Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 10:41 AM EDT

PDB ID	:	4RAP
Title	:	Crystal structure of bacterial iron-containing dodecameric glycosyltransferase TibC from enterotoxigenic E.coli H10407
Authors	:	Yao, Q.; Lu, Q.; Xu, Y.; Shao, F.
Deposited on	:	2014-09-10
Resolution	:	2.88 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:

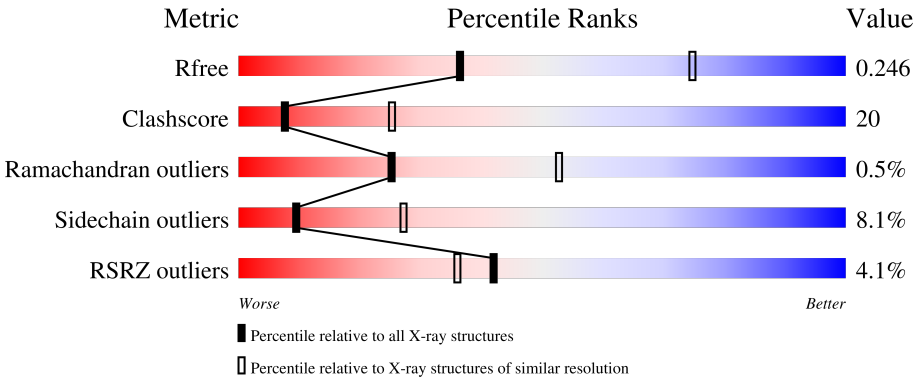
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 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.



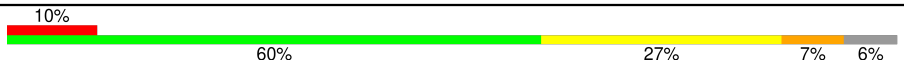
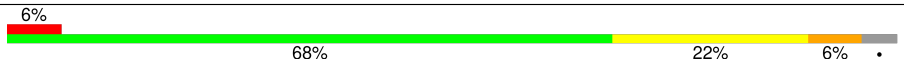
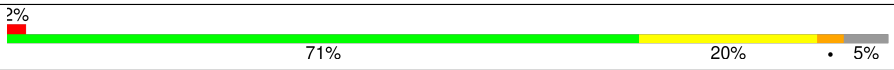
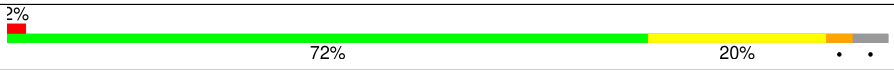
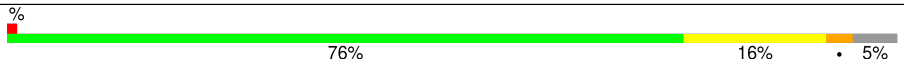
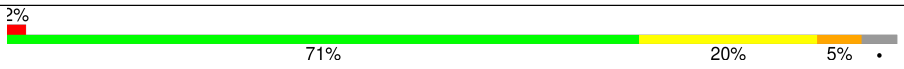
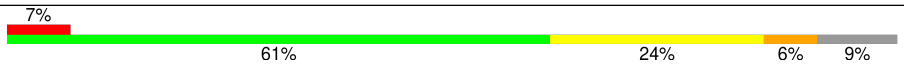
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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	406	2% 67% 23% • 6%
1	B	406	4% 70% 19% 5% 6%
1	C	406	3% 70% 21% 5% •
1	D	406	4% 67% 20% 6% 6%
1	E	406	3% 67% 24% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	406	
1	G	406	
1	H	406	
1	I	406	
1	J	406	
1	K	406	
1	L	406	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 37131 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 Glycosyltransferase TibC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	Se	0	0	0
			3069	1976	536	544	11	2			
1	B	383	Total	C	N	O	S	Se	0	0	0
			3085	1988	538	546	11	2			
1	C	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	D	381	Total	C	N	O	S	Se	0	0	0
			3067	1974	536	544	11	2			
1	E	390	Total	C	N	O	S	Se	0	0	0
			3132	2014	546	559	11	2			
1	F	382	Total	C	N	O	S	Se	0	0	0
			3071	1976	537	545	11	2			
1	G	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	H	385	Total	C	N	O	S	Se	0	0	0
			3096	1991	541	551	11	2			
1	I	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	J	384	Total	C	N	O	S	Se	0	0	0
			3092	1989	540	550	11	2			
1	K	389	Total	C	N	O	S	Se	0	0	0
			3124	2008	545	558	11	2			
1	L	371	Total	C	N	O	S	Se	0	0	0
			2988	1923	522	530	11	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	GLU	engineered mutation	UNP Q9S4K6
A	84	ALA	GLU	engineered mutation	UNP Q9S4K6
A	215	ALA	GLN	engineered mutation	UNP Q9S4K6
A	216	ALA	GLU	engineered mutation	UNP Q9S4K6
A	400	ALA	LYS	engineered mutation	UNP Q9S4K6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	ALA	LYS	engineered mutation	UNP Q9S4K6
B	83	ALA	GLU	engineered mutation	UNP Q9S4K6
B	84	ALA	GLU	engineered mutation	UNP Q9S4K6
B	215	ALA	GLN	engineered mutation	UNP Q9S4K6
B	216	ALA	GLU	engineered mutation	UNP Q9S4K6
B	400	ALA	LYS	engineered mutation	UNP Q9S4K6
B	401	ALA	LYS	engineered mutation	UNP Q9S4K6
C	83	ALA	GLU	engineered mutation	UNP Q9S4K6
C	84	ALA	GLU	engineered mutation	UNP Q9S4K6
C	215	ALA	GLN	engineered mutation	UNP Q9S4K6
C	216	ALA	GLU	engineered mutation	UNP Q9S4K6
C	400	ALA	LYS	engineered mutation	UNP Q9S4K6
C	401	ALA	LYS	engineered mutation	UNP Q9S4K6
D	83	ALA	GLU	engineered mutation	UNP Q9S4K6
D	84	ALA	GLU	engineered mutation	UNP Q9S4K6
D	215	ALA	GLN	engineered mutation	UNP Q9S4K6
D	216	ALA	GLU	engineered mutation	UNP Q9S4K6
D	400	ALA	LYS	engineered mutation	UNP Q9S4K6
D	401	ALA	LYS	engineered mutation	UNP Q9S4K6
E	83	ALA	GLU	engineered mutation	UNP Q9S4K6
E	84	ALA	GLU	engineered mutation	UNP Q9S4K6
E	215	ALA	GLN	engineered mutation	UNP Q9S4K6
E	216	ALA	GLU	engineered mutation	UNP Q9S4K6
E	400	ALA	LYS	engineered mutation	UNP Q9S4K6
E	401	ALA	LYS	engineered mutation	UNP Q9S4K6
F	83	ALA	GLU	engineered mutation	UNP Q9S4K6
F	84	ALA	GLU	engineered mutation	UNP Q9S4K6
F	215	ALA	GLN	engineered mutation	UNP Q9S4K6
F	216	ALA	GLU	engineered mutation	UNP Q9S4K6
F	400	ALA	LYS	engineered mutation	UNP Q9S4K6
F	401	ALA	LYS	engineered mutation	UNP Q9S4K6
G	83	ALA	GLU	engineered mutation	UNP Q9S4K6
G	84	ALA	GLU	engineered mutation	UNP Q9S4K6
G	215	ALA	GLN	engineered mutation	UNP Q9S4K6
G	216	ALA	GLU	engineered mutation	UNP Q9S4K6
G	400	ALA	LYS	engineered mutation	UNP Q9S4K6
G	401	ALA	LYS	engineered mutation	UNP Q9S4K6
H	83	ALA	GLU	engineered mutation	UNP Q9S4K6
H	84	ALA	GLU	engineered mutation	UNP Q9S4K6
H	215	ALA	GLN	engineered mutation	UNP Q9S4K6
H	216	ALA	GLU	engineered mutation	UNP Q9S4K6
H	400	ALA	LYS	engineered mutation	UNP Q9S4K6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	401	ALA	LYS	engineered mutation	UNP Q9S4K6
I	83	ALA	GLU	engineered mutation	UNP Q9S4K6
I	84	ALA	GLU	engineered mutation	UNP Q9S4K6
I	215	ALA	GLN	engineered mutation	UNP Q9S4K6
I	216	ALA	GLU	engineered mutation	UNP Q9S4K6
I	400	ALA	LYS	engineered mutation	UNP Q9S4K6
I	401	ALA	LYS	engineered mutation	UNP Q9S4K6
J	83	ALA	GLU	engineered mutation	UNP Q9S4K6
J	84	ALA	GLU	engineered mutation	UNP Q9S4K6
J	215	ALA	GLN	engineered mutation	UNP Q9S4K6
J	216	ALA	GLU	engineered mutation	UNP Q9S4K6
J	400	ALA	LYS	engineered mutation	UNP Q9S4K6
J	401	ALA	LYS	engineered mutation	UNP Q9S4K6
K	83	ALA	GLU	engineered mutation	UNP Q9S4K6
K	84	ALA	GLU	engineered mutation	UNP Q9S4K6
K	215	ALA	GLN	engineered mutation	UNP Q9S4K6
K	216	ALA	GLU	engineered mutation	UNP Q9S4K6
K	400	ALA	LYS	engineered mutation	UNP Q9S4K6
K	401	ALA	LYS	engineered mutation	UNP Q9S4K6
L	83	ALA	GLU	engineered mutation	UNP Q9S4K6
L	84	ALA	GLU	engineered mutation	UNP Q9S4K6
L	215	ALA	GLN	engineered mutation	UNP Q9S4K6
L	216	ALA	GLU	engineered mutation	UNP Q9S4K6
L	400	ALA	LYS	engineered mutation	UNP Q9S4K6
L	401	ALA	LYS	engineered mutation	UNP Q9S4K6

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

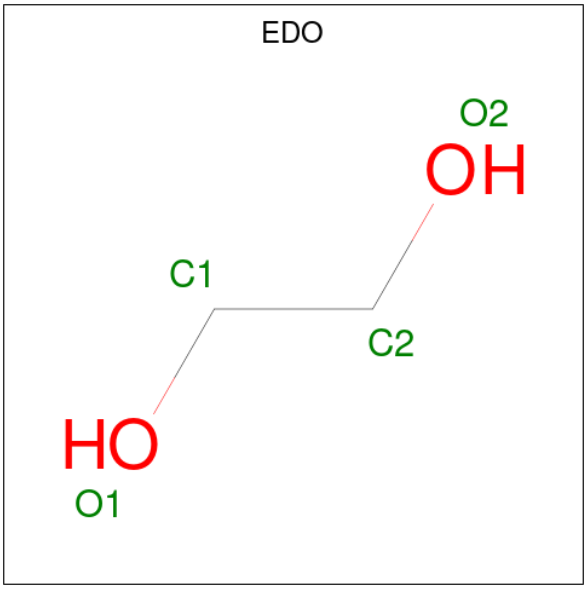
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

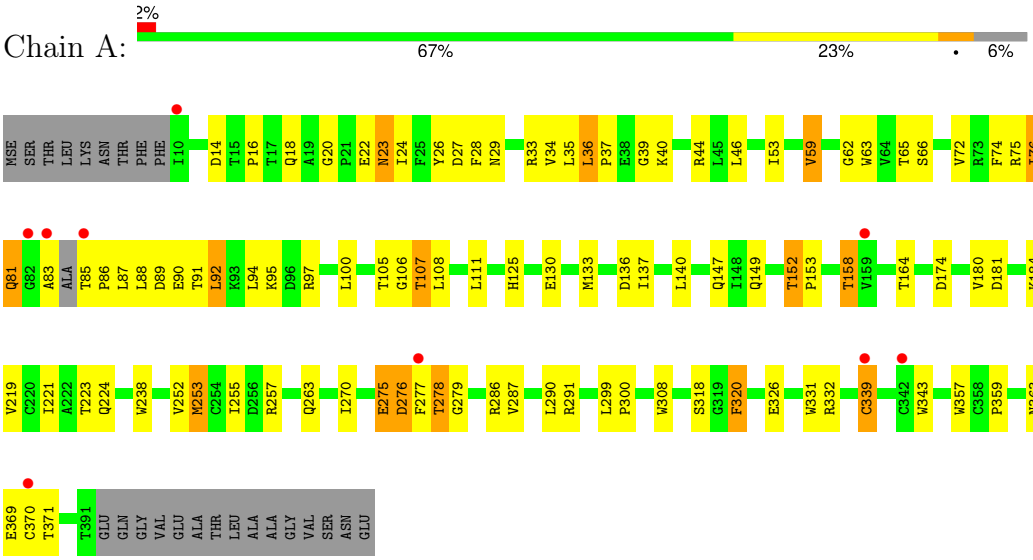
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	J	1	Total O 1 1	0	0

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.

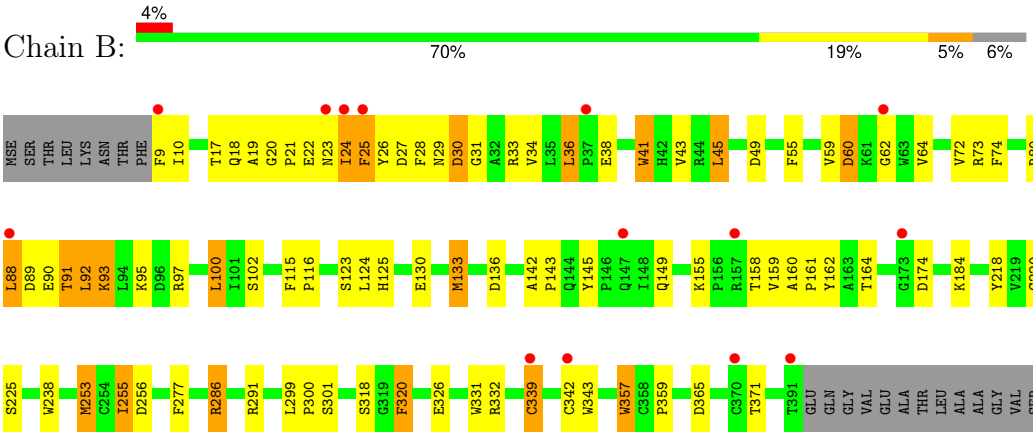
• Molecule 1: Glycosyltransferase TibC

Chain A:



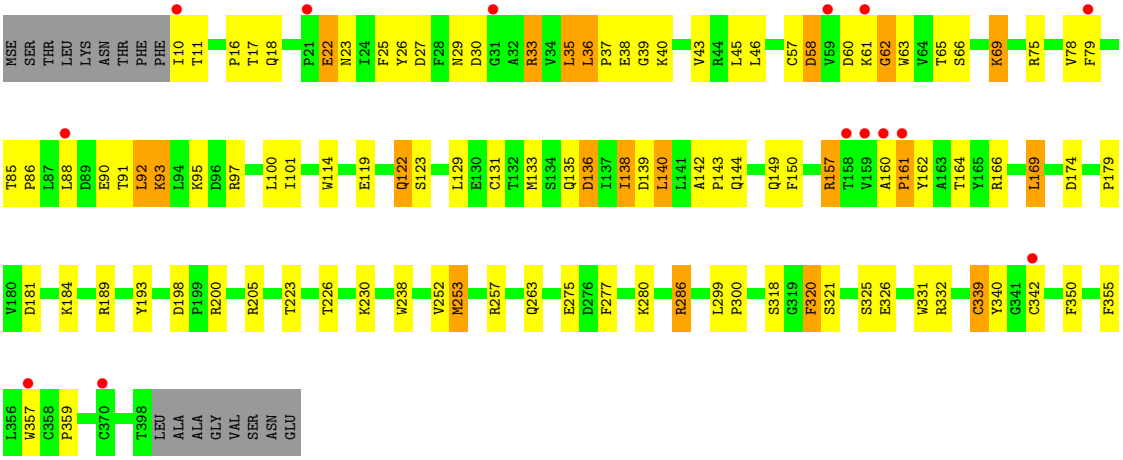
• Molecule 1: Glycosyltransferase TibC

Chain B:



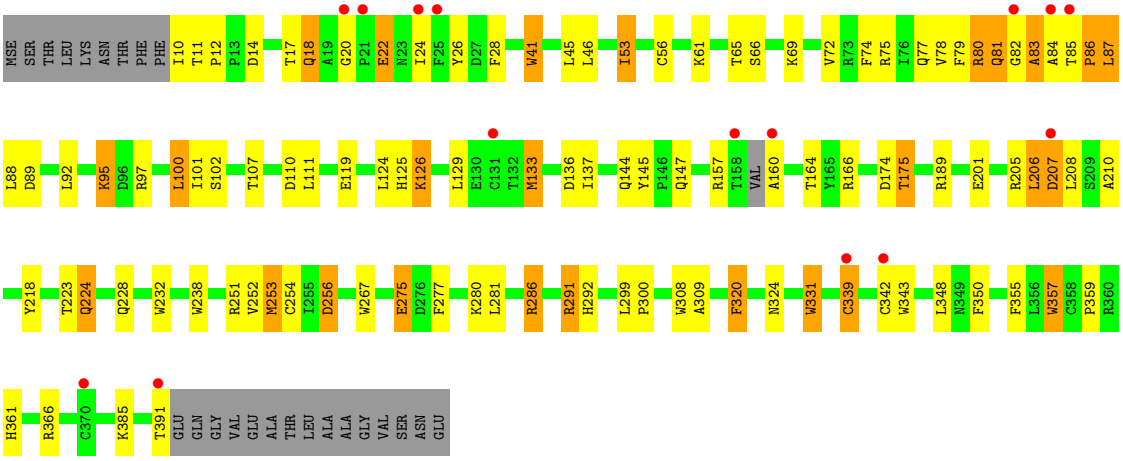
• Molecule 1: Glycosyltransferase TibC

Chain C:



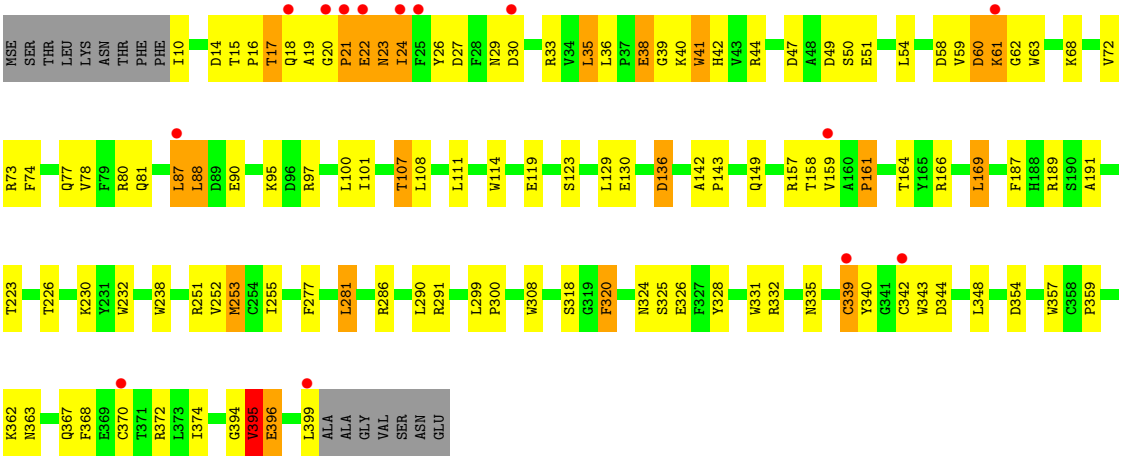
• Molecule 1: Glycosyltransferase TibC

Chain D:



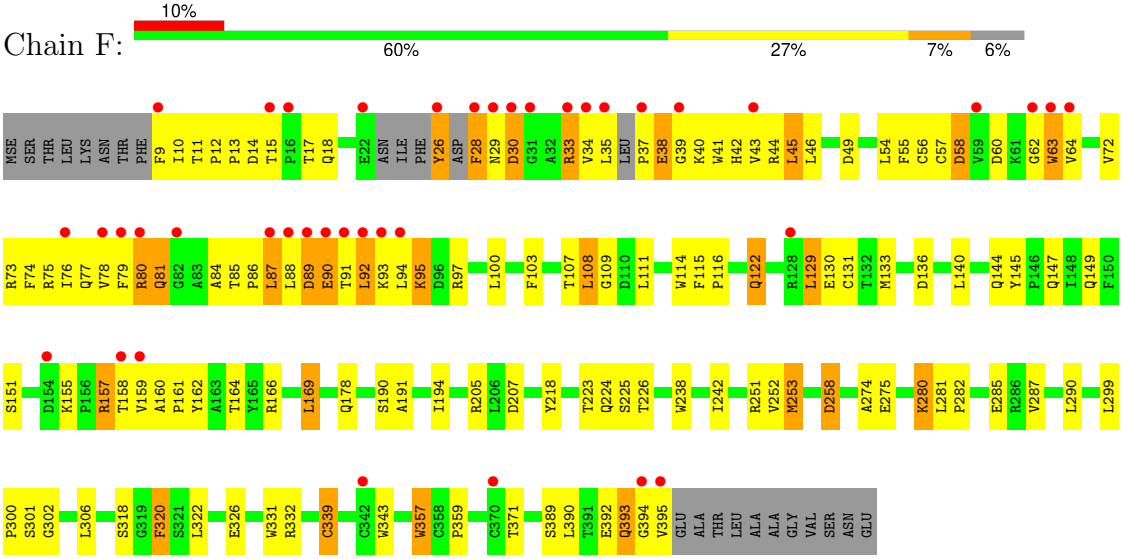
• Molecule 1: Glycosyltransferase TibC

Chain E:



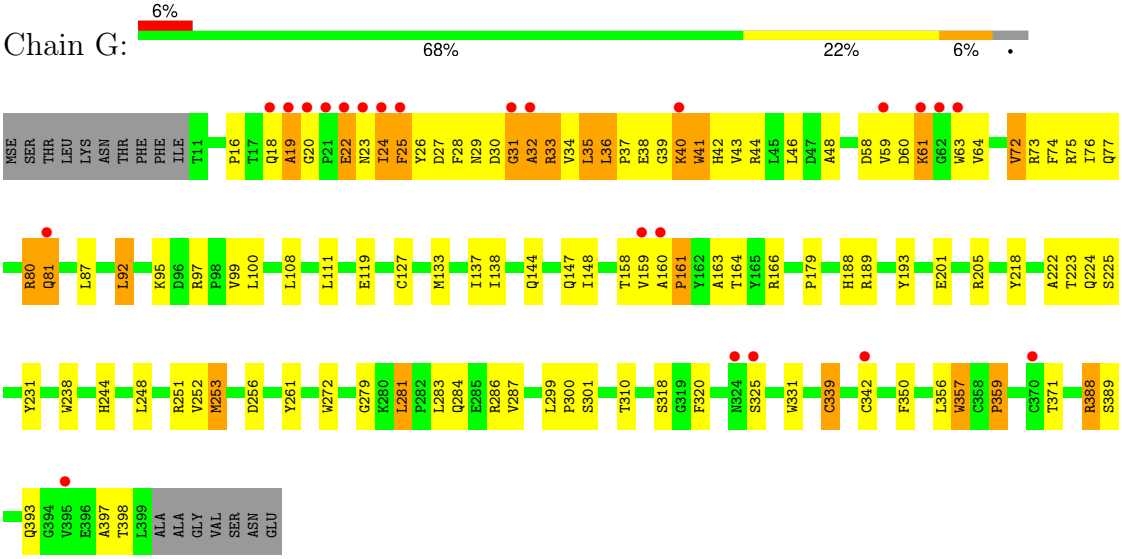
• Molecule 1: Glycosyltransferase TibC

Chain F:



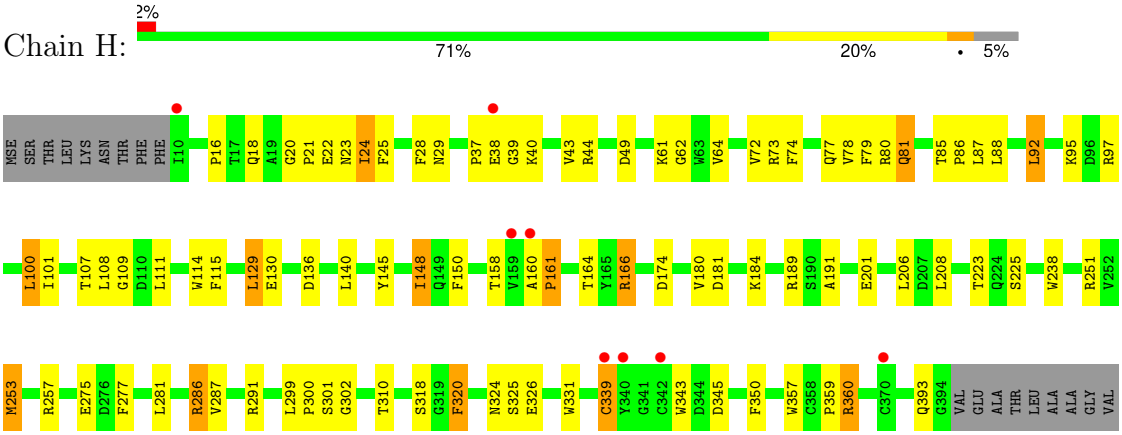
• Molecule 1: Glycosyltransferase TibC

Chain G:



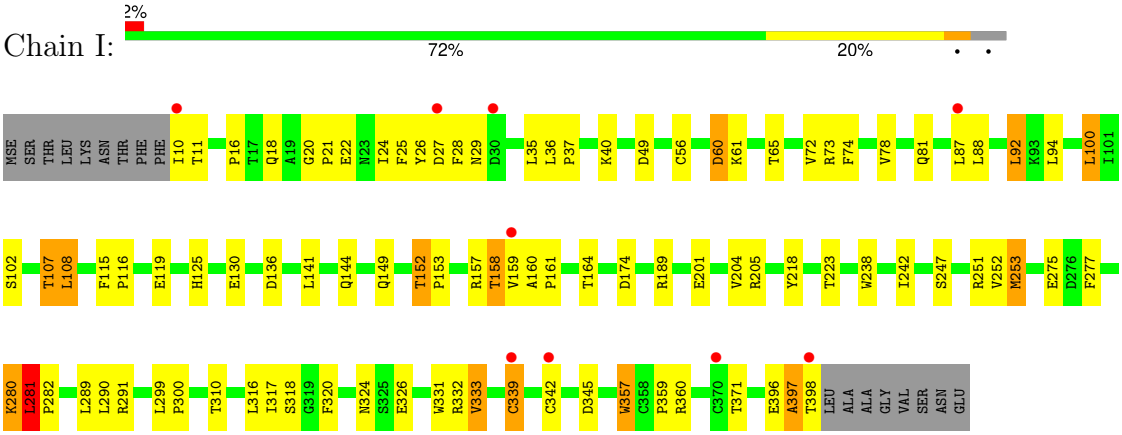
• Molecule 1: Glycosyltransferase TibC

Chain H:



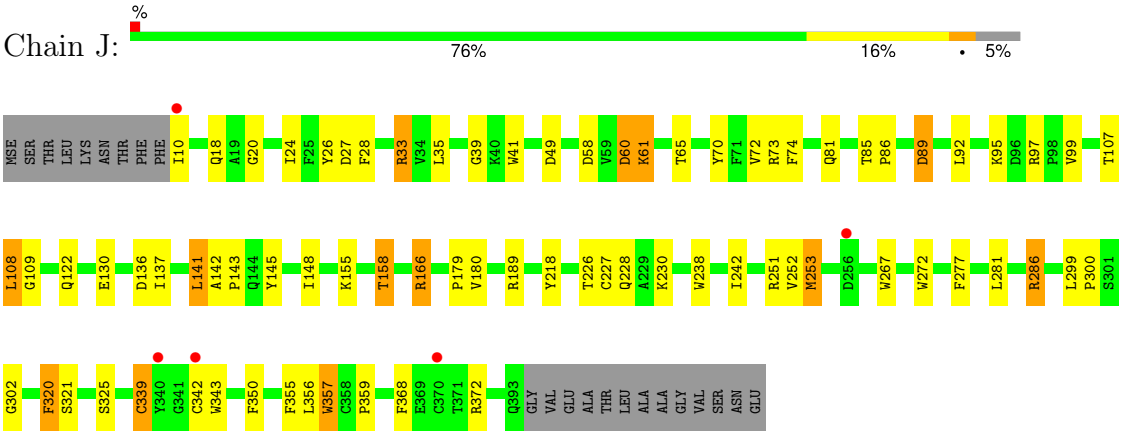
• Molecule 1: Glycosyltransferase TibC

Chain I:



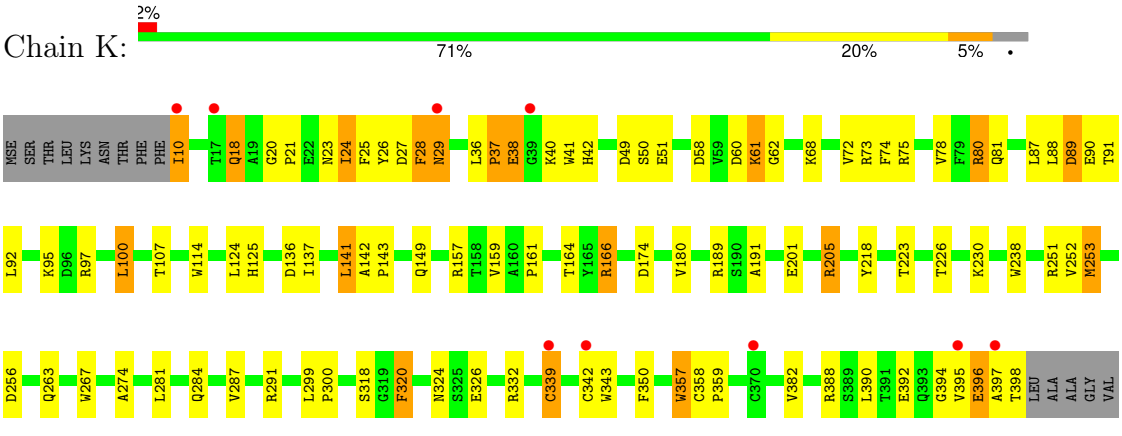
• Molecule 1: Glycosyltransferase TibC

Chain J:



• Molecule 1: Glycosyltransferase TibC

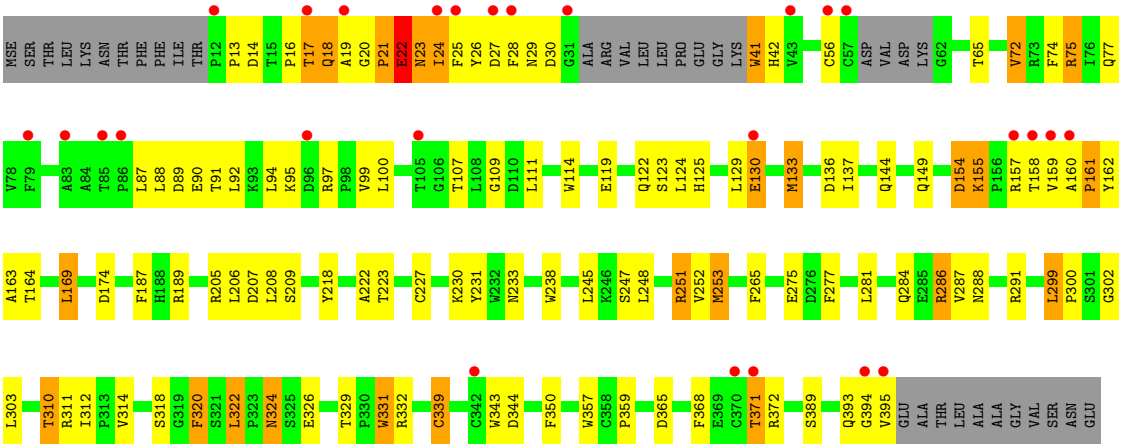
Chain K:



• Molecule 1: Glycosyltransferase TibC

Chain L:


7%
61%
24%
6%
9%


MSE SER THR LEU LYS ASN THR PHE PHE ILE THR P12 P13 D14 T15 P16 T17 Q18 A19 G20 P21 E22 N23 I24 F25 Y26 D27 F28 N29 D30 G31 ALA ARG VAL LEU LEU PRO GLU GLY LYS W41 H42 V43 C56 C57 ASP VAL ASP LYS G62 T65 V72 R73 F74 R75 I76 Q77
V78 F79 A83 A84 T85 P86 L87 L88 D89 E90 T91 L92 K93 L94 K95 D96 R97 P98 V99 L100 T105 G106 T107 L108 G109 D110 L111 W114 E119 Q122 S123 L124 H125 L129 E130 M133 D136 I137 Q144 Q149 D154 K155 P156 R157 T158 V159 A160 P161 Y162
A163 T164 L169 D174 F187 H188 R189 R205 L206 D207 L208 S209 Y218 A222 T223 C227 K230 Y231 W232 N233 W238 L245 K246 S247 L248 R251 V252 M253 F265 E275 D276 F277 L281 Q284 E285 R286 V287 N288 R291 L299 P300 S301 G302
L303 T310 R311 I312 P313 V314 S318 G319 F320 S321 L322 P323 N324 S325 E326 T329 P330 W331 R332 C339 C342 W343 D344 F350 W357 C358 P359 D365 F368 E369 C370 T371 R372 S389 Q393 G394 V395 GLU ALA THR LEU ALA ALA GLY VAL SER ASN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.79Å 314.37Å 164.53Å 90.00° 101.44° 90.00°	Depositor
Resolution (Å)	19.92 – 2.88 19.92 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.92-2.88) 99.0 (19.92-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.208 , 0.245 0.212 , 0.246	Depositor DCC
R_{free} test set	9781 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	37131	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

Bond lengths and bond angles in the following residue types are not validated in this section: FE, EDO

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	0.66	3/3164 (0.1%)	0.65	2/4310 (0.0%)
1	B	0.67	4/3182 (0.1%)	0.66	1/4336 (0.0%)
1	C	0.71	3/3220 (0.1%)	0.67	2/4388 (0.0%)
1	D	0.68	7/3162 (0.2%)	0.67	1/4307 (0.0%)
1	E	0.73	7/3228 (0.2%)	0.69	1/4399 (0.0%)
1	F	0.66	3/3164 (0.1%)	0.68	1/4305 (0.0%)
1	G	0.65	5/3220 (0.2%)	0.67	1/4388 (0.0%)
1	H	0.65	2/3192 (0.1%)	0.64	0/4349
1	I	0.66	5/3220 (0.2%)	0.64	1/4388 (0.0%)
1	J	0.70	5/3188 (0.2%)	0.68	1/4344 (0.0%)
1	K	0.74	6/3220 (0.2%)	0.74	8/4388 (0.2%)
1	L	0.69	3/3081 (0.1%)	0.68	2/4195 (0.0%)
All	All	0.68	53/38241 (0.1%)	0.67	21/52097 (0.0%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	29	ASN	C-O	-11.69	1.01	1.23
1	K	29	ASN	C-N	7.71	1.51	1.34
1	C	331	TRP	CD2-CE2	6.96	1.49	1.41
1	L	339	CYS	CB-SG	6.73	1.93	1.82
1	E	232	TRP	CD2-CE2	6.44	1.49	1.41
1	E	339	CYS	CB-SG	6.38	1.93	1.82
1	E	342	CYS	CB-SG	6.34	1.93	1.82
1	J	272	TRP	CD2-CE2	6.20	1.48	1.41
1	J	357	TRP	CD2-CE2	6.12	1.48	1.41
1	B	342	CYS	CB-SG	6.09	1.92	1.82
1	E	370	CYS	CB-SG	5.96	1.92	1.82
1	I	357	TRP	CD2-CE2	5.92	1.48	1.41
1	E	331	TRP	CD2-CE2	5.91	1.48	1.41
1	G	342	CYS	CB-SG	5.84	1.92	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	308	TRP	CD2-CE2	5.84	1.48	1.41
1	G	339	CYS	CB-SG	5.79	1.92	1.82
1	C	339	CYS	CB-SG	5.77	1.92	1.82
1	I	331	TRP	CD2-CE2	5.76	1.48	1.41
1	I	342	CYS	CB-SG	5.75	1.92	1.82
1	D	331	TRP	CD2-CE2	5.74	1.48	1.41
1	G	331	TRP	CD2-CE2	5.70	1.48	1.41
1	C	342	CYS	CB-SG	5.64	1.91	1.82
1	J	267	TRP	CD2-CE2	5.51	1.48	1.41
1	F	63	TRP	CD2-CE2	5.49	1.48	1.41
1	K	339	CYS	CB-SG	5.46	1.91	1.82
1	F	357	TRP	CD2-CE2	5.45	1.47	1.41
1	D	232	TRP	CD2-CE2	5.44	1.47	1.41
1	K	357	TRP	CD2-CE2	5.42	1.47	1.41
1	D	308	TRP	CD2-CE2	5.41	1.47	1.41
1	K	267	TRP	CD2-CE2	5.38	1.47	1.41
1	G	272	TRP	CD2-CE2	5.36	1.47	1.41
1	A	331	TRP	CD2-CE2	5.34	1.47	1.41
1	B	357	TRP	CD2-CE2	5.33	1.47	1.41
1	F	331	TRP	CD2-CE2	5.32	1.47	1.41
1	G	357	TRP	CD2-CE2	5.32	1.47	1.41
1	H	339	CYS	CB-SG	5.27	1.91	1.82
1	K	342	CYS	CB-SG	5.26	1.91	1.82
1	D	342	CYS	CB-SG	5.25	1.91	1.82
1	A	308	TRP	CD2-CE2	5.25	1.47	1.41
1	D	267	TRP	CD2-CE2	5.23	1.47	1.41
1	I	339	CYS	CB-SG	5.22	1.91	1.82
1	B	41	TRP	CD2-CE2	5.21	1.47	1.41
1	J	238	TRP	CD2-CE2	5.21	1.47	1.41
1	D	357	TRP	CD2-CE2	5.18	1.47	1.41
1	E	41	TRP	CD2-CE2	5.16	1.47	1.41
1	L	331	TRP	CD2-CE2	5.16	1.47	1.41
1	A	370	CYS	CB-SG	5.12	1.91	1.82
1	H	331	TRP	CD2-CE2	5.12	1.47	1.41
1	J	342	CYS	CA-CB	5.11	1.65	1.53
1	D	86	PRO	N-CD	5.10	1.54	1.47
1	L	13	PRO	N-CD	5.05	1.54	1.47
1	I	342	CYS	CA-CB	5.04	1.65	1.53
1	B	331	TRP	CD2-CE2	5.04	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	29	ASN	CA-C-O	12.00	145.29	120.10
1	K	29	ASN	O-C-N	-8.75	108.70	122.70
1	K	28	PHE	O-C-N	-8.01	109.89	122.70
1	C	339	CYS	CA-CB-SG	6.31	125.36	114.00
1	G	339	CYS	CA-CB-SG	6.30	125.34	114.00
1	I	281	LEU	CA-CB-CG	6.10	129.32	115.30
1	K	358	CYS	C-N-CD	5.86	140.69	128.40
1	A	39	GLY	N-CA-C	-5.83	98.52	113.10
1	K	339	CYS	CA-CB-SG	5.75	124.35	114.00
1	A	339	CYS	CA-CB-SG	5.75	124.35	114.00
1	K	28	PHE	C-N-CA	5.61	135.73	121.70
1	K	28	PHE	CA-C-N	5.55	129.42	117.20
1	J	339	CYS	CA-CB-SG	5.52	123.94	114.00
1	F	339	CYS	CA-CB-SG	5.39	123.71	114.00
1	D	339	CYS	CA-CB-SG	5.39	123.70	114.00
1	E	339	CYS	CA-CB-SG	5.36	123.65	114.00
1	B	339	CYS	CA-CB-SG	5.36	123.64	114.00
1	L	133	MSE	CB-CA-C	-5.26	99.87	110.40
1	K	29	ASN	CA-C-N	-5.24	105.67	117.20
1	L	339	CYS	CA-CB-SG	5.15	123.27	114.00
1	C	62	GLY	N-CA-C	5.05	125.73	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3069	0	2975	122	0
1	B	3085	0	2990	121	0
1	C	3124	0	3025	122	0
1	D	3067	0	2971	118	0
1	E	3132	0	3037	115	0
1	F	3071	0	2972	161	0
1	G	3124	0	3026	170	0
1	H	3096	0	2998	80	0
1	I	3124	0	3026	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3092	0	2996	74	0
1	K	3124	0	3025	96	0
1	L	2988	0	2880	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	C	4	0	6	2	0
3	I	8	0	12	0	0
3	J	4	0	6	1	0
3	L	4	0	6	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	J	1	0	0	0	0
All	All	37131	0	35951	1447	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 20.

All (1447) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MSE:HG2	1:A:277:PHE:CE2	1.42	1.53
1:J:108:LEU:HD21	1:J:302:GLY:C	1.33	1.48
1:C:138:ILE:CD1	1:C:150:PHE:HB3	1.45	1.47
1:G:24:ILE:CG2	1:G:37:PRO:HD3	1.42	1.47
1:A:253:MSE:CG	1:A:277:PHE:CE2	2.03	1.40
1:A:276:ASP:HB2	1:A:278:THR:CG2	1.48	1.39
1:L:21:PRO:CG	1:L:87:LEU:CD2	2.03	1.37
1:J:108:LEU:HD21	1:J:302:GLY:CA	1.54	1.34
1:C:138:ILE:HD11	1:C:150:PHE:CB	1.55	1.34
1:A:276:ASP:CB	1:A:278:THR:HG23	1.58	1.33
1:C:35:LEU:HD22	1:C:63:TRP:CZ3	1.62	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:GLN:HA	1:G:19:ALA:CB	1.59	1.30
1:C:85:THR:HG22	1:C:86:PRO:CD	1.60	1.30
1:H:130:GLU:OE1	1:H:158:THR:HG23	1.30	1.30
1:G:24:ILE:CG2	1:G:37:PRO:CD	2.11	1.27
1:D:206:LEU:O	1:D:208:LEU:CD1	1.81	1.27
1:L:21:PRO:CB	1:L:87:LEU:HD21	1.63	1.25
1:C:35:LEU:HA	1:C:62:GLY:O	1.37	1.24
1:F:130:GLU:OE2	1:F:157:ARG:HB2	1.32	1.24
1:L:16:PRO:HB2	1:L:25:PHE:O	1.34	1.24
1:D:83:ALA:HB1	1:D:84:ALA:CA	1.68	1.23
1:G:24:ILE:HG22	1:G:37:PRO:CD	1.69	1.23
1:J:108:LEU:CD1	1:J:302:GLY:HA3	1.65	1.23
1:F:78:VAL:HG23	1:F:88:LEU:CD1	1.68	1.21
1:B:92:LEU:HD23	1:B:92:LEU:O	1.36	1.21
1:L:133:MSE:CE	1:L:137:ILE:HB	1.72	1.20
1:F:282:PRO:HD2	1:F:285:GLU:OE2	1.43	1.19
1:G:18:GLN:O	1:G:25:PHE:HB3	1.40	1.17
1:G:32:ALA:O	1:G:33:ARG:HD3	1.43	1.17
1:K:394:GLY:HA2	1:K:395:VAL:HG22	1.27	1.16
1:L:21:PRO:HG2	1:L:87:LEU:CD2	1.70	1.16
1:J:108:LEU:CD2	1:J:302:GLY:CA	2.23	1.15
1:F:87:LEU:N	1:F:87:LEU:HD12	1.62	1.14
1:I:317:ILE:HA	1:I:333:VAL:HG23	1.16	1.14
1:G:133:MSE:HE3	1:G:137:ILE:HB	1.19	1.14
1:L:21:PRO:CG	1:L:87:LEU:HD21	1.71	1.14
1:A:76:ILE:HD12	1:A:90:GLU:O	1.44	1.13
1:F:78:VAL:CG2	1:F:88:LEU:CD1	2.25	1.13
1:F:108:LEU:HD21	1:F:302:GLY:HA3	1.20	1.13
1:I:24:ILE:HD12	1:I:37:PRO:HD3	1.29	1.13
1:A:276:ASP:HA	1:A:277:PHE:HB2	1.14	1.12
1:C:75:ARG:HG3	1:C:91:THR:HG22	1.23	1.13
1:D:83:ALA:CB	1:D:84:ALA:HA	1.64	1.12
1:J:108:LEU:HD11	1:J:302:GLY:HA3	1.19	1.12
1:L:21:PRO:HB2	1:L:87:LEU:HD21	1.18	1.12
1:A:253:MSE:CG	1:A:277:PHE:CD2	2.32	1.11
1:D:206:LEU:O	1:D:208:LEU:HD12	1.45	1.11
1:C:17:THR:CG2	1:C:160:ALA:HB1	1.81	1.10
1:K:78:VAL:HG22	1:K:88:LEU:HB2	1.19	1.10
1:L:251:ARG:HG2	1:L:253:MSE:HE1	1.18	1.10
1:F:122:GLN:HB2	1:F:129:LEU:HD23	1.34	1.09
1:J:108:LEU:CD2	1:J:302:GLY:HA3	1.80	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:THR:HG21	1:C:160:ALA:HB1	1.25	1.08
1:G:22:GLU:HG2	1:G:24:ILE:HD12	1.35	1.07
1:G:24:ILE:HB	1:G:35:LEU:O	1.53	1.07
1:F:281:LEU:HB3	1:F:285:GLU:OE2	1.54	1.07
1:G:32:ALA:O	1:G:33:ARG:CD	2.02	1.07
1:G:32:ALA:O	1:G:33:ARG:CG	2.02	1.06
1:F:26:TYR:HA	1:F:34:VAL:HA	1.11	1.06
1:L:322:LEU:HD23	1:L:344:ASP:OD2	1.54	1.06
1:A:78:VAL:HG22	1:A:88:LEU:HB3	1.36	1.06
1:J:108:LEU:HD13	1:J:109:GLY:H	1.13	1.06
1:G:18:GLN:HA	1:G:19:ALA:HB3	1.30	1.06
1:I:24:ILE:CD1	1:I:37:PRO:HD3	1.84	1.05
1:F:108:LEU:CD2	1:F:302:GLY:HA3	1.83	1.05
1:A:253:MSE:CG	1:A:277:PHE:HE2	1.51	1.05
1:G:18:GLN:CA	1:G:19:ALA:HB3	1.86	1.04
1:F:87:LEU:H	1:F:87:LEU:CD1	1.67	1.04
1:G:18:GLN:HA	1:G:19:ALA:HB2	1.36	1.04
1:F:17:THR:OG1	1:F:18:GLN:NE2	1.90	1.03
1:E:22:GLU:OE2	1:E:22:GLU:HA	1.58	1.03
1:F:78:VAL:HG23	1:F:88:LEU:HD13	1.35	1.03
1:F:79:PHE:CE1	1:F:86:PRO:HB3	1.93	1.03
1:A:253:MSE:HG3	1:A:277:PHE:CE2	1.89	1.03
1:B:21:PRO:HD3	1:B:88:LEU:HD12	1.36	1.03
1:C:85:THR:CG2	1:C:86:PRO:CD	2.37	1.02
1:I:317:ILE:HA	1:I:333:VAL:CG2	1.87	1.02
1:J:108:LEU:CD2	1:J:302:GLY:C	2.27	1.02
1:H:145:TYR:HB3	1:H:148:ILE:HD11	1.41	1.02
1:A:76:ILE:HD12	1:A:76:ILE:H	1.22	1.02
1:G:18:GLN:CA	1:G:19:ALA:CB	2.36	1.02
1:L:21:PRO:HG2	1:L:87:LEU:HD22	1.39	1.02
1:A:276:ASP:CG	1:A:278:THR:HG23	1.79	1.01
1:F:87:LEU:HD12	1:F:87:LEU:H	0.86	1.01
1:G:22:GLU:CG	1:G:24:ILE:HD12	1.89	1.01
1:K:40:LYS:HD3	1:K:60:ASP:OD1	1.59	1.01
1:A:276:ASP:HB2	1:A:278:THR:HG23	1.02	1.00
1:C:85:THR:CG2	1:C:86:PRO:HD2	1.90	1.00
1:F:79:PHE:CZ	1:F:86:PRO:HG3	1.95	1.00
1:C:10:ILE:HG23	1:C:11:THR:H	1.23	1.00
1:D:78:VAL:HG22	1:D:88:LEU:HB3	1.39	1.00
1:G:18:GLN:O	1:G:25:PHE:CB	2.08	1.00
1:L:21:PRO:HG3	1:L:87:LEU:HD23	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:OE1	1:C:39:GLY:N	1.95	0.99
1:L:233:ASN:H	1:L:371:THR:HB	1.24	0.99
1:B:34:VAL:HG12	1:B:64:VAL:CG2	1.91	0.99
1:F:78:VAL:HG23	1:F:88:LEU:HD12	1.42	0.99
1:L:21:PRO:HG3	1:L:87:LEU:CD2	1.91	0.99
1:L:19:ALA:HA	1:L:25:PHE:HA	1.42	0.98
1:D:277:PHE:O	1:D:286:ARG:NH2	1.96	0.98
1:C:85:THR:HG22	1:C:86:PRO:HD2	1.01	0.98
1:A:83:ALA:C	1:A:85:THR:N	2.17	0.98
1:G:23:ASN:O	1:G:25:PHE:CE1	2.16	0.97
1:K:10:ILE:O	1:K:166:ARG:NH1	1.97	0.97
1:A:253:MSE:HG2	1:A:277:PHE:CD2	1.99	0.97
1:J:108:LEU:CG	1:J:302:GLY:HA3	1.93	0.97
1:G:24:ILE:CG2	1:G:36:LEU:HA	1.94	0.97
1:G:34:VAL:CG2	1:G:64:VAL:CG1	2.42	0.97
1:A:133:MSE:CE	1:A:137:ILE:CG2	2.42	0.97
1:B:34:VAL:CG1	1:B:64:VAL:CG2	2.43	0.96
1:E:35:LEU:HA	1:E:62:GLY:O	1.64	0.96
1:L:231:TYR:O	1:L:371:THR:HG21	1.65	0.96
1:F:79:PHE:CZ	1:F:86:PRO:CG	2.47	0.95
1:J:108:LEU:HD21	1:J:302:GLY:HA3	1.38	0.95
1:C:10:ILE:O	1:C:166:ARG:NH1	1.99	0.95
1:J:108:LEU:HD11	1:J:302:GLY:CA	1.95	0.95
1:A:276:ASP:CA	1:A:277:PHE:HB2	1.94	0.95
1:A:276:ASP:OD2	1:A:278:THR:HG23	1.64	0.95
1:C:40:LYS:HE3	1:C:60:ASP:OD1	1.66	0.95
1:C:16:PRO:CG	1:C:35:LEU:HD21	1.97	0.95
1:E:21:PRO:O	1:E:24:ILE:CD1	2.15	0.95
1:F:122:GLN:CB	1:F:129:LEU:HD23	1.96	0.95
1:L:18:GLN:O	1:L:25:PHE:C	2.06	0.95
1:L:94:LEU:HD12	1:L:125:HIS:CD2	2.01	0.94
1:L:314:VAL:O	1:L:329:THR:HG21	1.65	0.94
1:A:276:ASP:HA	1:A:277:PHE:CB	1.91	0.94
1:I:20:GLY:HA3	1:I:24:ILE:CG2	1.97	0.94
1:I:317:ILE:HG12	1:I:333:VAL:HG21	1.47	0.94
1:G:80:ARG:HG3	1:G:80:ARG:HH11	1.32	0.94
1:L:322:LEU:CD2	1:L:344:ASP:OD2	2.14	0.94
1:J:108:LEU:HD13	1:J:109:GLY:N	1.82	0.94
1:A:253:MSE:HE2	1:A:253:MSE:N	1.81	0.93
1:G:133:MSE:HE3	1:G:137:ILE:CB	1.98	0.93
1:C:35:LEU:CD2	1:C:63:TRP:CZ3	2.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PRO:CD	1:C:35:LEU:HD21	1.99	0.93
1:A:253:MSE:HG3	1:A:277:PHE:CD2	2.01	0.93
1:E:130:GLU:OE1	1:E:158:THR:HG23	1.69	0.93
1:F:26:TYR:CA	1:F:34:VAL:HA	1.98	0.93
1:L:16:PRO:HB3	1:L:27:ASP:CB	1.99	0.93
1:H:145:TYR:CB	1:H:148:ILE:HD11	1.98	0.92
1:L:322:LEU:HD23	1:L:344:ASP:CG	1.90	0.92
1:B:29:ASN:O	1:B:164:THR:HB	1.69	0.92
1:F:78:VAL:CG2	1:F:88:LEU:HD12	1.93	0.92
1:C:93:LYS:HE3	1:C:93:LYS:HA	1.49	0.92
1:B:218:TYR:HB2	1:B:253:MSE:HE1	1.51	0.91
1:G:29:ASN:O	1:G:164:THR:HB	1.70	0.91
1:J:10:ILE:O	1:J:166:ARG:NH1	2.03	0.91
1:A:76:ILE:CD1	1:A:90:GLU:O	2.18	0.91
1:C:33:ARG:HG2	1:C:65:THR:HG22	1.50	0.91
1:I:20:GLY:N	1:I:24:ILE:O	2.03	0.91
1:L:133:MSE:CE	1:L:137:ILE:CB	2.49	0.91
1:E:18:GLN:OE1	1:E:97:ARG:NH2	2.04	0.91
1:E:19:ALA:HB1	1:E:20:GLY:HA3	1.51	0.91
1:F:122:GLN:HB3	1:F:129:LEU:CD2	2.01	0.91
1:I:20:GLY:HA3	1:I:24:ILE:HG22	1.51	0.90
1:A:363:ASN:H	1:A:367:GLN:NE2	1.70	0.90
1:I:24:ILE:CD1	1:I:37:PRO:CD	2.50	0.89
1:K:78:VAL:CG2	1:K:88:LEU:HB2	2.02	0.89
1:A:81:GLN:HE21	1:A:81:GLN:N	1.70	0.89
1:C:27:ASP:OD2	1:C:33:ARG:NH2	2.05	0.89
1:L:133:MSE:HE2	1:L:137:ILE:HB	1.55	0.89
1:F:79:PHE:CZ	1:F:86:PRO:HB3	2.07	0.89
1:G:18:GLN:O	1:G:25:PHE:CA	2.21	0.89
1:G:218:TYR:HB2	1:G:253:MSE:HE3	1.53	0.89
1:G:34:VAL:CG2	1:G:64:VAL:HG12	2.03	0.89
1:G:224:GLN:NE2	1:G:231:TYR:OH	2.06	0.88
1:D:206:LEU:O	1:D:208:LEU:HD13	1.73	0.88
1:G:34:VAL:HG22	1:G:64:VAL:HG13	1.55	0.88
1:L:100:LEU:HG	1:L:130:GLU:OE2	1.72	0.88
1:B:45:LEU:HD21	1:B:55:PHE:HB3	1.55	0.88
1:F:122:GLN:CB	1:F:129:LEU:CD2	2.51	0.88
1:F:73:ARG:HA	1:F:92:LEU:CD2	2.03	0.88
1:F:251:ARG:HB3	1:F:253:MSE:HE1	1.53	0.88
1:A:218:TYR:HB2	1:A:253:MSE:HE1	1.55	0.88
1:E:35:LEU:HD23	1:E:62:GLY:O	1.73	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:ILE:CG2	1:G:37:PRO:HD2	2.04	0.87
1:F:114:TRP:HZ2	1:F:169:LEU:HD13	1.37	0.87
1:H:21:PRO:HG2	1:H:87:LEU:CD2	2.04	0.87
1:L:18:GLN:O	1:L:25:PHE:HA	1.75	0.87
1:J:218:TYR:HB2	1:J:253:MSE:HE3	1.57	0.87
1:A:276:ASP:CB	1:A:278:THR:CG2	2.30	0.87
1:L:149:GLN:OE1	1:L:157:ARG:NH2	2.08	0.87
1:D:88:LEU:HD12	1:D:89:ASP:N	1.88	0.87
1:I:141:LEU:CD2	1:I:204:VAL:HG11	2.04	0.87
1:D:144:GLN:HE21	1:D:207:ASP:HB2	1.40	0.87
1:G:24:ILE:HG22	1:G:37:PRO:HD3	0.87	0.87
1:L:322:LEU:HD21	1:L:344:ASP:HB2	1.57	0.87
1:F:81:GLN:H	1:F:81:GLN:HE21	1.17	0.86
1:A:276:ASP:HB2	1:A:278:THR:HG22	1.52	0.86
1:D:144:GLN:NE2	1:D:207:ASP:HB2	1.90	0.86
1:A:100:LEU:HB3	1:A:164:THR:HG22	1.58	0.86
1:C:75:ARG:CG	1:C:91:THR:HG22	2.04	0.86
1:B:34:VAL:CG1	1:B:64:VAL:HG22	2.05	0.86
1:G:24:ILE:HG23	1:G:37:PRO:HD3	1.54	0.86
1:I:149:GLN:OE1	1:I:157:ARG:HD3	1.75	0.86
1:L:22:GLU:C	1:L:22:GLU:CD	2.32	0.86
1:F:42:HIS:O	1:F:79:PHE:N	2.08	0.86
1:A:75:ARG:HG3	1:A:91:THR:HG22	1.56	0.86
1:I:24:ILE:HD11	1:I:36:LEU:HA	1.58	0.86
1:E:35:LEU:HD23	1:E:62:GLY:C	1.97	0.85
1:G:27:ASP:O	1:G:32:ALA:HA	1.76	0.85
1:H:251:ARG:HB3	1:H:253:MSE:HE1	1.57	0.85
1:F:108:LEU:HD23	1:F:109:GLY:N	1.91	0.85
1:G:34:VAL:HG22	1:G:64:VAL:CG1	2.03	0.85
1:H:253:MSE:CG	1:H:277:PHE:CE1	2.60	0.85
1:L:251:ARG:CG	1:L:253:MSE:HE1	2.06	0.85
1:I:29:ASN:OD1	1:I:164:THR:OG1	1.93	0.85
1:L:41:TRP:N	1:L:41:TRP:CD1	2.44	0.85
1:C:36:LEU:HD21	1:C:61:LYS:O	1.76	0.85
1:C:40:LYS:CE	1:C:60:ASP:OD1	2.25	0.85
1:E:19:ALA:HB1	1:E:20:GLY:CA	2.07	0.85
1:H:145:TYR:HB3	1:H:148:ILE:CD1	2.06	0.84
1:D:254:CYS:SG	1:D:256:ASP:OD1	2.35	0.84
1:G:32:ALA:O	1:G:33:ARG:HG3	1.77	0.84
1:C:252:VAL:C	1:C:253:MSE:HE3	1.98	0.84
1:K:218:TYR:HB2	1:K:253:MSE:HE3	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:133:MSE:HE1	1:L:137:ILE:CG2	2.07	0.84
1:E:49:ASP:OD1	1:E:73:ARG:NH1	2.09	0.83
1:H:277:PHE:O	1:H:286:ARG:NH2	2.11	0.83
1:G:388:ARG:HG2	1:G:388:ARG:HH11	1.42	0.83
1:G:18:GLN:CB	1:G:19:ALA:HB3	2.07	0.83
1:D:87:LEU:HD12	1:D:87:LEU:O	1.78	0.83
1:D:251:ARG:HB3	1:D:253:MSE:HE1	1.60	0.83
1:G:284:GLN:HA	1:G:287:VAL:HG12	1.59	0.83
1:B:92:LEU:HD23	1:B:92:LEU:C	1.98	0.83
1:B:277:PHE:O	1:B:286:ARG:NH2	2.11	0.83
1:J:155:LYS:HG3	1:J:155:LYS:O	1.76	0.83
1:L:218:TYR:HB2	1:L:253:MSE:HE3	1.58	0.83
1:B:19:ALA:O	1:B:25:PHE:N	2.12	0.83
1:B:253:MSE:N	1:B:253:MSE:HE2	1.94	0.83
1:F:43:VAL:HG12	1:F:78:VAL:HG13	1.59	0.83
1:I:218:TYR:HB2	1:I:253:MSE:HE3	1.60	0.83
1:D:291:ARG:HH11	1:D:292:HIS:CE1	1.95	0.82
1:I:141:LEU:HD22	1:I:204:VAL:HG11	1.60	0.82
1:F:282:PRO:CD	1:F:285:GLU:OE2	2.25	0.82
1:G:389:SER:OG	1:G:398:THR:HG22	1.79	0.82
1:B:21:PRO:HD3	1:B:88:LEU:CD1	2.10	0.82
1:B:34:VAL:HG13	1:B:64:VAL:HG22	1.61	0.82
1:B:17:THR:C	1:B:18:GLN:OE1	2.19	0.82
1:B:45:LEU:H	1:B:45:LEU:HD22	1.43	0.82
1:F:13:PRO:O	1:F:14:ASP:HB3	1.79	0.82
1:H:130:GLU:OE1	1:H:158:THR:CG2	2.23	0.81
1:L:284:GLN:O	1:L:287:VAL:HG12	1.80	0.81
1:H:253:MSE:HG3	1:H:277:PHE:CE1	2.14	0.81
1:L:133:MSE:HE1	1:L:137:ILE:HG22	1.62	0.81
1:B:130:GLU:HB2	1:B:149:GLN:HE21	1.44	0.81
1:L:16:PRO:HB3	1:L:27:ASP:HB2	1.62	0.81
1:F:218:TYR:HB2	1:F:253:MSE:HE3	1.63	0.81
1:A:270:ILE:CD1	1:A:276:ASP:HB3	2.11	0.81
1:F:79:PHE:CE1	1:F:86:PRO:CB	2.63	0.81
1:D:46:LEU:CD2	1:D:53:ILE:HD13	2.11	0.80
1:F:79:PHE:CZ	1:F:86:PRO:CB	2.64	0.80
1:E:61:LYS:HG2	1:E:62:GLY:N	1.94	0.80
1:F:78:VAL:HG21	1:F:88:LEU:CD1	2.09	0.80
1:F:79:PHE:CD1	1:F:86:PRO:HB3	2.16	0.80
1:G:25:PHE:CD1	1:G:25:PHE:N	2.48	0.80
1:F:73:ARG:HA	1:F:92:LEU:HD23	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:GLN:NE2	1:G:97:ARG:HH22	1.79	0.80
1:G:244:HIS:O	1:G:248:LEU:CD2	2.30	0.80
1:L:277:PHE:O	1:L:286:ARG:NH2	2.15	0.80
1:A:276:ASP:OD2	1:A:278:THR:CG2	2.30	0.80
1:C:35:LEU:N	1:C:35:LEU:HD23	1.97	0.80
1:G:251:ARG:HB3	1:G:253:MSE:HE1	1.64	0.80
1:C:35:LEU:HD22	1:C:63:TRP:CH2	2.16	0.80
1:L:133:MSE:CE	1:L:137:ILE:CG2	2.60	0.80
1:D:218:TYR:HB2	1:D:253:MSE:HE3	1.63	0.80
1:F:108:LEU:HD21	1:F:302:GLY:CA	2.10	0.80
1:G:36:LEU:HD12	1:G:36:LEU:H	1.45	0.80
1:I:24:ILE:HD11	1:I:36:LEU:HD23	1.64	0.79
1:J:108:LEU:CD1	1:J:302:GLY:CA	2.53	0.79
1:J:251:ARG:HB3	1:J:253:MSE:HE1	1.65	0.79
1:I:27:ASP:CG	1:I:29:ASN:HD22	1.85	0.79
1:I:281:LEU:HB2	1:I:282:PRO:HD2	1.64	0.79
1:F:81:GLN:H	1:F:81:GLN:NE2	1.79	0.79
1:J:108:LEU:HD21	1:J:302:GLY:O	1.82	0.79
1:L:251:ARG:HG2	1:L:253:MSE:CE	2.09	0.79
1:E:21:PRO:O	1:E:24:ILE:HG12	1.83	0.79
1:K:326:GLU:OE1	1:K:332:ARG:NH2	2.14	0.79
1:C:119:GLU:OE1	1:C:205:ARG:NH2	2.16	0.79
1:E:21:PRO:HG2	1:E:88:LEU:HG	1.65	0.78
1:L:18:GLN:O	1:L:25:PHE:CA	2.30	0.78
1:A:133:MSE:CE	1:A:137:ILE:HG22	2.12	0.78
1:L:130:GLU:OE2	1:L:130:GLU:O	2.01	0.78
1:G:39:GLY:O	1:G:41:TRP:NE1	2.17	0.78
1:B:88:LEU:CD2	1:B:90:GLU:HG2	2.14	0.78
1:B:221:ILE:O	1:B:255:ILE:HD13	1.83	0.78
1:B:21:PRO:O	1:B:24:ILE:HD12	1.83	0.78
1:G:24:ILE:HG22	1:G:36:LEU:HA	1.62	0.77
1:E:21:PRO:O	1:E:24:ILE:HD13	1.85	0.77
1:A:253:MSE:HE2	1:A:253:MSE:H	1.47	0.77
1:J:60:ASP:O	1:J:61:LYS:HG3	1.84	0.77
1:L:94:LEU:HD12	1:L:125:HIS:HD2	1.43	0.77
1:B:21:PRO:CD	1:B:88:LEU:HD12	2.14	0.77
1:E:326:GLU:OE1	1:E:332:ARG:NH2	2.17	0.77
1:L:28:PHE:CD2	1:L:92:LEU:HD12	2.19	0.77
1:G:22:GLU:HG2	1:G:24:ILE:CD1	2.14	0.77
1:H:253:MSE:HG2	1:H:277:PHE:CE1	2.19	0.77
1:I:251:ARG:HB3	1:I:253:MSE:HE1	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:205:ARG:HG2	1:K:205:ARG:HH11	1.49	0.77
1:F:78:VAL:CG2	1:F:88:LEU:HD13	2.04	0.76
1:A:252:VAL:O	1:A:275:GLU:HG3	1.85	0.76
1:B:64:VAL:HG23	1:B:64:VAL:O	1.86	0.76
1:F:94:LEU:O	1:F:97:ARG:HG3	1.85	0.76
1:H:21:PRO:HG2	1:H:87:LEU:HD21	1.66	0.76
1:C:10:ILE:HG23	1:C:11:THR:N	2.00	0.76
1:F:17:THR:HG1	1:F:18:GLN:NE2	1.83	0.76
1:G:22:GLU:HG3	1:G:23:ASN:N	1.98	0.76
1:K:394:GLY:CA	1:K:395:VAL:HG22	2.12	0.76
1:C:277:PHE:O	1:C:286:ARG:NH2	2.18	0.76
1:G:24:ILE:HG21	1:G:36:LEU:HA	1.67	0.76
1:K:78:VAL:HG22	1:K:88:LEU:CB	2.11	0.76
1:L:322:LEU:HD22	1:L:322:LEU:H	1.51	0.76
1:D:124:LEU:HD23	1:D:125:HIS:NE2	2.01	0.76
1:J:49:ASP:OD1	1:J:73:ARG:NH1	2.19	0.76
1:K:394:GLY:O	1:K:397:ALA:HB2	1.86	0.76
1:H:49:ASP:OD1	1:H:73:ARG:NH1	2.18	0.75
1:D:65:THR:HG21	1:D:69:LYS:NZ	2.02	0.75
1:L:322:LEU:CD2	1:L:344:ASP:HB2	2.17	0.75
1:C:22:GLU:O	1:C:22:GLU:OE1	2.03	0.75
1:L:284:GLN:O	1:L:287:VAL:CG1	2.34	0.75
1:B:45:LEU:HD22	1:B:45:LEU:N	2.01	0.75
1:L:72:VAL:HG13	1:L:74:PHE:CE2	2.21	0.75
1:B:27:ASP:CG	1:B:29:ASN:HD22	1.89	0.75
1:H:115:PHE:HZ	1:H:148:ILE:HD12	1.51	0.75
1:D:119:GLU:OE1	1:D:145:TYR:CE2	2.40	0.75
1:G:18:GLN:OE1	1:G:26:TYR:OH	2.05	0.75
1:L:75:ARG:HG2	1:L:91:THR:OG1	1.87	0.75
1:G:22:GLU:CG	1:G:24:ILE:CD1	2.65	0.74
1:I:396:GLU:O	1:I:398:THR:N	2.20	0.74
1:H:145:TYR:HB3	1:H:148:ILE:CG1	2.17	0.74
1:E:22:GLU:OE2	1:E:22:GLU:CA	2.36	0.74
1:C:135:GLN:NE2	1:C:138:ILE:HG21	2.02	0.74
1:F:94:LEU:HD23	1:F:162:TYR:CD2	2.22	0.74
1:L:114:TRP:HZ2	1:L:169:LEU:HD13	1.52	0.74
1:L:100:LEU:HD12	1:L:158:THR:HG21	1.69	0.74
1:G:34:VAL:HG23	1:G:64:VAL:HG12	1.66	0.74
1:L:20:GLY:O	1:L:23:ASN:O	2.06	0.74
1:B:24:ILE:HD11	1:B:87:LEU:HD23	1.69	0.74
1:D:79:PHE:CE1	1:D:86:PRO:N	2.55	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:GLN:OE1	1:G:26:TYR:CZ	2.41	0.74
1:K:49:ASP:OD1	1:K:73:ARG:NH1	2.20	0.74
1:C:78:VAL:HG22	1:C:88:LEU:HB3	1.68	0.74
1:A:78:VAL:CG2	1:A:88:LEU:HB3	2.17	0.73
1:E:21:PRO:O	1:E:24:ILE:CG1	2.35	0.73
1:F:44:ARG:NH1	1:F:77:GLN:OE1	2.21	0.73
1:I:130:GLU:OE1	1:I:158:THR:OG1	2.06	0.73
1:K:284:GLN:O	1:K:287:VAL:CG2	2.36	0.73
1:G:24:ILE:HG23	1:G:37:PRO:CD	2.14	0.73
1:E:38:GLU:O	1:E:41:TRP:CZ2	2.40	0.73
1:J:277:PHE:O	1:J:286:ARG:NH1	2.21	0.73
1:C:16:PRO:HG2	1:C:35:LEU:CD2	2.18	0.73
1:G:28:PHE:HA	1:G:32:ALA:HA	1.71	0.73
1:I:317:ILE:CG1	1:I:333:VAL:HG21	2.18	0.73
1:F:280:LYS:HE3	1:F:280:LYS:O	1.89	0.73
1:E:22:GLU:HB2	1:E:24:ILE:HD11	1.69	0.72
1:C:35:LEU:HD22	1:C:63:TRP:CE3	2.23	0.72
1:I:94:LEU:HD12	1:I:125:HIS:ND1	2.04	0.72
1:B:357:TRP:CZ2	1:B:359:PRO:HG3	2.24	0.72
1:D:65:THR:CG2	1:D:69:LYS:NZ	2.51	0.72
1:A:133:MSE:CE	1:A:137:ILE:HG21	2.19	0.72
1:C:29:ASN:OD1	1:C:161:PRO:O	2.07	0.72
1:E:16:PRO:HD3	1:E:63:TRP:HH2	1.54	0.72
1:E:87:LEU:HD23	1:E:87:LEU:N	2.03	0.72
1:D:83:ALA:HB1	1:D:84:ALA:HA	0.80	0.72
1:E:251:ARG:HB3	1:E:253:MSE:HE1	1.70	0.72
1:B:357:TRP:CE2	1:B:359:PRO:HG3	2.25	0.72
1:B:34:VAL:HG12	1:B:64:VAL:HG23	1.72	0.71
1:K:394:GLY:HA2	1:K:395:VAL:CG2	2.14	0.71
1:C:253:MSE:HE2	1:C:275:GLU:HB2	1.72	0.71
1:F:87:LEU:N	1:F:87:LEU:CD1	2.38	0.71
1:G:284:GLN:HA	1:G:287:VAL:CG1	2.20	0.71
1:L:233:ASN:H	1:L:371:THR:CB	2.02	0.71
1:L:233:ASN:N	1:L:371:THR:HB	2.00	0.71
1:B:10:ILE:HG21	1:B:102:SER:OG	1.90	0.71
1:A:363:ASN:H	1:A:367:GLN:HE22	1.37	0.71
1:K:29:ASN:O	1:K:164:THR:HB	1.90	0.71
1:L:133:MSE:HE1	1:L:137:ILE:CB	2.20	0.71
1:A:133:MSE:HE2	1:A:137:ILE:HB	1.72	0.71
1:K:284:GLN:HA	1:K:287:VAL:HG22	1.71	0.71
1:H:145:TYR:CG	1:H:148:ILE:HD11	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD22	1:C:62:GLY:HA2	1.73	0.71
1:J:242:ILE:HG23	1:J:252:VAL:HG21	1.73	0.71
1:C:135:GLN:O	1:C:138:ILE:HG22	1.91	0.71
1:F:91:THR:HG22	1:F:92:LEU:N	2.06	0.71
1:I:21:PRO:HG2	1:I:87:LEU:HD13	1.73	0.71
1:I:24:ILE:HD13	1:I:37:PRO:CD	2.21	0.71
1:J:39:GLY:O	1:J:60:ASP:HB3	1.90	0.71
1:L:16:PRO:CB	1:L:27:ASP:HB2	2.21	0.71
1:F:39:GLY:O	1:F:60:ASP:HA	1.91	0.70
1:G:22:GLU:HG3	1:G:24:ILE:HD12	1.71	0.70
1:B:10:ILE:CG2	1:B:102:SER:OG	2.39	0.70
1:F:89:ASP:CG	1:F:89:ASP:O	2.30	0.70
1:I:49:ASP:OD1	1:I:73:ARG:NH1	2.24	0.70
1:C:114:TRP:HZ2	1:C:169:LEU:HD13	1.56	0.70
1:C:138:ILE:HD11	1:C:150:PHE:HB3	0.74	0.70
1:C:198:ASP:OD2	1:C:200:ARG:NH1	2.25	0.70
1:E:22:GLU:CB	1:E:24:ILE:CD1	2.70	0.70
1:K:26:TYR:OH	1:K:90:GLU:HG3	1.92	0.70
1:L:18:GLN:O	1:L:26:TYR:N	2.25	0.70
1:L:22:GLU:C	1:L:22:GLU:OE2	2.30	0.70
1:L:310:THR:CG2	1:L:310:THR:O	2.38	0.70
1:B:49:ASP:OD1	1:B:73:ARG:NH1	2.25	0.70
1:G:244:HIS:O	1:G:248:LEU:HD22	1.90	0.70
1:K:284:GLN:O	1:K:287:VAL:HG22	1.92	0.70
1:A:94:LEU:HD12	1:A:125:HIS:CG	2.27	0.70
1:B:72:VAL:HB	1:B:74:PHE:CE2	2.26	0.70
1:C:17:THR:HG22	1:C:160:ALA:HB1	1.71	0.70
1:C:135:GLN:NE2	1:C:138:ILE:CG2	2.55	0.70
1:A:81:GLN:HE21	1:A:81:GLN:CA	2.03	0.70
1:L:24:ILE:HG22	1:L:25:PHE:N	2.07	0.70
1:G:24:ILE:HG21	1:G:37:PRO:HD2	1.73	0.70
1:J:20:GLY:N	1:J:24:ILE:O	2.24	0.70
1:E:255:ILE:HB	1:E:286:ARG:HH21	1.56	0.69
1:G:28:PHE:HA	1:G:32:ALA:H	1.57	0.69
1:L:133:MSE:HE1	1:L:137:ILE:HB	1.72	0.69
1:E:16:PRO:HD3	1:E:63:TRP:CH2	2.26	0.69
1:G:25:PHE:N	1:G:25:PHE:HD1	1.87	0.69
1:L:21:PRO:CB	1:L:87:LEU:CD2	2.47	0.69
1:L:22:GLU:CD	1:L:22:GLU:O	2.30	0.69
1:B:222:ALA:HA	1:B:256:ASP:OD1	1.92	0.69
1:D:119:GLU:OE1	1:D:145:TYR:HE2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:TYR:HB3	1:F:34:VAL:HG23	1.74	0.69
1:C:16:PRO:CG	1:C:35:LEU:CD2	2.70	0.69
1:F:49:ASP:OD1	1:F:73:ARG:NH1	2.25	0.69
1:B:30:ASP:OD1	1:B:31:GLY:N	2.24	0.69
1:E:252:VAL:C	1:E:253:MSE:HE2	2.12	0.69
1:F:108:LEU:HD23	1:F:109:GLY:H	1.57	0.69
1:G:18:GLN:O	1:G:25:PHE:HA	1.90	0.69
1:B:38:GLU:O	1:B:60:ASP:O	2.11	0.69
1:C:35:LEU:CA	1:C:62:GLY:O	2.30	0.69
1:G:36:LEU:HD12	1:G:36:LEU:N	2.07	0.69
1:L:41:TRP:N	1:L:41:TRP:HD1	1.89	0.69
1:C:138:ILE:CD1	1:C:150:PHE:CB	2.37	0.69
1:F:79:PHE:CE1	1:F:86:PRO:HG3	2.27	0.68
1:A:76:ILE:HD12	1:A:76:ILE:N	2.04	0.68
1:D:10:ILE:O	1:D:166:ARG:NH1	2.26	0.68
1:F:94:LEU:HD23	1:F:162:TYR:CE2	2.28	0.68
1:B:17:THR:HG21	1:B:161:PRO:O	1.94	0.68
1:E:394:GLY:O	1:E:395:VAL:HG22	1.93	0.68
1:K:40:LYS:CD	1:K:60:ASP:OD1	2.40	0.68
1:K:89:ASP:OD1	1:K:89:ASP:C	2.30	0.68
1:I:141:LEU:HD22	1:I:204:VAL:CG1	2.24	0.68
1:A:46:LEU:HD12	1:A:75:ARG:HD3	1.74	0.68
1:A:133:MSE:HE3	1:A:137:ILE:HG21	1.75	0.68
1:E:17:THR:HG21	1:E:161:PRO:O	1.94	0.68
1:F:73:ARG:HA	1:F:92:LEU:HD22	1.73	0.68
1:L:299:LEU:HB3	1:L:300:PRO:HD2	1.75	0.68
1:B:36:LEU:H	1:B:36:LEU:HD12	1.58	0.68
1:I:24:ILE:CD1	1:I:36:LEU:HA	2.24	0.68
1:K:75:ARG:HG3	1:K:91:THR:OG1	1.94	0.68
1:A:208:LEU:O	1:A:291:ARG:NH1	2.27	0.67
1:G:40:LYS:HE2	1:G:60:ASP:OD2	1.93	0.67
1:I:253:MSE:HB3	1:I:277:PHE:CD1	2.29	0.67
1:L:207:ASP:OD1	1:L:209:SER:OG	2.13	0.67
1:L:394:GLY:O	1:L:395:VAL:HG23	1.95	0.67
1:K:40:LYS:HB3	1:K:81:GLN:HG3	1.76	0.67
1:E:101:ILE:HG12	1:E:129:LEU:HD11	1.75	0.67
1:G:41:TRP:CD1	1:G:41:TRP:N	2.61	0.67
1:L:311:ARG:HG3	1:L:311:ARG:O	1.94	0.67
1:C:93:LYS:O	1:C:162:TYR:HE2	1.78	0.67
1:I:317:ILE:CA	1:I:333:VAL:CG2	2.68	0.67
1:A:35:LEU:HD12	1:A:62:GLY:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LEU:C	1:C:92:LEU:HD23	2.14	0.67
1:J:61:LYS:HD2	1:J:61:LYS:O	1.95	0.67
1:L:16:PRO:CA	1:L:27:ASP:HB2	2.24	0.67
1:A:94:LEU:HD12	1:A:125:HIS:ND1	2.10	0.67
1:H:100:LEU:HD12	1:H:100:LEU:H	1.60	0.67
1:D:46:LEU:HD21	1:D:53:ILE:HD13	1.76	0.67
1:G:31:GLY:O	1:G:32:ALA:HB3	1.94	0.67
1:J:137:ILE:HG22	1:J:141:LEU:HD22	1.76	0.67
1:K:396:GLU:OE2	1:K:396:GLU:N	2.27	0.67
1:L:322:LEU:HD22	1:L:322:LEU:N	2.10	0.67
1:G:80:ARG:HG3	1:G:80:ARG:NH1	2.04	0.66
1:F:114:TRP:CZ2	1:F:169:LEU:HD13	2.27	0.66
1:E:29:ASN:O	1:E:33:ARG:HD3	1.95	0.66
1:I:326:GLU:OE1	1:I:332:ARG:NH1	2.28	0.66
1:D:80:ARG:O	1:D:83:ALA:N	2.29	0.66
1:J:39:GLY:O	1:J:60:ASP:CB	2.44	0.66
1:H:129:LEU:HD13	1:H:148:ILE:HG22	1.77	0.66
1:I:141:LEU:HD21	1:I:204:VAL:HG11	1.77	0.66
1:C:36:LEU:CD2	1:C:61:LYS:O	2.43	0.66
1:G:32:ALA:O	1:G:33:ARG:CB	2.43	0.66
1:A:133:MSE:HE2	1:A:137:ILE:CG2	2.24	0.66
1:F:392:GLU:O	1:F:393:GLN:HG2	1.95	0.66
1:L:322:LEU:CD2	1:L:344:ASP:CB	2.74	0.66
1:D:22:GLU:CG	1:D:87:LEU:HD21	2.25	0.66
1:F:281:LEU:CB	1:F:285:GLU:OE2	2.41	0.66
1:H:29:ASN:O	1:H:166:ARG:NH2	2.28	0.66
1:E:59:VAL:HG11	1:E:61:LYS:HE2	1.78	0.66
1:K:251:ARG:CB	1:K:253:MSE:HE1	2.25	0.65
1:G:284:GLN:CA	1:G:287:VAL:HG12	2.26	0.65
1:L:23:ASN:O	1:L:24:ILE:HB	1.97	0.65
1:L:75:ARG:NH1	1:L:77:GLN:OE1	2.29	0.65
1:L:100:LEU:HG	1:L:130:GLU:CD	2.16	0.65
1:L:329:THR:HG22	1:L:331:TRP:H	1.59	0.65
1:C:85:THR:CG2	1:C:86:PRO:HD3	2.24	0.65
1:L:252:VAL:C	1:L:253:MSE:HE2	2.15	0.65
1:D:10:ILE:HG21	1:D:102:SER:OG	1.96	0.65
1:I:291:ARG:HA	1:I:310:THR:CG2	2.26	0.65
1:A:253:MSE:HG3	1:A:277:PHE:HE2	1.42	0.65
1:K:78:VAL:HG23	1:K:87:LEU:HD12	1.79	0.65
1:B:21:PRO:HG2	1:B:24:ILE:HD13	1.77	0.65
1:G:24:ILE:HG21	1:G:37:PRO:CD	2.21	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:GLN:CB	1:L:26:TYR:O	2.44	0.65
1:C:299:LEU:HB3	1:C:300:PRO:HD2	1.79	0.65
1:E:21:PRO:CG	1:E:88:LEU:HG	2.27	0.65
1:G:279:GLY:O	1:G:286:ARG:NH2	2.25	0.65
1:D:22:GLU:HG3	1:D:87:LEU:HD21	1.78	0.64
1:E:24:ILE:HG22	1:E:36:LEU:HA	1.78	0.64
1:E:114:TRP:HZ2	1:E:169:LEU:HD13	1.62	0.64
1:L:16:PRO:HB3	1:L:27:ASP:HB3	1.78	0.64
1:F:122:GLN:HB3	1:F:129:LEU:HD21	1.80	0.64
1:G:133:MSE:HE1	1:G:137:ILE:HG22	1.78	0.64
1:K:40:LYS:NZ	1:K:60:ASP:OD2	2.30	0.64
1:F:90:GLU:HA	1:F:90:GLU:OE1	1.96	0.64
1:K:189:ARG:NH1	1:K:201:GLU:OE1	2.30	0.64
1:L:75:ARG:NH1	1:L:89:ASP:OD2	2.30	0.64
1:L:154:ASP:OD1	1:L:154:ASP:N	2.30	0.64
1:A:27:ASP:HB3	1:A:33:ARG:HG2	1.80	0.64
1:C:136:ASP:N	1:C:136:ASP:OD1	2.30	0.64
1:D:17:THR:OG1	1:D:160:ALA:HB1	1.98	0.64
1:L:27:ASP:OD1	1:L:28:PHE:N	2.30	0.64
1:I:189:ARG:NH1	1:I:201:GLU:OE1	2.30	0.64
1:B:45:LEU:CD2	1:B:55:PHE:HB3	2.26	0.64
1:G:81:GLN:HA	1:G:81:GLN:HE21	1.63	0.64
1:L:149:GLN:HG3	1:L:157:ARG:HH21	1.62	0.64
1:A:133:MSE:HE3	1:A:137:ILE:CG2	2.26	0.63
1:A:326:GLU:OE1	1:A:332:ARG:NH1	2.31	0.63
1:E:281:LEU:HD22	1:E:286:ARG:NH1	2.11	0.63
1:B:92:LEU:O	1:B:92:LEU:CD2	2.30	0.63
1:D:252:VAL:C	1:D:253:MSE:HE2	2.18	0.63
1:F:252:VAL:C	1:F:253:MSE:HE2	2.18	0.63
1:G:23:ASN:O	1:G:25:PHE:CD1	2.52	0.63
1:K:189:ARG:NH2	1:K:324:ASN:O	2.31	0.63
1:K:252:VAL:C	1:K:253:MSE:HE2	2.18	0.63
1:G:28:PHE:HA	1:G:32:ALA:CA	2.26	0.63
1:H:189:ARG:NH2	1:H:324:ASN:O	2.32	0.63
1:B:88:LEU:HD22	1:B:90:GLU:HG2	1.79	0.63
1:F:91:THR:CG2	1:F:92:LEU:N	2.62	0.63
1:C:35:LEU:CD2	1:C:63:TRP:CH2	2.80	0.63
1:E:101:ILE:CG1	1:E:129:LEU:HD11	2.29	0.63
1:G:72:VAL:HG13	1:G:74:PHE:CE2	2.33	0.63
1:L:18:GLN:HB2	1:L:26:TYR:O	1.98	0.63
1:D:41:TRP:N	1:D:81:GLN:NE2	2.47	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:VAL:CG2	1:D:88:LEU:HB3	2.24	0.63
1:F:34:VAL:HG22	1:F:35:LEU:HG	1.81	0.63
1:A:133:MSE:HE2	1:A:137:ILE:CB	2.29	0.62
1:B:36:LEU:HD12	1:B:36:LEU:N	2.13	0.62
1:H:253:MSE:CG	1:H:277:PHE:CD1	2.82	0.62
1:I:20:GLY:CA	1:I:24:ILE:HG22	2.27	0.62
1:D:101:ILE:HG13	1:D:129:LEU:HD11	1.80	0.62
1:I:20:GLY:HA3	1:I:24:ILE:HG23	1.77	0.62
1:B:253:MSE:HG3	1:B:277:PHE:CE1	2.34	0.62
1:E:136:ASP:OD1	1:E:136:ASP:N	2.31	0.62
1:F:28:PHE:CZ	1:F:92:LEU:CD1	2.82	0.62
1:F:40:LYS:O	1:F:81:GLN:NE2	2.33	0.62
1:G:28:PHE:HA	1:G:32:ALA:N	2.14	0.62
1:A:40:LYS:O	1:A:81:GLN:NE2	2.30	0.62
1:C:189:ARG:NE	3:C:502:EDO:O1	2.32	0.62
1:L:393:GLN:N	1:L:393:GLN:OE1	2.31	0.62
1:A:83:ALA:O	1:A:85:THR:N	2.32	0.62
1:G:18:GLN:HB3	1:G:19:ALA:HB3	1.81	0.62
1:C:253:MSE:HE1	1:C:275:GLU:CD	2.20	0.62
1:E:22:GLU:HB3	1:E:24:ILE:CD1	2.29	0.62
1:I:189:ARG:NH2	1:I:324:ASN:O	2.32	0.62
1:L:133:MSE:HE3	1:L:137:ILE:HB	1.73	0.62
1:B:220:CYS:HB3	1:B:255:ILE:HD12	1.81	0.62
1:D:79:PHE:CE1	1:D:85:THR:C	2.73	0.62
1:L:124:LEU:HD22	1:L:125:HIS:CE1	2.34	0.62
1:F:29:ASN:HD22	1:F:33:ARG:HH11	1.47	0.62
1:I:242:ILE:HG23	1:I:252:VAL:HG11	1.82	0.62
1:B:60:ASP:OD1	1:B:60:ASP:N	2.31	0.62
1:C:92:LEU:HD23	1:C:92:LEU:O	1.99	0.62
1:E:95:LYS:O	1:E:97:ARG:HG2	2.00	0.62
1:E:335:ASN:HB2	1:E:374:ILE:HD13	1.82	0.62
1:I:251:ARG:CB	1:I:253:MSE:HE1	2.30	0.62
1:B:85:THR:CG2	1:B:86:PRO:HD2	2.30	0.61
1:E:78:VAL:HG12	1:E:88:LEU:CB	2.30	0.61
1:J:251:ARG:CB	1:J:253:MSE:HE1	2.30	0.61
1:D:189:ARG:NH1	1:D:201:GLU:OE1	2.34	0.61
1:D:189:ARG:NH2	1:D:324:ASN:O	2.33	0.61
1:D:208:LEU:HD12	1:D:208:LEU:N	2.15	0.61
1:D:228:GLN:HG2	1:D:355:PHE:CE2	2.35	0.61
1:E:281:LEU:HD22	1:E:286:ARG:HH11	1.65	0.61
1:F:251:ARG:CB	1:F:253:MSE:HE1	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MSE:CE	1:A:137:ILE:HB	2.29	0.61
1:G:16:PRO:HB3	1:G:27:ASP:HB2	1.81	0.61
1:G:284:GLN:O	1:G:287:VAL:CG1	2.48	0.61
1:K:299:LEU:HB3	1:K:300:PRO:HD2	1.82	0.61
1:L:326:GLU:OE1	1:L:332:ARG:NH2	2.33	0.61
1:A:253:MSE:CG	1:A:277:PHE:HD2	2.09	0.61
1:C:23:ASN:O	1:C:37:PRO:HD3	2.01	0.61
1:F:44:ARG:HG2	1:F:77:GLN:HB2	1.83	0.61
1:F:108:LEU:HD23	1:F:302:GLY:HA3	1.81	0.61
1:A:75:ARG:CG	1:A:91:THR:HG22	2.27	0.61
1:F:37:PRO:HG2	1:F:38:GLU:H	1.66	0.61
1:G:188:HIS:HE1	1:G:325:SER:O	1.83	0.61
1:L:24:ILE:CG2	1:L:25:PHE:N	2.64	0.61
1:B:88:LEU:HD23	1:B:89:ASP:H	1.63	0.61
1:F:26:TYR:HB3	1:F:34:VAL:CG2	2.31	0.61
1:I:316:LEU:O	1:I:333:VAL:CG2	2.49	0.61
1:C:253:MSE:HE1	1:C:275:GLU:OE2	2.01	0.61
1:I:24:ILE:HD13	1:I:37:PRO:HD2	1.81	0.61
1:B:253:MSE:HE2	1:B:253:MSE:H	1.63	0.60
1:D:65:THR:HG21	1:D:69:LYS:HZ1	1.66	0.60
1:F:190:SER:O	1:F:194:ILE:HG12	2.01	0.60
1:L:19:ALA:HB2	1:L:25:PHE:CE1	2.36	0.60
1:A:33:ARG:HB3	1:A:65:THR:HG23	1.83	0.60
1:F:252:VAL:HG23	1:F:252:VAL:O	2.00	0.60
1:H:189:ARG:NH1	1:H:201:GLU:OE1	2.34	0.60
1:I:16:PRO:HB3	1:I:27:ASP:HB2	1.83	0.60
1:J:252:VAL:C	1:J:253:MSE:HE2	2.21	0.60
1:L:322:LEU:CD2	1:L:322:LEU:H	2.13	0.60
1:D:144:GLN:NE2	1:D:207:ASP:H	1.99	0.60
1:F:79:PHE:CE1	1:F:86:PRO:CG	2.85	0.60
1:K:61:LYS:HG3	1:K:62:GLY:N	2.17	0.60
1:G:18:GLN:HB2	1:G:26:TYR:O	2.02	0.60
1:J:108:LEU:CD2	1:J:302:GLY:O	2.44	0.60
1:B:18:GLN:O	1:B:25:PHE:HA	2.01	0.60
1:G:252:VAL:C	1:G:253:MSE:HE2	2.21	0.60
1:D:83:ALA:CB	1:D:84:ALA:CA	2.46	0.60
1:G:81:GLN:HE21	1:G:81:GLN:CA	2.15	0.60
1:H:23:ASN:O	1:H:37:PRO:HG3	2.02	0.60
1:K:284:GLN:NE2	1:K:287:VAL:HG21	2.17	0.60
1:D:46:LEU:HD23	1:D:53:ILE:HD13	1.84	0.59
1:D:291:ARG:HH11	1:D:292:HIS:HE2	1.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:GLU:OE2	1:F:157:ARG:CB	2.28	0.59
1:H:61:LYS:HG2	1:H:62:GLY:N	2.17	0.59
1:H:87:LEU:HD23	1:H:87:LEU:O	2.02	0.59
1:B:21:PRO:HG2	1:B:87:LEU:HD21	1.84	0.59
1:B:34:VAL:CG1	1:B:64:VAL:HG21	2.32	0.59
1:B:64:VAL:CG2	1:B:64:VAL:O	2.49	0.59
1:F:225:SER:OG	1:F:301:SER:OG	2.17	0.59
1:J:27:ASP:OD1	1:J:33:ARG:HG3	2.01	0.59
1:K:395:VAL:HG23	1:K:395:VAL:O	2.01	0.59
1:C:138:ILE:CG1	1:C:150:PHE:HB3	2.29	0.59
1:L:149:GLN:OE1	1:L:157:ARG:CZ	2.49	0.59
1:A:275:GLU:O	1:A:277:PHE:HB2	2.02	0.59
1:B:22:GLU:O	1:B:23:ASN:CG	2.40	0.59
1:F:26:TYR:HB3	1:F:34:VAL:CB	2.31	0.59
1:A:27:ASP:OD2	1:A:33:ARG:NH1	2.36	0.59
1:H:101:ILE:HG12	1:H:129:LEU:HD21	1.84	0.59
1:B:27:ASP:OD2	1:B:29:ASN:ND2	2.32	0.59
1:G:24:ILE:CB	1:G:35:LEU:O	2.40	0.59
1:G:393:GLN:HB3	1:G:397:ALA:HB3	1.85	0.59
1:B:326:GLU:OE1	1:B:332:ARG:NH1	2.36	0.59
1:F:122:GLN:HB2	1:F:129:LEU:CD2	2.17	0.59
1:L:28:PHE:CE2	1:L:92:LEU:HA	2.38	0.59
1:A:253:MSE:CB	1:A:277:PHE:CD2	2.86	0.58
1:D:41:TRP:CA	1:D:81:GLN:HE21	2.15	0.58
1:H:253:MSE:HE3	1:H:275:GLU:CD	2.23	0.58
1:A:46:LEU:HD22	1:A:53:ILE:HG13	1.85	0.58
1:A:133:MSE:CE	1:A:137:ILE:CB	2.81	0.58
1:A:152:THR:HG22	1:A:153:PRO:HD2	1.83	0.58
1:B:18:GLN:O	1:B:26:TYR:N	2.34	0.58
1:F:72:VAL:O	1:F:92:LEU:CD2	2.51	0.58
1:A:46:LEU:CD2	1:A:53:ILE:HG13	2.33	0.58
1:C:181:ASP:HB3	1:C:184:LYS:HD2	1.84	0.58
1:I:316:LEU:O	1:I:333:VAL:HG22	2.03	0.58
1:D:299:LEU:HB3	1:D:300:PRO:HD2	1.85	0.58
1:G:100:LEU:HD12	1:G:158:THR:HG21	1.84	0.58
1:B:18:GLN:OE1	1:B:18:GLN:N	2.36	0.58
1:C:36:LEU:N	1:C:36:LEU:HD13	2.18	0.58
1:D:20:GLY:N	1:D:24:ILE:O	2.36	0.58
1:H:325:SER:HB3	1:H:326:GLU:OE1	2.02	0.58
1:K:251:ARG:HB3	1:K:253:MSE:HE1	1.85	0.58
1:L:284:GLN:C	1:L:287:VAL:HG12	2.23	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:LEU:HB2	1:G:286:ARG:NH1	2.19	0.58
1:K:223:THR:N	1:K:256:ASP:OD2	2.34	0.58
1:I:18:GLN:O	1:I:25:PHE:HA	2.03	0.58
1:G:299:LEU:HB3	1:G:300:PRO:HD2	1.86	0.58
1:K:27:ASP:OD2	1:K:29:ASN:ND2	2.34	0.58
1:C:40:LYS:CD	1:C:60:ASP:OD1	2.51	0.58
1:J:145:TYR:HB3	1:J:148:ILE:HD13	1.85	0.58
1:A:76:ILE:H	1:A:76:ILE:CD1	2.02	0.57
1:C:93:LYS:O	1:C:162:TYR:CE2	2.56	0.57
1:L:133:MSE:HE3	1:L:137:ILE:CG2	2.34	0.57
1:G:119:GLU:OE2	1:G:205:ARG:NH2	2.36	0.57
1:L:324:ASN:HD22	1:L:324:ASN:H	1.50	0.57
1:G:16:PRO:HD3	1:G:63:TRP:CH2	2.40	0.57
1:K:40:LYS:N	1:K:80:ARG:HH12	2.02	0.57
1:A:253:MSE:HG3	1:A:277:PHE:HD2	1.66	0.57
1:B:17:THR:O	1:B:18:GLN:OE1	2.21	0.57
1:C:40:LYS:HD2	1:C:60:ASP:OD1	2.05	0.57
1:G:251:ARG:CB	1:G:253:MSE:HE1	2.32	0.57
1:H:136:ASP:N	1:H:136:ASP:OD1	2.37	0.57
1:A:130:GLU:OE1	1:A:158:THR:OG1	2.20	0.57
1:A:363:ASN:N	1:A:367:GLN:NE2	2.47	0.57
1:B:184:LYS:HE3	1:F:322:LEU:HD11	1.86	0.57
1:B:299:LEU:HB3	1:B:300:PRO:HD2	1.86	0.57
1:F:79:PHE:CZ	1:F:86:PRO:CD	2.87	0.57
1:I:152:THR:HG22	1:I:153:PRO:HD2	1.87	0.57
1:K:394:GLY:HA3	1:K:395:VAL:C	2.24	0.57
1:C:16:PRO:HD3	1:C:35:LEU:HD21	1.83	0.57
1:G:22:GLU:HG3	1:G:24:ILE:CD1	2.33	0.57
1:G:244:HIS:O	1:G:248:LEU:HD23	2.03	0.57
1:B:38:GLU:HB2	1:B:41:TRP:HE1	1.70	0.57
1:G:22:GLU:CG	1:G:23:ASN:N	2.68	0.57
1:H:100:LEU:HD11	1:H:161:PRO:CG	2.34	0.57
1:L:18:GLN:HG2	1:L:26:TYR:CZ	2.39	0.57
1:F:77:GLN:HB3	1:F:79:PHE:HE1	1.69	0.57
1:F:115:PHE:HE2	1:F:145:TYR:CE2	2.22	0.57
1:G:388:ARG:HG2	1:G:388:ARG:NH1	2.12	0.57
1:D:95:LYS:O	1:D:97:ARG:HG2	2.05	0.56
1:E:10:ILE:HG22	1:E:166:ARG:NH1	2.19	0.56
1:E:35:LEU:CD2	1:E:62:GLY:CA	2.83	0.56
1:G:284:GLN:O	1:G:287:VAL:HG13	2.05	0.56
1:K:284:GLN:CA	1:K:287:VAL:HG22	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:310:THR:HG22	1:L:312:ILE:HG23	1.87	0.56
1:A:133:MSE:HE2	1:A:137:ILE:HG22	1.85	0.56
1:A:133:MSE:HE1	1:A:137:ILE:HG22	1.87	0.56
1:D:87:LEU:HD12	1:D:87:LEU:C	2.25	0.56
1:F:178:GLN:HA	1:F:194:ILE:HD13	1.87	0.56
1:G:222:ALA:HA	1:G:256:ASP:OD1	2.05	0.56
1:H:100:LEU:HD12	1:H:100:LEU:N	2.20	0.56
1:A:27:ASP:HB3	1:A:33:ARG:CG	2.35	0.56
1:A:76:ILE:HD13	1:A:90:GLU:HB3	1.87	0.56
1:C:40:LYS:HE3	1:C:60:ASP:CG	2.24	0.56
1:G:99:VAL:HG21	1:G:127:CYS:SG	2.46	0.56
1:H:95:LYS:O	1:H:97:ARG:HG2	2.05	0.56
1:J:89:ASP:OD1	1:J:89:ASP:O	2.23	0.56
1:H:225:SER:OG	1:H:301:SER:OG	2.18	0.56
1:J:33:ARG:HB3	1:J:65:THR:HG22	1.86	0.56
1:J:228:GLN:HG2	1:J:355:PHE:CE2	2.40	0.56
1:L:251:ARG:HG3	1:L:275:GLU:OE1	2.05	0.56
1:A:14:ASP:O	1:A:63:TRP:HH2	1.88	0.56
1:A:16:PRO:HB3	1:A:27:ASP:HB2	1.88	0.56
1:B:24:ILE:CD1	1:B:87:LEU:HD23	2.35	0.56
1:D:253:MSE:HB3	1:D:277:PHE:CD1	2.41	0.56
1:G:27:ASP:O	1:G:32:ALA:CA	2.53	0.56
1:L:322:LEU:HD23	1:L:344:ASP:CB	2.35	0.56
1:E:22:GLU:O	1:E:24:ILE:HD13	2.05	0.56
1:G:24:ILE:N	1:G:24:ILE:HD13	2.21	0.56
1:J:108:LEU:HD11	1:J:302:GLY:N	2.20	0.56
1:A:299:LEU:HB3	1:A:300:PRO:HD2	1.87	0.56
1:B:136:ASP:OD1	1:B:136:ASP:N	2.36	0.56
1:G:80:ARG:HH11	1:G:80:ARG:CG	2.11	0.56
1:I:157:ARG:O	1:I:159:VAL:HG23	2.06	0.56
1:J:89:ASP:O	1:J:89:ASP:CG	2.44	0.56
1:L:287:VAL:HG13	1:L:288:ASN:N	2.21	0.56
1:C:85:THR:HG22	1:C:86:PRO:N	2.19	0.56
1:C:90:GLU:OE2	1:C:90:GLU:HA	2.06	0.56
1:C:326:GLU:OE1	1:C:332:ARG:NH2	2.38	0.56
1:E:59:VAL:HG12	1:E:60:ASP:N	2.21	0.56
1:K:284:GLN:O	1:K:287:VAL:HG23	2.04	0.56
1:C:16:PRO:HG2	1:C:35:LEU:HD23	1.88	0.56
1:A:79:PHE:CE1	1:A:86:PRO:HB3	2.41	0.56
1:C:17:THR:CG2	1:C:160:ALA:CB	2.72	0.56
1:F:28:PHE:CZ	1:F:92:LEU:HD13	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:ASP:HA	1:F:166:ARG:HH21	1.71	0.56
1:I:218:TYR:HB2	1:I:253:MSE:CE	2.35	0.56
1:E:367:GLN:O	1:E:372:ARG:NH2	2.39	0.55
1:I:317:ILE:CA	1:I:333:VAL:HG23	2.11	0.55
1:J:299:LEU:HB3	1:J:300:PRO:HD2	1.88	0.55
1:C:35:LEU:HD23	1:C:35:LEU:H	1.69	0.55
1:F:79:PHE:HZ	1:F:86:PRO:HG3	1.60	0.55
1:J:95:LYS:O	1:J:97:ARG:HG2	2.06	0.55
1:K:284:GLN:HA	1:K:287:VAL:CG2	2.35	0.55
1:K:284:GLN:C	1:K:287:VAL:HG22	2.26	0.55
1:D:41:TRP:CA	1:D:81:GLN:NE2	2.70	0.55
1:D:79:PHE:CD1	1:D:85:THR:C	2.79	0.55
1:I:281:LEU:HB2	1:I:282:PRO:CD	2.33	0.55
1:I:299:LEU:HB3	1:I:300:PRO:HD2	1.89	0.55
1:B:27:ASP:HB2	1:B:29:ASN:ND2	2.22	0.55
1:C:33:ARG:CG	1:C:65:THR:HG22	2.29	0.55
1:C:138:ILE:HD12	1:C:150:PHE:HB3	1.72	0.55
1:H:100:LEU:HD13	1:H:164:THR:HG23	1.89	0.55
1:B:100:LEU:CD1	1:B:164:THR:HG23	2.37	0.55
1:C:10:ILE:CG2	1:C:11:THR:H	2.08	0.55
1:E:47:ASP:O	1:E:51:GLU:N	2.36	0.55
1:F:389:SER:O	1:F:392:GLU:O	2.25	0.55
1:I:158:THR:O	1:I:160:ALA:N	2.39	0.55
1:A:29:ASN:O	1:A:33:ARG:HD3	2.06	0.55
1:B:34:VAL:HG13	1:B:64:VAL:CG2	2.27	0.55
1:E:299:LEU:HB3	1:E:300:PRO:HD2	1.86	0.55
1:L:119:GLU:OE2	1:L:205:ARG:NH2	2.39	0.55
1:F:28:PHE:HZ	1:F:92:LEU:HD13	1.72	0.55
1:E:363:ASN:H	1:E:367:GLN:NE2	2.05	0.55
1:F:79:PHE:CE2	1:F:86:PRO:HB3	2.40	0.55
1:H:16:PRO:HB2	1:H:25:PHE:HB3	1.89	0.55
1:H:100:LEU:HD11	1:H:161:PRO:CB	2.36	0.55
1:L:22:GLU:OE2	1:L:22:GLU:CA	2.55	0.55
1:L:310:THR:O	1:L:310:THR:HG23	2.06	0.55
1:D:88:LEU:HD12	1:D:89:ASP:H	1.69	0.54
1:D:210:ALA:O	1:D:291:ARG:NH1	2.40	0.54
1:E:78:VAL:HG12	1:E:88:LEU:HB2	1.88	0.54
1:I:291:ARG:HA	1:I:310:THR:HG21	1.88	0.54
1:D:100:LEU:HB3	1:D:164:THR:HG23	1.88	0.54
1:F:78:VAL:HG21	1:F:88:LEU:HD11	1.90	0.54
1:I:252:VAL:C	1:I:253:MSE:HE2	2.27	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:137:ILE:HG22	1:K:141:LEU:HD22	1.90	0.54
1:L:252:VAL:CA	1:L:253:MSE:HE2	2.37	0.54
1:A:136:ASP:N	1:A:136:ASP:OD1	2.38	0.54
1:B:130:GLU:HB2	1:B:149:GLN:NE2	2.17	0.54
1:C:138:ILE:HD11	1:C:150:PHE:CA	2.31	0.54
1:D:251:ARG:CB	1:D:253:MSE:HE1	2.35	0.54
1:C:92:LEU:O	1:C:93:LYS:HE3	2.07	0.54
1:A:181:ASP:HB3	1:A:184:LYS:HD2	1.90	0.54
1:F:45:LEU:HD23	1:F:55:PHE:HB3	1.90	0.54
1:G:25:PHE:HD1	1:G:25:PHE:H	1.54	0.54
1:H:129:LEU:HD13	1:H:148:ILE:CG2	2.37	0.54
1:I:136:ASP:OD1	1:I:136:ASP:N	2.36	0.54
1:L:42:HIS:NE2	1:L:56:CYS:SG	2.81	0.54
1:B:28:PHE:CE2	1:B:92:LEU:HB2	2.43	0.54
1:K:395:VAL:H	1:K:397:ALA:N	2.06	0.54
1:B:45:LEU:N	1:B:45:LEU:CD2	2.71	0.54
1:B:253:MSE:HG3	1:B:277:PHE:CD1	2.42	0.54
1:F:84:ALA:O	1:F:85:THR:HG22	2.07	0.54
1:D:101:ILE:CG1	1:D:129:LEU:HD11	2.38	0.54
1:E:26:TYR:CZ	1:E:90:GLU:HG2	2.43	0.54
1:G:158:THR:O	1:G:160:ALA:N	2.38	0.54
1:K:357:TRP:CE2	1:K:359:PRO:HD3	2.43	0.54
1:F:136:ASP:N	1:F:136:ASP:OD1	2.39	0.53
1:G:20:GLY:O	1:G:22:GLU:O	2.25	0.53
1:L:189:ARG:NH2	1:L:324:ASN:O	2.41	0.53
1:C:144:GLN:O	1:C:205:ARG:NH1	2.40	0.53
1:I:24:ILE:CD1	1:I:37:PRO:HD2	2.33	0.53
1:L:16:PRO:HA	1:L:27:ASP:HB2	1.90	0.53
1:F:26:TYR:HB3	1:F:34:VAL:HB	1.88	0.53
1:G:44:ARG:HB3	1:G:77:GLN:HB2	1.91	0.53
1:D:275:GLU:HB3	1:D:277:PHE:CE1	2.44	0.53
1:F:58:ASP:OD1	1:F:58:ASP:N	2.41	0.53
1:G:72:VAL:HG13	1:G:74:PHE:CZ	2.44	0.53
1:H:208:LEU:O	1:H:291:ARG:NE	2.36	0.53
1:L:158:THR:HG23	1:L:159:VAL:N	2.23	0.53
1:H:88:LEU:C	1:H:88:LEU:HD23	2.29	0.53
1:I:60:ASP:N	1:I:60:ASP:OD1	2.41	0.53
1:E:26:TYR:OH	1:E:90:GLU:HG2	2.08	0.53
1:F:13:PRO:O	1:F:14:ASP:CB	2.52	0.53
1:J:189:ARG:HE	3:J:502:EDO:H21	1.73	0.53
1:K:95:LYS:O	1:K:97:ARG:HG2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:VAL:CA	1:K:253:MSE:HE2	2.39	0.53
1:F:300:PRO:HD3	1:F:318:SER:HB2	1.91	0.53
1:B:85:THR:HG22	1:B:86:PRO:HD2	1.90	0.53
1:F:357:TRP:CZ2	1:F:359:PRO:HG3	2.44	0.53
1:J:41:TRP:HD1	1:J:60:ASP:HA	1.74	0.53
1:L:368:PHE:O	1:L:372:ARG:HG3	2.08	0.53
1:B:24:ILE:HD11	1:B:87:LEU:CD2	2.38	0.53
1:E:40:LYS:HG2	1:E:60:ASP:OD1	2.09	0.53
1:F:326:GLU:OE1	1:F:332:ARG:NH2	2.42	0.53
1:H:253:MSE:HE2	1:H:275:GLU:OE1	2.08	0.53
1:J:227:CYS:SG	1:J:230:LYS:HG3	2.49	0.53
1:K:252:VAL:HG23	1:K:252:VAL:O	2.09	0.53
1:C:189:ARG:HE	3:C:502:EDO:HO1	1.57	0.52
1:G:188:HIS:CE1	1:G:325:SER:O	2.62	0.52
1:L:21:PRO:O	1:L:22:GLU:C	2.47	0.52
1:L:22:GLU:O	1:L:22:GLU:CG	2.56	0.52
1:G:22:GLU:OE1	1:G:37:PRO:HG3	2.10	0.52
1:G:34:VAL:HG11	1:G:76:ILE:HG21	1.90	0.52
1:C:230:LYS:HE3	1:C:320:PHE:CZ	2.45	0.52
1:D:46:LEU:HD11	1:D:77:GLN:NE2	2.23	0.52
1:E:78:VAL:HG12	1:E:88:LEU:HB3	1.91	0.52
1:G:80:ARG:NH1	1:G:80:ARG:CG	2.71	0.52
1:L:75:ARG:CG	1:L:91:THR:OG1	2.57	0.52
1:A:255:ILE:HA	1:A:277:PHE:O	2.10	0.52
1:G:95:LYS:O	1:G:97:ARG:HG2	2.10	0.52
1:F:157:ARG:HG2	1:F:157:ARG:NH2	2.24	0.52
1:G:133:MSE:CE	1:G:137:ILE:HG22	2.39	0.52
1:C:95:LYS:O	1:C:97:ARG:HG3	2.09	0.52
1:K:149:GLN:OE1	1:K:157:ARG:HD2	2.10	0.52
1:K:284:GLN:NE2	1:K:287:VAL:CG2	2.73	0.52
1:L:19:ALA:HB2	1:L:25:PHE:CZ	2.45	0.52
1:A:81:GLN:CA	1:A:81:GLN:NE2	2.69	0.52
1:B:95:LYS:O	1:B:97:ARG:HG2	2.09	0.52
1:E:24:ILE:HD13	1:E:24:ILE:H	1.75	0.52
1:H:72:VAL:HB	1:H:74:PHE:CE2	2.43	0.52
1:L:100:LEU:HG	1:L:130:GLU:OE1	2.10	0.52
1:B:100:LEU:HD12	1:B:164:THR:HG23	1.91	0.52
1:C:17:THR:HG22	1:C:160:ALA:CB	2.39	0.52
1:E:38:GLU:O	1:E:41:TRP:HZ2	1.93	0.52
1:H:87:LEU:HD23	1:H:87:LEU:C	2.29	0.52
1:L:20:GLY:O	1:L:21:PRO:C	2.48	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:72:VAL:HG13	1:L:74:PHE:CZ	2.45	0.52
1:G:133:MSE:CE	1:G:137:ILE:CG2	2.87	0.52
1:B:218:TYR:HD2	1:B:253:MSE:HE3	1.75	0.52
1:C:16:PRO:HB3	1:C:27:ASP:HB2	1.92	0.52
1:D:88:LEU:HD12	1:D:88:LEU:C	2.28	0.52
1:E:300:PRO:HD3	1:E:318:SER:HB2	1.91	0.52
1:G:18:GLN:HE22	1:G:97:ARG:HH22	1.52	0.52
1:J:60:ASP:C	1:J:61:LYS:HG3	2.30	0.52
1:D:79:PHE:HE1	1:D:86:PRO:N	2.06	0.51
1:F:64:VAL:O	1:F:64:VAL:HG13	2.08	0.51
1:K:136:ASP:N	1:K:136:ASP:OD1	2.38	0.51
1:L:223:THR:HG22	1:L:238:TRP:CE2	2.45	0.51
1:E:29:ASN:O	1:E:33:ARG:CD	2.57	0.51
1:E:320:PHE:CE2	1:E:343:TRP:HB2	2.45	0.51
1:K:40:LYS:CB	1:K:81:GLN:HG3	2.40	0.51
1:L:322:LEU:HD22	1:L:344:ASP:OD2	2.07	0.51
1:B:30:ASP:HB3	1:B:33:ARG:HD3	1.92	0.51
1:E:22:GLU:HB2	1:E:24:ILE:CD1	2.34	0.51
1:E:22:GLU:CB	1:E:24:ILE:HD13	2.40	0.51
1:F:26:TYR:CD1	1:F:26:TYR:N	2.79	0.51
1:H:44:ARG:NH1	1:H:77:GLN:OE1	2.42	0.51
1:H:299:LEU:HB3	1:H:300:PRO:HD2	1.92	0.51
1:F:299:LEU:HB3	1:F:300:PRO:HD2	1.92	0.51
1:G:16:PRO:HG2	1:G:25:PHE:O	2.11	0.51
1:D:41:TRP:HA	1:D:81:GLN:HE21	1.75	0.51
1:E:39:GLY:O	1:E:60:ASP:HB3	2.10	0.51
1:G:39:GLY:O	1:G:41:TRP:CD1	2.64	0.51
1:I:280:LYS:O	1:I:280:LYS:HG2	2.11	0.51
1:L:136:ASP:OD1	1:L:136:ASP:N	2.39	0.51
1:E:27:ASP:OD2	1:E:33:ARG:NH1	2.44	0.51
1:C:252:VAL:O	1:C:253:MSE:HE3	2.11	0.51
1:G:43:VAL:HG11	1:G:64:VAL:HG21	1.92	0.51
1:L:122:GLN:HG3	1:L:123:SER:N	2.24	0.51
1:B:21:PRO:HG2	1:B:87:LEU:CD2	2.41	0.51
1:F:74:PHE:H	1:F:92:LEU:HD22	1.76	0.51
1:G:133:MSE:HE3	1:G:137:ILE:CG2	2.39	0.51
1:K:29:ASN:HA	1:K:164:THR:N	2.26	0.51
1:D:206:LEU:C	1:D:208:LEU:HD12	2.24	0.51
1:D:291:ARG:O	1:D:292:HIS:HB2	2.10	0.51
1:D:331:TRP:HZ3	1:D:385:LYS:HG2	1.76	0.51
1:F:94:LEU:O	1:F:95:LYS:C	2.49	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLY:O	1:G:32:ALA:CB	2.59	0.51
1:G:158:THR:HG23	1:G:159:VAL:N	2.25	0.51
1:K:100:LEU:HB3	1:K:164:THR:HG23	1.93	0.51
1:L:284:GLN:HA	1:L:287:VAL:HG12	1.93	0.51
1:D:65:THR:HG22	1:D:69:LYS:HZ3	1.76	0.51
1:E:61:LYS:CG	1:E:62:GLY:N	2.72	0.51
1:G:284:GLN:C	1:G:287:VAL:HG12	2.30	0.51
1:H:43:VAL:HG11	1:H:64:VAL:HG21	1.92	0.51
1:I:204:VAL:HG12	1:I:205:ARG:N	2.26	0.51
1:J:108:LEU:CD2	1:J:302:GLY:HA2	2.30	0.51
1:A:44:ARG:HG3	1:A:79:PHE:HE2	1.75	0.50
1:A:218:TYR:HB2	1:A:253:MSE:CE	2.36	0.50
1:C:35:LEU:HD13	1:C:63:TRP:CZ2	2.46	0.50
1:E:357:TRP:CZ2	1:E:359:PRO:HG3	2.46	0.50
1:G:24:ILE:CD1	1:G:24:ILE:N	2.74	0.50
1:G:34:VAL:CG1	1:G:76:ILE:HG21	2.41	0.50
1:G:252:VAL:CA	1:G:253:MSE:HE2	2.42	0.50
1:L:389:SER:O	1:L:393:GLN:O	2.29	0.50
1:C:93:LYS:HA	1:C:93:LYS:CE	2.20	0.50
1:K:388:ARG:O	1:K:392:GLU:HG3	2.11	0.50
1:A:46:LEU:CD2	1:A:53:ILE:CG1	2.89	0.50
1:A:46:LEU:HB2	1:A:75:ARG:HB3	1.94	0.50
1:I:291:ARG:HA	1:I:310:THR:HG22	1.93	0.50
1:K:29:ASN:C	1:K:164:THR:HB	2.31	0.50
1:A:88:LEU:HD12	1:A:89:ASP:N	2.26	0.50
1:B:19:ALA:O	1:B:24:ILE:N	2.45	0.50
1:F:85:THR:HG23	1:F:85:THR:O	2.11	0.50
1:G:284:GLN:O	1:G:287:VAL:HG12	2.11	0.50
1:L:18:GLN:CA	1:L:18:GLN:HE21	2.25	0.50
1:A:72:VAL:HB	1:A:74:PHE:CE2	2.46	0.50
1:A:357:TRP:CZ2	1:A:359:PRO:HG3	2.47	0.50
1:D:18:GLN:HA	1:D:18:GLN:NE2	2.26	0.50
1:D:46:LEU:HB2	1:D:75:ARG:HB3	1.93	0.50
1:D:206:LEU:HD11	1:D:309:ALA:CB	2.41	0.50
1:E:142:ALA:HB3	1:E:143:PRO:HD3	1.92	0.50
1:F:252:VAL:HG23	1:F:274:ALA:HA	1.93	0.50
1:I:119:GLU:OE2	1:I:205:ARG:NH2	2.43	0.50
1:L:357:TRP:CZ2	1:L:359:PRO:HG3	2.46	0.50
1:A:276:ASP:OD1	1:A:276:ASP:O	2.30	0.50
1:K:159:VAL:HG12	1:K:159:VAL:O	2.12	0.50
1:E:87:LEU:HD23	1:E:87:LEU:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:GLU:HG2	1:H:39:GLY:N	2.26	0.50
1:H:253:MSE:HG2	1:H:277:PHE:CD1	2.46	0.50
1:K:251:ARG:HB2	1:K:253:MSE:HE1	1.94	0.50
1:L:19:ALA:CA	1:L:25:PHE:HA	2.30	0.50
1:D:79:PHE:CE1	1:D:86:PRO:HD3	2.47	0.50
1:D:136:ASP:OD1	1:D:136:ASP:N	2.42	0.50
1:D:252:VAL:CA	1:D:253:MSE:HE2	2.42	0.50
1:I:27:ASP:OD2	1:I:29:ASN:ND2	2.40	0.50
1:A:270:ILE:HD12	1:A:276:ASP:HB3	1.90	0.50
1:D:79:PHE:CE1	1:D:86:PRO:CD	2.95	0.50
1:D:175:THR:HG23	1:D:175:THR:O	2.12	0.50
1:H:253:MSE:HG3	1:H:277:PHE:CD1	2.45	0.50
1:J:72:VAL:HB	1:J:74:PHE:CE2	2.47	0.50
1:K:90:GLU:OE1	1:K:90:GLU:HA	2.10	0.50
1:K:395:VAL:N	1:K:397:ALA:N	2.60	0.50
1:A:36:LEU:HD11	1:A:59:VAL:CG1	2.41	0.49
1:C:138:ILE:CG1	1:C:150:PHE:CB	2.90	0.49
1:G:189:ARG:NH2	1:G:201:GLU:OE1	2.45	0.49
1:L:310:THR:O	1:L:310:THR:HG22	2.11	0.49
1:A:18:GLN:HB2	1:A:26:TYR:O	2.12	0.49
1:E:61:LYS:HG2	1:E:62:GLY:H	1.76	0.49
1:F:72:VAL:HB	1:F:74:PHE:CE2	2.47	0.49
1:G:256:ASP:OD1	1:G:256:ASP:N	2.45	0.49
1:H:40:LYS:C	1:H:81:GLN:OE1	2.51	0.49
1:L:20:GLY:O	1:L:21:PRO:O	2.30	0.49
1:L:23:ASN:O	1:L:24:ILE:CB	2.61	0.49
1:C:131:CYS:HB3	1:C:133:MSE:CE	2.42	0.49
1:F:94:LEU:O	1:F:97:ARG:CG	2.57	0.49
1:F:115:PHE:N	1:F:116:PRO:CD	2.75	0.49
1:J:107:THR:OG1	1:J:108:LEU:HD12	2.12	0.49
1:J:251:ARG:C	1:J:253:MSE:CE	2.80	0.49
1:K:26:TYR:CZ	1:K:90:GLU:HG3	2.47	0.49
1:D:82:GLY:O	1:D:83:ALA:HB3	2.13	0.49
1:F:394:GLY:O	1:F:395:VAL:C	2.50	0.49
1:I:252:VAL:CA	1:I:253:MSE:HE2	2.42	0.49
1:B:23:ASN:OD1	1:B:23:ASN:O	2.30	0.49
1:D:275:GLU:HB3	1:D:277:PHE:CD1	2.48	0.49
1:E:77:GLN:HA	1:E:88:LEU:O	2.13	0.49
1:G:300:PRO:HD3	1:G:318:SER:HB2	1.95	0.49
1:H:28:PHE:CD2	1:H:92:LEU:HD12	2.47	0.49
1:I:27:ASP:OD1	1:I:29:ASN:ND2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:365:ASP:O	1:L:372:ARG:NH2	2.45	0.49
1:F:43:VAL:CG1	1:F:78:VAL:HG13	2.38	0.49
1:G:18:GLN:HE21	1:G:97:ARG:HH22	1.59	0.49
1:B:22:GLU:O	1:B:23:ASN:OD1	2.30	0.49
1:J:155:LYS:O	1:J:155:LYS:CG	2.55	0.49
1:K:230:LYS:HE3	1:K:320:PHE:CZ	2.48	0.49
1:B:223:THR:HG22	1:B:238:TRP:CE2	2.47	0.49
1:E:19:ALA:CB	1:E:20:GLY:CA	2.80	0.49
1:I:144:GLN:O	1:I:205:ARG:NH1	2.42	0.49
1:K:72:VAL:HB	1:K:74:PHE:CE2	2.48	0.49
1:D:65:THR:HG22	1:D:69:LYS:NZ	2.27	0.49
1:C:58:ASP:OD1	1:C:58:ASP:N	2.46	0.48
1:C:79:PHE:CE1	1:C:86:PRO:HB3	2.48	0.48
1:E:251:ARG:C	1:E:253:MSE:HE3	2.34	0.48
1:H:206:LEU:O	1:H:208:LEU:HD12	2.12	0.48
1:L:87:LEU:HD23	1:L:87:LEU:O	2.12	0.48
1:D:206:LEU:HD11	1:D:309:ALA:HB3	1.95	0.48
1:F:38:GLU:OE2	1:F:38:GLU:O	2.30	0.48
1:J:108:LEU:HD22	1:J:109:GLY:N	2.27	0.48
1:L:21:PRO:O	1:L:22:GLU:O	2.30	0.48
1:D:41:TRP:C	1:D:81:GLN:NE2	2.67	0.48
1:F:159:VAL:O	1:F:160:ALA:HB3	2.13	0.48
1:I:100:LEU:HB3	1:I:164:THR:HG23	1.94	0.48
1:K:205:ARG:HH11	1:K:205:ARG:CG	2.23	0.48
1:L:16:PRO:CB	1:L:27:ASP:CB	2.79	0.48
1:L:114:TRP:CZ2	1:L:169:LEU:HD13	2.42	0.48
1:B:357:TRP:CZ2	1:B:359:PRO:CG	2.95	0.48
1:D:208:LEU:CD1	1:D:208:LEU:N	2.76	0.48
1:E:22:GLU:C	1:E:24:ILE:HD13	2.34	0.48
1:F:46:LEU:HB2	1:F:75:ARG:HB3	1.95	0.48
1:F:74:PHE:N	1:F:92:LEU:HD22	2.28	0.48
1:H:24:ILE:HG23	1:H:37:PRO:CD	2.44	0.48
1:J:18:GLN:HB2	1:J:26:TYR:O	2.14	0.48
1:L:24:ILE:HG22	1:L:25:PHE:H	1.76	0.48
1:A:133:MSE:HE1	1:A:137:ILE:CG2	2.37	0.48
1:A:366:ARG:O	1:A:369:GLU:HB2	2.14	0.48
1:J:252:VAL:CA	1:J:253:MSE:HE2	2.44	0.48
1:B:253:MSE:CG	1:B:277:PHE:CE1	2.96	0.48
1:C:149:GLN:OE1	1:C:157:ARG:HD3	2.14	0.48
1:C:357:TRP:CZ2	1:C:359:PRO:HG3	2.49	0.48
1:C:257:ARG:HD2	1:C:280:LYS:HD3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LYS:O	1:D:280:LYS:HG3	2.13	0.48
1:G:158:THR:O	1:G:159:VAL:HB	2.14	0.48
1:C:161:PRO:O	1:C:162:TYR:C	2.52	0.48
1:G:27:ASP:HB3	1:G:33:ARG:HE	1.79	0.48
1:I:10:ILE:HD11	1:I:102:SER:OG	2.14	0.48
1:L:95:LYS:O	1:L:97:ARG:HG2	2.14	0.48
1:G:179:PRO:HG2	1:G:193:TYR:HB3	1.96	0.48
1:B:43:VAL:HG11	1:B:64:VAL:HG11	1.95	0.47
1:B:85:THR:HG23	1:B:86:PRO:HD2	1.95	0.47
1:E:14:ASP:O	1:E:63:TRP:HZ2	1.97	0.47
1:I:357:TRP:CZ2	1:I:359:PRO:HG3	2.49	0.47
1:J:357:TRP:CZ2	1:J:359:PRO:HG3	2.49	0.47
1:D:11:THR:HG22	1:D:12:PRO:O	2.15	0.47
1:E:47:ASP:HB3	1:E:50:SER:OG	2.14	0.47
1:F:144:GLN:NE2	1:F:207:ASP:HB2	2.29	0.47
1:G:108:LEU:HD11	1:G:283:LEU:HD22	1.97	0.47
1:C:35:LEU:CD2	1:C:35:LEU:N	2.73	0.47
1:C:85:THR:HG23	1:C:86:PRO:HD3	1.95	0.47
1:D:101:ILE:CD1	1:D:129:LEU:HD11	2.44	0.47
1:E:149:GLN:HE22	1:E:157:ARG:HD3	1.78	0.47
1:F:108:LEU:HD23	1:F:108:LEU:C	2.34	0.47
1:I:251:ARG:C	1:I:253:MSE:CE	2.83	0.47
1:D:83:ALA:HB1	1:D:84:ALA:CB	2.40	0.47
1:D:291:ARG:O	1:D:292:HIS:CB	2.62	0.47
1:F:157:ARG:HG2	1:F:157:ARG:HH21	1.78	0.47
1:F:252:VAL:CA	1:F:253:MSE:HE2	2.45	0.47
1:F:392:GLU:O	1:F:393:GLN:CG	2.61	0.47
1:G:218:TYR:HB2	1:G:253:MSE:CE	2.34	0.47
1:I:252:VAL:O	1:I:275:GLU:HG3	2.15	0.47
1:L:28:PHE:HE2	1:L:92:LEU:HA	1.79	0.47
1:F:160:ALA:N	1:F:161:PRO:HD3	2.29	0.47
1:I:316:LEU:O	1:I:333:VAL:HG23	2.15	0.47
1:J:230:LYS:HE3	1:J:320:PHE:CZ	2.49	0.47
1:L:133:MSE:HE3	1:L:137:ILE:HG21	1.96	0.47
1:L:158:THR:CG2	1:L:159:VAL:N	2.78	0.47
1:C:263:GLN:HG3	1:C:355:PHE:CB	2.45	0.47
1:D:65:THR:HG22	1:D:66:SER:O	2.14	0.47
1:D:223:THR:HG22	1:D:238:TRP:CE2	2.50	0.47
1:F:79:PHE:CG	1:F:86:PRO:HB3	2.49	0.47
1:G:224:GLN:N	1:G:256:ASP:OD2	2.42	0.47
1:G:357:TRP:CZ2	1:G:359:PRO:HG3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:THR:C	1:I:159:VAL:HG23	2.34	0.47
1:J:85:THR:CG2	1:J:86:PRO:HD2	2.44	0.47
1:J:321:SER:HB2	1:J:325:SER:OG	2.15	0.47
1:K:80:ARG:HA	1:K:80:ARG:HD2	1.50	0.47
1:K:394:GLY:CA	1:K:395:VAL:CG2	2.85	0.47
1:L:130:GLU:OE2	1:L:130:GLU:C	2.53	0.47
1:B:38:GLU:HB2	1:B:41:TRP:NE1	2.28	0.47
1:D:72:VAL:HB	1:D:74:PHE:CE2	2.50	0.47
1:D:320:PHE:CE2	1:D:343:TRP:HB2	2.50	0.47
1:H:320:PHE:CE2	1:H:343:TRP:HB2	2.50	0.47
1:J:286:ARG:N	1:J:286:ARG:HD2	2.30	0.47
1:K:252:VAL:HG23	1:K:274:ALA:HA	1.97	0.47
1:L:29:ASN:O	1:L:30:ASP:CB	2.63	0.47
1:A:279:GLY:O	1:A:286:ARG:NH2	2.48	0.47
1:B:115:PHE:HE2	1:B:145:TYR:CE2	2.33	0.47
1:C:66:SER:O	1:C:69:LYS:HE3	2.15	0.47
1:D:291:ARG:NH1	1:D:292:HIS:HE2	2.13	0.47
1:E:251:ARG:HB3	1:E:253:MSE:CE	2.40	0.47
1:F:37:PRO:HG2	1:F:41:TRP:HE1	1.80	0.47
1:L:87:LEU:HD23	1:L:87:LEU:C	2.35	0.47
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.95	0.47
1:C:135:GLN:HE22	1:C:138:ILE:HG21	1.76	0.47
1:E:35:LEU:HD23	1:E:62:GLY:CA	2.45	0.47
1:B:88:LEU:HD23	1:B:89:ASP:N	2.30	0.46
1:B:124:LEU:HD23	1:B:125:HIS:CE1	2.50	0.46
1:E:158:THR:O	1:E:159:VAL:HB	2.16	0.46
1:E:328:TYR:HE2	1:E:399:LEU:HD11	1.80	0.46
1:F:75:ARG:HG3	1:F:90:GLU:O	2.15	0.46
1:G:350:PHE:HA	1:G:357:TRP:CZ2	2.50	0.46
1:L:324:ASN:H	1:L:324:ASN:ND2	2.12	0.46
1:D:18:GLN:HB2	1:D:26:TYR:O	2.16	0.46
1:D:144:GLN:O	1:D:205:ARG:NH1	2.40	0.46
1:H:253:MSE:CE	1:H:275:GLU:CD	2.83	0.46
1:J:350:PHE:HA	1:J:357:TRP:CZ2	2.50	0.46
1:K:320:PHE:CE2	1:K:343:TRP:HB2	2.50	0.46
1:B:27:ASP:CB	1:B:29:ASN:ND2	2.79	0.46
1:D:357:TRP:CZ2	1:D:359:PRO:HG3	2.50	0.46
1:F:37:PRO:CG	1:F:38:GLU:H	2.27	0.46
1:L:253:MSE:HE2	1:L:253:MSE:N	2.31	0.46
1:D:119:GLU:OE1	1:D:145:TYR:CD2	2.69	0.46
1:E:22:GLU:HB3	1:E:24:ILE:HD13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:THR:O	1:H:160:ALA:N	2.46	0.46
1:G:59:VAL:CG1	1:G:61:LYS:O	2.62	0.46
1:J:108:LEU:CD1	1:J:109:GLY:N	2.68	0.46
1:A:24:ILE:HD11	1:A:34:VAL:CG2	2.46	0.46
1:D:385:LYS:HE3	1:D:385:LYS:HB2	1.40	0.46
1:E:101:ILE:HG12	1:E:129:LEU:CD1	2.43	0.46
1:F:41:TRP:HA	1:F:81:GLN:HE22	1.79	0.46
1:I:223:THR:HG22	1:I:238:TRP:CE2	2.50	0.46
1:K:23:ASN:O	1:K:37:PRO:HG3	2.15	0.46
1:K:398:THR:HG22	1:K:398:THR:O	2.16	0.46
1:L:158:THR:O	1:L:160:ALA:N	2.45	0.46
1:F:29:ASN:O	1:F:164:THR:HB	2.16	0.46
1:H:79:PHE:CE1	1:H:85:THR:C	2.88	0.46
1:L:218:TYR:HB2	1:L:253:MSE:CE	2.38	0.46
1:J:108:LEU:HD22	1:J:302:GLY:CA	2.37	0.46
1:K:142:ALA:N	1:K:143:PRO:HD2	2.30	0.46
1:K:205:ARG:HG2	1:K:205:ARG:NH1	2.26	0.46
1:C:138:ILE:CG2	1:C:139:ASP:N	2.79	0.46
1:H:345:ASP:OD2	1:H:360:ARG:NH2	2.49	0.46
1:D:18:GLN:HB3	1:D:26:TYR:CE1	2.51	0.46
1:J:39:GLY:O	1:J:60:ASP:HB2	2.14	0.46
1:E:38:GLU:O	1:E:41:TRP:CE2	2.68	0.45
1:G:133:MSE:HE2	1:G:138:ILE:HA	1.98	0.45
1:B:17:THR:OG1	1:B:160:ALA:HB1	2.16	0.45
1:B:17:THR:CG2	1:B:29:ASN:HD21	2.29	0.45
1:B:21:PRO:CD	1:B:88:LEU:CD1	2.87	0.45
1:E:396:GLU:N	1:E:396:GLU:OE2	2.49	0.45
1:F:84:ALA:O	1:F:85:THR:CG2	2.64	0.45
1:G:48:ALA:HB1	1:G:73:ARG:HH21	1.81	0.45
1:G:389:SER:HG	1:G:398:THR:HG22	1.81	0.45
1:L:16:PRO:HB3	1:L:27:ASP:N	2.30	0.45
1:L:19:ALA:HB2	1:L:25:PHE:CD1	2.52	0.45
1:A:36:LEU:HD11	1:A:59:VAL:HG11	1.97	0.45
1:A:276:ASP:OD2	1:A:278:THR:OG1	2.30	0.45
1:E:291:ARG:HG3	1:E:291:ARG:HH11	1.81	0.45
1:G:30:ASP:HB3	1:G:33:ARG:HD2	1.99	0.45
1:H:24:ILE:HG23	1:H:37:PRO:HD3	1.98	0.45
1:I:28:PHE:CD2	1:I:92:LEU:HD12	2.51	0.45
1:K:114:TRP:CD1	1:K:191:ALA:HB2	2.51	0.45
1:L:144:GLN:O	1:L:205:ARG:NH1	2.46	0.45
1:L:206:LEU:O	1:L:208:LEU:HD12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:VAL:HG11	1:E:61:LYS:CE	2.45	0.45
1:F:79:PHE:CZ	1:F:86:PRO:HD3	2.51	0.45
1:I:22:GLU:HB2	1:I:87:LEU:HD11	1.99	0.45
1:J:218:TYR:HB2	1:J:253:MSE:CE	2.36	0.45
1:K:36:LEU:HD22	1:K:41:TRP:CG	2.51	0.45
1:A:95:LYS:O	1:A:97:ARG:HG2	2.16	0.45
1:F:26:TYR:CB	1:F:34:VAL:HG23	2.43	0.45
1:F:90:GLU:OE1	1:F:90:GLU:CA	2.63	0.45
1:I:345:ASP:OD2	1:I:360:ARG:NH1	2.49	0.45
1:L:291:ARG:HA	1:L:310:THR:HG23	1.99	0.45
1:A:75:ARG:HG3	1:A:91:THR:CG2	2.37	0.45
1:C:30:ASP:O	1:C:69:LYS:HE2	2.16	0.45
1:E:226:THR:OG1	1:E:230:LYS:NZ	2.34	0.45
1:F:223:THR:HG22	1:F:238:TRP:CE2	2.52	0.45
1:G:24:ILE:CD1	1:G:24:ILE:H	2.29	0.45
1:I:253:MSE:HB3	1:I:277:PHE:CE1	2.50	0.45
1:L:17:THR:OG1	1:L:18:GLN:NE2	2.50	0.45
1:C:321:SER:HB2	1:C:325:SER:OG	2.17	0.45
1:D:251:ARG:C	1:D:253:MSE:CE	2.85	0.45
1:D:224:GLN:N	1:D:256:ASP:OD2	2.41	0.45
1:G:158:THR:CG2	1:G:159:VAL:N	2.79	0.45
1:H:21:PRO:O	1:H:24:ILE:CG1	2.65	0.45
1:H:140:LEU:HD11	1:H:287:VAL:HG21	1.99	0.45
1:I:281:LEU:CB	1:I:282:PRO:HD2	2.42	0.45
1:K:38:GLU:OE1	1:K:38:GLU:HA	2.16	0.45
1:K:350:PHE:HA	1:K:357:TRP:CZ2	2.52	0.45
1:L:133:MSE:HE3	1:L:137:ILE:CB	2.36	0.45
1:L:155:LYS:HB2	1:L:155:LYS:HE2	1.73	0.45
1:L:251:ARG:C	1:L:253:MSE:CE	2.85	0.45
1:B:221:ILE:O	1:B:255:ILE:CD1	2.61	0.45
1:K:251:ARG:C	1:K:253:MSE:CE	2.85	0.45
1:L:27:ASP:OD1	1:L:29:ASN:OD1	2.34	0.45
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.98	0.45
1:F:26:TYR:HA	1:F:33:ARG:O	2.17	0.45
1:J:320:PHE:CE2	1:J:343:TRP:HB2	2.52	0.45
1:F:33:ARG:O	1:F:33:ARG:HG2	2.16	0.44
1:G:42:HIS:ND1	1:G:58:ASP:OD1	2.41	0.44
1:H:357:TRP:CZ2	1:H:359:PRO:HG3	2.51	0.44
1:L:189:ARG:NH1	3:L:502:EDO:O1	2.41	0.44
1:H:350:PHE:HA	1:H:357:TRP:CZ2	2.52	0.44
1:E:100:LEU:HB3	1:E:164:THR:HG23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:PHE:O	1:E:286:ARG:NH2	2.43	0.44
1:F:77:GLN:HB3	1:F:79:PHE:CE1	2.51	0.44
1:G:38:GLU:HG3	1:G:39:GLY:N	2.32	0.44
1:L:222:ALA:O	1:L:299:LEU:HD22	2.16	0.44
1:B:91:THR:HG22	1:B:91:THR:O	2.18	0.44
1:B:130:GLU:CB	1:B:149:GLN:HG3	2.48	0.44
1:C:18:GLN:HB2	1:C:26:TYR:O	2.16	0.44
1:C:198:ASP:OD1	1:C:200:ARG:HD3	2.18	0.44
1:E:223:THR:HG22	1:E:238:TRP:CE2	2.52	0.44
1:F:28:PHE:CE2	1:F:92:LEU:CD1	3.00	0.44
1:K:223:THR:HG22	1:K:238:TRP:CE2	2.53	0.44
1:B:218:TYR:HB2	1:B:253:MSE:CE	2.36	0.44
1:F:34:VAL:O	1:F:35:LEU:C	2.54	0.44
1:F:252:VAL:O	1:F:252:VAL:CG2	2.65	0.44
1:A:26:TYR:OH	1:A:90:GLU:HG2	2.18	0.44
1:D:133:MSE:HE3	1:D:137:ILE:CG2	2.47	0.44
1:F:73:ARG:CA	1:F:92:LEU:HD22	2.44	0.44
1:I:72:VAL:HB	1:I:74:PHE:CE2	2.53	0.44
1:J:108:LEU:HD11	1:J:302:GLY:H	1.81	0.44
1:K:124:LEU:HD23	1:K:125:HIS:CE1	2.53	0.44
1:L:28:PHE:HB2	1:L:162:TYR:O	2.18	0.44
1:L:149:GLN:CG	1:L:157:ARG:HH21	2.31	0.44
1:A:14:ASP:O	1:A:63:TRP:CH2	2.71	0.44
1:A:28:PHE:CD2	1:A:92:LEU:HD12	2.52	0.44
1:C:179:PRO:HG2	1:C:193:TYR:HB3	2.00	0.44
1:E:114:TRP:CD1	1:E:191:ALA:HB2	2.52	0.44
1:G:225:SER:OG	1:G:301:SER:OG	2.25	0.44
1:A:223:THR:HG22	1:A:238:TRP:CE2	2.52	0.44
1:B:320:PHE:CE2	1:B:343:TRP:HB2	2.52	0.44
1:F:14:ASP:O	1:F:14:ASP:CG	2.56	0.44
1:F:17:THR:HG21	1:F:161:PRO:O	2.18	0.44
1:H:253:MSE:HG3	1:H:277:PHE:HE1	1.76	0.44
1:J:85:THR:HG23	1:J:86:PRO:HD2	2.00	0.44
1:A:29:ASN:O	1:A:33:ARG:CD	2.66	0.44
1:A:79:PHE:CD1	1:A:86:PRO:HB3	2.53	0.44
1:B:225:SER:OG	1:B:301:SER:OG	2.24	0.44
1:D:28:PHE:CD2	1:D:92:LEU:HD12	2.53	0.44
1:D:80:ARG:HA	1:D:80:ARG:HD2	1.78	0.44
1:E:189:ARG:NH2	1:E:324:ASN:O	2.51	0.44
1:F:251:ARG:HD2	1:F:275:GLU:OE1	2.18	0.44
1:H:20:GLY:N	1:H:24:ILE:O	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:ILE:HG13	1:H:150:PHE:HE1	1.83	0.44
1:H:181:ASP:HB3	1:H:184:LYS:HG3	2.00	0.44
1:B:115:PHE:N	1:B:116:PRO:CD	2.81	0.43
1:H:253:MSE:CE	1:H:275:GLU:OE1	2.65	0.43
1:B:17:THR:HG22	1:B:29:ASN:HD21	1.83	0.43
1:F:12:PRO:O	1:F:13:PRO:C	2.56	0.43
1:F:100:LEU:HB3	1:F:164:THR:HG23	2.00	0.43
1:H:87:LEU:CD2	1:H:87:LEU:C	2.87	0.43
1:H:114:TRP:CD1	1:H:191:ALA:HB2	2.53	0.43
1:H:223:THR:HG22	1:H:238:TRP:CE2	2.53	0.43
1:I:152:THR:CG2	1:I:153:PRO:HD2	2.48	0.43
1:C:101:ILE:HG13	1:C:129:LEU:HD11	2.00	0.43
1:D:291:ARG:HD2	1:D:292:HIS:NE2	2.34	0.43
1:K:40:LYS:N	1:K:80:ARG:NH1	2.65	0.43
1:D:252:VAL:O	1:D:275:GLU:HB2	2.18	0.43
1:J:28:PHE:CD2	1:J:92:LEU:HD12	2.53	0.43
1:L:144:GLN:NE2	1:L:207:ASP:HB2	2.34	0.43
1:A:77:GLN:OE1	1:A:79:PHE:HZ	2.02	0.43
1:E:325:SER:OG	1:E:344:ASP:OD2	2.36	0.43
1:D:174:ASP:OD1	1:D:175:THR:N	2.51	0.43
1:E:130:GLU:OE1	1:E:158:THR:CG2	2.54	0.43
1:G:30:ASP:CB	1:G:33:ARG:HD2	2.48	0.43
1:J:368:PHE:O	1:J:372:ARG:HG3	2.18	0.43
1:K:50:SER:O	1:K:51:GLU:HB2	2.18	0.43
1:A:23:ASN:HB3	1:A:37:PRO:HG3	2.01	0.43
1:G:224:GLN:NE2	1:G:261:TYR:HB3	2.33	0.43
1:L:169:LEU:HD11	1:L:187:PHE:HB2	2.00	0.43
1:D:126:LYS:HD2	1:D:126:LYS:HA	1.58	0.43
1:E:61:LYS:HE2	1:E:61:LYS:HB3	1.76	0.43
1:F:258:ASP:OD1	1:F:258:ASP:N	2.51	0.43
1:F:320:PHE:CE2	1:F:343:TRP:HB2	2.53	0.43
1:H:18:GLN:O	1:H:25:PHE:HA	2.18	0.43
1:H:291:ARG:HG2	1:H:291:ARG:HH11	1.83	0.43
1:L:350:PHE:HA	1:L:357:TRP:CZ2	2.54	0.43
1:B:93:LYS:HB2	1:B:93:LYS:HE3	1.65	0.43
1:C:46:LEU:HB2	1:C:75:ARG:HB3	2.01	0.43
1:C:340:TYR:CD1	1:C:340:TYR:C	2.91	0.43
1:E:169:LEU:HD11	1:E:187:PHE:HB2	1.99	0.43
1:I:300:PRO:HD3	1:I:318:SER:HB2	2.00	0.43
1:J:61:LYS:O	1:J:61:LYS:CD	2.64	0.43
1:K:29:ASN:HA	1:K:164:THR:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLN:N	1:B:256:ASP:OD2	2.43	0.43
1:C:43:VAL:HG22	1:C:57:CYS:O	2.18	0.43
1:C:300:PRO:HD3	1:C:318:SER:HB2	2.00	0.43
1:D:79:PHE:HE1	1:D:85:THR:C	2.19	0.43
1:F:131:CYS:HB3	1:F:133:MSE:HE3	2.01	0.43
1:G:64:VAL:HG13	1:G:64:VAL:O	2.18	0.43
1:G:99:VAL:HG12	1:G:163:ALA:HB3	2.00	0.43
1:L:22:GLU:O	1:L:23:ASN:C	2.57	0.43
1:B:21:PRO:O	1:B:24:ILE:CD1	2.62	0.42
1:B:59:VAL:HG12	1:B:60:ASP:N	2.33	0.42
1:C:140:LEU:O	1:C:140:LEU:HD22	2.19	0.42
1:D:291:ARG:NH1	1:D:292:HIS:CE1	2.76	0.42
1:D:361:HIS:CE1	1:D:366:ARG:HH21	2.37	0.42
1:E:44:ARG:NH1	1:E:77:GLN:OE1	2.52	0.42
1:F:242:ILE:HG23	1:F:252:VAL:HG21	2.01	0.42
1:A:300:PRO:HD3	1:A:318:SER:HB2	2.01	0.42
1:B:27:ASP:CG	1:B:29:ASN:ND2	2.66	0.42
1:C:16:PRO:HB2	1:C:25:PHE:HB3	2.01	0.42
1:C:263:GLN:HB2	1:C:355:PHE:CD2	2.55	0.42
1:G:133:MSE:CE	1:G:137:ILE:CB	2.84	0.42
1:G:287:VAL:HG23	1:G:310:THR:HG22	2.01	0.42
1:H:115:PHE:CZ	1:H:148:ILE:HD12	2.41	0.42
1:K:284:GLN:CD	1:K:287:VAL:HG21	2.40	0.42
1:C:36:LEU:HD13	1:C:36:LEU:H	1.83	0.42
1:H:208:LEU:HD21	1:H:310:THR:HA	2.00	0.42
1:H:286:ARG:N	1:H:286:ARG:HD2	2.33	0.42
1:L:109:GLY:CA	1:L:302:GLY:HA2	2.49	0.42
1:B:300:PRO:HD3	1:B:318:SER:HB2	2.01	0.42
1:C:350:PHE:HA	1:C:357:TRP:CZ2	2.54	0.42
1:F:114:TRP:CD1	1:F:191:ALA:HB2	2.54	0.42
1:I:29:ASN:OD1	1:I:161:PRO:HG2	2.19	0.42
1:L:99:VAL:HG23	1:L:163:ALA:O	2.20	0.42
1:A:276:ASP:CG	1:A:278:THR:CG2	2.66	0.42
1:I:78:VAL:HG23	1:I:88:LEU:HD23	2.01	0.42
1:L:233:ASN:HB2	1:L:371:THR:OG1	2.20	0.42
1:C:100:LEU:HB3	1:C:164:THR:HG23	2.02	0.42
1:D:252:VAL:N	1:D:253:MSE:HE2	2.33	0.42
1:E:42:HIS:CD2	1:E:58:ASP:OD1	2.73	0.42
1:L:19:ALA:HA	1:L:25:PHE:CA	2.31	0.42
1:B:93:LYS:O	1:B:162:TYR:HE2	2.02	0.42
1:E:35:LEU:CD2	1:E:62:GLY:C	2.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:PRO:O	1:G:41:TRP:HZ2	2.03	0.42
1:J:108:LEU:CD1	1:J:108:LEU:N	2.82	0.42
1:A:79:PHE:HE1	1:A:86:PRO:HG3	1.84	0.42
1:G:46:LEU:HB2	1:G:75:ARG:HB3	2.01	0.42
1:G:286:ARG:HG2	1:G:286:ARG:HH11	1.85	0.42
1:H:79:PHE:CE2	1:H:86:PRO:HB3	2.54	0.42
1:I:115:PHE:N	1:I:116:PRO:CD	2.82	0.42
1:A:26:TYR:CZ	1:A:90:GLU:HG2	2.54	0.42
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.85	0.42
1:E:252:VAL:C	1:E:253:MSE:CE	2.84	0.42
1:K:390:LEU:HD23	1:K:390:LEU:HA	1.88	0.42
1:A:253:MSE:HB3	1:A:277:PHE:CD2	2.55	0.41
1:A:320:PHE:CE2	1:A:343:TRP:HB2	2.55	0.41
1:B:115:PHE:CD1	1:B:133:MSE:HE1	2.55	0.41
1:B:286:ARG:N	1:B:286:ARG:HD2	2.35	0.41
1:C:286:ARG:N	1:C:286:ARG:HD2	2.34	0.41
1:D:101:ILE:HD12	1:D:129:LEU:HD11	2.01	0.41
1:E:35:LEU:CD2	1:E:62:GLY:O	2.57	0.41
1:E:368:PHE:HD2	1:L:265:PHE:CG	2.38	0.41
1:J:130:GLU:OE1	1:J:158:THR:OG1	2.30	0.41
1:K:42:HIS:ND1	1:K:58:ASP:OD1	2.52	0.41
1:K:300:PRO:HD3	1:K:318:SER:HB2	2.03	0.41
1:C:223:THR:HG22	1:C:238:TRP:CE2	2.55	0.41
1:D:17:THR:HG23	1:D:160:ALA:HB3	2.02	0.41
1:D:107:THR:O	1:D:110:ASP:HB2	2.21	0.41
1:G:29:ASN:HA	1:G:164:THR:H	1.85	0.41
1:I:397:ALA:O	1:I:398:THR:C	2.58	0.41
1:J:107:THR:OG1	1:J:108:LEU:CD1	2.68	0.41
1:A:219:VAL:O	1:A:253:MSE:CE	2.68	0.41
1:B:59:VAL:CG1	1:B:60:ASP:N	2.83	0.41
1:B:174:ASP:OD1	1:B:174:ASP:C	2.58	0.41
1:D:22:GLU:HG2	1:D:87:LEU:HD21	2.02	0.41
1:E:72:VAL:HB	1:E:74:PHE:CE2	2.55	0.41
1:I:204:VAL:CG1	1:I:205:ARG:N	2.83	0.41
1:L:27:ASP:OD2	1:L:29:ASN:OD1	2.38	0.41
1:L:29:ASN:ND2	1:L:161:PRO:HG2	2.35	0.41
1:L:100:LEU:CD1	1:L:130:GLU:OE1	2.68	0.41
1:L:227:CYS:SG	1:L:230:LYS:HG3	2.60	0.41
1:B:20:GLY:HA3	1:B:24:ILE:HB	2.02	0.41
1:L:99:VAL:HG13	1:L:129:LEU:HD13	2.02	0.41
1:K:218:TYR:HB2	1:K:253:MSE:CE	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HA	1:E:340:TYR:OH	2.21	0.41
1:D:350:PHE:HA	1:D:357:TRP:CZ2	2.55	0.41
1:F:218:TYR:HB2	1:F:253:MSE:CE	2.42	0.41
1:G:28:PHE:CA	1:G:32:ALA:H	2.31	0.41
1:G:30:ASP:HA	1:G:166:ARG:HH12	1.84	0.41
1:H:109:GLY:CA	1:H:302:GLY:HA2	2.51	0.41
1:I:149:GLN:CD	1:I:157:ARG:HD3	2.39	0.41
1:L:29:ASN:ND2	1:L:164:THR:OG1	2.48	0.41
1:L:149:GLN:CD	1:L:157:ARG:NH2	2.74	0.41
1:B:365:ASP:OD1	1:B:365:ASP:N	2.41	0.41
1:H:23:ASN:O	1:H:37:PRO:CG	2.69	0.41
1:H:78:VAL:HG23	1:H:88:LEU:HD22	2.02	0.41
1:K:20:GLY:N	1:K:24:ILE:O	2.36	0.41
1:K:29:ASN:OD1	1:K:161:PRO:HG2	2.21	0.41
1:L:284:GLN:O	1:L:287:VAL:HG13	2.17	0.41
1:B:19:ALA:O	1:B:24:ILE:HG22	2.20	0.41
1:B:24:ILE:HG22	1:B:25:PHE:N	2.35	0.41
1:E:17:THR:HG21	1:E:29:ASN:HD21	1.85	0.41
1:G:133:MSE:HE2	1:G:138:ILE:N	2.36	0.41
1:K:149:GLN:HG2	1:K:157:ARG:NH1	2.35	0.41
1:L:284:GLN:HA	1:L:287:VAL:CG1	2.50	0.41
1:A:140:LEU:HD11	1:A:287:VAL:HG21	2.03	0.41
1:B:255:ILE:HD13	1:B:255:ILE:H	1.85	0.41
1:D:144:GLN:NE2	1:D:207:ASP:N	2.67	0.41
1:E:68:LYS:HA	1:E:68:LYS:HD3	1.81	0.41
1:E:80:ARG:O	1:E:81:GLN:C	2.60	0.41
1:E:354:ASP:OD2	1:E:362:LYS:NZ	2.46	0.41
1:F:103:PHE:CD2	1:F:133:MSE:HE2	2.56	0.41
1:F:281:LEU:HB3	1:F:285:GLU:CD	2.34	0.41
1:G:28:PHE:CD2	1:G:92:LEU:HD12	2.56	0.41
1:G:144:GLN:O	1:G:205:ARG:NH1	2.46	0.41
1:G:147:GLN:HG2	1:G:148:ILE:HG13	2.02	0.41
1:I:18:GLN:HB2	1:I:26:TYR:O	2.21	0.41
1:I:21:PRO:HG2	1:I:87:LEU:CD1	2.45	0.41
1:L:26:TYR:CZ	1:L:90:GLU:HG3	2.55	0.41
1:L:174:ASP:C	1:L:174:ASP:OD1	2.59	0.41
1:L:284:GLN:CA	1:L:287:VAL:HG12	2.49	0.41
1:D:89:ASP:OD1	1:D:89:ASP:C	2.59	0.41
1:E:87:LEU:H	1:E:87:LEU:CD2	2.34	0.41
1:E:107:THR:OG1	1:E:108:LEU:N	2.53	0.41
1:F:80:ARG:H	1:F:80:ARG:HG2	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:LEU:HD22	1:G:164:THR:HG23	2.03	0.41
1:G:251:ARG:C	1:G:253:MSE:CE	2.89	0.41
1:K:253:MSE:HE2	1:K:253:MSE:N	2.36	0.41
1:K:395:VAL:N	1:K:396:GLU:C	2.74	0.41
1:B:92:LEU:HA	1:B:162:TYR:OH	2.20	0.40
1:B:253:MSE:CG	1:B:277:PHE:CD1	3.04	0.40
1:C:122:GLN:HG3	1:C:123:SER:N	2.37	0.40
1:C:161:PRO:HG2	1:C:164:THR:OG1	2.21	0.40
1:E:21:PRO:O	1:E:24:ILE:HD11	2.13	0.40
1:E:21:PRO:O	1:E:24:ILE:N	2.43	0.40
1:F:18:GLN:HB2	1:F:26:TYR:CE1	2.56	0.40
1:G:223:THR:HG22	1:G:238:TRP:CE2	2.56	0.40
1:I:107:THR:OG1	1:I:108:LEU:N	2.54	0.40
1:J:142:ALA:HB3	1:J:143:PRO:HD3	2.03	0.40
1:L:320:PHE:CE2	1:L:343:TRP:HB2	2.57	0.40
1:A:20:GLY:N	1:A:24:ILE:O	2.48	0.40
1:A:76:ILE:CD1	1:A:76:ILE:N	2.72	0.40
1:D:46:LEU:HD21	1:D:53:ILE:CD1	2.49	0.40
1:G:80:ARG:NH1	1:G:87:LEU:HD21	2.36	0.40
1:J:253:MSE:HE2	1:J:253:MSE:N	2.36	0.40
1:K:18:GLN:O	1:K:25:PHE:HA	2.21	0.40
1:K:89:ASP:OD1	1:K:89:ASP:O	2.39	0.40
1:K:252:VAL:N	1:K:253:MSE:HE2	2.37	0.40
1:J:20:GLY:CA	1:J:24:ILE:O	2.68	0.40
1:J:70:TYR:CE2	1:J:179:PRO:HA	2.56	0.40
1:L:21:PRO:HB2	1:L:87:LEU:CD2	2.13	0.40
1:A:106:GLY:O	1:A:107:THR:C	2.60	0.40
1:D:286:ARG:N	1:D:286:ARG:HD2	2.37	0.40
1:F:78:VAL:CB	1:F:88:LEU:HD12	2.48	0.40
1:F:140:LEU:HD11	1:F:287:VAL:HG21	2.04	0.40
1:G:16:PRO:HB2	1:G:25:PHE:C	2.42	0.40
1:G:393:GLN:HB3	1:G:397:ALA:CB	2.51	0.40
1:I:174:ASP:OD1	1:I:174:ASP:C	2.60	0.40
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.78	0.40
1:E:30:ASP:HB3	1:E:33:ARG:HD2	2.04	0.40
1:E:59:VAL:CG1	1:E:60:ASP:N	2.84	0.40
1:E:394:GLY:C	1:E:395:VAL:HG13	2.42	0.40
1:F:253:MSE:HE2	1:F:253:MSE:N	2.37	0.40
1:G:160:ALA:HA	1:G:161:PRO:HD3	1.86	0.40
1:H:300:PRO:HD3	1:H:318:SER:HB2	2.02	0.40
1:K:28:PHE:CD2	1:K:92:LEU:HD13	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:300:PRO:HD3	1:L:318:SER:HB2	2.02	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	377/406 (93%)	369 (98%)	8 (2%)	0	100	100
1	B	381/406 (94%)	368 (97%)	11 (3%)	2 (0%)	25	53
1	C	387/406 (95%)	373 (96%)	13 (3%)	1 (0%)	37	63
1	D	377/406 (93%)	363 (96%)	12 (3%)	2 (0%)	25	53
1	E	388/406 (96%)	369 (95%)	15 (4%)	4 (1%)	13	36
1	F	375/406 (92%)	358 (96%)	15 (4%)	2 (0%)	25	53
1	G	387/406 (95%)	370 (96%)	12 (3%)	5 (1%)	10	30
1	H	383/406 (94%)	370 (97%)	12 (3%)	1 (0%)	37	63
1	I	387/406 (95%)	373 (96%)	13 (3%)	1 (0%)	37	63
1	J	382/406 (94%)	371 (97%)	10 (3%)	1 (0%)	37	63
1	K	387/406 (95%)	376 (97%)	9 (2%)	2 (0%)	25	53
1	L	365/406 (90%)	345 (94%)	16 (4%)	4 (1%)	12	34
All	All	4576/4872 (94%)	4405 (96%)	146 (3%)	25 (0%)	25	53

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	21	PRO
1	E	23	ASN
1	E	395	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	33	ARG
1	I	397	ALA
1	F	62	GLY
1	L	21	PRO
1	L	22	GLU
1	B	25	PHE
1	C	161	PRO
1	G	161	PRO
1	L	161	PRO
1	E	161	PRO
1	F	95	LYS
1	G	31	GLY
1	J	81	GLN
1	B	62	GLY
1	D	207	ASP
1	G	19	ALA
1	G	32	ALA
1	K	21	PRO
1	L	23	ASN
1	D	83	ALA
1	K	37	PRO
1	H	161	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	331/347 (95%)	300 (91%)	31 (9%)	7 21
1	B	332/347 (96%)	308 (93%)	24 (7%)	12 32
1	C	336/347 (97%)	315 (94%)	21 (6%)	15 39
1	D	330/347 (95%)	299 (91%)	31 (9%)	7 21
1	E	337/347 (97%)	311 (92%)	26 (8%)	10 29
1	F	330/347 (95%)	282 (86%)	48 (14%)	2 7
1	G	336/347 (97%)	315 (94%)	21 (6%)	15 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	333/347 (96%)	311 (93%)	22 (7%)	14 36
1	I	336/347 (97%)	312 (93%)	24 (7%)	12 33
1	J	333/347 (96%)	312 (94%)	21 (6%)	15 39
1	K	336/347 (97%)	312 (93%)	24 (7%)	12 33
1	L	321/347 (92%)	290 (90%)	31 (10%)	6 19
All	All	3991/4164 (96%)	3667 (92%)	324 (8%)	9 27

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	23	ASN
1	A	36	LEU
1	A	59	VAL
1	A	66	SER
1	A	76	ILE
1	A	80	ARG
1	A	81	GLN
1	A	87	LEU
1	A	92	LEU
1	A	105	THR
1	A	107	THR
1	A	108	LEU
1	A	111	LEU
1	A	147	GLN
1	A	149	GLN
1	A	152	THR
1	A	158	THR
1	A	174	ASP
1	A	221	ILE
1	A	224	GLN
1	A	253	MSE
1	A	257	ARG
1	A	263	GLN
1	A	275	GLU
1	A	276	ASP
1	A	278	THR
1	A	290	LEU
1	A	320	PHE
1	A	339	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	371	THR
1	B	9	PHE
1	B	24	ILE
1	B	30	ASP
1	B	36	LEU
1	B	45	LEU
1	B	60	ASP
1	B	80	ARG
1	B	88	LEU
1	B	91	THR
1	B	92	LEU
1	B	93	LYS
1	B	100	LEU
1	B	123	SER
1	B	133	MSE
1	B	158	THR
1	B	159	VAL
1	B	224	GLN
1	B	253	MSE
1	B	255	ILE
1	B	286	ARG
1	B	291	ARG
1	B	320	PHE
1	B	339	CYS
1	B	371	THR
1	C	22	GLU
1	C	33	ARG
1	C	35	LEU
1	C	36	LEU
1	C	45	LEU
1	C	58	ASP
1	C	69	LYS
1	C	92	LEU
1	C	93	LYS
1	C	122	GLN
1	C	136	ASP
1	C	138	ILE
1	C	140	LEU
1	C	157	ARG
1	C	169	LEU
1	C	174	ASP
1	C	226	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	253	MSE
1	C	286	ARG
1	C	320	PHE
1	C	339	CYS
1	D	14	ASP
1	D	18	GLN
1	D	22	GLU
1	D	41	TRP
1	D	45	LEU
1	D	53	ILE
1	D	56	CYS
1	D	61	LYS
1	D	80	ARG
1	D	81	GLN
1	D	87	LEU
1	D	95	LYS
1	D	100	LEU
1	D	111	LEU
1	D	126	LYS
1	D	133	MSE
1	D	147	GLN
1	D	157	ARG
1	D	175	THR
1	D	206	LEU
1	D	224	GLN
1	D	253	MSE
1	D	256	ASP
1	D	275	GLU
1	D	281	LEU
1	D	286	ARG
1	D	291	ARG
1	D	320	PHE
1	D	339	CYS
1	D	348	LEU
1	D	391	THR
1	E	15	THR
1	E	17	THR
1	E	22	GLU
1	E	23	ASN
1	E	24	ILE
1	E	35	LEU
1	E	38	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	54	LEU
1	E	60	ASP
1	E	61	LYS
1	E	87	LEU
1	E	88	LEU
1	E	107	THR
1	E	111	LEU
1	E	119	GLU
1	E	123	SER
1	E	136	ASP
1	E	169	LEU
1	E	253	MSE
1	E	281	LEU
1	E	290	LEU
1	E	320	PHE
1	E	339	CYS
1	E	348	LEU
1	E	395	VAL
1	E	396	GLU
1	F	9	PHE
1	F	10	ILE
1	F	11	THR
1	F	15	THR
1	F	26	TYR
1	F	28	PHE
1	F	30	ASP
1	F	33	ARG
1	F	38	GLU
1	F	45	LEU
1	F	54	LEU
1	F	56	CYS
1	F	57	CYS
1	F	58	ASP
1	F	63	TRP
1	F	76	ILE
1	F	80	ARG
1	F	81	GLN
1	F	87	LEU
1	F	89	ASP
1	F	90	GLU
1	F	92	LEU
1	F	93	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	107	THR
1	F	108	LEU
1	F	111	LEU
1	F	122	GLN
1	F	129	LEU
1	F	147	GLN
1	F	149	GLN
1	F	151	SER
1	F	155	LYS
1	F	157	ARG
1	F	158	THR
1	F	169	LEU
1	F	205	ARG
1	F	224	GLN
1	F	226	THR
1	F	253	MSE
1	F	258	ASP
1	F	280	LYS
1	F	290	LEU
1	F	306	LEU
1	F	320	PHE
1	F	339	CYS
1	F	371	THR
1	F	390	LEU
1	F	393	GLN
1	G	22	GLU
1	G	24	ILE
1	G	25	PHE
1	G	35	LEU
1	G	36	LEU
1	G	40	LYS
1	G	41	TRP
1	G	61	LYS
1	G	72	VAL
1	G	80	ARG
1	G	81	GLN
1	G	92	LEU
1	G	111	LEU
1	G	253	MSE
1	G	281	LEU
1	G	320	PHE
1	G	339	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	356	LEU
1	G	359	PRO
1	G	371	THR
1	G	388	ARG
1	H	22	GLU
1	H	24	ILE
1	H	80	ARG
1	H	81	GLN
1	H	92	LEU
1	H	100	LEU
1	H	107	THR
1	H	108	LEU
1	H	111	LEU
1	H	129	LEU
1	H	148	ILE
1	H	166	ARG
1	H	174	ASP
1	H	180	VAL
1	H	253	MSE
1	H	257	ARG
1	H	281	LEU
1	H	286	ARG
1	H	320	PHE
1	H	339	CYS
1	H	360	ARG
1	H	393	GLN
1	I	11	THR
1	I	35	LEU
1	I	40	LYS
1	I	56	CYS
1	I	60	ASP
1	I	61	LYS
1	I	65	THR
1	I	81	GLN
1	I	92	LEU
1	I	100	LEU
1	I	107	THR
1	I	108	LEU
1	I	152	THR
1	I	158	THR
1	I	247	SER
1	I	253	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	280	LYS
1	I	281	LEU
1	I	289	LEU
1	I	290	LEU
1	I	320	PHE
1	I	333	VAL
1	I	339	CYS
1	I	371	THR
1	J	33	ARG
1	J	35	LEU
1	J	58	ASP
1	J	60	ASP
1	J	61	LYS
1	J	89	ASP
1	J	99	VAL
1	J	108	LEU
1	J	122	GLN
1	J	136	ASP
1	J	141	LEU
1	J	158	THR
1	J	166	ARG
1	J	180	VAL
1	J	226	THR
1	J	253	MSE
1	J	281	LEU
1	J	286	ARG
1	J	320	PHE
1	J	339	CYS
1	J	356	LEU
1	K	10	ILE
1	K	18	GLN
1	K	24	ILE
1	K	38	GLU
1	K	61	LYS
1	K	68	LYS
1	K	80	ARG
1	K	89	ASP
1	K	100	LEU
1	K	107	THR
1	K	141	LEU
1	K	166	ARG
1	K	174	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	180	VAL
1	K	205	ARG
1	K	226	THR
1	K	253	MSE
1	K	263	GLN
1	K	281	LEU
1	K	291	ARG
1	K	320	PHE
1	K	339	CYS
1	K	382	VAL
1	K	396	GLU
1	L	14	ASP
1	L	17	THR
1	L	18	GLN
1	L	22	GLU
1	L	24	ILE
1	L	41	TRP
1	L	65	THR
1	L	72	VAL
1	L	75	ARG
1	L	88	LEU
1	L	107	THR
1	L	111	LEU
1	L	130	GLU
1	L	154	ASP
1	L	155	LYS
1	L	169	LEU
1	L	245	LEU
1	L	247	SER
1	L	248	LEU
1	L	251	ARG
1	L	253	MSE
1	L	281	LEU
1	L	286	ARG
1	L	299	LEU
1	L	303	LEU
1	L	310	THR
1	L	320	PHE
1	L	322	LEU
1	L	324	ASN
1	L	339	CYS
1	L	371	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	149	GLN
1	A	367	GLN
1	B	29	ASN
1	B	122	GLN
1	B	125	HIS
1	B	149	GLN
1	B	178	GLN
1	C	81	GLN
1	C	135	GLN
1	D	81	GLN
1	D	144	GLN
1	D	268	ASN
1	D	335	ASN
1	E	42	HIS
1	E	149	GLN
1	E	349	ASN
1	E	367	GLN
1	F	18	GLN
1	F	29	ASN
1	F	81	GLN
1	F	149	GLN
1	F	176	ASN
1	F	284	GLN
1	G	23	ASN
1	G	81	GLN
1	G	224	GLN
1	H	228	GLN
1	H	244	HIS
1	H	268	ASN
1	J	18	GLN
1	J	176	ASN
1	K	23	ASN
1	K	177	ASN
1	K	244	HIS
1	L	18	GLN
1	L	29	ASN
1	L	81	GLN
1	L	324	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	C	502	-	3,3,3	0.28	0	2,2,2	0.77	0
3	EDO	I	502	-	3,3,3	0.29	0	2,2,2	0.61	0
3	EDO	I	503	-	3,3,3	0.57	0	2,2,2	0.46	0
3	EDO	L	502	-	3,3,3	0.25	0	2,2,2	0.91	0
3	EDO	J	502	-	3,3,3	0.30	0	2,2,2	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	I	502	-	-	1/1/1/1	-
3	EDO	I	503	-	-	1/1/1/1	-
3	EDO	L	502	-	-	1/1/1/1	-
3	EDO	J	502	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	502	EDO	O1-C1-C2-O2
3	L	502	EDO	O1-C1-C2-O2
3	I	503	EDO	O1-C1-C2-O2
3	J	502	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	EDO	2	0
3	L	502	EDO	1	0
3	J	502	EDO	1	0

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	379/406 (93%)	-0.03	10 (2%)	57	52	44, 69, 108, 132	0
1	B	381/406 (93%)	-0.09	15 (3%)	44	38	42, 64, 114, 148	0
1	C	387/406 (95%)	-0.18	14 (3%)	46	41	34, 56, 114, 146	0
1	D	379/406 (93%)	-0.05	15 (3%)	43	37	25, 66, 108, 129	0
1	E	388/406 (95%)	-0.14	14 (3%)	46	41	26, 59, 109, 131	0
1	F	380/406 (93%)	0.21	40 (10%)	13	12	25, 66, 125, 151	0
1	G	387/406 (95%)	-0.02	23 (5%)	29	25	30, 65, 114, 150	0
1	H	383/406 (94%)	-0.12	8 (2%)	63	58	44, 66, 106, 128	0
1	I	387/406 (95%)	-0.13	9 (2%)	61	55	40, 65, 108, 125	0
1	J	382/406 (94%)	-0.31	5 (1%)	74	70	35, 59, 97, 117	0
1	K	387/406 (95%)	-0.28	9 (2%)	61	55	37, 57, 98, 124	0
1	L	369/406 (90%)	0.17	27 (7%)	22	19	37, 67, 116, 132	0
All	All	4589/4872 (94%)	-0.08	189 (4%)	42	36	25, 64, 112, 151	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	35	LEU	8.2
1	F	34	VAL	6.7
1	L	31	GLY	6.2
1	K	10	ILE	6.0
1	G	21	PRO	6.0
1	I	30	ASP	5.9
1	G	32	ALA	5.9
1	E	21	PRO	5.6
1	G	62	GLY	5.5
1	A	79	PHE	5.2
1	C	159	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	324	ASN	5.1
1	G	395	VAL	4.9
1	F	87	LEU	4.8
1	A	342	CYS	4.7
1	L	342	CYS	4.7
1	F	29	ASN	4.7
1	F	92	LEU	4.6
1	F	88	LEU	4.6
1	F	9	PHE	4.5
1	E	22	GLU	4.5
1	F	395	VAL	4.4
1	L	12	PRO	4.4
1	F	28	PHE	4.4
1	C	160	ALA	4.3
1	F	22	GLU	4.3
1	B	88	LEU	4.3
1	G	325	SER	4.3
1	G	61	LYS	4.2
1	L	57	CYS	4.2
1	F	31	GLY	4.1
1	C	161	PRO	4.0
1	F	37	PRO	4.0
1	G	20	GLY	4.0
1	H	342	CYS	3.9
1	A	10	ILE	3.9
1	D	24	ILE	3.9
1	G	23	ASN	3.9
1	D	85	THR	3.9
1	E	342	CYS	3.8
1	L	371	THR	3.8
1	B	9	PHE	3.8
1	D	342	CYS	3.8
1	F	89	ASP	3.8
1	E	20	GLY	3.8
1	B	342	CYS	3.8
1	F	342	CYS	3.7
1	K	29	ASN	3.7
1	I	342	CYS	3.7
1	G	18	GLN	3.6
1	H	10	ILE	3.6
1	D	25	PHE	3.6
1	G	342	CYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	79	PHE	3.5
1	I	398	THR	3.5
1	K	342	CYS	3.5
1	A	159	VAL	3.5
1	B	370	CYS	3.4
1	K	397	ALA	3.4
1	H	370	CYS	3.4
1	A	370	CYS	3.4
1	C	342	CYS	3.4
1	G	159	VAL	3.3
1	F	39	GLY	3.3
1	J	342	CYS	3.3
1	A	83	ALA	3.3
1	E	370	CYS	3.3
1	C	158	THR	3.3
1	G	25	PHE	3.2
1	D	207	ASP	3.2
1	G	22	GLU	3.2
1	F	94	LEU	3.2
1	D	84	ALA	3.1
1	F	78	VAL	3.1
1	G	59	VAL	3.1
1	F	159	VAL	3.1
1	L	85	THR	3.1
1	F	33	ARG	3.1
1	E	399	LEU	3.1
1	E	24	ILE	3.1
1	G	24	ILE	3.1
1	E	18	GLN	3.0
1	F	158	THR	3.0
1	C	357	TRP	3.0
1	C	370	CYS	2.9
1	D	370	CYS	2.9
1	B	24	ILE	2.9
1	H	38	GLU	2.9
1	G	31	GLY	2.9
1	C	61	LYS	2.8
1	F	394	GLY	2.8
1	C	21	PRO	2.8
1	D	158	THR	2.8
1	D	391	THR	2.8
1	I	10	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	93	LYS	2.8
1	G	370	CYS	2.8
1	L	25	PHE	2.8
1	L	43	VAL	2.7
1	L	159	VAL	2.7
1	F	370	CYS	2.7
1	F	62	GLY	2.7
1	F	63	TRP	2.7
1	G	63	TRP	2.7
1	H	160	ALA	2.7
1	B	37	PRO	2.7
1	H	339	CYS	2.6
1	F	76	ILE	2.6
1	J	10	ILE	2.6
1	L	130	GLU	2.6
1	I	370	CYS	2.6
1	D	82	GLY	2.6
1	E	159	VAL	2.6
1	F	80	ARG	2.6
1	F	26	TYR	2.6
1	F	43	VAL	2.6
1	E	339	CYS	2.5
1	L	86	PRO	2.5
1	I	87	LEU	2.5
1	L	27	ASP	2.5
1	L	370	CYS	2.5
1	B	62	GLY	2.5
1	C	59	VAL	2.5
1	B	339	CYS	2.5
1	I	339	CYS	2.5
1	J	370	CYS	2.5
1	K	370	CYS	2.5
1	H	340	TYR	2.5
1	I	27	ASP	2.4
1	F	64	VAL	2.4
1	D	160	ALA	2.4
1	E	25	PHE	2.4
1	G	81	GLN	2.4
1	H	159	VAL	2.4
1	G	160	ALA	2.4
1	J	256	ASP	2.4
1	K	395	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	339	CYS	2.4
1	F	82	GLY	2.3
1	G	19	ALA	2.3
1	L	160	ALA	2.3
1	F	15	THR	2.3
1	D	21	PRO	2.3
1	E	61	LYS	2.3
1	D	20	GLY	2.3
1	L	83	ALA	2.3
1	B	147	GLN	2.3
1	L	395	VAL	2.3
1	F	90	GLU	2.3
1	L	28	PHE	2.3
1	E	87	LEU	2.3
1	L	157	ARG	2.2
1	F	30	ASP	2.2
1	I	159	VAL	2.2
1	B	157	ARG	2.2
1	B	87	LEU	2.2
1	G	40	LYS	2.2
1	L	56	CYS	2.2
1	C	88	LEU	2.2
1	L	17	THR	2.2
1	B	25	PHE	2.2
1	D	131	CYS	2.2
1	F	16	PRO	2.2
1	F	154	ASP	2.2
1	L	96	ASP	2.2
1	L	24	ILE	2.2
1	L	158	THR	2.1
1	L	79	PHE	2.1
1	B	23	ASN	2.1
1	B	173	GLY	2.1
1	C	31	GLY	2.1
1	E	30	ASP	2.1
1	K	39	GLY	2.1
1	F	91	THR	2.1
1	L	19	ALA	2.1
1	J	340	TYR	2.1
1	A	82	GLY	2.1
1	F	128	ARG	2.1
1	A	277	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	339	CYS	2.1
1	A	85	THR	2.0
1	L	105	THR	2.0
1	C	10	ILE	2.0
1	B	391	THR	2.0
1	K	17	THR	2.0
1	F	59	VAL	2.0
1	C	79	PHE	2.0
1	L	394	GLY	2.0
1	K	339	CYS	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	I	503	4/4	0.81	0.19	61,75,76,77	0
3	EDO	I	502	4/4	0.87	0.18	57,59,72,80	0
2	FE	B	501	1/1	0.87	0.35	60,60,60,60	0
2	FE	H	501	1/1	0.88	0.38	60,60,60,60	0
2	FE	E	1400	1/1	0.89	0.34	57,57,57,57	0
2	FE	K	501	1/1	0.89	0.34	59,59,59,59	0
2	FE	J	501	1/1	0.90	0.38	56,56,56,56	0
2	FE	G	1400	1/1	0.90	0.36	57,57,57,57	0
2	FE	A	501	1/1	0.91	0.34	59,59,59,59	0
2	FE	I	501	1/1	0.91	0.36	58,58,58,58	0
2	FE	D	501	1/1	0.91	0.34	63,63,63,63	0
2	FE	L	501	1/1	0.92	0.35	55,55,55,55	0
2	FE	F	501	1/1	0.92	0.33	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	C	501	1/1	0.92	0.36	54,54,54,54	0
3	EDO	L	502	4/4	0.92	0.14	51,52,59,62	0
3	EDO	C	502	4/4	0.94	0.13	40,43,48,59	0
3	EDO	J	502	4/4	0.96	0.11	48,49,52,57	0

6.5 Other polymers (i)

There are no such residues in this entry.