



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:37 PM GMT

PDB ID : 2H2P
Title : Crystal structure of CLC-ec1 in complex with Fab fragment in SeCN-
Authors : Nguitragool, W.; Miller, C.
Deposited on : 2006-05-19
Resolution : 3.10 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>

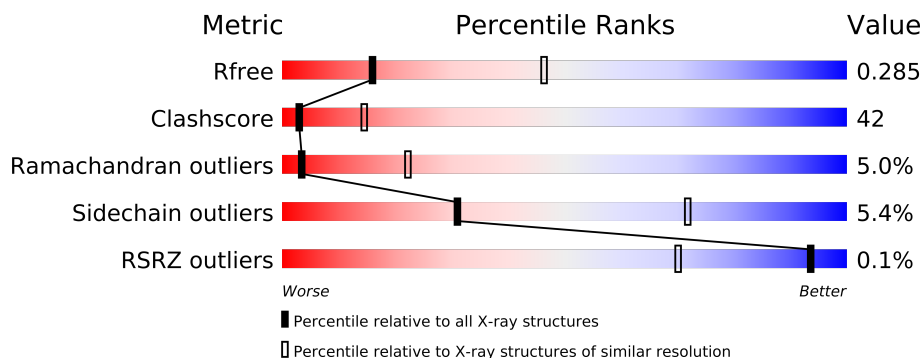
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **FAILED**
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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	465	
1	B	465	
2	C	221	
2	E	221	
3	D	211	
3	F	211	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13231 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 CLC Cl transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

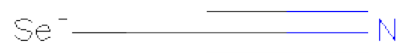
- Molecule 2 is a protein called FAB fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called FAB fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is SELENOCYANATE ION (three-letter code: SEK) (formula: CNSe).



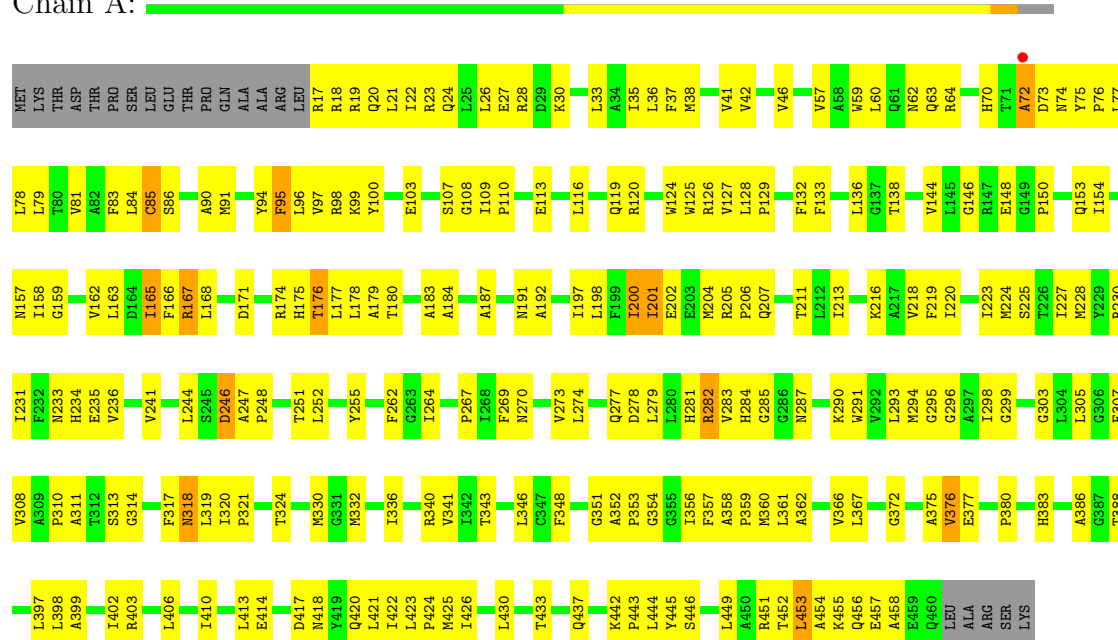
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Se 1	0	0
4	B	1	Total 1	Se 1	0	0
4	A	1	Total 1	Se 1	1	0
4	B	1	Total 1	Se 1	1	0
4	A	1	Total 1	Se 1	1	0
4	B	1	Total 1	Se 1	1	0
4	A	1	Total 1	Se 1	1	0
4	B	1	Total 1	Se 1	1	0

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.

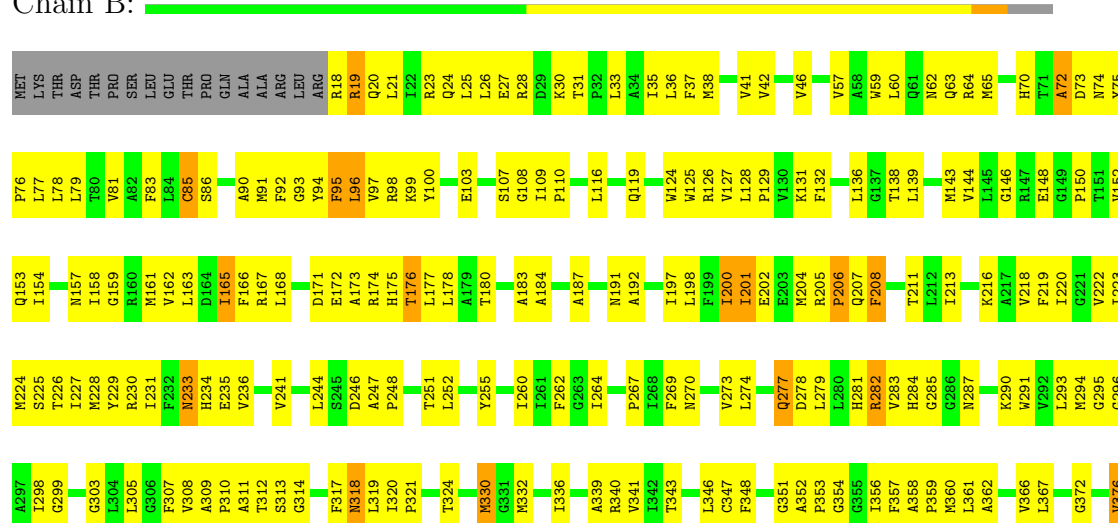
• Molecule 1: CLC Cl transporter

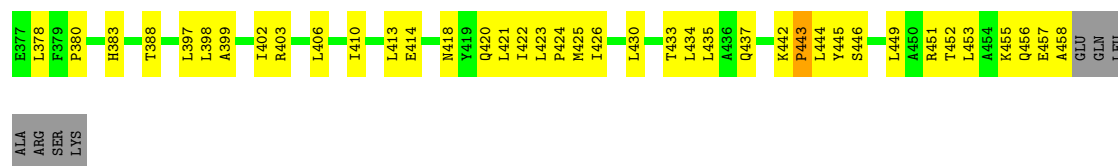
Chain A:



• Molecule 1: CLC Cl transporter

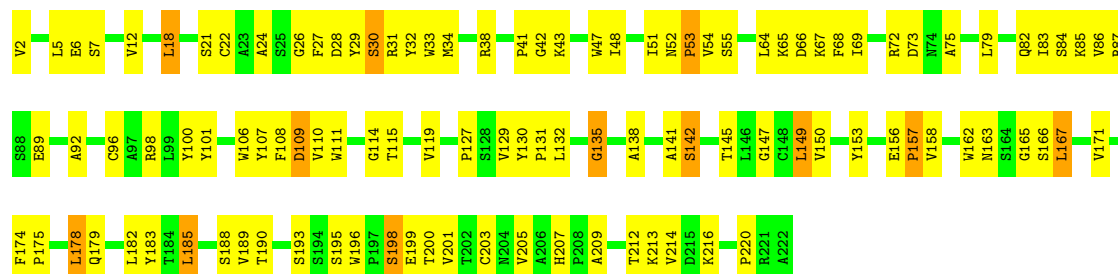
Chain B:





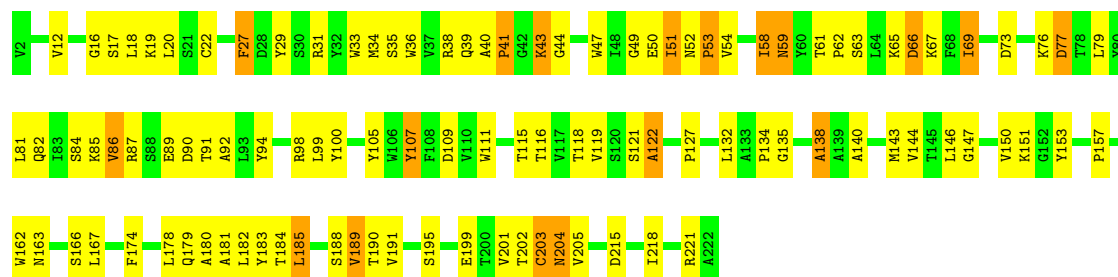
- Molecule 2: FAB fragment, heavy chain

Chain C:



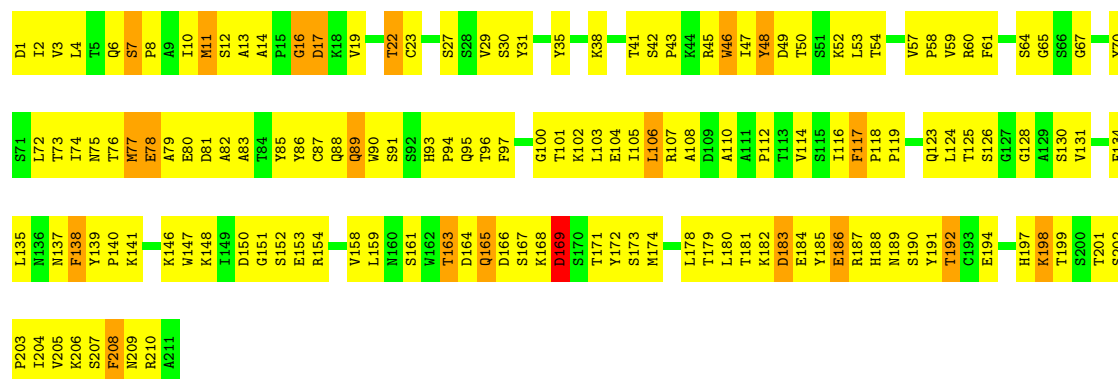
- Molecule 2: FAB fragment, heavy chain

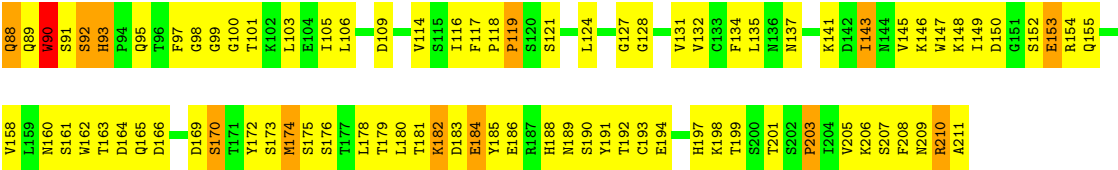
Chain E:



- Molecule 3: FAB fragment, light chain

Chain D:





4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.58Å 121.58Å 151.24Å 90.00° 128.25° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 37.67 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.10) 98.0 (37.67-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.278 , 0.280 0.281 , 0.285	Depositor DCC
R_{free} test set	3070 reflections (5.27%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.48	0/3405	0.64	0/4621
1	B	0.48	0/3376	0.63	0/4583
2	C	0.52	0/1721	0.76	0/2355
2	E	0.52	0/1721	0.78	0/2355
3	D	0.48	0/1660	0.73	1/2257 (0.0%)
3	F	0.52	0/1660	0.77	0/2257
All	All	0.49	0/13543	0.70	1/18428 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	16	GLY	N-CA-C	-6.80	96.11	113.10

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	3333	0	3482	267	0
1	B	3304	0	3456	274	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1672	0	1654	122	0
2	E	1672	0	1654	125	0
3	D	1621	0	1544	230	0
3	F	1621	0	1546	172	0
4	A	4	0	0	2	0
4	B	4	0	0	2	0
All	All	13231	0	13336	1109	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 42.

All (1109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:107:TYR:CE1	3:D:45:ARG:NH1	1.70	1.56
1:A:274:LEU:CD2	1:A:451:ARG:NH1	1.71	1.53
3:D:186:GLU:HA	3:D:210:ARG:NH2	1.27	1.45
2:E:163:ASN:HD22	2:E:167:LEU:CD1	1.35	1.39
1:A:18:ARG:NH1	1:B:456:GLN:OE1	1.62	1.30
1:A:274:LEU:HD22	1:A:451:ARG:NH1	0.94	1.25
3:D:75:ASN:O	3:D:76:THR:HG22	1.35	1.22
2:E:143:MET:CE	2:E:190:THR:HG22	1.70	1.21
3:D:188:HIS:O	3:D:210:ARG:HD2	1.36	1.20
1:A:119:GLN:NE2	1:B:18:ARG:HD3	1.55	1.19
3:F:38:LYS:O	3:F:41:THR:HG22	1.01	1.18
3:D:107:ARG:HG2	3:D:108:ALA:H	1.06	1.18
3:D:6:GLN:HG3	3:D:100:GLY:H	1.01	1.18
1:A:171:ASP:O	1:A:175:HIS:CD2	2.02	1.12
3:F:38:LYS:O	3:F:41:THR:CG2	1.97	1.12
3:D:16:GLY:HA2	3:D:76:THR:OG1	1.49	1.10
3:D:186:GLU:CA	3:D:210:ARG:NH2	2.14	1.10
1:B:171:ASP:O	1:B:175:HIS:ND1	1.82	1.09
2:E:163:ASN:ND2	2:E:167:LEU:HD13	1.67	1.09
3:D:74:ILE:HG21	3:D:77:MET:CB	1.81	1.09
3:D:186:GLU:CA	3:D:210:ARG:HH22	1.66	1.08
3:D:74:ILE:HG21	3:D:77:MET:HB2	1.07	1.07
2:E:35:SER:HB2	2:E:99:LEU:HD11	1.35	1.07
3:F:7:SER:HB2	3:F:22:THR:HB	1.10	1.07
3:D:192:THR:HA	3:D:207:SER:HB3	1.36	1.06
3:D:107:ARG:HG2	3:D:108:ALA:N	1.60	1.05
2:E:143:MET:HE3	2:E:190:THR:HG22	1.37	1.04
3:D:74:ILE:CG2	3:D:77:MET:HB2	1.86	1.04
2:E:143:MET:HE3	2:E:190:THR:CG2	1.88	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.39	1.02
2:E:163:ASN:ND2	2:E:167:LEU:CD1	2.18	1.02
2:E:143:MET:CE	2:E:190:THR:CG2	2.37	1.02
1:A:171:ASP:O	1:A:175:HIS:HD2	1.41	1.00
2:E:163:ASN:HD22	2:E:167:LEU:HD13	0.87	1.00
2:C:167:LEU:HD23	2:C:189:VAL:HG21	1.42	0.99
3:F:2:ILE:CD1	3:F:27:SER:OG	2.11	0.99
3:D:6:GLN:HG3	3:D:100:GLY:N	1.78	0.98
3:D:107:ARG:CG	3:D:108:ALA:H	1.75	0.98
3:F:191:TYR:O	3:F:207:SER:HB2	1.63	0.98
3:F:188:HIS:O	3:F:210:ARG:HD3	1.64	0.97
3:D:17:ASP:H	3:D:76:THR:HA	1.26	0.97
3:D:188:HIS:C	3:D:210:ARG:HD2	1.86	0.95
3:F:158:VAL:HG22	3:F:178:LEU:HD13	1.49	0.94
2:E:204:ASN:HB3	2:E:215:ASP:OD1	1.67	0.93
3:F:150:ASP:OD2	3:F:188:HIS:HB3	1.68	0.93
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.50	0.93
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.50	0.93
3:D:75:ASN:O	3:D:76:THR:CG2	2.16	0.93
1:B:107:SER:H	4:B:466:SEK:SE	2.01	0.93
3:F:7:SER:HB2	3:F:22:THR:CB	1.97	0.92
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.48	0.92
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.52	0.92
3:F:7:SER:CB	3:F:22:THR:HB	1.99	0.92
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.51	0.92
3:F:2:ILE:HD12	3:F:27:SER:OG	1.70	0.91
3:D:89:GLN:NE2	3:D:91:SER:H	1.68	0.90
3:D:79:ALA:HA	3:D:105:ILE:HD11	1.54	0.90
1:A:119:GLN:NE2	1:B:18:ARG:CD	2.34	0.90
3:F:54:THR:HG22	3:F:55:SER:H	1.34	0.89
3:F:32:ILE:HD11	3:F:70:TYR:CG	2.07	0.89
3:F:90:TRP:HH2	3:F:93:HIS:HD1	1.16	0.89
3:D:188:HIS:O	3:D:210:ARG:CD	2.20	0.89
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.73	0.89
2:C:6:GLU:OE1	2:C:114:GLY:HA2	1.70	0.88
3:F:201:THR:O	3:F:203:PRO:HD3	1.74	0.88
2:E:163:ASN:HD22	2:E:167:LEU:HD11	1.38	0.88
2:C:132:LEU:HB2	2:C:147:GLY:O	1.73	0.88
2:C:6:GLU:HG2	2:C:96:CYS:SG	2.14	0.88
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.07	0.87
3:D:112:PRO:HG2	3:D:204:ILE:HD12	1.55	0.87
1:B:180:THR:HG22	1:B:218:VAL:HA	1.55	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:7:SER:CB	3:F:8:PRO:HD3	2.05	0.87
1:B:244:LEU:H	1:B:418:ASN:HD21	1.23	0.87
3:D:6:GLN:NE2	3:D:86:TYR:HA	1.90	0.86
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.54	0.86
2:E:201:VAL:HG13	2:E:218:ILE:HB	1.57	0.86
3:D:185:TYR:O	3:D:210:ARG:NH1	2.08	0.86
1:B:287:ASN:ND2	1:B:290:LYS:H	1.73	0.85
3:F:95:GLN:OE1	3:F:95:GLN:N	2.10	0.85
2:E:91:THR:HG23	2:E:118:THR:HA	1.59	0.85
1:A:207:GLN:HG3	1:B:28:ARG:HH11	1.41	0.85
3:D:166:ASP:OD2	3:D:169:ASP:HB3	1.77	0.85
2:C:7:SER:HA	2:C:115:THR:HG21	1.59	0.85
2:E:29:TYR:HD1	2:E:34:MET:HE3	1.41	0.84
1:A:28:ARG:HH11	1:B:207:GLN:HG3	1.40	0.84
2:E:29:TYR:CD1	2:E:34:MET:CE	2.60	0.84
3:D:202:SER:HB3	3:D:203:PRO:HD2	1.60	0.84
1:A:107:SER:H	4:A:466:SEK:SE	2.11	0.84
2:C:107:TYR:HE1	3:D:45:ARG:NH1	1.35	0.84
3:F:143:ILE:HG13	3:F:197:HIS:HD2	1.42	0.84
3:F:191:TYR:HB2	3:F:208:PHE:CE2	2.12	0.84
1:A:274:LEU:HD23	1:A:451:ARG:NH1	1.88	0.83
2:E:29:TYR:CD1	2:E:34:MET:HE3	2.13	0.83
2:E:29:TYR:HD1	2:E:34:MET:CE	1.90	0.83
1:A:274:LEU:HA	1:A:277:GLN:HE21	1.43	0.83
3:D:192:THR:HA	3:D:207:SER:CB	2.08	0.83
1:B:59:TRP:O	1:B:63:GLN:HG2	1.78	0.83
1:A:287:ASN:ND2	1:A:290:LYS:H	1.75	0.83
3:D:201:THR:HG23	3:D:202:SER:N	1.94	0.83
3:F:38:LYS:C	3:F:41:THR:HG22	1.99	0.82
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.61	0.82
3:D:89:GLN:HE22	3:D:91:SER:H	1.21	0.82
3:D:146:LYS:HD3	3:D:153:GLU:HG3	1.60	0.82
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.44	0.82
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.15	0.82
3:F:194:GLU:HA	3:F:205:VAL:HG12	1.60	0.82
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.62	0.81
3:D:114:VAL:HG22	3:D:135:LEU:HD13	1.63	0.81
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.45	0.81
2:E:143:MET:HE2	2:E:190:THR:HG22	1.57	0.81
1:B:234:HIS:ND1	1:B:235:GLU:HG2	1.95	0.81
1:A:457:GLU:HB3	1:B:19:ARG:CZ	2.10	0.80
1:A:234:HIS:ND1	1:A:235:GLU:HG2	1.95	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:87:ARG:O	2:C:119:VAL:HG11	1.82	0.80
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.64	0.80
3:D:54:THR:O	3:D:57:VAL:HG23	1.82	0.80
2:E:143:MET:HE2	2:E:190:THR:CG2	2.08	0.80
1:A:244:LEU:H	1:A:418:ASN:HD21	1.25	0.80
3:D:139:TYR:CD1	3:D:140:PRO:HA	2.16	0.79
3:D:107:ARG:NH1	3:D:108:ALA:O	2.16	0.79
1:B:449:LEU:HD12	1:B:452:THR:HG21	1.62	0.79
3:D:182:LYS:O	3:D:186:GLU:HG2	1.83	0.79
3:D:125:THR:HG22	3:D:125:THR:O	1.83	0.79
3:F:7:SER:HB3	3:F:8:PRO:CD	2.12	0.79
1:A:180:THR:HG22	1:A:218:VAL:HA	1.63	0.79
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.16	0.79
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.62	0.79
1:A:59:TRP:O	1:A:63:GLN:HG2	1.83	0.79
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.64	0.78
3:D:140:PRO:HD3	3:D:198:LYS:HD3	1.65	0.77
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.15	0.77
2:C:107:TYR:CD1	3:D:45:ARG:NH1	2.49	0.77
3:D:31:TYR:HA	3:D:50:THR:OG1	1.84	0.77
1:A:332:MET:O	1:A:336:ILE:HG13	1.85	0.77
1:A:273:VAL:O	1:A:277:GLN:HG3	1.85	0.76
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.16	0.76
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.20	0.76
1:A:274:LEU:HA	1:A:277:GLN:NE2	2.01	0.75
3:D:74:ILE:HG21	3:D:77:MET:CA	2.16	0.75
1:B:99:LYS:HG2	1:B:100:TYR:CE2	2.20	0.75
1:A:18:ARG:NH1	1:B:456:GLN:CD	2.39	0.75
1:B:154:ILE:O	1:B:158:ILE:HG12	1.87	0.75
1:A:154:ILE:O	1:A:158:ILE:HG12	1.87	0.75
1:A:119:GLN:HE22	1:B:18:ARG:HD3	1.52	0.74
1:A:99:LYS:HG2	1:A:100:TYR:CE2	2.22	0.74
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.51	0.74
3:D:61:PHE:CE2	3:D:74:ILE:HG12	2.22	0.74
2:E:31:ARG:HH11	2:E:31:ARG:HG2	1.52	0.74
2:C:107:TYR:CZ	3:D:45:ARG:NH1	2.52	0.74
3:F:88:GLN:HG2	3:F:89:GLN:N	2.02	0.74
2:E:38:ARG:HD3	2:E:94:TYR:HE1	1.52	0.74
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.02	0.74
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.22	0.73
3:F:38:LYS:HB2	3:F:41:THR:HG21	1.68	0.73
3:F:2:ILE:HD11	3:F:27:SER:OG	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:73:ASP:OD2	2:E:76:LYS:HD2	1.86	0.73
3:F:121:SER:HA	3:F:124:LEU:HD12	1.70	0.73
2:C:66:ASP:OD1	2:C:69:ILE:HD11	1.89	0.73
3:F:188:HIS:O	3:F:210:ARG:CD	2.36	0.73
2:C:5:LEU:O	2:C:22:CYS:HA	1.89	0.73
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.54	0.73
3:D:124:LEU:HD23	3:D:128:GLY:O	1.89	0.73
3:D:154:ARG:NH2	3:D:184:GLU:OE2	2.16	0.72
2:C:149:LEU:O	2:C:149:LEU:HD23	1.89	0.72
1:B:311:ALA:O	1:B:340:ARG:NH1	2.21	0.72
2:E:144:VAL:HG13	2:E:191:VAL:HG23	1.71	0.72
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.53	0.72
2:E:73:ASP:OD2	2:E:76:LYS:CD	2.36	0.72
3:D:186:GLU:HA	3:D:210:ARG:CZ	2.16	0.72
3:F:119:PRO:HD3	3:F:131:VAL:HG12	1.71	0.72
3:D:7:SER:CB	3:D:8:PRO:HD3	2.18	0.72
1:A:216:LYS:HE2	1:B:433:THR:HG22	1.71	0.72
1:B:449:LEU:O	1:B:452:THR:HG22	1.89	0.72
2:E:39:GLN:O	2:E:92:ALA:HB1	1.89	0.72
2:C:145:THR:HG22	2:C:190:THR:OG1	1.91	0.71
3:D:74:ILE:CG2	3:D:77:MET:CA	2.68	0.71
3:D:90:TRP:CH2	3:D:95:GLN:NE2	2.59	0.71
3:D:79:ALA:C	3:D:81:ASP:H	1.94	0.71
2:E:29:TYR:CD1	2:E:34:MET:HE2	2.25	0.71
3:F:7:SER:OG	3:F:8:PRO:HD3	1.91	0.71
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.26	0.71
3:D:74:ILE:CG2	3:D:77:MET:CB	2.58	0.70
1:B:235:GLU:OE1	2:C:100:TYR:HE2	1.72	0.70
3:F:182:LYS:HG2	3:F:186:GLU:OE1	1.92	0.70
3:D:138:PHE:N	3:D:171:THR:HB	2.07	0.70
1:B:332:MET:O	1:B:336:ILE:HG13	1.91	0.70
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.74	0.70
3:D:6:GLN:HE21	3:D:86:TYR:HA	1.54	0.70
3:D:12:SER:HA	3:D:104:GLU:O	1.92	0.69
3:F:186:GLU:HA	3:F:210:ARG:HD2	1.73	0.69
2:C:130:TYR:HB2	2:C:149:LEU:CD2	2.22	0.69
1:A:311:ALA:O	1:A:340:ARG:NH2	2.25	0.69
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.27	0.69
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.73	0.69
3:F:189:ASN:ND2	3:F:210:ARG:HB3	2.08	0.69
3:D:7:SER:HB3	3:D:8:PRO:CD	2.22	0.69
3:F:90:TRP:HH2	3:F:93:HIS:ND1	1.89	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:89:GLN:HE21	3:F:95:GLN:HA	1.57	0.69
2:C:131:PRO:HD3	2:C:216:LYS:NZ	2.07	0.69
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.73	0.69
1:A:372:GLY:O	1:A:376:VAL:HG23	1.92	0.69
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.75	0.69
3:D:6:GLN:NE2	3:D:87:CYS:H	1.90	0.68
3:D:13:ALA:HB3	3:D:77:MET:SD	2.33	0.68
3:D:201:THR:HG23	3:D:202:SER:H	1.56	0.68
1:A:81:VAL:O	1:A:85:CYS:HB2	1.94	0.68
3:F:4:LEU:HD22	3:F:23:CYS:SG	2.34	0.68
3:F:54:THR:HG22	3:F:55:SER:N	2.07	0.68
2:C:147:GLY:HA2	2:C:162:TRP:CZ2	2.28	0.68
3:D:74:ILE:CG2	3:D:77:MET:HA	2.23	0.68
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.29	0.68
2:C:178:LEU:HD12	2:C:179:GLN:N	2.09	0.68
3:F:77:MET:HG2	3:F:78:GLU:N	2.07	0.68
2:E:163:ASN:ND2	2:E:167:LEU:HD11	1.99	0.68
2:E:61:THR:O	2:E:63:SER:N	2.27	0.67
1:A:442:LYS:HE3	1:B:26:LEU:O	1.94	0.67
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.75	0.67
3:F:32:ILE:HG22	3:F:89:GLN:HA	1.76	0.67
1:A:282:ARG:O	1:A:285:GLY:N	2.27	0.67
1:A:192:ALA:HB1	1:A:414:GLU:OE1	1.93	0.67
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.63	0.67
3:D:79:ALA:O	3:D:81:ASP:N	2.28	0.67
2:E:201:VAL:CG1	2:E:218:ILE:HB	2.24	0.67
1:A:78:LEU:HA	1:A:81:VAL:HG22	1.77	0.67
3:D:201:THR:CG2	3:D:202:SER:H	2.06	0.67
3:F:169:ASP:O	3:F:170:SER:HB2	1.94	0.67
2:C:42:GLY:O	2:C:43:LYS:HG2	1.94	0.67
2:C:207:HIS:NE2	2:C:209:ALA:HB3	2.10	0.67
3:D:81:ASP:O	3:D:103:LEU:HD23	1.95	0.67
3:D:201:THR:CG2	3:D:202:SER:N	2.57	0.67
2:E:143:MET:HE3	2:E:190:THR:HG23	1.75	0.67
1:B:449:LEU:HA	1:B:452:THR:HG22	1.74	0.67
1:B:330:MET:HE3	1:B:330:MET:HA	1.77	0.67
1:A:287:ASN:HD22	1:A:290:LYS:H	1.43	0.67
1:B:305:LEU:C	1:B:307:PHE:H	1.97	0.67
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.77	0.67
1:B:281:HIS:ND1	1:B:284:HIS:HE1	1.93	0.66
2:C:87:ARG:HH11	2:C:87:ARG:HG3	1.59	0.66
1:A:274:LEU:HD23	1:A:277:GLN:NE2	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:89:GLN:HE22	3:D:91:SER:N	1.93	0.66
1:A:26:LEU:O	1:B:442:LYS:HE3	1.96	0.66
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.26	0.66
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.76	0.66
3:D:146:LYS:HD3	3:D:153:GLU:CG	2.26	0.66
2:C:166:SER:O	2:C:167:LEU:HD12	1.95	0.66
1:A:305:LEU:C	1:A:307:PHE:H	1.99	0.66
2:E:17:SER:HB3	2:E:84:SER:HA	1.78	0.66
3:D:138:PHE:H	3:D:171:THR:HB	1.60	0.66
2:E:121:SER:O	2:E:122:ALA:O	2.13	0.66
1:B:287:ASN:HD22	1:B:290:LYS:H	1.41	0.65
3:F:189:ASN:HA	3:F:210:ARG:HB2	1.77	0.65
3:F:77:MET:HE3	3:F:103:LEU:HD21	1.78	0.65
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.78	0.65
3:F:116:ILE:HD12	3:F:193:CYS:HB2	1.78	0.65
3:D:205:VAL:O	3:D:206:LYS:HG2	1.97	0.65
3:D:8:PRO:O	3:D:101:THR:HG23	1.97	0.65
3:D:150:ASP:HA	3:D:190:SER:HB3	1.78	0.65
3:F:33:HIS:CE1	3:F:49:ASP:H	2.15	0.65
1:B:282:ARG:O	1:B:285:GLY:N	2.29	0.65
2:E:132:LEU:HB2	2:E:147:GLY:O	1.97	0.65
1:A:75:TYR:HB3	1:A:76:PRO:CD	2.25	0.65
3:F:90:TRP:HA	3:F:95:GLN:HB3	1.78	0.65
3:F:7:SER:CB	3:F:8:PRO:CD	2.70	0.65
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.30	0.65
1:A:281:HIS:ND1	1:A:284:HIS:HE1	1.94	0.65
2:E:163:ASN:HB2	2:E:166:SER:OG	1.98	0.64
2:C:6:GLU:OE1	2:C:114:GLY:CA	2.45	0.64
3:F:158:VAL:CG2	3:F:178:LEU:HD13	2.25	0.64
1:A:18:ARG:NH2	1:B:457:GLU:OE1	2.28	0.64
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.80	0.64
2:E:195:SER:O	2:E:199:GLU:HB2	1.97	0.64
2:E:132:LEU:HD11	3:F:132:VAL:HG21	1.79	0.64
2:E:38:ARG:HD3	2:E:94:TYR:CE1	2.33	0.64
2:E:105:TYR:CE1	3:F:31:TYR:HD2	2.15	0.64
3:D:89:GLN:NE2	3:D:90:TRP:N	2.46	0.63
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.79	0.63
1:B:81:VAL:O	1:B:85:CYS:HB2	1.97	0.63
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.80	0.63
3:F:143:ILE:HG13	3:F:197:HIS:CD2	2.30	0.63
3:D:123:GLN:HE22	3:D:130:SER:HB2	1.64	0.63
3:F:37:GLN:O	3:F:83:ALA:HB1	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:32:TYR:CE2	2:C:98:ARG:HD2	2.33	0.63
3:D:192:THR:CA	3:D:207:SER:HB3	2.23	0.63
3:F:149:ILE:HD12	3:F:154:ARG:CZ	2.27	0.63
3:F:146:LYS:CB	3:F:194:GLU:HB2	2.28	0.63
1:A:330:MET:HE3	1:A:330:MET:HA	1.79	0.63
3:F:72:LEU:HD23	3:F:72:LEU:C	2.19	0.63
1:B:294:MET:O	1:B:298:ILE:HG13	1.99	0.63
1:A:18:ARG:O	1:A:18:ARG:HG2	1.97	0.62
3:D:141:LYS:HB3	3:D:172:TYR:CG	2.34	0.62
2:E:162:TRP:HA	2:E:202:THR:O	1.99	0.62
2:C:30:SER:C	2:C:32:TYR:H	2.03	0.62
3:D:74:ILE:HG21	3:D:77:MET:HA	1.80	0.62
2:C:6:GLU:OE2	2:C:96:CYS:N	2.27	0.62
3:F:149:ILE:HD13	3:F:191:TYR:HE2	1.65	0.62
1:A:430:LEU:HD13	1:B:219:PHE:HB3	1.81	0.62
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.35	0.62
3:D:117:PHE:CD1	3:D:117:PHE:N	2.66	0.62
3:D:17:ASP:N	3:D:76:THR:HA	2.09	0.62
3:D:110:ALA:HB3	3:D:138:PHE:HA	1.82	0.62
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.80	0.62
1:A:120:ARG:NH1	1:A:452:THR:HG22	2.14	0.62
3:F:197:HIS:O	3:F:199:THR:N	2.32	0.61
1:B:336:ILE:O	1:B:340:ARG:HG3	1.99	0.61
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.35	0.61
2:C:18:LEU:HD21	2:C:83:ILE:HD12	1.82	0.61
3:F:13:ALA:HB3	3:F:77:MET:HE1	1.82	0.61
1:A:205:ARG:HG2	1:A:206:PRO:HD2	1.81	0.61
3:D:138:PHE:CE1	3:D:172:TYR:HB2	2.35	0.61
1:A:294:MET:O	1:A:298:ILE:HG13	2.00	0.61
2:C:6:GLU:HA	2:C:21:SER:O	2.01	0.61
2:E:132:LEU:CD1	3:F:132:VAL:HG21	2.30	0.61
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.28	0.61
1:A:433:THR:HG22	1:B:216:LYS:HE2	1.82	0.61
1:B:205:ARG:HG2	1:B:206:PRO:HD2	1.82	0.61
1:A:274:LEU:HD23	1:A:277:GLN:HE22	1.63	0.61
3:D:118:PRO:HG3	3:D:208:PHE:CD2	2.36	0.61
1:B:38:MET:O	1:B:41:VAL:HG12	2.01	0.61
2:E:67:LYS:NZ	2:E:85:LYS:O	2.34	0.61
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.83	0.61
1:A:274:LEU:O	1:A:277:GLN:HB2	2.01	0.60
3:D:107:ARG:HH21	3:D:171:THR:CG2	2.13	0.60
3:F:190:SER:HB2	3:F:209:ASN:OD1	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:MET:HG2	1:A:397:LEU:HD23	1.83	0.60
3:D:184:GLU:HA	3:D:187:ARG:HH21	1.65	0.60
3:F:32:ILE:HD11	3:F:70:TYR:CB	2.31	0.60
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.83	0.60
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.66	0.60
1:A:457:GLU:OE1	1:B:19:ARG:NH2	2.33	0.60
3:F:186:GLU:O	3:F:210:ARG:HD2	2.01	0.60
1:B:159:GLY:O	1:B:162:VAL:HG22	2.01	0.60
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.83	0.60
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.82	0.60
1:A:109:ILE:HG21	1:A:445:TYR:CD2	2.36	0.60
1:A:205:ARG:HG3	1:A:213:ILE:HD12	1.81	0.60
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.84	0.60
3:F:12:SER:HB3	3:F:106:LEU:HD21	1.84	0.60
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.37	0.60
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.16	0.60
2:C:109:ASP:OD1	2:C:110:VAL:HG23	2.01	0.60
2:C:52:ASN:HB2	2:C:53:PRO:HD2	1.83	0.59
3:D:38:LYS:HB2	3:D:41:THR:CG2	2.31	0.59
3:F:141:LYS:HD3	3:F:172:TYR:CE2	2.37	0.59
1:B:372:GLY:O	1:B:376:VAL:HG23	2.02	0.59
2:C:6:GLU:O	2:C:115:THR:HG23	2.02	0.59
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.84	0.59
1:B:205:ARG:CG	1:B:206:PRO:HD2	2.33	0.59
1:B:360:MET:HG2	1:B:397:LEU:HD23	1.85	0.59
3:D:6:GLN:NE2	3:D:87:CYS:N	2.50	0.59
3:F:186:GLU:O	3:F:210:ARG:CD	2.50	0.59
1:B:205:ARG:HG3	1:B:213:ILE:HD12	1.84	0.59
3:F:131:VAL:HG23	3:F:178:LEU:HB3	1.83	0.59
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.84	0.59
1:A:90:ALA:HB2	1:A:299:GLY:HA3	1.85	0.59
1:B:198:LEU:HD12	1:B:406:LEU:HG	1.83	0.59
3:D:179:THR:O	3:D:180:LEU:HD23	2.03	0.59
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.18	0.59
1:A:42:VAL:O	1:A:46:VAL:HG23	2.02	0.59
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.18	0.58
1:B:449:LEU:HD12	1:B:452:THR:CG2	2.32	0.58
1:A:270:ASN:OD1	1:A:444:LEU:HD13	2.03	0.58
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.18	0.58
2:C:2:VAL:O	2:C:2:VAL:HG23	2.02	0.58
3:D:7:SER:CB	3:D:8:PRO:CD	2.80	0.58
2:E:43:LYS:HD3	2:E:44:GLY:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:31:TYR:HA	3:F:50:THR:OG1	2.03	0.58
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.85	0.58
3:D:58:PRO:HB2	3:D:60:ARG:NH1	2.18	0.58
3:D:79:ALA:CA	3:D:105:ILE:HD11	2.31	0.58
1:A:216:LYS:HE2	1:B:433:THR:HG21	1.85	0.58
1:B:42:VAL:O	1:B:46:VAL:HG23	2.03	0.58
1:B:90:ALA:HB2	1:B:299:GLY:HA3	1.85	0.58
1:B:109:ILE:HG21	1:B:445:TYR:CD2	2.39	0.58
3:F:33:HIS:HD2	3:F:88:GLN:OE1	1.84	0.58
3:D:130:SER:HA	3:D:178:LEU:O	2.03	0.58
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.84	0.58
2:C:163:ASN:HD21	2:C:201:VAL:HA	1.69	0.58
3:F:90:TRP:CE3	3:F:90:TRP:O	2.57	0.58
2:C:64:LEU:O	2:C:66:ASP:N	2.37	0.58
1:A:205:ARG:CG	1:A:206:PRO:HD2	2.33	0.58
3:F:24:SER:HA	3:F:68:THR:O	2.03	0.58
3:F:180:LEU:HD13	3:F:184:GLU:HG3	1.85	0.58
1:B:136:LEU:HD12	1:B:136:LEU:H	1.67	0.58
1:B:319:LEU:HD12	1:B:319:LEU:C	2.24	0.58
1:B:18:ARG:O	1:B:21:LEU:N	2.37	0.58
2:E:31:ARG:NH1	2:E:31:ARG:HG2	2.17	0.58
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.04	0.58
1:A:380:PRO:HG2	3:D:93:HIS:HB2	1.85	0.58
3:F:145:VAL:HA	3:F:194:GLU:O	2.03	0.58
3:D:48:TYR:HE1	3:D:52:LYS:HE3	1.69	0.58
2:E:65:LYS:O	2:E:66:ASP:HB2	2.02	0.58
2:E:22:CYS:SG	2:E:22:CYS:O	2.61	0.58
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.39	0.57
1:B:270:ASN:OD1	1:B:444:LEU:HD13	2.03	0.57
1:B:192:ALA:HB1	1:B:414:GLU:OE1	2.03	0.57
2:C:30:SER:O	2:C:32:TYR:N	2.37	0.57
1:A:18:ARG:HB2	1:B:119:GLN:NE2	2.19	0.57
3:F:150:ASP:OD2	3:F:188:HIS:CB	2.50	0.57
2:C:130:TYR:HB2	2:C:149:LEU:HD23	1.87	0.57
1:B:358:ALA:O	1:B:361:LEU:HB2	2.05	0.57
3:F:114:VAL:O	3:F:206:LYS:HE2	2.04	0.57
3:D:107:ARG:HH21	3:D:171:THR:HG23	1.69	0.57
3:D:125:THR:O	3:D:125:THR:CG2	2.53	0.57
1:B:413:LEU:HD22	1:B:422:ILE:HD13	1.86	0.57
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.22	0.57
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.40	0.57
1:B:305:LEU:C	1:B:307:PHE:N	2.58	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:148:LYS:HB3	3:D:151:GLY:O	2.05	0.57
2:E:35:SER:CB	2:E:99:LEU:HD11	2.22	0.57
2:C:131:PRO:HD3	2:C:216:LYS:HE2	1.87	0.57
2:C:87:ARG:HG3	2:C:87:ARG:NH1	2.18	0.56
1:A:305:LEU:HA	1:A:308:VAL:CG2	2.34	0.56
3:F:141:LYS:HD3	3:F:172:TYR:CD2	2.40	0.56
3:D:6:GLN:NE2	3:D:86:TYR:CA	2.67	0.56
1:B:180:THR:HG22	1:B:218:VAL:CA	2.33	0.56
1:A:216:LYS:CE	1:B:433:THR:HG22	2.34	0.56
3:F:124:LEU:O	3:F:127:GLY:N	2.36	0.56
2:C:131:PRO:HD3	2:C:216:LYS:CE	2.36	0.56
1:B:73:ASP:OD1	1:B:74:ASN:N	2.34	0.56
2:C:32:TYR:CZ	2:C:98:ARG:HD2	2.40	0.56
1:A:97:VAL:HG21	1:A:353:PRO:HD3	1.87	0.56
2:E:151:LYS:HG3	2:E:184:THR:OG1	2.05	0.56
3:D:208:PHE:CD1	3:D:208:PHE:C	2.78	0.56
3:D:118:PRO:HG3	3:D:208:PHE:CE2	2.40	0.56
3:F:146:LYS:HD3	3:F:194:GLU:OE1	2.05	0.56
1:A:202:GLU:O	1:A:202:GLU:HG2	2.06	0.56
1:A:159:GLY:O	1:A:162:VAL:HG22	2.06	0.56
2:E:87:ARG:HG3	2:E:89:GLU:H	1.70	0.56
3:D:107:ARG:HG2	3:D:107:ARG:HH11	1.70	0.56
3:D:58:PRO:HG2	3:D:61:PHE:CD1	2.40	0.56
1:B:33:LEU:HD23	1:B:33:LEU:O	2.06	0.56
2:E:39:GLN:HE22	3:F:37:GLN:HE22	1.51	0.56
2:E:146:LEU:CD1	2:E:201:VAL:HG11	2.35	0.56
2:E:73:ASP:OD2	2:E:76:LYS:CE	2.54	0.56
2:E:29:TYR:CE2	2:E:77:ASP:HA	2.41	0.56
3:F:22:THR:CG2	3:F:23:CYS:N	2.68	0.56
3:D:140:PRO:CD	3:D:198:LYS:HD3	2.34	0.56
1:A:248:PRO:HB2	1:A:251:THR:HG23	1.88	0.56
3:D:4:LEU:HD11	3:D:89:GLN:CG	2.36	0.56
3:D:82:ALA:HB2	3:D:105:ILE:HG13	1.88	0.56
3:D:139:TYR:HA	3:D:140:PRO:O	2.06	0.56
2:C:129:VAL:HG12	2:C:205:VAL:HG21	1.88	0.55
1:A:38:MET:O	1:A:41:VAL:HG12	2.06	0.55
3:D:76:THR:HG23	3:D:76:THR:O	2.06	0.55
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.88	0.55
1:A:100:TYR:O	1:A:126:ARG:HD3	2.06	0.55
3:F:6:GLN:NE2	3:F:100:GLY:H	2.05	0.55
1:A:211:THR:HG22	1:A:213:ILE:HG13	1.89	0.55
1:A:437:GLN:NE2	1:B:30:LYS:HA	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:ARG:HD2	1:B:207:GLN:HG3	1.87	0.55
1:B:100:TYR:O	1:B:126:ARG:HD3	2.07	0.55
3:F:189:ASN:CG	3:F:210:ARG:HB3	2.26	0.55
1:B:421:LEU:O	1:B:424:PRO:HD2	2.07	0.55
3:D:50:THR:HG22	3:D:64:SER:HA	1.87	0.55
1:B:305:LEU:HA	1:B:308:VAL:CG2	2.36	0.55
3:D:154:ARG:NH2	3:D:180:LEU:HD22	2.20	0.55
2:E:73:ASP:OD2	2:E:76:LYS:HE3	2.07	0.55
1:B:99:LYS:CG	1:B:100:TYR:CE2	2.89	0.55
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.88	0.55
1:B:18:ARG:O	1:B:20:GLN:N	2.40	0.55
3:D:107:ARG:HG2	3:D:107:ARG:NH1	2.22	0.55
1:A:421:LEU:O	1:A:424:PRO:HD2	2.07	0.55
1:A:99:LYS:CG	1:A:100:TYR:CE2	2.90	0.55
3:F:15:PRO:HD3	3:F:105:ILE:HG23	1.89	0.55
2:C:185:LEU:HD12	2:C:185:LEU:C	2.27	0.55
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.07	0.55
3:F:92:SER:O	3:F:93:HIS:C	2.45	0.54
3:F:209:ASN:O	3:F:211:ALA:N	2.40	0.54
3:D:90:TRP:CZ3	3:D:95:GLN:OE1	2.60	0.54
1:A:33:LEU:O	1:A:33:LEU:HD23	2.07	0.54
1:B:455:LYS:C	1:B:457:GLU:H	2.10	0.54
3:F:166:ASP:HB3	3:F:169:ASP:OD1	2.06	0.54
1:A:205:ARG:HG3	1:A:213:ILE:CD1	2.37	0.54
2:C:196:TRP:HA	2:C:198:SER:N	2.22	0.54
3:F:146:LYS:HB3	3:F:194:GLU:CB	2.33	0.54
1:A:413:LEU:HD22	1:A:422:ILE:HD13	1.88	0.54
1:B:227:ILE:O	1:B:231:ILE:HG13	2.08	0.54
2:E:29:TYR:CE1	2:E:34:MET:CE	2.90	0.54
1:A:235:GLU:OE1	2:E:100:TYR:HE2	1.90	0.54
1:A:305:LEU:C	1:A:307:PHE:N	2.60	0.54
1:B:148:GLU:H	1:B:148:GLU:CD	2.09	0.54
1:B:362:ALA:O	1:B:366:VAL:HG23	2.06	0.54
2:C:167:LEU:HD23	2:C:189:VAL:CG2	2.28	0.54
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.90	0.54
2:C:147:GLY:HA2	2:C:162:TRP:CH2	2.41	0.54
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.90	0.54
1:A:273:VAL:O	1:A:277:GLN:NE2	2.39	0.54
3:D:16:GLY:HA2	3:D:76:THR:HG1	1.66	0.54
1:B:202:GLU:HG2	1:B:202:GLU:O	2.07	0.54
1:A:28:ARG:HH11	1:B:207:GLN:CG	2.18	0.54
3:F:90:TRP:HA	3:F:95:GLN:CB	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:142:SER:O	2:C:193:SER:HB2	2.08	0.53
1:A:148:GLU:H	1:A:148:GLU:CD	2.10	0.53
2:E:163:ASN:HB2	2:E:167:LEU:HD13	1.90	0.53
3:D:58:PRO:HG2	3:D:61:PHE:CE1	2.43	0.53
2:C:212:THR:HG22	2:C:213:LYS:N	2.23	0.53
2:C:51:ILE:CD1	2:C:72:ARG:HG2	2.37	0.53
3:F:77:MET:CE	3:F:103:LEU:HD21	2.38	0.53
3:D:10:ILE:O	3:D:11:MET:HB3	2.09	0.53
1:A:340:ARG:O	1:A:341:VAL:C	2.47	0.53
3:D:19:VAL:O	3:D:73:THR:HA	2.09	0.53
2:C:171:VAL:CG2	2:C:189:VAL:HG23	2.37	0.53
1:A:73:ASP:OD1	1:A:74:ASN:N	2.36	0.53
1:B:211:THR:HG22	1:B:213:ILE:HG13	1.90	0.53
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.91	0.53
1:A:136:LEU:HD12	1:A:136:LEU:H	1.72	0.53
2:C:127:PRO:HB3	2:C:153:TYR:CB	2.30	0.53
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.31	0.53
3:D:53:LEU:HD22	3:D:57:VAL:HB	1.91	0.53
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.38	0.53
3:D:48:TYR:CE1	3:D:52:LYS:HE3	2.44	0.53
2:C:174:PHE:H	2:C:174:PHE:HD2	1.56	0.53
3:D:189:ASN:HA	3:D:210:ARG:CD	2.39	0.53
3:F:109:ASP:HB3	3:F:199:THR:HG22	1.91	0.53
1:A:358:ALA:O	1:A:361:LEU:HB2	2.09	0.53
1:A:357:PHE:CE1	1:A:398:LEU:HD22	2.43	0.53
2:C:2:VAL:HG12	2:C:26:GLY:O	2.09	0.53
1:B:449:LEU:CA	1:B:452:THR:HG22	2.39	0.53
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.90	0.52
3:D:146:LYS:CD	3:D:153:GLU:HG3	2.37	0.52
3:D:146:LYS:NZ	3:D:153:GLU:OE2	2.42	0.52
1:A:418:ASN:ND2	1:A:420:GLN:HE22	2.06	0.52
2:E:87:ARG:CZ	2:E:89:GLU:HB2	2.40	0.52
2:E:33:TRP:O	2:E:99:LEU:HD12	2.09	0.52
2:E:204:ASN:CB	2:E:215:ASP:OD1	2.49	0.52
2:C:131:PRO:HD3	2:C:216:LYS:HZ1	1.74	0.52
3:D:186:GLU:C	3:D:210:ARG:NH2	2.62	0.52
3:D:79:ALA:C	3:D:81:ASP:N	2.62	0.52
3:F:134:PHE:O	3:F:135:LEU:HG	2.09	0.52
3:F:131:VAL:CG2	3:F:178:LEU:HB3	2.40	0.52
1:A:319:LEU:C	1:A:319:LEU:HD12	2.28	0.52
1:A:171:ASP:C	1:A:175:HIS:HD2	2.12	0.52
3:F:180:LEU:HD22	3:F:184:GLU:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:65:GLY:O	3:F:66:SER:HB3	2.09	0.52
1:B:163:LEU:HD22	1:B:174:ARG:HA	1.92	0.52
1:B:241:VAL:O	1:B:241:VAL:HG12	2.10	0.52
1:B:163:LEU:CD1	1:B:168:LEU:HB2	2.38	0.52
3:D:53:LEU:HD22	3:D:57:VAL:CG1	2.40	0.52
3:F:153:GLU:OE2	3:F:155:GLN:HG3	2.10	0.52
3:D:186:GLU:HA	3:D:210:ARG:HH22	0.71	0.51
3:F:149:ILE:HD12	3:F:154:ARG:NE	2.25	0.51
3:F:183:ASP:O	3:F:186:GLU:N	2.43	0.51
3:D:89:GLN:NE2	3:D:91:SER:N	2.50	0.51
2:E:47:TRP:CG	3:F:95:GLN:NE2	2.77	0.51
1:B:418:ASN:ND2	1:B:420:GLN:HE22	2.08	0.51
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.90	0.51
1:B:357:PHE:CE1	1:B:398:LEU:HD22	2.45	0.51
2:E:163:ASN:CB	2:E:166:SER:OG	2.58	0.51
2:C:129:VAL:HG21	2:C:214:VAL:HG21	1.90	0.51
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.91	0.51
1:A:22:ILE:HG12	1:B:453:LEU:HB3	1.93	0.51
3:D:48:TYR:C	3:D:48:TYR:CD1	2.83	0.51
1:A:317:PHE:O	1:A:319:LEU:N	2.43	0.51
3:D:46:TRP:CE3	3:D:46:TRP:HA	2.45	0.51
3:D:180:LEU:HD22	3:D:184:GLU:OE2	2.11	0.51
3:D:11:MET:HG3	3:D:11:MET:O	2.10	0.51
3:D:60:ARG:NE	3:D:78:GLU:HG2	2.26	0.51
3:F:90:TRP:CH2	3:F:93:HIS:ND1	2.66	0.51
1:A:388:THR:HG22	1:A:421:LEU:HD21	1.92	0.51
1:A:278:ASP:O	1:A:281:HIS:N	2.43	0.51
1:B:248:PRO:HB2	1:B:251:THR:HG23	1.92	0.51
1:B:183:ALA:HB2	1:B:200:ILE:CG1	2.41	0.51
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.92	0.51
2:E:143:MET:HA	2:E:191:VAL:O	2.10	0.51
3:F:89:GLN:O	3:F:91:SER:N	2.43	0.51
1:A:150:PRO:O	1:A:154:ILE:HG13	2.11	0.51
2:C:178:LEU:HB2	2:C:183:TYR:HE2	1.73	0.51
2:E:98:ARG:NH2	2:E:109:ASP:OD2	2.40	0.51
2:C:29:TYR:OH	2:C:79:LEU:HB2	2.10	0.51
2:C:53:PRO:HA	2:C:72:ARG:NH1	2.25	0.51
1:A:90:ALA:CB	1:A:299:GLY:HA3	2.41	0.51
1:A:17:ARG:C	1:A:19:ARG:N	2.64	0.51
2:E:144:VAL:N	2:E:191:VAL:O	2.35	0.51
2:E:51:ILE:O	2:E:51:ILE:HG23	2.11	0.51
1:A:362:ALA:O	1:A:366:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:ARG:HG3	1:B:213:ILE:CD1	2.40	0.50
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.92	0.50
1:B:148:GLU:CD	1:B:357:PHE:HB3	2.31	0.50
2:E:40:ALA:O	2:E:43:LYS:HB2	2.10	0.50
1:B:317:PHE:O	1:B:319:LEU:N	2.45	0.50
2:E:189:VAL:HG13	2:E:189:VAL:O	2.11	0.50
2:E:179:GLN:O	2:E:180:ALA:HB3	2.12	0.50
3:D:117:PHE:N	3:D:117:PHE:HD1	2.08	0.50
3:D:123:GLN:HE22	3:D:130:SER:CB	2.23	0.50
3:D:10:ILE:HA	3:D:102:LYS:HB3	1.93	0.50
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.42	0.50
1:B:388:THR:HG22	1:B:421:LEU:HD21	1.93	0.50
2:E:40:ALA:HA	2:E:92:ALA:CB	2.42	0.50
1:A:399:ALA:O	1:A:403:ARG:HA	2.10	0.50
1:A:433:THR:HG21	1:B:216:LYS:HE2	1.92	0.50
2:C:174:PHE:N	2:C:174:PHE:CD2	2.79	0.50
3:D:47:ILE:HD13	3:D:72:LEU:HD11	1.92	0.50
3:D:185:TYR:C	3:D:187:ARG:H	2.15	0.50
1:A:241:VAL:HG12	1:A:241:VAL:O	2.11	0.50
1:B:340:ARG:O	1:B:341:VAL:C	2.49	0.50
3:D:189:ASN:OD1	3:D:209:ASN:HB3	2.12	0.50
3:F:191:TYR:HB2	3:F:208:PHE:HE2	1.73	0.50
1:B:83:PHE:CD1	1:B:83:PHE:C	2.84	0.50
1:B:171:ASP:HB3	1:B:175:HIS:CE1	2.47	0.50
3:F:145:VAL:HG11	3:F:176:SER:OG	2.12	0.50
3:F:72:LEU:HD23	3:F:73:THR:N	2.27	0.50
1:B:252:LEU:HD11	1:B:423:LEU:HD23	1.93	0.50
1:A:70:HIS:O	1:A:70:HIS:ND1	2.45	0.50
1:B:402:ILE:HG22	1:B:402:ILE:O	2.11	0.50
3:F:27:SER:O	3:F:68:THR:HG22	2.11	0.49
1:B:107:SER:N	4:B:466:SEK:SE	2.83	0.49
3:D:88:GLN:HG2	3:D:89:GLN:N	2.27	0.49
2:C:6:GLU:CG	2:C:96:CYS:SG	2.96	0.49
1:A:207:GLN:HG3	1:B:28:ARG:HD2	1.93	0.49
2:C:53:PRO:O	2:C:55:SER:N	2.45	0.49
1:A:163:LEU:HD22	1:A:174:ARG:HA	1.93	0.49
3:F:38:LYS:H	3:F:41:THR:CG2	2.25	0.49
3:D:74:ILE:HG22	3:D:77:MET:CA	2.40	0.49
1:A:360:MET:CG	1:A:397:LEU:HD23	2.42	0.49
1:A:163:LEU:CD1	1:A:168:LEU:HB2	2.42	0.49
1:B:399:ALA:O	1:B:403:ARG:HA	2.13	0.49
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:24:ALA:HB1	2:C:27:PHE:CZ	2.48	0.49
3:D:16:GLY:O	3:D:17:ASP:HB2	2.13	0.49
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.47	0.49
2:C:195:SER:C	2:C:198:SER:HB2	2.32	0.49
3:D:208:PHE:HD1	3:D:209:ASN:N	2.10	0.49
1:B:457:GLU:O	1:B:458:ALA:HB2	2.13	0.49
3:D:166:ASP:C	3:D:168:LYS:H	2.16	0.49
1:A:17:ARG:C	1:A:19:ARG:H	2.15	0.49
1:B:131:LYS:HE2	1:B:153:GLN:NE2	2.28	0.49
3:D:188:HIS:O	3:D:210:ARG:CG	2.60	0.49
1:B:422:ILE:HG23	1:B:423:LEU:N	2.27	0.49
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.12	0.49
1:B:330:MET:HE3	1:B:330:MET:CA	2.42	0.49
1:A:298:ILE:HG23	1:A:346:LEU:HD23	1.95	0.49
1:B:205:ARG:CD	1:B:213:ILE:HD12	2.43	0.49
1:B:97:VAL:HG21	1:B:353:PRO:HD3	1.95	0.49
2:E:143:MET:HB3	2:E:190:THR:HG23	1.93	0.49
3:F:192:THR:HA	3:F:207:SER:CB	2.43	0.49
2:C:207:HIS:CD2	2:C:209:ALA:HB3	2.47	0.49
3:F:32:ILE:HG22	3:F:89:GLN:CA	2.42	0.49
1:B:163:LEU:HD21	1:B:174:ARG:HG3	1.95	0.49
3:F:148:LYS:HA	3:F:152:SER:O	2.12	0.49
1:B:75:TYR:CE2	1:B:79:LEU:HD11	2.47	0.49
3:D:85:TYR:HE1	3:D:103:LEU:HD23	1.78	0.49
3:D:35:TYR:O	3:D:85:TYR:HA	2.12	0.49
3:F:90:TRP:O	3:F:90:TRP:HE3	1.94	0.49
3:F:143:ILE:HG22	3:F:174:MET:CE	2.42	0.49
1:A:422:ILE:HG23	1:A:423:LEU:N	2.27	0.49
2:C:30:SER:C	2:C:32:TYR:N	2.65	0.49
1:A:163:LEU:HD21	1:A:174:ARG:HG3	1.95	0.49
1:B:165:ILE:HG22	1:B:166:PHE:N	2.26	0.49
1:A:98:ARG:HD2	1:A:291:TRP:CD2	2.47	0.49
3:D:189:ASN:O	3:D:209:ASN:HA	2.13	0.49
1:A:18:ARG:O	1:A:22:ILE:HG13	2.13	0.49
1:B:449:LEU:HA	1:B:452:THR:CG2	2.42	0.49
1:B:360:MET:CG	1:B:397:LEU:HD23	2.43	0.49
1:A:108:GLY:CA	1:A:153:GLN:NE2	2.76	0.49
1:A:383:HIS:CE1	3:D:90:TRP:CZ2	3.01	0.49
1:B:90:ALA:CB	1:B:299:GLY:HA3	2.43	0.49
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.48	0.49
3:F:8:PRO:O	3:F:101:THR:HG23	2.13	0.48
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:32:ILE:HG22	3:F:88:GLN:O	2.13	0.48
2:E:36:TRP:CZ2	2:E:81:LEU:HB2	2.48	0.48
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.42	0.48
1:A:165:ILE:HG22	1:A:166:PHE:N	2.28	0.48
1:A:183:ALA:HB2	1:A:200:ILE:CG1	2.42	0.48
3:F:189:ASN:HA	3:F:210:ARG:CB	2.41	0.48
3:D:114:VAL:HG22	3:D:135:LEU:CD1	2.39	0.48
1:A:205:ARG:CD	1:A:213:ILE:HD12	2.43	0.48
1:B:38:MET:HA	1:B:41:VAL:HG12	1.95	0.48
3:D:47:ILE:CD1	3:D:72:LEU:HD11	2.43	0.48
1:B:95:PHE:O	1:B:97:VAL:N	2.45	0.48
3:D:29:VAL:HG23	3:D:70:TYR:CE1	2.47	0.48
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.95	0.48
3:F:76:THR:HG22	3:F:76:THR:O	2.12	0.48
3:D:107:ARG:NH1	3:D:108:ALA:HB3	2.29	0.48
2:C:150:VAL:HG22	2:C:205:VAL:HG21	1.94	0.48
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.94	0.48
1:B:150:PRO:O	1:B:154:ILE:HG13	2.13	0.48
1:A:86:SER:OG	1:A:303:GLY:HA3	2.13	0.48
1:B:356:ILE:O	1:B:356:ILE:HG12	2.13	0.48
1:A:330:MET:CA	1:A:330:MET:HE3	2.44	0.48
3:D:6:GLN:HE22	3:D:87:CYS:N	2.10	0.48
2:C:158:VAL:HG12	2:C:207:HIS:HB2	1.95	0.48
3:F:77:MET:CE	3:F:103:LEU:HD11	2.44	0.48
2:E:16:GLY:O	2:E:85:LYS:N	2.47	0.48
1:A:36:LEU:HD13	1:B:434:LEU:CD2	2.44	0.48
2:E:150:VAL:HG22	2:E:205:VAL:HG21	1.96	0.48
3:F:186:GLU:O	3:F:210:ARG:NE	2.47	0.48
1:B:278:ASP:O	1:B:281:HIS:N	2.42	0.48
3:D:102:LYS:HG3	3:D:104:GLU:HG3	1.96	0.48
1:A:433:THR:HG22	1:B:216:LYS:CE	2.43	0.48
2:E:135:GLY:O	2:E:138:ALA:HB2	2.14	0.48
2:C:106:TRP:HD1	2:C:106:TRP:H	1.56	0.48
1:A:356:ILE:HG12	1:A:356:ILE:O	2.13	0.48
1:A:230:ARG:CG	1:A:230:ARG:HH11	2.26	0.48
1:A:37:PHE:HD2	1:A:38:MET:CE	2.27	0.48
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.96	0.48
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.95	0.48
3:D:17:ASP:O	3:D:76:THR:HA	2.13	0.48
2:C:185:LEU:CD1	2:C:185:LEU:C	2.83	0.48
2:C:72:ARG:O	2:C:72:ARG:HG3	2.14	0.48
1:B:126:ARG:HH11	1:B:126:ARG:HG2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:108:GLY:CA	1:B:153:GLN:NE2	2.77	0.48
1:B:93:GLY:O	1:B:97:VAL:HG23	2.13	0.48
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.49	0.48
3:F:53:LEU:HD21	3:F:61:PHE:O	2.13	0.48
3:D:146:LYS:HD3	3:D:153:GLU:CD	2.34	0.47
1:B:144:VAL:HG12	1:B:144:VAL:O	2.14	0.47
2:C:200:THR:HG23	2:C:200:THR:O	2.14	0.47
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.28	0.47
1:B:86:SER:HB3	1:B:299:GLY:O	2.14	0.47
1:A:83:PHE:C	1:A:83:PHE:CD1	2.86	0.47
3:F:6:GLN:NE2	3:F:98:GLY:HA3	2.29	0.47
1:B:183:ALA:HB2	1:B:200:ILE:HG12	1.95	0.47
1:A:183:ALA:HB2	1:A:200:ILE:HG12	1.95	0.47
1:B:229:TYR:CE1	1:B:233:ASN:ND2	2.78	0.47
3:D:135:LEU:HG	3:D:174:MET:CE	2.44	0.47
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.96	0.47
1:A:77:LEU:O	1:A:81:VAL:HG13	2.14	0.47
3:D:164:ASP:O	3:D:165:GLN:O	2.31	0.47
3:F:143:ILE:HG12	3:F:197:HIS:HB2	1.96	0.47
1:A:180:THR:HG22	1:A:218:VAL:CA	2.39	0.47
1:B:247:ALA:CB	1:B:424:PRO:HG2	2.44	0.47
1:B:298:ILE:HG23	1:B:346:LEU:HD23	1.95	0.47
3:D:181:THR:O	3:D:182:LYS:C	2.53	0.47
3:D:57:VAL:CG1	3:D:58:PRO:HD2	2.45	0.47
1:A:247:ALA:CB	1:A:424:PRO:HG2	2.44	0.47
1:A:418:ASN:HD22	1:A:420:GLN:HE22	1.62	0.47
3:F:169:ASP:OD1	3:F:170:SER:N	2.48	0.47
2:E:174:PHE:CD1	3:F:163:THR:HG23	2.50	0.47
2:C:18:LEU:CD2	2:C:18:LEU:H	2.27	0.47
2:C:165:GLY:C	2:C:167:LEU:H	2.18	0.47
3:F:186:GLU:CA	3:F:210:ARG:HD2	2.41	0.47
1:A:219:PHE:HB3	1:B:430:LEU:CD1	2.42	0.47
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.96	0.47
3:D:106:LEU:HA	3:D:139:TYR:OH	2.14	0.47
3:D:139:TYR:HA	3:D:140:PRO:C	2.35	0.47
2:C:69:ILE:N	2:C:69:ILE:HD12	2.30	0.47
1:A:202:GLU:OE2	1:A:406:LEU:HB3	2.15	0.47
1:B:86:SER:OG	1:B:303:GLY:HA3	2.15	0.47
2:E:181:ALA:O	2:E:182:LEU:HD23	2.15	0.47
1:A:144:VAL:HG21	1:A:343:THR:HB	1.96	0.47
2:E:18:LEU:HG	2:E:19:LYS:N	2.29	0.47
1:B:226:THR:O	1:B:230:ARG:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:146:LEU:HD23	2:E:146:LEU:N	2.30	0.47
3:F:143:ILE:HG22	3:F:174:MET:HE3	1.96	0.47
3:D:154:ARG:NH2	3:D:180:LEU:CD2	2.78	0.47
3:F:54:THR:CG2	3:F:55:SER:H	2.17	0.47
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.35	0.47
1:A:144:VAL:O	1:A:144:VAL:HG12	2.15	0.47
3:D:158:VAL:HG12	3:D:159:LEU:N	2.30	0.47
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.96	0.47
1:B:24:GLN:O	1:B:27:GLU:N	2.40	0.47
2:C:129:VAL:CG2	2:C:214:VAL:HG21	2.44	0.46
2:C:178:LEU:CD1	2:C:182:LEU:H	2.28	0.46
2:E:50:GLU:OE2	2:E:59:ASN:ND2	2.48	0.46
1:A:27:GLU:HA	1:A:27:GLU:OE1	2.15	0.46
3:D:75:ASN:C	3:D:76:THR:HG22	2.24	0.46
1:A:421:LEU:O	1:A:425:MET:HG3	2.15	0.46
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.50	0.46
2:C:178:LEU:HD12	2:C:178:LEU:C	2.36	0.46
1:A:457:GLU:HB3	1:B:19:ARG:NH2	2.30	0.46
3:F:4:LEU:HA	3:F:24:SER:O	2.15	0.46
3:D:114:VAL:HG11	3:D:206:LYS:HB2	1.97	0.46
1:A:38:MET:HA	1:A:41:VAL:HG12	1.96	0.46
3:D:107:ARG:NH2	3:D:171:THR:CG2	2.78	0.46
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.30	0.46
2:E:190:THR:O	2:E:191:VAL:HG13	2.16	0.46
3:F:183:ASP:O	3:F:184:GLU:C	2.54	0.46
3:F:33:HIS:O	3:F:87:CYS:HA	2.16	0.46
1:A:62:ASN:O	1:A:63:GLN:C	2.54	0.46
3:D:123:GLN:HG2	3:D:128:GLY:C	2.36	0.46
1:B:108:GLY:HA3	1:B:153:GLN:NE2	2.30	0.46
1:B:35:ILE:CG2	1:B:176:THR:HG21	2.45	0.46
1:A:201:ILE:HG13	1:A:201:ILE:O	2.16	0.46
1:A:22:ILE:CD1	1:B:453:LEU:HB3	2.46	0.46
1:B:456:GLN:O	1:B:456:GLN:HG2	2.15	0.46
3:F:21:MET:HG2	3:F:21:MET:H	1.66	0.46
3:F:188:HIS:O	3:F:210:ARG:NE	2.47	0.46
2:C:147:GLY:HA2	2:C:162:TRP:HZ2	1.79	0.46
1:A:207:GLN:CG	1:B:28:ARG:HH11	2.19	0.46
1:B:309:ALA:O	1:B:311:ALA:N	2.49	0.46
2:E:105:TYR:CE1	3:F:31:TYR:CD2	3.02	0.46
1:B:148:GLU:OE1	1:B:357:PHE:CB	2.64	0.46
2:E:143:MET:HE3	2:E:191:VAL:N	2.30	0.46
1:A:423:LEU:HB3	1:A:424:PRO:CD	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:70:HIS:ND1	1:B:70:HIS:O	2.49	0.46
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.45	0.46
1:B:451:ARG:C	1:B:453:LEU:H	2.20	0.46
3:D:107:ARG:HH11	3:D:108:ALA:HB3	1.81	0.46
1:B:376:VAL:HG12	1:B:376:VAL:O	2.16	0.46
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.46
1:A:35:ILE:CG2	1:A:176:THR:HG21	2.46	0.46
3:D:163:THR:OG1	3:D:173:SER:HB2	2.16	0.46
3:D:14:ALA:O	3:D:17:ASP:HB3	2.16	0.45
3:D:16:GLY:CA	3:D:76:THR:OG1	2.42	0.45
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.81	0.45
2:E:40:ALA:O	2:E:43:LYS:CB	2.65	0.45
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.97	0.45
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.50	0.45
2:C:175:PRO:HD2	3:D:161:SER:OG	2.16	0.45
1:A:124:TRP:CA	1:A:157:ASN:HD22	2.24	0.45
1:B:109:ILE:N	1:B:110:PRO:CD	2.79	0.45
1:B:136:LEU:N	1:B:136:LEU:HD12	2.31	0.45
1:B:274:LEU:O	1:B:277:GLN:HB2	2.16	0.45
3:D:77:MET:HE2	3:D:77:MET:O	2.16	0.45
1:B:127:VAL:O	1:B:128:LEU:C	2.55	0.45
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.16	0.45
3:F:6:GLN:HE21	3:F:99:GLY:N	2.14	0.45
1:A:126:ARG:HG2	1:A:126:ARG:HH11	1.82	0.45
1:A:205:ARG:CG	1:A:213:ILE:HD12	2.47	0.45
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.99	0.45
3:F:73:THR:CG2	3:F:74:ILE:N	2.79	0.45
1:A:269:PHE:O	1:A:273:VAL:HG12	2.16	0.45
3:F:188:HIS:N	3:F:188:HIS:ND1	2.64	0.45
2:E:36:TRP:NE1	2:E:81:LEU:HB2	2.32	0.45
1:A:30:LYS:HA	1:B:437:GLN:NE2	2.31	0.45
1:B:77:LEU:O	1:B:81:VAL:HG13	2.17	0.45
1:B:27:GLU:HA	1:B:27:GLU:OE1	2.16	0.45
1:B:312:THR:HG22	1:B:339:ALA:CB	2.46	0.45
3:F:6:GLN:O	3:F:7:SER:O	2.34	0.45
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.52	0.45
1:B:269:PHE:O	1:B:273:VAL:HG12	2.17	0.45
3:D:2:ILE:HG22	3:D:3:VAL:N	2.32	0.45
3:F:38:LYS:O	3:F:39:SER:C	2.55	0.45
3:D:53:LEU:HD22	3:D:57:VAL:HG11	1.99	0.45
1:A:109:ILE:HG21	1:A:445:TYR:CE2	2.51	0.45
1:B:455:LYS:C	1:B:457:GLU:N	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:68:PHE:CE2	2:C:83:ILE:HG23	2.51	0.45
3:F:205:VAL:O	3:F:205:VAL:HG23	2.16	0.45
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.23	0.45
1:A:252:LEU:HD11	1:A:423:LEU:HD23	1.98	0.45
1:B:200:ILE:HD13	1:B:204:MET:HG3	1.98	0.45
3:D:89:GLN:C	3:D:89:GLN:NE2	2.71	0.44
1:B:235:GLU:OE1	2:C:100:TYR:CE2	2.61	0.44
3:D:54:THR:HB	3:D:57:VAL:CG2	2.47	0.44
3:F:149:ILE:HD13	3:F:191:TYR:CE2	2.48	0.44
3:F:192:THR:HA	3:F:207:SER:HB2	1.98	0.44
3:F:33:HIS:CD2	3:F:88:GLN:OE1	2.69	0.44
3:F:124:LEU:HD23	3:F:128:GLY:O	2.17	0.44
1:A:230:ARG:NH1	1:A:230:ARG:HG3	2.27	0.44
1:A:317:PHE:O	1:A:318:ASN:C	2.54	0.44
1:B:176:THR:HG22	1:B:177:LEU:N	2.31	0.44
2:C:158:VAL:HG23	2:C:185:LEU:HD21	2.00	0.44
1:B:59:TRP:CE3	1:B:60:LEU:HD23	2.52	0.44
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.47	0.44
2:E:174:PHE:CE1	3:F:163:THR:HG23	2.53	0.44
2:E:221:ARG:NH1	3:F:118:PRO:HG2	2.32	0.44
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.47	0.44
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.86	0.44
3:D:29:VAL:HG23	3:D:70:TYR:HE1	1.81	0.44
1:A:24:GLN:O	1:A:27:GLU:N	2.39	0.44
1:B:260:ILE:HG23	1:B:435:LEU:HG	2.00	0.44
1:A:313:SER:OG	1:A:314:GLY:N	2.51	0.44
3:D:141:LYS:CB	3:D:172:TYR:CD1	2.93	0.44
2:C:132:LEU:CB	2:C:147:GLY:O	2.57	0.44
2:E:29:TYR:CE1	2:E:34:MET:HE2	2.52	0.44
1:A:74:ASN:O	1:A:78:LEU:HD13	2.17	0.44
2:C:109:ASP:C	2:C:109:ASP:OD1	2.56	0.44
1:A:264:ILE:O	1:A:267:PRO:HD2	2.18	0.44
3:D:60:ARG:HG2	3:D:60:ARG:HH11	1.82	0.44
2:E:47:TRP:CZ2	2:E:49:GLY:CA	3.01	0.44
3:D:189:ASN:HA	3:D:210:ARG:HD3	2.00	0.44
3:D:17:ASP:C	3:D:17:ASP:OD1	2.56	0.44
1:B:421:LEU:O	1:B:425:MET:HG3	2.18	0.44
2:E:86:VAL:HG12	2:E:90:ASP:HB2	2.00	0.44
3:F:154:ARG:HE	3:F:154:ARG:HB2	1.71	0.44
3:F:192:THR:HG22	3:F:207:SER:CB	2.48	0.44
2:C:127:PRO:HB2	2:C:150:VAL:HG13	1.99	0.44
3:D:7:SER:HB2	3:D:22:THR:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.24	0.44
1:B:62:ASN:O	1:B:63:GLN:C	2.56	0.44
2:E:153:TYR:CE1	2:E:183:TYR:HB2	2.53	0.44
1:B:74:ASN:O	1:B:78:LEU:HD13	2.18	0.44
1:B:224:MET:O	1:B:228:MET:HG2	2.17	0.44
2:C:18:LEU:HD22	2:C:18:LEU:H	1.81	0.44
1:A:60:LEU:O	1:A:64:ARG:HG3	2.17	0.44
3:D:46:TRP:HB3	3:D:47:ILE:H	1.61	0.44
1:B:35:ILE:HG21	1:B:176:THR:HG21	1.99	0.44
2:C:135:GLY:N	2:C:138:ALA:HB2	2.33	0.44
2:C:86:VAL:O	2:C:86:VAL:HG23	2.17	0.44
3:F:164:ASP:O	3:F:165:GLN:C	2.55	0.44
1:B:18:ARG:O	1:B:19:ARG:C	2.54	0.43
3:F:135:LEU:HB2	3:F:174:MET:HB3	2.00	0.43
3:D:10:ILE:HG22	3:D:11:MET:N	2.33	0.43
1:B:37:PHE:HD2	1:B:38:MET:CE	2.31	0.43
3:D:6:GLN:HE22	3:D:86:TYR:CA	2.32	0.43
3:D:6:GLN:HG3	3:D:100:GLY:CA	2.46	0.43
3:F:21:MET:HB3	3:F:101:THR:HG21	2.00	0.43
1:A:59:TRP:CE3	1:A:60:LEU:HD23	2.53	0.43
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.52	0.43
1:B:99:LYS:CG	1:B:100:TYR:CD2	3.01	0.43
1:B:270:ASN:OD1	1:B:444:LEU:HB2	2.18	0.43
1:A:227:ILE:O	1:A:231:ILE:HG13	2.18	0.43
2:E:163:ASN:ND2	2:E:167:LEU:CD2	2.81	0.43
3:D:57:VAL:HG13	3:D:58:PRO:HD2	2.00	0.43
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.48	0.43
3:D:38:LYS:O	3:D:41:THR:HG22	2.17	0.43
1:A:86:SER:HB3	1:A:299:GLY:O	2.18	0.43
3:F:90:TRP:CE3	3:F:90:TRP:HA	2.54	0.43
2:C:52:ASN:CB	2:C:53:PRO:CD	2.89	0.43
2:E:162:TRP:CZ3	2:E:203:CYS:CB	2.96	0.43
1:A:376:VAL:HG12	1:A:376:VAL:O	2.17	0.43
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.99	0.43
2:C:34:MET:HB3	2:C:79:LEU:HD22	2.01	0.43
2:C:67:LYS:NZ	2:C:85:LYS:O	2.52	0.43
3:D:185:TYR:O	3:D:187:ARG:N	2.51	0.43
2:C:18:LEU:CD2	2:C:18:LEU:N	2.81	0.43
3:F:109:ASP:HB3	3:F:199:THR:CG2	2.48	0.43
3:F:134:PHE:O	3:F:135:LEU:CG	2.66	0.43
1:B:37:PHE:HD2	1:B:38:MET:HE2	1.84	0.43
2:C:84:SER:O	2:C:85:LYS:C	2.55	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:150:ASP:OD2	3:D:188:HIS:HB3	2.19	0.43
1:A:207:GLN:HE21	1:B:28:ARG:HD2	1.84	0.43
1:A:107:SER:HB2	1:A:348:PHE:CZ	2.53	0.43
1:A:216:LYS:NZ	1:B:433:THR:HG22	2.33	0.43
3:F:169:ASP:O	3:F:170:SER:CB	2.64	0.43
1:B:205:ARG:CG	1:B:213:ILE:HD12	2.49	0.43
1:A:176:THR:O	1:A:179:ALA:N	2.52	0.43
1:A:116:LEU:CD2	1:A:178:LEU:HD23	2.48	0.43
2:E:185:LEU:O	2:E:185:LEU:HD12	2.19	0.43
1:B:208:PHE:CD1	1:B:208:PHE:N	2.87	0.43
1:A:184:ALA:HB1	1:A:225:SER:HB2	2.00	0.43
3:D:208:PHE:HD1	3:D:208:PHE:C	2.22	0.43
3:D:53:LEU:HD22	3:D:57:VAL:CB	2.49	0.43
1:B:270:ASN:HA	1:B:273:VAL:CG1	2.49	0.43
1:A:36:LEU:HD13	1:B:434:LEU:HD21	2.01	0.43
1:A:402:ILE:O	1:A:402:ILE:HG22	2.19	0.43
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.48	0.43
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.49	0.43
2:C:2:VAL:CG2	2:C:2:VAL:O	2.67	0.43
1:B:109:ILE:HG21	1:B:445:TYR:CE2	2.53	0.43
1:B:124:TRP:CA	1:B:157:ASN:HD22	2.25	0.43
1:B:270:ASN:O	1:B:273:VAL:CG1	2.67	0.43
1:B:264:ILE:O	1:B:267:PRO:HD2	2.19	0.43
1:B:423:LEU:HB3	1:B:424:PRO:CD	2.43	0.42
2:C:69:ILE:HB	2:C:82:GLN:HB2	2.01	0.42
1:B:317:PHE:O	1:B:318:ASN:C	2.57	0.42
1:A:246:ASP:O	1:A:248:PRO:HD3	2.19	0.42
3:D:47:ILE:HD13	3:D:72:LEU:CD1	2.49	0.42
2:C:111:TRP:N	2:C:111:TRP:CD1	2.86	0.42
1:A:433:THR:HG22	1:B:216:LYS:NZ	2.34	0.42
2:E:16:GLY:C	2:E:86:VAL:HG23	2.39	0.42
1:A:91:MET:HG3	1:A:296:GLY:CA	2.48	0.42
1:B:116:LEU:CD2	1:B:178:LEU:HD23	2.49	0.42
1:B:378:LEU:HD23	1:B:378:LEU:N	2.33	0.42
2:C:108:PHE:CE1	3:D:97:PHE:CZ	3.08	0.42
1:A:136:LEU:HD12	1:A:136:LEU:N	2.34	0.42
1:A:449:LEU:O	1:A:453:LEU:HB2	2.19	0.42
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.80	0.42
1:B:418:ASN:HD22	1:B:420:GLN:HE22	1.66	0.42
3:D:30:SER:O	3:D:31:TYR:HB2	2.20	0.42
3:D:48:TYR:O	3:D:49:ASP:HB2	2.19	0.42
2:E:178:LEU:HD12	2:E:182:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:MET:O	1:B:161:MET:HG2	2.19	0.42
1:B:222:VAL:O	1:B:225:SER:HB3	2.18	0.42
1:A:270:ASN:OD1	1:A:444:LEU:HB2	2.19	0.42
3:F:183:ASP:O	3:F:185:TYR:N	2.51	0.42
1:A:28:ARG:HE	1:B:443:PRO:HG2	1.84	0.42
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.49	0.42
1:B:403:ARG:HD2	1:B:433:THR:HG23	2.02	0.42
1:A:35:ILE:HG21	1:A:176:THR:HG21	2.01	0.42
1:A:456:GLN:C	1:A:458:ALA:H	2.21	0.42
1:B:279:LEU:HD23	1:B:279:LEU:C	2.40	0.42
2:C:153:TYR:CE1	2:C:158:VAL:HG13	2.55	0.42
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.87	0.42
3:D:4:LEU:HD11	3:D:89:GLN:HG2	2.02	0.42
2:E:20:LEU:HD13	2:E:115:THR:CG2	2.50	0.42
1:B:163:LEU:CD2	1:B:174:ARG:HA	2.49	0.42
3:F:15:PRO:HD3	3:F:105:ILE:CG2	2.49	0.42
2:E:111:TRP:N	2:E:111:TRP:CD1	2.87	0.42
3:D:210:ARG:HH11	3:D:210:ARG:HG2	1.84	0.42
2:E:31:ARG:NH1	2:E:31:ARG:CG	2.83	0.42
3:F:116:ILE:HD12	3:F:193:CYS:CB	2.47	0.42
2:C:212:THR:CG2	2:C:213:LYS:N	2.82	0.42
2:C:106:TRP:CD1	2:C:106:TRP:N	2.79	0.42
3:D:147:TRP:O	3:D:154:ARG:HB3	2.19	0.42
1:A:244:LEU:N	1:A:418:ASN:HD21	2.04	0.42
1:B:72:ALA:HA	1:B:78:LEU:HD21	2.02	0.42
1:B:136:LEU:H	1:B:136:LEU:CD1	2.32	0.42
1:A:417:ASP:O	1:A:417:ASP:OD1	2.37	0.42
3:D:90:TRP:CE3	3:D:95:GLN:OE1	2.73	0.42
3:F:88:GLN:HG2	3:F:89:GLN:H	1.81	0.42
1:B:380:PRO:HG2	3:F:93:HIS:HB3	2.02	0.42
2:E:91:THR:O	2:E:91:THR:HG22	2.20	0.42
2:E:76:LYS:O	2:E:77:ASP:HB2	2.20	0.42
1:B:109:ILE:HD13	1:B:445:TYR:HE2	1.84	0.42
3:F:65:GLY:O	3:F:66:SER:CB	2.67	0.42
2:E:98:ARG:O	2:E:109:ASP:HB3	2.20	0.42
1:A:108:GLY:HA3	1:A:153:GLN:HE21	1.84	0.42
2:C:41:PRO:HD3	2:C:92:ALA:HA	2.01	0.42
1:A:293:LEU:C	1:A:295:GLY:N	2.72	0.42
1:B:451:ARG:C	1:B:453:LEU:N	2.73	0.42
3:D:74:ILE:HG22	3:D:77:MET:N	2.35	0.42
1:B:60:LEU:O	1:B:64:ARG:HG3	2.20	0.42
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:139:TYR:CA	3:D:140:PRO:O	2.66	0.42
3:D:47:ILE:HD12	3:D:47:ILE:N	2.35	0.42
1:A:224:MET:O	1:A:228:MET:HG2	2.20	0.42
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.95	0.41
3:D:183:ASP:OD2	3:D:187:ARG:NH2	2.53	0.41
3:F:7:SER:HB2	3:F:22:THR:CA	2.49	0.41
1:A:127:VAL:O	1:A:128:LEU:C	2.58	0.41
1:A:403:ARG:HD2	1:A:433:THR:HG23	2.01	0.41
2:E:150:VAL:HB	2:E:185:LEU:HD12	2.02	0.41
1:A:187:ALA:O	1:A:191:ASN:N	2.53	0.41
3:F:85:TYR:CD1	3:F:85:TYR:N	2.88	0.41
1:B:313:SER:OG	1:B:314:GLY:N	2.53	0.41
2:E:40:ALA:HA	2:E:92:ALA:HB2	2.02	0.41
1:B:31:THR:HB	1:B:36:LEU:HD21	2.02	0.41
3:D:78:GLU:N	3:D:78:GLU:OE2	2.53	0.41
1:A:348:PHE:CD2	1:A:356:ILE:HD12	2.55	0.41
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.20	0.41
1:A:57:VAL:O	1:A:57:VAL:HG12	2.21	0.41
3:D:185:TYR:C	3:D:187:ARG:N	2.74	0.41
1:A:28:ARG:NH2	1:B:443:PRO:HB3	2.35	0.41
1:A:235:GLU:O	1:A:236:VAL:CG2	2.69	0.41
2:C:87:ARG:HB3	2:C:89:GLU:OE1	2.20	0.41
1:A:150:PRO:CG	1:A:354:GLY:HA2	2.50	0.41
2:C:141:ALA:O	2:C:193:SER:HB2	2.21	0.41
1:B:184:ALA:HB1	1:B:225:SER:HB2	2.01	0.41
1:A:279:LEU:C	1:A:279:LEU:HD23	2.40	0.41
3:D:131:VAL:O	3:D:147:TRP:CH2	2.73	0.41
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.38	0.41
1:A:223:ILE:CD1	1:B:426:ILE:HG22	2.49	0.41
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.55	0.41
1:B:293:LEU:C	1:B:295:GLY:N	2.73	0.41
1:A:274:LEU:CA	1:A:277:GLN:HE21	2.24	0.41
3:D:119:PRO:HG3	3:D:131:VAL:HG22	2.00	0.41
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.51	0.41
1:A:109:ILE:N	1:A:110:PRO:CD	2.83	0.41
1:B:148:GLU:OE1	1:B:357:PHE:HB3	2.21	0.41
1:B:57:VAL:CG1	1:B:139:LEU:HB3	2.50	0.41
3:D:48:TYR:CD1	3:D:48:TYR:O	2.73	0.41
1:A:358:ALA:HA	1:A:361:LEU:HD12	2.02	0.41
1:B:91:MET:HG3	1:B:296:GLY:CA	2.50	0.41
1:A:95:PHE:O	1:A:97:VAL:N	2.54	0.41
1:A:113:GLU:HG3	1:A:204:MET:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:42:SER:HA	3:D:43:PRO:HD3	1.85	0.41
3:D:110:ALA:C	3:D:199:THR:HG21	2.40	0.41
3:F:147:TRP:CG	3:F:178:LEU:HD22	2.56	0.41
1:B:107:SER:HB2	1:B:348:PHE:CZ	2.55	0.41
1:A:197:ILE:HD13	1:A:219:PHE:CZ	2.56	0.41
3:D:95:GLN:H	3:D:95:GLN:HG2	1.59	0.41
2:E:91:THR:OG1	2:E:119:VAL:CG2	2.58	0.41
1:A:28:ARG:HH21	1:B:443:PRO:HB3	1.85	0.41
3:D:202:SER:HB3	3:D:203:PRO:CD	2.40	0.41
1:B:143:MET:HB3	1:B:347:CYS:SG	2.60	0.41
1:B:187:ALA:O	1:B:191:ASN:N	2.54	0.41
1:B:92:PHE:CZ	1:B:96:LEU:HD11	2.56	0.41
1:B:20:GLN:O	1:B:23:ARG:HB3	2.20	0.41
3:F:38:LYS:H	3:F:41:THR:HG23	1.84	0.41
3:D:86:TYR:CE2	3:D:100:GLY:HA3	2.56	0.41
3:F:180:LEU:HD22	3:F:184:GLU:CG	2.51	0.41
3:D:89:GLN:C	3:D:89:GLN:CD	2.79	0.41
1:B:410:ILE:O	1:B:410:ILE:HG22	2.21	0.41
1:A:176:THR:HG22	1:A:177:LEU:N	2.35	0.41
1:B:57:VAL:HG12	1:B:57:VAL:O	2.21	0.41
2:C:73:ASP:C	2:C:75:ALA:N	2.74	0.41
3:F:22:THR:HG22	3:F:23:CYS:N	2.36	0.41
2:C:108:PHE:CZ	3:D:95:GLN:OE1	2.74	0.41
3:D:112:PRO:HG2	3:D:204:ILE:CD1	2.39	0.41
1:B:235:GLU:O	1:B:236:VAL:CG2	2.69	0.41
1:A:72:ALA:HA	1:A:78:LEU:HD21	2.03	0.41
1:A:200:ILE:HD13	1:A:204:MET:HG3	2.03	0.41
1:B:144:VAL:HG21	1:B:343:THR:HB	2.02	0.41
2:E:12:VAL:HG11	2:E:18:LEU:HB2	2.03	0.41
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.78	0.41
2:E:27:PHE:N	2:E:27:PHE:CD1	2.89	0.41
3:D:210:ARG:HG3	3:D:210:ARG:H	1.63	0.40
3:D:197:HIS:O	3:D:199:THR:N	2.55	0.40
3:F:181:THR:O	3:F:182:LYS:C	2.59	0.40
2:E:107:TYR:C	2:E:107:TYR:CD1	2.95	0.40
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.56	0.40
2:C:6:GLU:OE2	2:C:96:CYS:SG	2.79	0.40
2:E:201:VAL:HG13	2:E:201:VAL:O	2.21	0.40
3:D:134:PHE:C	3:D:135:LEU:HD22	2.42	0.40
1:B:423:LEU:HD12	1:B:423:LEU:HA	1.94	0.40
2:E:20:LEU:HD11	2:E:94:TYR:CD2	2.56	0.40
3:F:121:SER:HA	3:F:124:LEU:CD1	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:37:GLN:HE21	3:F:86:TYR:HE1	1.68	0.40
1:B:108:GLY:HA3	1:B:153:GLN:HE21	1.86	0.40
1:B:201:ILE:O	1:B:201:ILE:HG13	2.21	0.40
3:D:185:TYR:HA	3:D:191:TYR:OH	2.21	0.40
1:A:270:ASN:O	1:A:273:VAL:CG1	2.70	0.40
1:A:21:LEU:HD23	1:B:119:GLN:HG3	2.03	0.40
1:A:171:ASP:HB3	1:A:175:HIS:CD2	2.56	0.40
2:C:185:LEU:HD12	2:C:185:LEU:O	2.22	0.40
2:E:134:PRO:HD3	2:E:146:LEU:HD22	2.02	0.40
1:A:348:PHE:CZ	4:A:466:SEK:SE	3.24	0.40
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.52	0.40
1:A:281:HIS:ND1	1:A:284:HIS:CE1	2.82	0.40
1:A:166:PHE:O	1:A:167:ARG:O	2.39	0.40
1:B:148:GLU:O	1:B:152:VAL:HG23	2.21	0.40
1:A:20:GLN:O	1:A:23:ARG:HB3	2.21	0.40
1:A:375:ALA:O	1:A:377:GLU:N	2.54	0.40
2:C:101:TYR:CD2	2:C:101:TYR:N	2.89	0.40
2:C:38:ARG:NH1	2:C:68:PHE:HZ	2.20	0.40
1:B:281:HIS:ND1	1:B:284:HIS:CE1	2.82	0.40
1:B:100:TYR:N	1:B:100:TYR:CD2	2.89	0.40
1:B:24:GLN:O	1:B:25:LEU:C	2.59	0.40
1:B:172:GLU:O	1:B:173:ALA:C	2.59	0.40
2:C:28:ASP:C	2:C:28:ASP:OD1	2.60	0.40
3:D:185:TYR:C	3:D:210:ARG:HH12	2.24	0.40
3:D:22:THR:HG22	3:D:23:CYS:H	1.87	0.40
1:B:284:HIS:HA	1:B:290:LYS:HB3	2.04	0.40
1:A:167:ARG:O	1:A:168:LEU:HG	2.21	0.40
1:A:133:PHE:HA	1:A:136:LEU:HD13	2.04	0.40
1:A:375:ALA:C	1:A:377:GLU:H	2.24	0.40
3:D:116:ILE:HG23	3:D:116:ILE:O	2.22	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	442/465 (95%)	344 (78%)	80 (18%)	18 (4%)	4	27
1	B	439/465 (94%)	336 (76%)	85 (19%)	18 (4%)	4	27
2	C	219/221 (99%)	187 (85%)	22 (10%)	10 (5%)	4	24
2	E	219/221 (99%)	184 (84%)	24 (11%)	11 (5%)	3	22
3	D	209/211 (99%)	153 (73%)	40 (19%)	16 (8%)	1	11
3	F	209/211 (99%)	168 (80%)	28 (13%)	13 (6%)	2	16
All	All	1737/1794 (97%)	1372 (79%)	279 (16%)	86 (5%)	3	22

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	283	VAL
1	B	201	ILE
1	B	283	VAL
2	C	53	PRO
2	C	65	LYS
2	C	199	GLU
3	D	7	SER
3	D	126	SER
3	D	137	ASN
3	D	152	SER
3	D	165	GLN
3	D	169	ASP
3	D	198	LYS
2	E	41	PRO
2	E	51	ILE
2	E	66	ASP
2	E	122	ALA
2	E	189	VAL
3	F	7	SER
3	F	66	SER
3	F	90	TRP
3	F	92	SER
3	F	198	LYS
3	F	210	ARG
1	A	72	ALA
1	A	165	ILE
1	A	167	ARG
1	A	318	ASN
1	B	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	ILE
1	B	318	ASN
2	C	31	ARG
2	C	54	VAL
2	C	135	GLY
2	C	198	SER
3	D	17	ASP
3	D	67	GLY
3	D	80	GLU
2	E	58	ILE
1	A	132	PHE
1	A	455	LYS
1	B	72	ALA
1	B	132	PHE
1	B	167	ARG
1	B	310	PRO
1	B	351	GLY
2	C	109	ASP
3	D	11	MET
2	E	62	PRO
2	E	140	ALA
3	F	137	ASN
1	A	96	LEU
1	A	282	ARG
1	A	386	ALA
1	B	19	ARG
1	B	95	PHE
1	B	176	THR
1	B	282	ARG
2	C	142	SER
3	D	167	SER
3	D	186	GLU
2	E	138	ALA
3	F	182	LYS
3	F	184	GLU
1	A	95	PHE
1	A	176	THR
1	A	310	PRO
2	C	220	PRO
3	D	27	SER
3	D	83	ALA
2	E	53	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	93	HIS
3	F	170	SER
1	A	376	VAL
1	A	454	ALA
3	F	39	SER
1	A	351	GLY
1	B	200	ILE
3	D	59	VAL
1	A	200	ILE
2	E	69	ILE
3	F	203	PRO
1	B	206	PRO
1	B	376	VAL
1	B	443	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	335/353 (95%)	328 (98%)	7 (2%)	66	92
1	B	332/353 (94%)	323 (97%)	9 (3%)	57	89
2	C	181/181 (100%)	172 (95%)	9 (5%)	34	75
2	E	181/181 (100%)	165 (91%)	16 (9%)	14	49
3	D	185/185 (100%)	168 (91%)	17 (9%)	13	45
3	F	185/185 (100%)	168 (91%)	17 (9%)	13	45
All	All	1399/1438 (97%)	1324 (95%)	75 (5%)	31	72

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	85	CYS
1	A	103	GLU
1	A	138	THR
1	A	233	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	246	ASP
1	A	453	LEU
1	B	65	MET
1	B	85	CYS
1	B	103	GLU
1	B	138	THR
1	B	208	PHE
1	B	233	ASN
1	B	246	ASP
1	B	277	GLN
1	B	330	MET
2	C	18	LEU
2	C	30	SER
2	C	149	LEU
2	C	157	PRO
2	C	167	LEU
2	C	178	LEU
2	C	185	LEU
2	C	188	SER
2	C	203	CYS
3	D	1	ASP
3	D	22	THR
3	D	46	TRP
3	D	48	TYR
3	D	77	MET
3	D	78	GLU
3	D	89	GLN
3	D	94	PRO
3	D	96	THR
3	D	106	LEU
3	D	117	PHE
3	D	138	PHE
3	D	163	THR
3	D	169	ASP
3	D	183	ASP
3	D	192	THR
3	D	208	PHE
2	E	27	PHE
2	E	41	PRO
2	E	43	LYS
2	E	52	ASN
2	E	53	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	54	VAL
2	E	59	ASN
2	E	77	ASP
2	E	86	VAL
2	E	107	TYR
2	E	116	THR
2	E	157	PRO
2	E	185	LEU
2	E	188	SER
2	E	203	CYS
2	E	204	ASN
3	F	1	ASP
3	F	15	PRO
3	F	21	MET
3	F	68	THR
3	F	77	MET
3	F	88	GLN
3	F	90	TRP
3	F	119	PRO
3	F	143	ILE
3	F	153	GLU
3	F	160	ASN
3	F	161	SER
3	F	162	TRP
3	F	173	SER
3	F	174	MET
3	F	175	SER
3	F	179	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	153	GLN
1	A	157	ASN
1	A	175	HIS
1	A	207	GLN
1	A	277	GLN
1	A	284	HIS
1	A	287	ASN
1	A	327	ASN
1	A	383	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	ASN
1	A	437	GLN
1	B	119	GLN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
1	B	277	GLN
1	B	284	HIS
1	B	287	ASN
1	B	327	ASN
1	B	418	ASN
1	B	437	GLN
2	C	163	ASN
2	C	172	HIS
3	D	6	GLN
3	D	89	GLN
3	D	137	ASN
2	E	39	GLN
2	E	163	ASN
3	F	6	GLN
3	F	33	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	444/465 (95%)	-0.17	1 (0%) 93 61	77, 77, 77, 77	0
1	B	441/465 (94%)	-0.12	0 100 100	77, 77, 77, 77	0
2	C	221/221 (100%)	-0.16	0 100 100	77, 77, 77, 77	0
2	E	221/221 (100%)	-0.15	0 100 100	77, 77, 77, 77	0
3	D	211/211 (100%)	-0.17	0 100 100	77, 77, 77, 77	0
3	F	211/211 (100%)	-0.13	0 100 100	77, 77, 77, 77	0
All	All	1749/1794 (97%)	-0.15	1 (0%) 93 70	77, 77, 77, 77	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
4	SEK	A	468	1/3	-	-	76,76,76,76	1
4	SEK	B	466	1/3	0.46	-	76,76,76,76	0
4	SEK	A	466	1/3	0.36	-	76,76,76,76	0
4	SEK	B	468	1/3	-	-	76,76,76,76	1
4	SEK	B	467	1/3	-	-	76,76,76,76	1
4	SEK	A	467	1/3	-	-	76,76,76,76	1
4	SEK	A	469	1/3	-	-	76,76,76,76	1
4	SEK	B	469	1/3	-	-	76,76,76,76	1

6.5 Other polymers ⓘ

There are no such residues in this entry.