE:HD11	1.91	0.51
2:D:392:HIS:HD2	2:D:416:LEU:HD13	1.74	0.51
2:G:514:VAL:HG13	2:G:533:MET:HB2	1.93	0.51
2:H:420:VAL:HG22	2:H:459:VAL:HB	1.92	0.51
1:A:396:ILE:HG22	1:A:401:GLU:HB2	1.92	0.51
2:H:266:VAL:HB	2:H:270:SER:O	2.10	0.51
2:I:181:GLY:O	2:I:183:SER:N	2.36	0.51
2:J:117:ASN:OD1	2:J:117:ASN:N	2.27	0.51
1:B:608:ALA:O	1:B:610:LEU:N	2.39	0.51
3:L:22:ALA:HB1	3:L:80:LEU:HD11	1.90	0.51
1:A:147:LEU:HD13	1:A:154:TYR:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:H	1:B:38:ASP:HB2	1.75	0.51
2:I:75:ASN:ND2	2:I:100:LYS:O	2.40	0.51
2:I:80:ALA:HB2	2:I:88:LYS:HG3	1.92	0.51
1:C:235:ASP:HB2	1:C:459:HIS:CE1	2.45	0.51
1:C:456:GLY:HA2	1:C:471:GLN:OE1	2.10	0.51
2:D:484:THR:HA	2:D:493:ARG:HH22	1.74	0.51
2:H:467:LYS:HE3	2:H:487:ARG:HD3	1.92	0.51
2:I:312:SER:N	2:I:466:LEU:HD21	2.23	0.51
1:B:484:LEU:HD22	1:B:529:LEU:HD21	1.92	0.51
1:C:484:LEU:HD22	1:C:529:LEU:HD21	1.93	0.51
2:E:324:GLN:HG3	2:E:356:LEU:HD21	1.92	0.51
2:F:162:MET:O	2:F:166:MET:HE1	2.10	0.51
1:B:496:TYR:CZ	1:B:505:ILE:HD11	2.45	0.51
2:E:308:ILE:HB	2:E:461:VAL:HG22	1.93	0.51
2:F:397:PHE:CD2	2:G:451:GLY:HA2	2.46	0.51
2:F:266:VAL:HA	2:F:268:ALA:H	1.75	0.51
2:H:70:ASN:HB3	2:H:73:GLU:HB2	1.93	0.51
2:I:289:PHE:N	2:I:296:ASN:OD1	2.44	0.51
2:D:514:VAL:HG13	2:D:533:MET:HB2	1.92	0.51
2:E:233:LEU:HB3	2:E:241:CYS:SG	2.51	0.51
2:I:152:LYS:HE3	2:I:255:TRP:CH2	2.46	0.51
2:J:147:TRP:CE2	2:J:174:PRO:HA	2.46	0.51
2:J:229:ARG:HB2	2:J:257:ALA:HB1	1.93	0.51
2:G:492:LEU:O	2:G:496:SER:OG	2.27	0.51
2:I:409:LEU:HD23	2:I:421:ILE:HG21	1.92	0.51
2:F:217:GLU:HA	2:F:261:ILE:HD11	1.92	0.50
2:I:338:GLY:O	2:I:422:ILE:N	2.40	0.50
1:B:573:LEU:HD22	1:B:590:ARG:HG3	1.92	0.50
2:E:266:VAL:HG11	2:E:271:LEU:HG	1.92	0.50
2:F:346:VAL:HG13	2:F:395:ASP:HB2	1.93	0.50
2:H:283:GLU:HG3	2:H:303:ARG:HG3	1.92	0.50
2:I:447:THR:HG22	2:I:495:LEU:HD21	1.93	0.50
1:C:85:ARG:HD2	1:C:219:ARG:HA	1.94	0.50
2:I:225:ALA:HA	2:I:228:VAL:HG22	1.94	0.50
2:I:473:LYS:HB2	2:I:477:GLU:HB2	1.93	0.50
2:H:476:GLU:HG3	2:I:529:ILE:HG12	1.92	0.50
1:B:85:ARG:HG3	1:B:222:TRP:CG	2.46	0.50
1:C:471:GLN:NE2	1:C:657:GLN:OE1	2.37	0.50
2:I:490:GLY:HA2	2:I:493:ARG:NE	2.26	0.50
1:A:584:GLN:HG2	1:A:586:VAL:HG22	1.92	0.50
1:B:566:ARG:O	1:B:570:GLN:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HA	1:C:57:VAL:HB	1.94	0.50
2:D:221:GLN:NE2	2:D:266:VAL:HA	2.26	0.50
2:F:393:LEU:O	2:G:267:SER:HB2	2.12	0.50
2:G:345:SER:O	2:G:349:THR:HG23	2.12	0.50
2:D:425:HIS:ND1	2:D:428:ILE:HG13	2.27	0.50
2:F:515:LEU:HD11	2:F:529:ILE:HD13	1.94	0.50
2:H:421:ILE:HG12	2:H:458:VAL:HG21	1.94	0.50
2:I:84:ARG:HH21	2:I:160:ILE:HG21	1.75	0.50
1:C:588:TRP:CE3	1:C:591:ARG:HG2	2.46	0.50
2:D:147:TRP:CE2	2:D:174:PRO:HA	2.46	0.50
2:E:151:LYS:HD2	2:E:152:LYS:HG3	1.94	0.50
2:E:194:GLU:H	2:E:194:GLU:CD	2.14	0.50
2:F:282:GLU:CD	2:F:285:VAL:HG22	2.31	0.50
2:I:340:ALA:N	2:I:422:ILE:O	2.44	0.50
1:B:66:VAL:HG22	1:B:83:LEU:HD12	1.94	0.50
2:D:413:ARG:NH2	2:D:456:THR:O	2.30	0.50
2:F:86:ILE:HA	2:F:167:GLU:OE2	2.12	0.50
2:H:180:HIS:HB2	2:H:184:ALA:HB3	1.94	0.50
2:H:302:ALA:HB2	2:H:308:ILE:HD11	1.94	0.50
2:I:426:ILE:HG22	2:I:464:CYS:HA	1.94	0.50
2:J:371:GLU:O	2:J:375:ASN:ND2	2.45	0.50
1:C:496:TYR:CZ	1:C:505:ILE:HD11	2.47	0.49
2:F:260:TRP:HA	2:F:261:ILE:CB	2.41	0.49
2:H:78:TYR:CE1	2:H:97:TRP:HB3	2.47	0.49
2:I:411:TYR:HE2	2:J:266:VAL:HG11	1.76	0.49
1:B:363:VAL:HG13	1:B:365:ASP:H	1.76	0.49
1:C:26:TYR:CD1	1:C:199:THR:HG21	2.47	0.49
2:E:140:ALA:HB3	2:E:179:GLY:HA3	1.94	0.49
2:E:339:LEU:N	2:E:392:HIS:O	2.43	0.49
2:E:84:ARG:HA	2:E:243:LEU:HD11	1.94	0.49
2:F:152:LYS:HG2	2:F:201:GLN:HB2	1.94	0.49
2:H:260:TRP:C	2:H:262:PRO:HD3	2.33	0.49
2:I:306:GLU:HB3	2:I:450:LYS:HD3	1.93	0.49
1:C:645:ASP:HB3	1:C:665:ILE:HD13	1.95	0.49
2:D:534:GLU:HG3	2:D:545:SER:HB2	1.94	0.49
2:G:151:LYS:HD2	2:G:152:LYS:HG3	1.92	0.49
2:G:292:CYS:HA	2:G:544:PRO:HB3	1.93	0.49
2:G:316:MET:HA	2:G:504:ARG:HH11	1.77	0.49
2:E:203:ILE:HD12	2:E:229:ARG:HD2	1.94	0.49
2:F:220:ALA:HB2	2:F:261:ILE:CG2	2.43	0.49
2:D:340:ALA:HA	2:D:394:TYR:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:THR:HG21	1:B:363:VAL:HB	1.93	0.49
1:B:368:VAL:O	1:B:372:VAL:HG23	2.12	0.49
2:G:512:ASN:N	2:G:512:ASN:OD1	2.37	0.49
2:I:272:ARG:O	2:I:274:ARG:N	2.40	0.49
2:I:311:THR:O	2:I:318:LYS:CE	2.60	0.49
3:L:24:LEU:HB2	3:L:53:LEU:HD11	1.93	0.49
1:B:678:ARG:NH1	1:B:691:ASP:OD1	2.46	0.49
2:D:420:VAL:HG22	2:D:459:VAL:HB	1.94	0.49
2:F:484:THR:HA	2:F:493:ARG:HH22	1.78	0.49
2:I:313:GLY:HA3	2:I:475:HIS:HB3	1.93	0.49
1:A:85:ARG:HD2	1:A:219:ARG:HA	1.94	0.49
1:B:25:ASP:HB3	1:B:28:THR:OG1	2.12	0.49
2:G:80:ALA:HB2	2:G:88:LYS:HG3	1.94	0.49
2:I:318:LYS:NZ	2:I:502:LEU:HB2	2.27	0.49
2:I:299:THR:HA	2:I:521:CYS:SG	2.53	0.49
2:J:75:ASN:HB2	2:J:100:LYS:HG2	1.95	0.49
3:L:37:MET:N	3:L:37:MET:SD	2.85	0.49
1:A:128:TRP:CE3	1:A:131:ARG:HD2	2.48	0.49
1:A:154:TYR:HB2	1:A:158:MET:SD	2.52	0.49
2:D:412:MET:O	2:D:417:GLY:N	2.46	0.49
2:E:80:ALA:HB2	2:E:88:LYS:HG3	1.95	0.49
1:A:578:GLN:HB3	1:A:587:LYS:HZ1	1.78	0.49
1:B:363:VAL:HG22	1:B:364:VAL:HG12	1.95	0.49
1:B:423:ASN:OD1	1:B:599:ARG:NH2	2.45	0.49
1:B:608:ALA:C	1:B:610:LEU:H	2.15	0.49
1:A:103:LYS:HD3	1:A:120:PHE:CG	2.48	0.48
1:A:15:VAL:HG22	1:A:72:LEU:HD21	1.93	0.48
2:G:110:ASP:OD1	2:G:121:GLN:NE2	2.38	0.48
2:H:153:ILE:HA	2:H:174:PRO:HB2	1.94	0.48
2:H:314:SER:OG	2:I:527:THR:OG1	2.25	0.48
2:I:344:GLU:HA	2:J:454:LYS:HZ1	1.77	0.48
2:I:510:MET:N	2:I:511:PRO:HD2	2.27	0.48
2:J:204:LEU:N	2:J:229:ARG:O	2.43	0.48
1:A:588:TRP:CZ2	1:A:591:ARG:HD3	2.49	0.48
2:D:286:GLY:O	2:D:302:ALA:N	2.43	0.48
2:G:290:SER:N	2:G:325:GLN:OE1	2.43	0.48
2:H:283:GLU:HA	2:H:285:VAL:N	2.28	0.48
2:G:142:PHE:HB3	2:G:177:SER:HB3	1.94	0.48
2:H:77:ARG:HH22	2:H:100:LYS:HZ3	1.61	0.48
1:C:376:ASP:HB3	1:C:379:LYS:HB2	1.96	0.48
2:F:153:ILE:HA	2:F:174:PRO:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:392:HIS:HB3	2:F:266:VAL:HG12	1.95	0.48
2:G:147:TRP:CD2	2:G:174:PRO:HA	2.49	0.48
2:G:397:PHE:CE2	2:H:450:LYS:HE2	2.49	0.48
2:I:284:SER:HA	2:I:523:PHE:CZ	2.45	0.48
3:K:24:LEU:HD11	3:K:78:LEU:HB3	1.95	0.48
1:C:59:HIS:CD2	1:C:125:LEU:HG	2.48	0.48
2:F:412:MET:HB3	2:F:418:CYS:SG	2.54	0.48
2:I:235:CYS:HB2	2:I:241:CYS:SG	2.54	0.48
2:I:340:ALA:HA	2:I:394:TYR:HB3	1.95	0.48
2:D:162:MET:HG2	2:D:175:VAL:HG12	1.95	0.48
2:D:474:ALA:HA	2:D:479:ARG:HD2	1.95	0.48
2:G:333:MET:O	2:G:335:LYS:N	2.46	0.48
2:I:283:GLU:HG3	2:I:303:ARG:HG3	1.96	0.48
2:I:477:GLU:HA	2:I:507:GLN:HE22	1.78	0.48
3:L:13:ASP:O	3:L:18:LYS:HD3	2.14	0.48
1:A:575:GLU:HG3	1:A:589:LYS:HE3	1.96	0.48
1:C:24:TYR:HB2	1:C:31:TYR:CD2	2.49	0.48
2:E:502:LEU:HD23	2:E:514:VAL:HG21	1.94	0.48
2:E:397:PHE:HD2	2:F:451:GLY:HA2	1.79	0.48
2:F:77:ARG:HH21	2:F:98:ILE:HG21	1.79	0.48
2:G:84:ARG:O	2:G:239:ASN:ND2	2.45	0.48
3:K:90:LYS:HA	3:K:90:LYS:NZ	2.29	0.48
2:D:341:MET:HG3	2:D:349:THR:HB	1.96	0.48
1:B:578:GLN:HG3	1:B:585:GLN:HB2	1.95	0.48
1:C:473:GLY:HA3	1:C:703:CYS:HB3	1.96	0.48
2:D:221:GLN:HE21	2:D:266:VAL:HA	1.78	0.48
2:D:506:GLN:HB2	2:E:527:THR:OG1	2.14	0.48
2:G:124:ARG:HA	2:G:129:ASN:O	2.14	0.48
2:I:392:HIS:ND1	2:J:266:VAL:O	2.46	0.48
2:J:292:CYS:HB2	2:J:533:MET:HG2	1.95	0.48
2:E:242:HIS:ND1	2:E:247:ASP:OD1	2.32	0.48
2:E:393:LEU:O	2:F:265:VAL:HB	2.13	0.48
2:E:351:GLU:HG3	2:F:279:LEU:HD21	1.96	0.48
2:H:194:GLU:H	2:H:194:GLU:CD	2.16	0.48
2:I:504:ARG:HH11	2:I:512:ASN:HA	1.79	0.48
1:B:453:ALA:O	1:B:459:HIS:NE2	2.33	0.47
2:G:75:ASN:ND2	2:G:100:LYS:O	2.47	0.47
2:I:223:LEU:HD21	2:I:228:VAL:HG13	1.95	0.47
2:I:286:GLY:O	2:I:303:ARG:NH1	2.47	0.47
1:A:108:GLY:O	1:A:112:SER:OG	2.28	0.47
1:B:584:GLN:HG2	1:B:586:VAL:HG23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:474:ALA:O	2:D:476:GLU:N	2.47	0.47
2:E:312:SER:OG	2:E:318:LYS:HG3	2.15	0.47
2:F:345:SER:O	2:F:349:THR:HG23	2.14	0.47
2:G:425:HIS:ND1	2:G:428:ILE:HG13	2.28	0.47
2:G:395:ASP:CG	2:H:274:ARG:HH12	2.17	0.47
2:J:295:ILE:HD12	2:J:295:ILE:H	1.79	0.47
1:A:143:PHE:HE2	1:A:158:MET:HG3	1.79	0.47
1:B:677:MET:HG2	1:B:692:THR:HG23	1.95	0.47
2:F:207:ASP:O	2:F:213:ARG:NH2	2.37	0.47
2:F:397:PHE:HD2	2:G:451:GLY:HA2	1.79	0.47
2:F:379:ASP:OD1	2:G:272:ARG:NH1	2.47	0.47
2:G:305:GLY:HA2	2:G:454:LYS:HA	1.95	0.47
3:L:45:ILE:HG23	3:L:49:TYR:HD1	1.78	0.47
1:A:235:ASP:HB2	1:A:459:HIS:CE1	2.49	0.47
2:D:248:ARG:HH21	2:E:138:SER:HB2	1.79	0.47
2:F:166:MET:H	2:F:166:MET:CE	2.27	0.47
2:H:100:LYS:HG3	2:H:105:MET:SD	2.54	0.47
2:H:365:SER:HB3	2:H:368:LEU:HB2	1.97	0.47
2:I:318:LYS:NZ	2:I:502:LEU:CA	2.75	0.47
2:J:94:ALA:HA	2:J:146:LEU:HD11	1.96	0.47
1:A:341:HIS:CG	1:A:342:ILE:N	2.82	0.47
2:G:107:GLN:HB2	2:G:124:ARG:HG3	1.97	0.47
2:F:393:LEU:H	2:G:267:SER:HB2	1.78	0.47
2:G:425:HIS:HE1	2:G:427:SER:HB2	1.77	0.47
1:C:59:HIS:CG	1:C:125:LEU:HG	2.49	0.47
1:C:401:GLU:OE1	1:C:404:LYS:HB3	2.14	0.47
2:D:522:ARG:NH2	2:J:343:GLU:OE1	2.47	0.47
2:G:412:MET:HG2	2:G:416:LEU:HD12	1.96	0.47
2:H:283:GLU:N	2:H:284:SER:HB3	2.30	0.47
2:H:402:THR:HG21	2:H:448:LYS:HZ1	1.79	0.47
1:A:429:ARG:HD3	1:A:653:HIS:CG	2.49	0.47
1:C:368:VAL:O	1:C:372:VAL:HG23	2.15	0.47
2:I:151:LYS:HD2	2:I:152:LYS:HG3	1.96	0.47
2:I:272:ARG:CZ	2:I:276:ARG:HE	2.28	0.47
2:J:421:ILE:HG12	2:J:458:VAL:HG21	1.96	0.47
1:A:588:TRP:CE2	1:A:591:ARG:HD3	2.50	0.47
1:B:143:PHE:O	1:B:147:LEU:HG	2.14	0.47
1:B:515:LEU:HD12	1:B:520:ASN:HB3	1.96	0.47
1:C:604:ARG:HE	1:C:606:PRO:HD3	1.79	0.47
1:C:99:HIS:HB3	1:C:102:LEU:HG	1.97	0.47
2:F:259:PRO:HA	2:F:260:TRP:CB	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:326:ALA:HB1	2:H:337:VAL:HG11	1.96	0.47
1:B:190:HIS:NE2	1:B:598:GLY:O	2.48	0.47
2:D:96:TYR:CE1	2:D:107:GLN:HB3	2.50	0.47
2:F:169:GLN:NE2	2:F:173:TYR:HB2	2.30	0.47
2:F:309:MET:O	2:F:500:ILE:N	2.42	0.47
2:G:194:GLU:CD	2:G:194:GLU:H	2.17	0.47
2:H:106:TYR:CE2	2:H:125:ASP:HB3	2.50	0.47
1:A:217:GLU:OE2	1:A:423:ASN:ND2	2.31	0.47
1:B:3:VAL:HA	1:B:57:VAL:HB	1.96	0.47
2:D:475:HIS:H	2:D:479:ARG:HD2	1.79	0.47
2:H:162:MET:HB2	2:H:177:SER:HB2	1.97	0.47
2:H:229:ARG:HA	2:H:259:PRO:HD2	1.97	0.47
2:D:267:SER:HB2	2:J:393:LEU:H	1.80	0.47
1:A:233:PRO:HB2	1:A:456:GLY:O	2.15	0.47
1:C:338:SER:HB3	1:C:341:HIS:CG	2.49	0.47
1:C:485:ALA:HA	1:C:488:MET:HG2	1.97	0.47
2:D:69:TRP:CH2	2:D:123:VAL:HG11	2.50	0.47
2:D:412:MET:HB3	2:D:418:CYS:SG	2.55	0.47
2:E:162:MET:HB2	2:E:177:SER:HB2	1.97	0.47
2:G:84:ARG:HA	2:G:243:LEU:HD11	1.97	0.47
2:I:487:ARG:HG2	2:I:488:GLY:H	1.80	0.47
2:J:287:LEU:HG	2:J:329:TRP:CG	2.50	0.47
1:B:489:ALA:HA	1:B:492:ASP:OD1	2.16	0.46
1:C:18:PHE:HB2	1:C:72:LEU:HD13	1.97	0.46
2:F:170:ASP:O	2:F:170:ASP:CG	2.52	0.46
1:A:35:ARG:H	1:A:38:ASP:HB2	1.80	0.46
1:B:603:VAL:HG13	1:B:604:ARG:N	2.30	0.46
1:C:538:GLY:HA3	1:C:544:GLY:O	2.15	0.46
2:I:401:GLU:HG2	2:I:402:THR:HG22	1.96	0.46
3:L:37:MET:O	3:L:40:PRO:HD2	2.16	0.46
1:B:574:VAL:HG13	1:B:586:VAL:HG13	1.97	0.46
1:C:106:ASP:CG	1:C:131:ARG:HH22	2.17	0.46
1:C:193:PRO:O	1:C:198:PHE:HZ	1.97	0.46
2:D:276:ARG:HD2	2:J:373:ILE:HG23	1.96	0.46
2:G:307:VAL:HG22	2:G:460:LEU:HB3	1.96	0.46
2:H:271:LEU:HB3	2:H:275:ILE:CD1	2.45	0.46
2:I:287:LEU:HD21	2:I:335:LYS:HG3	1.96	0.46
2:D:233:LEU:HB3	2:D:241:CYS:SG	2.55	0.46
2:D:274:ARG:O	2:D:278:HIS:N	2.46	0.46
2:E:147:TRP:CE2	2:E:174:PRO:HA	2.49	0.46
2:E:412:MET:HE1	2:E:421:ILE:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:261:ILE:H	2:F:262:PRO:CD	2.28	0.46
2:G:339:LEU:O	2:G:393:LEU:HA	2.16	0.46
2:J:299:THR:O	2:J:303:ARG:NH1	2.29	0.46
2:G:236:LYS:H	2:G:240:GLU:HG2	1.81	0.46
2:J:139:ASP:HB2	2:J:192:ASN:ND2	2.30	0.46
1:A:106:ASP:OD1	1:A:131:ARG:NH2	2.49	0.46
1:A:428:GLY:HA3	1:A:619:ALA:HB3	1.98	0.46
2:F:105:MET:HG2	2:F:126:LYS:NZ	2.31	0.46
2:F:80:ALA:HB2	2:F:88:LYS:HG3	1.96	0.46
2:H:391:PHE:O	2:I:268:ALA:HB3	2.15	0.46
2:I:318:LYS:HE3	2:I:502:LEU:CB	2.32	0.46
1:A:330:GLU:HG3	3:K:31:TRP:CH2	2.51	0.46
1:B:139:TYR:OH	1:B:164:ASN:ND2	2.34	0.46
1:C:429:ARG:H	1:C:619:ALA:HB1	1.81	0.46
2:H:341:MET:HG3	2:H:349:THR:HG21	1.97	0.46
2:I:287:LEU:HD23	2:I:329:TRP:CD2	2.50	0.46
2:J:345:SER:O	2:J:349:THR:HG23	2.16	0.46
1:A:578:GLN:NE2	1:A:579:TRP:O	2.49	0.46
2:D:313:GLY:O	2:D:318:LYS:NZ	2.49	0.46
2:E:203:ILE:HG13	2:E:254:VAL:HG13	1.97	0.46
2:F:155:VAL:HB	2:F:204:LEU:HD23	1.97	0.46
2:J:319:SER:HB3	2:J:323:ARG:NH2	2.31	0.46
1:C:454:ALA:C	1:C:459:HIS:HE2	2.19	0.46
1:C:489:ALA:O	2:H:288:LEU:HD23	2.16	0.46
2:D:339:LEU:HB2	2:D:393:LEU:HA	1.98	0.46
2:D:292:CYS:HB2	2:D:533:MET:HG2	1.98	0.46
2:F:514:VAL:HG13	2:F:533:MET:HB2	1.98	0.46
2:F:361:ARG:NH1	2:F:535:TYR:OH	2.48	0.46
2:H:84:ARG:HH21	2:H:160:ILE:HG21	1.80	0.46
2:H:272:ARG:CZ	2:H:273:GLU:HA	2.45	0.46
2:J:205:MET:HG3	2:J:233:LEU:HD11	1.97	0.46
1:A:209:GLU:OE2	2:D:375:ASN:ND2	2.49	0.46
1:B:139:TYR:HB2	1:B:170:TYR:CB	2.46	0.46
1:C:462:ASP:OD2	1:C:465:THR:OG1	2.28	0.46
2:E:373:ILE:HD11	2:F:280:SER:HA	1.97	0.46
2:F:411:TYR:CE2	2:G:262:PRO:HA	2.51	0.46
2:I:287:LEU:HB2	2:I:303:ARG:HH12	1.81	0.46
2:I:510:MET:O	2:I:512:ASN:N	2.48	0.46
2:J:311:THR:HG21	2:J:486:LEU:HD21	1.97	0.46
2:J:290:SER:N	2:J:325:GLN:OE1	2.46	0.46
3:K:23:ILE:HD13	3:K:54:THR:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:34:PRO:HB2	3:M:76:PRO:HD3	1.98	0.46
2:D:151:LYS:HD2	2:D:152:LYS:HG3	1.98	0.45
2:D:542:LEU:HA	2:D:542:LEU:HD13	1.75	0.45
2:E:124:ARG:HH22	2:E:159:GLU:HB2	1.80	0.45
2:E:430:VAL:HG11	2:F:447:THR:HG21	1.98	0.45
2:H:229:ARG:HE	2:H:229:ARG:HB3	1.57	0.45
2:H:77:ARG:HH22	2:H:100:LYS:NZ	2.13	0.45
2:I:497:ASP:OD1	2:I:522:ARG:HB3	2.16	0.45
2:E:382:PHE:HE2	2:F:272:ARG:HG3	1.82	0.45
2:F:333:MET:O	2:F:335:LYS:HG2	2.16	0.45
2:F:421:ILE:HG12	2:F:458:VAL:HG21	1.96	0.45
1:B:22:VAL:HG23	1:B:171:ASN:ND2	2.27	0.45
1:C:237:LYS:O	1:C:241:GLU:HB2	2.16	0.45
1:C:405:ALA:O	1:C:407:LEU:N	2.41	0.45
2:F:413:ARG:NH2	2:F:457:GLY:O	2.49	0.45
2:G:421:ILE:HG12	2:G:458:VAL:HG21	1.98	0.45
2:I:77:ARG:HH12	2:I:100:LYS:HB2	1.81	0.45
2:I:311:THR:C	2:I:318:LYS:CE	2.85	0.45
2:I:486:LEU:HD22	2:I:487:ARG:H	1.80	0.45
2:J:194:GLU:H	2:J:194:GLU:CD	2.20	0.45
2:J:432:ALA:N	2:J:433:SER:HA	2.32	0.45
1:A:341:HIS:CD2	1:A:342:ILE:HG13	2.50	0.45
1:B:143:PHE:CE2	1:B:147:LEU:HD11	2.51	0.45
1:C:257:LEU:HD21	1:C:385:LEU:HB2	1.98	0.45
2:F:194:GLU:CD	2:F:194:GLU:H	2.20	0.45
2:H:246:HIS:HB3	2:H:249:GLU:OE1	2.16	0.45
1:A:57:VAL:HG13	1:A:89:ILE:HD11	1.98	0.45
1:C:128:TRP:CE3	1:C:131:ARG:HD2	2.51	0.45
1:C:427:THR:HA	1:C:601:VAL:HG13	1.98	0.45
2:E:260:TRP:HA	2:E:261:ILE:HA	1.45	0.45
2:E:301:GLY:O	2:E:303:ARG:NH1	2.50	0.45
1:A:495:GLU:OE2	2:E:546:SER:HB3	2.17	0.45
2:G:162:MET:HB2	2:G:177:SER:HB2	1.98	0.45
3:M:41:ILE:HD12	3:M:96:LYS:HB2	1.97	0.45
2:G:242:HIS:ND1	2:G:247:ASP:OD1	2.38	0.45
2:I:269:LEU:HD22	2:I:270:SER:HA	1.98	0.45
2:J:256:ASN:O	2:J:256:ASN:ND2	2.49	0.45
1:A:50:VAL:HG13	1:A:87:ASN:ND2	2.31	0.45
1:C:140:LYS:HG2	1:C:144:LYS:HE3	1.99	0.45
1:C:397:GLY:HA2	1:C:401:GLU:HB3	1.99	0.45
2:D:75:ASN:HD22	2:D:100:LYS:HB3	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:481:VAL:HG23	2:D:485:ASP:HB2	1.98	0.45
2:E:232:VAL:O	2:E:253:GLN:NE2	2.50	0.45
2:G:426:ILE:HD12	2:G:462:VAL:HG11	1.99	0.45
2:H:363:ARG:O	2:H:365:SER:N	2.41	0.45
2:J:108:VAL:HG13	2:J:123:VAL:HG22	1.98	0.45
2:J:261:ILE:C	2:J:263:ASP:H	2.20	0.45
2:J:394:TYR:HE2	2:J:408:LYS:HD2	1.81	0.45
1:A:6:ILE:HG12	1:A:65:ASP:OD2	2.17	0.45
2:D:229:ARG:HB3	2:D:257:ALA:HB3	1.99	0.45
2:D:309:MET:O	2:D:500:ILE:N	2.45	0.45
2:D:411:TYR:OH	2:E:260:TRP:O	2.26	0.45
2:G:97:TRP:CZ3	2:G:99:ALA:HB2	2.51	0.45
1:A:495:GLU:O	1:A:499:GLU:HG2	2.17	0.45
1:A:57:VAL:HG22	1:A:89:ILE:HD11	1.99	0.45
1:B:102:LEU:HD13	1:B:121:GLY:HA2	1.97	0.45
1:B:678:ARG:NE	1:B:689:LEU:HD11	2.32	0.45
2:E:533:MET:HA	2:E:544:PRO:HA	1.98	0.45
2:F:316:MET:HB2	2:F:504:ARG:HH11	1.82	0.45
2:G:140:ALA:HB3	2:G:179:GLY:HA3	1.98	0.45
2:G:232:VAL:HG23	2:G:260:TRP:CE3	2.51	0.45
2:H:392:HIS:CD2	2:H:416:LEU:HD13	2.52	0.45
2:I:311:THR:O	2:I:311:THR:CG2	2.65	0.45
2:J:515:LEU:HD11	2:J:529:ILE:HD13	1.99	0.45
1:A:236:THR:O	1:A:240:GLU:HG3	2.17	0.45
2:E:397:PHE:CD2	2:F:451:GLY:HA2	2.52	0.45
2:G:502:LEU:HD23	2:G:514:VAL:HG21	1.98	0.45
2:I:194:GLU:H	2:I:194:GLU:CD	2.18	0.45
2:I:244:ASN:HB3	2:I:246:HIS:CE1	2.52	0.45
2:J:147:TRP:CD2	2:J:174:PRO:HA	2.52	0.45
3:M:17:LEU:HA	3:M:84:GLY:HA2	1.99	0.45
1:A:368:VAL:O	1:A:372:VAL:HG23	2.17	0.44
1:A:482:ARG:HG2	1:A:500:ILE:HG21	1.98	0.44
1:B:235:ASP:HB2	1:B:459:HIS:CD2	2.52	0.44
1:C:491:PHE:O	2:H:333:MET:HG3	2.17	0.44
2:F:166:MET:HE3	2:F:166:MET:H	1.82	0.44
2:F:403:ASP:HA	2:F:404:ARG:HA	1.61	0.44
2:H:147:TRP:CE2	2:H:174:PRO:HA	2.52	0.44
2:I:535:TYR:CD2	2:I:541:TRP:HB2	2.50	0.44
2:J:486:LEU:HD13	2:J:492:LEU:HD13	1.98	0.44
3:L:28:TRP:HB2	3:L:35:CYS:SG	2.57	0.44
1:A:147:LEU:HD13	1:A:154:TYR:CB	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LYS:HA	1:B:192:PHE:O	2.17	0.44
2:D:320:THR:HG21	2:D:535:TYR:HE1	1.83	0.44
2:E:402:THR:HG21	2:E:448:LYS:HZ2	1.82	0.44
2:H:278:HIS:O	2:H:282:GLU:N	2.50	0.44
2:H:369:LYS:NZ	2:I:284:SER:HB3	2.31	0.44
3:K:3:LYS:HD2	3:K:47:ASP:OD1	2.18	0.44
3:L:45:ILE:HG23	3:L:49:TYR:CD1	2.51	0.44
2:D:78:TYR:CE1	2:D:97:TRP:HB3	2.51	0.44
2:E:84:ARG:O	2:E:239:ASN:ND2	2.42	0.44
2:F:124:ARG:NH2	2:F:159:GLU:HB2	2.28	0.44
2:G:107:GLN:O	2:G:123:VAL:HA	2.17	0.44
2:G:124:ARG:NH2	2:G:159:GLU:HB2	2.31	0.44
2:H:205:MET:HG3	2:H:231:ALA:HB3	1.98	0.44
2:H:282:GLU:C	2:H:284:SER:HB3	2.37	0.44
1:B:339:ARG:H	1:B:339:ARG:HD2	1.82	0.44
2:D:375:ASN:OD1	2:D:376:GLY:N	2.51	0.44
2:F:484:THR:HA	2:F:493:ARG:NH2	2.33	0.44
2:H:347:GLU:HG2	2:H:347:GLU:H	1.42	0.44
2:I:311:THR:C	2:I:318:LYS:HD2	2.37	0.44
2:J:114:GLN:OE1	2:J:148:ASN:ND2	2.50	0.44
2:J:139:ASP:HB2	2:J:192:ASN:HD21	1.82	0.44
2:I:411:TYR:CE1	2:J:260:TRP:HA	2.52	0.44
1:A:338:SER:O	1:A:341:HIS:ND1	2.50	0.44
1:A:640:HIS:CD2	1:A:647:ALA:HA	2.53	0.44
1:B:59:HIS:CG	1:B:125:LEU:HG	2.53	0.44
2:D:252:GLU:O	2:D:256:ASN:HB2	2.18	0.44
2:D:271:LEU:O	2:D:275:ILE:HG13	2.18	0.44
2:E:229:ARG:NH1	2:E:254:VAL:O	2.42	0.44
2:F:166:MET:HB3	2:F:166:MET:HE2	1.83	0.44
3:L:38:ILE:HG21	3:L:93:ALA:HA	2.00	0.44
1:A:261:PHE:HA	1:A:262:GLY:HA3	1.76	0.44
1:B:491:PHE:CE2	1:B:565:LEU:HA	2.53	0.44
2:E:138:SER:HA	2:E:180:HIS:NE2	2.32	0.44
2:E:369:LYS:O	2:E:373:ILE:HG13	2.16	0.44
1:C:491:PHE:HA	2:H:333:MET:HE2	1.99	0.44
1:A:489:ALA:HA	1:A:492:ASP:OD1	2.18	0.44
1:B:235:ASP:HB2	1:B:459:HIS:CE1	2.52	0.44
2:D:100:LYS:HG3	2:D:105:MET:SD	2.58	0.44
2:D:251:MET:O	2:D:255:TRP:HD1	1.99	0.44
2:F:320:THR:HG21	2:F:535:TYR:HE1	1.83	0.44
2:G:182:ALA:HB1	2:G:215:ALA:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:402:THR:HG21	2:G:448:LYS:HZ1	1.82	0.44
2:E:113:ASP:HB3	2:E:117:ASN:O	2.18	0.44
2:I:311:THR:C	2:I:318:LYS:CD	2.86	0.44
2:J:278:HIS:O	2:J:282:GLU:HB2	2.18	0.44
2:J:74:SER:HB2	2:J:99:ALA:HB1	1.99	0.44
2:F:475:HIS:H	2:F:479:ARG:HD2	1.82	0.44
2:H:250:ILE:O	2:H:254:VAL:HG23	2.18	0.44
2:I:410:ALA:HA	2:I:452:PHE:CE1	2.52	0.44
1:A:535:GLU:O	1:A:539:GLN:HG3	2.18	0.43
1:B:676:ALA:O	1:B:680:VAL:HG23	2.17	0.43
1:C:351:TRP:CZ3	1:C:353:PRO:HG3	2.53	0.43
1:C:475:ASP:HA	1:C:655:GLU:HA	2.00	0.43
2:D:121:GLN:HB2	2:D:133:THR:OG1	2.18	0.43
2:G:147:TRP:CE2	2:G:174:PRO:HA	2.52	0.43
2:G:357:HIS:ND1	2:G:385:LEU:HB2	2.32	0.43
2:I:312:SER:HB3	2:I:318:LYS:NZ	2.30	0.43
3:L:23:ILE:HB	3:L:81:PHE:HB2	1.99	0.43
1:A:103:LYS:HD3	1:A:120:PHE:CD1	2.53	0.43
1:A:429:ARG:HH11	1:A:653:HIS:N	2.17	0.43
2:D:154:VAL:HA	2:D:203:ILE:HB	2.00	0.43
2:F:162:MET:CB	2:F:177:SER:HB2	2.48	0.43
2:G:426:ILE:O	2:G:426:ILE:HG12	2.18	0.43
3:K:32:CYS:SG	3:K:34:PRO:HD2	2.58	0.43
1:A:547:ARG:O	1:A:551:LEU:HB2	2.18	0.43
1:B:388:GLU:O	1:B:392:ILE:HG12	2.19	0.43
2:D:250:ILE:H	2:D:250:ILE:HG13	1.44	0.43
2:D:402:THR:HG21	2:D:448:LYS:HZ1	1.83	0.43
2:D:307:VAL:HB	2:D:496:SER:HA	2.01	0.43
2:I:427:SER:HB2	2:I:465:HIS:CE1	2.53	0.43
2:J:258:GLY:HA3	2:J:260:TRP:CH2	2.54	0.43
2:J:316:MET:HE3	2:J:504:ARG:HG2	1.99	0.43
2:J:78:TYR:CD2	2:J:92:GLN:HG2	2.53	0.43
1:B:603:VAL:HG21	1:B:609:ALA:HA	2.01	0.43
1:A:388:GLU:O	1:A:392:ILE:HG12	2.18	0.43
1:B:13:GLU:OE1	1:B:13:GLU:N	2.51	0.43
2:D:229:ARG:NH2	2:D:257:ALA:H	2.15	0.43
2:D:267:SER:HB2	2:J:392:HIS:HA	1.99	0.43
2:F:311:THR:HG21	2:F:486:LEU:HD21	1.99	0.43
2:F:84:ARG:HH21	2:F:160:ILE:HG21	1.82	0.43
2:G:162:MET:HG2	2:G:175:VAL:HG12	2.01	0.43
2:G:284:SER:O	2:G:303:ARG:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:512:ASN:OD1	2:H:512:ASN:N	2.47	0.43
2:I:251:MET:O	2:I:254:VAL:HB	2.18	0.43
2:J:122:LYS:HB3	2:J:122:LYS:HE2	1.79	0.43
2:J:420:VAL:HG22	2:J:459:VAL:HB	2.01	0.43
3:K:22:ALA:HB1	3:K:53:LEU:HD12	2.01	0.43
3:M:34:PRO:HB3	3:M:93:ALA:HB2	2.00	0.43
1:A:490:ARG:NH1	1:A:568:SER:OG	2.52	0.43
1:A:530:TYR:CD1	1:A:611:ASN:HB2	2.54	0.43
2:D:164:THR:O	2:D:168:LEU:HG	2.17	0.43
2:D:221:GLN:HE21	2:D:266:VAL:HG22	1.82	0.43
2:E:77:ARG:HH12	2:E:100:LYS:HB2	1.84	0.43
2:F:111:TYR:CZ	2:F:142:PHE:HB2	2.53	0.43
2:H:80:ALA:HB2	2:H:88:LYS:HG3	2.00	0.43
2:I:269:LEU:HA	2:I:270:SER:HA	1.66	0.43
2:I:303:ARG:NE	2:I:303:ARG:HA	2.33	0.43
2:I:443:ASP:O	2:I:447:THR:HG23	2.18	0.43
1:A:533:GLY:O	1:A:537:ILE:HG12	2.19	0.43
2:D:426:ILE:O	2:D:426:ILE:HG12	2.19	0.43
2:E:504:ARG:NH1	2:E:506:GLN:HE21	2.16	0.43
2:E:534:GLU:HG3	2:E:545:SER:HB2	2.00	0.43
2:F:166:MET:HG2	2:F:171:CYS:SG	2.58	0.43
2:G:287:LEU:HG	2:G:329:TRP:CE2	2.54	0.43
2:H:329:TRP:CZ3	2:H:420:VAL:HG11	2.54	0.43
2:H:405:LEU:O	2:H:409:LEU:HG	2.19	0.43
2:H:484:THR:HA	2:H:493:ARG:NH2	2.32	0.43
2:J:178:LEU:HD11	2:J:206:PHE:CZ	2.53	0.43
1:C:535:GLU:O	1:C:539:GLN:HG3	2.19	0.43
2:D:169:GLN:HB3	2:D:173:TYR:HD2	1.84	0.43
2:G:367:SER:HA	2:G:370:ARG:NH1	2.32	0.43
2:I:330:GLY:HA3	2:I:391:PHE:CZ	2.53	0.43
2:I:340:ALA:HB3	2:I:423:LEU:HA	2.01	0.43
2:I:298:LYS:HG2	2:I:526:ASP:OD2	2.19	0.43
2:J:429:VAL:HG23	2:J:438:GLU:OE1	2.19	0.43
3:L:76:PRO:HG2	3:L:92:GLY:O	2.18	0.43
1:A:330:GLU:HG3	3:K:31:TRP:HH2	1.84	0.43
1:C:426:VAL:HB	1:C:602:HIS:HB2	2.00	0.43
2:E:356:LEU:O	2:E:541:TRP:NE1	2.46	0.43
2:E:324:GLN:NE2	2:E:542:LEU:HB2	2.27	0.43
2:F:140:ALA:HB3	2:F:179:GLY:HA3	2.01	0.43
2:F:408:LYS:HE2	2:G:217:GLU:HG3	2.00	0.43
2:G:382:PHE:CE2	2:H:272:ARG:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:542:LEU:HD12	2:G:542:LEU:HA	1.83	0.43
2:H:492:LEU:H	2:H:492:LEU:HG	1.63	0.43
2:I:401:GLU:HA	2:I:430:VAL:O	2.19	0.43
1:A:478:GLY:O	1:A:482:ARG:HG3	2.19	0.43
1:A:688:CYS:SG	1:A:689:LEU:N	2.92	0.43
1:B:112:SER:HB2	1:B:114:LYS:HG2	2.01	0.43
1:C:129:GLY:HA3	1:C:135:MET:HG2	2.00	0.43
1:C:425:ALA:O	1:C:427:THR:N	2.52	0.43
1:C:59:HIS:ND1	1:C:91:THR:OG1	2.35	0.43
2:E:311:THR:HG21	2:E:486:LEU:HD21	2.01	0.43
2:F:412:MET:C	2:F:414:SER:H	2.20	0.43
2:I:142:PHE:HB3	2:I:177:SER:HB3	2.01	0.43
1:A:143:PHE:CD2	1:A:159:GLU:HB3	2.54	0.42
1:A:48:ALA:HB1	1:A:52:ARG:HH12	1.84	0.42
1:A:603:VAL:HG23	1:A:612:THR:HB	2.01	0.42
1:B:351:TRP:NE1	1:B:372:VAL:HG22	2.35	0.42
1:C:66:VAL:HG22	1:C:83:LEU:HD12	2.01	0.42
2:F:313:GLY:O	2:F:316:MET:HG2	2.18	0.42
2:F:397:PHE:CE2	2:G:450:LYS:HG3	2.53	0.42
2:I:91:CYS:HB3	2:I:96:TYR:O	2.19	0.42
2:J:429:VAL:HG22	2:J:430:VAL:N	2.34	0.42
1:B:461:LEU:HD13	1:B:466:GLY:HA2	2.00	0.42
1:B:427:THR:HG23	1:B:616:SER:HA	2.01	0.42
1:C:335:ASN:HB3	1:C:341:HIS:ND1	2.34	0.42
1:C:402:GLY:HA2	1:C:408:ARG:HE	1.83	0.42
2:D:258:GLY:HA2	2:D:259:PRO:HD3	1.91	0.42
2:F:534:GLU:HG3	2:F:545:SER:HB2	2.00	0.42
2:H:518:ILE:HD13	2:H:530:ALA:HB2	2.01	0.42
2:I:201:GLN:HE21	2:I:203:ILE:HD11	1.84	0.42
2:I:78:TYR:CE1	2:I:97:TRP:HB3	2.54	0.42
1:A:676:ALA:O	1:A:680:VAL:HG23	2.19	0.42
1:B:233:PRO:HB2	1:B:456:GLY:O	2.19	0.42
2:D:194:GLU:CD	2:D:194:GLU:H	2.22	0.42
2:F:425:HIS:HB3	2:F:428:ILE:HD11	2.01	0.42
2:F:292:CYS:HB2	2:F:533:MET:HG2	2.01	0.42
2:F:78:TYR:CE1	2:F:97:TRP:HB3	2.54	0.42
2:G:333:MET:O	2:G:335:LYS:HG2	2.19	0.42
2:G:81:LEU:HD21	2:G:96:TYR:CE2	2.53	0.42
2:I:413:ARG:HD3	2:I:458:VAL:HB	2.00	0.42
2:I:493:ARG:HG2	2:I:493:ARG:H	1.52	0.42
1:B:485:ALA:HA	1:B:488:MET:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ASP:O	1:B:538:GLY:N	2.43	0.42
1:C:573:LEU:HD22	1:C:590:ARG:O	2.19	0.42
2:E:392:HIS:HB3	2:F:266:VAL:CG1	2.49	0.42
2:F:373:ILE:HD11	2:G:279:LEU:HB3	2.02	0.42
2:G:344:GLU:HG3	2:G:349:THR:HG22	2.01	0.42
2:H:233:LEU:HB3	2:H:241:CYS:SG	2.59	0.42
2:I:401:GLU:HG3	2:I:431:SER:O	2.19	0.42
2:J:193:TYR:OH	2:J:224:PRO:O	2.23	0.42
1:A:575:GLU:HB2	1:A:589:LYS:N	2.35	0.42
1:A:603:VAL:HG23	1:A:612:THR:CB	2.50	0.42
1:C:393:GLN:O	1:C:397:GLY:N	2.43	0.42
1:C:85:ARG:HG3	1:C:222:TRP:CG	2.54	0.42
2:F:250:ILE:O	2:F:254:VAL:HG23	2.19	0.42
2:G:265:VAL:O	2:G:266:VAL:HG22	2.20	0.42
2:G:309:MET:HB3	2:G:499:ILE:HG12	2.02	0.42
2:G:91:CYS:HB3	2:G:96:TYR:O	2.19	0.42
2:I:140:ALA:HB3	2:I:179:GLY:HA3	2.01	0.42
2:I:395:ASP:N	2:J:265:VAL:HG11	2.33	0.42
1:B:351:TRP:CD1	1:B:372:VAL:HG13	2.55	0.42
2:D:263:ASP:HA	2:D:264:GLY:HA2	1.51	0.42
2:E:333:MET:O	2:E:335:LYS:HG2	2.19	0.42
2:F:105:MET:HG2	2:F:126:LYS:HZ3	1.85	0.42
2:H:124:ARG:HH22	2:H:159:GLU:HB2	1.85	0.42
2:H:284:SER:OG	2:H:284:SER:O	2.37	0.42
2:H:347:GLU:OE2	2:I:274:ARG:NH2	2.53	0.42
2:I:361:ARG:HB3	2:I:364:GLN:HB2	2.00	0.42
3:K:4:ILE:HG23	3:K:55:VAL:HG12	2.01	0.42
2:F:300:LEU:HD12	2:F:524:THR:HG22	2.01	0.42
2:G:325:GLN:HG3	2:G:329:TRP:CZ2	2.54	0.42
2:H:284:SER:O	2:H:285:VAL:HB	2.20	0.42
2:I:306:GLU:O	2:I:496:SER:HA	2.20	0.42
2:I:465:HIS:HB2	2:I:487:ARG:NH1	2.34	0.42
1:B:624:LEU:HD12	1:B:684:TRP:CH2	2.53	0.42
1:C:98:ILE:HD12	1:C:185:LEU:HD22	2.02	0.42
1:C:674:GLN:NE2	1:C:678:ARG:HH22	2.10	0.42
2:D:402:THR:HG21	2:D:448:LYS:NZ	2.35	0.42
2:E:104:VAL:HB	2:E:106:TYR:CE1	2.54	0.42
2:F:256:ASN:HB3	2:F:257:ALA:H	1.56	0.42
2:F:324:GLN:HE22	2:F:542:LEU:N	2.18	0.42
2:H:343:GLU:HG3	2:H:428:ILE:HD11	2.01	0.42
2:H:514:VAL:HG13	2:H:533:MET:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:124:ARG:HA	2:I:129:ASN:O	2.20	0.42
1:B:24:TYR:HB2	1:B:31:TYR:CD2	2.55	0.42
1:B:687:ARG:HB3	1:B:687:ARG:HH11	1.84	0.42
1:C:534:ASP:O	1:C:548:GLY:HA3	2.20	0.42
2:F:542:LEU:HA	2:F:542:LEU:HD13	1.76	0.42
2:G:347:GLU:HG3	2:H:278:HIS:CG	2.55	0.42
2:H:476:GLU:HG3	2:I:529:ILE:CG1	2.49	0.42
2:J:78:TYR:O	2:J:88:LYS:HG3	2.19	0.42
3:K:23:ILE:O	3:K:81:PHE:N	2.41	0.42
3:K:22:ALA:HB3	3:K:53:LEU:HA	2.01	0.42
1:A:334:PHE:CE1	1:A:341:HIS:HB3	2.55	0.42
1:C:189:LYS:HA	1:C:192:PHE:O	2.19	0.42
2:D:252:GLU:O	2:D:256:ASN:N	2.52	0.42
2:D:272:ARG:HD3	2:J:382:PHE:CG	2.54	0.42
2:D:308:ILE:HB	2:D:461:VAL:HG22	2.01	0.42
2:E:295:ILE:H	2:E:295:ILE:HD12	1.84	0.42
2:E:346:VAL:CG1	2:E:395:ASP:HB2	2.50	0.42
2:E:78:TYR:O	2:E:88:LYS:HE3	2.20	0.42
2:G:413:ARG:NH2	2:G:456:THR:O	2.34	0.42
2:I:287:LEU:HD13	2:I:303:ARG:HH22	1.84	0.42
2:I:345:SER:O	2:I:349:THR:HG22	2.19	0.42
2:I:437:ASP:OD1	2:I:439:ARG:HG3	2.20	0.42
2:J:248:ARG:O	2:J:252:GLU:HG3	2.20	0.42
1:A:217:GLU:OE1	1:A:423:ASN:HB2	2.19	0.41
1:A:429:ARG:NH1	1:A:653:HIS:HB2	2.35	0.41
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.77	0.41
1:B:475:ASP:HA	1:B:655:GLU:HA	2.01	0.41
1:C:421:ASN:HA	1:C:422:PRO:HD2	1.91	0.41
2:E:288:LEU:HB3	2:E:296:ASN:ND2	2.35	0.41
2:H:486:LEU:HG	2:H:486:LEU:H	1.73	0.41
2:H:78:TYR:O	2:H:88:LYS:HE3	2.20	0.41
2:J:118:ILE:O	2:J:118:ILE:HG12	2.20	0.41
2:D:98:ILE:HG13	2:D:107:GLN:HG2	2.03	0.41
1:A:493:ASN:ND2	2:E:293:THR:O	2.48	0.41
2:E:312:SER:H	2:E:318:LYS:HD3	1.85	0.41
2:F:233:LEU:HB3	2:F:241:CYS:SG	2.60	0.41
2:E:373:ILE:CD1	2:F:280:SER:HA	2.49	0.41
2:J:413:ARG:HE	2:J:456:THR:HB	1.85	0.41
1:B:236:THR:O	1:B:240:GLU:HG3	2.20	0.41
2:E:327:LEU:HA	2:E:391:PHE:CE1	2.55	0.41
2:F:154:VAL:HA	2:F:203:ILE:HB	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:324:GLN:OE1	2:G:542:LEU:N	2.53	0.41
2:H:208:MET:HE1	2:H:231:ALA:O	2.21	0.41
2:G:392:HIS:HA	2:H:266:VAL:CG2	2.51	0.41
2:I:505:ASN:C	2:I:507:GLN:H	2.23	0.41
2:J:99:ALA:N	2:J:106:TYR:O	2.44	0.41
2:J:288:LEU:H	2:J:288:LEU:HD12	1.85	0.41
1:B:698:PRO:HD2	1:B:702:ILE:HG13	2.01	0.41
1:B:93:VAL:CG1	1:B:217:GLU:HB3	2.50	0.41
2:D:217:GLU:O	2:D:221:GLN:HG3	2.19	0.41
2:E:124:ARG:HA	2:E:129:ASN:O	2.19	0.41
2:E:75:ASN:HD22	2:E:100:LYS:HB3	1.84	0.41
2:F:260:TRP:CE3	2:F:261:ILE:HG22	2.56	0.41
2:I:272:ARG:NH1	2:I:276:ARG:HB2	2.35	0.41
2:I:272:ARG:NH2	2:I:276:ARG:HH21	2.18	0.41
2:I:469:PRO:HD3	2:I:475:HIS:NE2	2.35	0.41
2:J:140:ALA:HB3	2:J:179:GLY:HA3	2.02	0.41
3:M:32:CYS:SG	3:M:34:PRO:HD2	2.61	0.41
1:A:253:LEU:O	1:A:257:LEU:N	2.45	0.41
1:C:506:HIS:CG	1:C:522:LYS:HG2	2.56	0.41
2:D:159:GLU:N	2:D:159:GLU:OE1	2.50	0.41
2:D:162:MET:HB2	2:D:177:SER:HB2	2.03	0.41
2:D:182:ALA:HB1	2:D:215:ALA:HB2	2.02	0.41
2:F:78:TYR:O	2:F:88:LYS:HE3	2.21	0.41
1:C:678:ARG:NH2	2:G:371:GLU:OE2	2.47	0.41
2:I:315:GLY:C	2:I:317:GLY:H	2.24	0.41
2:I:473:LYS:O	2:I:479:ARG:NE	2.51	0.41
2:J:141:LEU:HD23	2:J:192:ASN:ND2	2.35	0.41
2:I:411:TYR:CZ	2:J:260:TRP:HA	2.55	0.41
3:L:52:LYS:NZ	3:L:107:LEU:HD13	2.35	0.41
1:A:86:GLU:HG2	1:A:86:GLU:H	1.72	0.41
1:B:66:VAL:HG11	1:B:222:TRP:CH2	2.56	0.41
2:E:182:ALA:HB1	2:E:215:ALA:HB2	2.02	0.41
2:F:205:MET:HA	2:F:231:ALA:HB3	2.03	0.41
2:F:492:LEU:HG	2:F:492:LEU:H	1.58	0.41
2:G:269:LEU:C	2:G:271:LEU:H	2.24	0.41
2:I:154:VAL:HB	2:I:175:VAL:HG22	2.03	0.41
2:I:310:VAL:HB	2:I:463:ILE:HD13	2.02	0.41
2:J:319:SER:O	2:J:323:ARG:HB2	2.20	0.41
3:L:28:TRP:HE1	3:L:57:LYS:HB3	1.86	0.41
1:C:154:TYR:HA	1:C:158:MET:SD	2.61	0.41
2:G:290:SER:OG	2:G:328:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:230:VAL:H	2:H:259:PRO:HG2	1.86	0.41
2:J:112:ARG:HG2	2:J:118:ILE:HG22	2.03	0.41
1:B:482:ARG:HD3	1:B:689:LEU:O	2.21	0.41
1:C:143:PHE:CE2	1:C:147:LEU:HD11	2.55	0.41
1:C:467:LYS:HA	1:C:468:PRO:HD2	1.92	0.41
1:C:652:VAL:O	1:C:654:ASP:N	2.53	0.41
2:D:361:ARG:NH1	2:D:535:TYR:OH	2.53	0.41
2:F:446:MET:SD	2:F:492:LEU:HB3	2.61	0.41
2:G:338:GLY:O	2:G:422:ILE:N	2.51	0.41
2:I:444:ASN:O	2:I:447:THR:OG1	2.25	0.41
1:A:102:LEU:O	1:A:106:ASP:N	2.54	0.41
1:C:547:ARG:O	1:C:551:LEU:HB2	2.20	0.41
1:C:602:HIS:CG	1:C:603:VAL:N	2.84	0.41
1:C:61:GLY:N	1:C:90:ASP:OD2	2.54	0.41
2:D:97:TRP:CZ3	2:D:99:ALA:HB2	2.56	0.41
2:E:453:ALA:HB2	2:E:460:LEU:HD22	2.03	0.41
2:F:124:ARG:HA	2:F:129:ASN:O	2.21	0.41
2:G:319:SER:O	2:G:323:ARG:HB2	2.21	0.41
2:G:347:GLU:HG3	2:H:278:HIS:CE1	2.56	0.41
2:G:475:HIS:H	2:G:479:ARG:HD2	1.85	0.41
2:H:474:ALA:O	2:H:476:GLU:HG2	2.21	0.41
2:I:298:LYS:HB3	2:I:526:ASP:O	2.21	0.41
2:I:97:TRP:CZ3	2:I:99:ALA:HB2	2.56	0.41
2:D:272:ARG:HG3	2:J:378:PHE:CE2	2.56	0.41
1:A:159:GLU:HG2	1:A:160:TRP:CD1	2.55	0.41
1:A:94:LEU:HD21	1:A:214:VAL:HG13	2.03	0.41
1:A:43:LEU:HD22	1:A:81:PHE:CG	2.56	0.41
1:A:440:ILE:HG22	1:A:452:ARG:HE	1.85	0.41
2:E:186:LYS:O	2:E:222:VAL:HG21	2.21	0.41
2:E:258:GLY:N	2:E:259:PRO:HD2	2.36	0.41
2:E:338:GLY:HA2	2:E:392:HIS:HB2	2.02	0.41
2:F:430:VAL:HG13	2:G:444:ASN:ND2	2.35	0.41
2:H:182:ALA:HB1	2:H:215:ALA:HB2	2.03	0.41
2:H:295:ILE:H	2:H:295:ILE:HD12	1.86	0.41
2:H:488:GLY:O	2:H:493:ARG:NH2	2.54	0.41
2:H:545:SER:OG	2:H:546:SER:N	2.53	0.41
2:H:97:TRP:CZ3	2:H:99:ALA:HB2	2.55	0.41
2:I:173:TYR:HA	2:I:174:PRO:HD3	1.98	0.41
2:I:251:MET:O	2:I:255:TRP:HD1	2.04	0.41
2:I:506:GLN:O	2:J:527:THR:OG1	2.31	0.41
1:A:351:TRP:CZ3	1:A:353:PRO:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:SER:OG	1:B:341:HIS:HB2	2.21	0.41
1:A:208:SER:HB2	2:D:375:ASN:HB2	2.02	0.41
2:D:340:ALA:HB3	2:D:423:LEU:HA	2.01	0.41
2:E:542:LEU:HA	2:E:542:LEU:HD12	1.69	0.41
2:F:172:LYS:HB3	2:F:172:LYS:HE2	1.68	0.41
2:F:426:ILE:O	2:F:426:ILE:HG12	2.20	0.41
2:F:467:LYS:HE3	2:F:487:ARG:HA	2.02	0.41
2:G:329:TRP:CZ3	2:G:420:VAL:HG11	2.56	0.41
2:H:203:ILE:HD12	2:H:229:ARG:CZ	2.50	0.41
2:J:220:ALA:HA	2:J:223:LEU:HD11	2.03	0.41
2:J:521:CYS:O	2:J:525:GLY:N	2.50	0.41
1:A:608:ALA:C	1:A:610:LEU:H	2.23	0.40
1:B:591:ARG:HB3	1:B:602:HIS:CE1	2.56	0.40
1:B:573:LEU:HD11	1:B:593:ILE:HG12	2.03	0.40
1:B:597:ASP:OD1	1:B:597:ASP:N	2.51	0.40
1:B:91:THR:HB	1:B:181:LEU:HD12	2.02	0.40
2:D:492:LEU:O	2:D:496:SER:OG	2.25	0.40
2:G:235:CYS:HB3	2:G:240:GLU:CG	2.51	0.40
2:G:312:SER:H	2:G:318:LYS:HD3	1.86	0.40
2:J:229:ARG:HE	2:J:229:ARG:HB3	1.72	0.40
2:J:284:SER:HA	2:J:303:ARG:HG3	2.03	0.40
1:A:103:LYS:HE3	1:A:106:ASP:CG	2.42	0.40
1:A:159:GLU:N	1:A:159:GLU:OE1	2.43	0.40
1:A:50:VAL:HG13	1:A:87:ASN:HD21	1.86	0.40
1:C:537:ILE:HG13	1:C:552:LYS:HD2	2.03	0.40
1:C:640:HIS:CD2	1:C:647:ALA:HA	2.56	0.40
2:D:429:VAL:HG23	2:D:430:VAL:H	1.85	0.40
2:E:165:VAL:HB	2:E:175:VAL:HG11	2.02	0.40
2:E:259:PRO:CA	2:E:260:TRP:HB3	2.46	0.40
2:F:166:MET:CG	2:F:171:CYS:HA	2.51	0.40
2:G:203:ILE:HA	2:G:229:ARG:HB2	2.03	0.40
2:I:107:GLN:O	2:I:123:VAL:HA	2.21	0.40
2:I:271:LEU:HD23	2:I:271:LEU:HA	1.86	0.40
1:A:678:ARG:NH1	1:A:691:ASP:OD1	2.55	0.40
1:B:476:ALA:HA	1:B:692:THR:HG22	2.03	0.40
1:C:101:ASN:C	1:C:103:LYS:H	2.24	0.40
1:C:114:LYS:O	1:C:130:TYR:HB3	2.21	0.40
2:E:228:VAL:HG11	2:E:260:TRP:CD1	2.55	0.40
2:E:395:ASP:H	2:F:265:VAL:HG21	1.87	0.40
2:G:368:LEU:HD23	2:G:368:LEU:HA	1.97	0.40
2:H:272:ARG:NH2	2:H:276:ARG:HB3	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:319:SER:HB3	2:I:323:ARG:NH1	2.36	0.40
2:I:318:LYS:NZ	2:I:502:LEU:CB	2.84	0.40
2:J:77:ARG:HB2	2:J:77:ARG:HE	1.77	0.40
2:D:357:HIS:ND1	2:D:385:LEU:HD13	2.37	0.40
2:E:262:PRO:O	2:E:264:GLY:N	2.54	0.40
2:G:261:ILE:H	2:G:262:PRO:CD	2.35	0.40
2:H:329:TRP:HZ3	2:H:420:VAL:HG11	1.85	0.40
2:J:111:TYR:CD2	2:J:140:ALA:HB1	2.57	0.40
1:B:382:ALA:O	1:B:386:ILE:HG13	2.21	0.40
1:B:498:HIS:NE2	2:G:543:GLU:HG2	2.37	0.40
1:C:155:VAL:O	1:C:157:GLY:N	2.55	0.40
2:E:268:ALA:HA	2:E:271:LEU:HD12	2.04	0.40
2:E:346:VAL:HG11	2:F:265:VAL:CG1	2.51	0.40
2:F:396:SER:C	2:F:398:ALA:H	2.25	0.40
2:H:347:GLU:HB3	2:I:275:ILE:CG1	2.48	0.40
2:J:258:GLY:HA2	2:J:259:PRO:HD3	1.91	0.40
2:J:316:MET:HA	2:J:504:ARG:HH11	1.85	0.40
2:J:287:LEU:HD11	2:J:335:LYS:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:ASN:O	3:L:73:ARG:NH2[2_455]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	635/704 (90%)	579 (91%)	44 (7%)	12 (2%)	10	53
1	B	632/704 (90%)	577 (91%)	44 (7%)	11 (2%)	11	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	629/704 (89%)	568 (90%)	50 (8%)	11 (2%)	11	56
2	D	483/486 (99%)	418 (86%)	52 (11%)	13 (3%)	6	46
2	E	483/486 (99%)	414 (86%)	51 (11%)	18 (4%)	4	39
2	F	484/486 (100%)	403 (83%)	60 (12%)	21 (4%)	3	34
2	G	482/486 (99%)	411 (85%)	52 (11%)	19 (4%)	4	37
2	H	484/486 (100%)	409 (84%)	56 (12%)	19 (4%)	4	37
2	I	468/486 (96%)	382 (82%)	63 (14%)	23 (5%)	3	31
2	J	481/486 (99%)	413 (86%)	51 (11%)	17 (4%)	4	40
3	K	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
3	L	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
3	M	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
All	All	5570/5829 (96%)	4862 (87%)	544 (10%)	164 (3%)	6	44

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	PRO
1	A	426	VAL
1	A	586	VAL
1	B	346	LEU
1	C	156	ASP
1	C	426	VAL
2	D	490	GLY
2	E	228	VAL
2	E	229	ARG
2	E	261	ILE
2	E	334	GLY
2	E	475	HIS
2	F	261	ILE
2	F	334	GLY
2	F	429	VAL
2	F	475	HIS
2	G	244	ASN
2	G	266	VAL
2	G	334	GLY
2	G	399	GLU
2	G	475	HIS
2	H	257	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	265	VAL
2	H	285	VAL
2	H	334	GLY
2	H	398	ALA
2	H	475	HIS
2	I	430	VAL
2	I	511	PRO
2	J	265	VAL
2	J	430	VAL
1	A	339	ARG
1	A	603	VAL
1	B	422	PRO
1	B	461	LEU
1	C	104	ASP
1	C	404	LYS
1	C	588	TRP
1	C	605	SER
1	C	653	HIS
2	D	244	ASN
2	D	399	GLU
2	D	489	SER
2	E	244	ASN
2	E	425	HIS
2	E	489	SER
2	E	490	GLY
2	F	244	ASN
2	F	412	MET
2	F	490	GLY
2	G	257	ALA
2	G	261	ILE
2	G	396	SER
2	G	398	ALA
2	G	546	SER
2	H	244	ASN
2	H	260	TRP
2	H	266	VAL
2	H	283	GLU
2	H	364	GLN
2	I	244	ASN
2	I	273	GLU
2	I	306	GLU
2	I	396	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	397	PHE
2	I	506	GLN
2	I	536	ASN
2	J	75	ASN
2	J	256	ASN
2	J	264	GLY
2	J	334	GLY
2	J	490	GLY
1	A	157	GLY
1	A	338	SER
1	A	653	HIS
1	B	156	ASP
1	B	263	SER
1	B	603	VAL
1	B	604	ARG
1	C	462	ASP
2	D	263	ASP
2	D	265	VAL
2	D	437	ASP
2	D	475	HIS
2	E	437	ASP
2	E	479	ARG
2	F	101	VAL
2	F	262	PRO
2	F	269	LEU
2	F	284	SER
2	F	314	SER
2	F	399	GLU
2	F	425	HIS
2	F	437	ASP
2	F	479	ARG
2	G	260	TRP
2	G	272	ARG
2	G	425	HIS
2	G	437	ASP
2	H	287	LEU
2	H	437	ASP
2	I	227	LYS
2	I	287	LEU
2	I	425	HIS
2	I	434	GLY
2	I	479	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	224	PRO
2	J	425	HIS
2	J	429	VAL
2	J	437	ASP
2	J	475	HIS
2	J	479	ARG
1	A	156	ASP
1	A	333	VAL
1	C	429	ARG
1	C	606	PRO
1	C	609	ALA
2	D	425	HIS
2	E	258	GLY
2	E	287	LEU
2	F	288	LEU
2	F	396	SER
2	G	375	ASN
2	G	413	ARG
2	G	479	ARG
2	H	425	HIS
2	H	479	ARG
2	I	272	ARG
2	I	307	VAL
2	I	315	GLY
2	I	467	LYS
2	J	262	PRO
2	J	396	SER
2	J	399	GLU
1	A	152	GLU
1	B	436	ASN
2	D	262	PRO
2	D	479	ARG
2	E	266	VAL
2	E	267	SER
2	E	268	ALA
2	E	396	SER
2	F	318	LYS
2	G	269	LEU
2	H	101	VAL
2	H	430	VAL
2	I	182	ALA
2	I	269	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	413	ARG
2	I	428	ILE
2	I	497	ASP
2	J	263	ASP
1	B	653	HIS
2	D	396	SER
2	H	413	ARG
2	H	488	GLY
1	A	336	PRO
1	B	533	GLY
2	F	428	ILE
1	B	361	ALA
2	D	266	VAL
2	E	428	ILE
2	F	430	VAL
2	G	430	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/582 (90%)	492 (93%)	35 (7%)	21	59
1	B	524/582 (90%)	502 (96%)	22 (4%)	36	71
1	C	521/582 (90%)	505 (97%)	16 (3%)	47	78
2	D	403/403 (100%)	381 (94%)	22 (6%)	27	65
2	E	403/403 (100%)	372 (92%)	31 (8%)	16	54
2	F	403/403 (100%)	379 (94%)	24 (6%)	24	63
2	G	402/403 (100%)	381 (95%)	21 (5%)	29	67
2	H	403/403 (100%)	383 (95%)	20 (5%)	30	67
2	I	391/403 (97%)	344 (88%)	47 (12%)	6	33
2	J	401/403 (100%)	369 (92%)	32 (8%)	15	52
3	K	85/85 (100%)	81 (95%)	4 (5%)	32	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	85/85 (100%)	79 (93%)	6 (7%)	18	57
3	M	85/85 (100%)	83 (98%)	2 (2%)	57	83
All	All	4633/4822 (96%)	4351 (94%)	282 (6%)	23	62

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	85	ARG
1	A	106	ASP
1	A	110	LEU
1	A	119	ARG
1	A	154	TYR
1	A	162	ASN
1	A	163	PHE
1	A	171	ASN
1	A	173	GLN
1	A	181	LEU
1	A	232	PHE
1	A	241	GLU
1	A	261	PHE
1	A	332	VAL
1	A	334	PHE
1	A	341	HIS
1	A	420	VAL
1	A	426	VAL
1	A	427	THR
1	A	429	ARG
1	A	470	VAL
1	A	554	LYS
1	A	573	LEU
1	A	574	VAL
1	A	585	GLN
1	A	586	VAL
1	A	587	LYS
1	A	605	SER
1	A	607	HIS
1	A	624	LEU
1	A	652	VAL
1	A	653	HIS
1	A	664	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	686	PHE
1	B	75	LEU
1	B	85	ARG
1	B	102	LEU
1	B	120	PHE
1	B	173	GLN
1	B	232	PHE
1	B	241	GLU
1	B	339	ARG
1	B	341	HIS
1	B	364	VAL
1	B	366	ASP
1	B	426	VAL
1	B	427	THR
1	B	461	LEU
1	B	464	ILE
1	B	470	VAL
1	B	534	ASP
1	B	554	LYS
1	B	572	THR
1	B	607	HIS
1	B	624	LEU
1	B	686	PHE
1	C	75	LEU
1	C	110	LEU
1	C	173	GLN
1	C	195	GLU
1	C	232	PHE
1	C	241	GLU
1	C	346	LEU
1	C	427	THR
1	C	458	GLU
1	C	467	LYS
1	C	470	VAL
1	C	554	LYS
1	C	604	ARG
1	C	624	LEU
1	C	653	HIS
1	C	686	PHE
2	D	77	ARG
2	D	96	TYR
2	D	104	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	167	GLU
2	D	194	GLU
2	D	250	ILE
2	D	251	MET
2	D	261	ILE
2	D	267	SER
2	D	269	LEU
2	D	284	SER
2	D	303	ARG
2	D	325	GLN
2	D	328	GLN
2	D	346	VAL
2	D	349	THR
2	D	406	LEU
2	D	429	VAL
2	D	468	ASN
2	D	476	GLU
2	D	492	LEU
2	D	507	GLN
2	E	77	ARG
2	E	96	TYR
2	E	113	ASP
2	E	114	GLN
2	E	115	ASN
2	E	167	GLU
2	E	193	TYR
2	E	194	GLU
2	E	251	MET
2	E	252	GLU
2	E	253	GLN
2	E	261	ILE
2	E	263	ASP
2	E	269	LEU
2	E	270	SER
2	E	283	GLU
2	E	285	VAL
2	E	303	ARG
2	E	328	GLN
2	E	347	GLU
2	E	349	THR
2	E	368	LEU
2	E	379	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	427	SER
2	E	428	ILE
2	E	429	VAL
2	E	431	SER
2	E	476	GLU
2	E	492	LEU
2	E	512	ASN
2	E	542	LEU
2	F	77	ARG
2	F	105	MET
2	F	166	MET
2	F	168	LEU
2	F	170	ASP
2	F	193	TYR
2	F	194	GLU
2	F	218	GLU
2	F	260	TRP
2	F	261	ILE
2	F	265	VAL
2	F	303	ARG
2	F	328	GLN
2	F	395	ASP
2	F	401	GLU
2	F	406	LEU
2	F	418	CYS
2	F	429	VAL
2	F	437	ASP
2	F	468	ASN
2	F	476	GLU
2	F	487	ARG
2	F	492	LEU
2	F	512	ASN
2	G	77	ARG
2	G	167	GLU
2	G	194	GLU
2	G	261	ILE
2	G	266	VAL
2	G	269	LEU
2	G	282	GLU
2	G	287	LEU
2	G	303	ARG
2	G	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	375	ASN
2	G	393	LEU
2	G	397	PHE
2	G	406	LEU
2	G	429	VAL
2	G	468	ASN
2	G	470	ASP
2	G	476	GLU
2	G	512	ASN
2	G	542	LEU
2	G	547	TYR
2	H	77	ARG
2	H	167	GLU
2	H	261	ILE
2	H	266	VAL
2	H	269	LEU
2	H	272	ARG
2	H	282	GLU
2	H	283	GLU
2	H	288	LEU
2	H	303	ARG
2	H	333	MET
2	H	347	GLU
2	H	406	LEU
2	H	429	VAL
2	H	454	LYS
2	H	476	GLU
2	H	486	LEU
2	H	492	LEU
2	H	512	ASN
2	H	542	LEU
2	I	77	ARG
2	I	96	TYR
2	I	126	LYS
2	I	193	TYR
2	I	194	GLU
2	I	223	LEU
2	I	250	ILE
2	I	251	MET
2	I	271	LEU
2	I	272	ARG
2	I	285	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	300	LEU
2	I	303	ARG
2	I	306	GLU
2	I	309	MET
2	I	316	MET
2	I	349	THR
2	I	370	ARG
2	I	371	GLU
2	I	397	PHE
2	I	399	GLU
2	I	402	THR
2	I	404	ARG
2	I	419	ASP
2	I	425	HIS
2	I	426	ILE
2	I	429	VAL
2	I	435	GLU
2	I	440	LYS
2	I	441	MET
2	I	442	ILE
2	I	470	ASP
2	I	471	LYS
2	I	477	GLU
2	I	479	ARG
2	I	492	LEU
2	I	493	ARG
2	I	497	ASP
2	I	504	ARG
2	I	506	GLN
2	I	507	GLN
2	I	512	ASN
2	I	514	VAL
2	I	516	VAL
2	I	532	TYR
2	I	534	GLU
2	I	539	THR
2	J	100	LYS
2	J	117	ASN
2	J	118	ILE
2	J	119	VAL
2	J	124	ARG
2	J	126	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	148	ASN
2	J	167	GLU
2	J	200	GLU
2	J	213	ARG
2	J	214	LYS
2	J	218	GLU
2	J	223	LEU
2	J	229	ARG
2	J	243	LEU
2	J	249	GLU
2	J	261	ILE
2	J	263	ASP
2	J	287	LEU
2	J	303	ARG
2	J	325	GLN
2	J	347	GLU
2	J	368	LEU
2	J	429	VAL
2	J	468	ASN
2	J	470	ASP
2	J	476	GLU
2	J	492	LEU
2	J	507	GLN
2	J	512	ASN
2	J	542	LEU
2	J	546	SER
3	K	53	LEU
3	K	89	THR
3	K	90	LYS
3	K	99	LEU
3	L	10	ASP
3	L	35	CYS
3	L	37	MET
3	L	73	ARG
3	L	89	THR
3	L	95	SER
3	M	89	THR
3	M	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	502	ASN
1	B	171	ASN
2	D	107	GLN
2	D	221	GLN
2	D	425	HIS
2	E	425	HIS
2	F	328	GLN
2	F	375	ASN
2	G	364	GLN
2	H	425	HIS
2	I	506	GLN
2	J	192	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	639/704 (90%)	0.31	31 (4%) 33 28	137, 214, 280, 318	0
1	B	636/704 (90%)	0.26	16 (2%) 61 52	135, 192, 256, 283	0
1	C	633/704 (89%)	0.45	37 (5%) 26 21	180, 240, 332, 354	0
2	D	485/486 (99%)	0.56	51 (10%) 8 8	190, 241, 349, 382	0
2	E	485/486 (99%)	0.33	20 (4%) 41 34	174, 220, 262, 278	0
2	F	486/486 (100%)	0.49	39 (8%) 15 13	177, 230, 274, 298	0
2	G	484/486 (99%)	0.53	47 (9%) 10 9	170, 238, 358, 443	0
2	H	486/486 (100%)	0.46	28 (5%) 26 21	158, 232, 285, 346	0
2	I	472/486 (97%)	0.58	39 (8%) 14 12	207, 282, 332, 359	0
2	J	483/486 (99%)	0.33	22 (4%) 36 30	174, 244, 298, 378	0
3	K	105/105 (100%)	1.27	23 (21%) 1 3	219, 359, 416, 451	0
3	L	105/105 (100%)	0.53	3 (2%) 55 45	225, 255, 277, 292	0
3	M	105/105 (100%)	1.40	27 (25%) 1 2	242, 345, 382, 388	0
All	All	5604/5829 (96%)	0.46	383 (6%) 20 16	135, 233, 335, 451	0

All (383) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	472	GLY	7.7
3	K	22	ALA	7.1
1	A	584	GLN	6.6
2	D	102	ASP	5.9
2	I	433	SER	5.8
3	K	55	VAL	5.7
2	D	67	ASN	5.7
2	D	69	TRP	5.7
1	C	642	TRP	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	546	GLU	5.6
2	D	66	TYR	5.5
2	G	180	HIS	5.5
2	I	436	SER	5.4
1	C	375	ASP	5.4
3	K	6	HIS	5.3
2	F	433	SER	5.3
1	C	54	GLY	5.1
2	D	70	ASN	5.1
3	K	5	ILE	5.0
2	H	69	TRP	4.7
2	D	435	GLU	4.7
2	I	285	VAL	4.6
1	C	376	ASP	4.5
2	H	110	ASP	4.5
1	A	586	VAL	4.4
3	M	55	VAL	4.4
2	G	181	GLY	4.4
2	F	434	GLY	4.3
1	C	638	LEU	4.3
2	I	435	GLU	4.3
2	D	434	GLY	4.3
3	K	21	GLY	4.2
2	G	433	SER	4.2
2	F	435	GLU	4.1
2	G	234	PRO	4.0
1	A	54	GLY	4.0
2	D	122	LYS	4.0
2	G	207	ASP	4.0
3	M	94	LEU	3.9
1	A	55	LEU	3.9
3	K	106	ASN	3.9
2	I	284	SER	3.9
2	F	436	SER	3.9
3	M	74	GLY	3.9
2	E	434	GLY	3.9
2	H	473	LYS	3.8
2	F	112	ARG	3.8
3	K	94	LEU	3.8
2	H	435	GLU	3.8
2	E	433	SER	3.8
3	K	7	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	54	THR	3.7
3	M	104	ASP	3.7
2	G	249	GLU	3.7
2	H	467	LYS	3.7
2	I	473	LYS	3.7
1	A	582	GLY	3.7
2	D	84	ARG	3.7
3	K	82	LYS	3.7
2	D	94	ALA	3.7
2	F	118	ILE	3.7
2	F	473	LYS	3.6
3	M	31	TRP	3.6
3	M	12	PHE	3.6
3	L	32	CYS	3.6
2	H	141	LEU	3.6
1	C	515	LEU	3.6
2	I	64	MET	3.5
3	K	53	LEU	3.5
1	B	575	GLU	3.5
1	C	379	LYS	3.5
2	D	152	LYS	3.5
2	G	136	HIS	3.5
2	D	79	SER	3.5
2	D	109	ALA	3.5
2	I	182	ALA	3.5
2	G	202	ILE	3.5
1	A	165	GLU	3.4
2	J	138	SER	3.4
2	J	136	HIS	3.4
1	B	354	THR	3.4
2	F	432	ALA	3.4
1	C	234	PHE	3.4
2	F	131	LYS	3.4
2	G	233	LEU	3.4
2	D	433	SER	3.4
2	I	122	LYS	3.4
2	G	531	GLY	3.3
2	G	138	SER	3.3
2	I	112	ARG	3.3
2	D	110	ASP	3.3
2	G	206	PHE	3.3
2	F	69	TRP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	96	TYR	3.3
3	L	94	LEU	3.3
3	M	24	LEU	3.3
1	A	363	VAL	3.3
2	J	179	GLY	3.3
2	H	96	TYR	3.3
1	A	541	VAL	3.3
2	D	238	ALA	3.2
1	C	378	GLU	3.2
2	J	111	TYR	3.2
2	I	334	GLY	3.2
3	M	96	LYS	3.2
1	A	355	LYS	3.2
2	D	134	GLY	3.2
2	H	144	LYS	3.2
2	J	84	ARG	3.2
3	K	104	ASP	3.1
3	M	73	ARG	3.1
2	I	145	HIS	3.1
2	J	113	ASP	3.1
2	G	115	ASN	3.1
2	H	131	LYS	3.1
3	M	53	LEU	3.1
2	G	255	TRP	3.0
2	I	434	GLY	3.0
2	J	233	LEU	3.0
2	G	200	GLU	3.0
2	D	103	GLY	3.0
2	I	532	TYR	3.0
2	F	134	GLY	3.0
2	D	98	ILE	3.0
3	M	54	THR	3.0
1	C	115	LEU	3.0
2	I	431	SER	3.0
2	D	432	ALA	3.0
2	F	168	LEU	3.0
1	B	355	LYS	3.0
2	D	95	GLY	3.0
1	A	583	GLU	3.0
2	D	436	SER	3.0
2	F	114	GLN	3.0
2	G	217	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	94	ALA	3.0
1	A	373	ARG	2.9
1	C	377	PRO	2.9
2	F	65	THR	2.9
2	G	228	VAL	2.9
2	F	144	LYS	2.9
2	F	195	TYR	2.9
1	B	163	PHE	2.9
1	C	352	VAL	2.9
2	D	101	VAL	2.9
2	H	432	ALA	2.9
2	F	64	MET	2.9
3	M	60	ILE	2.9
3	M	106	ASN	2.9
2	F	122	LYS	2.9
2	H	471	LYS	2.9
2	E	122	LYS	2.9
2	D	124	ARG	2.9
2	G	84	ARG	2.9
2	J	69	TRP	2.9
1	A	585	GLN	2.9
2	J	144	LYS	2.9
2	D	179	GLY	2.9
2	E	435	GLU	2.8
2	I	69	TRP	2.8
1	B	1	MET	2.8
3	M	10	ASP	2.8
1	A	56	ILE	2.8
2	E	471	LYS	2.8
2	F	399	GLU	2.8
2	I	114	GLN	2.8
2	F	68	VAL	2.8
1	A	1	MET	2.8
1	C	457	ALA	2.8
2	I	136	HIS	2.8
2	D	99	ALA	2.8
3	M	56	ALA	2.8
3	K	74	GLY	2.8
2	G	188	THR	2.7
1	C	506	HIS	2.7
2	E	157	GLU	2.7
3	M	52	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	2.7
2	F	196	PHE	2.7
1	C	355	LYS	2.7
2	G	139	ASP	2.7
2	I	509	ASP	2.7
1	A	579	TRP	2.7
2	I	254	VAL	2.7
1	C	516	PRO	2.7
2	D	104	VAL	2.7
2	F	130	PHE	2.7
2	J	94	ALA	2.7
2	E	531	GLY	2.7
2	H	436	SER	2.7
2	J	68	VAL	2.7
2	D	130	PHE	2.7
2	I	151	LYS	2.7
3	K	103	LEU	2.7
3	K	56	ALA	2.6
2	G	257	ALA	2.6
1	C	696	MET	2.6
3	M	57	LYS	2.6
2	D	97	TRP	2.6
1	C	577	SER	2.6
2	G	250	ILE	2.6
2	J	247	ASP	2.6
1	B	642	TRP	2.6
3	K	93	ALA	2.6
1	C	540	ILE	2.6
2	D	105	MET	2.6
2	H	121	GLN	2.6
3	K	12	PHE	2.6
2	D	121	GLN	2.6
1	B	577	SER	2.6
1	C	547	ARG	2.5
2	H	68	VAL	2.5
2	F	67	ASN	2.5
3	K	96	LYS	2.5
2	I	152	LYS	2.5
1	B	166	GLU	2.5
1	C	645	ASP	2.5
3	L	10	ASP	2.5
2	H	115	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	9	ASP	2.5
2	D	65	THR	2.5
2	E	65	THR	2.5
2	G	261	ILE	2.5
1	A	354	THR	2.5
2	D	364	GLN	2.5
2	I	113	ASP	2.5
2	I	335	LYS	2.5
2	G	159	GLU	2.5
2	H	434	GLY	2.5
2	F	79	SER	2.5
3	K	52	LYS	2.5
1	C	541	VAL	2.4
2	E	469	PRO	2.4
2	E	470	ASP	2.4
1	C	114	LYS	2.4
2	I	432	ALA	2.4
2	G	239	ASN	2.4
3	K	15	ASP	2.4
2	H	135	SER	2.4
2	G	432	ALA	2.4
2	I	115	ASN	2.4
2	D	399	GLU	2.4
3	M	102	PHE	2.4
1	A	540	ILE	2.4
1	A	152	GLU	2.4
2	E	238	ALA	2.4
2	G	242	HIS	2.4
1	C	358	ASP	2.4
2	E	233	LEU	2.4
2	G	179	GLY	2.4
1	A	149	GLU	2.4
2	F	468	ASN	2.4
2	E	432	ALA	2.4
1	A	163	PHE	2.4
2	F	141	LEU	2.4
2	I	287	LEU	2.4
2	D	389	ASP	2.3
2	I	234	PRO	2.3
2	D	178	LEU	2.3
2	D	144	LYS	2.3
2	H	526	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	26	TYR	2.3
1	C	350	GLY	2.3
2	J	98	ILE	2.3
2	D	83	ALA	2.3
2	E	436	SER	2.3
2	D	242	HIS	2.3
1	A	358	ASP	2.3
1	A	550	GLU	2.3
2	F	291	GLY	2.3
1	C	261	PHE	2.3
1	C	472	ALA	2.3
2	F	147	TRP	2.3
2	J	137	LYS	2.3
2	E	178	LEU	2.3
2	D	136	HIS	2.3
2	D	386	PHE	2.3
3	K	102	PHE	2.3
1	B	606	PRO	2.3
2	H	267	SER	2.3
2	I	65	THR	2.3
2	D	388	ASN	2.3
2	G	94	ALA	2.3
1	B	589	LYS	2.3
2	D	133	THR	2.3
2	G	149	GLY	2.3
2	J	149	GLY	2.3
2	G	148	ASN	2.3
2	G	152	LYS	2.3
2	H	122	LYS	2.3
2	G	260	TRP	2.3
2	F	481	VAL	2.3
2	H	134	GLY	2.3
2	I	200	GLU	2.3
2	E	131	LYS	2.3
1	A	547	ARG	2.3
2	F	135	SER	2.3
2	D	127	ASP	2.2
2	G	315	GLY	2.2
2	I	488	GLY	2.2
3	M	15	ASP	2.2
2	I	116	GLY	2.2
2	G	103	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	205	MET	2.2
3	M	20	ASP	2.2
2	H	231	ALA	2.2
3	M	98	GLN	2.2
2	J	110	ASP	2.2
2	J	145	HIS	2.2
2	I	144	LYS	2.2
2	I	286	GLY	2.2
2	H	120	SER	2.2
1	B	26	TYR	2.2
2	G	98	ILE	2.2
2	D	74	SER	2.2
3	M	61	ASP	2.2
1	B	353	PRO	2.2
2	E	508	GLY	2.2
2	G	69	TRP	2.2
2	J	100	LYS	2.2
1	A	34	TYR	2.2
2	F	437	ASP	2.2
1	A	524	PHE	2.1
2	J	232	VAL	2.1
3	K	107	LEU	2.1
2	G	182	ALA	2.1
1	C	55	LEU	2.1
1	B	532	ALA	2.1
2	D	132	THR	2.1
2	D	175	VAL	2.1
2	G	227	LYS	2.1
2	J	236	LYS	2.1
1	C	31	TYR	2.1
2	E	179	GLY	2.1
1	A	374	VAL	2.1
1	C	3	VAL	2.1
2	D	236	LYS	2.1
3	M	49	TYR	2.1
2	F	99	ALA	2.1
2	I	233	LEU	2.1
1	A	372	VAL	2.1
2	F	438	GLU	2.1
2	H	433	SER	2.1
2	J	504	ARG	2.1
1	A	537	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	206	PHE	2.1
1	B	387	LYS	2.1
2	F	276	ARG	2.1
1	B	447	TYR	2.1
1	C	385	LEU	2.1
2	D	78	TYR	2.1
2	F	115	ASN	2.1
2	H	106	TYR	2.1
2	F	110	ASP	2.1
2	I	533	MET	2.1
2	J	114	GLN	2.1
2	F	145	HIS	2.1
2	H	431	SER	2.1
2	G	317	GLY	2.1
1	C	246	LEU	2.1
2	E	64	MET	2.1
2	G	216	VAL	2.1
2	G	230	VAL	2.0
1	A	2	ILE	2.0
3	M	50	GLN	2.0
3	K	3	LYS	2.0
2	H	142	PHE	2.0
1	B	470	VAL	2.0
1	A	379	LYS	2.0
1	C	139	TYR	2.0
2	F	509	ASP	2.0
2	G	252	GLU	2.0
2	D	131	LYS	2.0
2	I	508	GLY	2.0
2	G	251	MET	2.0
2	G	263	ASP	2.0
3	M	81	PHE	2.0
1	C	662	THR	2.0
2	G	157	GLU	2.0
1	C	357	THR	2.0
2	F	113	ASP	2.0
2	I	538	GLU	2.0
3	M	13	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.