Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:31 am BST

PDB ID	:	1KNX
Title	:	HPr kinase/phosphatase from Mycoplasma pneumoniae
Authors	:	Allen, G.S.
Deposited on	:	2001-12-19
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

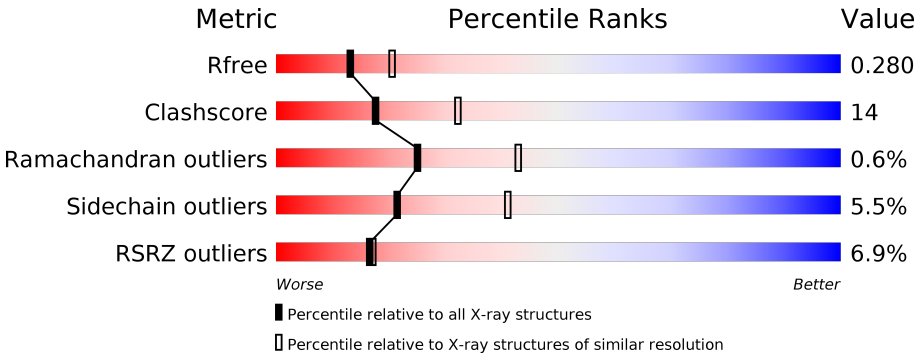
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	312	14% 58% 35%
1	B	312	2% 67% 29%
1	C	312	5% 65% 29%
1	D	312	11% 66% 29%
1	E	312	4% 73% 24%
1	F	312	4% 71% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14717 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 Probable HPr(Ser) kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2392	1546	404	436	6			
1	B	304	Total	C	N	O	S	0	0	0
			2415	1559	409	441	6			
1	C	300	Total	C	N	O	S	0	0	0
			2375	1532	403	434	6			
1	D	304	Total	C	N	O	S	0	0	0
			2400	1548	408	438	6			
1	E	310	Total	C	N	O	S	0	0	0
			2446	1576	414	450	6			
1	F	306	Total	C	N	O	S	0	0	0
			2407	1555	404	442	6			

- Molecule 2 is water.

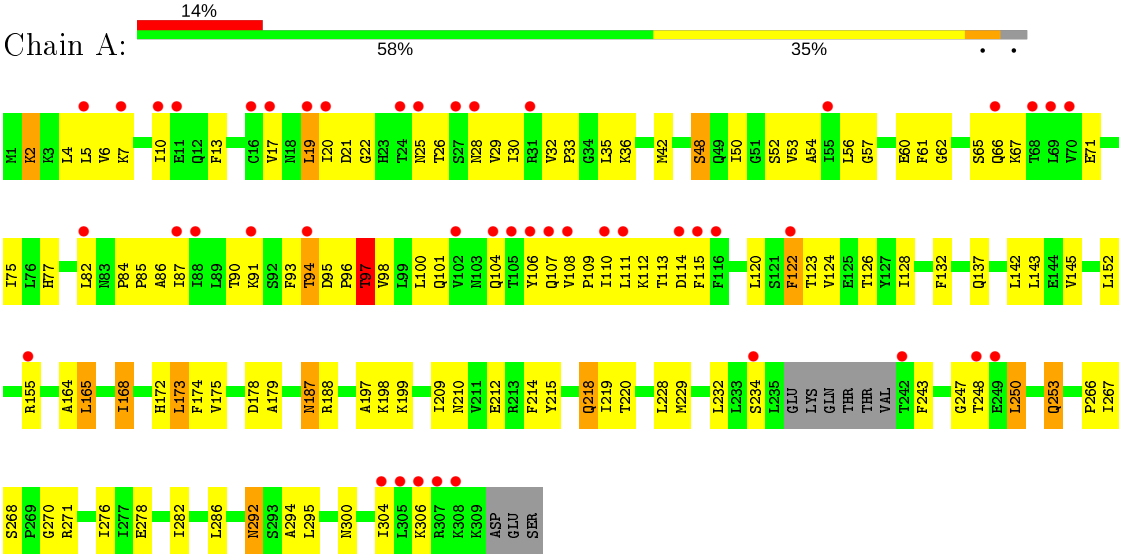
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	55	Total	O	0	0
			55	55		
2	C	38	Total	O	0	0
			38	38		
2	D	39	Total	O	0	0
			39	39		
2	E	61	Total	O	0	0
			61	61		
2	F	55	Total	O	0	0
			55	55		

3 Residue-property plots (i)

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

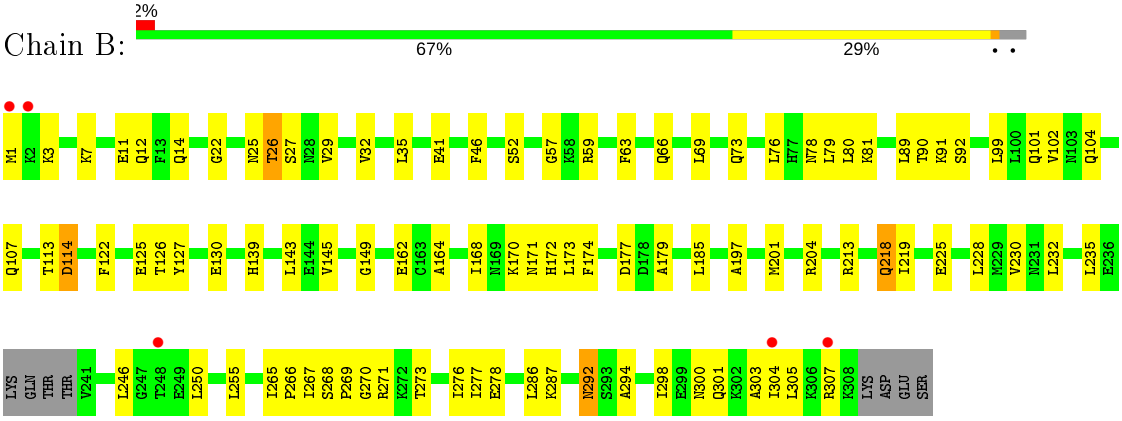
- Molecule 1: Probable HPr(Ser) kinase/phosphatase

Chain A:



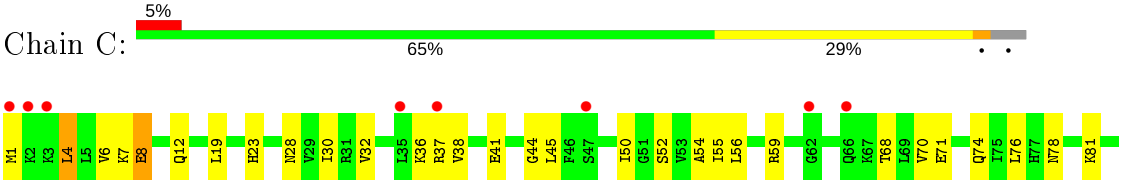
- Molecule 1: Probable HPr(Ser) kinase/phosphatase

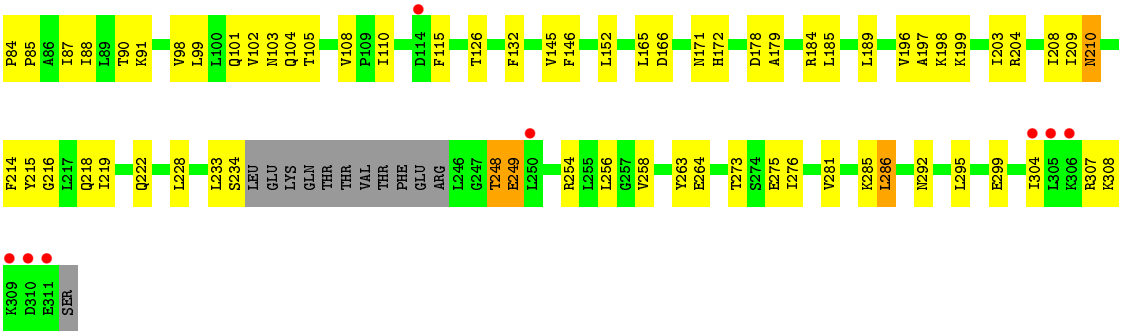
Chain B:



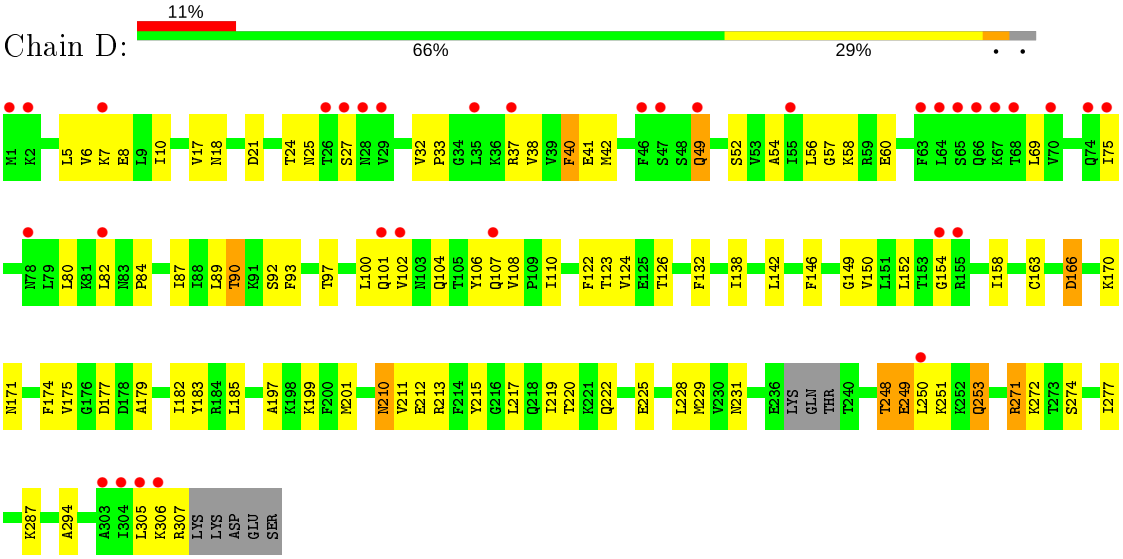
- Molecule 1: Probable HPr(Ser) kinase/phosphatase

Chain C:

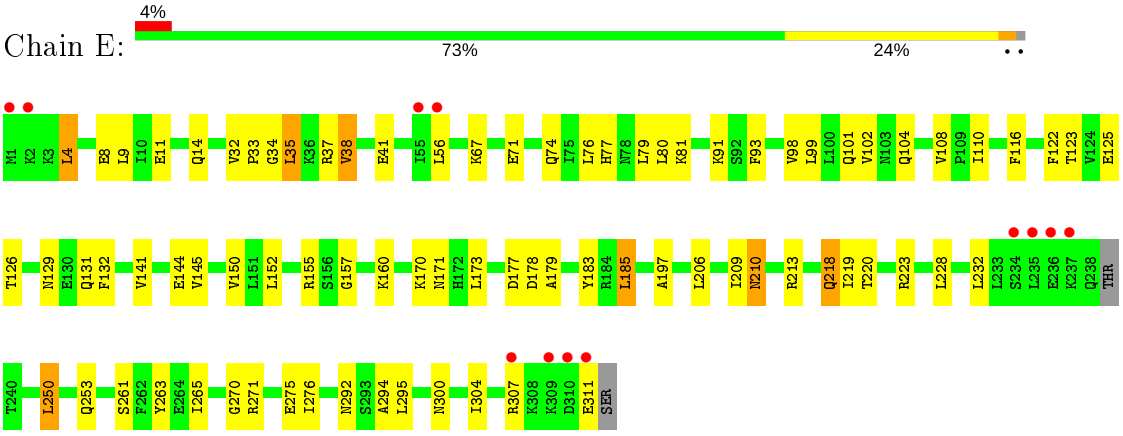




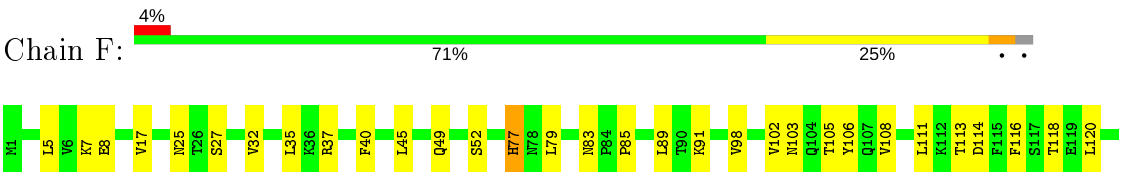
• Molecule 1: Probable HPr(Ser) kinase/phosphatase

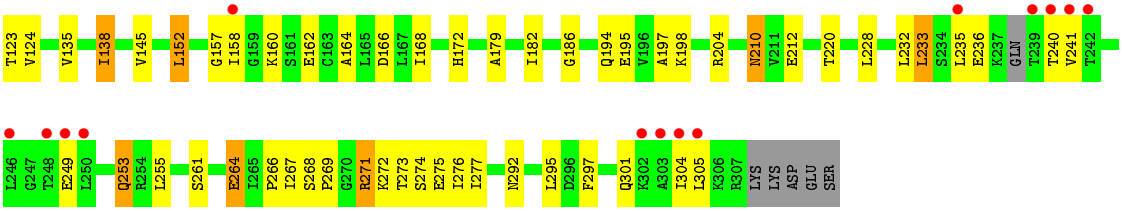


• Molecule 1: Probable HPr(Ser) kinase/phosphatase



• Molecule 1: Probable HPr(Ser) kinase/phosphatase




T123 V124 V135 I138 V145 L152 G157 I158 G159 K160 S161 E162 C163 A164 L165 D166 L167 I168 H172 A179 I182 G186 Q194 E195 V196 A197 K198 R204 N210 V211 E212 T220 L228 L232 L233 S234 L235 E236 K237 GLN T239 T240 V241 T242
L246 G247 T248 E249 L250 Q253 R254 L255 S261 E264 I265 P266 I267 S268 P269 G270 R271 K272 T273 S274 E275 I276 I277 N292 L295 D296 F297 Q301 K302 A303 I304 L305 K306 R307 LYS LYS ASP GLU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.73Å 127.84Å 170.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.22 – 2.50 29.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.22-2.50) 89.8 (29.22-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.280 0.229 , 0.280	Depositor DCC
R_{free} test set	4908 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14717	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/2427	0.55	0/3270
1	B	0.41	0/2450	0.62	0/3301
1	C	0.39	0/2409	0.59	0/3245
1	D	0.41	0/2435	0.59	0/3283
1	E	0.46	0/2481	0.61	0/3346
1	F	0.48	1/2442 (0.0%)	0.66	1/3295 (0.0%)
All	All	0.42	1/14644 (0.0%)	0.60	1/19740 (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	F	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	233	LEU	C-N	-6.51	1.19	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	235	LEU	C-N-CA	5.16	134.61	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	236	GLU	Mainchain,Peptide

5.2 Too-close contacts (i)

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	2392	0	2488	106	0
1	B	2415	0	2520	62	0
1	C	2375	0	2478	70	0
1	D	2400	0	2490	70	0
1	E	2446	0	2528	55	0
1	F	2407	0	2491	59	0
2	A	34	0	0	0	0
2	B	55	0	0	3	0
2	C	38	0	0	3	0
2	D	39	0	0	0	0
2	E	61	0	0	2	0
2	F	55	0	0	1	0
All	All	14717	0	14995	402	0

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 (402) 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:282:ILE:HG12	1:B:218:GLN:HG2	1.21	1.11
1:E:292:ASN:HD22	1:E:295:LEU:H	1.05	0.98
1:B:90:THR:HG23	1:B:92:SER:H	1.28	0.97
1:E:292:ASN:ND2	1:E:295:LEU:H	1.64	0.95
1:A:218:GLN:NE2	1:A:218:GLN:H	1.62	0.95
1:A:218:GLN:HE21	1:A:218:GLN:H	0.94	0.93
1:C:78:ASN:HA	1:C:81:LYS:HE2	1.51	0.93
1:A:218:GLN:HE21	1:A:218:GLN:N	1.69	0.90
1:C:292:ASN:HD22	1:C:295:LEU:H	1.21	0.89
1:B:168:ILE:HD11	1:B:174:PHE:HB2	1.55	0.88
1:A:187:ASN:H	1:A:187:ASN:HD22	1.22	0.86
1:C:32:VAL:HB	1:C:52:SER:HB3	1.56	0.86
1:F:49:GLN:HE22	1:F:83:ASN:HD22	1.21	0.84
1:A:250:LEU:HD23	1:A:250:LEU:H	1.41	0.84
1:A:113:THR:HG22	1:A:115:PHE:H	1.44	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HG12	1:B:218:GLN:CG	2.08	0.83
1:E:108:VAL:O	1:E:110:ILE:HD12	1.79	0.83
1:F:103:ASN:HD21	1:F:108:VAL:H	1.24	0.82
1:E:218:GLN:H	1:E:218:GLN:HE21	1.29	0.81
1:F:292:ASN:HD22	1:F:295:LEU:H	1.30	0.80
1:A:25:ASN:HB2	1:A:109:PRO:HD3	1.64	0.79
1:F:166:ASP:HB3	1:F:274:SER:HB3	1.63	0.79
1:B:273:THR:O	1:B:276:ILE:HG22	1.83	0.78
1:B:89:LEU:O	1:B:113:THR:HG22	1.84	0.78
1:E:210:ASN:C	1:E:210:ASN:HD22	1.88	0.77
1:B:22:GLY:HA2	1:B:107:GLN:HG3	1.67	0.77
1:A:19:LEU:HD23	1:A:19:LEU:H	1.48	0.76
1:D:179:ALA:HB3	1:D:197:ALA:HB2	1.68	0.75
1:A:187:ASN:H	1:A:187:ASN:ND2	1.85	0.74
1:C:55:ILE:HD13	1:C:88:ILE:HG23	1.70	0.74
1:B:1:MET:HG2	1:B:3:LYS:H	1.54	0.72
1:B:35:LEU:HG	1:B:125:GLU:HG2	1.69	0.72
1:F:157:GLY:HA2	1:F:160:LYS:NZ	2.04	0.72
1:D:271:ARG:HG2	1:D:272:LYS:N	2.04	0.72
1:F:273:THR:O	1:F:276:ILE:HG22	1.89	0.72
1:D:183:TYR:HD2	1:D:185:LEU:HD13	1.55	0.71
1:A:126:THR:HG23	1:B:122:PHE:CE2	2.25	0.71
1:A:35:LEU:HD13	1:A:120:LEU:HD23	1.73	0.70
1:A:97:THR:HG23	1:A:98:VAL:H	1.56	0.70
1:F:212:GLU:HG3	1:F:220:THR:HG21	1.73	0.69
1:A:271:ARG:NH2	1:A:276:ILE:HG13	2.08	0.68
1:B:76:LEU:HD13	1:B:99:LEU:HA	1.76	0.68
1:B:162:GLU:HG2	1:E:271:ARG:HD2	1.77	0.67
1:B:90:THR:HG23	1:B:92:SER:N	2.06	0.67
1:C:90:THR:HG21	2:C:313:HOH:O	1.96	0.66
1:A:56:LEU:HA	1:A:60:GLU:HG3	1.78	0.66
1:D:123:THR:HG22	1:D:124:VAL:N	2.10	0.66
1:A:126:THR:HG23	1:B:122:PHE:HE2	1.60	0.65
1:B:270:GLY:HA2	1:D:271:ARG:O	1.96	0.65
1:B:246:LEU:HD22	1:B:298:ILE:HD11	1.78	0.65
1:D:56:LEU:HD23	1:D:60:GLU:HG2	1.79	0.65
1:C:90:THR:HG22	1:C:91:LYS:N	2.12	0.65
1:C:233:LEU:HD11	1:C:264:GLU:OE2	1.97	0.64
1:F:77:HIS:CE1	1:F:102:VAL:HG13	2.32	0.64
1:A:57:GLY:HA2	1:A:90:THR:HG22	1.79	0.64
1:C:292:ASN:ND2	1:C:295:LEU:H	1.94	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ILE:HD12	1:C:56:LEU:H	1.63	0.64
1:D:174:PHE:CD2	1:D:211:VAL:HG21	2.32	0.64
1:C:165:LEU:HD22	1:C:203:ILE:HD13	1.80	0.64
1:B:32:VAL:HB	1:B:52:SER:HB3	1.79	0.63
1:A:36:LYS:HE3	1:B:59:ARG:HD2	1.80	0.63
1:D:32:VAL:HB	1:D:52:SER:HB3	1.80	0.63
1:B:170:LYS:O	1:B:171:ASN:HB2	1.99	0.62
1:B:301:GLN:O	1:B:305:LEU:HD13	1.99	0.62
1:B:300:ASN:O	1:B:304:ILE:HG12	2.00	0.62
1:C:198:LYS:O	1:C:199:LYS:HD2	1.99	0.61
1:D:228:LEU:HD23	1:D:229:MET:N	2.15	0.61
1:C:171:ASN:HA	1:C:219:ILE:HD11	1.81	0.61
1:E:292:ASN:HD22	1:E:295:LEU:N	1.88	0.61
1:C:228:LEU:HD11	1:C:263:TYR:CE1	2.36	0.61
1:D:80:LEU:HD22	1:D:108:VAL:HG21	1.83	0.60
1:E:219:ILE:HD12	1:E:220:THR:HG23	1.82	0.60
1:D:38:VAL:HG22	1:D:41:GLU:HB2	1.82	0.60
1:C:145:VAL:HG13	1:C:172:HIS:CD2	2.37	0.60
1:E:35:LEU:HD22	1:E:125:GLU:HB2	1.82	0.60
1:F:5:LEU:HD23	1:F:7:LYS:HE2	1.83	0.60
1:A:232:LEU:HB3	1:A:267:ILE:HD11	1.83	0.60
1:A:32:VAL:HB	1:A:52:SER:HB3	1.82	0.60
1:B:292:ASN:HD22	1:B:292:ASN:C	2.05	0.59
1:B:7:LYS:HB3	1:B:26:THR:HG23	1.84	0.59
1:A:17:VAL:HB	1:A:111:LEU:HD23	1.85	0.59
1:B:12:GLN:HG3	1:B:127:TYR:CE1	2.38	0.59
1:E:179:ALA:HB3	1:E:197:ALA:HB2	1.85	0.58
1:A:179:ALA:HB3	1:A:197:ALA:HB2	1.85	0.58
1:A:67:LYS:HG3	1:A:71:GLU:OE2	2.03	0.58
1:A:22:GLY:HA2	1:A:107:GLN:HG3	1.85	0.58
1:F:52:SER:O	1:F:85:PRO:HD2	2.04	0.58
1:A:292:ASN:HD21	1:A:294:ALA:HB3	1.69	0.57
1:B:177:ASP:OD1	1:B:201:MET:HG3	2.04	0.57
1:A:61:PHE:HB2	1:A:93:PHE:HD1	1.69	0.57
1:A:209:ILE:HG13	1:A:214:PHE:CZ	2.39	0.57
1:B:179:ALA:HB3	1:B:197:ALA:HB2	1.86	0.57
1:C:228:LEU:HD11	1:C:263:TYR:CD1	2.40	0.57
1:E:37:ARG:HD3	2:E:342:HOH:O	2.04	0.57
1:E:157:GLY:HA2	1:E:160:LYS:HE3	1.85	0.57
1:F:138:ILE:HD11	1:F:182:ILE:HG23	1.86	0.57
1:F:158:ILE:HG21	1:F:204:ARG:HG3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLN:O	1:C:104:GLN:HG2	2.05	0.56
1:E:34:GLY:HA2	1:E:129:ASN:HD21	1.69	0.56
1:D:57:GLY:HA2	1:D:90:THR:OG1	2.04	0.56
1:D:150:VAL:HG12	1:D:152:LEU:HD12	1.86	0.56
1:F:179:ALA:O	1:F:194:GLN:HG3	2.06	0.56
1:E:292:ASN:HD21	1:E:294:ALA:HB3	1.70	0.56
1:C:90:THR:HG22	1:C:91:LYS:H	1.70	0.56
1:A:292:ASN:ND2	1:A:295:LEU:H	2.04	0.56
1:A:93:PHE:O	1:A:94:THR:HG22	2.06	0.56
1:D:6:VAL:O	1:D:10:ILE:HG13	2.06	0.56
1:A:54:ALA:HB3	1:A:87:ILE:HD13	1.88	0.56
1:A:110:ILE:C	1:A:111:LEU:HD12	2.26	0.56
1:C:248:THR:HG22	1:C:295:LEU:HG	1.87	0.55
1:D:305:LEU:C	1:D:307:ARG:H	2.09	0.55
1:E:210:ASN:ND2	1:E:210:ASN:C	2.59	0.55
1:E:228:LEU:HD12	1:E:261:SER:HB2	1.87	0.55
1:B:69:LEU:O	1:B:73:GLN:HG3	2.06	0.55
1:D:199:LYS:O	1:D:211:VAL:HG22	2.07	0.55
1:A:152:LEU:HG	1:A:232:LEU:HD21	1.89	0.55
1:F:210:ASN:C	1:F:210:ASN:HD22	2.10	0.55
1:D:210:ASN:HD21	1:D:212:GLU:HB3	1.72	0.55
1:A:172:HIS:HE1	1:A:278:GLU:OE2	1.89	0.54
1:C:55:ILE:HD12	1:C:56:LEU:N	2.22	0.54
1:A:271:ARG:CZ	1:A:276:ILE:HG13	2.36	0.54
1:B:168:ILE:CD1	1:B:174:PHE:HB2	2.31	0.54
1:B:145:VAL:HG13	1:B:172:HIS:CD2	2.42	0.54
1:D:249:GLU:HG3	1:D:250:LEU:H	1.71	0.54
1:A:33:PRO:HB3	1:A:132:PHE:CD1	2.43	0.54
1:D:84:PRO:HG3	1:D:87:ILE:HD11	1.89	0.54
1:E:218:GLN:N	1:E:218:GLN:HE21	2.02	0.54
1:D:42:MET:O	1:D:75:ILE:HG23	2.07	0.54
1:A:143:LEU:HD21	1:A:164:ALA:HB1	1.90	0.54
1:A:268:SER:HB3	1:F:204:ARG:HH22	1.73	0.54
1:C:210:ASN:C	1:C:210:ASN:HD22	2.11	0.54
1:E:206:LEU:HD23	1:E:209:ILE:HG21	1.90	0.54
1:E:67:LYS:HB3	1:E:71:GLU:HB2	1.89	0.54
1:B:265:ILE:HG23	1:B:266:PRO:HD2	1.90	0.53
1:D:110:ILE:O	1:D:110:ILE:HG13	2.09	0.53
1:E:250:LEU:H	1:E:250:LEU:HD12	1.72	0.53
1:E:304:ILE:O	1:E:307:ARG:HG2	2.08	0.53
1:D:166:ASP:HB3	1:D:274:SER:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASN:N	1:A:187:ASN:HD22	1.90	0.53
1:B:294:ALA:O	1:B:298:ILE:HG12	2.07	0.53
1:B:41:GLU:HG3	1:B:46:PHE:HB2	1.91	0.52
1:F:233:LEU:HD11	1:F:264:GLU:HG2	1.92	0.52
1:A:7:LYS:HG3	1:A:26:THR:O	2.09	0.52
1:D:38:VAL:HG22	1:D:38:VAL:O	2.09	0.52
1:A:145:VAL:HG13	1:A:172:HIS:CD2	2.44	0.52
1:C:36:LYS:HB2	1:C:52:SER:OG	2.09	0.52
1:D:183:TYR:CD2	1:D:185:LEU:HD13	2.38	0.52
1:B:139:HIS:HB3	2:B:353:HOH:O	2.09	0.52
1:C:68:THR:HG22	1:C:70:VAL:H	1.74	0.52
1:C:41:GLU:CD	1:C:41:GLU:H	2.12	0.52
1:A:56:LEU:HD13	1:A:60:GLU:HG3	1.90	0.52
1:C:54:ALA:O	1:C:87:ILE:HA	2.10	0.52
1:D:33:PRO:HB3	1:D:132:PHE:CD1	2.46	0.51
1:C:19:LEU:HD21	1:C:23:HIS:HA	1.91	0.51
1:A:168:ILE:HG13	1:A:219:ILE:HB	1.93	0.51
1:C:76:LEU:HD13	1:C:99:LEU:HA	1.92	0.51
1:D:54:ALA:HB3	1:D:87:ILE:HG12	1.92	0.51
1:F:164:ALA:O	1:F:168:ILE:HG13	2.10	0.51
1:A:168:ILE:CG1	1:A:219:ILE:HD13	2.41	0.51
1:B:130:GLU:HG2	1:B:185:LEU:HD11	1.93	0.51
1:F:32:VAL:HB	1:F:52:SER:HB3	1.93	0.51
1:B:91:LYS:HE2	1:B:114:ASP:OD1	2.11	0.51
1:C:98:VAL:O	1:C:102:VAL:HG23	2.11	0.51
1:E:76:LEU:HD13	1:E:99:LEU:HA	1.92	0.51
1:A:152:LEU:HG	1:A:232:LEU:CD2	2.41	0.50
1:D:248:THR:HG22	1:D:294:ALA:HB1	1.93	0.50
1:D:41:GLU:HG2	1:D:82:LEU:CD1	2.41	0.50
1:E:101:GLN:O	1:E:104:GLN:HG3	2.11	0.50
1:F:301:GLN:O	1:F:305:LEU:HG	2.12	0.50
1:F:123:THR:OG1	1:F:124:VAL:N	2.43	0.50
1:E:34:GLY:H	1:E:129:ASN:ND2	2.10	0.50
1:A:247:GLY:H	1:A:294:ALA:HB2	1.76	0.50
1:D:248:THR:HG22	1:D:294:ALA:CB	2.42	0.49
1:A:188:ARG:HH11	1:A:188:ARG:HG2	1.77	0.49
1:A:292:ASN:HD22	1:A:295:LEU:H	1.59	0.49
1:C:44:GLY:C	1:C:45:LEU:HD12	2.33	0.49
1:B:218:GLN:NE2	1:B:218:GLN:H	2.10	0.49
1:A:96:PRO:O	1:A:100:LEU:HG	2.11	0.49
1:B:3:LYS:HE3	1:B:29:VAL:HG11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LEU:HD22	1:D:69:LEU:N	2.27	0.49
1:E:228:LEU:HD11	1:E:263:TYR:CE2	2.47	0.49
1:A:7:LYS:HG2	1:A:26:THR:HB	1.94	0.49
1:C:295:LEU:O	1:C:299:GLU:HG2	2.13	0.49
1:A:270:GLY:HA2	1:F:271:ARG:O	2.13	0.49
1:D:219:ILE:HD12	1:D:220:THR:HG23	1.94	0.49
1:A:56:LEU:HD23	1:A:87:ILE:HG23	1.95	0.49
1:E:11:GLU:O	1:E:14:GLN:HG3	2.12	0.48
1:F:49:GLN:NE2	1:F:83:ASN:HD22	2.02	0.48
1:F:228:LEU:HD12	1:F:261:SER:HB2	1.94	0.48
1:F:292:ASN:ND2	1:F:295:LEU:HG	2.28	0.48
1:A:4:LEU:HG	1:A:30:ILE:HD12	1.95	0.48
1:C:249:GLU:CD	1:C:249:GLU:H	2.16	0.48
1:A:228:LEU:HD23	1:A:229:MET:N	2.28	0.48
1:A:187:ASN:N	1:A:187:ASN:ND2	2.48	0.48
1:B:271:ARG:HG2	1:D:166:ASP:OD1	2.13	0.48
1:C:204:ARG:NH2	1:F:268:SER:HB2	2.28	0.48
1:A:42:MET:HB3	1:A:75:ILE:CG2	2.44	0.48
1:F:89:LEU:O	1:F:113:THR:HG22	2.14	0.48
1:F:91:LYS:HB3	1:F:114:ASP:HA	1.96	0.48
1:B:228:LEU:CD1	1:B:230:VAL:HG23	2.44	0.47
1:D:177:ASP:OD1	1:D:201:MET:HG3	2.14	0.47
1:A:57:GLY:HA2	1:A:90:THR:CG2	2.43	0.47
1:C:68:THR:HB	1:C:71:GLU:HG3	1.96	0.47
1:F:77:HIS:HD2	1:F:106:TYR:OH	1.97	0.47
1:A:48:SER:O	1:A:82:LEU:HD13	2.14	0.47
1:D:102:VAL:O	1:D:106:TYR:HD1	1.97	0.47
1:B:303:ALA:O	1:B:307:ARG:HG3	2.14	0.47
1:C:90:THR:CG2	1:C:91:LYS:N	2.77	0.47
1:F:138:ILE:CD1	1:F:182:ILE:HG23	2.45	0.47
1:A:271:ARG:HD2	1:F:162:GLU:HB3	1.95	0.47
1:C:108:VAL:O	1:C:110:ILE:HG13	2.14	0.47
1:B:11:GLU:O	1:B:14:GLN:HG3	2.14	0.47
1:B:78:ASN:HA	1:B:81:LYS:HE2	1.95	0.47
1:C:90:THR:HG23	1:C:115:PHE:O	2.15	0.47
1:F:91:LYS:HD3	1:F:116:PHE:CZ	2.50	0.47
1:D:7:LYS:HA	1:D:10:ILE:HD12	1.97	0.47
1:D:69:LEU:HD22	1:D:69:LEU:H	1.80	0.47
1:A:168:ILE:HG13	1:A:219:ILE:HD13	1.96	0.47
1:C:184:ARG:O	1:C:185:LEU:HD12	2.15	0.47
1:C:4:LEU:HD22	1:C:30:ILE:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:HA	2:E:316:HOH:O	2.15	0.46
1:B:101:GLN:O	1:B:104:GLN:HB2	2.15	0.46
1:D:60:GLU:N	1:D:60:GLU:OE2	2.48	0.46
1:C:204:ARG:HH22	1:F:268:SER:HB2	1.80	0.46
1:A:32:VAL:CB	1:A:52:SER:HB3	2.46	0.46
1:B:168:ILE:HG23	1:B:219:ILE:HG12	1.98	0.46
1:E:250:LEU:N	1:E:250:LEU:HD12	2.31	0.46
1:C:281:VAL:O	1:C:285:LYS:HG3	2.16	0.46
1:E:183:TYR:CD1	1:E:185:LEU:HD13	2.51	0.46
1:E:218:GLN:H	1:E:218:GLN:NE2	2.06	0.46
1:F:195:GLU:O	1:F:198:LYS:HG3	2.15	0.46
1:A:2:LYS:HA	1:A:2:LYS:HE3	1.97	0.46
1:C:254:ARG:HA	1:C:258:VAL:O	2.16	0.46
1:D:138:ILE:HD13	1:D:182:ILE:HD13	1.97	0.46
1:D:7:LYS:HG3	1:D:8:GLU:H	1.81	0.46
1:E:77:HIS:O	1:E:81:LYS:HB2	2.15	0.46
1:D:215:TYR:HB2	1:D:219:ILE:HG12	1.98	0.46
1:E:32:VAL:HG13	1:E:33:PRO:HD2	1.98	0.46
1:A:122:PHE:HD1	1:A:123:THR:HG23	1.80	0.46
1:F:272:LYS:HD2	1:F:275:GLU:OE2	2.15	0.46
1:B:80:LEU:HD12	1:B:102:VAL:HG12	1.97	0.45
1:C:179:ALA:HB3	1:C:197:ALA:HB2	1.98	0.45
1:C:50:ILE:O	1:C:85:PRO:HD3	2.16	0.45
1:A:33:PRO:HD3	1:A:132:PHE:CD2	2.52	0.45
1:B:232:LEU:HD21	1:B:277:ILE:HD11	1.98	0.45
1:A:101:GLN:HA	1:A:104:GLN:HE21	1.82	0.45
1:E:232:LEU:HA	1:E:265:ILE:O	2.16	0.45
1:C:273:THR:HA	1:C:276:ILE:HD12	1.98	0.45
1:C:209:ILE:HG13	1:C:209:ILE:O	2.17	0.45
1:C:59:ARG:NH2	1:D:40:PHE:HB2	2.32	0.45
1:C:218:GLN:HB2	1:D:146:PHE:CD2	2.51	0.45
1:F:77:HIS:ND1	1:F:102:VAL:HG13	2.32	0.45
1:A:243:PHE:CE2	1:A:266:PRO:HD3	2.52	0.45
1:D:170:LYS:O	1:D:171:ASN:HB2	2.15	0.45
1:F:118:THR:HG23	2:F:322:HOH:O	2.16	0.45
1:A:60:GLU:H	1:A:60:GLU:CD	2.20	0.45
1:C:1:MET:HE1	1:C:132:PHE:HA	1.98	0.45
1:C:55:ILE:CD1	1:C:88:ILE:HG23	2.44	0.45
1:D:69:LEU:H	1:D:69:LEU:CD2	2.30	0.45
1:A:10:ILE:HD13	1:A:111:LEU:HD21	1.99	0.45
1:A:19:LEU:CD2	1:A:19:LEU:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLU:HG3	1:B:46:PHE:CB	2.47	0.45
1:C:214:PHE:HB3	1:C:215:TYR:CE1	2.52	0.45
1:D:17:VAL:HG12	1:D:18:ASN:N	2.32	0.45
1:A:10:ILE:CD1	1:A:111:LEU:HD21	2.47	0.44
1:B:300:ASN:HB3	2:B:336:HOH:O	2.18	0.44
1:C:145:VAL:O	1:C:146:PHE:HB2	2.17	0.44
1:D:38:VAL:CG2	1:D:41:GLU:HB2	2.47	0.44
1:A:106:TYR:HB3	1:A:108:VAL:HG23	1.99	0.44
1:A:62:GLY:HA2	1:A:65:SER:HB3	1.98	0.44
1:F:157:GLY:HA2	1:F:160:LYS:HZ2	1.81	0.44
1:F:157:GLY:HA2	1:F:160:LYS:HZ3	1.79	0.44
1:A:6:VAL:O	1:A:10:ILE:HG12	2.17	0.44
1:D:58:LYS:HB2	1:D:92:SER:HB3	1.99	0.44
1:E:170:LYS:O	1:E:171:ASN:HB2	2.16	0.44
1:D:210:ASN:C	1:D:210:ASN:HD22	2.21	0.44
1:C:36:LYS:O	1:C:55:ILE:HG22	2.18	0.44
1:D:163:CYS:SG	1:D:277:ILE:HD12	2.58	0.44
1:C:208:ILE:HD13	1:F:297:PHE:CD2	2.53	0.44
1:D:101:GLN:O	1:D:104:GLN:HB3	2.18	0.44
1:A:124:VAL:O	1:A:128:ILE:HG13	2.18	0.44
1:D:154:GLY:HA2	1:D:231:ASN:ND2	2.33	0.44
1:F:49:GLN:HE22	1:F:83:ASN:ND2	2.01	0.44
1:A:212:GLU:HG3	1:A:220:THR:HG21	1.99	0.43
1:A:5:LEU:HD23	1:A:29:VAL:HG12	2.00	0.43
1:F:113:THR:HG21	1:F:120:LEU:HD11	2.00	0.43
1:B:63:PHE:O	1:B:66:GLN:HG2	2.18	0.43
1:C:90:THR:CG2	1:C:91:LYS:H	2.31	0.43
1:D:253:GLN:C	1:D:253:GLN:HE21	2.22	0.43
1:E:213:ARG:HD2	1:E:213:ARG:HA	1.77	0.43
1:E:271:ARG:HD2	1:E:276:ILE:HD11	2.01	0.43
1:A:248:THR:HG23	1:A:294:ALA:HB1	2.00	0.43
1:A:286:LEU:HD12	1:A:286:LEU:HA	1.87	0.43
1:C:286:LEU:HD12	1:C:286:LEU:HA	1.91	0.43
1:C:36:LYS:HD3	1:C:50:ILE:HG23	2.01	0.43
1:E:141:VAL:HG22	1:E:177:ASP:OD1	2.19	0.43
1:F:138:ILE:N	1:F:138:ILE:HD13	2.33	0.43
1:F:152:LEU:HD11	1:F:277:ILE:HD13	2.00	0.43
1:F:40:PHE:HD2	1:F:45:LEU:HD12	1.83	0.43
1:A:61:PHE:HB2	1:A:93:PHE:CD1	2.51	0.43
1:C:103:ASN:C	1:C:105:THR:H	2.22	0.43
1:A:17:VAL:HA	1:A:112:LYS:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:HB2	1:A:253:GLN:HE21	1.66	0.43
1:A:42:MET:HB3	1:A:75:ILE:HG23	2.01	0.43
1:E:183:TYR:HD1	1:E:185:LEU:HD13	1.82	0.43
1:C:216:GLY:O	1:C:219:ILE:HG22	2.18	0.43
1:C:55:ILE:HD11	1:C:90:THR:OG1	2.18	0.43
1:A:250:LEU:HD23	1:A:250:LEU:N	2.22	0.43
1:A:243:PHE:CZ	1:A:266:PRO:HB3	2.54	0.43
1:A:91:LYS:HD2	1:A:114:ASP:HA	2.00	0.43
1:E:91:LYS:HD3	1:E:116:PHE:CZ	2.54	0.43
1:B:267:ILE:CG2	1:E:270:GLY:HA2	2.48	0.43
1:F:240:THR:HG23	1:F:241:VAL:HG23	2.00	0.43
1:E:250:LEU:H	1:E:250:LEU:CD1	2.29	0.43
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.77	0.42
1:B:164:ALA:O	1:B:168:ILE:HD13	2.19	0.42
1:D:250:LEU:HD22	1:D:287:LYS:HD3	2.01	0.42
1:E:56:LEU:HB3	1:E:93:PHE:CE1	2.54	0.42
1:A:13:PHE:O	1:A:17:VAL:HG22	2.20	0.42
1:C:8:GLU:O	1:C:12:GLN:HB2	2.20	0.42
1:A:304:ILE:HD11	1:F:195:GLU:HG2	2.01	0.42
1:A:53:VAL:HG13	1:A:86:ALA:HB3	2.01	0.42
1:B:25:ASN:C	1:B:27:SER:H	2.23	0.42
1:B:250:LEU:HD13	1:B:287:LYS:HD2	2.01	0.42
1:E:300:ASN:O	1:E:304:ILE:HG13	2.19	0.42
1:F:253:GLN:HE21	1:F:253:GLN:HB2	1.64	0.42
1:F:25:ASN:C	1:F:27:SER:H	2.22	0.42
1:A:155:ARG:HG2	1:A:155:ARG:NH1	2.34	0.42
1:C:304:ILE:O	1:C:308:LYS:HG2	2.20	0.42
1:D:142:LEU:HB3	1:D:175:VAL:HB	2.02	0.42
1:D:210:ASN:ND2	1:D:213:ARG:H	2.17	0.42
1:E:38:VAL:HB	1:E:41:GLU:HG2	2.02	0.42
1:F:17:VAL:HG13	1:F:111:LEU:HB3	2.01	0.42
1:D:25:ASN:C	1:D:27:SER:N	2.72	0.42
1:F:145:VAL:HG13	1:F:172:HIS:CE1	2.54	0.42
1:A:168:ILE:HD12	1:A:172:HIS:O	2.20	0.42
1:A:95:ASP:C	1:A:97:THR:H	2.23	0.42
1:D:183:TYR:HD2	1:D:185:LEU:CD1	2.30	0.42
1:C:196:VAL:HG12	1:F:304:ILE:HD12	2.02	0.42
1:A:304:ILE:C	1:A:306:LYS:H	2.23	0.42
1:C:219:ILE:HA	1:C:219:ILE:HD12	1.77	0.42
1:C:7:LYS:HG3	1:C:8:GLU:N	2.34	0.42
1:E:123:THR:O	1:F:186:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HG3	2:B:361:HOH:O	2.19	0.42
1:D:58:LYS:HB2	1:D:92:SER:CB	2.49	0.42
1:A:91:LYS:C	1:A:93:PHE:H	2.23	0.41
1:E:35:LEU:HD12	1:E:35:LEU:HA	1.90	0.41
1:F:268:SER:HA	1:F:269:PRO:HD3	1.95	0.41
1:B:149:GLY:HA3	1:B:225:GLU:O	2.21	0.41
1:E:144:GLU:HB3	1:E:173:LEU:HB2	2.02	0.41
1:C:84:PRO:HA	1:C:85:PRO:HD3	1.90	0.41
1:E:76:LEU:HD12	1:E:98:VAL:HG12	2.02	0.41
1:A:35:LEU:CD1	1:A:120:LEU:HD23	2.48	0.41
1:B:57:GLY:HA2	1:B:90:THR:CG2	2.51	0.41
1:D:49:GLN:O	1:D:49:GLN:HG3	2.20	0.41
1:F:103:ASN:ND2	1:F:108:VAL:H	2.03	0.41
1:D:217:LEU:N	1:D:217:LEU:HD12	2.36	0.41
1:D:89:LEU:HD13	1:D:93:PHE:CD2	2.55	0.41
1:D:97:THR:O	1:D:101:GLN:HG3	2.21	0.41
1:E:34:GLY:N	1:E:129:ASN:ND2	2.68	0.41
1:A:173:LEU:HD12	1:A:219:ILE:HA	2.03	0.41
1:D:32:VAL:CB	1:D:52:SER:HB3	2.49	0.41
1:E:34:GLY:CA	1:E:129:ASN:HD21	2.32	0.41
1:F:179:ALA:HB3	1:F:197:ALA:HB2	2.02	0.41
1:A:28:ASN:ND2	1:A:85:PRO:HA	2.35	0.41
1:C:37:ARG:NH2	2:C:318:HOH:O	2.54	0.41
1:C:38:VAL:HB	1:C:41:GLU:HG2	2.01	0.41
1:D:122:PHE:HA	1:D:126:THR:OG1	2.21	0.41
1:D:149:GLY:HA3	1:D:225:GLU:O	2.21	0.41
1:D:163:CYS:SG	1:D:277:ILE:CD1	3.09	0.41
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.85	0.41
1:F:5:LEU:HB2	1:F:8:GLU:HG3	2.03	0.41
1:D:97:THR:HA	1:D:100:LEU:HD12	2.02	0.41
1:F:98:VAL:O	1:F:102:VAL:HG23	2.20	0.41
1:F:232:LEU:HB3	1:F:267:ILE:HD11	2.03	0.41
1:A:20:ILE:CD1	1:A:112:LYS:HE2	2.51	0.41
1:A:214:PHE:HB3	1:A:215:TYR:CD1	2.56	0.41
1:B:126:THR:O	1:B:130:GLU:HG3	2.19	0.41
1:B:145:VAL:HA	1:B:172:HIS:CD2	2.56	0.41
1:B:7:LYS:HB3	1:B:26:THR:CG2	2.49	0.41
1:C:228:LEU:HD11	1:C:263:TYR:HE1	1.86	0.41
1:E:150:VAL:HG12	1:E:152:LEU:HD12	2.03	0.41
1:F:35:LEU:HD23	1:F:35:LEU:HA	1.87	0.41
1:A:300:ASN:O	1:A:304:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:HD2	1:B:114:ASP:O	2.21	0.41
1:A:198:LYS:HB3	1:A:199:LYS:H	1.46	0.40
1:B:172:HIS:HE1	1:B:278:GLU:OE2	2.04	0.40
1:E:219:ILE:C	1:E:219:ILE:HD12	2.42	0.40
1:A:32:VAL:O	1:A:52:SER:HB3	2.21	0.40
1:C:6:VAL:HG23	1:C:28:ASN:O	2.21	0.40
1:D:5:LEU:HB2	1:D:8:GLU:OE2	2.21	0.40
1:E:80:LEU:HD12	1:E:102:VAL:HG12	2.03	0.40
1:A:168:ILE:HD11	1:A:174:PHE:HB2	2.03	0.40
1:A:50:ILE:HB	1:A:84:PRO:HA	2.03	0.40
1:C:307:ARG:HG2	1:C:307:ARG:HH11	1.87	0.40
1:C:36:LYS:NZ	2:C:344:HOH:O	2.54	0.40
1:E:4:LEU:HD12	1:E:132:PHE:CE1	2.56	0.40
1:D:25:ASN:ND2	1:D:107:GLN:HB3	2.37	0.40
1:D:7:LYS:HG3	1:D:8:GLU:N	2.36	0.40
1:A:142:LEU:CB	1:A:175:VAL:HB	2.52	0.40
1:B:268:SER:HA	1:B:269:PRO:HD3	1.93	0.40
1:E:122:PHE:HA	1:E:126:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	299/312 (96%)	263 (88%)	31 (10%)	5 (2%)	9 16
1	B	300/312 (96%)	288 (96%)	12 (4%)	0	100 100
1	C	296/312 (95%)	279 (94%)	16 (5%)	1 (0%)	41 61
1	D	300/312 (96%)	265 (88%)	32 (11%)	3 (1%)	15 28
1	E	306/312 (98%)	289 (94%)	16 (5%)	1 (0%)	41 61
1	F	302/312 (97%)	285 (94%)	17 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1803/1872 (96%)	1669 (93%)	124 (7%)	10 (1%)	25 43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	THR
1	A	94	THR
1	C	178	ASP
1	A	21	ASP
1	D	249	GLU
1	A	66	GLN
1	A	178	ASP
1	D	90	THR
1	D	306	LYS
1	E	178	ASP

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	265/279 (95%)	248 (94%)	17 (6%)	17 33
1	B	270/279 (97%)	259 (96%)	11 (4%)	30 55
1	C	265/279 (95%)	250 (94%)	15 (6%)	20 39
1	D	266/279 (95%)	253 (95%)	13 (5%)	25 47
1	E	271/279 (97%)	253 (93%)	18 (7%)	16 32
1	F	267/279 (96%)	253 (95%)	14 (5%)	23 44
All	All	1604/1674 (96%)	1516 (94%)	88 (6%)	21 41

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	48	SER
1	A	77	HIS
1	A	97	THR
1	A	122	PHE
1	A	137	GLN
1	A	165	LEU
1	A	168	ILE
1	A	173	LEU
1	A	187	ASN
1	A	210	ASN
1	A	218	GLN
1	A	234	SER
1	A	250	LEU
1	A	253	GLN
1	A	292	ASN
1	B	26	THR
1	B	79	LEU
1	B	114	ASP
1	B	143	LEU
1	B	173	LEU
1	B	213	ARG
1	B	218	GLN
1	B	235	LEU
1	B	255	LEU
1	B	286	LEU
1	B	292	ASN
1	C	4	LEU
1	C	8	GLU
1	C	74	GLN
1	C	126	THR
1	C	152	LEU
1	C	166	ASP
1	C	189	LEU
1	C	210	ASN
1	C	222	GLN
1	C	234	SER
1	C	248	THR
1	C	249	GLU
1	C	256	LEU
1	C	275	GLU
1	C	286	LEU
1	D	21	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	24	THR
1	D	37	ARG
1	D	40	PHE
1	D	49	GLN
1	D	158	ILE
1	D	166	ASP
1	D	210	ASN
1	D	222	GLN
1	D	248	THR
1	D	251	LYS
1	D	253	GLN
1	D	271	ARG
1	E	4	LEU
1	E	8	GLU
1	E	9	LEU
1	E	35	LEU
1	E	38	VAL
1	E	74	GLN
1	E	79	LEU
1	E	131	GLN
1	E	145	VAL
1	E	155	ARG
1	E	185	LEU
1	E	210	ASN
1	E	218	GLN
1	E	223	ARG
1	E	250	LEU
1	E	253	GLN
1	E	275	GLU
1	E	311	GLU
1	F	37	ARG
1	F	77	HIS
1	F	79	LEU
1	F	105	THR
1	F	135	VAL
1	F	138	ILE
1	F	152	LEU
1	F	210	ASN
1	F	249	GLU
1	F	253	GLN
1	F	255	LEU
1	F	264	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	266	PRO
1	F	271	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	49	GLN
1	A	66	GLN
1	A	83	ASN
1	A	104	GLN
1	A	137	GLN
1	A	171	ASN
1	A	172	HIS
1	A	187	ASN
1	A	210	ASN
1	A	218	GLN
1	A	222	GLN
1	A	231	ASN
1	A	253	GLN
1	A	292	ASN
1	B	72	GLN
1	B	101	GLN
1	B	104	GLN
1	B	169	ASN
1	B	171	ASN
1	B	172	HIS
1	B	218	GLN
1	B	292	ASN
1	C	28	ASN
1	C	66	GLN
1	C	131	GLN
1	C	169	ASN
1	C	172	HIS
1	C	210	ASN
1	C	231	ASN
1	C	292	ASN
1	D	25	ASN
1	D	49	GLN
1	D	107	GLN
1	D	210	ASN
1	D	253	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	28	ASN
1	E	72	GLN
1	E	73	GLN
1	E	129	ASN
1	E	131	GLN
1	E	137	GLN
1	E	171	ASN
1	E	210	ASN
1	E	218	GLN
1	E	292	ASN
1	F	12	GLN
1	F	28	ASN
1	F	77	HIS
1	F	83	ASN
1	F	103	ASN
1	F	104	GLN
1	F	107	GLN
1	F	194	GLN
1	F	210	ASN
1	F	222	GLN
1	F	253	GLN
1	F	292	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	233:LEU	C	234:SER	N	1.19

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, 95^{th} 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	303/312 (97%)	0.55	45 (14%) 2 2	25, 65, 131, 145	0
1	B	304/312 (97%)	-0.17	5 (1%) 72 74	24, 44, 66, 100	0
1	C	300/312 (96%)	0.16	16 (5%) 26 28	26, 50, 90, 125	0
1	D	304/312 (97%)	0.50	34 (11%) 5 4	26, 53, 100, 113	0
1	E	310/312 (99%)	-0.13	12 (3%) 39 42	25, 41, 68, 108	0
1	F	306/312 (98%)	-0.05	14 (4%) 32 34	24, 41, 90, 127	0
All	All	1827/1872 (97%)	0.14	126 (6%) 16 17	24, 46, 106, 145	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	5.6
1	E	236	GLU	5.6
1	C	311	GLU	5.1
1	D	107	GLN	5.0
1	A	115	PHE	4.9
1	D	75	ILE	4.8
1	E	235	LEU	4.6
1	D	68	THR	4.5
1	A	106	TYR	4.5
1	D	303	ALA	4.4
1	F	239	THR	4.3
1	A	19	LEU	4.3
1	D	47	SER	4.2
1	F	305	LEU	4.2
1	F	303	ALA	3.9
1	D	1	MET	3.9
1	F	235	LEU	3.9
1	A	10	ILE	3.7
1	D	49	GLN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	304	ILE	3.6
1	C	310	ASP	3.6
1	A	307	ARG	3.5
1	D	305	LEU	3.5
1	C	306	LYS	3.5
1	E	311	GLU	3.5
1	F	240	THR	3.5
1	F	241	VAL	3.5
1	D	63	PHE	3.5
1	F	158	ILE	3.4
1	E	1	MET	3.4
1	A	66	GLN	3.4
1	F	248	THR	3.3
1	A	87	ILE	3.3
1	C	114	ASP	3.3
1	A	24	THR	3.3
1	A	114	ASP	3.3
1	F	242	THR	3.2
1	B	1	MET	3.2
1	D	28	ASN	3.2
1	D	55	ILE	3.2
1	F	304	ILE	3.2
1	A	27	SER	3.2
1	A	11	GLU	3.2
1	A	25	ASN	3.2
1	E	237	LYS	3.1
1	A	68	THR	3.1
1	D	102	VAL	3.1
1	A	122	PHE	3.1
1	D	7	LYS	3.0
1	D	66	GLN	2.9
1	E	310	ASP	2.9
1	C	1	MET	2.9
1	C	62	GLY	2.9
1	A	305	LEU	2.9
1	E	307	ARG	2.8
1	D	2	LYS	2.8
1	A	69	LEU	2.8
1	A	308	LYS	2.8
1	C	37	ARG	2.8
1	A	105	THR	2.8
1	D	74	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.7
1	D	70	VAL	2.7
1	A	155	ARG	2.7
1	B	304	ILE	2.7
1	C	305	LEU	2.7
1	C	66	GLN	2.6
1	D	64	LEU	2.6
1	C	3	LYS	2.6
1	D	250	LEU	2.6
1	F	250	LEU	2.6
1	C	2	LYS	2.6
1	A	249	GLU	2.6
1	D	82	LEU	2.5
1	B	2	LYS	2.5
1	C	309	LYS	2.5
1	D	155	ARG	2.5
1	A	110	ILE	2.5
1	D	37	ARG	2.5
1	A	107	GLN	2.5
1	A	28	ASN	2.5
1	D	26	THR	2.5
1	E	55	ILE	2.5
1	D	78	ASN	2.5
1	D	65	SER	2.4
1	D	154	GLY	2.4
1	D	27	SER	2.4
1	D	67	LYS	2.4
1	A	31	ARG	2.4
1	A	104	GLN	2.4
1	A	242	THR	2.4
1	A	88	ILE	2.4
1	E	309	LYS	2.4
1	B	248	THR	2.4
1	A	94	THR	2.3
1	C	35	LEU	2.3
1	D	306	LYS	2.3
1	E	234	SER	2.3
1	A	55	ILE	2.3
1	A	20	ILE	2.3
1	D	35	LEU	2.3
1	A	116	PHE	2.3
1	A	7	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	102	VAL	2.2
1	D	101	GLN	2.2
1	A	5	LEU	2.2
1	F	249	GLU	2.2
1	A	306	LYS	2.2
1	D	304	ILE	2.2
1	A	248	THR	2.2
1	A	82	LEU	2.2
1	D	29	VAL	2.1
1	B	307	ARG	2.1
1	C	47	SER	2.1
1	A	108	VAL	2.1
1	F	246	LEU	2.1
1	A	234	SER	2.1
1	A	16	CYS	2.1
1	C	304	ILE	2.1
1	E	56	LEU	2.1
1	E	2	LYS	2.1
1	A	17	VAL	2.1
1	C	250	LEU	2.0
1	D	46	PHE	2.0
1	A	91	LYS	2.0
1	F	302	LYS	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 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.