Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2024 – 04:03 pm GMT

PDB ID	:	8RJ8
Title	:	CytK nanopore mutant
Authors	:	Whittaker, J.J.; Sauciuc, A.; Guskov, A.
Deposited on	:	2023-12-20
Resolution	:	4.32 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:

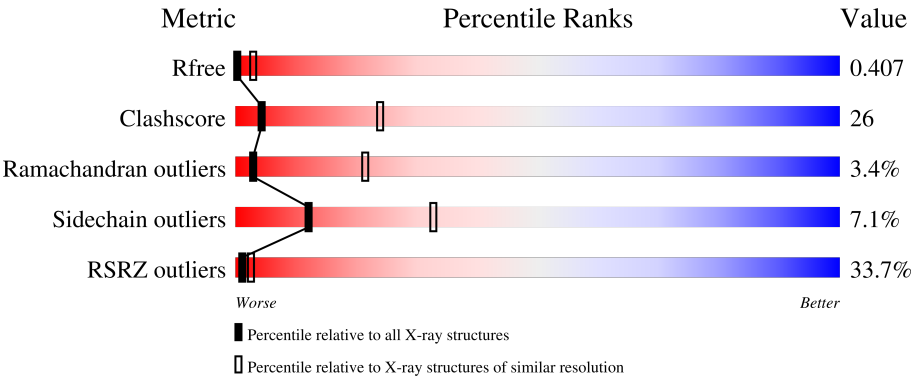
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 4.32 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.



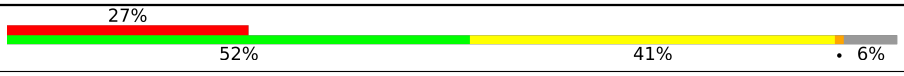
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1002 (4.76-3.88)
Clashscore	180529	1034 (4.72-3.90)
Ramachandran outliers	177936	1027 (4.80-3.84)
Sidechain outliers	177891	1010 (4.80-3.84)
RSRZ outliers	164620	1000 (4.76-3.88)

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%

Mol	Chain	Length	Quality of chain
1	A	310	32% 41% 44% 7% • 6%
1	B	310	29% 45% 39% • 12%
1	C	310	33% 49% 38% • 8%
1	D	310	41% 38% 42% 8% • 10%
1	E	310	37% 51% 38% • • 6%
1	F	310	21% 45% 48% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	310	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15699 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 Cytotoxin K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2267	1419	381	460	7			
1	B	272	Total	C	N	O	S	0	0	0
			2119	1324	357	431	7			
1	C	284	Total	C	N	O	S	0	0	0
			2227	1396	376	448	7			
1	D	279	Total	C	N	O	S	0	0	0
			2184	1371	368	438	7			
1	E	292	Total	C	N	O	S	0	0	0
			2267	1420	380	460	7			
1	F	302	Total	C	N	O	S	0	0	0
			2351	1472	393	478	8			
1	G	292	Total	C	N	O	S	0	0	0
			2284	1432	382	463	7			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q09KJ1
A	130	ASP	LYS	conflict	UNP Q09KJ1
A	149	ASP	THR	conflict	UNP Q09KJ1
A	157	ASP	LYS	conflict	UNP Q09KJ1
A	308	GLY	-	expression tag	UNP Q09KJ1
A	309	SER	-	expression tag	UNP Q09KJ1
A	310	ALA	-	expression tag	UNP Q09KJ1
B	1	MET	-	initiating methionine	UNP Q09KJ1
B	130	ASP	LYS	conflict	UNP Q09KJ1
B	149	ASP	THR	conflict	UNP Q09KJ1
B	157	ASP	LYS	conflict	UNP Q09KJ1
B	308	GLY	-	expression tag	UNP Q09KJ1
B	309	SER	-	expression tag	UNP Q09KJ1
B	310	ALA	-	expression tag	UNP Q09KJ1
C	1	MET	-	initiating methionine	UNP Q09KJ1

Continued on next page...

Continued from previous page...

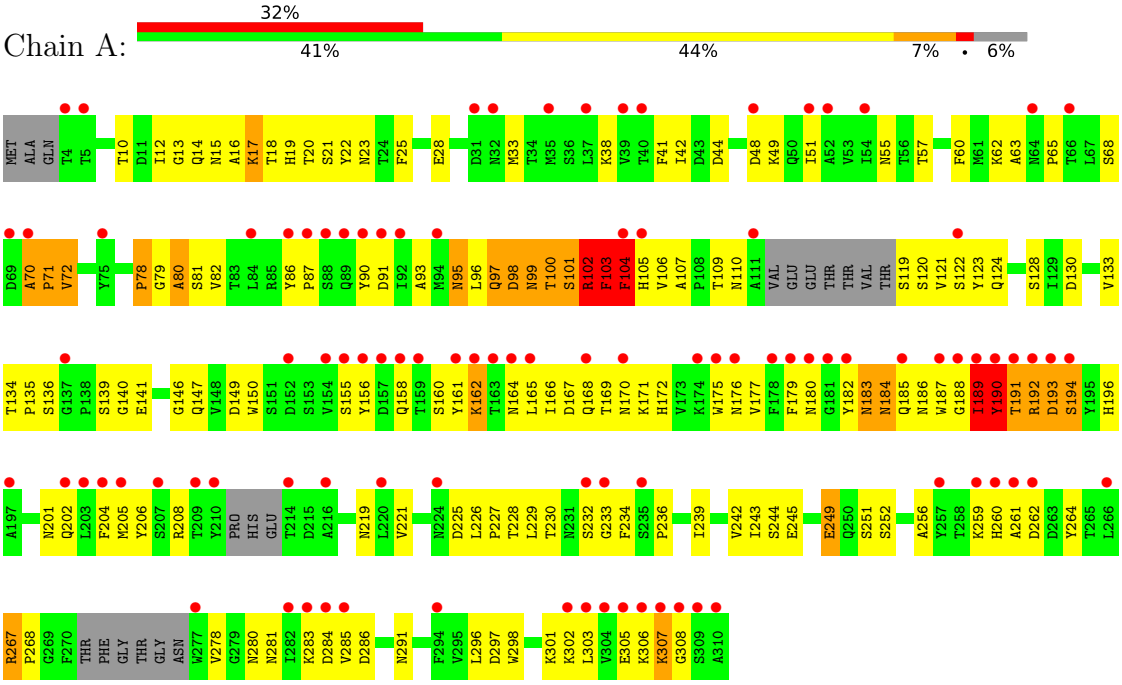
Chain	Residue	Modelled	Actual	Comment	Reference
C	130	ASP	LYS	conflict	UNP Q09KJ1
C	149	ASP	THR	conflict	UNP Q09KJ1
C	157	ASP	LYS	conflict	UNP Q09KJ1
C	308	GLY	-	expression tag	UNP Q09KJ1
C	309	SER	-	expression tag	UNP Q09KJ1
C	310	ALA	-	expression tag	UNP Q09KJ1
D	1	MET	-	initiating methionine	UNP Q09KJ1
D	130	ASP	LYS	conflict	UNP Q09KJ1
D	149	ASP	THR	conflict	UNP Q09KJ1
D	157	ASP	LYS	conflict	UNP Q09KJ1
D	308	GLY	-	expression tag	UNP Q09KJ1
D	309	SER	-	expression tag	UNP Q09KJ1
D	310	ALA	-	expression tag	UNP Q09KJ1
E	1	MET	-	initiating methionine	UNP Q09KJ1
E	130	ASP	LYS	conflict	UNP Q09KJ1
E	149	ASP	THR	conflict	UNP Q09KJ1
E	157	ASP	LYS	conflict	UNP Q09KJ1
E	308	GLY	-	expression tag	UNP Q09KJ1
E	309	SER	-	expression tag	UNP Q09KJ1
E	310	ALA	-	expression tag	UNP Q09KJ1
F	1	MET	-	initiating methionine	UNP Q09KJ1
F	130	ASP	LYS	conflict	UNP Q09KJ1
F	149	ASP	THR	conflict	UNP Q09KJ1
F	157	ASP	LYS	conflict	UNP Q09KJ1
F	308	GLY	-	expression tag	UNP Q09KJ1
F	309	SER	-	expression tag	UNP Q09KJ1
F	310	ALA	-	expression tag	UNP Q09KJ1
G	1	MET	-	initiating methionine	UNP Q09KJ1
G	130	ASP	LYS	conflict	UNP Q09KJ1
G	149	ASP	THR	conflict	UNP Q09KJ1
G	157	ASP	LYS	conflict	UNP Q09KJ1
G	308	GLY	-	expression tag	UNP Q09KJ1
G	309	SER	-	expression tag	UNP Q09KJ1
G	310	ALA	-	expression tag	UNP Q09KJ1

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. 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. 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.

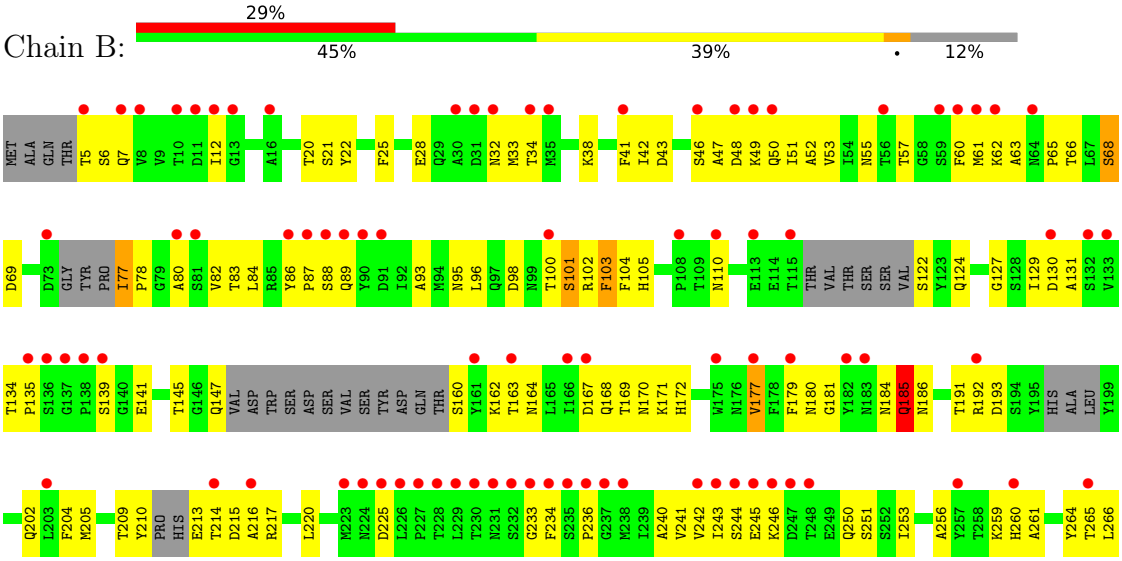
• Molecule 1: Cytotoxin K

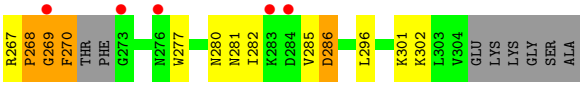
Chain A:



• Molecule 1: Cytotoxin K

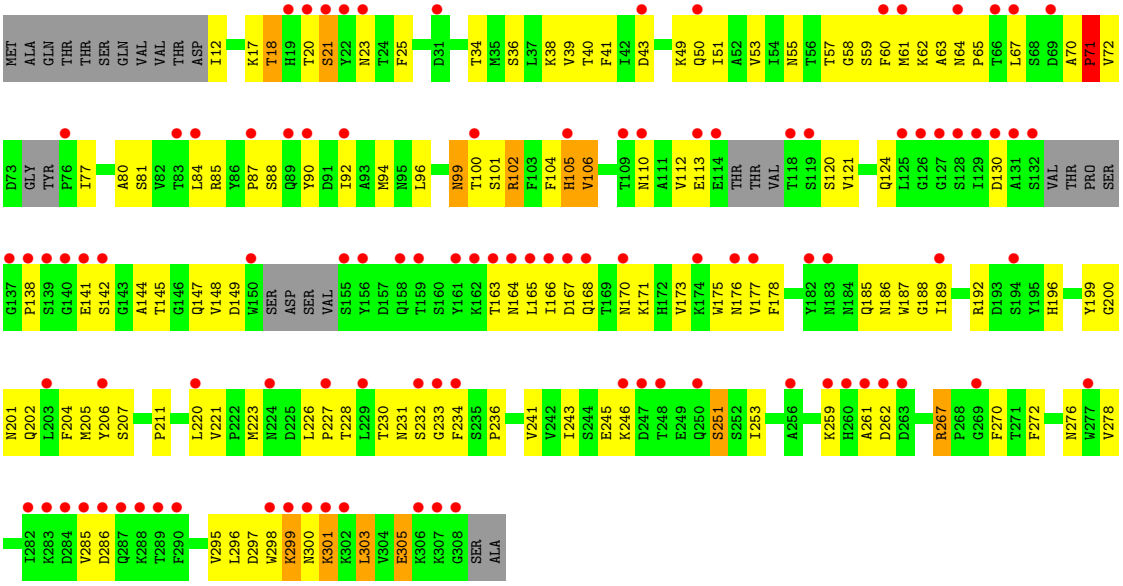
Chain B:





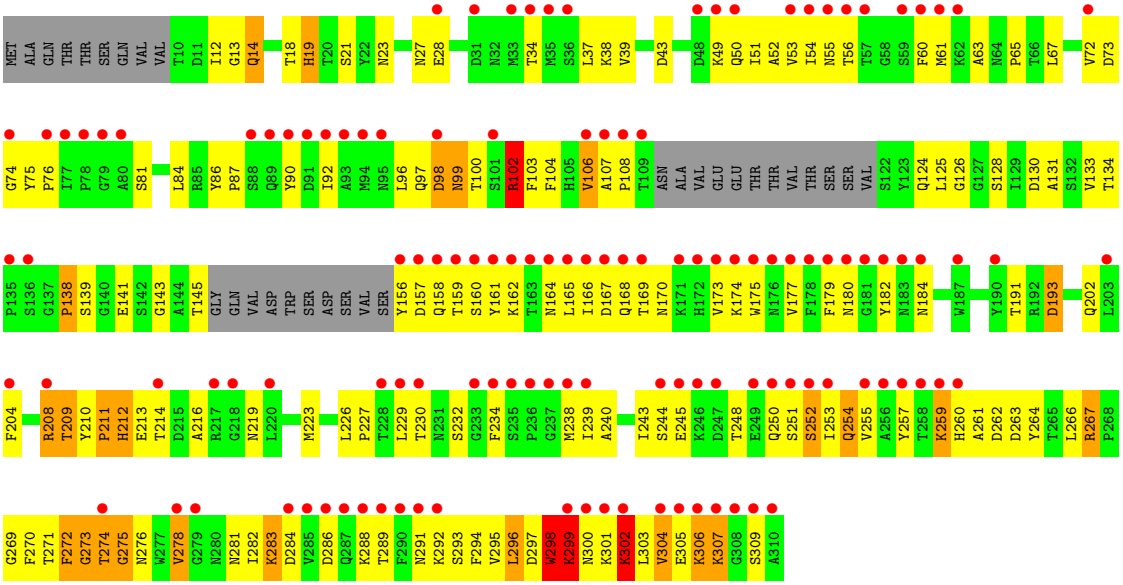
• Molecule 1: Cytotoxin K

Chain C:



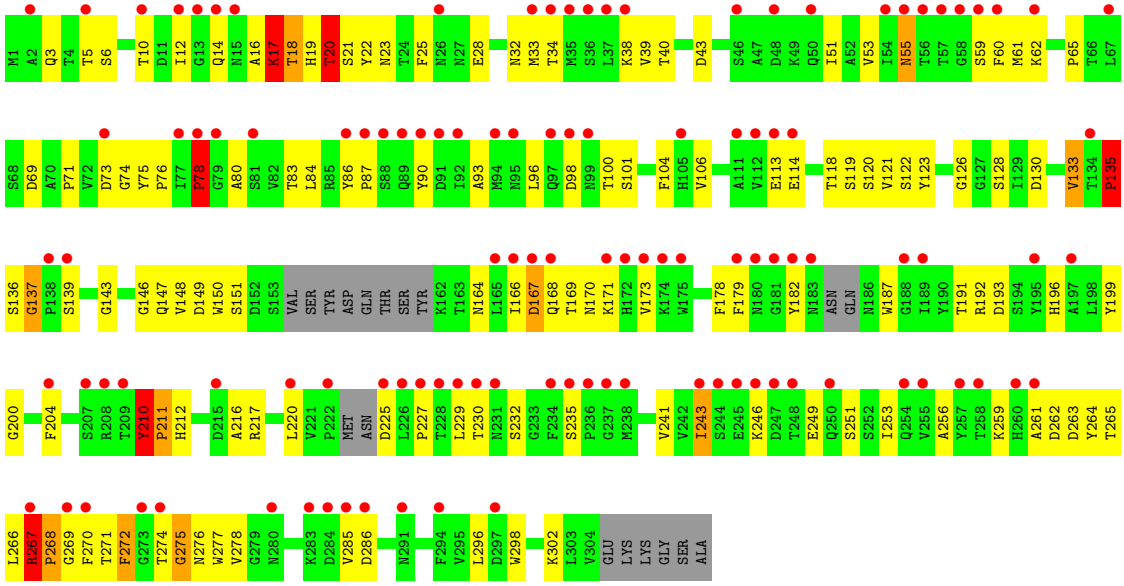
• Molecule 1: Cytotoxin K

Chain D:



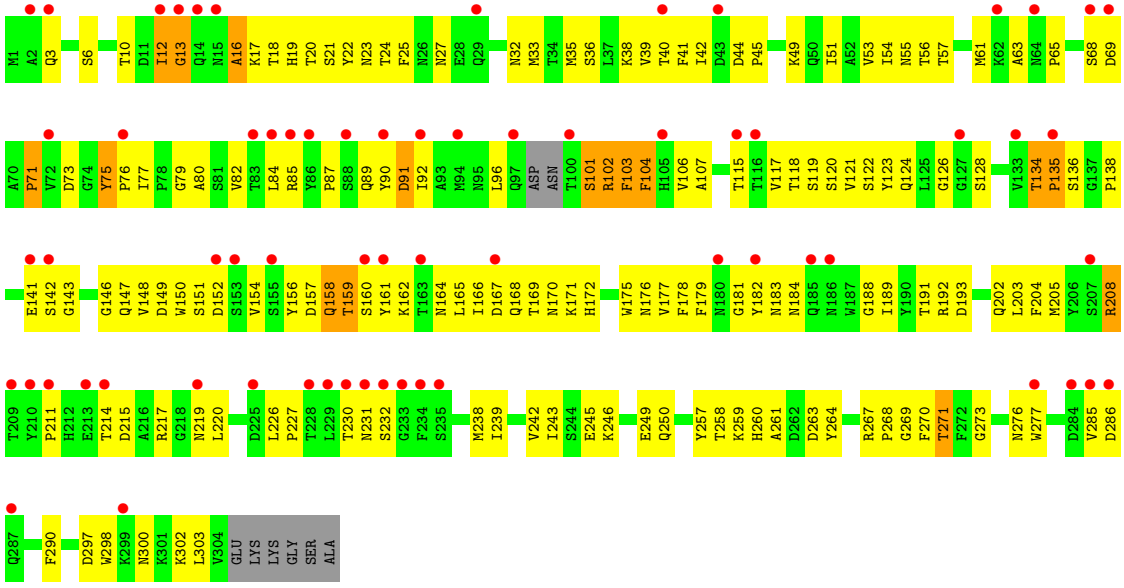
• Molecule 1: Cytotoxin K

Chain E:



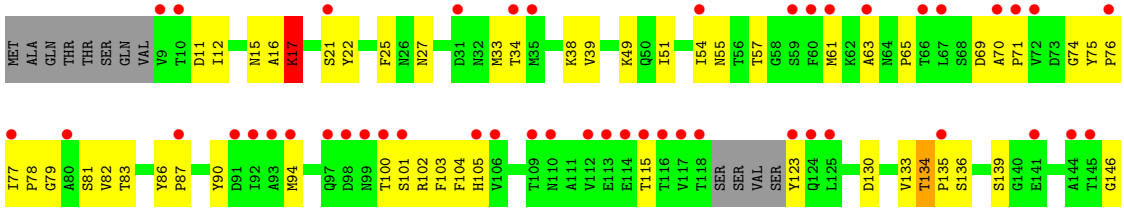
• Molecule 1: Cytotoxin K

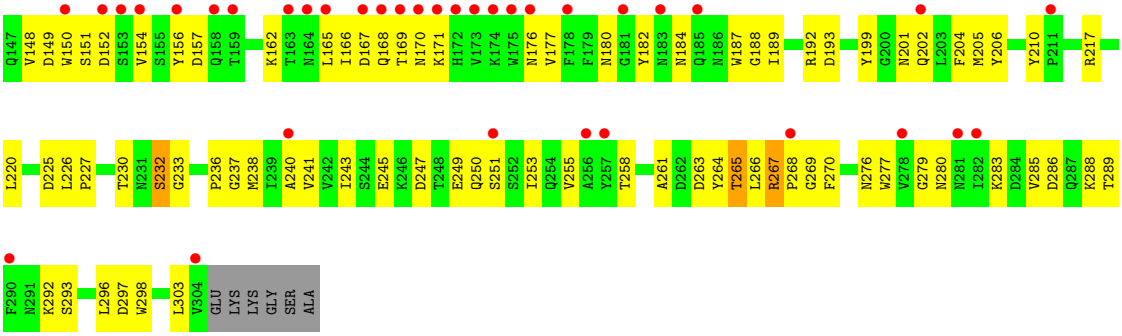
Chain F:



• Molecule 1: Cytotoxin K

Chain G:




Q147 V148 D149 W150 S151 D152 S153 V154 S155 Y156 D157 Q158 T159 K162 T163 N164 L165 I166 D167 Q168 T169 N170 K171 H172 V173 K174 W175 N176 V177 F178 F179 N180 G181 Y182 N183 N184 Q185 N186 W187 G188 I189 R192 D193 Y199 G200 N201 Q202 L203 F204 M205 Y206 Y210 P211 R217
L220 D225 L226 P227 T230 N231 S232 G233 P236 G237 M238 I239 A240 V241 V242 I243 S244 E245 K246 D247 T248 E249 Q250 S251 S252 I253 Q254 V255 A256 Y257 T258 A261 D262 D263 Y264 T265 L266 R267 P268 G269 F270 N276 W277 V278 G279 N280 N281 I282 K283 D284 V285 D286 Q287 K288 T289
P290 N291 K292 S293 L296 D297 W298 L303 V304 GLU LYS LYS GLY SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.23Å 186.22Å 104.53Å 90.00° 115.85° 90.00°	Depositor
Resolution (Å)	94.07 – 4.32 94.07 – 4.32	Depositor EDS
% Data completeness (in resolution range)	95.5 (94.07-4.32) 97.0 (94.07-4.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 4.30Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.322 , 0.407 0.322 , 0.407	Depositor DCC
R_{free} test set	1942 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å^2)	84.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 178.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	15699	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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	0.43	0/2318	0.68	1/3153 (0.0%)
1	B	0.33	0/2161	0.63	0/2933
1	C	0.37	0/2278	0.65	1/3093 (0.0%)
1	D	0.45	0/2237	0.69	0/3042
1	E	0.38	0/2319	0.67	2/3159 (0.1%)
1	F	0.32	0/2407	0.65	0/3282
1	G	0.33	0/2340	0.63	0/3191
All	All	0.38	0/16060	0.66	4/21853 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	78	PRO	N-CA-CB	-7.71	94.05	103.30
1	E	135	PRO	N-CA-CB	-7.28	94.56	103.30
1	C	71	PRO	N-CA-CB	-6.28	95.69	102.60
1	A	104	PHE	N-CA-CB	5.22	119.99	110.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	190	TYR	Mainchain
1	B	267	ARG	Sidechain
1	C	102	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	208	ARG	Sidechain
1	D	267	ARG	Sidechain
1	E	267	ARG	Sidechain
1	F	102	ARG	Sidechain
1	G	267	ARG	Sidechain

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	2267	0	2148	149	0
1	B	2119	0	2006	121	0
1	C	2227	0	2102	141	0
1	D	2184	0	2067	113	0
1	E	2267	0	2149	118	0
1	F	2351	0	2226	149	0
1	G	2284	0	2151	103	0
All	All	15699	0	14849	805	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 26.

All (805) 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:C:296:LEU:HA	1:C:303:LEU:HD23	1.28	1.12
1:D:87:PRO:HA	1:D:261:ALA:HA	1.12	1.11
1:A:72:VAL:HA	1:A:79:GLY:HA2	1.12	1.11
1:A:96:LEU:HD21	1:A:101:SER:H	1.21	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:THR:OG1	1:G:267:ARG:HG2	1.58	1.01
1:A:72:VAL:HA	1:A:79:GLY:CA	1.91	1.00
1:B:250:GLN:HA	1:B:296:LEU:O	1.64	0.97
1:E:270:PHE:HB2	1:E:278:VAL:HG21	1.47	0.96
1:C:20:THR:CB	1:C:301:LYS:HZ1	1.79	0.95
1:A:38:LYS:HB2	1:A:55:ASN:HB3	1.49	0.94
1:B:209:THR:O	1:B:210:TYR:HD1	1.49	0.94
1:C:251:SER:HB3	1:C:298:TRP:CZ3	2.06	0.90
1:C:20:THR:CB	1:C:301:LYS:NZ	2.35	0.90
1:D:81:SER:CB	1:D:267:ARG:HH21	1.84	0.89
1:B:167:ASP:HB3	1:C:61:MET:HB2	1.55	0.88
1:C:20:THR:HG21	1:C:301:LYS:NZ	1.90	0.87
1:D:295:VAL:H	1:D:304:VAL:HB	1.39	0.86
1:F:39:VAL:HG12	1:F:54:ILE:HG13	1.58	0.84
1:D:87:PRO:HA	1:D:261:ALA:CA	2.03	0.84
1:B:87:PRO:HA	1:B:261:ALA:HA	1.59	0.84
1:C:20:THR:HB	1:C:301:LYS:HZ1	1.42	0.83
1:D:108:PRO:HD2	1:D:175:TRP:CZ3	2.13	0.83
1:F:102:ARG:HB3	1:F:170:ASN:HB3	1.60	0.83
1:G:87:PRO:HA	1:G:261:ALA:HA	1.59	0.83
1:A:96:LEU:HD21	1:A:101:SER:N	1.94	0.83
1:A:98:ASP:HA	1:A:171:LYS:HD3	1.59	0.82
1:B:209:THR:O	1:B:210:TYR:CD1	2.33	0.82
1:A:169:THR:HA	1:E:34:THR:HG21	1.62	0.82
1:D:81:SER:HB2	1:D:267:ARG:HH21	1.43	0.81
1:B:102:ARG:HD2	1:B:170:ASN:HB3	1.64	0.79
1:F:115:THR:HB	1:G:156:TYR:HB2	1.65	0.79
1:A:87:PRO:HA	1:A:261:ALA:HA	1.64	0.79
1:F:159:THR:HB	1:F:181:GLY:H	1.47	0.79
1:D:34:THR:HG21	1:G:169:THR:HA	1.62	0.79
1:E:80:ALA:HA	1:E:268:PRO:HD3	1.64	0.78
1:D:267:ARG:NH1	1:D:270:PHE:CE1	2.52	0.78
1:G:100:THR:HG21	1:G:251:SER:HA	1.66	0.78
1:F:79:GLY:HA3	1:F:268:PRO:HG2	1.63	0.77
1:F:202:GLN:HB3	1:F:205:MET:HE2	1.67	0.77
1:C:20:THR:HG21	1:C:301:LYS:HZ3	1.51	0.76
1:C:20:THR:CG2	1:C:301:LYS:NZ	2.49	0.76
1:B:89:GLN:HB2	1:B:260:HIS:HB2	1.69	0.75
1:A:16:ALA:HB1	1:A:42:ILE:HD11	1.67	0.75
1:B:124:GLN:HG2	1:C:147:GLN:HG2	1.67	0.75
1:F:120:SER:HB2	1:F:149:ASP:HB3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:HD21	1:A:164:ASN:HA	1.50	0.74
1:G:81:SER:HB2	1:G:267:ARG:HH11	1.51	0.74
1:A:72:VAL:CA	1:A:79:GLY:HA2	2.07	0.74
1:F:71:PRO:HG3	1:F:217:ARG:HH22	1.53	0.73
1:F:87:PRO:HA	1:F:261:ALA:HA	1.70	0.73
1:G:130:ASP:HB2	1:G:139:SER:HB2	1.71	0.73
1:C:20:THR:CG2	1:C:301:LYS:HZ1	2.00	0.73
1:A:104:PHE:HA	1:E:25:PHE:CD2	2.23	0.73
1:E:121:VAL:HG22	1:E:148:VAL:HG13	1.70	0.73
1:A:133:VAL:HG11	1:E:137:GLY:HA2	1.71	0.73
1:F:89:GLN:HB2	1:F:260:HIS:HB2	1.68	0.73
1:A:21:SER:HB3	1:C:12:ILE:HG22	1.70	0.73
1:G:265:THR:OG1	1:G:267:ARG:CG	2.37	0.73
1:B:124:GLN:HG3	1:C:147:GLN:HA	1.70	0.72
1:C:43:ASP:OD1	1:C:246:LYS:NZ	2.22	0.72
1:E:114:GLU:HA	1:F:157:ASP:HA	1.71	0.72
1:F:261:ALA:HB3	1:F:286:ASP:HB2	1.69	0.72
1:B:163:THR:HA	1:B:177:VAL:HG13	1.72	0.72
1:D:184:ASN:ND2	1:D:202:GLN:O	2.23	0.72
1:F:42:ILE:HG23	1:F:51:ILE:HB	1.72	0.72
1:D:164:ASN:O	1:D:175:TRP:HB3	1.91	0.71
1:B:134:THR:HB	1:B:135:PRO:HD3	1.72	0.71
1:C:87:PRO:HA	1:C:261:ALA:HA	1.71	0.70
1:C:251:SER:CB	1:C:298:TRP:CZ3	2.73	0.70
1:G:81:SER:HB2	1:G:267:ARG:NH1	2.05	0.70
1:F:84:LEU:HD21	1:F:220:LEU:HD22	1.73	0.70
1:E:6:SER:OG	1:F:13:GLY:HA3	1.92	0.70
1:A:192:ARG:O	1:A:193:ASP:C	2.30	0.70
1:B:181:GLY:HA3	1:B:191:THR:HA	1.74	0.69
1:F:69:ASP:HB3	1:F:217:ARG:HH21	1.56	0.69
1:G:226:LEU:HG	1:G:227:PRO:HD2	1.73	0.69
1:C:106:VAL:HG11	1:C:173:VAL:HG11	1.72	0.69
1:F:161:TYR:HB3	1:F:177:VAL:HG22	1.74	0.69
1:F:267:ARG:HE	1:F:269:GLY:HA3	1.57	0.69
1:B:130:ASP:HB3	1:B:139:SER:HB2	1.74	0.69
1:G:77:ILE:HB	1:G:78:PRO:HD3	1.75	0.69
1:B:41:PHE:HB3	1:B:301:LYS:HE3	1.75	0.69
1:C:120:SER:HB3	1:C:149:ASP:HB2	1.75	0.68
1:C:165:LEU:HD21	1:C:168:GLN:HE22	1.56	0.68
1:B:96:LEU:HG	1:B:253:ILE:HG22	1.75	0.68
1:G:103:PHE:HB2	1:G:170:ASN:HA	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:PRO:O	1:G:270:PHE:N	2.25	0.68
1:C:270:PHE:HB2	1:C:278:VAL:HG22	1.76	0.68
1:B:95:ASN:HB3	1:B:172:HIS:CE1	2.29	0.67
1:C:20:THR:OG1	1:C:301:LYS:NZ	2.26	0.67
1:C:202:GLN:NE2	1:C:205:MET:SD	2.68	0.67
1:G:115:THR:HA	1:G:154:VAL:HG12	1.77	0.67
1:G:263:ASP:HB2	1:G:285:VAL:HG11	1.74	0.67
1:A:130:ASP:HB3	1:A:139:SER:HB2	1.77	0.67
1:A:161:TYR:HB2	1:C:112:VAL:HG12	1.77	0.67
1:E:87:PRO:HA	1:E:261:ALA:HA	1.76	0.67
1:B:88:SER:HA	1:B:179:PHE:CE2	2.29	0.67
1:E:17:LYS:HB2	1:E:43:ASP:HB3	1.77	0.67
1:B:42:ILE:HB	1:B:51:ILE:HG23	1.77	0.66
1:C:251:SER:HB3	1:C:298:TRP:CH2	2.31	0.66
1:D:138:PRO:HG2	1:G:133:VAL:HG23	1.78	0.66
1:D:161:TYR:HA	1:D:179:PHE:HA	1.78	0.66
1:A:202:GLN:NE2	1:A:205:MET:SD	2.67	0.66
1:A:226:LEU:HB3	1:A:230:THR:HG21	1.77	0.66
1:B:38:LYS:HB3	1:B:55:ASN:HB2	1.78	0.66
1:C:168:GLN:HB2	1:C:173:VAL:HA	1.77	0.66
1:A:189:ILE:HB	1:A:196:HIS:NE2	2.11	0.65
1:F:169:THR:HB	1:F:172:HIS:H	1.62	0.65
1:D:100:THR:HB	1:D:251:SER:HA	1.79	0.65
1:D:211:PRO:C	1:D:213:GLU:H	2.00	0.65
1:A:80:ALA:HB3	1:A:268:PRO:HD3	1.78	0.65
1:A:109:THR:HB	1:E:235:SER:HB3	1.79	0.65
1:B:251:SER:HB3	1:B:296:LEU:HB2	1.78	0.64
1:A:133:VAL:HG13	1:A:134:THR:H	1.63	0.64
1:D:102:ARG:HB3	1:D:104:PHE:CE2	2.32	0.64
1:D:133:VAL:HG12	1:D:134:THR:H	1.62	0.64
1:F:63:ALA:O	1:F:85:ARG:NH2	2.31	0.64
1:A:120:SER:HB3	1:A:149:ASP:HB3	1.79	0.64
1:B:6:SER:HB3	1:C:12:ILE:HD11	1.80	0.64
1:G:133:VAL:HG12	1:G:134:THR:H	1.63	0.64
1:A:20:THR:HB	1:A:22:TYR:CE2	2.33	0.64
1:D:175:TRP:CZ3	1:D:238:MET:HB3	2.33	0.64
1:E:130:ASP:HB2	1:E:139:SER:HB2	1.80	0.64
1:F:184:ASN:ND2	1:F:205:MET:O	2.31	0.64
1:A:160:SER:HB3	1:A:180:ASN:HB3	1.80	0.63
1:A:96:LEU:HD11	1:A:101:SER:HB3	1.81	0.63
1:C:120:SER:N	1:C:149:ASP:O	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ALA:HB3	1:E:286:ASP:HB2	1.79	0.63
1:F:123:TYR:HA	1:F:146:GLY:HA2	1.80	0.63
1:A:182:TYR:CE1	1:A:227:PRO:HD3	2.34	0.63
1:A:251:SER:HB3	1:A:296:LEU:HB2	1.81	0.63
1:E:270:PHE:HD2	1:E:278:VAL:HG11	1.64	0.63
1:E:43:ASP:OD1	1:E:246:LYS:NZ	2.25	0.63
1:E:73:ASP:OD1	1:E:74:GLY:N	2.32	0.63
1:C:38:LYS:HB3	1:C:55:ASN:HB3	1.80	0.62
1:B:186:ASN:HB3	1:G:150:TRP:HH2	1.64	0.62
1:C:84:LEU:HD21	1:C:220:LEU:HD22	1.81	0.62
1:C:296:LEU:HB2	1:C:298:TRP:CZ3	2.34	0.62
1:D:106:VAL:HG21	1:D:173:VAL:HG21	1.81	0.62
1:F:267:ARG:HG2	1:F:269:GLY:H	1.64	0.62
1:A:90:TYR:HB2	1:A:177:VAL:HG23	1.82	0.62
1:B:191:THR:HG23	1:B:193:ASP:H	1.63	0.62
1:G:245:GLU:HG3	1:G:247:ASP:H	1.65	0.62
1:B:162:LYS:NZ	1:C:226:LEU:O	2.32	0.62
1:B:261:ALA:HB3	1:B:286:ASP:HB2	1.81	0.62
1:F:92:ILE:HG12	1:F:257:TYR:HD1	1.65	0.62
1:A:189:ILE:HD11	1:A:208:ARG:HE	1.65	0.62
1:C:81:SER:HB3	1:C:267:ARG:HE	1.64	0.62
1:F:165:LEU:HD21	1:F:168:GLN:HE21	1.65	0.62
1:F:257:TYR:HB2	1:F:290:PHE:CZ	2.35	0.62
1:A:189:ILE:HB	1:A:196:HIS:CE1	2.35	0.62
1:D:156:TYR:HB3	1:D:158:GLN:HG2	1.82	0.62
1:A:201:ASN:HD22	1:A:281:ASN:HB3	1.64	0.61
1:B:162:LYS:HB2	1:C:228:THR:HG22	1.81	0.61
1:E:216:ALA:HB2	1:E:277:TRP:CZ3	2.35	0.61
1:D:165:LEU:HG	1:D:175:TRP:CD1	2.35	0.61
1:G:134:THR:O	1:G:136:SER:N	2.33	0.61
1:B:100:THR:OG1	1:B:101:SER:N	2.34	0.61
1:A:68:SER:O	1:A:82:VAL:HA	2.01	0.61
1:E:122:SER:O	1:E:147:GLN:N	2.27	0.61
1:G:22:TYR:CE2	1:G:303:LEU:HB3	2.36	0.61
1:F:226:LEU:HB3	1:F:230:THR:HG21	1.83	0.61
1:A:42:ILE:HG23	1:A:51:ILE:HB	1.83	0.60
1:F:75:TYR:HB2	1:F:76:PRO:HD3	1.82	0.60
1:F:159:THR:HG1	1:F:179:PHE:HD1	1.47	0.60
1:D:226:LEU:HB3	1:D:230:THR:HG21	1.82	0.60
1:F:27:ASN:ND2	1:F:33:MET:O	2.35	0.60
1:C:41:PHE:HE2	1:C:296:LEU:HD23	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:HIS:HB2	1:D:214:THR:HG22	1.84	0.60
1:C:21:SER:HA	1:C:40:THR:HG22	1.84	0.59
1:D:107:ALA:HB3	1:D:239:ILE:HB	1.84	0.59
1:D:126:GLY:N	1:D:143:GLY:O	2.34	0.59
1:C:251:SER:CB	1:C:298:TRP:HZ3	2.15	0.59
1:A:267:ARG:HG3	1:A:268:PRO:HD2	1.83	0.59
1:B:53:VAL:HG13	1:B:241:VAL:HG22	1.83	0.59
1:B:122:SER:O	1:B:147:GLN:N	2.25	0.59
1:B:202:GLN:HG2	1:B:205:MET:HB3	1.84	0.59
1:E:38:LYS:HG3	1:E:55:ASN:HB2	1.83	0.59
1:E:123:TYR:HA	1:E:146:GLY:HA2	1.83	0.59
1:G:86:TYR:CE1	1:G:230:THR:HG23	2.37	0.59
1:A:184:ASN:H	1:A:190:TYR:HE1	1.48	0.59
1:D:159:THR:O	1:D:227:PRO:HG3	2.03	0.59
1:E:249:GLU:O	1:E:298:TRP:N	2.35	0.59
1:A:158:GLN:C	1:A:160:SER:H	2.06	0.59
1:B:47:ALA:HA	1:C:21:SER:O	2.03	0.59
1:A:97:GLN:HB2	1:A:252:SER:OG	2.03	0.59
1:G:237:GLY:H	1:G:238:MET:HE3	1.68	0.59
1:A:48:ASP:HB2	1:E:22:TYR:CD1	2.38	0.58
1:B:180:ASN:O	1:B:192:ARG:N	2.35	0.58
1:E:263:ASP:OD1	1:E:285:VAL:HG21	2.03	0.58
1:A:232:SER:HB3	1:C:165:LEU:O	2.02	0.58
1:F:159:THR:O	1:F:160:SER:C	2.41	0.58
1:F:165:LEU:HD11	1:F:168:GLN:HE21	1.69	0.58
1:G:292:LYS:NZ	1:G:293:SER:O	2.35	0.58
1:A:189:ILE:CG1	1:A:208:ARG:HH21	2.15	0.58
1:A:192:ARG:HD2	1:E:225:ASP:OD2	2.04	0.58
1:B:103:PHE:N	1:B:170:ASN:O	2.34	0.58
1:B:213:GLU:HA	1:B:277:TRP:HZ2	1.69	0.58
1:F:36:SER:HB2	1:F:57:THR:O	2.04	0.58
1:A:103:PHE:N	1:A:170:ASN:OD1	2.36	0.57
1:A:190:TYR:HE2	1:A:208:ARG:HH22	1.51	0.57
1:D:81:SER:HB2	1:D:267:ARG:NH2	2.17	0.57
1:G:250:GLN:HG3	1:G:297:ASP:HA	1.86	0.57
1:B:46:SER:HB2	1:C:20:THR:HA	1.86	0.57
1:B:214:THR:HG22	1:B:215:ASP:H	1.69	0.57
1:A:103:PHE:O	1:A:242:VAL:HA	2.04	0.57
1:A:122:SER:O	1:A:147:GLN:N	2.31	0.57
1:B:204:PHE:CE2	1:B:264:TYR:HB3	2.39	0.57
1:D:294:PHE:HA	1:D:304:VAL:HG12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ILE:HG12	1:D:296:LEU:HD23	1.86	0.57
1:D:301:LYS:O	1:D:302:LYS:C	2.43	0.57
1:F:154:VAL:HB	1:F:156:TYR:CE2	2.39	0.57
1:G:182:TYR:OH	1:G:225:ASP:O	2.20	0.57
1:A:38:LYS:HE2	1:B:5:THR:CG2	2.34	0.57
1:A:249:GLU:HA	1:A:298:TRP:HB2	1.87	0.57
1:F:208:ARG:HH11	1:F:208:ARG:HB2	1.69	0.57
1:B:186:ASN:HB3	1:G:150:TRP:CH2	2.39	0.57
1:A:192:ARG:O	1:A:194:SER:N	2.38	0.57
1:D:175:TRP:CH2	1:D:238:MET:HB3	2.39	0.57
1:E:53:VAL:HG12	1:E:241:VAL:HG22	1.87	0.56
1:F:104:PHE:HB2	1:G:25:PHE:CE2	2.39	0.56
1:A:78:PRO:HD2	1:A:268:PRO:HG3	1.87	0.56
1:C:77:ILE:HB	1:C:80:ALA:HB3	1.88	0.56
1:F:38:LYS:HB3	1:F:55:ASN:HB2	1.88	0.56
1:F:121:VAL:HG22	1:F:148:VAL:HG13	1.87	0.56
1:E:10:THR:HA	1:F:40:THR:HG21	1.88	0.56
1:G:285:VAL:HG13	1:G:286:ASP:H	1.70	0.56
1:D:87:PRO:CA	1:D:261:ALA:HA	2.08	0.56
1:E:33:MET:HG3	1:E:60:PHE:HD1	1.70	0.56
1:E:120:SER:O	1:E:149:ASP:N	2.33	0.56
1:A:41:PHE:CG	1:A:301:LYS:HD2	2.40	0.56
1:G:75:TYR:O	1:G:79:GLY:HA2	2.05	0.56
1:F:80:ALA:O	1:F:267:ARG:HG3	2.06	0.56
1:G:27:ASN:ND2	1:G:33:MET:O	2.39	0.56
1:B:104:PHE:CE1	1:B:243:ILE:HG23	2.40	0.56
1:A:123:TYR:HA	1:A:146:GLY:HA2	1.88	0.56
1:B:34:THR:HG21	1:D:169:THR:HA	1.88	0.56
1:B:168:GLN:HB3	1:C:34:THR:HG21	1.87	0.56
1:G:69:ASP:HA	1:G:82:VAL:HG22	1.87	0.55
1:F:73:ASP:HB3	1:F:77:ILE:HB	1.87	0.55
1:A:121:VAL:HG13	1:E:150:TRP:HB2	1.89	0.55
1:A:190:TYR:HE2	1:A:208:ARG:NH2	2.05	0.55
1:C:34:THR:HG23	1:C:59:SER:H	1.71	0.55
1:D:90:TYR:CE1	1:D:259:LYS:HB2	2.41	0.55
1:D:174:LYS:C	1:D:175:TRP:CD1	2.80	0.55
1:D:244:SER:HB2	1:D:298:TRP:CD1	2.41	0.55
1:A:90:TYR:CE1	1:A:259:LYS:HG3	2.42	0.55
1:B:43:ASP:OD1	1:B:246:LYS:NZ	2.40	0.55
1:B:169:THR:OG1	1:B:172:HIS:O	2.21	0.55
1:C:88:SER:OG	1:C:192:ARG:NH2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ILE:HG23	1:D:257:TYR:CE1	2.42	0.55
1:G:123:TYR:HA	1:G:146:GLY:HA2	1.87	0.55
1:G:101:SER:OG	1:G:170:ASN:OD1	2.25	0.55
1:B:49:LYS:HD2	1:B:245:GLU:HA	1.87	0.55
1:B:204:PHE:HB2	1:B:220:LEU:HD23	1.89	0.55
1:E:84:LEU:HD22	1:E:220:LEU:HD13	1.88	0.55
1:E:113:GLU:OE1	1:E:113:GLU:N	2.39	0.55
1:A:260:HIS:HB3	1:A:284:ASP:OD1	2.07	0.55
1:B:33:MET:HB3	1:B:60:PHE:HD1	1.72	0.55
1:G:90:TYR:HB2	1:G:177:VAL:HG23	1.89	0.55
1:B:52:ALA:HB3	1:B:242:VAL:HG23	1.89	0.55
1:B:130:ASP:OD1	1:B:131:ALA:N	2.40	0.54
1:E:196:HIS:ND1	1:E:200:GLY:O	2.36	0.54
1:F:20:THR:OG1	1:F:41:PHE:HB2	2.07	0.54
1:G:51:ILE:HG22	1:G:243:ILE:HG12	1.88	0.54
1:E:106:VAL:HG21	1:E:168:GLN:OE1	2.07	0.54
1:C:65:PRO:HB2	1:C:67:LEU:HG	1.89	0.54
1:B:124:GLN:HG2	1:C:147:GLN:CG	2.37	0.54
1:A:166:ILE:HG12	1:A:167:ASP:H	1.72	0.54
1:G:82:VAL:HG11	1:G:217:ARG:HA	1.90	0.54
1:G:253:ILE:HG12	1:G:296:LEU:HD11	1.90	0.54
1:B:66:THR:HG21	1:B:217:ARG:HG3	1.90	0.54
1:F:25:PHE:CZ	1:F:36:SER:HB3	2.43	0.54
1:D:124:GLN:HG2	1:D:145:THR:HB	1.90	0.54
1:F:16:ALA:HB1	1:F:44:ASP:HA	1.90	0.54
1:F:68:SER:O	1:F:82:VAL:HA	2.08	0.54
1:A:107:ALA:HB3	1:A:239:ILE:HG13	1.89	0.53
1:B:61:MET:HB2	1:D:167:ASP:CG	2.28	0.53
1:C:196:HIS:N	1:C:200:GLY:O	2.38	0.53
1:F:184:ASN:HB3	1:F:208:ARG:NH2	2.23	0.53
1:G:94:MET:SD	1:G:255:VAL:HG12	2.49	0.53
1:A:158:GLN:C	1:A:160:SER:N	2.60	0.53
1:F:65:PRO:HD2	1:F:85:ARG:HB3	1.91	0.53
1:A:70:ALA:HB3	1:A:71:PRO:HD3	1.90	0.53
1:C:96:LEU:HD13	1:C:100:THR:HG22	1.91	0.53
1:E:19:HIS:O	1:E:21:SER:N	2.41	0.53
1:D:128:SER:HB3	1:D:141:GLU:HB3	1.90	0.53
1:C:92:ILE:HG23	1:C:175:TRP:CD1	2.44	0.53
1:F:38:LYS:N	1:F:55:ASN:O	2.42	0.53
1:F:166:ILE:HG13	1:F:176:ASN:HB2	1.90	0.53
1:G:74:GLY:HA3	1:G:78:PRO:HG2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ALA:HB3	1:B:256:ALA:HB3	1.89	0.53
1:D:97:GLN:O	1:D:99:ASN:N	2.42	0.53
1:F:120:SER:HA	1:G:150:TRP:O	2.09	0.53
1:D:56:THR:HG22	1:D:238:MET:O	2.09	0.52
1:A:160:SER:O	1:A:162:LYS:N	2.39	0.52
1:A:206:TYR:HB3	1:A:219:ASN:O	2.10	0.52
1:B:216:ALA:HB1	1:B:266:LEU:HD22	1.91	0.52
1:C:41:PHE:CE1	1:C:301:LYS:HB3	2.44	0.52
1:E:62:LYS:HG3	1:E:230:THR:HA	1.91	0.52
1:F:270:PHE:O	1:F:271:THR:OG1	2.26	0.52
1:A:97:GLN:O	1:A:99:ASN:N	2.42	0.52
1:F:102:ARG:CB	1:F:170:ASN:HB3	2.37	0.52
1:F:165:LEU:HD21	1:F:168:GLN:HG3	1.92	0.52
1:A:28:GLU:N	1:A:28:GLU:OE1	2.42	0.52
1:A:38:LYS:CE	1:B:5:THR:HG22	2.40	0.52
1:C:23:ASN:HB3	1:C:25:PHE:CE1	2.44	0.52
1:C:81:SER:HB3	1:C:267:ARG:NE	2.23	0.52
1:G:286:ASP:OD1	1:G:288:LYS:NZ	2.43	0.52
1:A:229:LEU:HD23	1:A:234:PHE:HB2	1.90	0.52
1:A:190:TYR:HD2	1:A:202:GLN:HB2	1.73	0.52
1:D:273:GLY:O	1:D:275:GLY:N	2.43	0.52
1:B:69:ASP:OD2	1:B:217:ARG:NH1	2.42	0.52
1:B:164:ASN:ND2	1:C:231:ASN:OD1	2.42	0.52
1:A:23:ASN:O	1:C:49:LYS:NZ	2.35	0.52
1:A:38:LYS:CB	1:A:55:ASN:HB3	2.33	0.52
1:A:187:TRP:HE1	1:A:191:THR:HA	1.75	0.52
1:C:39:VAL:HA	1:C:53:VAL:O	2.10	0.52
1:F:191:THR:HG23	1:F:193:ASP:H	1.75	0.52
1:B:68:SER:HB3	1:B:83:THR:HG22	1.91	0.52
1:C:63:ALA:O	1:C:65:PRO:HD3	2.10	0.52
1:D:108:PRO:HD2	1:D:175:TRP:CH2	2.45	0.52
1:D:251:SER:O	1:D:252:SER:C	2.48	0.52
1:C:96:LEU:HD13	1:C:100:THR:CG2	2.40	0.51
1:E:86:TYR:CZ	1:E:204:PHE:HD2	2.28	0.51
1:A:63:ALA:O	1:A:65:PRO:HD3	2.10	0.51
1:A:228:THR:HA	1:C:164:ASN:ND2	2.26	0.51
1:B:98:ASP:HA	1:B:171:LYS:HD2	1.92	0.51
1:C:297:ASP:O	1:C:298:TRP:C	2.49	0.51
1:D:81:SER:OG	1:D:267:ARG:NH2	2.42	0.51
1:F:17:LYS:O	1:F:19:HIS:N	2.38	0.51
1:F:204:PHE:CE2	1:F:264:TYR:HB3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ALA:HA	1:E:268:PRO:CD	2.38	0.51
1:C:50:GLN:HG3	1:C:246:LYS:HG2	1.90	0.51
1:F:90:TYR:CE1	1:F:259:LYS:HG3	2.45	0.51
1:F:117:VAL:HB	1:G:156:TYR:CE1	2.45	0.51
1:G:184:ASN:ND2	1:G:202:GLN:O	2.39	0.51
1:B:269:GLY:O	1:B:270:PHE:C	2.49	0.51
1:C:57:THR:HG22	1:C:58:GLY:H	1.74	0.51
1:F:96:LEU:HB3	1:F:171:LYS:HZ1	1.76	0.51
1:D:216:ALA:HA	1:D:219:ASN:HB3	1.92	0.51
1:G:81:SER:CB	1:G:267:ARG:HH11	2.20	0.51
1:B:127:GLY:O	1:C:144:ALA:N	2.44	0.51
1:F:227:PRO:O	1:F:231:ASN:ND2	2.44	0.51
1:E:266:LEU:HD11	1:E:277:TRP:HB3	1.93	0.51
1:F:126:GLY:N	1:F:143:GLY:O	2.44	0.51
1:E:169:THR:HG22	1:E:170:ASN:H	1.75	0.50
1:A:100:THR:C	1:A:102:ARG:H	2.14	0.50
1:C:295:VAL:H	1:C:305:GLU:HA	1.76	0.50
1:A:38:LYS:HE2	1:B:5:THR:HG22	1.94	0.50
1:D:38:LYS:HB3	1:D:55:ASN:HB3	1.92	0.50
1:E:33:MET:HG3	1:E:60:PHE:CD1	2.46	0.50
1:F:22:TYR:CD2	1:F:303:LEU:HB3	2.46	0.50
1:B:63:ALA:O	1:B:65:PRO:HD3	2.11	0.50
1:D:133:VAL:HG12	1:D:134:THR:N	2.27	0.50
1:G:39:VAL:HG22	1:G:54:ILE:HG22	1.93	0.50
1:A:10:THR:HG22	1:E:53:VAL:HG21	1.94	0.50
1:G:154:VAL:HG22	1:G:156:TYR:CE1	2.47	0.50
1:B:103:PHE:CE1	1:B:240:ALA:HB1	2.47	0.50
1:D:84:LEU:HD13	1:D:86:TYR:CD2	2.47	0.50
1:D:18:THR:O	1:D:19:HIS:HB3	2.12	0.50
1:D:175:TRP:HZ3	1:D:238:MET:SD	2.35	0.50
1:F:122:SER:HA	1:G:148:VAL:O	2.11	0.49
1:B:124:GLN:CG	1:C:147:GLN:HA	2.40	0.49
1:C:90:TYR:HB2	1:C:177:VAL:HG23	1.92	0.49
1:G:22:TYR:CZ	1:G:39:VAL:HB	2.47	0.49
1:G:70:ALA:H	1:G:82:VAL:HG22	1.77	0.49
1:A:168:GLN:HG2	1:E:59:SER:HB3	1.94	0.49
1:C:36:SER:HB2	1:C:57:THR:C	2.33	0.49
1:C:41:PHE:CE2	1:C:296:LEU:HD23	2.47	0.49
1:E:76:PRO:O	1:E:80:ALA:HB2	2.12	0.49
1:B:66:THR:HB	1:B:84:LEU:HG	1.94	0.49
1:B:253:ILE:HG12	1:B:296:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:SER:HB2	1:F:57:THR:C	2.33	0.49
1:A:104:PHE:CE2	1:E:23:ASN:HB3	2.47	0.49
1:B:22:TYR:OH	1:B:302:LYS:HG2	2.13	0.49
1:B:57:THR:HA	1:B:236:PRO:O	2.13	0.49
1:C:186:ASN:OD1	1:C:186:ASN:O	2.31	0.49
1:D:275:GLY:O	1:D:276:ASN:C	2.50	0.49
1:F:106:VAL:HG13	1:F:175:TRP:CZ2	2.47	0.49
1:F:118:THR:HA	1:G:152:ASP:O	2.11	0.49
1:G:49:LYS:HG2	1:G:245:GLU:HA	1.95	0.49
1:A:133:VAL:HG13	1:A:134:THR:N	2.28	0.49
1:F:250:GLN:HA	1:F:298:TRP:HD1	1.77	0.49
1:G:22:TYR:HE2	1:G:303:LEU:HD22	1.78	0.49
1:A:12:ILE:HD11	1:A:44:ASP:OD2	2.13	0.49
1:A:201:ASN:ND2	1:A:281:ASN:HB3	2.27	0.49
1:F:263:ASP:HB2	1:F:285:VAL:HG21	1.95	0.49
1:A:80:ALA:C	1:A:82:VAL:H	2.15	0.48
1:B:28:GLU:HG2	1:B:33:MET:HB2	1.95	0.48
1:E:120:SER:HB3	1:E:149:ASP:HB3	1.94	0.48
1:F:22:TYR:CG	1:F:23:ASN:N	2.81	0.48
1:F:63:ALA:O	1:F:65:PRO:HD3	2.13	0.48
1:F:90:TYR:HB2	1:F:177:VAL:HG13	1.94	0.48
1:G:210:TYR:HB3	1:G:277:TRP:HE1	1.76	0.48
1:F:17:LYS:C	1:F:19:HIS:H	2.12	0.48
1:F:54:ILE:HD13	1:F:242:VAL:HG23	1.93	0.48
1:G:16:ALA:O	1:G:17:LYS:C	2.51	0.48
1:C:105:HIS:HB3	1:C:241:VAL:CG1	2.43	0.48
1:G:296:LEU:HG	1:G:303:LEU:HD12	1.95	0.48
1:B:20:THR:OG1	1:B:41:PHE:HB2	2.12	0.48
1:C:296:LEU:HG	1:C:303:LEU:CD2	2.44	0.48
1:D:130:ASP:OD1	1:D:131:ALA:N	2.46	0.48
1:D:211:PRO:C	1:D:213:GLU:N	2.67	0.48
1:D:232:SER:HB3	1:G:165:LEU:O	2.13	0.48
1:E:121:VAL:HG13	1:E:148:VAL:HG22	1.94	0.48
1:E:251:SER:HB2	1:E:296:LEU:HB2	1.94	0.48
1:F:103:PHE:N	1:F:170:ASN:O	2.42	0.48
1:F:122:SER:O	1:F:147:GLN:N	2.26	0.48
1:A:96:LEU:HB3	1:A:171:LYS:HA	1.94	0.48
1:E:272:PHE:HD2	1:E:276:ASN:HB2	1.79	0.48
1:F:164:ASN:HD21	1:F:178:PHE:HD2	1.61	0.48
1:F:215:ASP:OD2	1:F:217:ARG:NH1	2.46	0.48
1:A:103:PHE:O	1:A:104:PHE:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:PRO:O	1:E:84:LEU:HD12	2.14	0.48
1:E:126:GLY:N	1:E:143:GLY:O	2.43	0.48
1:F:49:LYS:HG2	1:F:245:GLU:HA	1.96	0.48
1:A:48:ASP:HB2	1:E:22:TYR:CE1	2.49	0.48
1:A:165:LEU:O	1:E:232:SER:HB3	2.14	0.48
1:B:164:ASN:HB3	1:C:232:SER:OG	2.14	0.48
1:C:61:MET:HG2	1:C:63:ALA:N	2.29	0.48
1:E:166:ILE:HG13	1:E:167:ASP:H	1.79	0.48
1:F:96:LEU:HD13	1:F:171:LYS:NZ	2.29	0.48
1:E:28:GLU:N	1:E:28:GLU:OE1	2.47	0.48
1:E:199:TYR:CE1	1:E:276:ASN:HB3	2.48	0.48
1:A:49:LYS:HG2	1:A:245:GLU:HA	1.96	0.48
1:C:49:LYS:HD3	1:C:245:GLU:HG3	1.94	0.48
1:C:206:TYR:HA	1:C:221:VAL:HG13	1.96	0.48
1:G:149:ASP:OD1	1:G:150:TRP:N	2.46	0.48
1:C:297:ASP:O	1:C:301:LYS:N	2.39	0.47
1:F:56:THR:HG22	1:F:238:MET:O	2.13	0.47
1:G:166:ILE:HG13	1:G:176:ASN:ND2	2.30	0.47
1:G:202:GLN:O	1:G:202:GLN:HG2	2.14	0.47
1:D:19:HIS:CE1	1:G:12:ILE:HA	2.50	0.47
1:E:212:HIS:O	1:E:212:HIS:CG	2.67	0.47
1:F:128:SER:HB3	1:F:141:GLU:HB3	1.94	0.47
1:G:202:GLN:HG3	1:G:205:MET:HB3	1.95	0.47
1:B:110:ASN:ND2	1:C:233:GLY:O	2.33	0.47
1:F:32:ASN:HB2	1:F:61:MET:HE1	1.96	0.47
1:C:64:ASN:ND2	1:C:230:THR:O	2.47	0.47
1:D:51:ILE:HA	1:D:243:ILE:HG13	1.97	0.47
1:D:72:VAL:O	1:D:74:GLY:N	2.47	0.47
1:E:274:THR:O	1:E:275:GLY:C	2.52	0.47
1:A:133:VAL:CG1	1:E:137:GLY:HA2	2.43	0.47
1:C:104:PHE:CE1	1:C:243:ILE:HB	2.49	0.47
1:C:163:THR:HA	1:C:177:VAL:HG12	1.96	0.47
1:F:118:THR:HB	1:F:151:SER:HB2	1.96	0.47
1:G:204:PHE:CE2	1:G:264:TYR:HB3	2.50	0.47
1:A:19:HIS:HD2	1:A:42:ILE:HD13	1.80	0.47
1:B:104:PHE:HA	1:B:168:GLN:NE2	2.29	0.47
1:E:83:THR:HG22	1:E:265:THR:HB	1.96	0.47
1:A:49:LYS:HB3	1:A:244:SER:O	2.15	0.47
1:A:267:ARG:HB3	1:A:278:VAL:HB	1.96	0.47
1:B:77:ILE:HB	1:B:78:PRO:HD3	1.96	0.47
1:C:270:PHE:O	1:C:276:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:THR:HG22	1:E:170:ASN:N	2.30	0.47
1:F:166:ILE:HG22	1:F:167:ASP:H	1.79	0.47
1:C:207:SER:HB3	1:C:211:PRO:HD3	1.96	0.47
1:D:75:TYR:N	1:D:76:PRO:HD3	2.30	0.47
1:F:120:SER:O	1:F:149:ASP:N	2.33	0.47
1:B:261:ALA:N	1:B:286:ASP:O	2.48	0.47
1:A:104:PHE:HB3	1:A:105:HIS:H	1.42	0.46
1:A:167:ASP:HB3	1:E:61:MET:SD	2.56	0.46
1:B:50:GLN:HB2	1:B:301:LYS:HE2	1.97	0.46
1:C:227:PRO:O	1:C:230:THR:HG22	2.15	0.46
1:D:61:MET:HG2	1:D:63:ALA:N	2.30	0.46
1:D:96:LEU:HD23	1:D:103:PHE:CE1	2.50	0.46
1:D:267:ARG:HG2	1:D:269:GLY:H	1.80	0.46
1:G:285:VAL:HG13	1:G:286:ASP:N	2.29	0.46
1:A:140:GLY:O	1:C:130:ASP:HB3	2.14	0.46
1:A:307:LYS:HB3	1:A:308:GLY:H	1.55	0.46
1:E:268:PRO:O	1:E:269:GLY:C	2.52	0.46
1:F:6:SER:N	1:G:11:ASP:HB3	2.29	0.46
1:C:223:MET:HB3	1:C:231:ASN:HB3	1.98	0.46
1:A:190:TYR:CD2	1:A:202:GLN:HB2	2.50	0.46
1:B:164:ASN:ND2	1:C:228:THR:O	2.48	0.46
1:D:297:ASP:CG	1:D:300:ASN:HB3	2.36	0.46
1:D:305:GLU:HB3	1:D:306:LYS:H	1.36	0.46
1:D:305:GLU:C	1:D:307:LYS:H	2.19	0.46
1:E:86:TYR:CE2	1:E:264:TYR:HB3	2.51	0.46
1:D:60:PHE:CZ	1:D:234:PHE:HD2	2.33	0.46
1:F:167:ASP:HB3	1:G:61:MET:SD	2.56	0.46
1:B:62:LYS:HE2	1:B:233:GLY:HA2	1.97	0.46
1:E:98:ASP:HA	1:E:171:LYS:HD3	1.98	0.46
1:A:184:ASN:O	1:A:186:ASN:N	2.48	0.46
1:A:227:PRO:O	1:A:230:THR:HG22	2.14	0.46
1:C:20:THR:HG21	1:C:301:LYS:HZ1	1.64	0.46
1:C:100:THR:OG1	1:C:101:SER:N	2.48	0.46
1:C:251:SER:CB	1:C:298:TRP:CH2	2.96	0.46
1:E:119:SER:OG	1:F:152:ASP:HB2	2.16	0.46
1:G:74:GLY:O	1:G:79:GLY:N	2.49	0.46
1:B:160:SER:O	1:B:179:PHE:HB2	2.16	0.46
1:C:17:LYS:O	1:C:18:THR:OG1	2.28	0.46
1:F:157:ASP:O	1:F:158:GLN:C	2.54	0.46
1:F:203:LEU:HD11	1:F:264:TYR:CE2	2.51	0.46
1:E:168:GLN:HG2	1:E:173:VAL:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:MET:SD	1:D:223:MET:N	2.90	0.45
1:F:211:PRO:HB2	1:F:277:TRP:CD1	2.51	0.45
1:A:16:ALA:CB	1:A:42:ILE:HD11	2.41	0.45
1:C:60:PHE:HB2	1:C:259:LYS:HE2	1.98	0.45
1:E:199:TYR:HE1	1:E:276:ASN:HB3	1.82	0.45
1:A:91:ASP:HA	1:A:175:TRP:O	2.15	0.45
1:C:88:SER:HB2	1:C:262:ASP:OD2	2.16	0.45
1:E:128:SER:HA	1:F:142:SER:O	2.17	0.45
1:A:48:ASP:HB2	1:E:22:TYR:HD1	1.80	0.45
1:B:12:ILE:HG23	1:C:38:LYS:HZ1	1.82	0.45
1:F:159:THR:HB	1:F:181:GLY:N	2.24	0.45
1:B:7:GLN:HG3	1:C:105:HIS:CD2	2.51	0.45
1:C:94:MET:CG	1:C:173:VAL:HB	2.46	0.45
1:D:50:GLN:HG3	1:D:298:TRP:CZ3	2.51	0.45
1:E:84:LEU:HD23	1:E:86:TYR:OH	2.16	0.45
1:F:69:ASP:HB3	1:F:217:ARG:HE	1.80	0.45
1:F:89:GLN:HG3	1:F:178:PHE:CD1	2.52	0.45
1:F:192:ARG:HG3	1:F:193:ASP:OD1	2.17	0.45
1:G:104:PHE:CE1	1:G:243:ILE:HB	2.52	0.45
1:F:102:ARG:HA	1:F:170:ASN:O	2.16	0.45
1:A:190:TYR:H	1:A:196:HIS:HE1	1.65	0.45
1:B:48:ASP:C	1:B:49:LYS:HD3	2.37	0.45
1:B:61:MET:HG2	1:B:63:ALA:N	2.31	0.45
1:C:285:VAL:HG23	1:C:286:ASP:H	1.81	0.45
1:D:52:ALA:HB2	1:D:298:TRP:CH2	2.52	0.45
1:E:22:TYR:HB2	1:E:39:VAL:HG12	1.98	0.45
1:E:69:ASP:HB3	1:E:217:ARG:CZ	2.46	0.45
1:F:165:LEU:HD11	1:F:168:GLN:NE2	2.32	0.45
1:F:211:PRO:HD2	1:F:276:ASN:HA	1.98	0.45
1:B:61:MET:O	1:B:259:LYS:NZ	2.27	0.45
1:B:80:ALA:H	1:B:268:PRO:HD3	1.80	0.45
1:C:166:ILE:HG13	1:C:167:ASP:H	1.82	0.45
1:D:97:GLN:C	1:D:99:ASN:H	2.20	0.45
1:F:24:THR:C	1:F:25:PHE:HD1	2.21	0.45
1:F:128:SER:N	1:F:141:GLU:O	2.49	0.45
1:C:166:ILE:HB	1:C:176:ASN:CG	2.37	0.45
1:C:301:LYS:HB2	1:C:301:LYS:HE3	1.36	0.45
1:D:229:LEU:HD23	1:D:234:PHE:HB2	1.99	0.45
1:E:274:THR:O	1:E:276:ASN:N	2.50	0.45
1:F:134:THR:O	1:F:135:PRO:C	2.56	0.45
1:F:249:GLU:HB3	1:F:250:GLN:H	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:HD22	1:A:281:ASN:CB	2.28	0.45
1:E:191:THR:OG1	1:E:192:ARG:N	2.50	0.45
1:E:270:PHE:CD2	1:E:278:VAL:HG11	2.48	0.45
1:F:159:THR:HB	1:F:181:GLY:O	2.17	0.45
1:A:182:TYR:CG	1:A:183:ASN:N	2.85	0.44
1:C:164:ASN:ND2	1:C:178:PHE:HE2	2.14	0.44
1:C:188:GLY:HA3	1:C:189:ILE:HA	1.63	0.44
1:D:27:ASN:HB3	1:G:170:ASN:ND2	2.32	0.44
1:B:167:ASP:CB	1:C:61:MET:HB2	2.37	0.44
1:D:165:LEU:HG	1:D:175:TRP:NE1	2.32	0.44
1:G:38:LYS:HB3	1:G:55:ASN:HB2	1.98	0.44
1:A:51:ILE:HA	1:A:243:ILE:HG13	1.99	0.44
1:A:149:ASP:O	1:A:150:TRP:HD1	2.00	0.44
1:E:122:SER:HA	1:F:148:VAL:O	2.18	0.44
1:F:35:MET:HG3	1:F:257:TYR:CE2	2.51	0.44
1:A:25:PHE:CE1	1:C:170:ASN:HB3	2.52	0.44
1:A:57:THR:HA	1:A:236:PRO:O	2.18	0.44
1:A:96:LEU:N	1:A:171:LYS:O	2.50	0.44
1:A:133:VAL:HG22	1:A:134:THR:HG23	1.99	0.44
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.84	0.44
1:A:158:GLN:NE2	1:C:113:GLU:OE2	2.51	0.44
1:B:48:ASP:OD1	1:B:48:ASP:N	2.44	0.44
1:C:96:LEU:HB3	1:C:253:ILE:HD12	1.99	0.44
1:F:166:ILE:HG22	1:F:167:ASP:N	2.33	0.44
1:G:63:ALA:O	1:G:65:PRO:HD3	2.18	0.44
1:C:196:HIS:HB3	1:C:199:TYR:HB2	1.98	0.44
1:D:18:THR:HG21	1:D:43:ASP:H	1.82	0.44
1:D:159:THR:HG23	1:D:182:TYR:CD1	2.53	0.44
1:D:254:GLN:HA	1:D:293:SER:HA	2.00	0.44
1:F:214:THR:HB	1:F:219:ASN:HD21	1.82	0.44
1:B:51:ILE:HA	1:B:243:ILE:HG22	2.00	0.44
1:B:83:THR:HA	1:B:265:THR:HA	2.00	0.44
1:D:54:ILE:HG13	1:D:240:ALA:O	2.18	0.44
1:E:210:TYR:HA	1:E:211:PRO:HD3	1.88	0.44
1:F:160:SER:OG	1:F:161:TYR:N	2.51	0.44
1:C:20:THR:OG1	1:C:41:PHE:HB2	2.18	0.43
1:E:96:LEU:HD21	1:E:101:SER:H	1.83	0.43
1:E:133:VAL:HG23	1:F:138:PRO:HG3	2.00	0.43
1:E:261:ALA:O	1:E:285:VAL:N	2.41	0.43
1:F:96:LEU:CB	1:F:171:LYS:HZ1	2.31	0.43
1:F:227:PRO:O	1:F:230:THR:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:PRO:HA	1:F:273:GLY:HA3	2.00	0.43
1:G:54:ILE:HG13	1:G:240:ALA:O	2.18	0.43
1:A:86:TYR:N	1:A:262:ASP:O	2.50	0.43
1:B:96:LEU:O	1:B:172:HIS:NE2	2.52	0.43
1:F:183:ASN:HB3	1:F:189:ILE:HD13	2.00	0.43
1:G:21:SER:HA	1:G:39:VAL:O	2.18	0.43
1:C:165:LEU:HD12	1:C:175:TRP:CZ3	2.54	0.43
1:G:199:TYR:CE1	1:G:276:ASN:HB3	2.53	0.43
1:A:93:ALA:HB3	1:A:256:ALA:HB3	2.00	0.43
1:A:124:GLN:HA	1:E:147:GLN:HA	2.00	0.43
1:B:33:MET:HB3	1:B:60:PHE:CD1	2.51	0.43
1:C:96:LEU:HG	1:C:171:LYS:HA	2.00	0.43
1:C:121:VAL:HG12	1:C:148:VAL:HG22	1.99	0.43
1:C:124:GLN:HG2	1:C:145:THR:HB	1.99	0.43
1:C:298:TRP:O	1:C:299:LYS:C	2.56	0.43
1:D:204:PHE:HD1	1:D:226:LEU:HD21	1.83	0.43
1:G:201:ASN:N	1:G:279:GLY:O	2.52	0.43
1:A:14:GLN:O	1:A:15:ASN:C	2.55	0.43
1:A:182:TYR:CD1	1:A:227:PRO:HD3	2.53	0.43
1:B:216:ALA:O	1:B:266:LEU:HD13	2.19	0.43
1:C:251:SER:HG	1:C:298:TRP:HZ3	1.65	0.43
1:C:251:SER:OG	1:C:298:TRP:CZ3	2.70	0.43
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.79	0.43
1:E:86:TYR:N	1:E:262:ASP:O	2.51	0.43
1:E:267:ARG:HE	1:E:267:ARG:HB2	1.36	0.43
1:F:96:LEU:HD12	1:F:171:LYS:HA	1.99	0.43
1:F:191:THR:OG1	1:F:192:ARG:N	2.51	0.43
1:A:60:PHE:CZ	1:A:234:PHE:HD2	2.36	0.43
1:B:84:LEU:HD13	1:B:220:LEU:HD21	2.01	0.43
1:D:166:ILE:HB	1:D:174:LYS:O	2.19	0.43
1:D:227:PRO:O	1:D:230:THR:HG22	2.19	0.43
1:E:22:TYR:CE2	1:E:302:LYS:HA	2.53	0.43
1:E:90:TYR:CE1	1:E:259:LYS:HG3	2.53	0.43
1:F:101:SER:HB3	1:F:243:ILE:O	2.18	0.43
1:G:206:TYR:HB2	1:G:220:LEU:C	2.39	0.43
1:A:189:ILE:HD11	1:A:208:ARG:NE	2.34	0.43
1:B:6:SER:O	1:C:53:VAL:HB	2.19	0.43
1:B:25:PHE:HB2	1:D:104:PHE:CD1	2.54	0.43
1:D:103:PHE:HB2	1:D:170:ASN:HA	2.00	0.43
1:E:84:LEU:HD12	1:E:84:LEU:HA	1.84	0.43
1:G:57:THR:HA	1:G:236:PRO:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:GLY:HA3	1:G:189:ILE:HA	1.79	0.43
1:B:103:PHE:HD1	1:B:104:PHE:H	1.66	0.43
1:D:297:ASP:C	1:D:299:LYS:H	2.22	0.43
1:F:165:LEU:O	1:G:232:SER:HB3	2.18	0.43
1:B:145:THR:HA	1:D:125:LEU:O	2.19	0.43
1:B:280:ASN:OD1	1:B:281:ASN:N	2.52	0.43
1:C:92:ILE:HG23	1:C:175:TRP:HD1	1.84	0.43
1:D:271:THR:HG22	1:D:278:VAL:HG22	2.00	0.43
1:G:250:GLN:HA	1:G:298:TRP:HD1	1.83	0.43
1:A:189:ILE:HG12	1:A:208:ARG:HH21	1.84	0.43
1:A:285:VAL:HG23	1:A:286:ASP:H	1.84	0.43
1:C:58:GLY:O	1:C:236:PRO:HD2	2.18	0.43
1:C:70:ALA:O	1:C:72:VAL:N	2.52	0.43
1:C:70:ALA:O	1:C:71:PRO:C	2.57	0.43
1:D:49:LYS:HG2	1:D:245:GLU:HA	2.00	0.43
1:G:263:ASP:CB	1:G:285:VAL:HG11	2.45	0.43
1:A:256:ALA:HA	1:A:291:ASN:HB3	2.01	0.42
1:E:25:PHE:CE1	1:E:34:THR:HB	2.54	0.42
1:E:71:PRO:HG3	1:E:80:ALA:O	2.18	0.42
1:E:272:PHE:CD2	1:E:276:ASN:HB2	2.54	0.42
1:A:104:PHE:CE2	1:E:25:PHE:HB2	2.54	0.42
1:A:192:ARG:CZ	1:A:193:ASP:HB2	2.49	0.42
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.93	0.42
1:F:107:ALA:HB3	1:F:239:ILE:HB	2.00	0.42
1:G:83:THR:HB	1:G:263:ASP:OD1	2.19	0.42
1:G:166:ILE:HG22	1:G:167:ASP:OD1	2.19	0.42
1:A:100:THR:OG1	1:A:171:LYS:NZ	2.52	0.42
1:A:162:LYS:HE2	1:A:162:LYS:HB2	1.43	0.42
1:A:180:ASN:O	1:A:192:ARG:HB2	2.19	0.42
1:B:34:THR:HG21	1:D:168:GLN:O	2.18	0.42
1:E:20:THR:O	1:E:40:THR:HA	2.18	0.42
1:E:32:ASN:OD1	1:E:61:MET:HB2	2.19	0.42
1:F:162:LYS:O	1:F:177:VAL:HA	2.19	0.42
1:A:62:LYS:HE2	1:A:233:GLY:HA2	2.01	0.42
1:B:185:GLN:HE21	1:B:185:GLN:HB2	1.48	0.42
1:C:270:PHE:C	1:C:272:PHE:H	2.23	0.42
1:D:18:THR:O	1:D:19:HIS:CB	2.67	0.42
1:D:297:ASP:HB3	1:D:300:ASN:C	2.40	0.42
1:E:199:TYR:O	1:E:278:VAL:HG13	2.20	0.42
1:G:102:ARG:HB3	1:G:243:ILE:O	2.20	0.42
1:A:20:THR:HG21	1:A:41:PHE:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:PHE:CE1	1:C:226:LEU:HD22	2.54	0.42
1:D:63:ALA:O	1:D:65:PRO:HD3	2.18	0.42
1:F:119:SER:HA	1:F:150:TRP:CD1	2.54	0.42
1:F:250:GLN:HG3	1:F:297:ASP:HA	2.00	0.42
1:G:51:ILE:HG22	1:G:243:ILE:CG1	2.49	0.42
1:B:49:LYS:HB3	1:B:244:SER:O	2.19	0.42
1:B:127:GLY:HA2	1:B:141:GLU:O	2.20	0.42
1:C:57:THR:HA	1:C:236:PRO:O	2.20	0.42
1:D:209:THR:HB	1:D:210:TYR:H	1.67	0.42
1:D:267:ARG:NH1	1:D:270:PHE:CZ	2.87	0.42
1:D:274:THR:O	1:D:275:GLY:C	2.56	0.42
1:E:120:SER:HA	1:F:151:SER:HA	2.01	0.42
1:E:168:GLN:NE2	1:E:173:VAL:HB	2.34	0.42
1:F:124:GLN:HA	1:G:146:GLY:O	2.20	0.42
1:C:38:LYS:N	1:C:55:ASN:O	2.53	0.42
1:D:160:SER:HB3	1:D:227:PRO:HB3	2.01	0.42
1:E:75:TYR:N	1:E:76:PRO:HD3	2.35	0.42
1:A:28:GLU:HB2	1:A:33:MET:HB2	2.01	0.42
1:B:101:SER:OG	1:B:244:SER:HA	2.19	0.42
1:C:90:TYR:CE2	1:C:259:LYS:HG2	2.54	0.42
1:D:158:GLN:OE1	1:D:180:ASN:HB2	2.20	0.42
1:D:158:GLN:C	1:D:160:SER:H	2.21	0.42
1:E:14:GLN:HB2	1:F:19:HIS:CD2	2.54	0.42
1:D:84:LEU:HD11	1:D:264:TYR:HB3	2.02	0.42
1:D:272:PHE:O	1:D:274:THR:N	2.53	0.42
1:D:302:LYS:HD2	1:D:302:LYS:HA	1.48	0.42
1:F:91:ASP:HA	1:F:175:TRP:O	2.20	0.42
1:C:51:ILE:HA	1:C:243:ILE:HG13	2.02	0.42
1:C:166:ILE:HB	1:C:176:ASN:OD1	2.20	0.42
1:D:23:ASN:ND2	1:D:37:LEU:O	2.46	0.42
1:F:21:SER:HG	1:F:38:LYS:HZ2	1.56	0.42
1:F:166:ILE:HG13	1:F:176:ASN:CG	2.40	0.42
1:F:300:ASN:HD21	1:F:302:LYS:HD3	1.85	0.42
1:A:95:ASN:HA	1:A:172:HIS:HA	2.01	0.41
1:A:297:ASP:HB3	1:A:302:LYS:H	1.84	0.41
1:B:82:VAL:HG11	1:B:217:ARG:HA	2.01	0.41
1:C:41:PHE:CD1	1:C:301:LYS:HB3	2.55	0.41
1:C:164:ASN:HB2	1:C:176:ASN:OD1	2.20	0.41
1:F:89:GLN:HB2	1:F:260:HIS:CB	2.43	0.41
1:F:182:TYR:CE1	1:F:227:PRO:HD3	2.56	0.41
1:G:226:LEU:HD23	1:G:230:THR:HG21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:CE2	1:A:264:TYR:HB3	2.56	0.41
1:G:22:TYR:CZ	1:G:303:LEU:HB3	2.54	0.41
1:G:237:GLY:H	1:G:238:MET:CE	2.32	0.41
1:A:12:ILE:HD13	1:E:21:SER:HB2	2.02	0.41
1:A:166:ILE:HD12	1:A:176:ASN:ND2	2.35	0.41
1:B:86:TYR:HB2	1:B:264:TYR:CD1	2.55	0.41
1:B:129:ILE:HG13	1:C:142:SER:HB2	2.02	0.41
1:C:270:PHE:O	1:C:272:PHE:N	2.53	0.41
1:C:296:LEU:HG	1:C:303:LEU:HD23	2.01	0.41
1:D:191:THR:HG22	1:D:193:ASP:H	1.85	0.41
1:F:91:ASP:O	1:F:258:THR:OG1	2.23	0.41
1:F:161:TYR:CE2	1:F:179:PHE:HB2	2.55	0.41
1:A:107:ALA:HB3	1:A:239:ILE:CG1	2.51	0.41
1:A:189:ILE:CG2	1:A:196:HIS:NE2	2.84	0.41
1:B:98:ASP:HA	1:B:171:LYS:CD	2.51	0.41
1:B:102:ARG:HD2	1:B:170:ASN:CB	2.42	0.41
1:B:191:THR:OG1	1:B:192:ARG:N	2.54	0.41
1:B:205:MET:SD	1:B:277:TRP:HB3	2.60	0.41
1:C:199:TYR:HE1	1:C:276:ASN:HB3	1.85	0.41
1:E:168:GLN:O	1:F:61:MET:HE2	2.20	0.41
1:E:253:ILE:CG1	1:E:296:LEU:HD11	2.50	0.41
1:A:303:LEU:C	1:A:305:GLU:H	2.24	0.41
1:B:50:GLN:NE2	1:B:245:GLU:O	2.52	0.41
1:C:185:GLN:HE21	1:C:187:TRP:HB3	1.84	0.41
1:E:164:ASN:HB3	1:F:232:SER:OG	2.20	0.41
1:E:167:ASP:OD1	1:E:167:ASP:N	2.46	0.41
1:G:258:THR:HG22	1:G:289:THR:HG22	2.01	0.41
1:B:103:PHE:HE1	1:B:240:ALA:HB1	1.83	0.41
1:B:215:ASP:OD1	1:B:216:ALA:N	2.54	0.41
1:D:61:MET:HB2	1:G:167:ASP:HB3	2.02	0.41
1:E:51:ILE:HG13	1:E:243:ILE:HD11	2.03	0.41
1:F:102:ARG:HB3	1:F:170:ASN:CB	2.41	0.41
1:F:165:LEU:HD21	1:F:168:GLN:NE2	2.35	0.41
1:G:38:LYS:N	1:G:55:ASN:O	2.54	0.41
1:G:70:ALA:HA	1:G:71:PRO:HD3	1.94	0.41
1:A:86:TYR:HD2	1:A:264:TYR:CE2	2.39	0.41
1:D:244:SER:OG	1:D:248:THR:OG1	2.27	0.41
1:D:283:LYS:HB2	1:D:284:ASP:H	1.77	0.41
1:E:93:ALA:HB3	1:E:256:ALA:HB3	2.03	0.41
1:E:118:THR:N	1:E:151:SER:O	2.45	0.41
1:G:232:SER:HB2	1:G:233:GLY:H	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:SER:HB2	1:A:141:GLU:HB3	2.02	0.41
1:A:188:GLY:O	1:A:189:ILE:HG23	2.21	0.41
1:A:206:TYR:HB2	1:A:221:VAL:N	2.35	0.41
1:B:282:ILE:HD12	1:B:285:VAL:HG22	2.02	0.41
1:C:101:SER:O	1:C:102:ARG:HB2	2.21	0.41
1:D:34:THR:CG2	1:G:169:THR:HA	2.42	0.41
1:E:182:TYR:HE1	1:E:227:PRO:HG2	1.86	0.41
1:F:39:VAL:HA	1:F:53:VAL:O	2.20	0.41
1:A:17:LYS:HD3	1:A:17:LYS:HA	1.37	0.41
1:A:60:PHE:CE1	1:A:234:PHE:HB3	2.56	0.41
1:A:71:PRO:HB2	1:A:81:SER:HB2	2.03	0.41
1:B:104:PHE:HE1	1:B:243:ILE:HG23	1.83	0.41
1:B:214:THR:HG22	1:B:215:ASP:N	2.35	0.41
1:D:28:GLU:OE1	1:D:28:GLU:N	2.54	0.41
1:D:39:VAL:HA	1:D:53:VAL:O	2.21	0.41
1:E:86:TYR:CE2	1:E:204:PHE:HD2	2.39	0.41
1:F:169:THR:HG22	1:F:170:ASN:N	2.35	0.41
1:E:86:TYR:CD2	1:E:264:TYR:HB3	2.56	0.41
1:E:100:THR:HB	1:E:251:SER:OG	2.21	0.41
1:F:3:GLN:OE1	1:G:241:VAL:HG21	2.21	0.41
1:F:35:MET:HG2	1:F:36:SER:N	2.36	0.41
1:F:91:ASP:OD1	1:F:91:ASP:N	2.53	0.41
1:G:101:SER:OG	1:G:171:LYS:HD3	2.21	0.41
1:G:166:ILE:HG13	1:G:176:ASN:CG	2.42	0.41
1:G:192:ARG:NH1	1:G:283:LYS:HG2	2.36	0.41
1:C:60:PHE:CE1	1:C:234:PHE:HB3	2.56	0.40
1:C:105:HIS:HB3	1:C:241:VAL:HG12	2.03	0.40
1:D:96:LEU:HA	1:D:253:ILE:HA	2.02	0.40
1:E:178:PHE:CG	1:E:179:PHE:N	2.89	0.40
1:F:120:SER:N	1:F:149:ASP:O	2.33	0.40
1:G:168:GLN:HG2	1:G:169:THR:N	2.36	0.40
1:B:82:VAL:HB	1:B:216:ALA:HB3	2.03	0.40
1:C:110:ASN:OD1	1:C:165:LEU:N	2.55	0.40
1:C:201:ASN:N	1:C:201:ASN:OD1	2.51	0.40
1:C:226:LEU:HB3	1:C:227:PRO:HD2	2.02	0.40
1:D:14:GLN:HE21	1:D:14:GLN:H	1.69	0.40
1:E:16:ALA:O	1:E:18:THR:N	2.54	0.40
1:E:104:PHE:HA	1:F:25:PHE:CE2	2.56	0.40
1:E:274:THR:O	1:E:276:ASN:ND2	2.54	0.40
1:F:134:THR:O	1:F:136:SER:N	2.55	0.40
1:A:80:ALA:C	1:A:82:VAL:N	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:H	1:A:196:HIS:CE1	2.40	0.40
1:C:62:LYS:HE2	1:C:233:GLY:HA2	2.03	0.40
1:C:85:ARG:HA	1:C:262:ASP:O	2.21	0.40
1:F:12:ILE:HD11	1:G:38:LYS:HE2	2.04	0.40
1:F:119:SER:O	1:G:151:SER:HA	2.21	0.40
1:F:188:GLY:HA3	1:F:189:ILE:HA	1.83	0.40
1:G:249:GLU:OE1	1:G:250:GLN:HB2	2.21	0.40
1:B:96:LEU:HD13	1:B:171:LYS:O	2.22	0.40
1:C:168:GLN:CB	1:C:173:VAL:HA	2.48	0.40
1:D:273:GLY:O	1:D:274:THR:C	2.60	0.40
1:D:283:LYS:O	1:D:284:ASP:C	2.59	0.40
1:E:261:ALA:N	1:E:286:ASP:O	2.52	0.40
1:A:119:SER:HA	1:A:150:TRP:CD1	2.56	0.40
1:A:189:ILE:HD12	1:A:202:GLN:HG3	2.03	0.40
1:B:184:ASN:O	1:B:185:GLN:C	2.59	0.40
1:B:202:GLN:CG	1:B:205:MET:HB3	2.51	0.40
1:D:263:ASP:OD1	1:D:263:ASP:N	2.55	0.40
1:E:3:GLN:O	1:E:5:THR:HG23	2.21	0.40
1:E:22:TYR:HB2	1:E:39:VAL:CG1	2.52	0.40
1:E:130:ASP:CB	1:E:139:SER:HB2	2.51	0.40
1:E:179:PHE:HE2	1:E:182:TYR:HH	1.66	0.40
1:F:45:PRO:HA	1:F:246:LYS:NZ	2.37	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	283/310 (91%)	222 (78%)	42 (15%)	19 (7%)	1 12
1	B	258/310 (83%)	223 (86%)	31 (12%)	4 (2%)	8 37
1	C	274/310 (88%)	231 (84%)	37 (14%)	6 (2%)	5 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	273/310 (88%)	206 (76%)	52 (19%)	15 (6%)	1 15
1	E	284/310 (92%)	235 (83%)	38 (13%)	11 (4%)	2 19
1	F	298/310 (96%)	257 (86%)	34 (11%)	7 (2%)	5 29
1	G	288/310 (93%)	247 (86%)	36 (12%)	5 (2%)	7 36
All	All	1958/2170 (90%)	1621 (83%)	270 (14%)	67 (3%)	3 21

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	98	ASP
1	A	103	PHE
1	A	104	PHE
1	A	135	PRO
1	A	189	ILE
1	A	193	ASP
1	B	185	GLN
1	C	71	PRO
1	C	105	HIS
1	D	19	HIS
1	D	98	ASP
1	D	274	THR
1	D	299	LYS
1	D	302	LYS
1	E	20	THR
1	E	78	PRO
1	E	135	PRO
1	E	275	GLY
1	F	18	THR
1	F	75	TYR
1	F	135	PRO
1	G	17	LYS
1	G	105	HIS
1	A	190	TYR
1	D	73	ASP
1	D	273	GLY
1	F	16	ALA
1	G	135	PRO
1	A	70	ALA
1	A	80	ALA
1	A	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	101	SER
1	A	185	GLN
1	B	177	VAL
1	D	212	HIS
1	D	252	SER
1	E	211	PRO
1	F	271	THR
1	A	156	TYR
1	B	105	HIS
1	C	305	GLU
1	D	13	GLY
1	D	275	GLY
1	D	306	LYS
1	E	17	LYS
1	E	18	THR
1	E	136	SER
1	E	137	GLY
1	F	13	GLY
1	G	269	GLY
1	A	13	GLY
1	A	72	VAL
1	C	18	THR
1	C	99	ASN
1	D	138	PRO
1	D	298	TRP
1	G	76	PRO
1	A	18	THR
1	A	155	SER
1	E	133	VAL
1	E	210	TYR
1	B	269	GLY
1	C	138	PRO
1	D	211	PRO
1	A	71	PRO
1	F	71	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	254/270 (94%)	230 (91%)	24 (9%)	7 23
1	B	237/270 (88%)	225 (95%)	12 (5%)	20 42
1	C	247/270 (92%)	236 (96%)	11 (4%)	23 46
1	D	242/270 (90%)	203 (84%)	39 (16%)	2 12
1	E	254/270 (94%)	238 (94%)	16 (6%)	15 36
1	F	264/270 (98%)	254 (96%)	10 (4%)	28 50
1	G	255/270 (94%)	242 (95%)	13 (5%)	20 42
All	All	1753/1890 (93%)	1628 (93%)	125 (7%)	12 33

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	95	ASN
1	A	97	GLN
1	A	100	THR
1	A	102	ARG
1	A	103	PHE
1	A	106	VAL
1	A	136	SER
1	A	162	LYS
1	A	179	PHE
1	A	183	ASN
1	A	184	ASN
1	A	189	ILE
1	A	190	TYR
1	A	191	THR
1	A	192	ARG
1	A	194	SER
1	A	225	ASP
1	A	249	GLU
1	A	267	ARG
1	A	280	ASN
1	A	283	LYS
1	A	306	LYS
1	A	307	LYS
1	B	21	SER
1	B	32	ASN
1	B	68	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	ILE
1	B	101	SER
1	B	103	PHE
1	B	185	GLN
1	B	225	ASP
1	B	234	PHE
1	B	268	PRO
1	B	270	PHE
1	B	286	ASP
1	C	21	SER
1	C	71	PRO
1	C	99	ASN
1	C	106	VAL
1	C	141	GLU
1	C	251	SER
1	C	267	ARG
1	C	299	LYS
1	C	300	ASN
1	C	301	LYS
1	C	303	LEU
1	D	12	ILE
1	D	14	GLN
1	D	21	SER
1	D	98	ASP
1	D	99	ASN
1	D	102	ARG
1	D	106	VAL
1	D	139	SER
1	D	157	ASP
1	D	162	LYS
1	D	177	VAL
1	D	193	ASP
1	D	208	ARG
1	D	209	THR
1	D	250	GLN
1	D	254	GLN
1	D	255	VAL
1	D	259	LYS
1	D	260	HIS
1	D	262	ASP
1	D	266	LEU
1	D	272	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	278	VAL
1	D	281	ASN
1	D	282	ILE
1	D	283	LYS
1	D	286	ASP
1	D	288	LYS
1	D	289	THR
1	D	291	ASN
1	D	292	LYS
1	D	296	LEU
1	D	298	TRP
1	D	299	LYS
1	D	302	LYS
1	D	303	LEU
1	D	304	VAL
1	D	307	LYS
1	D	309	SER
1	E	12	ILE
1	E	17	LYS
1	E	20	THR
1	E	55	ASN
1	E	78	PRO
1	E	135	PRO
1	E	167	ASP
1	E	187	TRP
1	E	193	ASP
1	E	210	TYR
1	E	229	LEU
1	E	243	ILE
1	E	267	ARG
1	E	268	PRO
1	E	271	THR
1	E	272	PHE
1	F	10	THR
1	F	12	ILE
1	F	91	ASP
1	F	101	SER
1	F	103	PHE
1	F	104	PHE
1	F	134	THR
1	F	158	GLN
1	F	159	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	208	ARG
1	G	15	ASN
1	G	17	LYS
1	G	34	THR
1	G	134	THR
1	G	157	ASP
1	G	162	LYS
1	G	180	ASN
1	G	187	TRP
1	G	193	ASP
1	G	232	SER
1	G	265	THR
1	G	266	LEU
1	G	280	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	180	ASN
1	A	185	GLN
1	A	201	ASN
1	A	280	ASN
1	B	185	GLN
1	C	186	ASN
1	D	14	GLN
1	D	276	ASN
1	D	300	ASN
1	E	276	ASN
1	F	168	GLN

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 oligosaccharides 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

Warning: The R factor obtained from EDS is 0.376, which does not match the depositor's R factor of 0.322. Please interpret the results in this section carefully.

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	291/310 (93%)	1.79	98 (33%)	1	2	30, 84, 154, 262	0
1	B	272/310 (87%)	1.96	90 (33%)	1	2	39, 89, 150, 256	0
1	C	284/310 (91%)	2.20	102 (35%)	1	2	30, 93, 166, 237	0
1	D	279/310 (90%)	2.74	126 (45%)	1	1	30, 82, 141, 167	0
1	E	292/310 (94%)	2.19	114 (39%)	1	2	30, 80, 134, 204	0
1	F	302/310 (97%)	1.39	66 (21%)	3	5	30, 85, 137, 197	0
1	G	292/310 (94%)	1.81	83 (28%)	1	3	43, 80, 137, 203	0
All	All	2012/2170 (92%)	2.00	679 (33%)	1	2	30, 85, 145, 262	0

All (679) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	SER	23.3
1	C	140	GLY	19.4
1	C	130	ASP	18.4
1	C	141	GLU	18.4
1	D	165	LEU	16.8
1	G	110	ASN	16.4
1	C	129	ILE	16.2
1	D	176	ASN	16.1
1	D	109	THR	14.4
1	D	175	TRP	14.3
1	C	138	PRO	13.8
1	E	231	ASN	13.6
1	D	166	ILE	13.5
1	E	59	SER	13.2
1	D	163	THR	13.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	177	VAL	12.9
1	C	139	SER	12.7
1	D	229	LEU	12.7
1	C	127	GLY	12.5
1	G	165	LEU	12.0
1	E	56	THR	11.9
1	F	232	SER	11.8
1	B	235	SER	11.7
1	D	167	ASP	11.7
1	D	90	TYR	11.5
1	C	113	GLU	11.5
1	G	164	ASN	11.4
1	E	60	PHE	11.3
1	C	283	LYS	11.2
1	E	237	GLY	11.1
1	A	192	ARG	10.9
1	D	161	TYR	10.9
1	B	234	PHE	10.7
1	B	233	GLY	10.3
1	D	60	PHE	10.3
1	E	174	LYS	10.2
1	B	137	GLY	9.9
1	E	235	SER	9.5
1	D	230	THR	9.4
1	C	131	ALA	9.4
1	C	137	GLY	9.4
1	B	232	SER	9.4
1	D	157	ASP	9.3
1	D	159	THR	9.3
1	D	239	ILE	9.2
1	D	237	GLY	9.2
1	B	161	TYR	9.2
1	C	288	LYS	9.1
1	E	173	VAL	9.1
1	G	113	GLU	9.1
1	B	31	ASP	8.9
1	C	167	ASP	8.9
1	G	98	ASP	8.9
1	E	58	GLY	8.8
1	G	97	GLN	8.8
1	F	233	GLY	8.8
1	B	60	PHE	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	32	ASN	8.7
1	A	191	THR	8.7
1	B	228	THR	8.6
1	B	229	LEU	8.6
1	D	158	GLN	8.4
1	D	174	LYS	8.4
1	G	167	ASP	8.3
1	D	178	PHE	8.3
1	G	71	PRO	8.3
1	E	234	PHE	8.2
1	D	234	PHE	8.1
1	D	92	ILE	8.1
1	E	238	MET	8.0
1	D	91	ASP	8.0
1	D	238	MET	8.0
1	F	86	TYR	7.9
1	D	156	TYR	7.9
1	D	172	HIS	7.9
1	G	9	VAL	7.9
1	E	172	HIS	7.8
1	B	163	THR	7.8
1	D	235	SER	7.7
1	G	156	TYR	7.7
1	B	64	ASN	7.7
1	B	236	PRO	7.7
1	B	133	VAL	7.6
1	B	61	MET	7.6
1	D	168	GLN	7.6
1	E	86	TYR	7.6
1	C	287	GLN	7.5
1	F	234	PHE	7.5
1	B	182	TYR	7.4
1	A	284	ASP	7.4
1	A	162	LYS	7.3
1	D	173	VAL	7.3
1	D	56	THR	7.2
1	C	166	ILE	7.2
1	F	231	ASN	7.2
1	G	105	HIS	7.1
1	A	157	ASP	7.0
1	E	165	LEU	7.0
1	E	88	SER	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	35	MET	6.9
1	E	55	ASN	6.9
1	A	163	THR	6.9
1	E	225	ASP	6.9
1	F	69	ASP	6.8
1	G	172	HIS	6.8
1	B	62	LYS	6.8
1	G	109	THR	6.8
1	A	310	ALA	6.8
1	D	160	SER	6.7
1	A	179	PHE	6.7
1	A	31	ASP	6.7
1	C	125	LEU	6.6
1	B	86	TYR	6.6
1	A	309	SER	6.6
1	B	30	ALA	6.5
1	C	114	GLU	6.5
1	G	99	ASN	6.5
1	F	155	SER	6.4
1	E	36	SER	6.4
1	B	224	ASN	6.4
1	F	180	ASN	6.4
1	G	114	GLU	6.4
1	G	145	THR	6.4
1	B	136	SER	6.3
1	F	228	THR	6.3
1	F	225	ASP	6.2
1	F	229	LEU	6.2
1	D	31	ASP	6.2
1	A	285	VAL	6.2
1	G	112	VAL	6.2
1	G	106	VAL	6.1
1	G	116	THR	6.0
1	A	90	TYR	6.0
1	D	287	GLN	6.0
1	B	231	ASN	6.0
1	F	68	SER	6.0
1	A	260	HIS	5.9
1	F	235	SER	5.9
1	D	257	TYR	5.8
1	E	257	TYR	5.8
1	E	285	VAL	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	260	HIS	5.8
1	C	182	TYR	5.8
1	A	283	LYS	5.8
1	G	93	ALA	5.8
1	G	10	THR	5.8
1	E	90	TYR	5.7
1	E	99	ASN	5.7
1	B	90	TYR	5.7
1	G	169	THR	5.7
1	C	156	TYR	5.7
1	E	182	TYR	5.7
1	D	108	PRO	5.6
1	C	142	SER	5.6
1	C	155	SER	5.6
1	C	284	ASP	5.6
1	E	38	LYS	5.6
1	D	183	ASN	5.6
1	E	114	GLU	5.6
1	C	260	HIS	5.5
1	E	204	PHE	5.5
1	E	92	ILE	5.5
1	C	163	THR	5.5
1	A	193	ASP	5.5
1	F	152	ASP	5.5
1	E	37	LEU	5.4
1	E	57	THR	5.4
1	D	171	LYS	5.4
1	C	308	GLY	5.4
1	A	105	HIS	5.4
1	B	203	LEU	5.3
1	E	112	VAL	5.3
1	A	307	LYS	5.2
1	G	153	SER	5.2
1	A	257	TYR	5.2
1	A	190	TYR	5.1
1	A	156	TYR	5.1
1	G	117	VAL	5.1
1	G	202	GLN	5.1
1	A	165	LEU	5.1
1	A	189	ILE	5.1
1	A	39	VAL	5.1
1	G	124	GLN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	139	SER	5.0
1	G	240	ALA	5.0
1	A	176	ASN	5.0
1	D	182	TYR	4.9
1	B	113	GLU	4.9
1	C	233	GLY	4.9
1	D	34	THR	4.9
1	D	236	PRO	4.9
1	E	138	PRO	4.9
1	D	62	LYS	4.9
1	C	161	TYR	4.8
1	G	94	MET	4.8
1	C	83	THR	4.8
1	G	154	VAL	4.8
1	E	255	VAL	4.8
1	D	250	GLN	4.8
1	E	105	HIS	4.8
1	E	94	MET	4.7
1	D	169	THR	4.7
1	B	46	SER	4.7
1	D	284	ASP	4.7
1	A	180	ASN	4.7
1	B	59	SER	4.7
1	E	236	PRO	4.7
1	G	170	ASN	4.7
1	F	76	PRO	4.7
1	C	176	ASN	4.7
1	F	3	GLN	4.6
1	A	164	ASN	4.6
1	G	59	SER	4.6
1	F	85	ARG	4.6
1	C	224	ASN	4.6
1	G	173	VAL	4.6
1	D	94	MET	4.6
1	A	210	TYR	4.6
1	F	92	ILE	4.6
1	G	77	ILE	4.5
1	D	89	GLN	4.5
1	A	308	GLY	4.5
1	B	230	THR	4.5
1	G	163	THR	4.5
1	D	107	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	230	THR	4.5
1	E	95	ASN	4.5
1	B	260	HIS	4.5
1	A	178	PHE	4.5
1	G	176	ASN	4.5
1	G	70	ALA	4.4
1	A	187	TRP	4.4
1	F	287	GLN	4.4
1	C	298	TRP	4.4
1	D	55	ASN	4.4
1	E	34	THR	4.4
1	G	135	PRO	4.4
1	C	259	LYS	4.4
1	C	89	GLN	4.4
1	F	2	ALA	4.4
1	A	306	LYS	4.3
1	A	277	TRP	4.3
1	C	261	ALA	4.3
1	D	300	ASN	4.3
1	F	209	THR	4.3
1	E	97	GLN	4.3
1	C	165	LEU	4.2
1	D	228	THR	4.2
1	B	89	GLN	4.2
1	A	152	ASP	4.2
1	G	290	PHE	4.2
1	D	80	ALA	4.2
1	B	48	ASP	4.2
1	D	286	ASP	4.2
1	D	233	GLY	4.2
1	E	175	TRP	4.2
1	A	66	THR	4.2
1	C	189	ILE	4.1
1	A	37	LEU	4.1
1	D	218	GLY	4.1
1	B	226	LEU	4.1
1	G	171	LYS	4.1
1	D	252	SER	4.1
1	F	185	GLN	4.1
1	F	116	THR	4.1
1	E	111	ALA	4.1
1	A	168	GLN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	168	GLN	4.1
1	C	66	THR	4.1
1	D	285	VAL	4.1
1	G	34	THR	4.1
1	D	79	GLY	4.0
1	B	223	MET	4.0
1	D	106	VAL	4.0
1	E	167	ASP	4.0
1	D	33	MET	4.0
1	B	7	GLN	4.0
1	D	98	ASP	4.0
1	D	258	THR	4.0
1	A	86	TYR	4.0
1	D	61	MET	4.0
1	D	255	VAL	4.0
1	C	299	LYS	4.0
1	A	282	ILE	4.0
1	A	154	VAL	4.0
1	B	8	VAL	3.9
1	D	259	LYS	3.9
1	E	286	ASP	3.9
1	E	220	LEU	3.9
1	F	90	TYR	3.9
1	D	164	ASN	3.9
1	E	222	PRO	3.9
1	B	130	ASP	3.8
1	B	138	PRO	3.8
1	D	203	LEU	3.8
1	D	101	SER	3.8
1	G	150	TRP	3.8
1	B	87	PRO	3.8
1	B	238	MET	3.8
1	B	10	THR	3.8
1	F	210	TYR	3.8
1	E	14	GLN	3.8
1	E	183	ASN	3.7
1	B	214	THR	3.7
1	E	13	GLY	3.7
1	C	234	PHE	3.7
1	A	175	TRP	3.7
1	G	175	TRP	3.7
1	D	95	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	111	ALA	3.7
1	G	185	GLN	3.7
1	E	98	ASP	3.6
1	A	159	THR	3.6
1	F	163	THR	3.6
1	G	61	MET	3.6
1	B	88	SER	3.6
1	F	186	ASN	3.6
1	D	249	GLU	3.6
1	G	257	TYR	3.6
1	G	178	PHE	3.6
1	B	132	SER	3.6
1	A	89	GLN	3.6
1	F	97	GLN	3.6
1	A	4	THR	3.6
1	B	12	ILE	3.5
1	B	166	ILE	3.5
1	A	88	SER	3.5
1	D	309	SER	3.5
1	F	207	SER	3.5
1	D	299	LYS	3.5
1	D	136	SER	3.5
1	A	52	ALA	3.5
1	D	35	MET	3.5
1	B	135	PRO	3.5
1	A	182	TYR	3.5
1	C	183	ASN	3.5
1	C	300	ASN	3.5
1	A	185	GLN	3.5
1	E	226	LEU	3.4
1	E	291	ASN	3.4
1	B	11	ASP	3.4
1	D	93	ALA	3.4
1	D	244	SER	3.4
1	E	166	ILE	3.4
1	F	83	THR	3.4
1	B	257	TYR	3.4
1	A	158	GLN	3.4
1	E	227	PRO	3.4
1	G	168	GLN	3.4
1	E	46	SER	3.4
1	F	13	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	3.4
1	F	182	TYR	3.4
1	E	62	LYS	3.4
1	C	23	ASN	3.3
1	C	285	VAL	3.3
1	G	21	SER	3.3
1	C	307	LYS	3.3
1	B	227	PRO	3.3
1	C	132	SER	3.3
1	A	233	GLY	3.3
1	C	164	ASN	3.3
1	F	142	SER	3.3
1	C	269	GLY	3.3
1	C	31	ASP	3.3
1	A	48	ASP	3.3
1	D	135	PRO	3.3
1	E	26	ASN	3.3
1	E	244	SER	3.2
1	C	61	MET	3.2
1	E	33	MET	3.2
1	F	40	THR	3.2
1	C	64	ASN	3.2
1	F	64	ASN	3.2
1	F	100	THR	3.2
1	D	247	ASP	3.2
1	B	5	THR	3.2
1	G	118	THR	3.2
1	B	225	ASP	3.2
1	C	109	THR	3.2
1	E	134	THR	3.2
1	G	101	SER	3.2
1	E	254	GLN	3.2
1	F	214	THR	3.2
1	F	286	ASP	3.2
1	E	67	LEU	3.2
1	F	94	MET	3.1
1	F	285	VAL	3.1
1	C	84	LEU	3.1
1	E	81	SER	3.1
1	G	72	VAL	3.1
1	E	250	GLN	3.1
1	G	92	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	141	GLU	3.1
1	D	307	LYS	3.1
1	A	194	SER	3.1
1	E	195	TYR	3.1
1	G	256	ALA	3.1
1	B	245	GLU	3.1
1	G	174	LYS	3.1
1	C	229	LEU	3.1
1	A	51	ILE	3.1
1	F	160	SER	3.1
1	G	67	LEU	3.0
1	D	78	PRO	3.0
1	E	269	GLY	3.0
1	B	50	GLN	3.0
1	G	159	THR	3.0
1	C	43	ASP	3.0
1	E	79	GLY	3.0
1	E	189	ILE	3.0
1	G	35	MET	3.0
1	E	273	GLY	3.0
1	B	216	ALA	3.0
1	C	282	ILE	3.0
1	D	77	ILE	3.0
1	C	290	PHE	3.0
1	F	135	PRO	3.0
1	A	161	TYR	3.0
1	F	141	GLU	3.0
1	F	277	TRP	3.0
1	D	256	ALA	3.0
1	F	14	GLN	3.0
1	G	123	TYR	3.0
1	E	215	ASP	3.0
1	D	220	LEU	3.0
1	C	250	GLN	2.9
1	A	54	ILE	2.9
1	G	66	THR	2.9
1	E	247	ASP	2.9
1	C	306	LYS	2.9
1	D	50	GLN	2.9
1	E	15	ASN	2.9
1	F	12	ILE	2.9
1	B	56	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	115	THR	2.9
1	F	230	THR	2.9
1	D	187	TRP	2.9
1	D	88	SER	2.9
1	A	205	MET	2.9
1	D	245	GLU	2.9
1	E	77	ILE	2.9
1	D	288	LYS	2.9
1	B	179	PHE	2.9
1	G	60	PHE	2.9
1	E	91	ASP	2.9
1	B	237	GLY	2.9
1	F	213	GLU	2.9
1	C	50	GLN	2.9
1	D	54	ILE	2.9
1	D	278	VAL	2.9
1	A	261	ALA	2.8
1	D	204	PHE	2.8
1	B	175	TRP	2.8
1	F	43	ASP	2.8
1	C	246	LYS	2.8
1	E	228	THR	2.8
1	B	247	ASP	2.8
1	E	180	ASN	2.8
1	C	286	ASP	2.8
1	F	153	SER	2.8
1	D	289	THR	2.8
1	E	197	ALA	2.8
1	C	263	ASP	2.8
1	B	49	LYS	2.8
1	E	179	PHE	2.8
1	C	256	ALA	2.8
1	C	67	LEU	2.8
1	A	94	MET	2.8
1	C	301	LYS	2.8
1	E	280	ASN	2.8
1	C	203	LEU	2.8
1	B	243	ILE	2.8
1	E	261	ALA	2.8
1	C	248	THR	2.7
1	D	57	THR	2.7
1	D	48	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	235	SER	2.7
1	F	127	GLY	2.7
1	C	232	SER	2.7
1	E	139	SER	2.7
1	G	152	ASP	2.7
1	E	283	LYS	2.7
1	A	204	PHE	2.7
1	G	278	VAL	2.7
1	E	89	GLN	2.7
1	B	265	THR	2.7
1	G	91	ASP	2.7
1	D	304	VAL	2.7
1	G	181	GLY	2.7
1	B	108	PRO	2.7
1	C	118	THR	2.7
1	E	5	THR	2.7
1	A	170	ASN	2.7
1	E	208	ARG	2.6
1	F	72	VAL	2.6
1	E	10	THR	2.6
1	A	224	ASN	2.6
1	A	202	GLN	2.6
1	B	242	VAL	2.6
1	D	251	SER	2.6
1	A	188	GLY	2.6
1	D	74	GLY	2.6
1	C	247	ASP	2.6
1	D	301	LYS	2.6
1	C	277	TRP	2.6
1	A	262	ASP	2.6
1	A	305	GLU	2.6
1	A	32	ASN	2.5
1	D	246	LYS	2.5
1	E	274	THR	2.5
1	B	183	ASN	2.5
1	C	110	ASN	2.5
1	G	125	LEU	2.5
1	C	20	THR	2.5
1	D	290	PHE	2.5
1	D	49	LYS	2.5
1	B	276	ASN	2.5
1	A	69	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	SER	2.5
1	C	21	SER	2.5
1	C	289	THR	2.5
1	A	91	ASP	2.5
1	B	91	ASP	2.5
1	C	119	SER	2.5
1	E	284	ASP	2.5
1	C	206	TYR	2.5
1	C	302	LYS	2.5
1	A	40	THR	2.5
1	B	34	THR	2.5
1	C	87	PRO	2.5
1	E	270	PHE	2.5
1	C	168	GLN	2.5
1	D	184	ASN	2.5
1	A	220	LEU	2.4
1	E	12	ILE	2.5
1	D	308	GLY	2.4
1	A	104	PHE	2.4
1	B	273	GLY	2.4
1	D	180	ASN	2.4
1	B	100	THR	2.4
1	B	81	SER	2.4
1	B	244	SER	2.4
1	C	220	LEU	2.4
1	D	162	LYS	2.4
1	D	190	TYR	2.4
1	E	243	ILE	2.4
1	C	158	GLN	2.4
1	G	158	GLN	2.4
1	A	216	ALA	2.4
1	A	294	PHE	2.4
1	B	284	ASP	2.4
1	D	72	VAL	2.4
1	F	62	LYS	2.4
1	F	84	LEU	2.4
1	A	155	SER	2.4
1	B	16	ALA	2.4
1	E	54	ILE	2.4
1	F	211	PRO	2.4
1	G	268	PRO	2.4
1	E	73	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	167	ASP	2.4
1	E	294	PHE	2.4
1	A	75	TYR	2.4
1	C	227	PRO	2.4
1	B	110	ASN	2.4
1	C	262	ASP	2.4
1	G	80	ALA	2.3
1	F	161	TYR	2.3
1	B	192	ARG	2.3
1	E	209	THR	2.3
1	F	284	ASP	2.3
1	G	144	ALA	2.3
1	A	203	LEU	2.3
1	E	246	LYS	2.3
1	G	76	PRO	2.3
1	A	302	LYS	2.3
1	E	171	LYS	2.3
1	D	36	SER	2.3
1	D	181	GLY	2.3
1	D	302	LYS	2.3
1	C	105	HIS	2.3
1	D	217	ARG	2.3
1	E	258	THR	2.3
1	D	53	VAL	2.3
1	A	122	SER	2.3
1	C	150	TRP	2.3
1	D	291	ASN	2.3
1	F	219	ASN	2.3
1	C	19	HIS	2.3
1	A	181	GLY	2.3
1	D	274	THR	2.3
1	C	170	ASN	2.3
1	C	174	LYS	2.3
1	G	183	ASN	2.3
1	C	194	SER	2.3
1	D	279	GLY	2.3
1	C	76	PRO	2.2
1	D	76	PRO	2.2
1	G	281	ASN	2.2
1	C	60	PHE	2.2
1	D	208	ARG	2.2
1	B	283	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	303	LEU	2.2
1	C	22	TYR	2.2
1	E	48	ASP	2.2
1	E	297	ASP	2.2
1	C	126	GLY	2.2
1	C	177	VAL	2.2
1	B	35	MET	2.2
1	E	87	PRO	2.2
1	E	248	THR	2.2
1	D	28	GLU	2.2
1	A	64	ASN	2.2
1	A	259	LYS	2.2
1	A	209	THR	2.2
1	F	133	VAL	2.2
1	D	179	PHE	2.2
1	F	105	HIS	2.2
1	B	13	GLY	2.2
1	B	115	THR	2.2
1	B	80	ALA	2.2
1	E	245	GLU	2.2
1	A	137	GLY	2.2
1	A	5	THR	2.2
1	C	69	ASP	2.2
1	C	159	THR	2.2
1	C	162	LYS	2.2
1	D	214	THR	2.2
1	B	246	LYS	2.2
1	B	73	ASP	2.2
1	A	92	ILE	2.1
1	D	59	SER	2.1
1	F	29	GLN	2.1
1	A	70	ALA	2.1
1	B	248	THR	2.1
1	E	260	HIS	2.1
1	A	174	LYS	2.1
1	A	87	PRO	2.1
1	E	50	GLN	2.1
1	E	113	GLU	2.1
1	E	181	GLY	2.1
1	D	292	LYS	2.1
1	D	306	LYS	2.1
1	G	31	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	282	ILE	2.1
1	E	78	PRO	2.1
1	G	63	ALA	2.1
1	F	299	LYS	2.1
1	G	251	SER	2.1
1	A	304	VAL	2.1
1	G	304	VAL	2.1
1	C	100	THR	2.1
1	A	84	LEU	2.1
1	B	41	PHE	2.1
1	E	188	GLY	2.1
1	D	253	ILE	2.0
1	D	305	GLU	2.0
1	A	214	THR	2.0
1	B	269	GLY	2.0
1	D	310	ALA	2.0
1	C	90	TYR	2.0
1	A	266	LEU	2.0
1	C	92	ILE	2.0
1	E	229	LEU	2.0
1	A	207	SER	2.0
1	F	88	SER	2.0
1	F	15	ASN	2.0
1	B	167	ASP	2.0
1	G	100	THR	2.0
1	E	207	SER	2.0
1	G	87	PRO	2.0
1	G	115	THR	2.0
1	G	54	ILE	2.0
1	A	35	MET	2.0
1	A	197	ALA	2.0
1	E	2	ALA	2.0
1	E	267	ARG	2.0
1	G	211	PRO	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.