Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 01:58 AM EDT

PDB ID	:	2QLV
Title	:	Crystal structure of the heterotrimer core of the S. cerevisiae AMPK homolog SNF1
Authors	:	Amodeo, G.A.; Rudolph, M.J.; Tong, L.
Deposited on	:	2007-07-13
Resolution	:	2.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

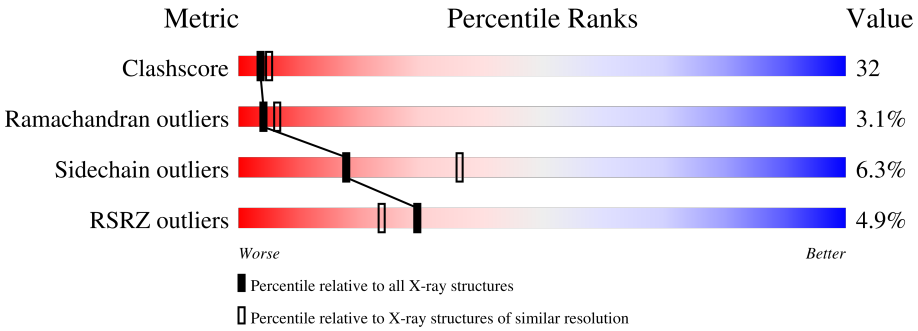
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	171	4% 35% 37% 5% 22%
1	D	171	9% 33% 40% 5% 22%
2	B	252	2% 27% 29% 38%
2	E	252	3% 32% 19% 44%
3	C	315	2% 52% 41% 5%
3	F	315	5% 50% 44%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9579 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 Carbon catabolite derepressing protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1079	704	177	192	6			
1	D	133	Total	C	N	O	S	0	0	0
			1079	704	177	192	6			

- Molecule 2 is a protein called Protein SIP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	0	0
			1264	815	219	225	5			
2	E	140	Total	C	N	O	S	0	0	0
			1131	731	198	198	4			

- Molecule 3 is a protein called Nuclear protein SNF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	310	Total	C	N	O	S	0	0	0
			2457	1570	412	465	10			
3	F	310	Total	C	N	O	S	0	0	0
			2458	1570	412	466	10			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	23	Total	O	0	0
			23	23		
4	C	28	Total	O	0	0
			28	28		
4	D	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

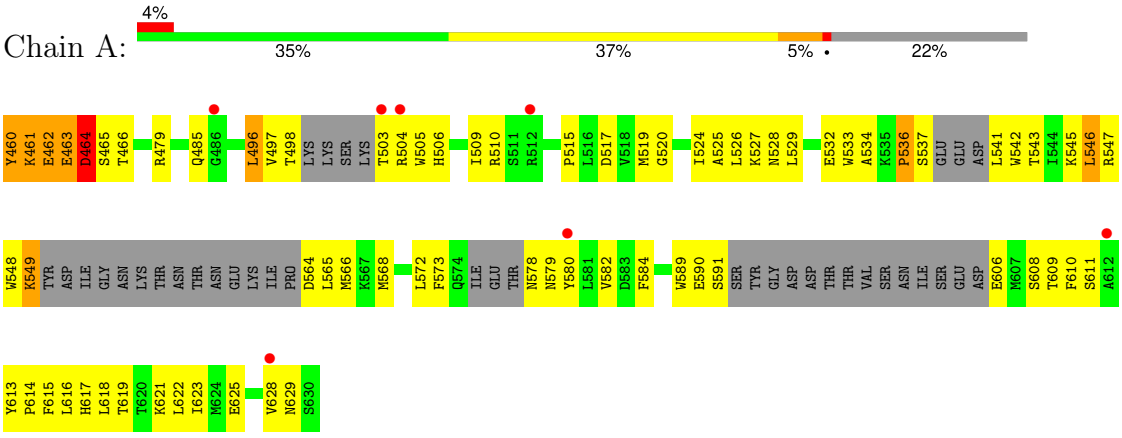
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	11	Total O 11 11	0	0
4	F	29	Total O 29 29	0	0

3 Residue-property plots (i)

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

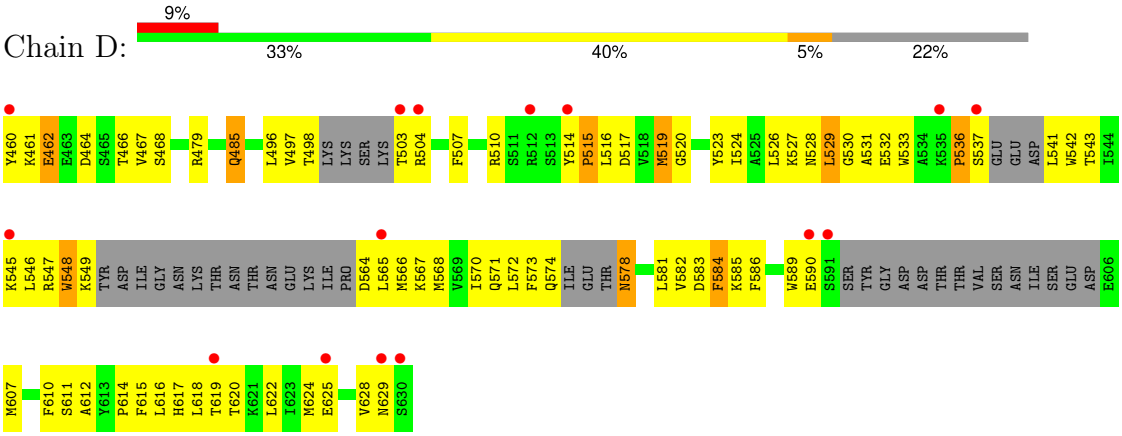
• Molecule 1: Carbon catabolite derepressing protein kinase

Chain A:



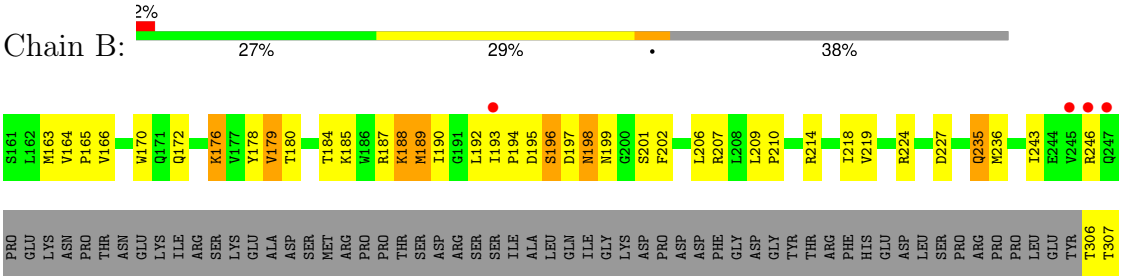
• Molecule 1: Carbon catabolite derepressing protein kinase

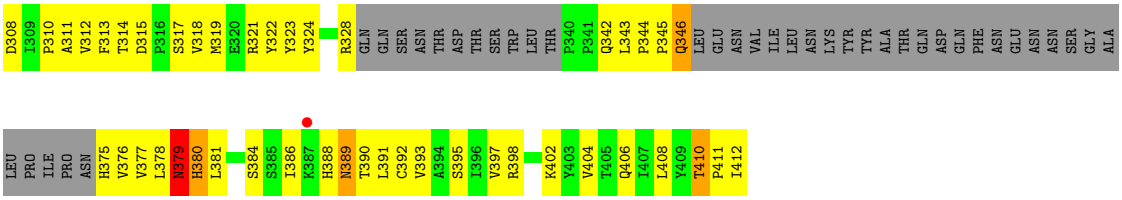
Chain D:



• Molecule 2: Protein SIP2

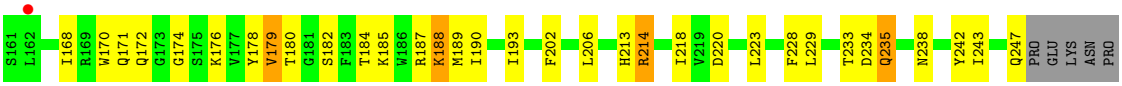
Chain B:

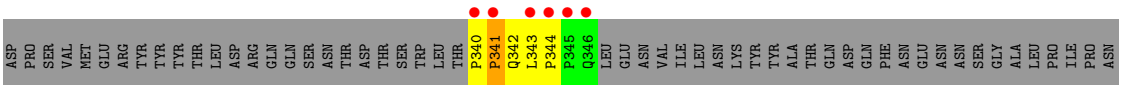


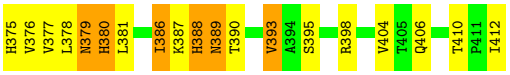


• Molecule 2: Protein SIP2

Chain E:

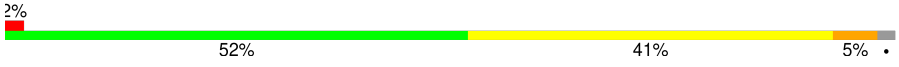


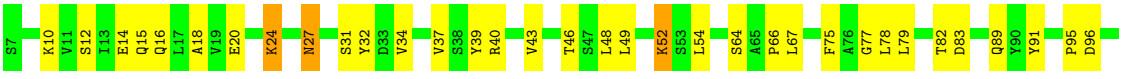


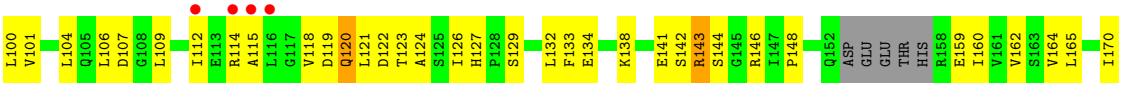


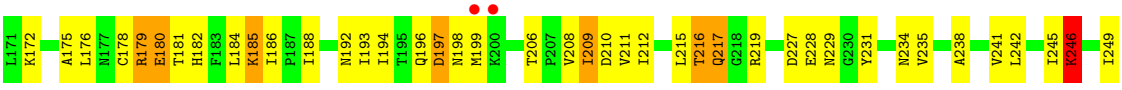
• Molecule 3: Nuclear protein SNF4

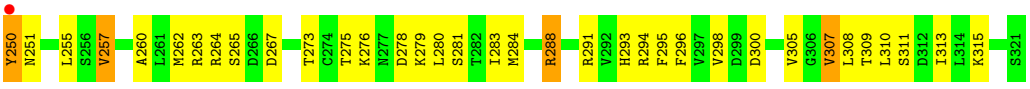
Chain C:





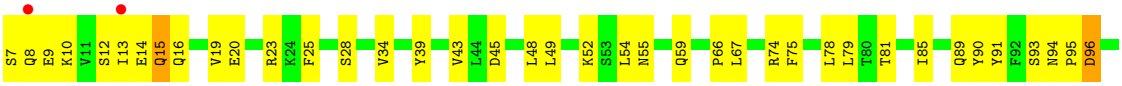


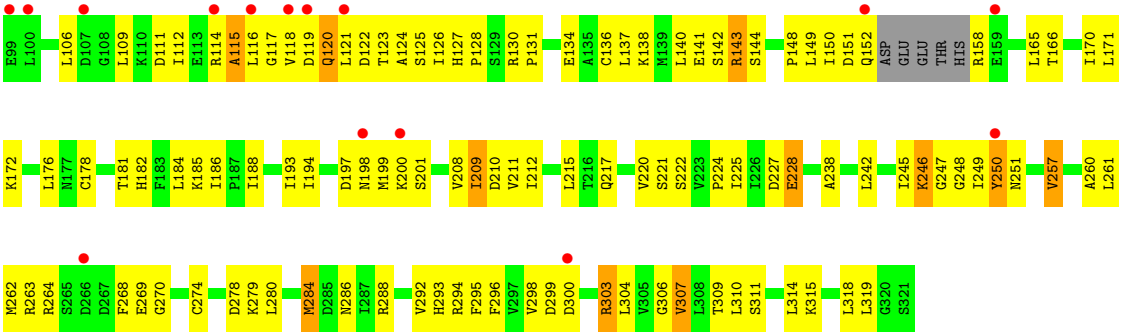




• Molecule 3: Nuclear protein SNF4

Chain F:




E99 L100 L106 D107 G108 L109 K110 D111 I112 E113 R114 A115 L116 G117 V118 D119 Q120 L121 D122 T123 A124 S125 I126 H127 P128 S129 R130 P131 E134 A135 C136 L137 K138 M139 L140 E141 S142 R143 S144 P148 L149 I150 D151 Q152 ASP GLU GLU THR HIS R158 E159 L165 T166 I170 L171
K172 L176 N177 C178 T181 H182 F183 L184 K185 I186 P187 I188 I193 I194 D197 N198 M199 K200 S201 V208 I209 D210 V211 I212 L215 T216 Q217 V220 S221 S222 V223 P224 I225 I226 D227 E228 A238 L242 I245 K246 G247 G248 I249 V250 N251 V257 A260 L261
M262 R263 R264 S265 D266 D267 F268 E269 G270 C274 D278 K279 L280 M284 D285 N286 I287 R288 V292 H293 R294 F295 F296 V297 V298 D299 D300 R303 L304 V305 G306 V307 L308 T309 L310 S311 L314 K315 L318 L319 G320 S321

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.33Å 81.84Å 174.74Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	29.54 – 2.60 29.54 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.54-2.60) 88.1 (29.54-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.299 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9579	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.41	0/1104	0.61	0/1490
1	D	0.40	0/1104	0.61	0/1490
2	B	0.45	0/1295	0.67	0/1759
2	E	0.44	0/1158	0.68	0/1572
3	C	0.44	0/2491	0.65	0/3371
3	F	0.44	0/2492	0.66	0/3371
All	All	0.43	0/9644	0.65	0/13053

There are no bond length outliers.

There are no bond angle outliers.

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	1079	0	1083	69	0
1	D	1079	0	1083	84	0
2	B	1264	0	1271	108	0
2	E	1131	0	1149	77	0
3	C	2457	0	2544	163	0
3	F	2458	0	2544	178	0
4	A	15	0	0	2	0
4	B	23	0	0	5	0
4	C	28	0	0	1	0
4	D	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	11	0	0	0	0
4	F	29	0	0	4	0
All	All	9579	0	9674	605	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 32.

All (605) 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)
3:C:114:ARG:HA	3:C:119:ASP:HB3	1.34	1.09
3:F:249:ILE:HG22	3:F:250:TYR:H	1.22	1.00
2:E:386:ILE:HD12	2:E:386:ILE:H	1.29	0.96
3:C:188:ILE:HD11	3:C:280:LEU:HG	1.44	0.95
3:C:82:THR:HG21	3:C:219:ARG:HH12	1.33	0.94
3:F:209:ILE:HD12	3:F:210:ASP:H	1.34	0.93
3:C:120:GLN:HG2	3:F:117:GLY:H	1.32	0.91
2:E:375:HIS:CD2	2:E:377:VAL:HG22	2.05	0.90
3:C:276:LYS:HE3	3:C:305:VAL:HG11	1.54	0.90
3:F:120:GLN:HE22	3:F:122:ASP:HB3	1.37	0.89
3:C:175:ALA:HB2	3:C:284:MET:HG3	1.55	0.89
3:C:211:VAL:HG21	3:C:257:VAL:CG1	2.04	0.87
1:D:616:LEU:HD22	2:E:393:VAL:HG13	1.56	0.87
2:E:184:THR:HG21	2:E:188:LYS:O	1.74	0.86
2:E:189:MET:CE	2:E:218:ILE:HD13	2.05	0.86
2:E:375:HIS:CG	2:E:376:VAL:H	1.93	0.86
3:F:95:PRO:O	3:F:96:ASP:HB2	1.77	0.84
2:E:375:HIS:HD2	2:E:377:VAL:HG22	1.41	0.84
2:B:184:THR:HG21	2:B:188:LYS:O	1.78	0.83
3:C:245:ILE:HA	3:C:249:ILE:HB	1.60	0.83
2:E:214:ARG:HH11	2:E:214:ARG:HB2	1.44	0.82
2:B:386:ILE:HD12	2:B:386:ILE:H	1.43	0.81
3:C:309:THR:HG22	3:C:311:SER:H	1.43	0.81
2:E:390:THR:HG21	3:F:48:LEU:HD11	1.61	0.81
3:F:165:LEU:HG	3:F:170:ILE:HD11	1.62	0.80
1:D:467:VAL:HG11	3:F:286:ASN:ND2	1.96	0.80
3:F:130:ARG:HH11	3:F:131:PRO:HD2	1.47	0.79
3:F:130:ARG:NH2	3:F:134:GLU:HG2	1.96	0.79
3:F:310:LEU:HD11	4:F:768:HOH:O	1.82	0.79
3:F:10:LYS:O	3:F:14:GLU:HG3	1.82	0.79
2:B:198:ASN:HD22	2:B:199:ASN:N	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:HIS:HD2	2:B:377:VAL:HG22	1.49	0.78
3:C:82:THR:CG2	3:C:219:ARG:HH12	1.97	0.77
3:C:196:GLN:HE22	3:C:305:VAL:HG12	1.50	0.77
3:C:211:VAL:HG21	3:C:257:VAL:HG11	1.66	0.77
2:E:185:LYS:HD3	2:E:187:ARG:NH1	1.99	0.77
3:C:91:TYR:HB2	3:C:101:VAL:HG21	1.66	0.77
2:B:176:LYS:NZ	2:B:176:LYS:HB3	2.00	0.76
3:C:127:HIS:CD2	3:C:129:SER:H	2.03	0.76
3:F:16:GLN:HE21	3:F:20:GLU:HG3	1.51	0.76
3:F:315:LYS:HG3	3:F:319:LEU:HD12	1.68	0.76
2:B:166:VAL:HG11	2:B:243:ILE:CD1	2.17	0.75
3:F:309:THR:HG22	3:F:311:SER:H	1.52	0.74
3:C:16:GLN:O	3:C:20:GLU:HG3	1.87	0.74
2:E:184:THR:HG23	2:E:188:LYS:HB3	1.68	0.73
2:B:376:VAL:HG23	2:B:398:ARG:HH22	1.52	0.73
2:E:375:HIS:CG	2:E:376:VAL:N	2.56	0.72
3:C:188:ILE:HD11	3:C:280:LEU:CG	2.17	0.72
3:F:188:ILE:HG13	3:F:193:ILE:HD11	1.70	0.72
3:F:152:GLN:HE21	3:F:152:GLN:HA	1.55	0.72
3:F:178:CYS:O	3:F:181:THR:HG23	1.89	0.72
2:B:377:VAL:C	2:B:378:LEU:HD12	2.08	0.72
2:E:184:THR:CG2	2:E:188:LYS:HB3	2.20	0.71
1:D:496:LEU:HD12	1:D:497:VAL:H	1.55	0.71
2:E:377:VAL:C	2:E:378:LEU:HD12	2.11	0.71
2:B:189:MET:CE	2:B:218:ILE:HD13	2.20	0.71
2:B:386:ILE:HG13	2:B:391:LEU:HD13	1.72	0.71
2:E:375:HIS:NE2	2:E:377:VAL:HG13	2.05	0.71
3:F:142:SER:O	3:F:144:SER:N	2.22	0.71
2:E:168:ILE:HD13	2:E:206:LEU:HD12	1.73	0.70
3:C:67:LEU:HD21	3:C:79:LEU:HB2	1.72	0.70
3:C:127:HIS:HD2	3:C:129:SER:H	1.36	0.70
3:F:199:MET:CE	3:F:304:LEU:HD21	2.20	0.70
2:B:178:TYR:HB3	2:B:189:MET:HB3	1.74	0.70
3:C:54:LEU:CD1	3:C:242:LEU:HD22	2.21	0.70
2:E:404:VAL:HG22	3:F:39:TYR:CZ	2.27	0.70
3:F:249:ILE:HG22	3:F:250:TYR:N	2.02	0.70
3:F:199:MET:HE1	3:F:304:LEU:HD21	1.74	0.69
2:E:189:MET:HE1	2:E:218:ILE:HD13	1.72	0.69
2:E:386:ILE:H	2:E:386:ILE:CD1	2.05	0.69
3:C:141:GLU:HB3	3:F:118:VAL:HB	1.74	0.69
3:C:120:GLN:N	3:F:116:LEU:HD22	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:ARG:O	1:D:548:TRP:HB2	1.93	0.68
2:B:209:LEU:HG	2:B:210:PRO:HD2	1.75	0.68
3:F:66:PRO:HA	3:F:78:LEU:HD23	1.74	0.68
2:E:386:ILE:HD12	2:E:386:ILE:N	2.08	0.68
3:F:120:GLN:NE2	3:F:122:ASP:HB3	2.09	0.68
3:C:211:VAL:HG21	3:C:257:VAL:HG13	1.74	0.68
3:F:176:LEU:HD13	3:F:288:ARG:HG3	1.75	0.68
3:C:199:MET:HE1	3:C:307:VAL:HG23	1.76	0.68
3:F:220:VAL:HG22	3:F:222:SER:H	1.58	0.68
3:F:209:ILE:HD12	3:F:210:ASP:N	2.09	0.67
3:F:209:ILE:CD1	3:F:210:ASP:H	2.07	0.67
3:C:49:LEU:HB3	3:C:52:LYS:HB2	1.77	0.67
2:B:375:HIS:CD2	2:B:377:VAL:HG22	2.28	0.67
3:C:67:LEU:HD22	3:C:106:LEU:HD13	1.77	0.67
3:C:10:LYS:O	3:C:14:GLU:HG3	1.95	0.66
3:C:118:VAL:HB	3:F:116:LEU:HG	1.77	0.66
2:B:172:GLN:HE22	2:B:227:ASP:H	1.44	0.66
3:F:16:GLN:O	3:F:20:GLU:HG3	1.96	0.66
2:B:318:VAL:HA	2:B:321:ARG:HD3	1.77	0.65
3:F:124:ALA:O	3:F:148:PRO:HD2	1.97	0.65
2:B:390:THR:HG23	4:B:747:HOH:O	1.95	0.65
1:D:532:GLU:HG3	1:D:547:ARG:HB3	1.78	0.65
3:F:245:ILE:O	3:F:247:GLY:N	2.29	0.65
3:F:128:PRO:HG3	3:F:149:LEU:HB3	1.79	0.65
3:C:118:VAL:O	3:F:116:LEU:HD21	1.97	0.65
3:F:309:THR:HG22	3:F:310:LEU:N	2.12	0.65
3:C:77:GLY:HA2	3:C:123:THR:HG21	1.77	0.64
3:C:118:VAL:HB	3:F:116:LEU:CG	2.27	0.64
3:C:196:GLN:NE2	3:C:305:VAL:HG12	2.12	0.64
1:D:572:LEU:HD13	1:D:582:VAL:HG22	1.78	0.64
1:D:566:MET:CE	1:D:618:LEU:HD12	2.28	0.64
1:D:485:GLN:OE1	1:D:485:GLN:HA	1.97	0.64
1:D:532:GLU:CD	1:D:547:ARG:HE	2.01	0.64
2:E:189:MET:HE2	2:E:218:ILE:HD13	1.80	0.64
3:F:249:ILE:HG12	4:F:720:HOH:O	1.97	0.64
1:D:467:VAL:HG23	3:F:278:ASP:OD1	1.97	0.64
3:F:188:ILE:HD11	3:F:280:LEU:HG	1.80	0.64
3:C:46:THR:HG22	3:C:107:ASP:HB2	1.80	0.64
1:D:607:MET:SD	3:F:158:ARG:NH2	2.71	0.63
1:A:590:GLU:HG3	1:A:591:SER:H	1.63	0.63
3:C:120:GLN:HG2	3:F:117:GLY:N	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:91:TYR:HE1	3:F:250:TYR:HB2	1.64	0.63
3:C:118:VAL:HG12	3:F:94:ASN:OD1	1.99	0.63
2:E:174:GLY:O	2:E:202:PHE:HZ	1.80	0.63
3:C:126:ILE:HD11	3:C:134:GLU:HG3	1.79	0.63
3:C:206:THR:O	3:C:257:VAL:HG22	1.99	0.63
2:E:176:LYS:HZ2	2:E:176:LYS:HB3	1.63	0.63
2:E:310:PRO:HG2	2:E:313:PHE:HD1	1.63	0.63
3:F:67:LEU:HD21	3:F:79:LEU:HB2	1.81	0.62
1:D:507:PHE:HE1	2:E:378:LEU:HD23	1.65	0.62
3:C:118:VAL:HB	3:F:116:LEU:CD1	2.29	0.62
3:F:185:LYS:HA	3:F:279:LYS:HD3	1.81	0.62
2:B:246:ARG:HH22	2:B:398:ARG:HH12	1.47	0.62
3:C:122:ASP:OD2	3:F:118:VAL:HG13	1.99	0.62
3:F:66:PRO:CA	3:F:78:LEU:HD23	2.29	0.61
3:F:114:ARG:HA	3:F:119:ASP:HB3	1.82	0.61
2:B:377:VAL:HG23	2:B:378:LEU:HD12	1.82	0.61
3:C:188:ILE:CD1	3:C:280:LEU:HG	2.25	0.61
3:C:114:ARG:CZ	3:C:121:LEU:HD11	2.30	0.61
3:C:118:VAL:HB	3:F:116:LEU:HD11	1.81	0.61
3:C:142:SER:O	3:C:144:SER:N	2.34	0.61
1:D:515:PRO:O	1:D:542:TRP:HZ3	1.84	0.61
3:F:130:ARG:CZ	3:F:134:GLU:HG2	2.30	0.61
2:B:386:ILE:HD12	2:B:386:ILE:N	2.15	0.61
2:B:381:LEU:HD11	2:B:393:VAL:CG2	2.31	0.61
1:D:514:TYR:HB2	1:D:517:ASP:OD2	2.01	0.61
3:F:228:GLU:CD	3:F:228:GLU:H	2.03	0.61
3:F:249:ILE:CG2	3:F:250:TYR:H	2.03	0.60
3:F:142:SER:C	3:F:144:SER:H	2.05	0.60
1:A:519:MET:HG2	2:B:313:PHE:CZ	2.37	0.60
2:B:376:VAL:HG23	2:B:398:ARG:NH2	2.16	0.60
3:C:142:SER:C	3:C:144:SER:H	2.05	0.60
3:C:208:VAL:HG11	3:C:260:ALA:HB2	1.84	0.60
3:C:276:LYS:CE	3:C:305:VAL:HG11	2.28	0.60
3:F:136:CYS:HB3	3:F:318:LEU:HD11	1.84	0.60
1:D:460:TYR:CD2	1:D:461:LYS:N	2.70	0.60
1:A:610:PHE:HA	3:C:160:ILE:HG13	1.82	0.59
2:E:410:THR:HG22	3:F:45:ASP:HB2	1.84	0.59
2:B:176:LYS:HB3	2:B:176:LYS:HZ2	1.64	0.59
2:B:307:THR:HG22	2:B:307:THR:O	2.02	0.59
1:D:585:LYS:HG3	2:E:380:HIS:CE1	2.37	0.59
3:F:74:ARG:HH11	3:F:74:ARG:HG2	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:ARG:HA	3:C:119:ASP:CB	2.21	0.59
2:E:381:LEU:HD11	2:E:393:VAL:HG21	1.84	0.59
2:B:306:THR:HG22	2:B:308:ASP:H	1.68	0.59
2:B:386:ILE:HG13	2:B:391:LEU:CD1	2.33	0.59
2:B:388:HIS:C	2:B:390:THR:H	2.06	0.59
1:D:574:GLN:HE22	1:D:578:ASN:HB3	1.66	0.59
3:F:199:MET:O	3:F:199:MET:HG3	2.02	0.59
2:B:187:ARG:O	2:B:187:ARG:HG3	2.03	0.59
2:B:402:LYS:NZ	3:C:32:TYR:O	2.35	0.59
1:D:497:VAL:HG12	1:D:498:THR:N	2.18	0.59
3:F:91:TYR:CE1	3:F:250:TYR:HB2	2.37	0.59
3:F:130:ARG:HD2	3:F:131:PRO:HD2	1.86	0.58
1:A:524:ILE:HG22	1:A:525:ALA:N	2.18	0.58
3:C:193:ILE:HD12	3:C:308:LEU:HD11	1.86	0.58
3:F:280:LEU:O	3:F:284:MET:HB2	2.04	0.58
2:B:190:ILE:HG21	2:B:206:LEU:HD21	1.86	0.58
3:C:142:SER:CA	3:F:118:VAL:HG12	2.34	0.58
1:D:573:PHE:HB3	2:E:343:LEU:HB2	1.86	0.58
2:E:184:THR:O	2:E:184:THR:HG22	2.03	0.58
2:B:346:GLN:H	2:B:346:GLN:NE2	2.02	0.57
3:C:43:VAL:HG22	3:C:66:PRO:HG2	1.86	0.57
3:C:104:LEU:HD22	3:C:112:ILE:HD12	1.85	0.57
2:E:176:LYS:HB3	2:E:176:LYS:NZ	2.19	0.57
2:E:187:ARG:O	2:E:187:ARG:HG3	2.03	0.57
1:A:460:TYR:HD2	1:A:461:LYS:N	2.01	0.57
3:F:120:GLN:HE22	3:F:122:ASP:CB	2.14	0.57
2:B:189:MET:HE3	2:B:218:ILE:HD13	1.86	0.57
2:B:386:ILE:H	2:B:386:ILE:CD1	2.15	0.57
1:D:566:MET:HG3	1:D:586:PHE:HE1	1.68	0.57
3:F:269:GLU:HG2	4:F:704:HOH:O	2.05	0.57
2:B:184:THR:HG22	2:B:184:THR:O	2.04	0.57
3:C:315:LYS:NZ	3:F:121:LEU:HB2	2.20	0.57
1:D:549:LYS:HB3	1:D:565:LEU:HG	1.85	0.57
2:E:377:VAL:HG23	2:E:377:VAL:O	2.05	0.56
3:C:118:VAL:C	3:F:116:LEU:HD21	2.25	0.56
1:A:466:THR:O	1:A:466:THR:HG22	2.06	0.56
2:E:170:TRP:CZ2	2:E:172:GLN:HB2	2.39	0.56
2:B:315:ASP:HB3	2:B:318:VAL:HG23	1.87	0.56
3:C:185:LYS:HA	3:C:279:LYS:HD3	1.86	0.56
2:E:187:ARG:O	2:E:188:LYS:HB2	2.06	0.56
3:C:24:LYS:HB2	3:C:24:LYS:NZ	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:PRO:O	3:C:96:ASP:HB2	2.05	0.56
1:D:543:THR:HG21	1:D:545:LYS:NZ	2.21	0.56
3:C:119:ASP:O	3:F:116:LEU:HD13	2.06	0.56
3:F:16:GLN:HE21	3:F:20:GLU:CG	2.18	0.56
2:B:306:THR:CG2	2:B:308:ASP:H	2.18	0.56
3:C:142:SER:N	3:F:118:VAL:HG12	2.21	0.55
2:B:180:THR:HG22	2:B:188:LYS:O	2.06	0.55
3:C:176:LEU:HD13	3:C:288:ARG:HG3	1.86	0.55
3:F:67:LEU:HD22	3:F:106:LEU:HD13	1.88	0.55
2:B:163:MET:HB3	2:B:207:ARG:O	2.07	0.55
2:B:184:THR:O	2:B:184:THR:CG2	2.54	0.55
2:B:389:ASN:HB3	3:C:52:LYS:NZ	2.21	0.55
3:C:309:THR:HG22	3:C:311:SER:N	2.18	0.55
2:E:410:THR:HG22	3:F:45:ASP:CB	2.36	0.55
3:F:188:ILE:HG22	3:F:194:ILE:HD11	1.87	0.55
2:E:168:ILE:HG21	2:E:179:VAL:HG11	1.88	0.55
3:C:197:ASP:O	3:C:198:ASN:HB2	2.07	0.55
1:D:526:LEU:HB3	1:D:531:ALA:HB3	1.87	0.55
3:F:208:VAL:HG11	3:F:260:ALA:HB2	1.87	0.55
1:D:615:PHE:O	1:D:619:THR:HG23	2.07	0.55
1:A:503:THR:HG22	1:A:504:ARG:H	1.72	0.54
3:C:54:LEU:HD11	3:C:242:LEU:HD22	1.89	0.54
2:B:311:ALA:HA	2:B:314:THR:OG1	2.07	0.54
2:B:312:VAL:HG23	4:B:725:HOH:O	2.06	0.54
2:B:189:MET:HE2	2:B:218:ILE:HD13	1.89	0.54
3:C:78:LEU:CD1	3:C:146:ARG:HD3	2.37	0.54
3:F:209:ILE:CD1	3:F:210:ASP:N	2.69	0.54
1:A:589:TRP:HE1	1:A:611:SER:HG	1.56	0.54
3:C:78:LEU:HD13	3:C:146:ARG:HD3	1.89	0.54
1:A:573:PHE:HB3	2:B:343:LEU:HB2	1.90	0.54
2:B:235:GLN:HG3	4:B:717:HOH:O	2.08	0.54
1:D:496:LEU:HD11	3:F:246:LYS:NZ	2.23	0.54
3:F:7:SER:CB	3:F:10:LYS:HB3	2.37	0.54
2:B:379:ASN:O	2:B:379:ASN:ND2	2.40	0.54
2:B:402:LYS:HD2	3:C:32:TYR:CE2	2.43	0.53
3:F:143:ARG:HG3	3:F:143:ARG:O	2.09	0.53
3:F:298:VAL:HA	3:F:303:ARG:O	2.09	0.53
2:E:376:VAL:HG23	2:E:398:ARG:HH21	1.74	0.53
3:F:54:LEU:CD1	3:F:242:LEU:HD22	2.39	0.53
1:A:524:ILE:O	1:A:528:ASN:ND2	2.42	0.53
3:C:208:VAL:HG11	3:C:260:ALA:CB	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:MET:HG3	2:E:412:ILE:HG23	1.88	0.53
1:A:496:LEU:HB2	3:C:263:ARG:NH2	2.24	0.53
3:F:201:SER:HB2	3:F:224:PRO:O	2.09	0.53
2:B:176:LYS:HB3	2:B:176:LYS:HZ3	1.73	0.53
1:D:566:MET:CG	1:D:586:PHE:HE1	2.22	0.53
1:A:616:LEU:HD21	2:B:395:SER:HB2	1.90	0.53
1:D:536:PRO:O	1:D:537:SER:CB	2.56	0.53
2:E:388:HIS:HB3	3:F:52:LYS:NZ	2.24	0.53
3:F:152:GLN:HA	3:F:152:GLN:NE2	2.22	0.53
3:F:268:PHE:CE2	3:F:270:GLY:HA2	2.43	0.53
3:C:251:ASN:HB2	4:C:782:HOH:O	2.09	0.52
1:D:566:MET:HE1	1:D:618:LEU:HD12	1.91	0.52
3:C:119:ASP:N	3:F:116:LEU:HD11	2.24	0.52
1:D:536:PRO:HB3	1:D:541:LEU:HB3	1.91	0.52
2:E:307:THR:HG22	2:E:307:THR:O	2.10	0.52
2:B:170:TRP:CZ2	2:B:172:GLN:HB2	2.44	0.52
3:C:219:ARG:HB3	3:F:114:ARG:HG2	1.90	0.52
2:B:166:VAL:HG11	2:B:243:ILE:HD11	1.92	0.52
3:C:227:ASP:OD2	3:C:231:TYR:HB2	2.09	0.52
3:F:7:SER:HB2	3:F:10:LYS:HB3	1.90	0.52
3:F:211:VAL:HG21	3:F:257:VAL:CG1	2.39	0.52
2:B:179:VAL:HG22	2:B:192:LEU:CD1	2.40	0.52
2:B:388:HIS:C	2:B:390:THR:N	2.63	0.52
3:C:27:ASN:ND2	3:C:133:PHE:HB3	2.25	0.52
3:C:309:THR:HG22	3:C:310:LEU:N	2.24	0.52
2:E:228:PHE:O	2:E:229:LEU:HD23	2.10	0.52
3:C:54:LEU:HD23	3:C:246:LYS:O	2.10	0.52
3:C:34:VAL:CG1	3:C:34:VAL:O	2.58	0.51
3:C:100:LEU:HD12	3:C:100:LEU:O	2.08	0.51
1:D:515:PRO:O	1:D:542:TRP:CZ3	2.63	0.51
3:F:211:VAL:HG21	3:F:257:VAL:HG13	1.92	0.51
1:A:525:ALA:O	1:A:529:LEU:HG	2.10	0.51
3:F:94:ASN:HD21	3:F:116:LEU:HD12	1.75	0.51
3:F:125:SER:CB	3:F:150:ILE:HD12	2.40	0.51
1:A:527:LYS:HG3	1:A:528:ASN:N	2.25	0.51
1:D:479:ARG:HG3	3:F:262:MET:HE3	1.92	0.51
3:C:179:ARG:NH1	3:C:182:HIS:CD2	2.78	0.51
1:D:497:VAL:HG12	1:D:498:THR:H	1.75	0.51
3:F:7:SER:C	3:F:9:GLU:H	2.13	0.51
3:F:81:THR:HG21	3:F:238:ALA:HB1	1.93	0.51
3:C:120:GLN:NE2	3:C:122:ASP:HB3	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:PRO:O	1:D:537:SER:HB3	2.11	0.51
1:A:529:LEU:HD11	1:A:622:LEU:HA	1.91	0.51
3:C:142:SER:C	3:C:144:SER:N	2.63	0.51
1:D:466:THR:O	3:F:274:CYS:HA	2.10	0.51
1:A:548:TRP:HD1	1:A:549:LYS:H	1.57	0.51
2:B:377:VAL:HG23	2:B:378:LEU:CD1	2.41	0.51
3:C:54:LEU:CD2	3:C:245:ILE:HG13	2.40	0.51
3:F:54:LEU:CD2	3:F:245:ILE:HG13	2.41	0.51
1:A:606:GLU:HG3	1:A:608:SER:H	1.76	0.50
2:B:319:MET:O	2:B:322:TYR:HB3	2.11	0.50
2:B:184:THR:O	2:B:185:LYS:HB2	2.11	0.50
3:C:27:ASN:ND2	3:C:133:PHE:CB	2.74	0.50
2:E:190:ILE:HD12	2:E:190:ILE:N	2.26	0.50
3:F:85:ILE:O	3:F:89:GLN:HG3	2.11	0.50
3:C:79:LEU:HA	3:C:83:ASP:OD1	2.11	0.50
3:C:142:SER:HA	3:F:118:VAL:HG12	1.91	0.50
3:C:188:ILE:HG13	3:C:193:ILE:HD11	1.93	0.50
1:D:461:LYS:HD2	1:D:462:GLU:H	1.76	0.50
2:E:185:LYS:HD3	2:E:187:ARG:HH12	1.77	0.50
3:F:7:SER:OG	3:F:10:LYS:HB3	2.12	0.50
2:B:187:ARG:O	2:B:188:LYS:HB2	2.12	0.50
3:F:212:ILE:O	3:F:215:LEU:HB2	2.11	0.50
2:B:236:MET:O	3:C:172:LYS:HE2	2.12	0.50
3:C:82:THR:HG21	3:C:219:ARG:NH1	2.15	0.50
1:D:461:LYS:O	1:D:462:GLU:HB3	2.11	0.50
3:F:199:MET:HE2	3:F:304:LEU:HD21	1.93	0.50
2:B:388:HIS:O	2:B:390:THR:N	2.44	0.50
3:C:79:LEU:HD12	3:C:83:ASP:OD1	2.11	0.50
3:F:245:ILE:HA	3:F:249:ILE:HD12	1.94	0.50
2:B:165:PRO:HG3	2:B:207:ARG:CG	2.42	0.50
2:B:319:MET:O	2:B:323:TYR:HD1	1.95	0.50
3:C:188:ILE:HD11	3:C:280:LEU:CD2	2.42	0.50
3:F:288:ARG:HG3	3:F:288:ARG:HH11	1.77	0.50
3:F:292:VAL:HG11	3:F:295:PHE:CZ	2.46	0.50
3:C:185:LYS:HD3	3:C:185:LYS:N	2.26	0.49
3:F:91:TYR:HE1	3:F:250:TYR:CB	2.25	0.49
2:B:163:MET:HG2	2:B:209:LEU:HD12	1.93	0.49
2:E:342:GLN:O	2:E:344:PRO:HD3	2.12	0.49
2:B:342:GLN:O	2:B:344:PRO:HD3	2.12	0.49
3:C:283:ILE:HG23	3:C:295:PHE:CE1	2.47	0.49
3:C:199:MET:CE	3:C:307:VAL:HG23	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:LEU:HD21	2:E:395:SER:HB2	1.93	0.49
1:A:506:HIS:CD2	1:A:510:ARG:HE	2.30	0.49
2:B:376:VAL:HG22	2:B:376:VAL:O	2.13	0.49
3:C:148:PRO:HA	3:C:164:VAL:HA	1.94	0.49
1:D:510:ARG:HG2	1:D:510:ARG:HH11	1.78	0.49
1:D:584:PHE:N	1:D:584:PHE:CD1	2.80	0.49
2:E:390:THR:CG2	3:F:48:LEU:HD11	2.37	0.49
3:F:90:TYR:O	3:F:94:ASN:HB2	2.12	0.49
3:C:91:TYR:O	3:C:91:TYR:CD2	2.66	0.49
1:D:507:PHE:CE1	2:E:378:LEU:HD23	2.47	0.49
1:D:612:ALA:CB	2:E:406:GLN:HE21	2.26	0.49
3:F:309:THR:HG22	3:F:311:SER:N	2.25	0.49
3:C:37:VAL:HG12	3:C:37:VAL:O	2.12	0.49
2:B:236:MET:HG2	3:C:176:LEU:HD21	1.95	0.48
1:D:549:LYS:CB	1:D:565:LEU:HG	2.43	0.48
3:F:54:LEU:HD11	3:F:242:LEU:HD22	1.95	0.48
1:A:506:HIS:NE2	1:A:510:ARG:NE	2.57	0.48
1:A:566:MET:HE3	1:A:615:PHE:HD1	1.79	0.48
1:A:617:HIS:CE1	1:A:621:LYS:HD2	2.48	0.48
1:D:519:MET:O	1:D:523:TYR:HD1	1.96	0.48
1:D:532:GLU:OE1	1:D:547:ARG:NH2	2.46	0.48
1:D:612:ALA:CB	2:E:406:GLN:NE2	2.76	0.48
3:C:112:ILE:O	3:C:115:ALA:HB3	2.13	0.48
3:C:185:LYS:CA	3:C:279:LYS:HD3	2.43	0.48
3:F:112:ILE:O	3:F:115:ALA:HB3	2.11	0.48
3:F:114:ARG:O	3:F:115:ALA:C	2.52	0.48
2:B:179:VAL:HG22	2:B:192:LEU:HD11	1.94	0.48
3:F:309:THR:CG2	3:F:310:LEU:N	2.75	0.48
1:A:628:VAL:HG23	1:A:629:ASN:N	2.27	0.48
3:C:120:GLN:HE22	3:C:122:ASP:HB3	1.78	0.48
2:E:187:ARG:O	2:E:188:LYS:CB	2.62	0.48
2:E:234:ASP:OD2	2:E:238:ASN:HB2	2.13	0.48
3:C:118:VAL:HG23	3:F:116:LEU:HD21	1.96	0.48
3:C:196:GLN:NE2	3:C:305:VAL:O	2.39	0.48
1:D:589:TRP:HE1	1:D:611:SER:CB	2.27	0.48
3:F:225:ILE:CD1	3:F:261:LEU:HD11	2.44	0.48
3:C:114:ARG:NE	3:C:119:ASP:OD1	2.46	0.48
3:C:134:GLU:OE2	3:C:138:LYS:HE2	2.13	0.48
3:C:212:ILE:O	3:C:215:LEU:HB2	2.13	0.48
2:E:233:THR:HA	2:E:238:ASN:O	2.13	0.48
1:A:526:LEU:O	1:A:529:LEU:N	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:TYR:HB2	1:A:614:PRO:HD3	1.95	0.48
3:F:7:SER:O	3:F:9:GLU:N	2.47	0.48
3:C:18:ALA:HB1	3:C:180:GLU:HB2	1.95	0.48
2:B:389:ASN:HB3	3:C:52:LYS:HZ3	1.77	0.47
3:C:275:THR:HG22	3:C:298:VAL:O	2.14	0.47
2:E:247:GLN:OE1	2:E:247:GLN:HA	2.14	0.47
3:F:151:ASP:OD1	3:F:152:GLN:N	2.44	0.47
1:A:463:GLU:HB3	1:A:464:ASP:H	1.42	0.47
2:B:310:PRO:HG2	2:B:313:PHE:HD1	1.79	0.47
3:C:12:SER:HA	3:C:186:ILE:HD11	1.97	0.47
3:F:201:SER:HB3	3:F:224:PRO:HG2	1.95	0.47
2:B:386:ILE:CG2	2:B:412:ILE:HD11	2.44	0.47
3:C:208:VAL:HG22	3:C:255:LEU:O	2.15	0.47
2:E:381:LEU:HD11	2:E:393:VAL:CG2	2.44	0.47
3:F:188:ILE:HD11	3:F:280:LEU:CG	2.42	0.47
1:A:547:ARG:NE	1:A:565:LEU:HD13	2.30	0.47
3:C:180:GLU:CD	3:C:180:GLU:H	2.18	0.47
1:D:524:ILE:O	1:D:527:LYS:HG2	2.14	0.47
1:D:528:ASN:C	1:D:530:GLY:H	2.17	0.47
1:D:546:LEU:HD11	1:D:568:MET:HB2	1.96	0.47
3:F:142:SER:C	3:F:144:SER:N	2.62	0.47
1:A:625:GLU:O	1:A:628:VAL:HG22	2.14	0.47
2:B:187:ARG:O	2:B:188:LYS:CB	2.62	0.47
2:B:243:ILE:O	2:B:243:ILE:HG13	2.15	0.47
1:D:617:HIS:O	1:D:620:THR:HB	2.14	0.47
1:A:520:GLY:HA3	4:A:791:HOH:O	2.14	0.47
1:A:609:THR:HG23	2:B:397:VAL:HG11	1.97	0.47
2:B:198:ASN:HD22	2:B:199:ASN:H	1.55	0.47
3:C:31:SER:HA	3:C:132:LEU:HD13	1.96	0.47
3:C:106:LEU:O	3:C:109:LEU:HB2	2.13	0.47
1:D:460:TYR:HD2	1:D:461:LYS:N	2.12	0.47
2:E:178:TYR:CB	2:E:189:MET:HB2	2.44	0.47
3:F:130:ARG:HH11	3:F:131:PRO:CD	2.21	0.47
2:B:219:VAL:HB	2:B:224:ARG:HH11	1.79	0.47
3:C:263:ARG:HH11	3:C:263:ARG:HG2	1.79	0.47
1:A:461:LYS:O	1:A:461:LYS:HG2	2.14	0.47
1:A:497:VAL:HG12	1:A:498:THR:N	2.29	0.47
3:C:238:ALA:O	3:C:241:VAL:HB	2.15	0.47
3:F:114:ARG:O	3:F:115:ALA:O	2.32	0.47
2:B:384:SER:OG	2:B:392:CYS:HB3	2.16	0.47
3:C:175:ALA:CB	3:C:284:MET:HG3	2.36	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:ILE:HG23	3:F:212:ILE:HG23	1.96	0.47
2:B:195:ASP:O	2:B:196:SER:C	2.54	0.46
3:C:245:ILE:HA	3:C:249:ILE:CB	2.39	0.46
1:D:496:LEU:HD11	3:F:246:LYS:HZ3	1.80	0.46
1:A:515:PRO:HB2	1:A:542:TRP:CZ3	2.50	0.46
2:B:184:THR:HG23	2:B:188:LYS:HB3	1.96	0.46
2:E:378:LEU:HD12	2:E:378:LEU:N	2.29	0.46
1:A:619:THR:O	1:A:623:ILE:HG13	2.14	0.46
3:F:25:PHE:CD1	3:F:178:CYS:SG	3.08	0.46
3:F:318:LEU:O	3:F:319:LEU:HD23	2.15	0.46
2:B:397:VAL:HG12	2:B:398:ARG:N	2.30	0.46
2:B:410:THR:HG22	2:B:411:PRO:HD2	1.97	0.46
3:C:104:LEU:CD2	3:C:112:ILE:HD12	2.46	0.46
2:E:193:ILE:N	2:E:193:ILE:HD12	2.30	0.46
1:A:590:GLU:CG	1:A:591:SER:H	2.27	0.46
1:D:628:VAL:HG23	1:D:629:ASN:N	2.29	0.46
1:A:461:LYS:O	1:A:462:GLU:HG2	2.15	0.46
1:A:463:GLU:C	1:A:465:SER:H	2.18	0.46
2:B:379:ASN:HD22	2:B:379:ASN:C	2.19	0.46
1:D:548:TRP:HD1	1:D:549:LYS:N	2.14	0.46
3:F:9:GLU:O	3:F:13:ILE:HB	2.15	0.46
3:F:19:VAL:HG12	3:F:23:ARG:HH21	1.80	0.46
1:A:547:ARG:CZ	1:A:565:LEU:HD13	2.46	0.46
1:D:529:LEU:HD11	1:D:622:LEU:HA	1.97	0.46
3:F:54:LEU:HD21	3:F:245:ILE:HG13	1.96	0.46
1:A:534:ALA:O	1:A:536:PRO:HD3	2.16	0.46
3:F:220:VAL:HG22	3:F:221:SER:N	2.31	0.46
2:E:214:ARG:HB2	2:E:214:ARG:NH1	2.22	0.46
1:A:510:ARG:HG2	1:A:510:ARG:HH11	1.81	0.45
1:A:536:PRO:O	1:A:537:SER:HB3	2.17	0.45
3:C:188:ILE:CG2	3:C:194:ILE:HD11	2.46	0.45
1:D:496:LEU:HD13	3:F:263:ARG:NH2	2.31	0.45
1:A:505:TRP:HH2	3:C:40:ARG:HE	1.64	0.45
2:B:324:TYR:OH	2:B:328:ARG:NH2	2.48	0.45
2:B:389:ASN:O	2:B:389:ASN:ND2	2.50	0.45
1:D:571:GLN:O	1:D:582:VAL:HA	2.16	0.45
1:A:517:ASP:HA	4:A:791:HOH:O	2.16	0.45
1:A:549:LYS:CB	1:A:565:LEU:HD23	2.46	0.45
3:F:248:GLY:C	3:F:249:ILE:HG13	2.36	0.45
1:A:524:ILE:O	1:A:527:LYS:HG2	2.16	0.45
1:A:527:LYS:HB3	1:A:533:TRP:HH2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:PRO:HG3	2:B:207:ARG:HG3	1.98	0.45
2:B:390:THR:HG21	3:C:48:LEU:HD11	1.97	0.45
3:C:293:HIS:O	3:C:294:ARG:HB3	2.15	0.45
3:F:296:PHE:CD2	3:F:307:VAL:HG13	2.52	0.45
1:A:462:GLU:OE1	1:A:462:GLU:HA	2.16	0.45
2:B:195:ASP:O	2:B:197:ASP:N	2.50	0.45
1:A:479:ARG:HG3	3:C:262:MET:HE2	1.97	0.45
1:A:548:TRP:CD2	1:A:618:LEU:HD13	2.51	0.45
1:D:547:ARG:HG2	1:D:548:TRP:H	1.82	0.45
1:D:567:LYS:HZ2	1:D:590:GLU:CD	2.20	0.45
3:F:12:SER:HA	3:F:186:ILE:HD11	1.98	0.45
3:F:55:ASN:O	3:F:59:GLN:HB2	2.16	0.45
2:B:189:MET:HE2	2:B:218:ILE:HG21	1.98	0.45
3:C:234:ASN:OD1	3:C:235:VAL:N	2.41	0.45
3:F:197:ASP:O	3:F:198:ASN:HB2	2.16	0.45
2:B:317:SER:O	2:B:321:ARG:HG3	2.16	0.45
2:B:406:GLN:HB3	4:B:808:HOH:O	2.17	0.45
2:E:202:PHE:N	2:E:202:PHE:CD1	2.85	0.45
1:A:506:HIS:CD2	1:A:510:ARG:NE	2.85	0.45
1:A:527:LYS:HE3	1:A:528:ASN:OD1	2.16	0.45
3:C:227:ASP:O	3:C:228:GLU:C	2.54	0.45
1:D:625:GLU:O	1:D:628:VAL:HG22	2.17	0.45
2:E:410:THR:CG2	3:F:45:ASP:HB2	2.46	0.45
1:A:497:VAL:O	1:A:498:THR:C	2.56	0.44
2:B:246:ARG:HH22	2:B:398:ARG:NH1	2.14	0.44
3:C:114:ARG:HH21	3:F:93:SER:HA	1.82	0.44
3:C:120:GLN:OE1	3:C:122:ASP:HB3	2.17	0.44
3:F:314:LEU:O	3:F:318:LEU:HG	2.17	0.44
2:E:178:TYR:HB3	2:E:189:MET:HB2	2.00	0.44
3:F:130:ARG:HH12	3:F:134:GLU:HB2	1.82	0.44
1:A:541:LEU:HG	1:A:543:THR:H	1.82	0.44
1:A:566:MET:CE	1:A:615:PHE:HD1	2.30	0.44
1:D:624:MET:CG	2:E:412:ILE:HG23	2.47	0.44
3:C:294:ARG:HD2	3:C:296:PHE:CE1	2.52	0.44
3:C:309:THR:CG2	3:C:310:LEU:N	2.80	0.44
3:F:171:LEU:HD12	3:F:310:LEU:HD22	2.00	0.44
3:F:250:TYR:O	3:F:251:ASN:C	2.55	0.44
3:F:296:PHE:CE2	3:F:307:VAL:HG13	2.52	0.44
3:C:120:GLN:CA	3:F:116:LEU:HD22	2.48	0.44
1:D:583:ASP:OD1	2:E:380:HIS:HB3	2.17	0.44
2:E:375:HIS:CE1	2:E:376:VAL:HG12	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:43:VAL:HG22	3:F:66:PRO:HG2	2.00	0.44
3:F:106:LEU:O	3:F:109:LEU:HB2	2.18	0.44
1:A:532:GLU:OE2	1:A:547:ARG:NH2	2.47	0.44
1:D:514:TYR:CD1	1:D:514:TYR:N	2.86	0.44
1:A:466:THR:HB	3:C:278:ASP:OD1	2.18	0.44
2:B:176:LYS:NZ	2:B:176:LYS:CB	2.72	0.44
2:B:195:ASP:OD1	2:B:201:SER:HB3	2.17	0.44
3:C:212:ILE:HA	3:C:215:LEU:HD12	2.00	0.44
1:D:479:ARG:HG3	3:F:262:MET:CE	2.47	0.44
1:D:529:LEU:CD1	1:D:622:LEU:HA	2.48	0.44
2:E:213:HIS:O	2:E:242:TYR:HA	2.17	0.44
3:F:85:ILE:HG23	3:F:212:ILE:CG2	2.47	0.44
1:D:572:LEU:HD12	1:D:581:LEU:O	2.18	0.43
2:E:189:MET:HE1	2:E:218:ILE:HG21	1.98	0.43
2:B:312:VAL:HG12	2:B:312:VAL:O	2.17	0.43
3:C:39:TYR:OH	3:C:162:VAL:HG12	2.17	0.43
3:C:109:LEU:HD12	3:C:109:LEU:HA	1.77	0.43
3:F:199:MET:SD	3:F:306:GLY:HA2	2.58	0.43
2:B:386:ILE:HG21	2:B:412:ILE:HD11	2.00	0.43
3:C:196:GLN:O	3:C:199:MET:HE3	2.18	0.43
1:A:510:ARG:HG2	1:A:510:ARG:NH1	2.33	0.43
3:F:34:VAL:CG1	3:F:34:VAL:O	2.66	0.43
2:B:346:GLN:H	2:B:346:GLN:HE21	1.66	0.43
1:D:497:VAL:HA	4:D:734:HOH:O	2.18	0.43
1:A:548:TRP:HD1	1:A:549:LYS:N	2.16	0.43
3:C:159:GLU:O	3:C:160:ILE:HG12	2.19	0.43
3:C:165:LEU:HD21	3:C:170:ILE:HD11	1.99	0.43
3:C:209:ILE:HD12	3:C:210:ASP:H	1.83	0.43
3:F:15:GLN:OE1	3:F:184:LEU:HA	2.18	0.43
3:F:182:HIS:O	3:F:182:HIS:ND1	2.51	0.43
1:D:543:THR:HG21	1:D:545:LYS:HZ2	1.83	0.43
3:F:126:ILE:HD12	3:F:138:LYS:HD2	2.01	0.43
1:A:572:LEU:CD1	1:A:582:VAL:HG22	2.49	0.43
1:A:613:TYR:O	1:A:614:PRO:C	2.55	0.43
3:C:217:GLN:C	3:C:219:ARG:H	2.22	0.43
1:D:570:ILE:HG22	1:D:582:VAL:HG12	2.00	0.43
3:C:178:CYS:O	3:C:181:THR:HG23	2.19	0.43
1:A:590:GLU:HG3	1:A:591:SER:N	2.32	0.42
1:D:527:LYS:HB3	1:D:533:TRP:HH2	1.83	0.42
2:E:174:GLY:O	2:E:202:PHE:CZ	2.66	0.42
3:F:293:HIS:O	3:F:294:ARG:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:TYR:CD1	1:A:580:TYR:N	2.86	0.42
3:C:127:HIS:CD2	3:C:129:SER:HB2	2.55	0.42
2:B:404:VAL:HG22	3:C:39:TYR:CZ	2.55	0.42
3:C:49:LEU:O	3:C:52:LYS:N	2.50	0.42
1:D:610:PHE:N	1:D:610:PHE:CD2	2.88	0.42
2:E:171:GLN:HG3	2:E:228:PHE:CD1	2.54	0.42
2:E:376:VAL:HG22	2:E:376:VAL:O	2.19	0.42
2:E:389:ASN:HD22	2:E:389:ASN:HA	1.55	0.42
3:F:111:ASP:O	3:F:115:ALA:HB2	2.20	0.42
1:A:519:MET:HB3	2:B:313:PHE:CD2	2.54	0.42
1:A:548:TRP:O	1:A:566:MET:N	2.42	0.42
1:D:520:GLY:O	1:D:524:ILE:HG13	2.18	0.42
3:F:25:PHE:HD1	3:F:178:CYS:SG	2.43	0.42
3:C:283:ILE:HD13	3:C:308:LEU:HD23	2.02	0.42
1:D:503:THR:HG22	1:D:504:ARG:HG2	2.00	0.42
3:F:172:LYS:O	3:F:176:LEU:HB2	2.19	0.42
3:F:188:ILE:CD1	3:F:280:LEU:HG	2.48	0.42
3:C:196:GLN:O	3:C:197:ASP:O	2.37	0.42
1:D:536:PRO:HA	1:D:541:LEU:HD23	2.01	0.42
3:C:75:PHE:HB3	3:C:159:GLU:OE1	2.20	0.42
3:F:197:ASP:CG	3:F:198:ASN:H	2.23	0.42
1:A:549:LYS:HB3	1:A:565:LEU:HD23	2.01	0.42
2:B:163:MET:HG2	2:B:209:LEU:CD1	2.50	0.42
3:C:249:ILE:HG22	3:C:250:TYR:N	2.35	0.42
1:D:514:TYR:HD1	1:D:514:TYR:H	1.67	0.42
3:F:293:HIS:CE1	4:F:768:HOH:O	2.73	0.42
1:A:609:THR:HA	2:B:397:VAL:HG11	2.01	0.42
1:A:519:MET:HG2	2:B:313:PHE:CE2	2.55	0.41
2:B:408:LEU:HG	4:B:757:HOH:O	2.19	0.41
3:C:119:ASP:C	3:F:116:LEU:HD22	2.40	0.41
3:C:143:ARG:HE	3:F:114:ARG:NH2	2.18	0.41
1:A:509:ILE:HD12	1:A:584:PHE:HZ	1.84	0.41
1:D:566:MET:HE2	1:D:618:LEU:HD12	1.99	0.41
3:F:138:LYS:O	3:F:141:GLU:HB2	2.20	0.41
3:F:140:LEU:HA	3:F:140:LEU:HD23	1.77	0.41
1:A:546:LEU:HG	1:A:568:MET:HB3	2.02	0.41
2:B:164:VAL:HA	2:B:165:PRO:HD3	1.84	0.41
2:B:198:ASN:ND2	2:B:199:ASN:N	2.59	0.41
1:D:514:TYR:O	1:D:516:LEU:N	2.40	0.41
1:D:533:TRP:HA	1:D:546:LEU:HA	2.02	0.41
1:A:527:LYS:CG	1:A:528:ASN:N	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:ILE:HG23	2:B:194:PRO:HD2	2.02	0.41
3:C:265:SER:HG	3:C:267:ASP:CG	2.24	0.41
1:D:611:SER:C	1:D:614:PRO:HD2	2.41	0.41
2:E:174:GLY:HA2	2:E:220:ASP:OD2	2.20	0.41
3:C:37:VAL:O	3:C:37:VAL:CG1	2.69	0.41
3:C:179:ARG:O	3:C:181:THR:N	2.54	0.41
3:F:227:ASP:OD1	3:F:227:ASP:C	2.59	0.41
2:B:377:VAL:CG2	2:B:378:LEU:HD12	2.48	0.41
3:C:27:ASN:HD22	3:C:133:PHE:HB3	1.84	0.41
3:C:27:ASN:HD22	3:C:27:ASN:HA	1.51	0.41
1:D:612:ALA:HB3	2:E:406:GLN:NE2	2.35	0.41
2:E:182:SER:C	2:E:184:THR:H	2.24	0.41
2:E:340:PRO:HA	2:E:341:PRO:HD2	1.88	0.41
3:C:15:GLN:OE1	3:C:184:LEU:HA	2.21	0.41
3:C:146:ARG:HA	3:C:165:LEU:O	2.21	0.41
1:D:543:THR:HG21	1:D:545:LYS:HZ3	1.85	0.41
2:E:235:GLN:H	2:E:235:GLN:HG2	1.69	0.41
2:B:192:LEU:HB3	2:B:202:PHE:HB3	2.03	0.41
2:B:380:HIS:ND1	2:B:380:HIS:N	2.68	0.41
3:C:89:GLN:HE22	3:C:216:THR:CB	2.34	0.41
3:C:141:GLU:CB	3:F:118:VAL:HB	2.44	0.41
3:F:7:SER:C	3:F:9:GLU:N	2.73	0.41
3:C:309:THR:O	3:C:313:ILE:HG13	2.20	0.41
1:D:464:ASP:O	1:D:464:ASP:OD1	2.37	0.40
3:F:137:LEU:HA	3:F:137:LEU:HD23	1.86	0.40
3:F:166:THR:O	3:F:170:ILE:HG12	2.21	0.40
3:F:188:ILE:CG2	3:F:194:ILE:HD11	2.51	0.40
2:B:377:VAL:O	2:B:378:LEU:HD12	2.20	0.40
3:C:64:SER:HA	3:C:79:LEU:O	2.21	0.40
3:C:315:LYS:HZ1	3:F:121:LEU:HB2	1.86	0.40
3:F:119:ASP:OD1	3:F:121:LEU:HD11	2.21	0.40
3:C:273:THR:HA	3:C:296:PHE:O	2.21	0.40
1:D:514:TYR:C	1:D:516:LEU:H	2.24	0.40
2:E:375:HIS:HB3	2:E:378:LEU:HD13	2.03	0.40
3:C:179:ARG:NH1	3:C:182:HIS:CG	2.90	0.40
3:F:19:VAL:HG12	3:F:23:ARG:NH2	2.35	0.40
3:F:123:THR:O	3:F:123:THR:HG22	2.22	0.40
3:F:299:ASP:OD1	3:F:303:ARG:HB2	2.21	0.40
2:B:189:MET:HG2	2:B:218:ILE:HD13	2.02	0.40
3:F:127:HIS:HA	3:F:128:PRO:HD3	1.86	0.40
3:F:141:GLU:OE1	3:F:141:GLU:HA	2.20	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	121/171 (71%)	105 (87%)	13 (11%)	3 (2%)	5 9
1	D	121/171 (71%)	105 (87%)	11 (9%)	5 (4%)	3 3
2	B	147/252 (58%)	125 (85%)	17 (12%)	5 (3%)	3 5
2	E	132/252 (52%)	115 (87%)	11 (8%)	6 (4%)	2 3
3	C	306/315 (97%)	265 (87%)	32 (10%)	9 (3%)	4 7
3	F	306/315 (97%)	272 (89%)	27 (9%)	7 (2%)	6 11
All	All	1133/1476 (77%)	987 (87%)	111 (10%)	35 (3%)	4 6

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	188	LYS
2	B	379	ASN
3	C	197	ASP
3	C	246	LYS
2	E	188	LYS
2	E	379	ASN
2	E	387	LYS
2	E	388	HIS
3	F	115	ALA
3	F	246	LYS
1	A	536	PRO
2	B	196	SER
3	C	143	ARG
3	C	180	GLU
3	C	217	GLN
3	C	229	ASN
1	D	548	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	8	GLN
3	F	143	ARG
3	F	250	TYR
2	B	389	ASN
3	C	250	TYR
1	D	462	GLU
1	D	529	LEU
1	D	536	PRO
2	E	386	ILE
3	F	96	ASP
3	C	124	ALA
3	C	216	THR
1	D	515	PRO
3	F	217	GLN
1	A	463	GLU
1	A	464	ASP
2	B	345	PRO
2	E	341	PRO

5.3.2 Protein sidechains (i)

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	119/155 (77%)	107 (90%)	12 (10%)	7 14
1	D	119/155 (77%)	113 (95%)	6 (5%)	24 47
2	B	145/234 (62%)	135 (93%)	10 (7%)	15 31
2	E	130/234 (56%)	120 (92%)	10 (8%)	13 25
3	C	285/290 (98%)	269 (94%)	16 (6%)	21 42
3	F	285/290 (98%)	271 (95%)	14 (5%)	25 48
All	All	1083/1358 (80%)	1015 (94%)	68 (6%)	18 36

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	TYR
1	A	461	LYS
1	A	462	GLU
1	A	464	ASP
1	A	485	GLN
1	A	496	LEU
1	A	545	LYS
1	A	546	LEU
1	A	549	LYS
1	A	564	ASP
1	A	578	ASN
1	A	579	ASN
2	B	176	LYS
2	B	179	VAL
2	B	189	MET
2	B	198	ASN
2	B	214	ARG
2	B	235	GLN
2	B	346	GLN
2	B	379	ASN
2	B	380	HIS
2	B	410	THR
3	C	24	LYS
3	C	27	ASN
3	C	52	LYS
3	C	120	GLN
3	C	179	ARG
3	C	185	LYS
3	C	192	ASN
3	C	209	ILE
3	C	246	LYS
3	C	257	VAL
3	C	264	ARG
3	C	281	SER
3	C	288	ARG
3	C	291	ARG
3	C	300	ASP
3	C	307	VAL
1	D	468	SER
1	D	485	GLN
1	D	519	MET
1	D	564	ASP
1	D	578	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	584	PHE
2	E	179	VAL
2	E	180	THR
2	E	214	ARG
2	E	223	LEU
2	E	235	GLN
2	E	243	ILE
2	E	379	ASN
2	E	380	HIS
2	E	389	ASN
2	E	393	VAL
3	F	15	GLN
3	F	28	SER
3	F	49	LEU
3	F	75	PHE
3	F	120	GLN
3	F	200	LYS
3	F	209	ILE
3	F	228	GLU
3	F	257	VAL
3	F	264	ARG
3	F	284	MET
3	F	300	ASP
3	F	303	ARG
3	F	307	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	GLN
2	B	172	GLN
2	B	198	ASN
2	B	221	ASN
2	B	235	GLN
2	B	238	ASN
2	B	346	GLN
2	B	375	HIS
2	B	389	ASN
3	C	27	ASN
3	C	94	ASN
3	C	127	HIS
3	C	152	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	192	ASN
3	C	196	GLN
3	C	213	GLN
3	C	217	GLN
1	D	506	HIS
1	D	571	GLN
1	D	574	GLN
1	D	617	HIS
2	E	172	GLN
2	E	235	GLN
2	E	346	GLN
2	E	389	ASN
2	E	406	GLN
3	F	16	GLN
3	F	60	ASN
3	F	127	HIS
3	F	152	GLN
3	F	167	GLN
3	F	192	ASN
3	F	196	GLN
3	F	213	GLN
3	F	217	GLN
3	F	286	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 monosaccharides in this entry.

5.6 Ligand geometry

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, 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	133/171 (77%)	0.34	7 (5%) 26 20	38, 75, 96, 99	0
1	D	133/171 (77%)	0.54	15 (11%) 5 3	40, 81, 100, 102	0
2	B	155/252 (61%)	0.16	5 (3%) 47 40	37, 65, 97, 101	0
2	E	140/252 (55%)	0.22	7 (5%) 28 23	39, 62, 101, 102	0
3	C	310/315 (98%)	-0.05	7 (2%) 60 54	37, 57, 93, 102	0
3	F	310/315 (98%)	0.11	17 (5%) 25 19	35, 59, 93, 102	0
All	All	1181/1476 (80%)	0.16	58 (4%) 29 23	35, 63, 97, 102	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	250	TYR	5.5
1	A	503	THR	4.8
1	D	537	SER	4.7
2	E	344	PRO	4.7
2	E	162	LEU	4.7
3	F	198	ASN	4.7
1	A	512	ARG	4.4
1	D	514	TYR	4.3
2	B	246	ARG	4.2
2	E	343	LEU	4.1
3	C	116	LEU	3.6
1	D	512	ARG	3.5
1	A	612	ALA	3.3
1	D	629	ASN	3.1
3	F	99	GLU	3.0
2	B	245	VAL	2.9
3	F	152	GLN	2.9
3	C	199	MET	2.9
3	C	250	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	345	PRO	2.9
3	F	8	GLN	2.8
3	F	121	LEU	2.8
3	F	266	ASP	2.8
1	D	460	TYR	2.7
3	F	159	GLU	2.7
1	D	535	LYS	2.7
2	E	346	GLN	2.6
2	B	387	LYS	2.5
2	E	340	PRO	2.5
2	B	193	ILE	2.5
2	B	247	GLN	2.5
1	D	565	LEU	2.5
1	D	591	SER	2.4
3	F	114	ARG	2.4
1	D	630	SER	2.4
2	E	341	PRO	2.4
1	D	590	GLU	2.3
1	D	545	LYS	2.3
3	F	119	ASP	2.3
3	F	100	LEU	2.3
1	A	504	ARG	2.2
3	C	200	LYS	2.2
1	D	503	THR	2.2
3	F	13	ILE	2.2
3	C	115	ALA	2.2
1	D	619	THR	2.2
3	F	200	LYS	2.2
3	F	116	LEU	2.1
1	A	486	GLY	2.1
3	F	300	ASP	2.1
1	D	504	ARG	2.1
1	A	628	VAL	2.1
3	C	114	ARG	2.1
1	D	625	GLU	2.1
1	A	580	TYR	2.1
3	F	118	VAL	2.0
3	F	107	ASP	2.0
3	C	112	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.