



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:47 pm GMT

PDB ID : 3UDB  
Title : Crystal structure of SnRK2.6  
Authors : Xie, T.; Ren, R.; Pang, Y.; Yan, C.  
Deposited on : 2011-10-27  
Resolution : 2.57 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

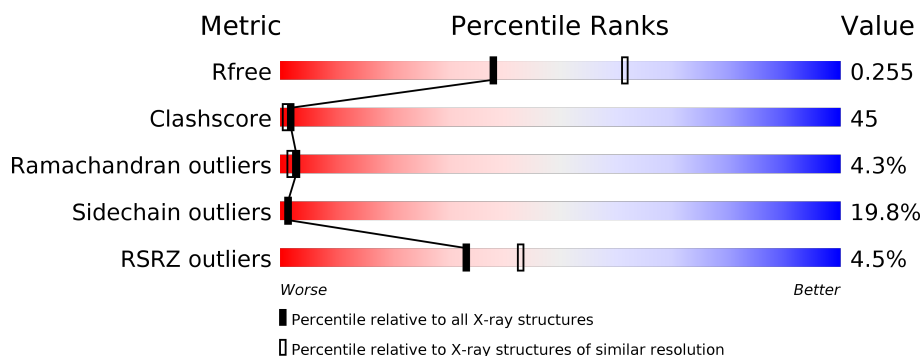
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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))
$R_{free}$	111664	1056 (2.58-2.54)
Clashscore	122126	1102 (2.58-2.54)
Ramachandran outliers	120053	1092 (2.58-2.54)
Sidechain outliers	120020	1092 (2.58-2.54)
RSRZ outliers	108989	1048 (2.58-2.54)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	
1	F	317	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13176 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein kinase SRK2E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2214	1418	386	401	9			
1	B	278	Total	C	N	O	S	0	1	0
			2245	1437	394	405	9			
1	C	261	Total	C	N	O	S	0	0	0
			2109	1351	367	381	10			
1	D	279	Total	C	N	O	S	0	0	0
			2235	1428	390	408	9			
1	E	255	Total	C	N	O	S	0	0	0
			2036	1304	360	363	9			
1	F	273	Total	C	N	O	S	0	0	0
			2202	1411	385	397	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
A	29	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
A	43	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
A	131	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
A	137	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
A	159	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
A	166	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
A	176	ALA	THR	ENGINEERED MUTATION	UNP Q940H6
B	7	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
B	29	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
B	43	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
B	131	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
B	137	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
B	159	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
B	166	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
B	176	ALA	THR	ENGINEERED MUTATION	UNP Q940H6
C	7	ALA	SER	ENGINEERED MUTATION	UNP Q940H6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
C	43	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
C	131	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
C	137	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
C	159	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
C	166	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
C	176	ALA	THR	ENGINEERED MUTATION	UNP Q940H6
D	7	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
D	29	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
D	43	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
D	131	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
D	137	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
D	159	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
D	166	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
D	176	ALA	THR	ENGINEERED MUTATION	UNP Q940H6
E	7	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
E	29	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
E	43	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
E	131	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
E	137	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
E	159	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
E	166	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
E	176	ALA	THR	ENGINEERED MUTATION	UNP Q940H6
F	7	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
F	29	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
F	43	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
F	131	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
F	137	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
F	159	ALA	CYS	ENGINEERED MUTATION	UNP Q940H6
F	166	ALA	SER	ENGINEERED MUTATION	UNP Q940H6
F	176	ALA	THR	ENGINEERED MUTATION	UNP Q940H6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0	0
2	F	1	Total 1	Cl 1	0	0

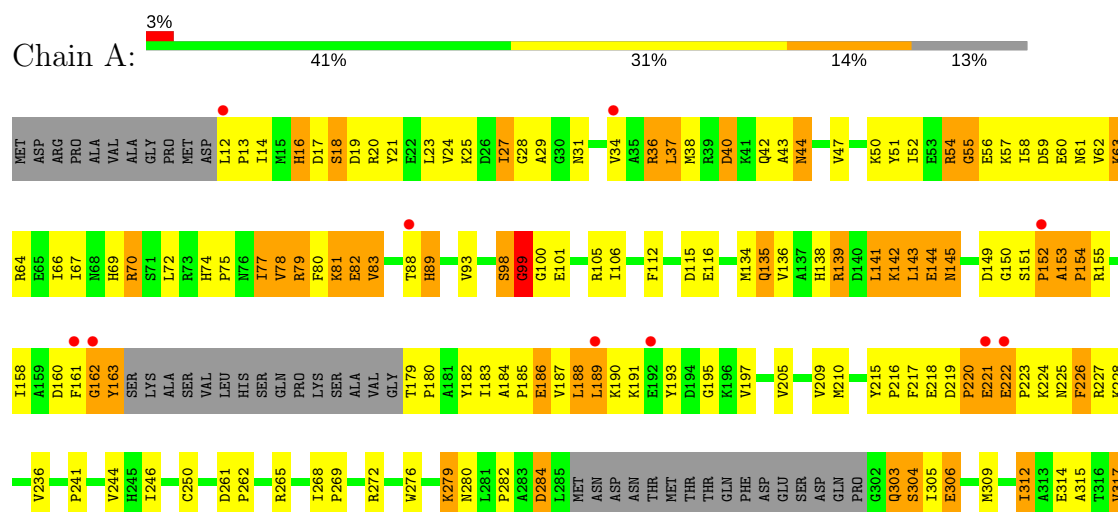
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	32	Total 32	O 32	0	0
3	C	32	Total 32	O 32	0	0
3	D	20	Total 20	O 20	0	0
3	E	13	Total 13	O 13	0	0
3	F	18	Total 18	O 18	0	0

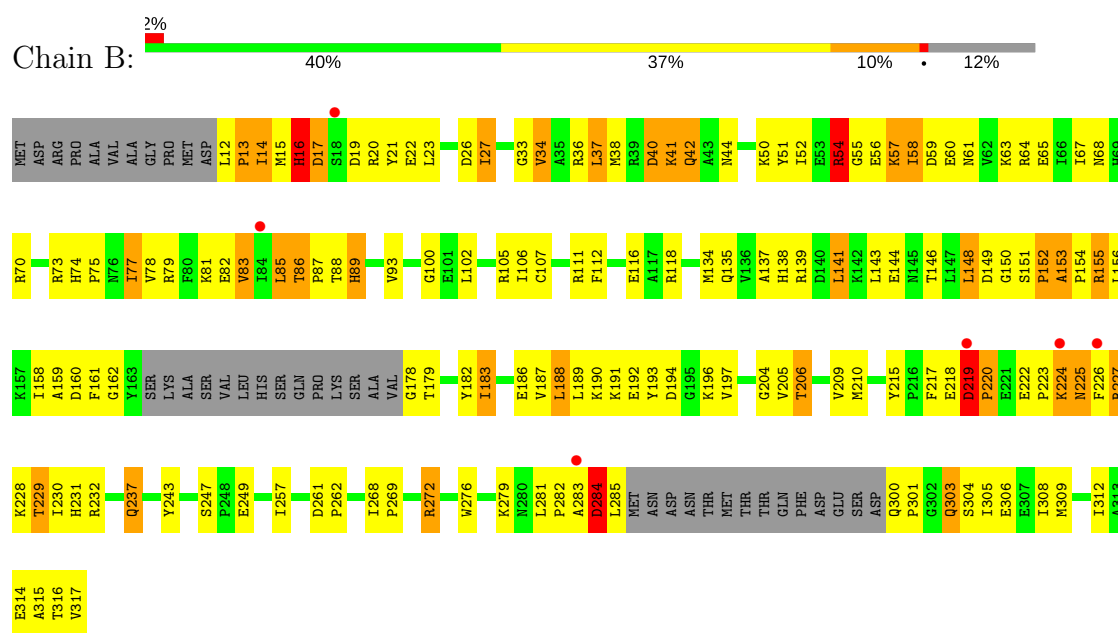
### 3 Residue-property plots

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

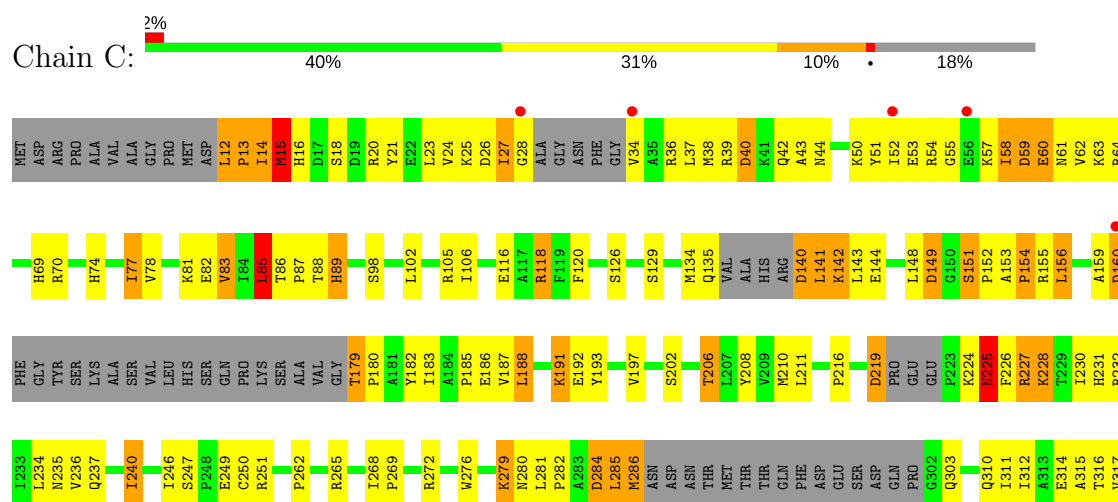
#### • Molecule 1: Serine/threonine-protein kinase SRK2E



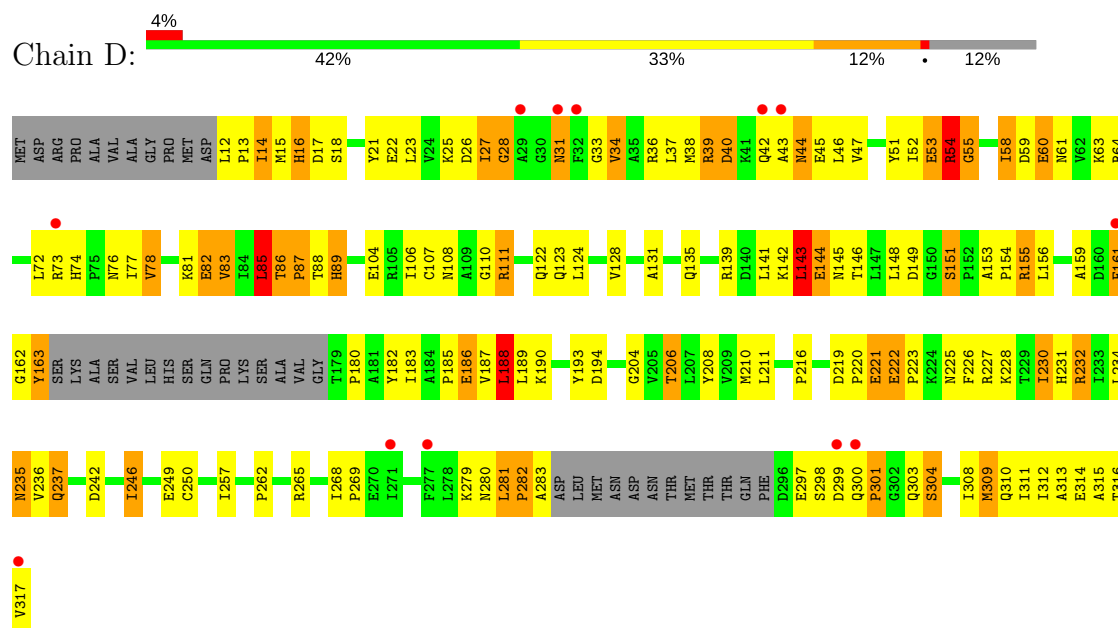
#### • Molecule 1: Serine/threonine-protein kinase SRK2E



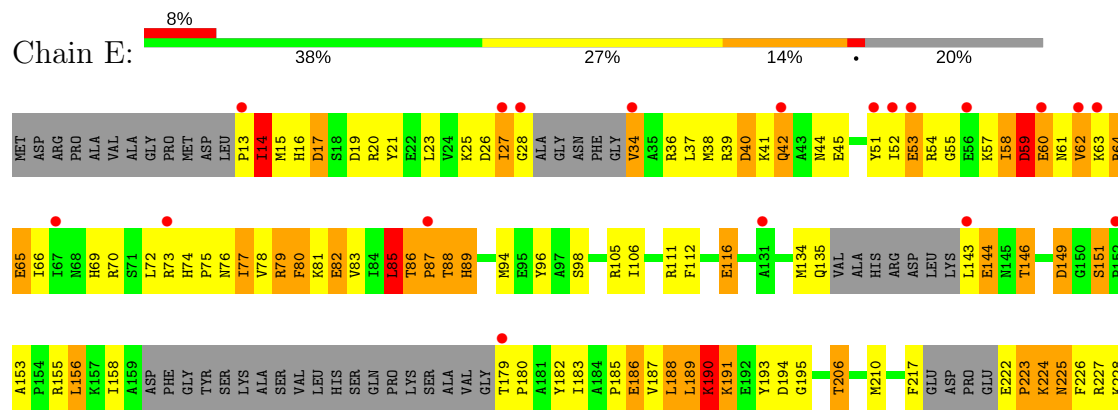
#### • Molecule 1: Serine/threonine-protein kinase SRK2E

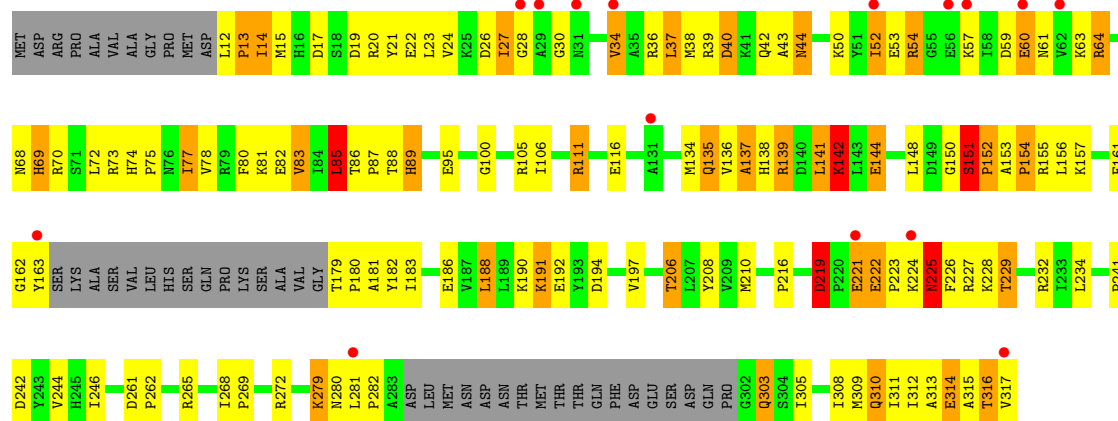


- Molecule 1: Serine/threonine-protein kinase SRK2E



- Molecule 1: Serine/threonine-protein kinase SRK2E







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.09Å 98.79Å 113.10Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	37.08 – 2.57 37.08 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.4 (37.08-2.57) 98.2 (37.08-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.236 , 0.259 0.230 , 0.255	Depositor DCC
$R_{free}$ test set	3932 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CL

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	0.47	0/2263	0.67	6/3062 (0.2%)
1	B	0.48	1/2295 (0.0%)	0.61	5/3104 (0.2%)
1	C	0.56	0/2150	0.69	6/2901 (0.2%)
1	D	0.56	2/2285 (0.1%)	0.89	8/3093 (0.3%)
1	E	0.46	0/2077	0.73	7/2805 (0.2%)
1	F	0.51	0/2251	0.69	5/3044 (0.2%)
All	All	0.51	3/13321 (0.0%)	0.72	37/18009 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	4
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	CYS	CB-SG	-5.66	1.72	1.81
1	D	282	PRO	CA-C	5.27	1.63	1.52
1	B	107	CYS	CB-SG	-5.12	1.73	1.81

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ARG	NE-CZ-NH1	-21.76	109.42	120.30
1	D	39	ARG	NE-CZ-NH2	20.71	130.65	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	219	ASP	N-CA-CB	-11.77	89.42	110.60
1	E	53	GLU	CB-CA-C	-11.38	87.65	110.40
1	D	39	ARG	CD-NE-CZ	10.36	138.11	123.60
1	E	59	ASP	CB-CA-C	-9.35	91.70	110.40
1	A	18	SER	CB-CA-C	9.34	127.85	110.10
1	C	59	ASP	CB-CA-C	-9.11	92.17	110.40
1	A	16	HIS	CB-CA-C	-8.95	92.50	110.40
1	F	219	ASP	N-CA-C	-8.54	87.95	111.00
1	E	87	PRO	CB-CA-C	8.36	132.91	112.00
1	C	285	LEU	CB-CA-C	-7.73	95.51	110.20
1	C	85	LEU	CA-CB-CG	7.26	132.00	115.30
1	F	85	LEU	CA-CB-CG	7.03	131.46	115.30
1	D	85	LEU	CA-CB-CG	6.94	131.26	115.30
1	B	17	ASP	CB-CA-C	-6.91	96.58	110.40
1	D	16	HIS	CB-CA-C	-6.71	96.98	110.40
1	E	85	LEU	CA-CB-CG	6.62	130.52	115.30
1	B	16	HIS	CB-CA-C	-6.54	97.31	110.40
1	E	53	GLU	N-CA-C	6.21	127.78	111.00
1	D	188	LEU	CA-CB-CG	6.15	129.44	115.30
1	F	135	GLN	CB-CA-C	5.96	122.32	110.40
1	D	282	PRO	CA-C-N	5.92	130.21	117.20
1	C	151	SER	CB-CA-C	5.73	120.98	110.10
1	C	39	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	39	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	E	59	ASP	C-N-CA	5.57	135.62	121.70
1	A	282	PRO	CB-CA-C	-5.56	98.09	112.00
1	A	99	GLY	N-CA-C	5.52	126.90	113.10
1	F	30	GLY	N-CA-C	-5.46	99.46	113.10
1	A	141	LEU	CB-CA-C	5.40	120.46	110.20
1	A	150	GLY	N-CA-C	5.30	126.35	113.10
1	B	137	ALA	N-CA-C	-5.15	97.10	111.00
1	E	86	THR	CB-CA-C	5.11	125.41	111.60
1	D	282	PRO	C-N-CA	5.10	134.46	121.70
1	B	150	GLY	N-CA-C	5.10	125.85	113.10
1	B	284	ASP	N-CA-C	5.07	124.68	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	281	LEU	Mainchain
1	E	57	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	E	59	ASP	Mainchain,Peptide
1	E	87	PRO	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2214	0	2210	203	0
1	B	2245	0	2243	205	0
1	C	2109	0	2128	193	0
1	D	2235	0	2212	221	0
1	E	2036	0	2035	216	1
1	F	2202	0	2206	150	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	14	0	0	1	0
3	B	32	0	0	5	1
3	C	32	0	0	3	0
3	D	20	0	0	4	0
3	E	13	0	0	2	0
3	F	18	0	0	5	0
All	All	13176	0	13034	1162	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:THR:CG2	1:E:89:HIS:HD2	1.03	1.62
1:C:126:SER:CB	1:C:286:MET:CE	1.74	1.60
1:E:88:THR:HG23	1:E:89:HIS:CD2	1.05	1.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:SER:HB2	1:C:286:MET:CE	0.98	1.43
1:A:88:THR:HG23	1:A:89:HIS:CD2	1.55	1.41
1:B:146:THR:CG2	1:B:156:LEU:HD11	1.54	1.38
1:B:88:THR:HG23	1:B:89:HIS:CD2	1.60	1.36
1:B:61:ASN:OD1	1:B:64:ARG:NH2	1.59	1.35
1:D:219:ASP:OD2	1:D:221:GLU:HG3	1.30	1.31
1:E:310:GLN:O	1:E:314:GLU:HB2	1.26	1.31
1:E:82:GLU:HG3	1:E:303:GLN:NE2	1.45	1.30
1:B:88:THR:CG2	1:B:89:HIS:HD2	1.46	1.28
1:B:152:PRO:O	1:B:154:PRO:HD3	1.33	1.28
1:C:140:ASP:C	1:C:141:LEU:HD13	1.54	1.27
1:E:88:THR:CG2	1:E:89:HIS:CD2	1.86	1.25
1:C:13:PRO:HG3	1:C:89:HIS:NE2	1.50	1.23
1:E:14:ILE:O	1:E:36:ARG:NH2	1.73	1.22
1:A:188:LEU:H	1:A:188:LEU:CD1	1.50	1.21
1:D:183:ILE:CG2	1:D:188:LEU:HD13	1.70	1.20
1:C:314:GLU:O	1:C:317:VAL:HG22	1.40	1.20
1:E:70:ARG:HG2	1:E:80:PHE:CE2	1.78	1.19
1:D:300:GLN:CB	1:D:301:PRO:HA	1.62	1.16
1:A:12:LEU:CD2	1:A:13:PRO:HD2	1.73	1.16
1:E:70:ARG:HG2	1:E:80:PHE:HE2	0.99	1.16
1:F:68:ASN:OD1	1:F:139:ARG:NH1	1.79	1.15
1:C:126:SER:HB2	1:C:286:MET:HE3	1.17	1.15
1:A:188:LEU:N	1:A:188:LEU:HD12	1.58	1.15
1:A:88:THR:CG2	1:A:89:HIS:CD2	2.30	1.14
1:C:284:ASP:OD2	3:C:326:HOH:O	1.61	1.14
1:C:83:VAL:H	1:C:303:GLN:NE2	1.47	1.13
1:E:14:ILE:HG23	1:E:15:MET:H	0.99	1.13
1:E:14:ILE:HG23	1:E:15:MET:N	1.54	1.13
1:F:221:GLU:OE1	1:F:221:GLU:HA	1.47	1.12
1:F:135:GLN:OE1	1:F:135:GLN:HA	1.44	1.12
1:C:126:SER:CA	1:C:286:MET:HE2	1.79	1.12
1:C:126:SER:CB	1:C:286:MET:HE2	1.71	1.11
1:A:151:SER:HB2	1:A:152:PRO:HD2	1.14	1.11
1:F:141:LEU:H	1:F:141:LEU:CD1	1.64	1.11
1:B:146:THR:HG21	1:B:156:LEU:CD1	1.79	1.10
1:B:146:THR:CG2	1:B:156:LEU:CD1	2.27	1.10
1:D:282:PRO:CB	1:D:283:ALA:HB3	1.81	1.10
1:F:141:LEU:HD12	1:F:141:LEU:N	1.62	1.10
1:E:313:ALA:HA	1:E:316:THR:OG1	1.50	1.10
1:E:186:GLU:HG2	1:E:262:PRO:HG3	1.29	1.10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:HG2	1:A:262:PRO:HG3	1.29	1.10
1:C:126:SER:CB	1:C:286:MET:HE1	1.52	1.09
1:C:142:LYS:H	1:C:142:LYS:CD	1.63	1.08
1:A:101:GLU:OE2	1:A:145:ASN:ND2	1.86	1.08
1:D:282:PRO:HB3	1:D:283:ALA:HB3	1.29	1.08
1:A:12:LEU:HD22	1:A:13:PRO:CD	1.82	1.07
1:A:220:PRO:O	1:A:223:PRO:HD3	1.54	1.07
1:C:27:ILE:CB	1:C:28:GLY:HA3	1.85	1.07
1:D:183:ILE:HG21	1:D:188:LEU:CD1	1.85	1.07
1:B:20:ARG:O	1:B:41:LYS:HG3	1.54	1.06
1:E:82:GLU:CG	1:E:303:GLN:NE2	2.16	1.06
1:C:16:HIS:HE1	1:C:51:TYR:OH	1.36	1.06
1:F:141:LEU:HD12	1:F:141:LEU:H	1.13	1.06
1:B:182:TYR:HE2	1:B:206:THR:HG22	1.17	1.06
1:E:310:GLN:O	1:E:314:GLU:CB	2.02	1.06
1:D:25:LYS:HE2	1:D:27:ILE:HD12	1.35	1.05
1:C:126:SER:HA	1:C:286:MET:HE2	1.34	1.05
1:A:88:THR:C	1:A:89:HIS:CD2	2.30	1.05
1:D:88:THR:HG22	1:D:89:HIS:CD2	1.91	1.05
1:E:58:ILE:HG21	1:E:316:THR:HG23	1.37	1.05
1:A:225:ASN:OD1	1:A:226:PHE:N	1.89	1.05
1:D:63:LYS:HD2	1:D:309:MET:HE2	1.35	1.05
1:D:88:THR:CG2	1:D:89:HIS:CD2	2.40	1.05
1:E:61:ASN:O	1:E:64:ARG:HD2	1.55	1.05
1:F:21:TYR:CE1	1:F:40:ASP:HB2	1.91	1.04
1:B:21:TYR:CE1	1:B:40:ASP:HB2	1.92	1.04
1:F:313:ALA:O	1:F:316:THR:OG1	1.72	1.04
1:A:135:GLN:HG2	1:A:138:HIS:HA	1.38	1.04
1:F:64:ARG:HH11	1:F:64:ARG:HB3	1.20	1.04
1:B:192:GLU:HG2	1:B:192:GLU:O	1.56	1.04
1:C:126:SER:CA	1:C:286:MET:CE	2.36	1.03
1:A:88:THR:CG2	1:A:89:HIS:HD2	1.69	1.03
1:A:27:ILE:HD11	1:A:29:ALA:O	1.56	1.03
1:C:27:ILE:HB	1:C:28:GLY:HA3	1.38	1.03
1:D:231:HIS:O	1:D:235:ASN:OD1	1.76	1.02
1:B:85:LEU:HD12	1:B:85:LEU:C	1.78	1.02
1:D:53:GLU:HA	1:D:89:HIS:HB3	1.05	1.02
1:F:310:GLN:NE2	1:F:314:GLU:OE2	1.93	1.01
1:D:63:LYS:HD2	1:D:309:MET:CE	1.90	1.01
1:F:219:ASP:OD1	1:F:221:GLU:HB2	1.59	1.01
1:A:40:ASP:OD2	1:A:42:GLN:O	1.78	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:O	1:B:70:ARG:HD3	1.61	1.01
1:C:88:THR:CG2	1:C:89:HIS:NE2	2.24	1.01
1:D:282:PRO:HB3	1:D:283:ALA:CB	1.90	1.01
1:B:88:THR:CG2	1:B:89:HIS:CD2	2.30	1.01
1:B:152:PRO:O	1:B:154:PRO:CD	2.09	1.00
1:E:77:ILE:HG12	1:E:158:ILE:HB	1.42	1.00
1:D:226:PHE:CE2	1:D:230:ILE:HD13	1.97	1.00
1:B:225:ASN:HD22	1:B:226:PHE:N	1.60	0.99
1:D:183:ILE:HG21	1:D:188:LEU:HD13	1.02	0.99
1:A:70:ARG:NH2	1:A:303:GLN:O	1.96	0.99
1:C:140:ASP:C	1:C:141:LEU:CD1	2.30	0.99
1:D:82:GLU:HB2	1:D:303:GLN:NE2	1.76	0.99
1:F:28:GLY:O	1:F:34:VAL:HA	1.62	0.98
1:E:82:GLU:HB2	1:E:303:GLN:NE2	1.79	0.98
1:B:58:ILE:HG22	1:B:58:ILE:O	1.61	0.98
1:D:12:LEU:N	1:D:13:PRO:HD2	1.77	0.98
1:D:182:TYR:HE2	1:D:206:THR:HG22	1.24	0.98
1:F:53:GLU:HA	1:F:89:HIS:HB3	1.44	0.98
1:F:134:MET:O	1:F:135:GLN:HG2	1.64	0.97
1:E:58:ILE:CG2	1:E:316:THR:HG23	1.94	0.97
1:A:12:LEU:HD22	1:A:13:PRO:HD2	0.99	0.97
1:C:142:LYS:H	1:C:142:LYS:HD3	1.25	0.97
1:A:219:ASP:OD1	1:A:220:PRO:HD2	1.64	0.97
1:A:60:GLU:OE2	1:A:63:LYS:NZ	1.97	0.97
1:A:81:LYS:HB2	1:A:93:VAL:O	1.65	0.96
1:A:188:LEU:H	1:A:188:LEU:HD12	0.81	0.96
1:C:141:LEU:HD13	1:C:141:LEU:N	1.80	0.96
1:B:219:ASP:HB2	1:B:232:ARG:CZ	1.95	0.96
1:E:189:LEU:H	1:E:189:LEU:HD23	1.24	0.96
1:B:85:LEU:HD12	1:B:86:THR:N	1.78	0.96
1:F:88:THR:C	1:F:89:HIS:HD2	1.68	0.96
1:B:300:GLN:N	1:B:301:PRO:HD2	1.80	0.95
1:E:112:PHE:CD2	1:E:116:GLU:HG2	1.99	0.95
1:C:236:VAL:O	1:C:236:VAL:HG12	1.62	0.95
1:D:300:GLN:CB	1:D:301:PRO:CA	2.44	0.95
1:D:53:GLU:HA	1:D:89:HIS:CB	1.97	0.95
1:B:300:GLN:N	1:B:301:PRO:CD	2.30	0.95
1:C:88:THR:HG22	1:C:89:HIS:CD2	2.01	0.95
1:A:88:THR:CB	1:A:89:HIS:HD2	1.79	0.95
1:C:142:LYS:CE	1:C:159:ALA:O	2.15	0.94
1:E:14:ILE:CG2	1:E:15:MET:H	1.79	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:HIS:CE1	1:E:76:ASN:HB2	2.02	0.94
1:E:85:LEU:HD23	1:E:315:ALA:HB2	1.46	0.94
1:F:310:GLN:HA	1:F:310:GLN:OE1	1.67	0.94
1:E:189:LEU:HD23	1:E:189:LEU:N	1.81	0.94
1:C:58:ILE:HG22	1:C:58:ILE:O	1.67	0.94
1:A:88:THR:HG1	1:A:89:HIS:CD2	1.86	0.94
1:B:272:ARG:HG2	1:B:272:ARG:HH11	1.33	0.94
1:D:88:THR:CG2	1:D:89:HIS:NE2	2.30	0.93
1:B:146:THR:HG21	1:B:156:LEU:HD11	0.96	0.93
1:E:26:ASP:OD2	1:E:36:ARG:HG3	1.68	0.93
1:C:27:ILE:CG1	1:C:28:GLY:HA3	1.98	0.93
1:D:143:LEU:O	1:D:146:THR:HG23	1.69	0.93
1:C:142:LYS:CD	1:C:142:LYS:N	2.30	0.93
1:D:52:ILE:O	1:D:89:HIS:HB2	1.70	0.92
1:D:88:THR:HG21	1:D:89:HIS:NE2	1.85	0.92
1:B:225:ASN:HD22	1:B:226:PHE:H	1.07	0.92
1:E:183:ILE:CG2	1:E:188:LEU:HD22	1.98	0.92
1:E:191:LYS:NZ	1:E:191:LYS:CB	2.30	0.92
1:B:20:ARG:O	1:B:41:LYS:CG	2.18	0.92
1:D:78:VAL:HG13	1:D:78:VAL:O	1.67	0.91
1:A:27:ILE:HG13	1:A:28:GLY:N	1.84	0.91
1:E:82:GLU:CG	1:E:303:GLN:HE22	1.82	0.91
1:A:151:SER:CB	1:A:152:PRO:HD2	1.95	0.91
1:C:83:VAL:N	1:C:303:GLN:HE22	1.67	0.91
1:B:146:THR:HG22	1:B:156:LEU:CD1	1.99	0.91
1:E:183:ILE:HG22	1:E:188:LEU:HD22	1.53	0.91
1:A:88:THR:C	1:A:89:HIS:HD2	1.69	0.91
1:D:144:GLU:HB3	1:D:182:TYR:CD1	2.05	0.90
1:D:141:LEU:HB3	1:D:143:LEU:HD23	1.54	0.90
1:C:16:HIS:CE1	1:C:51:TYR:OH	2.24	0.90
1:E:82:GLU:CB	1:E:303:GLN:NE2	2.34	0.90
1:C:191:LYS:HD2	1:C:191:LYS:O	1.71	0.89
1:B:225:ASN:O	1:B:229:THR:HG22	1.72	0.89
1:B:88:THR:HG23	1:B:89:HIS:HD2	0.74	0.89
1:D:219:ASP:OD2	1:D:221:GLU:CG	2.19	0.89
1:D:25:LYS:HE2	1:D:27:ILE:CD1	2.02	0.89
1:D:144:GLU:HB3	1:D:182:TYR:CE1	2.07	0.89
1:E:191:LYS:HB3	1:E:191:LYS:HZ3	1.36	0.89
1:D:26:ASP:OD2	1:D:36:ARG:HG3	1.73	0.89
1:B:182:TYR:CE2	1:B:206:THR:HG22	2.07	0.89
1:A:185:PRO:O	1:A:189:LEU:HB2	1.73	0.88

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:THR:CG2	1:C:89:HIS:CD2	2.55	0.88
1:A:12:LEU:CD2	1:A:13:PRO:CD	2.48	0.88
1:C:21:TYR:CE1	1:C:40:ASP:HB2	2.07	0.88
1:D:82:GLU:CB	1:D:303:GLN:NE2	2.37	0.88
1:E:82:GLU:HG3	1:E:303:GLN:HE22	1.06	0.88
1:C:88:THR:HG22	1:C:89:HIS:NE2	1.88	0.88
1:B:205:VAL:O	1:B:209:VAL:HG23	1.74	0.87
1:C:142:LYS:HE3	1:C:159:ALA:O	1.71	0.87
1:E:54:ARG:NH2	1:E:86:THR:O	2.07	0.87
1:E:58:ILE:HG23	1:E:58:ILE:O	1.72	0.87
1:D:12:LEU:N	1:D:13:PRO:CD	2.37	0.87
1:B:73:ARG:HG2	1:B:73:ARG:O	1.75	0.87
1:D:53:GLU:CA	1:D:89:HIS:HB3	2.00	0.87
1:F:180:PRO:HA	1:F:183:ILE:HD12	1.57	0.87
1:E:182:TYR:CE2	1:E:206:THR:HG22	2.10	0.87
1:B:314:GLU:OE1	3:B:347:HOH:O	1.93	0.86
1:D:63:LYS:CG	1:D:309:MET:HE1	2.05	0.86
1:B:225:ASN:ND2	1:B:226:PHE:N	2.22	0.86
1:F:63:LYS:HD2	1:F:309:MET:HE1	1.58	0.86
1:E:14:ILE:CG2	1:E:15:MET:N	2.30	0.86
1:B:219:ASP:OD2	1:B:232:ARG:NE	2.10	0.85
1:E:217:PHE:HB3	1:E:232:ARG:HB3	1.58	0.85
1:E:61:ASN:HA	1:E:64:ARG:NE	1.90	0.85
1:B:54:ARG:HD3	1:B:315:ALA:HA	1.57	0.85
1:D:72:LEU:O	3:D:325:HOH:O	1.94	0.85
1:F:317:VAL:O	1:F:317:VAL:HG12	1.75	0.85
1:A:60:GLU:CD	1:A:63:LYS:NZ	2.30	0.85
1:D:149:ASP:OD1	1:D:154:PRO:HA	1.75	0.85
1:A:27:ILE:HG13	1:A:28:GLY:H	1.41	0.85
1:D:211:LEU:HD13	1:D:246:ILE:HD11	1.56	0.85
1:E:80:PHE:O	1:E:80:PHE:CD2	2.30	0.85
1:E:191:LYS:NZ	1:E:191:LYS:HB3	1.89	0.85
1:C:83:VAL:N	1:C:303:GLN:NE2	2.24	0.85
1:B:232:ARG:NH2	1:B:237:GLN:HE21	1.76	0.84
1:C:83:VAL:H	1:C:303:GLN:HE22	0.88	0.84
1:D:58:ILE:HD13	1:D:316:THR:HA	1.59	0.84
1:A:135:GLN:HG2	1:A:138:HIS:CA	2.06	0.83
1:C:211:LEU:O	3:C:323:HOH:O	1.96	0.83
1:E:61:ASN:C	1:E:64:ARG:HD2	1.97	0.83
1:A:23:LEU:HD13	1:A:36:ARG:HD3	1.59	0.83
1:E:70:ARG:CG	1:E:80:PHE:CE2	2.59	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LYS:HB2	1:B:93:VAL:O	1.78	0.83
1:D:52:ILE:O	1:D:89:HIS:CB	2.26	0.83
1:A:187:VAL:O	1:C:227:ARG:NE	2.11	0.83
1:B:58:ILE:HG22	1:B:316:THR:HG22	1.61	0.82
1:C:88:THR:HG21	1:C:89:HIS:NE2	1.92	0.82
1:B:186:GLU:CG	1:B:262:PRO:HG3	2.08	0.82
1:E:88:THR:HG21	1:E:89:HIS:CD2	2.08	0.82
1:E:191:LYS:HZ3	1:E:191:LYS:CB	1.90	0.82
1:A:219:ASP:OD1	1:A:220:PRO:CD	2.28	0.82
1:F:63:LYS:HD2	1:F:309:MET:CE	2.09	0.82
1:D:16:HIS:HE1	1:D:51:TYR:OH	1.61	0.82
1:F:226:PHE:HA	1:F:229:THR:CG2	2.09	0.82
1:D:162:GLY:O	1:D:163:TYR:O	1.98	0.81
1:A:88:THR:CB	1:A:89:HIS:CD2	2.59	0.81
1:D:222:GLU:HG3	1:D:228:LYS:NZ	1.94	0.81
1:D:88:THR:HB	1:D:89:HIS:HD2	1.46	0.81
1:E:61:ASN:HA	1:E:64:ARG:CD	2.10	0.81
1:E:40:ASP:OD1	1:E:42:GLN:HB2	1.80	0.81
1:E:77:ILE:CG1	1:E:158:ILE:HB	2.11	0.81
1:C:27:ILE:CB	1:C:28:GLY:CA	2.59	0.81
1:E:135:GLN:HE21	1:E:135:GLN:HA	1.45	0.81
1:E:59:ASP:C	1:E:59:ASP:OD2	2.19	0.81
1:B:272:ARG:HG2	1:B:272:ARG:NH1	1.89	0.81
1:C:227:ARG:HG3	1:C:231:HIS:HD2	1.44	0.80
1:D:180:PRO:HA	1:D:183:ILE:HD12	1.63	0.80
1:B:85:LEU:CD1	1:B:85:LEU:C	2.50	0.80
1:D:303:GLN:O	1:D:304:SER:O	2.00	0.80
1:D:78:VAL:CG1	1:D:78:VAL:O	2.30	0.80
1:C:186:GLU:HG3	1:C:262:PRO:HG3	1.63	0.80
1:E:58:ILE:CG2	1:E:58:ILE:O	2.30	0.80
1:D:89:HIS:CD2	1:D:89:HIS:N	2.49	0.80
1:E:64:ARG:HG2	1:E:65:GLU:N	1.97	0.80
1:F:225:ASN:HD21	1:F:227:ARG:HB2	1.46	0.79
1:A:78:VAL:HG23	1:A:158:ILE:O	1.81	0.79
1:C:142:LYS:H	1:C:142:LYS:HD2	1.47	0.79
1:D:186:GLU:HG2	1:D:262:PRO:HG3	1.64	0.79
1:D:27:ILE:CG2	1:D:28:GLY:N	2.45	0.79
1:D:88:THR:HB	1:D:89:HIS:CD2	2.17	0.79
1:A:183:ILE:HG22	1:A:188:LEU:HD11	1.64	0.79
1:D:182:TYR:CE2	1:D:206:THR:HG22	2.15	0.79
1:D:83:VAL:H	1:D:303:GLN:HE22	1.30	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:VAL:O	1:F:317:VAL:CG1	2.30	0.79
1:F:70:ARG:HD3	3:F:329:HOH:O	1.81	0.79
1:B:139:ARG:NH1	1:B:160:ASP:OD2	2.16	0.78
1:B:58:ILE:CG2	1:B:58:ILE:O	2.30	0.78
1:C:140:ASP:O	1:C:141:LEU:CD1	2.30	0.78
1:A:88:THR:O	1:A:89:HIS:CD2	2.37	0.78
1:D:63:LYS:CD	1:D:309:MET:CE	2.61	0.78
1:A:88:THR:OG1	1:A:89:HIS:CD2	2.36	0.78
1:C:142:LYS:HE2	1:C:159:ALA:O	1.82	0.78
1:D:27:ILE:HG22	1:D:28:GLY:N	1.97	0.78
1:E:180:PRO:O	1:E:233:ILE:HD11	1.83	0.78
1:E:313:ALA:CA	1:E:316:THR:OG1	2.30	0.78
1:F:221:GLU:CA	1:F:221:GLU:OE1	2.30	0.78
1:F:310:GLN:OE1	1:F:310:GLN:CA	2.31	0.78
1:B:58:ILE:CG2	1:B:316:THR:HG22	2.13	0.77
1:B:13:PRO:HG3	1:B:51:TYR:CD1	2.18	0.77
1:D:183:ILE:CD1	1:F:226:PHE:HZ	1.98	0.77
1:E:16:HIS:NE2	1:E:51:TYR:OH	1.88	0.77
1:E:61:ASN:O	1:E:64:ARG:CD	2.30	0.77
1:E:88:THR:HG22	1:E:89:HIS:HD2	1.41	0.77
1:B:186:GLU:HG2	1:B:262:PRO:HG3	1.66	0.77
1:E:82:GLU:HG3	1:E:303:GLN:HE21	1.48	0.77
1:C:13:PRO:CG	1:C:89:HIS:NE2	2.41	0.77
1:B:88:THR:OG1	1:B:89:HIS:CD2	2.38	0.77
1:C:227:ARG:O	1:C:231:HIS:CD2	2.37	0.77
1:D:144:GLU:CB	1:D:182:TYR:CE1	2.67	0.77
1:D:222:GLU:HG3	1:D:228:LYS:HZ1	1.50	0.77
1:D:58:ILE:HD13	1:D:316:THR:CG2	2.15	0.77
1:A:60:GLU:CD	1:A:63:LYS:HZ1	1.87	0.77
1:D:58:ILE:HD13	1:D:316:THR:CA	2.15	0.77
1:E:61:ASN:HA	1:E:64:ARG:HD2	1.66	0.77
1:C:140:ASP:O	1:C:141:LEU:HD12	1.84	0.76
1:D:88:THR:CB	1:D:89:HIS:CD2	2.68	0.76
1:B:219:ASP:CB	1:B:232:ARG:CZ	2.63	0.76
1:F:64:ARG:NH1	1:F:64:ARG:HB3	1.98	0.76
1:F:89:HIS:N	1:F:89:HIS:CD2	2.51	0.76
1:C:183:ILE:HG21	1:C:188:LEU:CD1	2.15	0.76
1:F:21:TYR:HE1	1:F:40:ASP:HB2	1.47	0.76
1:F:88:THR:C	1:F:89:HIS:CD2	2.51	0.76
1:E:54:ARG:CD	1:E:315:ALA:HB1	2.15	0.76
1:B:183:ILE:N	1:B:183:ILE:CD1	2.49	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:O	1:D:111:ARG:HD3	1.85	0.76
1:C:227:ARG:HG3	1:C:231:HIS:CD2	2.21	0.76
1:D:226:PHE:CZ	1:D:230:ILE:HD13	2.20	0.76
1:E:61:ASN:CA	1:E:64:ARG:HD2	2.16	0.76
1:B:232:ARG:CZ	1:B:237:GLN:HE21	1.99	0.75
1:C:88:THR:HB	1:C:89:HIS:CD2	2.20	0.75
1:B:88:THR:HG1	1:B:89:HIS:CD2	2.05	0.75
1:E:182:TYR:HE2	1:E:206:THR:HG22	1.48	0.75
1:E:74:HIS:HE1	1:E:76:ASN:HB2	1.49	0.75
1:F:151:SER:HB2	1:F:152:PRO:HD2	1.68	0.75
1:C:27:ILE:HG13	1:C:28:GLY:N	2.00	0.75
1:C:52:ILE:O	1:C:89:HIS:HB2	1.87	0.75
1:E:135:GLN:NE2	1:E:135:GLN:HA	2.02	0.75
1:A:314:GLU:O	1:A:317:VAL:HG23	1.86	0.75
1:E:58:ILE:CG2	1:E:316:THR:CG2	2.65	0.75
1:E:179:THR:HB	1:E:180:PRO:HD3	1.69	0.74
1:A:151:SER:HB2	1:A:152:PRO:CD	2.08	0.74
1:B:304:SER:HB2	1:B:306:GLU:OE1	1.87	0.74
1:E:61:ASN:O	1:E:65:GLU:HG3	1.87	0.74
1:C:126:SER:CB	1:C:286:MET:HE3	1.84	0.74
1:C:53:GLU:HA	1:C:89:HIS:HB3	1.69	0.74
1:F:54:ARG:HG2	1:F:89:HIS:HA	1.69	0.74
1:B:21:TYR:HE1	1:B:40:ASP:HB2	1.50	0.74
1:C:58:ILE:CG2	1:C:58:ILE:O	2.35	0.74
1:D:46:LEU:O	3:D:324:HOH:O	2.04	0.74
1:E:13:PRO:HG2	1:E:51:TYR:CG	2.23	0.74
1:E:179:THR:HB	1:E:180:PRO:CD	2.18	0.74
1:B:146:THR:HG22	1:B:156:LEU:HD12	1.69	0.74
1:C:13:PRO:HG3	1:C:89:HIS:CE1	2.22	0.74
1:B:146:THR:HG22	1:B:156:LEU:HD11	1.58	0.74
1:C:126:SER:HB2	1:C:286:MET:HE1	0.74	0.73
1:A:116:GLU:OE1	3:A:319:HOH:O	2.05	0.73
1:D:303:GLN:O	1:D:308:ILE:HD12	1.88	0.73
1:D:63:LYS:CG	1:D:309:MET:CE	2.66	0.73
1:B:219:ASP:HB2	1:B:232:ARG:NH1	2.03	0.73
1:D:317:VAL:O	1:D:317:VAL:HG12	1.86	0.73
1:F:135:GLN:OE1	1:F:135:GLN:CA	2.30	0.73
1:A:27:ILE:CG1	1:A:28:GLY:N	2.51	0.73
1:B:85:LEU:CD1	1:B:86:THR:N	2.51	0.73
1:B:27:ILE:HD13	1:B:37:LEU:HD13	1.70	0.73
1:E:229:THR:HG22	1:E:230:ILE:N	2.01	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ARG:HD2	1:E:315:ALA:HB1	1.71	0.73
1:B:139:ARG:NH2	3:B:322:HOH:O	2.22	0.73
1:A:136:VAL:HG13	1:B:316:THR:HG21	1.70	0.73
1:C:27:ILE:CD1	1:C:28:GLY:HA3	2.19	0.73
1:A:63:LYS:HD2	1:A:309:MET:HE1	1.71	0.72
1:C:236:VAL:CG1	1:C:236:VAL:O	2.36	0.72
1:F:181:ALA:O	3:F:320:HOH:O	2.06	0.72
1:C:61:ASN:OD1	1:C:64:ARG:NH2	2.22	0.72
1:D:282:PRO:HB2	1:D:283:ALA:HB3	1.70	0.72
1:E:23:LEU:HD13	1:E:36:ARG:HD3	1.72	0.72
1:A:186:GLU:HG2	1:A:262:PRO:CG	2.16	0.72
1:B:272:ARG:CG	1:B:272:ARG:HH11	2.01	0.72
1:E:232:ARG:NH1	1:E:237:GLN:HE21	1.86	0.72
1:A:74:HIS:HB3	1:A:77:ILE:HG13	1.70	0.72
1:B:183:ILE:HD13	1:B:183:ILE:N	2.04	0.72
1:C:27:ILE:HB	1:C:28:GLY:CA	2.16	0.72
1:C:34:VAL:O	1:C:50:LYS:HE3	1.90	0.72
1:D:142:LYS:C	1:D:144:GLU:OE2	2.28	0.72
1:E:105:ARG:NH2	3:E:330:HOH:O	2.23	0.72
1:A:141:LEU:HD11	1:A:160:ASP:OD2	1.90	0.72
1:C:82:GLU:HA	1:C:303:GLN:HE21	1.54	0.72
1:E:236:VAL:O	1:E:236:VAL:HG12	1.90	0.72
1:B:281:LEU:HD12	1:B:282:PRO:HD2	1.71	0.71
1:D:110:GLY:O	3:D:327:HOH:O	2.06	0.71
1:D:23:LEU:HD13	1:D:36:ARG:HD3	1.72	0.71
1:E:61:ASN:O	1:E:65:GLU:CG	2.38	0.71
1:A:268:ILE:O	1:A:272:ARG:HG3	1.90	0.71
1:A:83:VAL:H	1:A:303:GLN:HE22	1.36	0.71
1:E:78:VAL:HG23	1:E:158:ILE:O	1.91	0.71
1:E:232:ARG:HH11	1:E:237:GLN:HE21	1.38	0.71
1:B:12:LEU:CD2	1:B:13:PRO:HD2	2.20	0.71
1:D:183:ILE:CD1	1:F:226:PHE:CZ	2.74	0.71
1:E:189:LEU:CD2	1:E:189:LEU:N	2.54	0.71
1:A:88:THR:HG23	1:A:89:HIS:CG	2.25	0.71
1:E:309:MET:O	1:E:311:ILE:N	2.24	0.71
1:A:186:GLU:CG	1:A:262:PRO:HG3	2.16	0.71
1:A:188:LEU:O	1:C:231:HIS:CE1	2.43	0.71
1:C:89:HIS:N	1:C:89:HIS:CD2	2.58	0.71
1:A:70:ARG:HD3	1:A:70:ARG:O	1.90	0.70
1:C:27:ILE:CG1	1:C:28:GLY:CA	2.69	0.70
1:B:88:THR:CB	1:B:89:HIS:CD2	2.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:N	1:C:141:LEU:CD1	2.49	0.70
1:C:23:LEU:HD13	1:C:36:ARG:HD3	1.73	0.70
1:D:74:HIS:HB3	1:D:77:ILE:HG13	1.71	0.70
1:E:13:PRO:HG2	1:E:51:TYR:CD1	2.26	0.70
1:F:53:GLU:CA	1:F:89:HIS:HB3	2.18	0.70
1:A:40:ASP:OD2	1:A:40:ASP:C	2.30	0.70
1:B:178:GLY:N	1:E:224:LYS:HB3	2.06	0.70
1:C:88:THR:CB	1:C:89:HIS:CD2	2.74	0.70
1:E:180:PRO:O	1:E:233:ILE:CD1	2.39	0.70
1:C:27:ILE:HD12	1:C:28:GLY:HA3	1.72	0.70
1:C:186:GLU:CG	1:C:262:PRO:HG3	2.21	0.70
1:C:219:ASP:OD1	1:C:219:ASP:C	2.30	0.70
1:C:126:SER:CA	1:C:286:MET:HE1	2.16	0.69
1:E:304:SER:O	1:E:306:GLU:N	2.26	0.69
1:F:74:HIS:HB3	1:F:77:ILE:HG13	1.73	0.69
1:F:229:THR:HG21	3:F:325:HOH:O	1.92	0.69
1:B:225:ASN:ND2	1:B:226:PHE:H	1.82	0.69
1:C:142:LYS:HD2	1:C:142:LYS:N	2.04	0.69
1:C:285:LEU:C	1:C:286:MET:HG2	2.12	0.69
1:F:151:SER:O	1:F:152:PRO:C	2.30	0.69
1:F:85:LEU:HB3	1:F:311:ILE:HG23	1.72	0.69
1:A:141:LEU:CD1	1:A:160:ASP:OD2	2.41	0.68
1:B:36:ARG:HD2	1:B:38:MET:CE	2.22	0.68
1:B:36:ARG:HD2	1:B:38:MET:HE2	1.74	0.68
1:A:36:ARG:HD2	1:A:38:MET:CE	2.23	0.68
1:D:83:VAL:N	1:D:303:GLN:HE22	1.91	0.68
1:E:112:PHE:CD2	1:E:116:GLU:CG	2.76	0.68
1:A:179:THR:HB	1:A:180:PRO:HD2	1.76	0.68
1:C:183:ILE:HG21	1:C:188:LEU:HD11	1.76	0.68
1:F:308:ILE:O	1:F:312:ILE:HG13	1.94	0.68
1:F:26:ASP:OD2	1:F:36:ARG:HG3	1.94	0.68
1:A:135:GLN:CG	1:A:138:HIS:HA	2.21	0.68
1:D:16:HIS:CE1	1:D:51:TYR:OH	2.47	0.68
1:A:138:HIS:CE1	1:A:195:GLY:HA3	2.28	0.68
1:D:88:THR:HG22	1:D:89:HIS:NE2	2.05	0.68
1:F:23:LEU:HD13	1:F:36:ARG:HD3	1.74	0.68
1:F:134:MET:O	1:F:135:GLN:CG	2.38	0.68
1:F:83:VAL:H	1:F:303:GLN:HE22	1.41	0.68
1:A:63:LYS:CD	1:A:309:MET:HE1	2.24	0.67
1:B:183:ILE:HD13	1:B:183:ILE:H	1.59	0.67
1:D:143:LEU:C	1:D:145:ASN:H	1.98	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:HIS:ND1	1:A:75:PRO:HD2	2.09	0.67
1:C:126:SER:OG	1:C:286:MET:CE	2.42	0.67
1:D:58:ILE:HG12	1:D:58:ILE:O	1.93	0.67
1:C:54:ARG:HG3	1:C:89:HIS:HA	1.76	0.67
1:D:142:LYS:O	1:D:144:GLU:N	2.27	0.67
1:E:310:GLN:O	1:E:314:GLU:N	2.28	0.67
1:F:141:LEU:C	1:F:142:LYS:HG2	2.14	0.67
1:C:88:THR:HG22	1:C:89:HIS:CE1	2.30	0.67
1:D:27:ILE:CG2	1:D:28:GLY:H	2.06	0.67
1:F:310:GLN:O	1:F:314:GLU:HG2	1.93	0.67
1:D:82:GLU:HB2	1:D:303:GLN:HE21	1.58	0.67
1:C:26:ASP:OD2	1:C:36:ARG:HG3	1.94	0.67
1:B:83:VAL:H	1:B:303:GLN:HE22	1.42	0.67
1:B:26:ASP:OD2	1:B:36:ARG:HG3	1.95	0.67
1:C:82:GLU:HA	1:C:303:GLN:NE2	2.10	0.66
1:E:80:PHE:HA	1:E:94:MET:HA	1.77	0.66
1:C:312:ILE:O	1:C:316:THR:HG23	1.95	0.66
1:D:282:PRO:CB	1:D:283:ALA:CB	2.57	0.66
1:A:63:LYS:CD	1:A:309:MET:CE	2.73	0.66
1:A:88:THR:CA	1:A:89:HIS:HD2	2.09	0.66
1:F:226:PHE:HA	1:F:229:THR:HG23	1.78	0.66
1:F:186:GLU:HG2	1:F:262:PRO:HG3	1.76	0.66
1:F:191:LYS:HG3	1:F:192:GLU:HG3	1.77	0.66
1:B:223:PRO:O	1:B:225:ASN:N	2.29	0.65
1:B:225:ASN:O	1:B:229:THR:CG2	2.45	0.65
1:C:182:TYR:HE2	1:C:206:THR:HG22	1.61	0.65
1:D:141:LEU:HD13	1:D:143:LEU:HD21	1.78	0.65
1:D:141:LEU:HB3	1:D:143:LEU:CD2	2.26	0.65
1:C:183:ILE:CG2	1:C:188:LEU:HD13	2.25	0.65
1:C:86:THR:O	1:C:88:THR:N	2.30	0.65
1:C:160:ASP:N	1:C:160:ASP:OD2	2.30	0.65
1:D:122:GLN:HG2	1:D:281:LEU:HD13	1.78	0.65
1:E:85:LEU:CD2	1:E:315:ALA:HB2	2.25	0.65
1:B:308:ILE:O	1:B:312:ILE:HG13	1.97	0.65
1:E:61:ASN:OD1	1:E:64:ARG:NH1	2.30	0.65
1:F:151:SER:O	1:F:153:ALA:N	2.30	0.65
1:A:220:PRO:O	1:A:222:GLU:N	2.30	0.65
1:B:74:HIS:HB3	1:B:77:ILE:HG13	1.79	0.65
1:B:89:HIS:N	1:B:89:HIS:CD2	2.64	0.65
1:A:70:ARG:CD	1:A:70:ARG:O	2.44	0.65
1:B:223:PRO:C	1:B:225:ASN:H	1.99	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LEU:HD13	1:F:188:LEU:O	1.97	0.65
1:E:307:GLU:O	1:E:309:MET:N	2.30	0.65
1:F:72:LEU:O	3:F:322:HOH:O	2.15	0.65
1:A:205:VAL:HG13	1:A:216:PRO:HG2	1.78	0.64
1:A:27:ILE:CD1	1:A:29:ALA:O	2.40	0.64
1:D:143:LEU:O	1:D:145:ASN:N	2.30	0.64
1:D:13:PRO:HB3	1:D:89:HIS:NE2	2.11	0.64
1:A:284:ASP:OD1	1:A:284:ASP:N	2.30	0.64
1:A:54:ARG:HH11	1:A:54:ARG:HG2	1.63	0.64
1:D:13:PRO:HG3	1:D:51:TYR:CD1	2.32	0.64
1:D:149:ASP:OD1	1:D:155:ARG:N	2.30	0.64
1:E:313:ALA:O	1:E:315:ALA:N	2.30	0.64
1:A:60:GLU:CD	1:A:63:LYS:HZ3	1.99	0.64
1:B:12:LEU:HD23	1:B:13:PRO:HD2	1.79	0.64
1:A:218:GLU:HG2	1:A:223:PRO:CB	2.28	0.64
1:B:284:ASP:OD1	1:B:284:ASP:N	2.30	0.64
1:D:303:GLN:O	1:D:304:SER:C	2.36	0.64
1:C:24:VAL:HA	1:D:111:ARG:HH11	1.62	0.64
1:C:86:THR:C	1:C:88:THR:H	2.01	0.64
1:D:82:GLU:CA	1:D:303:GLN:NE2	2.60	0.64
1:D:86:THR:O	1:D:88:THR:N	2.30	0.64
1:A:63:LYS:HD2	1:A:309:MET:CE	2.27	0.64
1:B:215:TYR:HB2	1:B:218:GLU:HG3	1.80	0.64
1:B:86:THR:O	1:B:88:THR:N	2.30	0.64
1:B:88:THR:OG1	1:B:89:HIS:NE2	2.30	0.64
1:C:52:ILE:O	1:C:89:HIS:CB	2.45	0.64
1:D:159:ALA:HB1	1:D:161:PHE:CE1	2.33	0.63
1:D:232:ARG:HA	1:D:237:GLN:HG3	1.79	0.63
1:D:297:GLU:C	1:D:299:ASP:H	2.01	0.63
1:C:281:LEU:HD12	1:C:282:PRO:HD2	1.80	0.63
1:D:226:PHE:CZ	1:D:230:ILE:CD1	2.82	0.63
1:A:54:ARG:O	1:A:315:ALA:O	2.16	0.63
1:C:59:ASP:OD2	1:C:59:ASP:O	2.17	0.63
1:D:58:ILE:HD13	1:D:316:THR:HG22	1.78	0.63
1:A:36:ARG:HD2	1:A:38:MET:HE2	1.78	0.63
1:B:23:LEU:HD13	1:B:36:ARG:HD3	1.79	0.63
1:E:85:LEU:HD23	1:E:315:ALA:CB	2.26	0.63
1:F:225:ASN:OD1	1:F:228:LYS:HG3	1.98	0.63
1:F:36:ARG:HD2	1:F:38:MET:CE	2.28	0.63
1:D:128:VAL:HG22	1:D:141:LEU:HD11	1.79	0.63
1:D:183:ILE:HG22	1:D:188:LEU:HD13	1.77	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ILE:CD1	1:D:316:THR:CG2	2.77	0.63
1:C:105:ARG:NH1	1:C:116:GLU:OE2	2.32	0.62
1:F:180:PRO:HA	1:F:183:ILE:CD1	2.28	0.62
1:B:149:ASP:C	1:B:149:ASP:OD1	2.37	0.62
1:D:58:ILE:HD11	1:D:312:ILE:O	1.99	0.62
1:D:63:LYS:HG3	1:D:309:MET:CE	2.29	0.62
1:E:185:PRO:O	1:E:189:LEU:HD23	1.99	0.62
1:A:162:GLY:O	1:A:163:TYR:C	2.37	0.62
1:C:70:ARG:NH2	1:C:303:GLN:O	2.25	0.62
1:C:60:GLU:O	1:C:63:LYS:N	2.33	0.62
1:E:230:ILE:HG22	1:E:231:HIS:N	2.14	0.62
1:A:220:PRO:O	1:A:221:GLU:C	2.37	0.62
1:C:36:ARG:HD2	1:C:38:MET:CE	2.30	0.62
1:E:45:GLU:OE1	1:E:81:LYS:NZ	2.26	0.62
1:B:34:VAL:O	1:B:50:LYS:HE3	2.00	0.62
1:B:83:VAL:H	1:B:303:GLN:NE2	1.98	0.62
1:D:55:GLY:O	1:D:58:ILE:HG22	1.99	0.62
1:A:141:LEU:O	1:A:142:LYS:CG	2.48	0.61
1:A:179:THR:HB	1:A:180:PRO:CD	2.30	0.61
1:A:63:LYS:HD3	1:A:309:MET:HE3	1.82	0.61
1:C:227:ARG:O	1:C:231:HIS:HD2	1.80	0.61
1:D:299:ASP:O	1:D:299:ASP:CG	2.38	0.61
1:C:54:ARG:NH2	1:C:85:LEU:HD21	2.15	0.61
1:D:142:LYS:O	1:D:143:LEU:C	2.38	0.61
1:D:180:PRO:HG3	1:D:226:PHE:CE1	2.35	0.61
1:A:138:HIS:CG	1:A:138:HIS:O	2.52	0.61
1:C:228:LYS:O	1:C:232:ARG:HG3	2.01	0.61
1:B:317:VAL:C	3:B:323:HOH:O	2.39	0.61
1:B:65:GLU:CD	1:B:162:GLY:O	2.39	0.61
1:F:21:TYR:CE1	1:F:40:ASP:CB	2.77	0.61
1:C:183:ILE:HG21	1:C:188:LEU:HD13	1.80	0.61
1:A:190:LYS:O	1:C:227:ARG:NH2	2.33	0.61
1:F:14:ILE:HG13	1:F:15:MET:N	2.15	0.61
1:F:13:PRO:HB3	1:F:88:THR:HG21	1.83	0.61
1:C:36:ARG:HD2	1:C:38:MET:HE3	1.83	0.60
1:F:105:ARG:NH1	1:F:116:GLU:OE2	2.34	0.60
1:D:27:ILE:HG23	1:D:28:GLY:H	1.67	0.60
1:A:13:PRO:HG3	1:A:51:TYR:CD1	2.36	0.60
1:A:54:ARG:HH11	1:A:54:ARG:CG	2.14	0.60
1:A:63:LYS:HD3	1:A:309:MET:CE	2.31	0.60
1:D:58:ILE:CD1	1:D:316:THR:N	2.65	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:THR:O	1:D:87:PRO:C	2.39	0.60
1:E:185:PRO:O	1:E:189:LEU:CD2	2.49	0.60
1:B:105:ARG:NH1	1:B:116:GLU:OE2	2.35	0.60
1:E:191:LYS:NZ	1:E:191:LYS:HB2	2.13	0.60
1:E:82:GLU:HB2	1:E:303:GLN:CD	2.22	0.60
1:F:305:ILE:O	1:F:309:MET:HG2	2.02	0.60
1:D:63:LYS:HG3	1:D:309:MET:HE1	1.81	0.60
1:B:186:GLU:HG3	1:B:262:PRO:HG3	1.81	0.60
1:B:54:ARG:NH2	1:B:85:LEU:HD11	2.17	0.60
1:E:58:ILE:HG22	1:E:316:THR:CG2	2.32	0.60
1:B:70:ARG:CD	1:B:70:ARG:O	2.46	0.59
1:F:219:ASP:OD2	1:F:228:LYS:HD2	2.02	0.59
1:E:224:LYS:O	1:E:225:ASN:C	2.39	0.59
1:E:58:ILE:HG21	1:E:316:THR:CG2	2.20	0.59
1:F:188:LEU:HD23	1:F:234:LEU:HD21	1.84	0.59
1:D:148:LEU:HB3	1:D:154:PRO:HB2	1.83	0.59
1:E:227:ARG:NH1	3:E:319:HOH:O	2.11	0.59
1:A:19:ASP:OD1	1:A:20:ARG:HG3	2.03	0.59
1:B:13:PRO:HG3	1:B:51:TYR:CE1	2.38	0.59
1:B:52:ILE:O	1:B:89:HIS:HB3	2.03	0.59
1:B:219:ASP:HB2	1:B:232:ARG:NE	2.17	0.59
1:F:151:SER:CB	1:F:152:PRO:HD2	2.33	0.59
1:B:102:LEU:O	1:B:106:ILE:HG13	2.03	0.59
1:E:183:ILE:HG21	1:E:188:LEU:HD22	1.82	0.59
1:A:74:HIS:CE1	1:A:75:PRO:HD2	2.38	0.58
1:E:242:ASP:N	1:E:242:ASP:OD2	2.36	0.58
1:A:88:THR:OG1	1:A:89:HIS:NE2	2.30	0.58
1:D:185:PRO:O	1:D:189:LEU:HD22	2.03	0.58
1:A:54:ARG:NH1	1:A:54:ARG:HG2	2.17	0.58
1:D:106:ILE:HD11	1:D:210:MET:HG2	1.85	0.58
1:E:146:THR:OG1	1:E:156:LEU:HD21	2.03	0.58
1:A:216:PRO:HB2	1:A:217:PHE:CD1	2.37	0.58
1:A:241:PRO:HG2	1:A:244:VAL:HG23	1.85	0.58
1:E:20:ARG:NH2	1:E:82:GLU:OE2	2.36	0.58
1:C:272:ARG:HH12	1:C:286:MET:HB3	1.67	0.58
1:E:52:ILE:O	1:E:89:HIS:HB3	2.04	0.58
1:E:149:ASP:CG	1:E:151:SER:HG	2.06	0.58
1:F:268:ILE:O	1:F:272:ARG:HG3	2.04	0.58
1:A:78:VAL:HG11	1:A:161:PHE:HZ	1.68	0.58
1:B:230:ILE:HD12	1:E:188:LEU:HD11	1.86	0.58
1:D:58:ILE:CD1	1:D:316:THR:HG23	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:PHE:O	1:B:232:ARG:HD3	2.04	0.58
1:B:86:THR:C	1:B:88:THR:H	2.07	0.58
1:E:187:VAL:O	1:E:187:VAL:HG12	2.03	0.58
1:A:78:VAL:HG11	1:A:161:PHE:CZ	2.38	0.58
1:D:151:SER:HB2	1:D:153:ALA:O	2.03	0.58
1:D:186:GLU:OE2	1:D:265:ARG:NH2	2.31	0.58
1:E:39:ARG:HD2	1:E:44:ASN:OD1	2.03	0.58
1:B:155[B]:ARG:CG	1:B:155[B]:ARG:HH11	2.18	0.57
1:B:78:VAL:HG23	1:B:158:ILE:O	2.04	0.57
1:E:307:GLU:C	1:E:309:MET:H	2.07	0.57
1:A:151:SER:CB	1:A:152:PRO:CD	2.77	0.57
1:F:225:ASN:O	1:F:229:THR:HG22	2.04	0.57
1:A:184:ALA:O	1:A:188:LEU:CD1	2.52	0.57
1:D:58:ILE:HD11	1:D:316:THR:HG23	1.86	0.57
1:E:268:ILE:O	1:E:272:ARG:HG3	2.04	0.57
1:F:69:HIS:HE1	1:F:78:VAL:O	1.88	0.57
1:B:151:SER:O	1:B:152:PRO:C	2.42	0.57
1:A:89:HIS:N	1:A:89:HIS:CD2	2.72	0.57
1:A:141:LEU:O	1:A:142:LYS:HG3	2.05	0.57
1:A:61:ASN:OD1	1:A:64:ARG:NH2	2.37	0.57
1:B:192:GLU:CG	1:B:192:GLU:O	2.40	0.57
1:B:261:ASP:OD1	1:B:262:PRO:HD2	2.03	0.57
1:C:187:VAL:HG22	1:C:193:TYR:CE2	2.40	0.57
1:D:282:PRO:HB3	1:D:283:ALA:HB2	1.83	0.57
1:B:70:ARG:NH2	1:B:303:GLN:O	2.38	0.57
1:D:78:VAL:HG11	1:D:161:PHE:CD1	2.40	0.57
1:D:31:ASN:ND2	1:D:31:ASN:H	2.03	0.57
1:F:141:LEU:H	1:F:141:LEU:HD13	1.64	0.57
1:D:54:ARG:CG	1:D:54:ARG:HH11	2.18	0.56
1:A:66:ILE:HD12	1:A:312:ILE:CD1	2.34	0.56
1:E:16:HIS:ND1	1:E:17:ASP:OD2	2.38	0.56
1:A:74:HIS:H	1:A:79:ARG:HD2	1.70	0.56
1:B:12:LEU:HD22	1:B:13:PRO:HD2	1.87	0.56
1:C:53:GLU:CA	1:C:89:HIS:HB3	2.36	0.56
1:C:88:THR:HB	1:C:89:HIS:HD2	1.67	0.56
1:F:54:ARG:NH1	1:F:314:GLU:O	2.38	0.56
1:A:72:LEU:HD11	1:A:139:ARG:HH12	1.70	0.56
1:D:55:GLY:O	1:D:58:ILE:CG2	2.53	0.56
1:A:66:ILE:HD12	1:A:312:ILE:HD13	1.87	0.56
1:B:218:GLU:O	1:B:223:PRO:HB3	2.05	0.56
1:D:162:GLY:O	1:D:163:TYR:C	2.44	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:TYR:HE1	1:F:40:ASP:CB	2.17	0.56
1:A:218:GLU:HG2	1:A:223:PRO:HB2	1.88	0.56
1:B:88:THR:CB	1:B:89:HIS:HD2	2.07	0.56
1:C:21:TYR:HE1	1:C:40:ASP:HB2	1.64	0.56
1:D:246:ILE:HG23	1:D:250:CYS:HB3	1.88	0.56
1:D:63:LYS:HG2	1:D:309:MET:HE1	1.85	0.56
1:A:135:GLN:HG2	1:A:138:HIS:N	2.20	0.56
1:D:128:VAL:HG22	1:D:141:LEU:CD1	2.36	0.56
1:E:304:SER:O	1:E:305:ILE:C	2.43	0.56
1:E:284:ASP:OD2	1:E:284:ASP:N	2.38	0.56
1:F:36:ARG:HD2	1:F:38:MET:HE2	1.88	0.56
1:A:13:PRO:HG3	1:A:51:TYR:CG	2.41	0.55
1:C:240:ILE:HD12	1:C:246:ILE:HD11	1.88	0.55
1:D:139:ARG:CB	1:D:139:ARG:HH11	2.19	0.55
1:E:189:LEU:O	1:E:190:LYS:HE3	2.06	0.55
1:A:52:ILE:O	1:A:89:HIS:HB3	2.07	0.55
1:C:60:GLU:HA	1:C:63:LYS:HB3	1.89	0.55
1:D:149:ASP:CG	1:D:155:ARG:H	2.10	0.55
1:F:226:PHE:O	1:F:229:THR:HG23	2.07	0.55
1:D:142:LYS:O	1:D:144:GLU:OE2	2.25	0.55
1:E:106:ILE:HA	1:E:112:PHE:CE1	2.42	0.55
1:C:74:HIS:HB3	1:C:77:ILE:HG13	1.88	0.55
1:D:222:GLU:HG3	1:D:228:LYS:HZ2	1.71	0.55
1:E:268:ILE:HB	1:E:269:PRO:HD3	1.88	0.55
1:A:13:PRO:HB3	1:A:88:THR:HG21	1.88	0.55
1:B:218:GLU:O	1:B:223:PRO:HA	2.07	0.55
1:B:27:ILE:CD1	1:B:37:LEU:HD13	2.35	0.55
1:C:27:ILE:HG13	1:C:28:GLY:CA	2.37	0.55
1:D:21:TYR:CE1	1:D:40:ASP:HB2	2.41	0.55
1:D:82:GLU:HA	1:D:303:GLN:NE2	2.22	0.55
1:B:65:GLU:OE2	1:B:162:GLY:O	2.24	0.55
1:C:82:GLU:CA	1:C:303:GLN:NE2	2.69	0.55
1:A:60:GLU:OE1	1:A:63:LYS:NZ	2.38	0.54
1:F:106:ILE:HD11	1:F:210:MET:HG2	1.89	0.54
1:A:193:TYR:O	1:A:193:TYR:CD1	2.60	0.54
1:A:21:TYR:CE1	1:A:40:ASP:HB2	2.42	0.54
1:F:182:TYR:HE2	1:F:206:THR:HG22	1.72	0.54
1:C:81:LYS:O	1:C:82:GLU:HB3	2.06	0.54
1:D:208:TYR:CE2	1:D:216:PRO:HA	2.42	0.54
1:E:16:HIS:HB2	1:E:17:ASP:OD2	2.07	0.54
1:F:219:ASP:HB2	1:F:232:ARG:HD2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ASP:OD2	1:D:36:ARG:NH1	2.41	0.54
1:E:149:ASP:OD1	1:E:149:ASP:C	2.46	0.54
1:E:307:GLU:C	1:E:309:MET:N	2.61	0.54
1:B:14:ILE:HG12	1:B:15:MET:N	2.22	0.54
1:C:225:ASN:HB3	1:C:228:LYS:HB2	1.89	0.54
1:C:179:THR:HB	1:C:180:PRO:HD3	1.90	0.54
1:A:223:PRO:O	1:A:225:ASN:N	2.39	0.54
1:C:118:ARG:HD3	1:C:276:TRP:O	2.07	0.54
1:D:222:GLU:N	1:D:223:PRO:CD	2.71	0.54
1:B:215:TYR:CB	1:B:218:GLU:HG3	2.37	0.53
1:C:120:PHE:HZ	1:C:154:PRO:HG2	1.73	0.53
1:D:131:ALA:O	1:D:135:GLN:HB2	2.08	0.53
1:D:189:LEU:HD21	1:D:234:LEU:HD22	1.91	0.53
1:E:21:TYR:CE1	1:E:40:ASP:HB2	2.43	0.53
1:A:279:LYS:O	1:A:280:ASN:HB2	2.08	0.53
1:B:222:GLU:O	1:B:222:GLU:HG3	2.07	0.53
1:B:237:GLN:O	1:B:237:GLN:HG2	2.07	0.53
1:C:54:ARG:NH2	1:C:85:LEU:CD2	2.71	0.53
1:E:227:ARG:O	1:E:231:HIS:HB2	2.08	0.53
1:E:309:MET:O	1:E:310:GLN:C	2.46	0.53
1:E:59:ASP:O	1:E:59:ASP:OD2	2.26	0.53
1:A:98:SER:O	1:A:100:GLY:N	2.42	0.53
1:E:82:GLU:CG	1:E:303:GLN:HE21	2.12	0.53
1:B:106:ILE:HD11	1:B:210:MET:HG2	1.90	0.53
1:C:179:THR:CB	1:C:180:PRO:CD	2.87	0.53
1:D:124:LEU:HD11	1:D:143:LEU:CD1	2.37	0.53
1:A:220:PRO:O	1:A:223:PRO:CD	2.43	0.53
1:B:21:TYR:CE1	1:B:40:ASP:CB	2.80	0.53
1:C:102:LEU:HA	1:C:148:LEU:HD11	1.91	0.53
1:C:27:ILE:HD12	1:C:28:GLY:CA	2.39	0.53
1:E:182:TYR:HE2	1:E:206:THR:CG2	2.19	0.53
1:B:83:VAL:HG22	1:B:303:GLN:HE22	1.73	0.53
1:E:188:LEU:HB3	1:E:189:LEU:CD2	2.39	0.53
1:F:86:THR:O	1:F:88:THR:N	2.42	0.53
1:B:58:ILE:HG21	1:B:316:THR:HG22	1.91	0.53
1:C:86:THR:C	1:C:88:THR:N	2.61	0.53
1:D:54:ARG:HH11	1:D:54:ARG:HG3	1.74	0.53
1:E:232:ARG:NH1	1:E:237:GLN:NE2	2.54	0.53
1:B:161:PHE:O	1:B:161:PHE:CD2	2.61	0.53
1:B:268:ILE:HB	1:B:269:PRO:HD3	1.90	0.53
1:D:268:ILE:HB	1:D:269:PRO:HD3	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:GLU:OE2	1:F:265:ARG:NH2	2.39	0.53
1:C:191:LYS:C	1:C:192:GLU:HG2	2.29	0.53
1:C:235:ASN:HB2	1:C:237:GLN:HG3	1.91	0.53
1:D:183:ILE:HD13	1:F:226:PHE:CZ	2.44	0.53
1:E:34:VAL:O	1:E:34:VAL:HG22	2.08	0.53
1:C:54:ARG:HH21	1:C:85:LEU:HD21	1.74	0.53
1:A:309:MET:CE	1:B:68:ASN:OD1	2.58	0.52
1:A:42:GLN:O	1:A:43:ALA:HB3	2.09	0.52
1:C:24:VAL:HA	1:D:111:ARG:NH1	2.24	0.52
1:D:82:GLU:HA	1:D:303:GLN:HE21	1.73	0.52
1:F:27:ILE:CG2	1:F:37:LEU:HD22	2.39	0.52
1:D:89:HIS:HD2	1:D:89:HIS:N	2.02	0.52
1:F:313:ALA:O	1:F:316:THR:N	2.28	0.52
1:F:59:ASP:CG	1:F:61:ASN:HB2	2.30	0.52
1:A:59:ASP:OD2	1:A:61:ASN:HB2	2.10	0.52
1:B:135:GLN:OE1	1:B:138:HIS:HA	2.09	0.52
1:C:53:GLU:HB2	1:C:57:LYS:HD3	1.91	0.52
1:E:88:THR:CG2	1:E:89:HIS:N	2.71	0.52
1:A:83:VAL:H	1:A:303:GLN:NE2	2.06	0.52
1:C:126:SER:HA	1:C:286:MET:CE	2.15	0.52
1:D:183:ILE:HD13	1:F:226:PHE:CE1	2.44	0.52
1:D:186:GLU:HG2	1:D:262:PRO:CG	2.39	0.52
1:F:225:ASN:ND2	1:F:227:ARG:HB2	2.20	0.52
1:B:54:ARG:CZ	1:B:85:LEU:HD11	2.40	0.52
1:C:54:ARG:HH21	1:C:85:LEU:CD2	2.23	0.52
1:D:36:ARG:HD2	1:D:38:MET:CE	2.39	0.52
1:E:62:VAL:O	1:E:66:ILE:HG13	2.09	0.52
1:F:69:HIS:CE1	1:F:78:VAL:O	2.63	0.52
1:C:140:ASP:CA	1:C:141:LEU:HD13	2.36	0.52
1:C:142:LYS:N	1:C:142:LYS:HD3	2.03	0.52
1:E:61:ASN:OD1	1:E:64:ARG:HD3	2.10	0.52
1:A:144:GLU:HB3	1:A:182:TYR:CE1	2.44	0.52
1:B:88:THR:C	1:B:89:HIS:CD2	2.83	0.52
1:B:187:VAL:HG22	1:B:193:TYR:CE1	2.45	0.52
1:B:15:MET:SD	1:B:23:LEU:HB2	2.50	0.52
1:C:60:GLU:HB2	1:C:63:LYS:HE2	1.92	0.52
1:D:232:ARG:NH1	1:D:232:ARG:HG2	2.23	0.52
1:A:193:TYR:C	1:A:193:TYR:CD1	2.83	0.51
1:A:220:PRO:HG2	1:A:221:GLU:H	1.74	0.51
1:A:219:ASP:OD1	1:A:220:PRO:N	2.42	0.51
1:A:54:ARG:HG3	1:A:315:ALA:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:O	1:B:219:ASP:C	2.48	0.51
1:C:42:GLN:O	1:C:43:ALA:HB3	2.10	0.51
1:A:216:PRO:HB2	1:A:217:PHE:CE1	2.45	0.51
1:D:225:ASN:HB3	1:D:228:LYS:HB2	1.93	0.51
1:F:136:VAL:C	1:F:137:ALA:O	2.49	0.51
1:E:229:THR:O	1:E:230:ILE:C	2.48	0.51
1:D:124:LEU:HD21	1:D:143:LEU:CD1	2.41	0.51
1:A:24:VAL:O	1:F:111:ARG:HD3	2.10	0.51
1:F:95:GLU:OE1	1:F:157:LYS:NZ	2.39	0.51
1:B:86:THR:C	1:B:88:THR:N	2.64	0.51
1:D:143:LEU:C	1:D:145:ASN:N	2.64	0.51
1:A:151:SER:O	1:A:152:PRO:C	2.48	0.51
1:E:229:THR:O	1:E:232:ARG:N	2.44	0.51
1:E:27:ILE:HG12	1:E:28:GLY:N	2.26	0.51
1:B:21:TYR:CD1	1:B:40:ASP:HB2	2.44	0.51
1:E:151:SER:HB2	1:E:153:ALA:O	2.11	0.51
1:B:268:ILE:HG22	1:B:272:ARG:HD2	1.93	0.51
1:B:36:ARG:CD	1:B:38:MET:HE2	2.41	0.51
1:D:149:ASP:OD1	1:D:154:PRO:CA	2.53	0.51
1:B:60:GLU:OE1	1:B:63:LYS:NZ	2.40	0.50
1:C:151:SER:HB2	1:C:152:PRO:HD2	1.93	0.50
1:B:230:ILE:HD12	1:E:188:LEU:CD1	2.40	0.50
1:A:16:HIS:NE2	1:A:51:TYR:OH	2.03	0.50
1:E:232:ARG:HG3	1:E:237:GLN:O	2.12	0.50
1:A:106:ILE:HD11	1:A:210:MET:HG2	1.93	0.50
1:B:102:LEU:HA	1:B:148:LEU:HD11	1.93	0.50
1:B:219:ASP:HB3	1:B:220:PRO:HB3	1.94	0.50
1:D:40:ASP:OD2	1:D:42:GLN:O	2.29	0.50
1:E:144:GLU:HB3	1:E:182:TYR:CG	2.46	0.50
1:F:136:VAL:O	1:F:137:ALA:O	2.30	0.50
1:A:80:PHE:CD1	1:A:81:LYS:N	2.78	0.50
1:C:120:PHE:CZ	1:C:154:PRO:HG2	2.46	0.50
1:C:88:THR:CG2	1:C:89:HIS:CE1	2.92	0.50
1:E:189:LEU:O	1:E:190:LYS:CB	2.60	0.50
1:B:88:THR:HG23	1:B:89:HIS:N	2.26	0.50
1:D:299:ASP:O	1:D:299:ASP:OD1	2.30	0.50
1:D:58:ILE:CD1	1:D:316:THR:CA	2.88	0.50
1:E:54:ARG:HB2	1:E:88:THR:O	2.11	0.50
1:D:52:ILE:O	1:D:89:HIS:HB3	2.04	0.50
1:E:85:LEU:HB3	1:E:311:ILE:HG23	1.93	0.50
1:E:96:TYR:CE2	1:E:98:SER:HB3	2.47	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ILE:HG21	1:F:188:LEU:HD11	1.94	0.50
1:F:310:GLN:O	1:F:310:GLN:OE1	2.30	0.50
1:A:268:ILE:HB	1:A:269:PRO:HD3	1.94	0.50
1:B:12:LEU:O	1:B:13:PRO:O	2.30	0.50
1:E:313:ALA:O	1:E:316:THR:N	2.44	0.50
1:F:60:GLU:HG3	1:F:61:ASN:N	2.27	0.50
1:F:64:ARG:CB	1:F:64:ARG:HH11	2.09	0.50
1:A:36:ARG:HD2	1:A:38:MET:HE3	1.92	0.50
1:C:12:LEU:O	1:C:13:PRO:O	2.30	0.50
1:E:16:HIS:NE2	1:E:51:TYR:CE1	2.79	0.50
1:E:59:ASP:C	1:E:61:ASN:H	2.08	0.50
1:B:218:GLU:O	1:B:219:ASP:O	2.30	0.49
1:C:14:ILE:O	1:C:15:MET:O	2.30	0.49
1:D:139:ARG:HB2	1:D:139:ARG:NH1	2.26	0.49
1:D:74:HIS:HE1	1:D:76:ASN:HD22	1.60	0.49
1:E:149:ASP:OD2	1:E:151:SER:OG	2.30	0.49
1:B:232:ARG:CZ	1:B:237:GLN:NE2	2.72	0.49
1:C:185:PRO:O	1:C:186:GLU:C	2.50	0.49
1:C:197:VAL:HG12	1:C:265:ARG:NH1	2.27	0.49
1:D:186:GLU:CG	1:D:262:PRO:HG3	2.40	0.49
1:C:126:SER:OG	1:C:286:MET:HE3	2.06	0.49
1:C:59:ASP:OD2	1:C:59:ASP:C	2.50	0.49
1:D:143:LEU:O	1:D:146:THR:CG2	2.53	0.49
1:D:220:PRO:HG2	1:D:221:GLU:HG2	1.94	0.49
1:D:236:VAL:O	1:D:236:VAL:HG12	2.13	0.49
1:D:144:GLU:OE2	1:D:144:GLU:N	2.43	0.49
1:C:106:ILE:HD11	1:C:210:MET:HG2	1.93	0.49
1:A:180:PRO:HA	1:A:183:ILE:HD12	1.94	0.49
1:B:305:ILE:O	1:B:309:MET:HB2	2.13	0.49
1:D:297:GLU:O	1:D:299:ASP:N	2.45	0.49
1:E:188:LEU:HB3	1:E:189:LEU:HD23	1.94	0.49
1:A:12:LEU:HD23	1:A:13:PRO:CD	2.39	0.49
1:A:219:ASP:OD2	1:A:228:LYS:HE3	2.12	0.49
1:D:232:ARG:HG2	1:D:237:GLN:HB2	1.94	0.49
1:C:14:ILE:O	1:C:15:MET:C	2.51	0.49
1:D:143:LEU:HB3	1:D:206:THR:HG21	1.94	0.49
1:F:26:ASP:OD2	1:F:36:ARG:NH1	2.45	0.49
1:F:36:ARG:HD2	1:F:38:MET:HE3	1.93	0.49
1:A:54:ARG:O	1:A:55:GLY:O	2.31	0.49
1:D:143:LEU:H	1:D:143:LEU:HD23	1.76	0.49
1:E:106:ILE:HD11	1:E:210:MET:HG2	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ASP:OD1	1:E:151:SER:OG	2.30	0.49
1:F:226:PHE:CA	1:F:229:THR:HG23	2.42	0.49
1:F:27:ILE:HG21	1:F:37:LEU:HD22	1.95	0.49
1:A:309:MET:HE1	1:B:68:ASN:OD1	2.13	0.49
1:B:14:ILE:O	1:B:16:HIS:ND1	2.46	0.49
1:B:223:PRO:C	1:B:225:ASN:N	2.65	0.49
1:C:179:THR:OG1	1:C:180:PRO:CD	2.60	0.49
1:E:309:MET:C	1:E:311:ILE:N	2.62	0.49
1:F:78:VAL:HG11	1:F:161:PHE:CE1	2.47	0.48
1:B:155[B]:ARG:CG	1:B:155[B]:ARG:NH1	2.76	0.48
1:C:179:THR:CB	1:C:180:PRO:HD3	2.42	0.48
1:C:268:ILE:HB	1:C:269:PRO:HD3	1.95	0.48
1:D:223:PRO:C	1:D:225:ASN:H	2.16	0.48
1:F:134:MET:O	1:F:135:GLN:CB	2.61	0.48
1:A:135:GLN:HG2	1:A:138:HIS:H	1.78	0.48
1:A:40:ASP:OD2	1:A:40:ASP:O	2.31	0.48
1:B:56:GLU:HG3	1:B:56:GLU:O	2.13	0.48
1:D:42:GLN:O	1:D:43:ALA:HB3	2.13	0.48
1:D:85:LEU:O	1:D:85:LEU:HD13	2.13	0.48
1:B:218:GLU:O	1:B:223:PRO:CB	2.61	0.48
1:D:279:LYS:O	1:D:280:ASN:HB2	2.13	0.48
1:E:310:GLN:O	1:E:314:GLU:CA	2.60	0.48
1:F:228:LYS:O	1:F:232:ARG:HG3	2.12	0.48
1:A:188:LEU:N	1:A:188:LEU:CD1	2.30	0.48
1:B:81:LYS:HB2	1:B:93:VAL:C	2.34	0.48
1:E:106:ILE:HA	1:E:112:PHE:HE1	1.77	0.48
1:E:313:ALA:C	1:E:315:ALA:N	2.65	0.48
1:A:136:VAL:HG13	1:B:316:THR:CG2	2.40	0.48
1:A:161:PHE:N	1:A:161:PHE:CD1	2.80	0.48
1:B:197:VAL:HG21	1:B:262:PRO:HB3	1.96	0.48
1:B:74:HIS:CG	1:B:75:PRO:HD2	2.49	0.48
1:D:124:LEU:HD11	1:D:143:LEU:HD13	1.96	0.48
1:A:226:PHE:HZ	1:C:226:PHE:CZ	2.31	0.48
1:C:40:ASP:OD2	1:C:42:GLN:O	2.31	0.48
1:D:141:LEU:CD1	1:D:143:LEU:HD21	2.44	0.48
1:D:149:ASP:OD2	1:D:151:SER:OG	2.30	0.48
1:D:144:GLU:HB2	1:D:182:TYR:CE1	2.45	0.48
1:B:21:TYR:HE1	1:B:40:ASP:CB	2.23	0.48
1:E:191:LYS:HZ2	1:E:191:LYS:CB	2.23	0.48
1:E:16:HIS:CD2	1:E:51:TYR:HH	2.11	0.48
1:C:144:GLU:HB2	1:C:182:TYR:CE1	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:LYS:O	1:F:280:ASN:HB2	2.13	0.48
1:B:194:ASP:C	1:B:194:ASP:OD2	2.52	0.47
1:C:285:LEU:HB3	1:C:286:MET:HG2	1.96	0.47
1:F:100:GLY:N	3:F:319:HOH:O	2.09	0.47
1:A:241:PRO:HG2	1:A:244:VAL:CG2	2.43	0.47
1:E:74:HIS:CG	1:E:75:PRO:HD2	2.49	0.47
1:F:54:ARG:HG3	1:F:88:THR:O	2.14	0.47
1:C:54:ARG:NH1	1:C:317:VAL:O	2.47	0.47
1:D:232:ARG:HH11	1:D:232:ARG:CG	2.27	0.47
1:E:74:HIS:ND1	1:E:76:ASN:HB2	2.26	0.47
1:F:188:LEU:N	1:F:188:LEU:HD13	2.28	0.47
1:D:14:ILE:HG23	1:D:15:MET:N	2.29	0.47
1:F:225:ASN:HD22	1:F:225:ASN:C	2.15	0.47
1:F:226:PHE:C	1:F:229:THR:HG23	2.34	0.47
1:F:40:ASP:OD2	1:F:42:GLN:O	2.33	0.47
1:B:56:GLU:O	1:B:56:GLU:CG	2.62	0.47
1:E:61:ASN:O	1:E:65:GLU:HG2	2.13	0.47
1:C:54:ARG:HD2	1:C:88:THR:C	2.35	0.47
1:C:224:LYS:O	1:C:226:PHE:N	2.48	0.47
1:D:58:ILE:HD12	1:D:316:THR:N	2.29	0.47
1:E:61:ASN:OD1	1:E:64:ARG:CD	2.63	0.47
1:E:69:HIS:HE1	1:E:79:ARG:HA	1.80	0.47
1:D:281:LEU:HD12	1:D:282:PRO:HD2	1.97	0.47
1:E:313:ALA:O	1:E:316:THR:OG1	2.33	0.47
1:E:313:ALA:HA	1:E:316:THR:HG1	1.74	0.47
1:A:141:LEU:C	1:A:142:LYS:HG2	2.35	0.47
1:A:179:THR:CB	1:A:180:PRO:CD	2.92	0.47
1:D:297:GLU:C	1:D:299:ASP:N	2.67	0.47
1:E:73:ARG:HD2	1:E:73:ARG:HA	1.62	0.47
1:A:205:VAL:HG13	1:A:216:PRO:CG	2.42	0.46
1:C:88:THR:HG22	1:C:89:HIS:CG	2.48	0.46
1:D:187:VAL:HG22	1:D:193:TYR:CE1	2.51	0.46
1:D:27:ILE:N	1:D:27:ILE:CD1	2.78	0.46
1:D:54:ARG:CG	1:D:54:ARG:NH1	2.78	0.46
1:F:161:PHE:N	1:F:161:PHE:CD1	2.83	0.46
1:F:224:LYS:O	1:F:225:ASN:C	2.54	0.46
1:C:227:ARG:NE	1:C:231:HIS:NE2	2.63	0.46
1:E:230:ILE:O	1:E:233:ILE:HB	2.15	0.46
1:F:225:ASN:HD22	1:F:227:ARG:H	1.63	0.46
1:B:247:SER:HB2	1:B:249:GLU:OE1	2.15	0.46
1:D:28:GLY:HA2	1:D:34:VAL:HA	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ASP:CG	1:E:151:SER:OG	2.54	0.46
1:F:316:THR:O	1:F:317:VAL:C	2.53	0.46
1:F:54:ARG:HD2	1:F:315:ALA:HA	1.96	0.46
1:B:40:ASP:OD1	1:B:42:GLN:HB2	2.15	0.46
1:D:36:ARG:HD2	1:D:38:MET:HE3	1.96	0.46
1:F:42:GLN:O	1:F:43:ALA:HB3	2.15	0.46
1:B:15:MET:CE	1:B:21:TYR:O	2.64	0.46
1:D:232:ARG:HG2	1:D:232:ARG:HH11	1.80	0.46
1:A:223:PRO:C	1:A:225:ASN:N	2.68	0.46
1:A:250:CYS:HB2	1:A:276:TRP:NE1	2.31	0.46
1:B:57:LYS:HE3	1:B:57:LYS:HB2	1.41	0.46
1:C:85:LEU:HB3	1:C:311:ILE:HG23	1.97	0.46
1:E:279:LYS:O	1:E:280:ASN:HB2	2.15	0.46
1:E:58:ILE:O	1:E:59:ASP:O	2.34	0.46
1:E:70:ARG:HD3	1:E:70:ARG:O	2.16	0.46
1:B:249:GLU:H	1:B:249:GLU:CD	2.19	0.46
1:C:187:VAL:HG22	1:C:193:TYR:CZ	2.51	0.46
1:D:139:ARG:CB	1:D:139:ARG:NH1	2.78	0.46
1:E:188:LEU:HD13	1:E:188:LEU:HA	1.81	0.46
1:F:74:HIS:CG	1:F:75:PRO:HD2	2.51	0.46
1:B:187:VAL:HG22	1:B:193:TYR:CZ	2.51	0.46
1:E:313:ALA:O	1:E:314:GLU:C	2.53	0.46
1:F:314:GLU:H	1:F:314:GLU:HG2	1.44	0.46
1:A:74:HIS:ND1	1:A:75:PRO:CD	2.78	0.46
1:C:250:CYS:HB2	1:C:276:TRP:NE1	2.31	0.46
1:C:281:LEU:O	1:C:282:PRO:C	2.52	0.46
1:E:189:LEU:O	1:E:190:LYS:CD	2.63	0.46
1:F:28:GLY:O	1:F:34:VAL:CA	2.49	0.46
1:A:28:GLY:O	1:A:29:ALA:HB2	2.16	0.45
1:B:70:ARG:HD3	1:B:70:ARG:C	2.30	0.45
1:C:284:ASP:HB3	3:C:350:HOH:O	2.15	0.45
1:C:58:ILE:HD12	1:C:315:ALA:HB1	1.97	0.45
1:E:80:PHE:CD2	1:E:80:PHE:C	2.90	0.45
1:F:138:HIS:ND1	1:F:138:HIS:O	2.49	0.45
1:F:241:PRO:HG2	1:F:244:VAL:HG23	1.99	0.45
1:A:54:ARG:NH1	1:A:54:ARG:CG	2.77	0.45
1:B:155[B]:ARG:HG3	1:B:155[B]:ARG:NH1	2.31	0.45
1:E:19:ASP:C	1:E:19:ASP:OD2	2.53	0.45
1:E:304:SER:C	1:E:306:GLU:N	2.69	0.45
1:F:225:ASN:ND2	1:F:227:ARG:H	2.14	0.45
1:A:187:VAL:O	1:C:227:ARG:CZ	2.64	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:CG2	1:A:188:LEU:HD11	2.40	0.45
1:D:211:LEU:O	3:D:319:HOH:O	2.20	0.45
1:A:101:GLU:CD	1:A:145:ASN:HD21	2.13	0.45
1:B:36:ARG:HD2	1:B:38:MET:HE3	1.96	0.45
1:B:50:LYS:NZ	3:B:327:HOH:O	2.50	0.45
1:C:148:LEU:C	1:C:149:ASP:O	2.53	0.45
1:C:149:ASP:C	1:C:149:ASP:OD1	2.53	0.45
1:D:142:LYS:O	1:D:145:ASN:N	2.49	0.45
1:E:187:VAL:CG1	1:E:187:VAL:O	2.65	0.45
1:E:61:ASN:OD1	1:E:64:ARG:CZ	2.64	0.45
1:B:22:GLU:OE1	3:B:324:HOH:O	2.21	0.45
1:B:85:LEU:HD12	1:B:86:THR:CA	2.46	0.45
1:C:129:SER:HB2	1:C:268:ILE:HG21	1.99	0.45
1:D:88:THR:HG22	1:D:89:HIS:CG	2.47	0.45
1:F:54:ARG:CG	1:F:89:HIS:HA	2.43	0.45
1:A:105:ARG:NH1	1:A:116:GLU:OE2	2.50	0.45
1:A:236:VAL:HG12	1:A:236:VAL:O	2.17	0.45
1:B:237:GLN:O	1:B:237:GLN:CG	2.64	0.45
1:B:81:LYS:O	1:B:82:GLU:HB3	2.16	0.45
1:C:182:TYR:CE2	1:C:206:THR:HG22	2.47	0.45
1:C:55:GLY:C	1:C:57:LYS:N	2.69	0.45
1:A:72:LEU:HD11	1:A:139:ARG:NH1	2.32	0.45
1:F:78:VAL:HG11	1:F:161:PHE:HE1	1.80	0.45
1:F:53:GLU:HA	1:F:89:HIS:CB	2.32	0.45
1:A:153:ALA:O	1:A:154:PRO:C	2.55	0.45
1:A:67:ILE:HG23	1:B:305:ILE:HD12	1.99	0.45
1:A:36:ARG:HB2	1:A:36:ARG:HE	1.49	0.44
1:A:58:ILE:O	1:A:58:ILE:HG22	2.16	0.44
1:A:67:ILE:HG22	1:B:305:ILE:HD11	1.99	0.44
1:F:12:LEU:HD12	1:F:26:ASP:CG	2.37	0.44
1:F:161:PHE:HB2	1:F:162:GLY:H	1.48	0.44
1:A:88:THR:C	1:A:89:HIS:CG	2.89	0.44
1:C:153:ALA:O	1:C:154:PRO:C	2.55	0.44
1:D:59:ASP:OD2	1:D:60:GLU:N	2.50	0.44
1:D:85:LEU:C	1:D:85:LEU:HD13	2.38	0.44
1:E:179:THR:CB	1:E:180:PRO:CD	2.93	0.44
1:E:222:GLU:CB	1:E:223:PRO:CD	2.95	0.44
1:F:226:PHE:HA	1:F:229:THR:HG21	1.94	0.44
1:F:86:THR:C	1:F:88:THR:N	2.70	0.44
1:F:52:ILE:O	1:F:89:HIS:CB	2.65	0.44
1:A:12:LEU:HD23	1:A:13:PRO:HD3	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ARG:HA	1:E:54:ARG:HD3	1.69	0.44
1:F:148:LEU:HD22	1:F:154:PRO:HB2	1.99	0.44
1:A:144:GLU:HB3	1:A:182:TYR:CD1	2.52	0.44
1:B:227:ARG:O	1:B:231:HIS:CD2	2.69	0.44
1:E:149:ASP:OD1	1:E:149:ASP:O	2.36	0.44
1:E:186:GLU:OE2	1:E:265:ARG:NH1	2.42	0.44
1:B:188:LEU:HA	1:B:188:LEU:HD12	1.62	0.44
1:A:24:VAL:HA	1:F:111:ARG:NH1	2.32	0.44
1:D:208:TYR:CG	1:D:216:PRO:HB3	2.53	0.44
1:D:249:GLU:CD	1:D:249:GLU:H	2.21	0.44
1:E:183:ILE:O	1:E:183:ILE:HG22	2.17	0.44
1:E:60:GLU:HG3	1:E:60:GLU:H	1.39	0.44
1:D:139:ARG:HB3	1:D:139:ARG:HH11	1.83	0.44
1:B:282:PRO:C	1:B:284:ASP:N	2.72	0.43
1:E:193:TYR:HE1	1:E:195:GLY:HA2	1.83	0.43
1:D:58:ILE:HD12	1:D:315:ALA:C	2.38	0.43
1:D:58:ILE:O	1:D:58:ILE:CG1	2.58	0.43
1:F:281:LEU:HD22	1:F:282:PRO:O	2.18	0.43
1:A:12:LEU:CD2	1:A:13:PRO:HD3	2.41	0.43
1:A:153:ALA:HA	1:A:154:PRO:HD2	1.77	0.43
1:B:152:PRO:HB2	1:B:153:ALA:H	1.70	0.43
1:D:204:GLY:HA3	1:D:257:ILE:HG21	2.00	0.43
1:D:27:ILE:N	1:D:27:ILE:HD13	2.33	0.43
1:E:180:PRO:HG2	1:E:229:THR:HG21	2.00	0.43
1:B:230:ILE:CD1	1:E:188:LEU:CD1	2.96	0.43
1:E:70:ARG:CG	1:E:80:PHE:CZ	2.99	0.43
1:F:194:ASP:HB3	1:F:197:VAL:HG22	1.98	0.43
1:F:34:VAL:O	1:F:50:LYS:HE3	2.18	0.43
1:B:225:ASN:ND2	1:B:225:ASN:C	2.68	0.43
1:F:14:ILE:HG13	1:F:15:MET:O	2.18	0.43
1:A:250:CYS:HB2	1:A:276:TRP:CD1	2.54	0.43
1:B:118:ARG:HD3	1:B:276:TRP:O	2.18	0.43
1:B:158:ILE:HG22	1:B:159:ALA:N	2.33	0.43
1:B:219:ASP:OD2	1:B:232:ARG:CZ	2.67	0.43
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.89	0.43
1:E:310:GLN:O	1:E:314:GLU:CG	2.65	0.43
1:E:40:ASP:OD1	1:E:42:GLN:CB	2.60	0.43
1:C:143:LEU:HD23	1:C:143:LEU:N	2.34	0.43
1:C:36:ARG:HD2	1:C:38:MET:HE2	2.00	0.43
1:D:33:GLY:O	1:D:34:VAL:C	2.57	0.43
1:F:144:GLU:HB3	1:F:182:TYR:CE1	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ALA:O	1:A:188:LEU:HD11	2.18	0.43
1:A:43:ALA:O	1:A:44:ASN:C	2.57	0.43
1:A:80:PHE:CD1	1:A:80:PHE:C	2.92	0.43
1:B:204:GLY:HA3	1:B:257:ILE:HG21	2.00	0.43
1:C:227:ARG:CZ	1:C:231:HIS:NE2	2.82	0.43
1:C:52:ILE:HD13	1:C:62:VAL:HG21	2.00	0.43
1:D:88:THR:C	1:D:89:HIS:CD2	2.92	0.43
1:F:186:GLU:OE2	1:F:265:ARG:NH1	2.52	0.43
1:F:52:ILE:O	1:F:89:HIS:HB3	2.18	0.43
1:A:141:LEU:O	1:A:142:LYS:HG2	2.19	0.43
1:A:17:ASP:C	1:A:19:ASP:H	2.22	0.43
1:A:261:ASP:HA	1:A:262:PRO:HD3	1.80	0.43
1:D:74:HIS:CE1	1:D:76:ASN:HD22	2.37	0.43
1:E:72:LEU:HD23	1:E:134:MET:HG2	2.01	0.43
1:E:189:LEU:O	1:E:190:LYS:HB2	2.19	0.43
1:E:36:ARG:HD2	1:E:38:MET:CE	2.49	0.43
1:F:150:GLY:O	1:F:151:SER:CB	2.66	0.43
1:A:78:VAL:HB	1:A:161:PHE:HE1	1.84	0.43
1:B:139:ARG:HH11	1:B:160:ASP:CG	2.22	0.43
1:C:55:GLY:C	1:C:57:LYS:H	2.22	0.43
1:A:17:ASP:C	1:A:19:ASP:N	2.72	0.42
1:C:134:MET:O	1:C:135:GLN:HG2	2.19	0.42
1:C:208:TYR:CE2	1:C:216:PRO:HA	2.54	0.42
1:C:226:PHE:O	1:C:230:ILE:HB	2.18	0.42
1:E:191:LYS:HZ2	1:E:191:LYS:HB2	1.84	0.42
1:E:232:ARG:CG	1:E:237:GLN:O	2.67	0.42
1:D:223:PRO:C	1:D:225:ASN:N	2.71	0.42
1:C:183:ILE:HG22	1:C:188:LEU:HD13	1.98	0.42
1:D:144:GLU:CB	1:D:182:TYR:CD1	2.90	0.42
1:D:303:GLN:O	1:D:308:ILE:CD1	2.64	0.42
1:E:232:ARG:HH11	1:E:237:GLN:NE2	2.10	0.42
1:A:62:VAL:O	1:A:66:ILE:HG13	2.20	0.42
1:A:63:LYS:CD	1:A:309:MET:HE3	2.43	0.42
1:A:69:HIS:O	1:A:69:HIS:CD2	2.72	0.42
1:B:20:ARG:O	1:B:41:LYS:HG2	2.16	0.42
1:C:153:ALA:O	1:C:154:PRO:O	2.37	0.42
1:C:98:SER:O	1:D:108:ASN:HB3	2.20	0.42
1:E:185:PRO:O	1:E:189:LEU:HD21	2.19	0.42
1:E:311:ILE:O	1:E:313:ALA:N	2.52	0.42
1:F:208:TYR:CD2	1:F:216:PRO:HG3	2.54	0.42
1:F:43:ALA:O	1:F:44:ASN:C	2.57	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ILE:HD11	1:B:309:MET:HE2	2.01	0.42
1:D:43:ALA:O	1:D:44:ASN:C	2.57	0.42
1:E:16:HIS:C	1:E:17:ASP:OD2	2.56	0.42
1:E:80:PHE:O	1:E:80:PHE:CG	2.71	0.42
1:A:180:PRO:HG3	1:A:226:PHE:CE2	2.54	0.42
1:A:99:GLY:HA3	1:A:149:ASP:O	2.19	0.42
1:B:141:LEU:N	1:B:141:LEU:HD13	2.35	0.42
1:B:281:LEU:O	1:B:282:PRO:C	2.57	0.42
1:C:58:ILE:HD12	1:C:315:ALA:CB	2.50	0.42
1:D:124:LEU:HD11	1:D:143:LEU:HD11	2.02	0.42
1:B:146:THR:HG21	1:B:156:LEU:CG	2.45	0.42
1:F:222:GLU:HA	1:F:223:PRO:HD2	1.86	0.42
1:B:186:GLU:OE1	1:B:186:GLU:N	2.49	0.42
1:B:261:ASP:HA	1:B:262:PRO:HD3	1.83	0.42
1:E:249:GLU:CD	1:E:249:GLU:H	2.23	0.42
1:E:70:ARG:NH2	1:E:303:GLN:O	2.53	0.42
1:A:141:LEU:C	1:A:142:LYS:CG	2.88	0.42
1:B:106:ILE:HA	1:B:112:PHE:CE1	2.55	0.42
1:B:160:ASP:O	1:B:161:PHE:HB3	2.19	0.42
1:E:183:ILE:HG22	1:E:188:LEU:CD2	2.37	0.42
1:F:54:ARG:HH11	1:F:315:ALA:HA	1.85	0.42
1:A:101:GLU:CD	1:A:145:ASN:ND2	2.66	0.42
1:B:152:PRO:O	1:B:154:PRO:N	2.51	0.42
1:F:21:TYR:CD1	1:F:40:ASP:HA	2.55	0.42
1:A:152:PRO:HG2	1:A:153:ALA:H	1.84	0.41
1:E:281:LEU:HD23	1:E:281:LEU:HA	1.75	0.41
1:F:63:LYS:HD2	1:F:309:MET:HE3	2.00	0.41
1:A:12:LEU:CB	1:A:13:PRO:HD2	2.49	0.41
1:A:141:LEU:HB2	1:A:143:LEU:CD2	2.51	0.41
1:A:219:ASP:OD1	1:A:219:ASP:C	2.57	0.41
1:D:313:ALA:O	1:D:316:THR:OG1	2.30	0.41
1:D:76:ASN:OD1	1:D:123:GLN:HB3	2.20	0.41
1:E:311:ILE:C	1:E:313:ALA:N	2.72	0.41
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.79	0.41
1:B:218:GLU:O	1:B:223:PRO:CA	2.67	0.41
1:B:70:ARG:CD	1:B:70:ARG:C	2.89	0.41
1:E:135:GLN:HE21	1:E:135:GLN:CA	2.16	0.41
1:F:268:ILE:HB	1:F:269:PRO:HD3	2.01	0.41
1:B:54:ARG:HB2	1:B:88:THR:O	2.21	0.41
1:C:156:LEU:HA	1:C:156:LEU:HD23	1.84	0.41
1:C:249:GLU:CD	1:C:249:GLU:H	2.24	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ARG:O	1:D:55:GLY:O	2.38	0.41
1:A:215:TYR:HA	1:A:216:PRO:HD3	1.74	0.41
1:A:59:ASP:OD2	1:A:59:ASP:C	2.59	0.41
1:A:70:ARG:O	1:A:70:ARG:HD2	2.20	0.41
1:F:224:LYS:O	1:F:226:PHE:N	2.53	0.41
1:F:59:ASP:OD1	1:F:61:ASN:HB2	2.20	0.41
1:B:16:HIS:O	1:B:17:ASP:HB2	2.19	0.41
1:C:21:TYR:CD1	1:C:40:ASP:HB2	2.51	0.41
1:D:161:PHE:N	1:D:161:PHE:CD1	2.89	0.41
1:E:312:ILE:O	1:E:316:THR:OG1	2.30	0.41
1:F:39:ARG:HD2	1:F:44:ASN:OD1	2.20	0.41
1:A:112:PHE:HB3	1:A:116:GLU:HB3	2.02	0.41
1:B:141:LEU:N	1:B:141:LEU:CD1	2.84	0.41
1:C:282:PRO:HD2	1:C:285:LEU:HD12	2.02	0.41
1:C:34:VAL:O	1:C:34:VAL:HG12	2.21	0.41
1:E:191:LYS:HG2	1:E:191:LYS:O	2.21	0.41
1:F:23:LEU:HD12	1:F:24:VAL:N	2.36	0.41
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.89	0.41
1:B:146:THR:CG2	1:B:156:LEU:HD12	2.30	0.41
1:B:186:GLU:HG2	1:B:262:PRO:CG	2.43	0.41
1:C:179:THR:OG1	1:C:180:PRO:HD2	2.20	0.41
1:C:247:SER:HB2	1:C:249:GLU:OE1	2.21	0.41
1:E:81:LYS:O	1:E:82:GLU:HB3	2.21	0.41
1:A:304:SER:HB2	1:A:306:GLU:HG2	2.03	0.41
1:A:81:LYS:HD2	1:A:81:LYS:HA	1.35	0.41
1:B:183:ILE:N	1:B:183:ILE:HD12	2.34	0.41
1:B:55:GLY:C	1:B:57:LYS:H	2.22	0.41
1:B:219:ASP:HA	1:B:220:PRO:HA	1.66	0.41
1:C:69:HIS:NE2	1:C:78:VAL:O	2.28	0.41
1:D:85:LEU:HB3	1:D:311:ILE:HG23	2.03	0.41
1:A:106:ILE:HD13	1:A:209:VAL:HG12	2.03	0.40
1:C:191:LYS:C	1:C:191:LYS:HD2	2.15	0.40
1:D:146:THR:HB	1:D:156:LEU:HD21	2.03	0.40
1:D:61:ASN:OD1	1:D:64:ARG:NH2	2.54	0.40
1:E:156:LEU:HA	1:E:156:LEU:HD23	1.80	0.40
1:A:152:PRO:O	1:A:154:PRO:HD3	2.21	0.40
1:A:55:GLY:C	1:A:57:LYS:H	2.25	0.40
1:C:279:LYS:O	1:C:280:ASN:HB2	2.21	0.40
1:D:54:ARG:HB2	1:D:88:THR:O	2.22	0.40
1:E:311:ILE:O	1:E:312:ILE:C	2.59	0.40
1:F:59:ASP:OD2	1:F:59:ASP:N	2.46	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:HD13	1:D:143:LEU:CD2	2.49	0.40
1:D:14:ILE:CG2	1:D:15:MET:N	2.83	0.40
1:E:246:ILE:HG23	1:E:250:CYS:HB3	2.03	0.40
1:A:197:VAL:HG12	1:A:265:ARG:NH1	2.36	0.40
1:B:14:ILE:O	1:B:15:MET:C	2.60	0.40
1:C:282:PRO:C	1:C:284:ASP:H	2.24	0.40
1:E:77:ILE:HG23	1:E:78:VAL:N	2.37	0.40
1:F:70:ARG:HA	1:F:80:PHE:HB3	2.03	0.40
1:A:63:LYS:HE2	1:A:63:LYS:HB3	1.30	0.40
1:B:183:ILE:HG21	1:B:188:LEU:HD13	2.03	0.40
1:E:193:TYR:C	1:E:193:TYR:CD1	2.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ARG:NH2	3:B:324:HOH:O[2_556]	2.16	0.04

## 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	269/317 (85%)	232 (86%)	24 (9%)	13 (5%)	2	1
1	B	273/317 (86%)	229 (84%)	31 (11%)	13 (5%)	2	1
1	C	249/317 (78%)	220 (88%)	22 (9%)	7 (3%)	5	5
1	D	273/317 (86%)	233 (85%)	28 (10%)	12 (4%)	3	2
1	E	243/317 (77%)	203 (84%)	26 (11%)	14 (6%)	2	0
1	F	267/317 (84%)	229 (86%)	29 (11%)	9 (3%)	4	3
All	All	1574/1902 (83%)	1346 (86%)	160 (10%)	68 (4%)	3	2

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	A	221	GLU
1	B	13	PRO
1	B	42	GLN
1	B	152	PRO
1	B	153	ALA
1	B	220	PRO
1	C	13	PRO
1	C	15	MET
1	C	225	ASN
1	D	87	PRO
1	D	143	LEU
1	D	304	SER
1	E	194	ASP
1	E	229	THR
1	E	305	ILE
1	E	310	GLN
1	F	137	ALA
1	F	152	PRO
1	A	55	GLY
1	A	162	GLY
1	A	224	LYS
1	B	100	GLY
1	B	224	LYS
1	D	34	VAL
1	D	55	GLY
1	D	144	GLU
1	D	298	SER
1	E	190	LYS
1	E	223	PRO
1	E	308	ILE
1	E	314	GLU
1	F	225	ASN
1	A	220	PRO
1	B	44	ASN
1	B	87	PRO
1	C	87	PRO
1	C	149	ASP
1	C	154	PRO
1	D	54	ARG
1	E	225	ASN
1	E	306	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	13	PRO
1	F	154	PRO
1	A	44	ASN
1	A	139	ARG
1	A	152	PRO
1	A	154	PRO
1	B	54	ARG
1	B	283	ALA
1	D	301	PRO
1	E	14	ILE
1	E	230	ILE
1	A	82	GLU
1	B	219	ASP
1	C	44	ASN
1	D	44	ASN
1	F	44	ASN
1	F	142	LYS
1	F	151	SER
1	A	153	ALA
1	D	28	GLY
1	E	55	GLY
1	B	33	GLY
1	F	87	PRO
1	D	78	VAL
1	E	312	ILE
1	A	78	VAL

### 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	237/274 (86%)	190 (80%)	47 (20%)	1	1
1	B	240/274 (88%)	193 (80%)	47 (20%)	1	1
1	C	229/274 (84%)	191 (83%)	38 (17%)	2	2
1	D	238/274 (87%)	192 (81%)	46 (19%)	1	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	216/274 (79%)	166 (77%)	50 (23%)	1	0
1	F	236/274 (86%)	187 (79%)	49 (21%)	1	1
All	All	1396/1644 (85%)	1119 (80%)	277 (20%)	1	1

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	18	SER
1	A	25	LYS
1	A	27	ILE
1	A	31	ASN
1	A	34	VAL
1	A	36	ARG
1	A	37	LEU
1	A	40	ASP
1	A	47	VAL
1	A	50	LYS
1	A	54	ARG
1	A	56	GLU
1	A	63	LYS
1	A	70	ARG
1	A	77	ILE
1	A	79	ARG
1	A	81	LYS
1	A	82	GLU
1	A	83	VAL
1	A	89	HIS
1	A	98	SER
1	A	115	ASP
1	A	134	MET
1	A	135	GLN
1	A	142	LYS
1	A	143	LEU
1	A	144	GLU
1	A	145	ASN
1	A	155	ARG
1	A	163	TYR
1	A	186	GLU
1	A	188	LEU
1	A	189	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	191	LYS
1	A	222	GLU
1	A	226	PHE
1	A	227	ARG
1	A	246	ILE
1	A	279	LYS
1	A	284	ASP
1	A	303	GLN
1	A	304	SER
1	A	305	ILE
1	A	306	GLU
1	A	312	ILE
1	A	317	VAL
1	B	14	ILE
1	B	16	HIS
1	B	19	ASP
1	B	27	ILE
1	B	34	VAL
1	B	37	LEU
1	B	40	ASP
1	B	41	LYS
1	B	54	ARG
1	B	57	LYS
1	B	58	ILE
1	B	59	ASP
1	B	67	ILE
1	B	77	ILE
1	B	79	ARG
1	B	83	VAL
1	B	85	LEU
1	B	86	THR
1	B	89	HIS
1	B	111	ARG
1	B	134	MET
1	B	141	LEU
1	B	143	LEU
1	B	144	GLU
1	B	148	LEU
1	B	155[A]	ARG
1	B	155[B]	ARG
1	B	179	THR
1	B	183	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	188	LEU
1	B	190	LYS
1	B	191	LYS
1	B	196	LYS
1	B	206	THR
1	B	219	ASP
1	B	224	LYS
1	B	225	ASN
1	B	227	ARG
1	B	228	LYS
1	B	229	THR
1	B	237	GLN
1	B	243	TYR
1	B	272	ARG
1	B	279	LYS
1	B	284	ASP
1	B	285	LEU
1	B	303	GLN
1	C	12	LEU
1	C	14	ILE
1	C	15	MET
1	C	18	SER
1	C	20	ARG
1	C	25	LYS
1	C	27	ILE
1	C	37	LEU
1	C	40	ASP
1	C	58	ILE
1	C	60	GLU
1	C	77	ILE
1	C	83	VAL
1	C	85	LEU
1	C	89	HIS
1	C	118	ARG
1	C	140	ASP
1	C	141	LEU
1	C	142	LYS
1	C	155	ARG
1	C	156	LEU
1	C	160	ASP
1	C	179	THR
1	C	188	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	191	LYS
1	C	202	SER
1	C	206	THR
1	C	219	ASP
1	C	225	ASN
1	C	227	ARG
1	C	228	LYS
1	C	234	LEU
1	C	240	ILE
1	C	251	ARG
1	C	279	LYS
1	C	284	ASP
1	C	286	MET
1	C	310	GLN
1	D	14	ILE
1	D	17	ASP
1	D	18	SER
1	D	22	GLU
1	D	27	ILE
1	D	31	ASN
1	D	37	LEU
1	D	39	ARG
1	D	40	ASP
1	D	45	GLU
1	D	47	VAL
1	D	53	GLU
1	D	54	ARG
1	D	58	ILE
1	D	60	GLU
1	D	73	ARG
1	D	81	LYS
1	D	82	GLU
1	D	83	VAL
1	D	85	LEU
1	D	86	THR
1	D	89	HIS
1	D	104	GLU
1	D	111	ARG
1	D	143	LEU
1	D	151	SER
1	D	155	ARG
1	D	161	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	163	TYR
1	D	186	GLU
1	D	188	LEU
1	D	190	LYS
1	D	194	ASP
1	D	206	THR
1	D	221	GLU
1	D	222	GLU
1	D	227	ARG
1	D	230	ILE
1	D	232	ARG
1	D	235	ASN
1	D	237	GLN
1	D	242	ASP
1	D	246	ILE
1	D	309	MET
1	D	310	GLN
1	D	314	GLU
1	E	14	ILE
1	E	17	ASP
1	E	25	LYS
1	E	27	ILE
1	E	34	VAL
1	E	37	LEU
1	E	40	ASP
1	E	41	LYS
1	E	42	GLN
1	E	53	GLU
1	E	58	ILE
1	E	60	GLU
1	E	62	VAL
1	E	63	LYS
1	E	64	ARG
1	E	65	GLU
1	E	77	ILE
1	E	79	ARG
1	E	80	PHE
1	E	82	GLU
1	E	83	VAL
1	E	85	LEU
1	E	88	THR
1	E	89	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	116	GLU
1	E	143	LEU
1	E	144	GLU
1	E	146	THR
1	E	149	ASP
1	E	151	SER
1	E	155	ARG
1	E	156	LEU
1	E	186	GLU
1	E	188	LEU
1	E	189	LEU
1	E	190	LYS
1	E	191	LYS
1	E	206	THR
1	E	224	LYS
1	E	226	PHE
1	E	228	LYS
1	E	230	ILE
1	E	232	ARG
1	E	234	LEU
1	E	240	ILE
1	E	242	ASP
1	E	279	LYS
1	E	281	LEU
1	E	284	ASP
1	E	316	THR
1	F	14	ILE
1	F	17	ASP
1	F	19	ASP
1	F	20	ARG
1	F	22	GLU
1	F	27	ILE
1	F	34	VAL
1	F	37	LEU
1	F	40	ASP
1	F	52	ILE
1	F	54	ARG
1	F	57	LYS
1	F	60	GLU
1	F	64	ARG
1	F	69	HIS
1	F	73	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	77	ILE
1	F	81	LYS
1	F	82	GLU
1	F	83	VAL
1	F	85	LEU
1	F	89	HIS
1	F	111	ARG
1	F	139	ARG
1	F	141	LEU
1	F	142	LYS
1	F	144	GLU
1	F	151	SER
1	F	155	ARG
1	F	156	LEU
1	F	163	TYR
1	F	179	THR
1	F	188	LEU
1	F	190	LYS
1	F	191	LYS
1	F	206	THR
1	F	219	ASP
1	F	221	GLU
1	F	222	GLU
1	F	225	ASN
1	F	229	THR
1	F	242	ASP
1	F	246	ILE
1	F	261	ASP
1	F	279	LYS
1	F	303	GLN
1	F	310	GLN
1	F	314	GLU
1	F	316	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	89	HIS
1	A	138	HIS
1	A	145	ASN
1	A	237	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	303	GLN
1	B	89	HIS
1	B	225	ASN
1	B	231	HIS
1	B	237	GLN
1	B	303	GLN
1	C	16	HIS
1	C	303	GLN
1	D	16	HIS
1	D	31	ASN
1	D	76	ASN
1	D	89	HIS
1	D	231	HIS
1	D	235	ASN
1	D	303	GLN
1	E	89	HIS
1	E	135	GLN
1	E	237	GLN
1	E	303	GLN
1	F	16	HIS
1	F	69	HIS
1	F	76	ASN
1	F	225	ASN
1	F	273	ASN
1	F	303	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - 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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/317 (86%)	0.19	10 (3%) 42 52	30, 53, 102, 178	0
1	B	278/317 (87%)	0.01	6 (2%) 62 70	32, 53, 103, 134	0
1	C	261/317 (82%)	0.03	5 (1%) 66 75	26, 50, 100, 121	0
1	D	279/317 (88%)	0.23	12 (4%) 35 44	31, 58, 105, 158	0
1	E	255/317 (80%)	0.37	25 (9%) 7 11	32, 63, 118, 161	0
1	F	273/317 (86%)	0.24	15 (5%) 25 32	31, 55, 106, 128	0
All	All	1621/1902 (85%)	0.18	73 (4%) 33 43	26, 55, 106, 178	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	GLU	8.4
1	E	87	PRO	5.2
1	D	299	ASP	4.5
1	E	56	GLU	4.4
1	E	302	GLY	4.3
1	F	317	VAL	4.3
1	A	189	LEU	4.2
1	A	162	GLY	4.1
1	D	31	ASN	3.9
1	A	12	LEU	3.8
1	F	62	VAL	3.7
1	F	163	TYR	3.6
1	E	62	VAL	3.6
1	D	300	GLN	3.6
1	F	60	GLU	3.4
1	F	52	ILE	3.3
1	B	224	LYS	3.3
1	E	53	GLU	3.3
1	C	34	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	222	GLU	3.2
1	A	88	THR	3.1
1	E	52	ILE	3.0
1	E	67	ILE	2.9
1	C	28	GLY	2.9
1	D	29	ALA	2.8
1	F	56	GLU	2.8
1	E	152	PRO	2.8
1	E	143	LEU	2.8
1	C	56	GLU	2.8
1	F	34	VAL	2.8
1	F	31	ASN	2.7
1	E	304	SER	2.7
1	B	18	SER	2.7
1	A	192	GLU	2.7
1	F	131	ALA	2.7
1	F	29	ALA	2.6
1	D	317	VAL	2.6
1	A	161	PHE	2.6
1	E	34	VAL	2.5
1	F	224	LYS	2.5
1	E	63	LYS	2.5
1	C	52	ILE	2.5
1	E	311	ILE	2.4
1	E	28	GLY	2.4
1	D	73	ARG	2.4
1	E	303	GLN	2.4
1	E	13	PRO	2.4
1	E	305	ILE	2.4
1	A	152	PRO	2.4
1	E	60	GLU	2.4
1	D	277	PHE	2.4
1	F	57	LYS	2.3
1	C	160	ASP	2.3
1	D	161	PHE	2.3
1	B	84	ILE	2.3
1	E	27	ILE	2.3
1	F	28	GLY	2.3
1	A	34	VAL	2.3
1	E	42	GLN	2.3
1	E	51	TYR	2.3
1	E	73	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	219	ASP	2.2
1	E	179	THR	2.2
1	B	226	PHE	2.2
1	D	271	ILE	2.1
1	D	43	ALA	2.1
1	E	131	ALA	2.1
1	D	42	GLN	2.1
1	B	283	ALA	2.1
1	D	32	PHE	2.1
1	F	281	LEU	2.1
1	F	221	GLU	2.0
1	E	259	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	B	318	1/1	0.81	0.13	87,87,87,87	0
2	CL	D	318	1/1	0.90	0.18	91,91,91,91	0
2	CL	F	318	1/1	0.90	0.29	88,88,88,88	0
2	CL	E	318	1/1	0.91	0.12	86,86,86,86	0
2	CL	C	318	1/1	0.93	0.25	86,86,86,86	0
2	CL	A	318	1/1	0.95	0.09	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.