



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:04 PM GMT

PDB ID : 3HGK
Title : crystal structure of effect protein AvrptoB complexed with kinase Pto
Authors : Dong, J.; Fan, F.; Gu, L.; Chai, J.
Deposited on : 2009-05-14
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

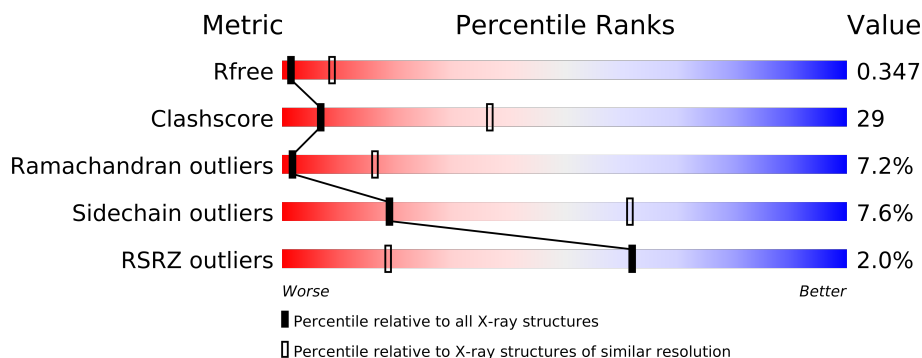
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	
1	C	327	
1	D	327	
2	E	85	
2	F	85	
2	G	85	
2	H	85	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11599 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2308	1462	398	435	2	11			
1	B	288	Total	C	N	O	P	S	0	0	0
			2306	1459	398	436	2	11			
1	C	286	Total	C	N	O	P	S	0	0	0
			2293	1451	396	433	2	11			
1	D	288	Total	C	N	O	P	S	0	0	0
			2308	1462	398	435	2	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	GLY	ASP	ENGINEERED	UNP Q40234
A	322	HIS	-	EXPRESSION TAG	UNP Q40234
A	323	HIS	-	EXPRESSION TAG	UNP Q40234
A	324	HIS	-	EXPRESSION TAG	UNP Q40234
A	325	HIS	-	EXPRESSION TAG	UNP Q40234
A	326	HIS	-	EXPRESSION TAG	UNP Q40234
A	327	HIS	-	EXPRESSION TAG	UNP Q40234
B	193	GLY	ASP	ENGINEERED	UNP Q40234
B	322	HIS	-	EXPRESSION TAG	UNP Q40234
B	323	HIS	-	EXPRESSION TAG	UNP Q40234
B	324	HIS	-	EXPRESSION TAG	UNP Q40234
B	325	HIS	-	EXPRESSION TAG	UNP Q40234
B	326	HIS	-	EXPRESSION TAG	UNP Q40234
B	327	HIS	-	EXPRESSION TAG	UNP Q40234
C	193	GLY	ASP	ENGINEERED	UNP Q40234
C	322	HIS	-	EXPRESSION TAG	UNP Q40234
C	323	HIS	-	EXPRESSION TAG	UNP Q40234
C	324	HIS	-	EXPRESSION TAG	UNP Q40234
C	325	HIS	-	EXPRESSION TAG	UNP Q40234
C	326	HIS	-	EXPRESSION TAG	UNP Q40234
C	327	HIS	-	EXPRESSION TAG	UNP Q40234

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	193	GLY	ASP	ENGINEERED	UNP Q40234
D	322	HIS	-	EXPRESSION TAG	UNP Q40234
D	323	HIS	-	EXPRESSION TAG	UNP Q40234
D	324	HIS	-	EXPRESSION TAG	UNP Q40234
D	325	HIS	-	EXPRESSION TAG	UNP Q40234
D	326	HIS	-	EXPRESSION TAG	UNP Q40234
D	327	HIS	-	EXPRESSION TAG	UNP Q40234

- Molecule 2 is a protein called Effector protein hopAB2.

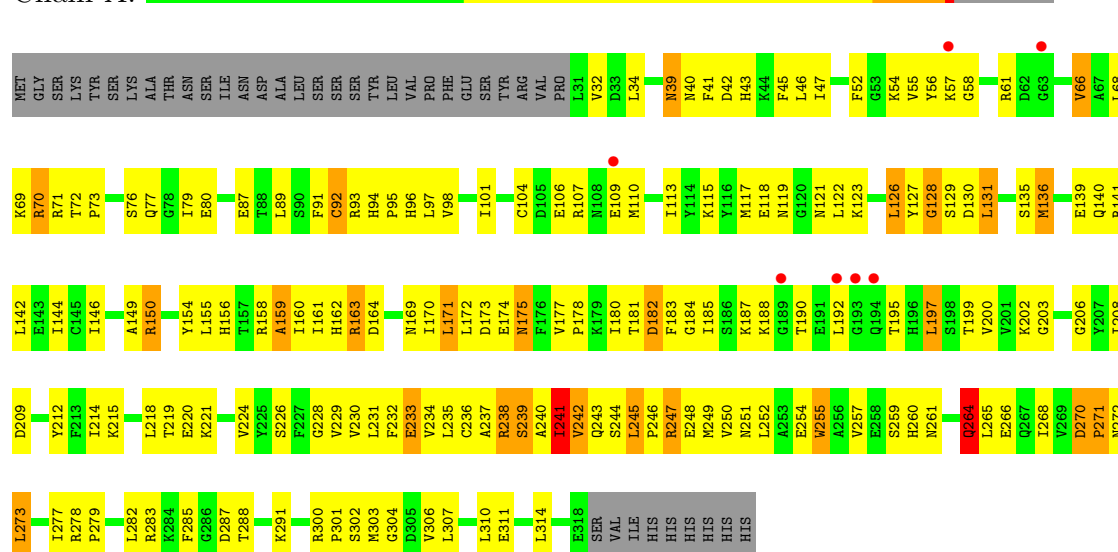
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			
2	F	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			
2	G	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			
2	H	77	Total	C	N	O	S	0	0	0
			596	363	121	108	4			

3 Residue-property plots

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

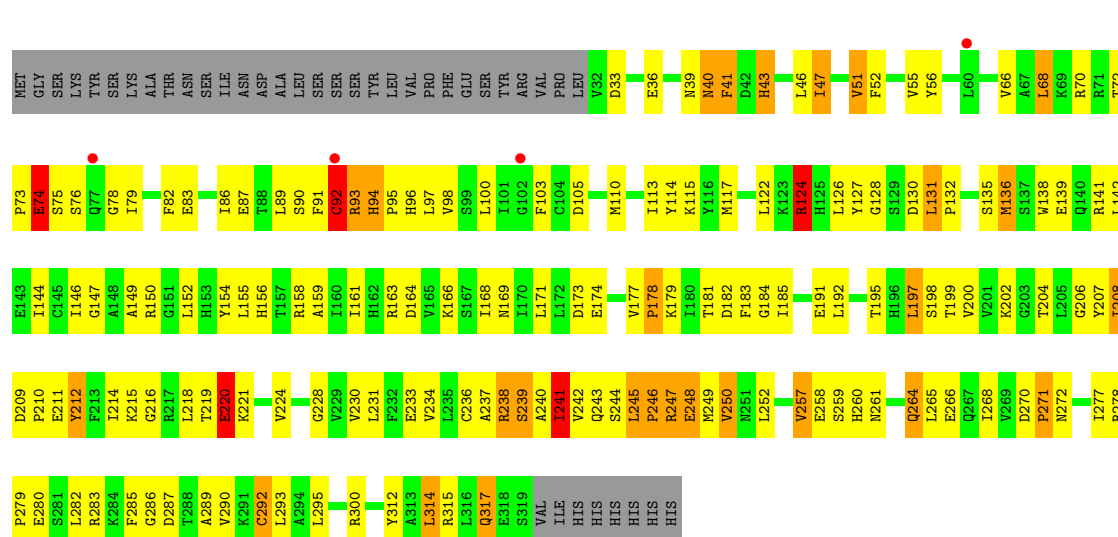
• Molecule 1: Protein kinase

Chain A:



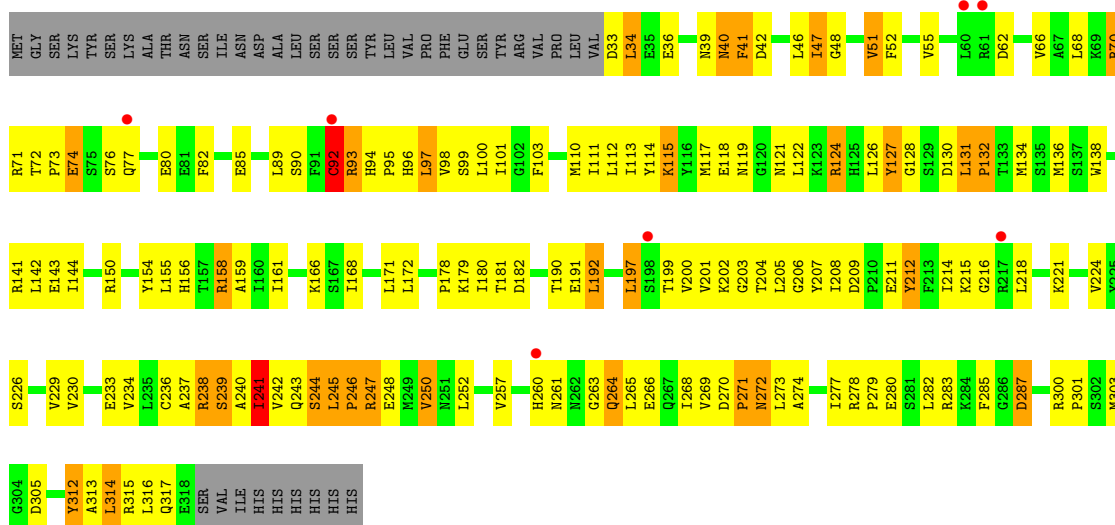
• Molecule 1: Protein kinase

Chain B:



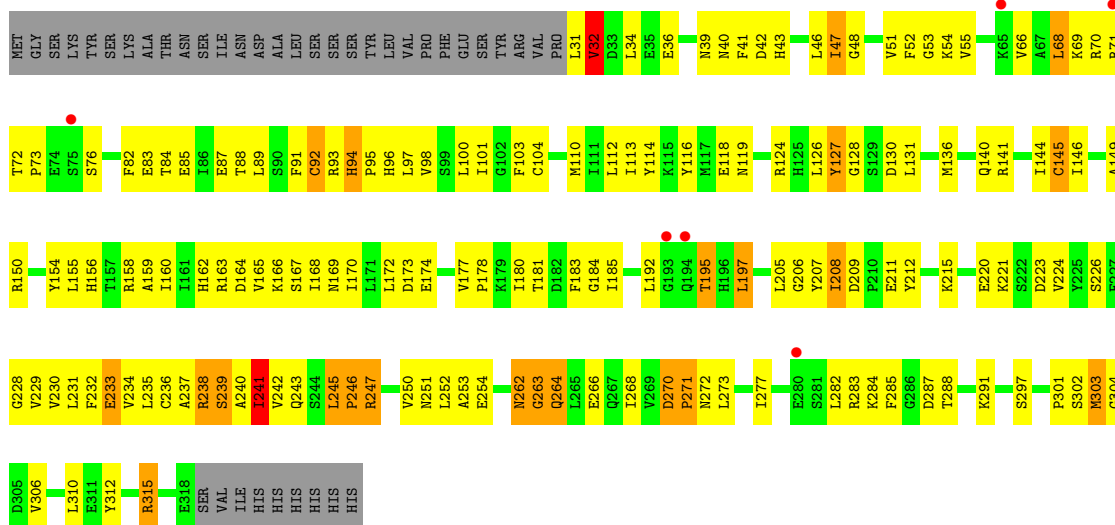
• Molecule 1: Protein kinase

Chain C:



- Molecule 1: Protein kinase

Chain D:



- Molecule 2: Effector protein hopAB2

Chain E:



- Molecule 2: Effector protein hopAB2

Chain F:



- Molecule 2: Effector protein hopAB2

Chain G: 

PRO	ARG	ARG	G124	A125	V126	N130	S131	V132	V133	Q134	Q135	L136	R147	D157	V164	E165	Q166	N167	I168	Q171	M176	P177	G180	I181	S182	R183	E190	L195	R196	V199	GLN	ALA	ALA	SER
-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

● Molecule 2: Effector protein hopAB2

Chain H: 

PRO	ARG	G124	A125	V126	V133	L136	A141	S144	R147	R151	N155	M176	G180	I181	S182	R183	E186	T189	E190	L191	R192	G193	A194	L195	R196	R197	H200	GLN	GLN	ALA	ALA	SER
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.07Å 104.47Å 298.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 44.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.30) 99.6 (44.96-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.317 , 0.331 0.331 , 0.347	Depositor DCC
R_{free} test set	1508 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	95.1	Xtriage
Anisotropy	0.895	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 18.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 29705 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11599	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7970e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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	0.51	1/2331 (0.0%)	0.66	0/3143
1	B	0.51	0/2329	0.68	1/3140 (0.0%)
1	C	0.49	0/2316	0.67	0/3122
1	D	0.50	0/2331	0.65	0/3143
2	E	0.38	0/605	0.50	0/814
2	F	0.41	0/605	0.51	0/814
2	G	0.59	2/605 (0.3%)	0.58	1/814 (0.1%)
2	H	0.40	0/605	0.51	0/814
All	All	0.49	3/11727 (0.0%)	0.64	2/15804 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	124	GLY	C-O	-7.03	1.12	1.23
2	G	124	GLY	CA-C	-5.72	1.42	1.51
1	A	126	LEU	C-N	-5.23	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	124	GLY	N-CA-C	-7.49	94.38	113.10
1	B	47	ILE	N-CA-C	6.44	128.40	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2308	0	2301	172	0
1	B	2306	0	2295	156	0
1	C	2293	0	2281	175	0
1	D	2308	0	2301	141	0
2	E	596	0	585	18	0
2	F	596	0	585	17	0
2	G	596	0	585	18	0
2	H	596	0	585	17	0
All	All	11599	0	11518	671	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (671) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:245:LEU:HB3	1:D:240:ALA:HB2	1.38	1.06
1:B:240:ALA:HB2	1:D:245:LEU:HB3	1.40	1.03
1:C:238:ARG:HD2	1:C:252:LEU:HD13	1.43	0.98
1:A:203:GLY:HA3	1:A:208:ILE:HD11	1.43	0.97
1:C:77:GLN:HE21	1:C:80:GLU:HB2	1.26	0.97
1:A:268:ILE:HD13	1:C:268:ILE:HD13	1.45	0.96
1:A:240:ALA:HB2	1:C:245:LEU:HB3	1.47	0.95
1:B:247:ARG:HG3	1:B:248:GLU:H	1.29	0.95
1:D:127:TYR:HB3	1:D:239:SER:HB3	1.47	0.94
1:D:89:LEU:O	1:D:92:CYS:SG	2.28	0.92
1:B:159:ALA:HB2	1:B:192:LEU:HA	1.49	0.92
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.35	0.91
1:C:278:ARG:H	1:C:317:GLN:HE21	1.12	0.90
1:C:278:ARG:H	1:C:317:GLN:NE2	1.67	0.90
1:B:268:ILE:HD13	1:D:268:ILE:HD13	1.54	0.90
1:A:245:LEU:HB3	1:C:240:ALA:HB2	1.51	0.90
1:A:89:LEU:O	1:A:92:CYS:SG	2.31	0.88
1:B:247:ARG:HG3	1:B:248:GLU:N	1.87	0.87
1:C:159:ALA:HB2	1:C:192:LEU:HA	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:230:VAL:O	1:C:234:VAL:HG23	1.74	0.87
2:E:183:ARG:NH1	2:H:183:ARG:HB2	1.91	0.85
1:A:203:GLY:CA	1:A:208:ILE:HD11	2.06	0.85
1:A:118:GLU:HG3	1:A:174:GLU:HG2	1.58	0.85
2:E:183:ARG:HB2	2:H:183:ARG:NH1	1.91	0.83
1:B:97:LEU:HD21	1:B:155:LEU:HD11	1.60	0.83
1:B:277:ILE:HG21	1:B:282:LEU:HB2	1.59	0.82
1:B:259:SER:HB3	1:B:266:GLU:HB2	1.60	0.82
1:A:123:LYS:HG3	1:A:239:SER:OG	1.79	0.82
1:B:240:ALA:HB1	1:B:243:GLN:HB2	1.59	0.82
1:D:52:PHE:CE2	1:D:76:SER:HB2	2.14	0.82
1:D:126:LEU:HD13	1:D:233:GLU:O	1.80	0.81
1:B:224:VAL:HG12	1:B:292:CYS:HB3	1.62	0.81
1:B:66:VAL:HG21	1:B:113:ILE:CG2	2.10	0.81
1:B:209:ASP:HB3	1:B:212:TYR:HB2	1.62	0.81
1:C:144:ILE:HG23	1:C:178:PRO:HG3	1.61	0.80
2:E:183:ARG:HD3	2:H:183:ARG:HD3	1.64	0.80
1:D:94:HIS:ND1	1:D:95:PRO:HD2	1.97	0.79
1:A:91:PHE:HB3	1:A:158:ARG:HH12	1.45	0.79
1:C:209:ASP:HB3	1:C:212:TYR:CB	2.13	0.79
1:C:266:GLU:HB3	1:C:269:VAL:HG23	1.63	0.79
1:B:244:SER:O	1:D:127:TYR:HE2	1.65	0.79
1:B:277:ILE:CG2	1:B:282:LEU:HB2	2.12	0.79
1:B:243:GLN:HG3	1:B:246:PRO:HD3	1.65	0.78
1:B:247:ARG:CG	1:B:248:GLU:H	1.93	0.78
2:F:183:ARG:NH1	2:G:183:ARG:HB2	1.98	0.78
1:B:94:HIS:ND1	1:B:95:PRO:HD2	1.99	0.78
1:B:244:SER:O	1:D:127:TYR:CE2	2.39	0.76
1:B:127:TYR:HB3	1:B:239:SER:HB3	1.67	0.76
1:B:245:LEU:HD12	1:D:243:GLN:OE1	1.85	0.76
1:B:52:PHE:CE2	1:B:76:SER:HB2	2.20	0.76
1:C:77:GLN:NE2	1:C:80:GLU:HB2	2.00	0.75
1:A:136:MET:CG	1:A:140:GLN:HG2	2.16	0.75
1:B:241:ILE:HG12	1:B:242:VAL:N	2.02	0.75
1:A:271:PRO:HB3	1:C:247:ARG:HG3	1.69	0.74
1:C:238:ARG:O	1:C:238:ARG:HD3	1.86	0.74
1:A:146:ILE:HG12	1:A:310:LEU:HB3	1.69	0.74
1:A:238:ARG:C	1:A:240:ALA:H	1.86	0.74
1:A:161:ILE:HG22	1:A:163:ARG:HG3	1.69	0.74
1:C:94:HIS:HB3	1:C:97:LEU:HB2	1.69	0.74
1:C:209:ASP:HB3	1:C:212:TYR:HB2	1.69	0.73
1:B:178:PRO:O	1:B:179:LYS:HG2	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:264:GLN:HB3	1:C:266:GLU:HG3	1.70	0.73
1:D:240:ALA:O	1:D:242:VAL:N	2.21	0.72
1:B:260:HIS:HA	1:B:265:LEU:HA	1.70	0.72
1:D:136:MET:HG3	1:D:140:GLN:HG2	1.71	0.72
1:D:270:ASP:HB2	1:D:271:PRO:HD2	1.72	0.71
1:B:278:ARG:H	1:B:317:GLN:HE21	1.39	0.71
1:D:127:TYR:HB3	1:D:239:SER:CB	2.21	0.71
2:E:183:ARG:CZ	2:H:183:ARG:HB2	2.20	0.71
1:D:91:PHE:HB3	1:D:158:ARG:HH12	1.56	0.71
1:B:238:ARG:NH2	1:B:250:VAL:O	2.24	0.71
1:A:91:PHE:CB	1:A:158:ARG:HH12	2.03	0.71
1:C:117:MET:HG3	1:C:171:LEU:HD23	1.72	0.71
1:B:230:VAL:O	1:B:234:VAL:HG23	1.91	0.70
1:B:271:PRO:HB3	1:D:247:ARG:HG3	1.74	0.70
1:A:271:PRO:CB	1:C:247:ARG:HG3	2.22	0.70
1:A:170:ILE:O	1:A:170:ILE:HG22	1.90	0.70
1:A:197:LEU:H	1:A:197:LEU:HD23	1.56	0.70
1:A:271:PRO:HB3	1:C:247:ARG:CG	2.22	0.69
1:B:243:GLN:OE1	1:D:245:LEU:HD12	1.92	0.69
1:A:270:ASP:HB2	1:A:271:PRO:HD2	1.74	0.69
1:B:66:VAL:HG23	1:B:114:TYR:O	1.92	0.69
1:C:236:CYS:HA	1:C:270:ASP:HA	1.73	0.69
1:C:205:LEU:HD21	2:G:180:GLY:HA3	1.73	0.69
1:A:155:LEU:HD21	1:A:183:PHE:HE2	1.57	0.69
1:A:136:MET:HG3	1:A:140:GLN:HG2	1.74	0.69
1:C:154:TYR:O	1:C:158:ARG:HG3	1.93	0.69
1:B:283:ARG:O	1:B:287:ASP:HB2	1.92	0.68
1:A:247:ARG:HG3	1:A:248:GLU:H	1.58	0.68
1:B:127:TYR:HB3	1:B:239:SER:CB	2.24	0.68
1:B:238:ARG:HD2	1:B:252:LEU:HD13	1.75	0.68
1:A:52:PHE:CE2	1:A:76:SER:HB2	2.29	0.68
1:A:117:MET:HG3	1:A:171:LEU:HD23	1.75	0.68
1:B:214:ILE:HG13	1:B:215:LYS:HG3	1.76	0.68
1:C:94:HIS:ND1	1:C:95:PRO:HD2	2.09	0.68
1:C:197:LEU:H	1:C:197:LEU:HD23	1.59	0.68
1:A:127:TYR:HB3	1:A:239:SER:HB3	1.77	0.67
1:A:240:ALA:HB1	1:A:243:GLN:HB2	1.76	0.67
1:D:228:GLY:HA2	1:D:231:LEU:HD12	1.76	0.67
1:B:209:ASP:HB3	1:B:212:TYR:CB	2.23	0.67
1:B:135:SER:HB3	1:D:247:ARG:HH22	1.60	0.67
1:A:240:ALA:O	1:A:242:VAL:N	2.28	0.67
1:A:135:SER:HB3	1:C:247:ARG:HH22	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:277:ILE:CG2	1:D:282:LEU:HB2	2.24	0.66
1:D:209:ASP:HB3	1:D:212:TYR:HB3	1.78	0.66
1:B:141:ARG:HD3	1:B:234:VAL:HG12	1.78	0.66
1:D:83:GLU:O	1:D:87:GLU:HG2	1.96	0.66
1:B:156:HIS:CD2	1:B:220:GLU:HB2	2.31	0.66
1:B:124:ARG:HG3	1:B:124:ARG:NH1	2.06	0.66
1:D:226:SER:O	1:D:230:VAL:HG23	1.96	0.66
1:C:238:ARG:C	1:C:240:ALA:H	1.98	0.66
1:C:243:GLN:HG3	1:C:246:PRO:HD3	1.78	0.65
1:D:277:ILE:HG21	1:D:282:LEU:HB2	1.77	0.65
1:A:195:THR:HB	1:A:197:LEU:HD22	1.78	0.65
1:D:238:ARG:C	1:D:240:ALA:H	1.99	0.65
1:B:277:ILE:HD13	1:B:282:LEU:HD13	1.77	0.65
2:H:186:GLU:HA	2:H:189:ILE:HD12	1.78	0.65
1:A:206:GLY:C	1:A:241:ILE:HD11	2.16	0.65
1:D:243:GLN:HE21	1:D:245:LEU:N	1.94	0.65
1:C:130:ASP:O	1:C:131:LEU:HB3	1.95	0.65
1:D:238:ARG:HB3	1:D:252:LEU:HD12	1.79	0.65
1:C:126:LEU:HD13	1:C:233:GLU:O	1.95	0.65
1:C:283:ARG:O	1:C:287:ASP:HB2	1.96	0.65
1:B:166:LYS:HB2	1:B:207:TYR:CZ	2.32	0.65
1:D:52:PHE:HE2	1:D:76:SER:HB2	1.57	0.64
1:B:236:CYS:SG	1:B:252:LEU:HD11	2.37	0.64
1:D:206:GLY:C	1:D:241:ILE:HD11	2.17	0.64
1:C:171:LEU:HD11	1:C:181:THR:HG21	1.78	0.64
1:B:66:VAL:CG2	1:B:113:ILE:CG2	2.75	0.64
1:B:314:LEU:O	1:B:314:LEU:HD12	1.98	0.64
1:C:66:VAL:CG2	1:C:113:ILE:HG22	2.28	0.64
1:A:54:LYS:HG3	1:A:73:PRO:HG2	1.79	0.64
2:G:176:MET:HA	2:G:180:GLY:HA2	1.79	0.64
1:C:209:ASP:HB3	1:C:212:TYR:HB3	1.79	0.64
1:B:210:PRO:O	1:B:214:ILE:HG23	1.98	0.64
1:D:238:ARG:HD2	1:D:252:LEU:HD12	1.80	0.64
1:A:230:VAL:O	1:A:234:VAL:HG23	1.97	0.64
1:C:313:ALA:HA	1:C:316:LEU:HD12	1.80	0.64
1:B:66:VAL:HG21	1:B:113:ILE:HG22	1.79	0.63
1:A:161:ILE:HG21	1:A:218:LEU:HD11	1.80	0.63
1:C:166:LYS:HE3	1:C:168:ILE:HD12	1.81	0.63
2:G:133:VAL:HG22	2:G:195:LEU:HD12	1.81	0.63
1:D:54:LYS:HG3	1:D:73:PRO:HG2	1.79	0.63
1:C:221:LYS:NZ	1:C:300:ARG:O	2.32	0.63
1:A:209:ASP:HB3	1:A:212:TYR:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:43:HIS:CE1	1:D:70:ARG:HH21	2.17	0.63
1:A:68:LEU:HD12	1:A:113:ILE:HG12	1.81	0.62
1:A:43:HIS:CE1	1:A:70:ARG:HH21	2.16	0.62
1:D:230:VAL:O	1:D:234:VAL:HG23	1.99	0.62
1:A:158:ARG:O	1:A:160:ILE:HG13	1.99	0.62
1:A:135:SER:CB	1:C:247:ARG:HH22	2.13	0.62
1:D:236:CYS:HA	1:D:270:ASP:HA	1.82	0.62
1:D:263:GLY:O	1:D:264:GLN:HB2	1.99	0.62
1:B:241:ILE:HG12	1:B:242:VAL:H	1.64	0.61
1:B:166:LYS:HE3	1:B:168:ILE:HD12	1.82	0.61
1:A:301:PRO:HG2	1:A:306:VAL:CG2	2.30	0.61
1:A:58:GLY:O	1:A:66:VAL:HG12	2.00	0.61
2:E:176:MET:HA	2:E:180:GLY:HA2	1.81	0.61
1:B:66:VAL:CG2	1:B:113:ILE:HG22	2.30	0.61
2:H:176:MET:HA	2:H:180:GLY:HA2	1.82	0.61
1:B:243:GLN:HE21	1:B:245:LEU:N	1.98	0.61
1:D:243:GLN:HG3	1:D:246:PRO:HD2	1.82	0.61
1:C:278:ARG:N	1:C:317:GLN:NE2	2.46	0.61
1:A:243:GLN:O	1:A:250:VAL:HG23	2.01	0.61
1:D:270:ASP:HB2	1:D:271:PRO:CD	2.30	0.61
1:C:90:SER:C	1:C:92:CYS:H	2.03	0.61
1:B:183:PHE:O	1:B:185:ILE:N	2.34	0.60
1:B:43:HIS:CE1	1:B:70:ARG:HH21	2.19	0.60
1:A:238:ARG:NH2	1:A:250:VAL:O	2.35	0.60
1:D:96:HIS:O	1:D:97:LEU:HD12	2.01	0.60
1:C:171:LEU:HD12	1:C:171:LEU:N	2.15	0.60
1:B:197:LEU:CD2	1:B:197:LEU:H	2.15	0.60
1:C:229:VAL:HG11	1:C:241:ILE:HD12	1.83	0.60
1:C:89:LEU:CD2	1:C:100:LEU:HB2	2.32	0.60
1:C:89:LEU:HD23	1:C:100:LEU:HB2	1.84	0.60
1:A:243:GLN:OE1	1:C:245:LEU:HD12	2.01	0.60
1:A:126:LEU:HD13	1:A:233:GLU:O	2.02	0.60
1:C:156:HIS:CE1	1:C:303:MET:HG2	2.37	0.60
1:B:96:HIS:O	1:B:97:LEU:HD12	2.01	0.59
1:D:69:LYS:HD3	1:D:71:ARG:HH21	1.68	0.59
1:A:238:ARG:O	1:A:240:ALA:N	2.34	0.59
1:C:240:ALA:HB1	1:C:243:GLN:HB2	1.85	0.59
1:C:238:ARG:O	1:C:240:ALA:N	2.35	0.59
1:B:86:ILE:O	1:B:90:SER:N	2.28	0.59
1:C:178:PRO:O	1:C:179:LYS:HG2	2.03	0.59
1:A:203:GLY:HA3	1:A:208:ILE:CD1	2.25	0.58
1:A:214:ILE:HG13	1:A:215:LYS:HG3	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:127:TYR:CB	1:D:239:SER:HB3	2.26	0.58
1:B:171:LEU:N	1:B:171:LEU:HD12	2.17	0.58
1:C:312:TYR:O	1:C:315:ARG:HB3	2.02	0.58
1:B:241:ILE:CG1	1:B:242:VAL:N	2.67	0.58
1:A:175:ASN:N	1:A:175:ASN:OD1	2.37	0.58
1:C:93:ARG:O	1:C:94:HIS:HB2	2.01	0.58
1:D:284:LYS:HE2	1:D:312:TYR:HD2	1.68	0.58
1:A:245:LEU:HD12	1:C:243:GLN:OE1	2.03	0.58
1:B:292:CYS:O	1:B:300:ARG:HD3	2.03	0.58
1:C:260:HIS:HA	1:C:265:LEU:HA	1.86	0.58
1:A:236:CYS:O	1:A:237:ALA:HB3	2.03	0.58
1:D:236:CYS:O	1:D:237:ALA:HB3	2.03	0.58
1:A:301:PRO:HG2	1:A:306:VAL:HG23	1.86	0.58
1:C:278:ARG:N	1:C:317:GLN:HE21	1.93	0.57
1:C:197:LEU:H	1:C:197:LEU:CD2	2.17	0.57
1:B:245:LEU:HB3	1:D:240:ALA:CB	2.24	0.57
1:B:72:THR:N	1:B:73:PRO:CD	2.67	0.57
1:B:154:TYR:O	1:B:158:ARG:HG3	2.04	0.57
1:B:238:ARG:HD3	1:B:238:ARG:O	2.04	0.57
1:B:130:ASP:O	1:B:131:LEU:HB3	2.02	0.57
1:A:91:PHE:O	1:A:93:ARG:N	2.37	0.57
1:A:122:LEU:HD13	1:A:144:ILE:HG21	1.86	0.57
1:B:238:ARG:C	1:B:240:ALA:H	2.06	0.57
1:D:264:GLN:OE1	1:D:266:GLU:HA	2.05	0.57
1:C:214:ILE:HG13	1:C:215:LYS:HG3	1.86	0.57
1:C:214:ILE:HG13	1:C:215:LYS:N	2.19	0.57
1:A:159:ALA:HB2	1:A:192:LEU:HA	1.86	0.57
1:C:270:ASP:HB2	1:C:271:PRO:HD2	1.86	0.57
1:A:283:ARG:O	1:A:287:ASP:HB2	2.04	0.57
1:B:271:PRO:CB	1:D:247:ARG:HG3	2.35	0.56
1:C:314:LEU:O	1:C:314:LEU:HD12	2.05	0.56
1:A:264:GLN:OE1	1:A:266:GLU:HG2	2.05	0.56
1:B:124:ARG:HD3	1:B:124:ARG:O	2.04	0.56
1:A:162:HIS:HE1	1:A:182:ASP:O	1.88	0.56
1:C:212:TYR:O	1:C:216:GLY:N	2.33	0.56
1:D:166:LYS:HE3	1:D:168:ILE:HD12	1.88	0.56
1:A:155:LEU:HD21	1:A:183:PHE:CE2	2.40	0.56
1:A:97:LEU:HD21	1:A:155:LEU:HD11	1.88	0.56
1:C:241:ILE:HG12	1:C:242:VAL:N	2.20	0.56
1:D:312:TYR:O	1:D:315:ARG:HB3	2.05	0.56
2:F:133:VAL:HG22	2:F:195:LEU:HD12	1.87	0.56
1:C:52:PHE:CE2	1:C:76:SER:HB2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:238:ARG:HD2	1:D:252:LEU:HB2	1.88	0.55
1:A:155:LEU:HD23	1:A:160:ILE:HG21	1.88	0.55
1:A:161:ILE:CG2	1:A:163:ARG:HG3	2.34	0.55
1:A:119:ASN:ND2	1:A:173:ASP:O	2.38	0.55
1:C:97:LEU:HD11	1:C:155:LEU:HD13	1.88	0.55
1:B:221:LYS:NZ	1:B:300:ARG:O	2.37	0.55
1:C:94:HIS:HD2	1:C:154:TYR:CD2	2.25	0.55
1:C:98:VAL:HG21	1:C:181:THR:HB	1.87	0.55
1:B:135:SER:CB	1:D:247:ARG:HH22	2.19	0.55
1:A:162:HIS:ND1	1:A:162:HIS:O	2.34	0.55
1:A:45:PHE:HA	1:A:56:TYR:HE2	1.72	0.55
1:D:232:PHE:C	1:D:234:VAL:H	2.09	0.55
1:B:94:HIS:ND1	1:B:95:PRO:CD	2.68	0.55
1:D:149:ALA:HA	1:D:303:MET:CE	2.37	0.55
1:B:163:ARG:NH2	1:B:199:TPO:O1P	2.37	0.55
1:D:232:PHE:HB2	1:D:252:LEU:HD21	1.88	0.55
1:C:161:ILE:CD1	1:C:197:LEU:HD21	2.37	0.55
1:C:257:VAL:O	1:C:261:ASN:HB3	2.07	0.55
1:B:155:LEU:HD21	1:B:183:PHE:HE2	1.73	0.54
1:A:136:MET:HG2	1:A:140:GLN:HG2	1.89	0.54
1:C:171:LEU:CD1	1:C:171:LEU:H	2.20	0.54
1:A:66:VAL:HG23	1:A:101:ILE:HD12	1.88	0.54
1:A:104:CYS:O	1:A:110:MET:HA	2.08	0.54
1:B:126:LEU:HD13	1:B:233:GLU:O	2.07	0.54
1:C:72:THR:N	1:C:73:PRO:CD	2.71	0.54
1:D:197:LEU:HD23	1:D:197:LEU:H	1.73	0.54
1:B:197:LEU:H	1:B:197:LEU:HD23	1.72	0.54
1:D:162:HIS:ND1	1:D:162:HIS:O	2.38	0.54
1:A:229:VAL:HG11	1:A:241:ILE:HD12	1.89	0.54
1:D:209:ASP:HB3	1:D:212:TYR:CB	2.37	0.54
1:D:96:HIS:HD2	1:D:150:ARG:HB3	1.71	0.54
1:C:277:ILE:HG21	1:C:282:LEU:HD13	1.88	0.54
1:A:130:ASP:O	1:A:131:LEU:HB3	2.06	0.54
1:D:48:GLY:HA3	1:D:55:VAL:HB	1.88	0.54
1:C:51:VAL:HG22	2:G:157:ASP:HB3	1.90	0.54
1:D:232:PHE:CB	1:D:252:LEU:HD21	2.38	0.54
1:A:238:ARG:HD2	1:A:252:LEU:HB2	1.90	0.53
1:B:161:ILE:HG21	1:B:218:LEU:HD11	1.90	0.53
2:G:130:ASN:O	2:G:134:GLN:HG2	2.08	0.53
1:B:236:CYS:O	1:B:271:PRO:HD3	2.08	0.53
2:E:183:ARG:HB2	2:H:183:ARG:CZ	2.37	0.53
2:F:183:ARG:HD3	2:G:183:ARG:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:238:ARG:C	1:C:240:ALA:N	2.61	0.53
2:F:176:MET:HA	2:F:180:GLY:HA2	1.89	0.53
1:A:238:ARG:C	1:A:240:ALA:N	2.57	0.53
1:B:169:ASN:O	1:B:181:THR:HG22	2.08	0.53
2:H:133:VAL:HG22	2:H:195:LEU:HD12	1.91	0.53
1:C:277:ILE:CG2	1:C:282:LEU:HB2	2.38	0.53
1:A:127:TYR:CD2	1:A:128:GLY:N	2.77	0.53
1:C:89:LEU:HD23	1:C:100:LEU:HD12	1.92	0.52
1:D:72:THR:N	1:D:73:PRO:CD	2.72	0.52
1:A:136:MET:O	1:A:141:ARG:NH1	2.43	0.52
1:A:66:VAL:HG21	1:A:113:ILE:CG2	2.39	0.52
1:D:238:ARG:O	1:D:240:ALA:N	2.28	0.52
1:C:209:ASP:O	1:C:212:TYR:HB3	2.09	0.52
1:A:232:PHE:HB2	1:A:252:LEU:HD21	1.92	0.52
1:D:119:ASN:HB2	1:D:172:LEU:HB2	1.91	0.52
1:C:66:VAL:HG21	1:C:113:ILE:CG2	2.39	0.52
1:B:211:GLU:O	1:B:215:LYS:HB2	2.09	0.52
1:A:238:ARG:HD2	1:A:252:LEU:CD1	2.39	0.52
1:C:117:MET:CG	1:C:171:LEU:HD23	2.38	0.52
1:A:180:ILE:N	1:A:180:ILE:HD13	2.24	0.52
2:E:167:ASN:O	2:E:171:GLN:HG3	2.10	0.52
1:B:238:ARG:C	1:B:240:ALA:N	2.64	0.52
1:C:94:HIS:ND1	1:C:95:PRO:CD	2.73	0.52
1:D:271:PRO:HD2	1:D:273:LEU:HD12	1.91	0.52
1:C:171:LEU:CD1	1:C:181:THR:HG21	2.39	0.52
1:C:221:LYS:O	1:C:224:VAL:HB	2.09	0.52
1:B:289:ALA:O	1:B:293:LEU:HG	2.10	0.52
1:D:159:ALA:HB2	1:D:192:LEU:HA	1.92	0.52
1:B:259:SER:O	1:B:264:GLN:N	2.41	0.52
1:C:94:HIS:HD2	1:C:154:TYR:CG	2.28	0.52
2:H:151:ARG:HG2	2:H:155:ASN:ND2	2.25	0.52
1:D:170:ILE:HG22	1:D:170:ILE:O	2.10	0.52
1:C:94:HIS:CD2	1:C:154:TYR:CG	2.98	0.51
1:D:166:LYS:HB2	1:D:207:TYR:CZ	2.44	0.51
1:B:240:ALA:CB	1:D:245:LEU:HB3	2.26	0.51
1:A:163:ARG:NH2	1:A:202:LYS:HD2	2.26	0.51
1:A:270:ASP:CB	1:A:271:PRO:HD2	2.40	0.51
2:E:195:LEU:O	2:E:199:VAL:HG23	2.10	0.51
1:D:94:HIS:CD2	1:D:154:TYR:CG	2.98	0.51
1:C:117:MET:HG3	1:C:171:LEU:CD2	2.41	0.51
2:F:148:ASN:HA	2:F:151:ARG:NH1	2.25	0.51
1:A:232:PHE:CB	1:A:252:LEU:HD21	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:THR:N	1:A:73:PRO:CD	2.74	0.51
1:B:240:ALA:O	1:B:241:ILE:HG23	2.11	0.51
1:C:243:GLN:HG3	1:C:246:PRO:CD	2.40	0.51
2:F:151:ARG:HG2	2:F:155:ASN:HD21	1.75	0.51
1:A:139:GLU:O	1:A:142:LEU:N	2.43	0.51
1:A:277:ILE:CG2	1:A:282:LEU:HB2	2.41	0.51
1:D:91:PHE:CB	1:D:158:ARG:HH12	2.22	0.51
1:A:150:ARG:HD3	1:A:307:LEU:HD21	1.94	0.50
1:A:180:ILE:HG22	1:A:181:THR:N	2.26	0.50
2:H:151:ARG:HG2	2:H:155:ASN:HD21	1.77	0.50
1:C:82:PHE:CE2	1:C:112:LEU:HG	2.46	0.50
1:B:94:HIS:HB3	1:B:97:LEU:HB2	1.93	0.50
1:C:171:LEU:HD12	1:C:171:LEU:H	1.76	0.50
1:C:90:SER:C	1:C:92:CYS:N	2.65	0.50
1:B:72:THR:H	1:B:73:PRO:HD3	1.77	0.50
2:G:147:ARG:NH1	2:G:196:ARG:HG3	2.27	0.50
1:B:236:CYS:O	1:B:237:ALA:HB3	2.12	0.50
1:B:66:VAL:CG2	1:B:114:TYR:O	2.60	0.50
1:B:164:ASP:O	1:B:169:ASN:ND2	2.45	0.50
1:C:221:LYS:CE	1:C:300:ARG:O	2.60	0.50
1:D:146:ILE:HG12	1:D:310:LEU:HB3	1.92	0.50
1:B:89:LEU:HD23	1:B:100:LEU:HB2	1.93	0.50
1:B:135:SER:HB3	1:D:247:ARG:NH2	2.25	0.49
1:B:43:HIS:HD2	1:B:56:TYR:CE1	2.30	0.49
1:C:66:VAL:HG21	1:C:113:ILE:HG22	1.94	0.49
1:C:127:TYR:O	1:C:239:SER:CB	2.61	0.49
1:C:166:LYS:HB2	1:C:207:TYR:CZ	2.47	0.49
1:A:66:VAL:CG2	1:A:113:ILE:CG2	2.90	0.49
1:A:55:VAL:HA	1:A:68:LEU:O	2.12	0.49
1:B:238:ARG:O	1:B:240:ALA:N	2.45	0.49
1:D:238:ARG:C	1:D:240:ALA:N	2.63	0.49
1:A:155:LEU:HD23	1:A:160:ILE:CG2	2.42	0.49
1:A:270:ASP:HB2	1:A:271:PRO:CD	2.42	0.49
1:C:66:VAL:CG2	1:C:113:ILE:CG2	2.90	0.49
1:D:156:HIS:CD2	1:D:220:GLU:HB2	2.47	0.49
1:B:79:ILE:HG13	1:B:110:MET:CE	2.42	0.49
1:D:85:GLU:O	1:D:89:LEU:HB3	2.12	0.49
1:C:240:ALA:O	1:C:241:ILE:HG23	2.13	0.49
1:C:240:ALA:O	1:C:242:VAL:N	2.44	0.49
1:C:236:CYS:SG	1:C:269:VAL:HG12	2.51	0.49
1:C:171:LEU:N	1:C:171:LEU:CD1	2.75	0.49
1:D:97:LEU:HD11	1:D:155:LEU:CD1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:224:VAL:HG21	1:D:301:PRO:O	2.12	0.49
1:B:228:GLY:O	1:B:231:LEU:HB2	2.12	0.49
1:D:89:LEU:HD23	1:D:100:LEU:HD12	1.95	0.49
1:B:171:LEU:HD11	1:B:181:THR:HG21	1.94	0.49
1:A:251:ASN:HB3	1:A:254:GLU:HB2	1.95	0.49
1:C:89:LEU:HD11	1:C:98:VAL:O	2.12	0.48
1:A:162:HIS:HD2	1:A:180:ILE:HG21	1.76	0.48
1:B:51:VAL:HG22	2:E:157:ASP:HB3	1.95	0.48
1:A:195:THR:HB	1:A:197:LEU:CD2	2.43	0.48
1:D:264:GLN:CD	1:D:266:GLU:HG2	2.34	0.48
1:A:264:GLN:HB3	1:A:266:GLU:CG	2.43	0.48
1:B:270:ASP:HB2	1:B:271:PRO:HD2	1.95	0.48
1:B:257:VAL:HG12	1:B:258:GLU:N	2.29	0.48
1:A:94:HIS:CD2	1:A:154:TYR:CD1	3.01	0.48
1:B:240:ALA:O	1:B:242:VAL:N	2.46	0.48
1:D:238:ARG:HD2	1:D:252:LEU:CD1	2.42	0.48
1:A:98:VAL:HG23	1:A:180:ILE:O	2.13	0.48
1:B:286:GLY:O	1:B:290:VAL:HG23	2.12	0.48
1:A:221:LYS:HD2	1:A:300:ARG:HB2	1.95	0.48
1:A:127:TYR:CD1	1:C:246:PRO:O	2.67	0.48
1:D:98:VAL:HG23	1:D:180:ILE:O	2.13	0.48
1:D:232:PHE:O	1:D:234:VAL:N	2.47	0.48
1:B:247:ARG:HG3	1:B:249:MET:H	1.79	0.48
1:B:206:GLY:C	1:B:241:ILE:HD11	2.33	0.48
1:B:265:LEU:HD11	1:B:283:ARG:HG3	1.96	0.48
2:H:189:ILE:HG23	2:H:192:ARG:HH12	1.78	0.48
1:D:306:VAL:O	1:D:310:LEU:HG	2.14	0.48
1:D:232:PHE:C	1:D:234:VAL:N	2.66	0.47
1:B:219:THR:O	1:B:221:LYS:N	2.47	0.47
1:D:262:ASN:O	1:D:264:GLN:N	2.41	0.47
1:B:90:SER:C	1:B:92:CYS:H	2.16	0.47
2:F:133:VAL:O	2:F:137:VAL:HG23	2.14	0.47
1:D:211:GLU:HG3	1:D:215:LYS:HD2	1.96	0.47
1:C:36:GLU:HB2	1:C:103:PHE:CE1	2.48	0.47
1:B:74:GLU:N	1:B:74:GLU:CD	2.68	0.47
1:B:171:LEU:CD1	1:B:171:LEU:N	2.77	0.47
1:C:55:VAL:HA	1:C:68:LEU:O	2.13	0.47
2:F:148:ASN:HA	2:F:151:ARG:HH12	1.77	0.47
1:B:136:MET:O	1:B:141:ARG:NH1	2.46	0.47
1:C:98:VAL:HG23	1:C:180:ILE:O	2.13	0.47
1:A:247:ARG:C	1:A:249:MET:H	2.17	0.47
1:B:72:THR:N	1:B:73:PRO:HD3	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:302:SER:O	1:D:304:GLY:N	2.48	0.47
1:D:238:ARG:HB3	1:D:252:LEU:CD1	2.43	0.47
1:A:238:ARG:HD3	1:A:238:ARG:O	2.14	0.47
1:B:144:ILE:HA	1:B:178:PRO:CG	2.45	0.47
2:F:133:VAL:HA	2:F:136:LEU:HD12	1.95	0.47
1:A:156:HIS:CD2	1:A:220:GLU:HB2	2.50	0.47
1:D:55:VAL:HA	1:D:68:LEU:O	2.15	0.47
1:C:203:GLY:HA3	1:C:208:ILE:HD11	1.97	0.47
1:C:122:LEU:HD21	1:C:234:VAL:HG22	1.96	0.47
1:C:161:ILE:HD11	1:C:197:LEU:HD21	1.96	0.47
1:B:144:ILE:HA	1:B:178:PRO:HG3	1.96	0.47
1:C:171:LEU:O	1:C:172:LEU:HD23	2.15	0.47
1:A:260:HIS:HA	1:A:265:LEU:HA	1.96	0.47
1:A:45:PHE:HA	1:A:56:TYR:CE2	2.49	0.47
1:B:83:GLU:O	1:B:87:GLU:HG2	2.15	0.47
1:D:277:ILE:HG22	1:D:282:LEU:HB2	1.96	0.46
1:C:161:ILE:HG21	1:C:218:LEU:HD11	1.97	0.46
2:E:134:GLN:NE2	2:E:134:GLN:HA	2.30	0.46
1:D:104:CYS:O	1:D:110:MET:HA	2.15	0.46
1:D:273:LEU:HD13	1:D:277:ILE:HD11	1.97	0.46
1:C:48:GLY:HA3	1:C:55:VAL:HB	1.97	0.46
1:C:68:LEU:HD13	1:C:113:ILE:HG23	1.98	0.46
1:A:149:ALA:HB3	1:A:307:LEU:HD13	1.97	0.46
1:D:164:ASP:OD2	1:D:169:ASN:ND2	2.46	0.46
1:C:247:ARG:HB3	1:C:248:GLU:H	1.39	0.46
1:C:93:ARG:HH11	1:C:93:ARG:HG3	1.80	0.46
2:G:131:SER:O	2:G:134:GLN:HB2	2.16	0.46
1:A:228:GLY:HA2	1:A:231:LEU:HD12	1.97	0.46
1:C:199:TPO:OG1	1:C:200:VAL:N	2.48	0.46
1:C:266:GLU:CB	1:C:269:VAL:HG23	2.42	0.46
1:A:221:LYS:O	1:A:224:VAL:N	2.48	0.46
1:C:142:LEU:HD21	1:C:285:PHE:CD1	2.49	0.46
1:D:144:ILE:HG23	1:D:178:PRO:HB3	1.97	0.46
1:D:145:CYS:SG	1:D:231:LEU:HD23	2.55	0.46
1:B:55:VAL:HA	1:B:68:LEU:O	2.15	0.46
1:A:146:ILE:CD1	1:A:311:GLU:HA	2.46	0.46
1:A:162:HIS:CE1	1:A:182:ASP:O	2.69	0.46
1:B:199:TPO:OG1	1:B:200:VAL:N	2.49	0.46
1:A:251:ASN:HD22	2:F:178:MET:HB3	1.79	0.46
1:D:288:THR:O	1:D:291:LYS:N	2.49	0.46
1:A:240:ALA:O	1:A:241:ILE:HG23	2.15	0.46
1:C:277:ILE:HG21	1:C:282:LEU:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:180:ILE:HG22	1:D:181:THR:N	2.30	0.46
1:D:31:LEU:O	1:D:32:VAL:HG23	2.16	0.46
1:C:144:ILE:HA	1:C:178:PRO:CG	2.46	0.46
1:B:211:GLU:CG	1:B:215:LYS:HD2	2.46	0.45
1:A:77:GLN:C	1:A:79:ILE:H	2.20	0.45
1:A:77:GLN:HE21	1:A:80:GLU:H	1.65	0.45
1:A:208:ILE:HG22	1:A:209:ASP:O	2.16	0.45
1:A:249:MET:HB2	1:A:255:TRP:NE1	2.30	0.45
2:H:147:ARG:NH1	2:H:196:ARG:HG3	2.31	0.45
1:A:242:VAL:CG2	2:F:179:HIS:HA	2.47	0.45
1:A:209:ASP:HB3	1:A:212:TYR:CB	2.47	0.45
1:A:96:HIS:O	1:A:97:LEU:HD12	2.17	0.45
1:B:135:SER:CB	1:D:247:ARG:NH2	2.79	0.45
1:B:122:LEU:HD21	1:B:234:VAL:HG22	1.99	0.45
1:A:277:ILE:HG21	1:A:282:LEU:HB2	1.98	0.45
1:C:47:ILE:HG13	1:C:48:GLY:H	1.82	0.45
2:F:147:ARG:NH1	2:F:196:ARG:HG3	2.31	0.45
1:D:243:GLN:O	1:D:250:VAL:HG23	2.17	0.45
1:A:270:ASP:CB	1:A:271:PRO:CD	2.94	0.45
1:A:162:HIS:CD2	1:A:180:ILE:HG21	2.52	0.45
1:A:177:VAL:HA	1:A:178:PRO:HD2	1.83	0.45
1:C:40:ASN:CG	1:C:41:PHE:N	2.71	0.45
1:B:66:VAL:HG13	1:B:68:LEU:HD21	1.99	0.45
1:B:166:LYS:NZ	1:B:204:THR:OG1	2.35	0.45
1:C:301:PRO:HB2	1:C:305:ASP:HB2	1.99	0.45
1:C:77:GLN:HE21	1:C:80:GLU:CB	2.13	0.44
1:D:236:CYS:O	1:D:237:ALA:CB	2.64	0.44
1:A:264:GLN:HB3	1:A:266:GLU:HG2	1.99	0.44
2:E:133:VAL:HG22	2:E:195:LEU:HD12	1.99	0.44
1:D:118:GLU:HG3	1:D:174:GLU:HG2	1.99	0.44
1:A:69:LYS:HD3	1:A:71:ARG:HH21	1.82	0.44
1:C:101:ILE:HD11	1:C:115:LYS:HG3	1.99	0.44
1:B:36:GLU:HB2	1:B:103:PHE:CE1	2.52	0.44
1:B:247:ARG:HG2	1:B:249:MET:HG2	1.99	0.44
1:A:121:ASN:HA	1:A:171:LEU:HA	1.97	0.44
1:A:119:ASN:HB2	1:A:172:LEU:HB2	1.99	0.44
2:E:166:GLN:HE21	2:E:170:ARG:HH21	1.65	0.44
1:D:221:LYS:CB	1:D:297:SER:HB2	2.47	0.44
1:B:117:MET:HG3	1:B:171:LEU:HB3	2.00	0.44
1:B:211:GLU:HG3	1:B:215:LYS:HD2	1.98	0.44
1:C:82:PHE:HE2	1:C:112:LEU:HG	1.80	0.44
1:A:232:PHE:C	1:A:234:VAL:N	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:190:THR:C	1:C:192:LEU:H	2.20	0.44
1:D:94:HIS:HD2	1:D:154:TYR:CD2	2.35	0.44
1:B:117:MET:HG3	1:B:171:LEU:HD23	2.00	0.44
2:G:195:LEU:O	2:G:199:VAL:HG23	2.17	0.44
1:C:72:THR:N	1:C:73:PRO:HD3	2.32	0.44
1:A:302:SER:C	1:A:304:GLY:H	2.21	0.44
1:C:144:ILE:HA	1:C:178:PRO:HG3	1.99	0.44
1:A:170:ILE:O	1:A:170:ILE:CG2	2.62	0.44
1:A:190:THR:N	1:A:195:THR:HG21	2.33	0.44
1:D:68:LEU:HD22	1:D:68:LEU:N	2.32	0.44
2:G:126:VAL:HG22	2:G:190:GLU:CD	2.38	0.44
1:D:232:PHE:O	1:D:235:LEU:N	2.50	0.44
1:C:270:ASP:HB2	1:C:271:PRO:CD	2.47	0.44
1:C:206:GLY:C	1:C:241:ILE:HD11	2.38	0.44
1:C:96:HIS:O	1:C:97:LEU:HD12	2.18	0.44
1:B:138:TRP:CH2	1:B:285:PHE:CD1	3.06	0.44
1:D:270:ASP:CB	1:D:271:PRO:CD	2.95	0.44
2:G:176:MET:N	2:G:177:PRO:CD	2.81	0.44
2:G:133:VAL:HA	2:G:136:LEU:HD12	2.00	0.44
1:C:211:GLU:HG2	1:C:215:LYS:HD2	2.00	0.44
2:H:193:GLY:HA2	2:H:196:ARG:NH1	2.33	0.43
1:D:251:ASN:O	1:D:254:GLU:N	2.43	0.43
1:C:236:CYS:O	1:C:271:PRO:HD3	2.18	0.43
1:C:271:PRO:C	1:C:273:LEU:H	2.22	0.43
1:D:158:ARG:O	1:D:160:ILE:HG13	2.18	0.43
1:C:171:LEU:CD1	1:C:181:THR:CG2	2.96	0.43
1:C:92:CYS:SG	1:C:99:SER:HA	2.58	0.43
1:C:156:HIS:HE1	1:C:303:MET:HG2	1.78	0.43
1:A:142:LEU:HD13	1:A:314:LEU:HA	2.00	0.43
2:F:186:GLU:HA	2:F:189:ILE:HD12	2.00	0.43
1:A:278:ARG:HG2	1:A:279:PRO:HD2	2.00	0.43
1:C:212:TYR:CD1	1:C:212:TYR:C	2.90	0.43
1:D:47:ILE:HG13	1:D:48:GLY:H	1.83	0.43
1:C:204:THR:O	1:C:208:ILE:HG12	2.18	0.43
1:B:173:ASP:OD1	1:B:177:VAL:HG23	2.18	0.43
1:A:243:GLN:HE21	1:A:245:LEU:N	2.17	0.43
1:C:203:GLY:CA	1:C:208:ILE:HD11	2.49	0.43
1:D:66:VAL:HG23	1:D:101:ILE:HD12	2.00	0.43
1:D:165:VAL:HB	1:D:226:SER:HB3	2.01	0.43
1:B:98:VAL:HG21	1:B:181:THR:HB	2.00	0.43
1:D:284:LYS:HE2	1:D:312:TYR:CD2	2.50	0.43
1:C:41:PHE:C	1:C:41:PHE:CD1	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:136:MET:O	1:C:141:ARG:NH1	2.50	0.43
1:B:93:ARG:HD2	1:B:93:ARG:HA	1.22	0.43
1:D:94:HIS:HD2	1:D:154:TYR:CG	2.36	0.43
1:C:74:GLU:C	1:C:76:SER:H	2.22	0.43
1:A:150:ARG:HD3	1:A:307:LEU:HD11	2.00	0.43
1:A:302:SER:O	1:A:304:GLY:N	2.51	0.43
1:B:139:GLU:O	1:B:142:LEU:N	2.51	0.43
1:D:231:LEU:O	1:D:234:VAL:HB	2.19	0.43
1:A:245:LEU:HD13	1:C:240:ALA:HA	2.00	0.43
1:C:238:ARG:NH2	1:C:250:VAL:O	2.52	0.43
1:C:156:HIS:CE1	1:C:303:MET:CG	3.01	0.43
1:C:201:VAL:HB	2:G:166:GLN:OE1	2.18	0.43
2:H:136:LEU:O	2:H:141:ALA:N	2.52	0.43
1:A:164:ASP:OD2	1:A:169:ASN:ND2	2.48	0.43
1:A:70:ARG:HD2	1:A:109:GLU:OE1	2.18	0.43
1:A:265:LEU:HD21	1:A:283:ARG:HG3	2.01	0.43
1:C:41:PHE:C	1:C:41:PHE:HD1	2.21	0.43
1:B:146:ILE:O	1:B:149:ALA:HB3	2.18	0.43
1:D:242:VAL:HG13	1:D:242:VAL:O	2.18	0.43
1:B:94:HIS:CD2	1:B:154:TYR:CG	3.07	0.43
1:D:136:MET:CG	1:D:140:GLN:HG2	2.45	0.43
1:D:263:GLY:O	1:D:264:GLN:CB	2.66	0.43
1:A:46:LEU:HD13	1:A:57:LYS:HB3	2.01	0.43
1:C:158:ARG:HB3	1:C:158:ARG:HE	1.63	0.42
1:A:190:THR:H	1:A:195:THR:HG21	1.85	0.42
1:D:47:ILE:HD13	1:D:116:TYR:HE1	1.84	0.42
1:C:127:TYR:C	1:C:127:TYR:CD2	2.92	0.42
1:D:84:THR:O	1:D:88:THR:HB	2.18	0.42
2:E:154:MET:HG2	2:E:181:ILE:HG22	2.01	0.42
1:D:85:GLU:HG3	1:D:183:PHE:HB2	2.00	0.42
1:B:96:HIS:HD2	1:B:150:ARG:HB3	1.82	0.42
1:D:53:GLY:HA2	1:D:73:PRO:HD2	2.01	0.42
1:B:89:LEU:C	1:B:91:PHE:N	2.71	0.42
2:F:135:GLN:O	2:F:139:GLU:N	2.44	0.42
2:H:126:VAL:HG22	2:H:190:GLU:CD	2.40	0.42
1:D:36:GLU:HB2	1:D:103:PHE:CE1	2.54	0.42
2:E:147:ARG:NH1	2:E:196:ARG:HG3	2.34	0.42
1:D:240:ALA:O	1:D:241:ILE:HG23	2.19	0.42
1:A:243:GLN:NE2	1:A:244:SER:N	2.67	0.42
1:B:89:LEU:CD2	1:B:100:LEU:HB2	2.49	0.42
2:G:164:VAL:O	2:G:168:ILE:HG13	2.19	0.42
1:A:226:SER:O	1:A:230:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:245:LEU:H	1:C:246:PRO:CD	2.31	0.42
1:C:96:HIS:HD2	1:C:150:ARG:HB3	1.83	0.42
1:A:117:MET:CG	1:A:171:LEU:HD23	2.46	0.42
1:C:221:LYS:HE2	1:C:300:ARG:O	2.19	0.42
1:A:235:LEU:HB2	1:A:285:PHE:HE2	1.84	0.42
1:C:33:ASP:OD1	1:C:34:LEU:N	2.52	0.42
1:A:232:PHE:O	1:A:234:VAL:N	2.52	0.42
1:A:241:ILE:HG12	1:A:242:VAL:N	2.33	0.42
1:B:96:HIS:NE2	1:B:147:GLY:HA2	2.34	0.42
1:A:158:ARG:HB3	1:A:158:ARG:HE	1.49	0.42
1:A:187:LYS:HG2	1:A:197:LEU:HD11	2.01	0.42
1:B:198:SEP:HB3	1:B:216:GLY:O	2.19	0.42
1:A:238:ARG:HD2	1:A:252:LEU:HD13	2.01	0.42
1:A:273:LEU:HD13	1:A:277:ILE:HD11	2.00	0.42
2:E:136:LEU:O	2:E:141:ALA:N	2.51	0.42
1:A:183:PHE:O	1:A:185:ILE:N	2.52	0.42
1:A:236:CYS:O	1:A:237:ALA:CB	2.66	0.42
1:D:283:ARG:O	1:D:287:ASP:HB2	2.20	0.42
1:D:252:LEU:HD23	1:D:252:LEU:C	2.40	0.42
1:C:236:CYS:O	1:C:237:ALA:HB3	2.18	0.42
1:B:74:GLU:O	1:B:76:SER:N	2.46	0.42
1:B:278:ARG:O	1:B:280:GLU:N	2.53	0.42
1:B:202:LYS:O	1:B:208:ILE:CD1	2.67	0.42
1:D:238:ARG:HD3	1:D:238:ARG:O	2.19	0.42
1:B:94:HIS:HD2	1:B:154:TYR:CD2	2.38	0.42
1:C:278:ARG:HA	1:C:279:PRO:HD2	1.72	0.42
1:C:117:MET:HG3	1:C:171:LEU:HB3	2.01	0.42
1:A:187:LYS:HG3	1:A:188:LYS:N	2.35	0.42
1:D:97:LEU:HD11	1:D:155:LEU:HD11	2.02	0.42
1:C:74:GLU:N	1:C:74:GLU:CD	2.73	0.42
1:D:85:GLU:OE2	1:D:114:TYR:OH	2.31	0.41
1:C:126:LEU:HD21	1:C:234:VAL:HG13	2.02	0.41
1:C:93:ARG:HA	1:C:93:ARG:HD3	1.27	0.41
1:A:288:THR:O	1:A:291:LYS:N	2.53	0.41
1:D:68:LEU:HD12	1:D:113:ILE:HG12	2.01	0.41
2:F:151:ARG:HG2	2:F:155:ASN:ND2	2.35	0.41
1:D:285:PHE:CD2	1:D:285:PHE:C	2.94	0.41
1:A:68:LEU:CD1	1:A:113:ILE:HG12	2.49	0.41
1:B:142:LEU:HD21	1:B:285:PHE:CD1	2.56	0.41
1:A:238:ARG:HB3	1:A:252:LEU:CD1	2.51	0.41
1:C:238:ARG:HH11	1:C:238:ARG:HG3	1.85	0.41
1:B:219:THR:C	1:B:221:LYS:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:146:ILE:HD13	1:A:311:GLU:HA	2.00	0.41
1:B:200:VAL:O	1:B:202:LYS:HG3	2.20	0.41
1:A:302:SER:C	1:A:304:GLY:N	2.73	0.41
2:G:167:ASN:O	2:G:171:GLN:HG3	2.19	0.41
1:A:98:VAL:HG21	1:A:181:THR:HB	2.03	0.41
2:F:147:ARG:CG	2:F:195:LEU:HB3	2.50	0.41
1:B:78:GLY:O	1:B:82:PHE:HB2	2.20	0.41
1:B:245:LEU:H	1:B:246:PRO:CD	2.33	0.41
1:A:163:ARG:NH1	1:A:185:ILE:O	2.53	0.41
1:C:205:LEU:HD21	2:G:180:GLY:CA	2.45	0.41
1:B:197:LEU:HD23	1:B:218:LEU:O	2.20	0.41
2:E:133:VAL:O	2:E:137:VAL:HG23	2.21	0.41
1:B:89:LEU:C	1:B:91:PHE:H	2.23	0.41
1:C:36:GLU:HB2	1:C:103:PHE:CZ	2.56	0.41
1:B:259:SER:O	1:B:265:LEU:N	2.46	0.41
1:C:85:GLU:O	1:C:89:LEU:HB3	2.20	0.41
1:D:195:THR:HB	1:D:197:LEU:CD2	2.51	0.41
1:D:220:GLU:O	1:D:223:ASP:HB2	2.21	0.41
1:A:278:ARG:CG	1:A:279:PRO:HD2	2.50	0.41
1:B:40:ASN:CG	1:B:41:PHE:N	2.73	0.41
1:A:257:VAL:O	1:A:261:ASN:HB3	2.20	0.41
1:D:141:ARG:O	1:D:145:CYS:HB2	2.21	0.41
1:C:226:SER:O	1:C:230:VAL:HG23	2.21	0.41
1:A:287:ASP:O	1:A:291:LYS:HG3	2.21	0.41
1:D:91:PHE:O	1:D:93:ARG:N	2.54	0.41
1:A:94:HIS:ND1	1:A:95:PRO:HD2	2.36	0.41
1:C:71:ARG:HB2	1:C:110:MET:HG3	2.02	0.41
1:A:127:TYR:CE2	1:C:244:SER:O	2.73	0.41
1:B:161:ILE:HD13	1:B:218:LEU:HG	2.03	0.41
1:A:259:SER:HB3	1:A:266:GLU:HB2	2.03	0.41
1:C:138:TRP:CD1	1:C:277:ILE:HG12	2.56	0.41
2:H:133:VAL:HG21	2:H:194:ALA:HB1	2.02	0.41
1:B:142:LEU:HD21	1:B:285:PHE:HD1	1.86	0.41
1:D:82:PHE:CE2	1:D:112:LEU:HG	2.55	0.41
1:A:106:GLU:HG2	1:A:107:ARG:HG3	2.03	0.41
1:A:39:ASN:ND2	1:A:106:GLU:OE2	2.54	0.41
1:D:229:VAL:HG22	1:D:253:ALA:HB2	2.01	0.41
1:A:32:VAL:HG12	1:A:32:VAL:O	2.21	0.41
1:B:122:LEU:HD13	1:B:144:ILE:HG21	2.03	0.41
1:D:207:TYR:O	1:D:208:ILE:C	2.59	0.41
1:C:70:ARG:HG2	1:C:111:ILE:HG12	2.03	0.41
1:C:271:PRO:HB2	1:C:272:ASN:H	1.71	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:98:VAL:HG12	1:C:114:TYR:HD2	1.86	0.40
1:A:199:TPO:OG1	1:A:200:VAL:N	2.54	0.40
1:C:240:ALA:CB	1:C:243:GLN:HB2	2.50	0.40
1:C:117:MET:O	1:C:119:ASN:N	2.55	0.40
1:C:132:PRO:C	1:C:134:MET:N	2.74	0.40
1:D:205:LEU:HA	1:D:205:LEU:HD12	1.96	0.40
1:D:173:ASP:OD2	1:D:177:VAL:HB	2.21	0.40
1:B:245:LEU:H	1:B:246:PRO:HD3	1.85	0.40
2:F:183:ARG:HB2	2:G:183:ARG:NH1	2.36	0.40
1:B:98:VAL:HG22	1:B:179:LYS:HB3	2.03	0.40
2:H:176:MET:HA	2:H:180:GLY:CA	2.49	0.40
1:C:200:VAL:O	1:C:202:LYS:HG3	2.22	0.40
1:A:39:ASN:ND2	1:A:106:GLU:CD	2.75	0.40
2:E:164:VAL:O	2:E:168:ILE:HG13	2.21	0.40
2:E:182:SER:HB3	2:E:185:SER:HB2	2.02	0.40
1:D:238:ARG:HD3	1:D:240:ALA:HB3	2.03	0.40
1:A:197:LEU:H	1:A:197:LEU:CD2	2.30	0.40
1:D:251:ASN:HB3	1:D:254:GLU:HB2	2.04	0.40
1:C:132:PRO:C	1:C:134:MET:H	2.24	0.40
1:C:238:ARG:O	1:C:238:ARG:CD	2.64	0.40
1:C:121:ASN:HA	1:C:171:LEU:HA	2.03	0.40
1:B:161:ILE:CD1	1:B:197:LEU:HD21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	284/327 (87%)	209 (74%)	54 (19%)	21 (7%)	2 15
1	B	284/327 (87%)	194 (68%)	63 (22%)	27 (10%)	1 9
1	C	282/327 (86%)	201 (71%)	60 (21%)	21 (7%)	2 15
1	D	284/327 (87%)	209 (74%)	49 (17%)	26 (9%)	1 9
2	E	75/85 (88%)	62 (83%)	11 (15%)	2 (3%)	8 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	75/85 (88%)	62 (83%)	11 (15%)	2 (3%)	8	49
2	G	75/85 (88%)	61 (81%)	12 (16%)	2 (3%)	8	49
2	H	75/85 (88%)	67 (89%)	6 (8%)	2 (3%)	8	49
All	All	1434/1648 (87%)	1065 (74%)	266 (18%)	103 (7%)	2	16

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	47	ILE
1	A	92	CYS
1	B	39	ASN
1	B	47	ILE
1	B	51	VAL
1	B	184	GLY
1	C	39	ASN
1	C	47	ILE
1	C	51	VAL
1	C	127	TYR
1	C	263	GLY
1	D	39	ASN
1	D	47	ILE
1	D	92	CYS
1	D	239	SER
1	D	264	GLN
2	E	181	ILE
2	F	181	ILE
2	G	181	ILE
2	H	181	ILE
1	A	128	GLY
1	A	129	SER
1	A	159	ALA
1	A	171	LEU
1	A	184	GLY
1	A	239	SER
1	A	241	ILE
1	A	247	ARG
1	A	264	GLN
1	B	40	ASN
1	B	74	GLU
1	B	92	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	124	ARG
1	B	128	GLY
1	B	220	GLU
1	B	239	SER
1	B	241	ILE
1	B	246	PRO
1	B	261	ASN
1	C	40	ASN
1	C	92	CYS
1	C	118	GLU
1	C	192	LEU
1	C	239	SER
1	C	241	ILE
1	C	245	LEU
1	C	246	PRO
1	D	51	VAL
1	D	128	GLY
1	D	163	ARG
1	D	241	ILE
1	D	247	ARG
1	D	263	GLY
1	D	303	MET
2	E	180	GLY
2	F	180	GLY
2	H	180	GLY
1	A	163	ARG
1	A	245	LEU
1	B	43	HIS
1	B	182	ASP
1	B	271	PRO
1	B	295	LEU
1	C	124	ARG
1	C	128	GLY
1	C	132	PRO
1	C	182	ASP
1	C	191	GLU
1	D	34	LEU
1	D	184	GLY
1	D	233	GLU
1	D	245	LEU
2	G	180	GLY
1	A	40	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	ASP
1	A	233	GLU
1	A	271	PRO
1	A	303	MET
1	B	245	LEU
1	C	131	LEU
1	C	271	PRO
1	C	274	ALA
1	D	40	ASN
1	D	130	ASP
1	D	131	LEU
1	D	167	SER
1	D	262	ASN
1	A	246	PRO
1	B	131	LEU
1	B	174	GLU
1	B	191	GLU
1	D	271	PRO
1	A	131	LEU
1	B	75	SER
1	D	32	VAL
1	D	127	TYR
1	B	178	PRO
1	D	208	ILE
1	D	246	PRO
1	B	132	PRO
1	B	208	ILE
1	B	279	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/287 (88%)	230 (92%)	21 (8%)	16	55
1	B	251/287 (88%)	221 (88%)	30 (12%)	7	33
1	C	249/287 (87%)	222 (89%)	27 (11%)	9	39
1	D	251/287 (88%)	235 (94%)	16 (6%)	25	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	62/68 (91%)	62 (100%)	0	100	100
2	F	62/68 (91%)	62 (100%)	0	100	100
2	G	62/68 (91%)	62 (100%)	0	100	100
2	H	62/68 (91%)	61 (98%)	1 (2%)	75	94
All	All	1250/1420 (88%)	1155 (92%)	95 (8%)	19	61

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	41	PHE
1	A	42	ASP
1	A	61	ARG
1	A	66	VAL
1	A	70	ARG
1	A	87	GLU
1	A	115	LYS
1	A	136	MET
1	A	150	ARG
1	A	175	ASN
1	A	197	LEU
1	A	219	THR
1	A	238	ARG
1	A	241	ILE
1	A	242	VAL
1	A	255	TRP
1	A	264	GLN
1	A	270	ASP
1	A	272	ASN
1	A	273	LEU
1	B	33	ASP
1	B	41	PHE
1	B	46	LEU
1	B	68	LEU
1	B	74	GLU
1	B	92	CYS
1	B	93	ARG
1	B	94	HIS
1	B	105	ASP
1	B	115	LYS
1	B	124	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	MET
1	B	152	LEU
1	B	195	THR
1	B	197	LEU
1	B	212	TYR
1	B	220	GLU
1	B	238	ARG
1	B	241	ILE
1	B	247	ARG
1	B	248	GLU
1	B	250	VAL
1	B	257	VAL
1	B	264	GLN
1	B	272	ASN
1	B	292	CYS
1	B	312	TYR
1	B	314	LEU
1	B	315	ARG
1	B	317	GLN
1	C	34	LEU
1	C	41	PHE
1	C	42	ASP
1	C	46	LEU
1	C	62	ASP
1	C	70	ARG
1	C	74	GLU
1	C	92	CYS
1	C	93	ARG
1	C	97	LEU
1	C	115	LYS
1	C	124	ARG
1	C	143	GLU
1	C	158	ARG
1	C	197	LEU
1	C	212	TYR
1	C	238	ARG
1	C	241	ILE
1	C	244	SER
1	C	247	ARG
1	C	250	VAL
1	C	264	GLN
1	C	272	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	280	GLU
1	C	287	ASP
1	C	312	TYR
1	C	314	LEU
1	D	32	VAL
1	D	41	PHE
1	D	42	ASP
1	D	46	LEU
1	D	68	LEU
1	D	94	HIS
1	D	124	ARG
1	D	145	CYS
1	D	185	ILE
1	D	195	THR
1	D	197	LEU
1	D	238	ARG
1	D	241	ILE
1	D	270	ASP
1	D	272	ASN
1	D	315	ARG
2	H	144	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	77	GLN
1	A	262	ASN
1	B	39	ASN
1	B	77	GLN
1	B	243	GLN
1	B	272	ASN
1	B	317	GLN
1	C	39	ASN
1	C	77	GLN
1	C	96	HIS
1	C	156	HIS
1	C	272	ASN
1	C	317	GLN
1	D	77	GLN
1	D	94	HIS
1	D	96	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	119	ASN
1	D	243	GLN
1	D	262	ASN
1	D	272	ASN
2	E	130	ASN
2	E	134	GLN
2	E	155	ASN
2	E	175	ASN
2	F	130	ASN
2	F	134	GLN
2	F	155	ASN
2	G	130	ASN
2	G	134	GLN
2	G	155	ASN
2	H	134	GLN
2	H	155	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	SEP	A	198	1	9,9,10	7.42	5 (55%)	10,12,14	1.20	0
1	TPO	A	199	1	10,10,11	6.12	2 (20%)	12,14,16	1.03	0
1	SEP	B	198	1	9,9,10	7.39	5 (55%)	10,12,14	2.10	2 (20%)
1	TPO	B	199	1	10,10,11	6.34	2 (20%)	12,14,16	1.20	0
1	SEP	C	198	1	9,9,10	7.55	5 (55%)	10,12,14	1.47	2 (20%)
1	TPO	C	199	1	10,10,11	6.13	2 (20%)	12,14,16	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	D	198	1	9,9,10	7.26	5 (55%)	10,12,14	1.24	1 (10%)
1	TPO	D	199	1	10,10,11	6.27	2 (20%)	12,14,16	1.12	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
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0
1	TPO	A	199	1	-	1/9/11/13	0/0/0/0
1	SEP	B	198	1	-	0/6/8/10	0/0/0/0
1	TPO	B	199	1	-	1/9/11/13	0/0/0/0
1	SEP	C	198	1	-	0/6/8/10	0/0/0/0
1	TPO	C	199	1	-	1/9/11/13	0/0/0/0
1	SEP	D	198	1	-	0/6/8/10	0/0/0/0
1	TPO	D	199	1	-	1/9/11/13	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	SEP	O-C	21.45	1.26	1.11
1	A	198	SEP	O-C	21.31	1.26	1.11
1	B	198	SEP	O-C	21.00	1.25	1.11
1	D	198	SEP	O-C	20.91	1.25	1.11
1	B	199	TPO	O-C	19.73	1.25	1.11
1	D	199	TPO	O-C	19.50	1.24	1.11
1	C	199	TPO	O-C	19.08	1.24	1.11
1	A	199	TPO	O-C	18.97	1.24	1.11
1	B	198	SEP	CA-C	4.71	1.57	1.48
1	C	198	SEP	CA-C	4.38	1.56	1.48
1	C	198	SEP	P-O1P	4.27	1.65	1.51
1	A	198	SEP	CA-C	4.16	1.56	1.48
1	D	198	SEP	CA-C	4.00	1.55	1.48
1	B	198	SEP	P-O1P	3.82	1.64	1.51
1	A	198	SEP	P-O1P	3.47	1.62	1.51
1	D	198	SEP	P-O1P	3.35	1.62	1.51
1	A	199	TPO	CA-C	3.09	1.54	1.48
1	C	198	SEP	P-O2P	2.91	1.65	1.54
1	D	199	TPO	CA-C	2.77	1.53	1.48
1	C	199	TPO	CA-C	2.67	1.53	1.48
1	B	199	TPO	CA-C	2.66	1.53	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	SEP	P-O3P	2.49	1.63	1.54
1	B	198	SEP	P-O3P	2.49	1.63	1.54
1	B	198	SEP	P-O2P	2.41	1.63	1.54
1	A	198	SEP	P-O3P	2.32	1.63	1.54
1	A	198	SEP	P-O2P	2.32	1.63	1.54
1	D	198	SEP	P-O2P	2.23	1.62	1.54
1	D	198	SEP	P-O3P	2.21	1.62	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	SEP	C-CA-N	5.00	118.83	113.83
1	B	198	SEP	P-OG-CB	-3.51	108.03	118.19
1	C	198	SEP	P-OG-CB	-3.17	109.03	118.19
1	C	198	SEP	C-CA-N	3.07	116.90	113.83
1	D	198	SEP	P-OG-CB	-2.36	111.36	118.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	199	TPO	OG1-CB-CA-N
1	D	199	TPO	OG1-CB-CA-N
1	B	199	TPO	OG1-CB-CA-N
1	C	199	TPO	OG1-CB-CA-N

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	288/327 (88%)	0.34	7 (2%)	56	15	48, 81, 109, 115	0
1	B	288/327 (88%)	0.21	4 (1%)	72	25	50, 75, 98, 107	0
1	C	286/327 (87%)	0.22	7 (2%)	56	15	47, 75, 99, 110	0
1	D	288/327 (88%)	0.33	6 (2%)	60	17	50, 82, 103, 109	0
2	E	77/85 (90%)	0.28	0	100	100	74, 90, 105, 107	0
2	F	77/85 (90%)	0.32	3 (3%)	37	8	72, 85, 109, 113	0
2	G	77/85 (90%)	0.32	1 (1%)	74	27	83, 102, 113, 115	0
2	H	77/85 (90%)	0.27	1 (1%)	74	27	76, 85, 95, 101	0
All	All	1458/1648 (88%)	0.28	29 (1%)	62	19	47, 81, 105, 115	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	194	ALA	4.0
1	A	57	LYS	3.0
1	A	63	GLY	2.9
2	G	132	ILE	2.8
1	B	77	GLN	2.8
1	B	92	CYS	2.6
1	D	193	GLY	2.5
1	D	194	GLN	2.5
1	A	194	GLN	2.5
1	C	92	CYS	2.5
1	C	60	LEU	2.4
1	D	280	GLU	2.4
1	A	192	LEU	2.3
1	C	77	GLN	2.3
1	A	193	GLY	2.3
2	H	197	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	75	SER	2.2
1	A	189	GLY	2.2
2	F	195	LEU	2.2
1	D	65	LYS	2.2
1	C	260	HIS	2.1
1	B	60	LEU	2.1
1	D	71	ARG	2.1
1	C	198	SEP	2.0
1	A	109	GLU	2.0
2	F	191	LEU	2.0
1	C	61	ARG	2.0
1	B	102	GLY	2.0
1	C	217	ARG	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	B	198	10/11	0.45	0.76	78,82,83,88	0
1	SEP	C	198	10/11	0.50	0.69	82,85,86,89	0
1	TPO	C	199	11/12	0.26	-0.56	82,83,85,88	0
1	SEP	D	198	10/11	0.22	-0.64	78,79,81,85	0
1	TPO	D	199	11/12	0.16	-1.18	79,80,81,82	0
1	SEP	A	198	10/11	0.20	-1.22	84,85,86,90	0
1	TPO	B	199	11/12	0.17	-1.58	79,79,80,80	0
1	TPO	A	199	11/12	0.16	-2.17	83,83,85,87	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.