



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:36 PM GMT

PDB ID : 5D98  
Title : Influenza C Virus RNA-dependent RNA Polymerase - Space group P43212  
Authors : Hengrung, N.; El Omari, K.; Serna Martin, I.; Vreede, F.T.; Cusack, S.; Rambo, R.P.; Vornrhein, C.; Bricogne, G.; Stuart, D.I.; Grimes, J.M.; Fodor, E.  
Deposited on : 2015-08-18  
Resolution : 3.90 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  
<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

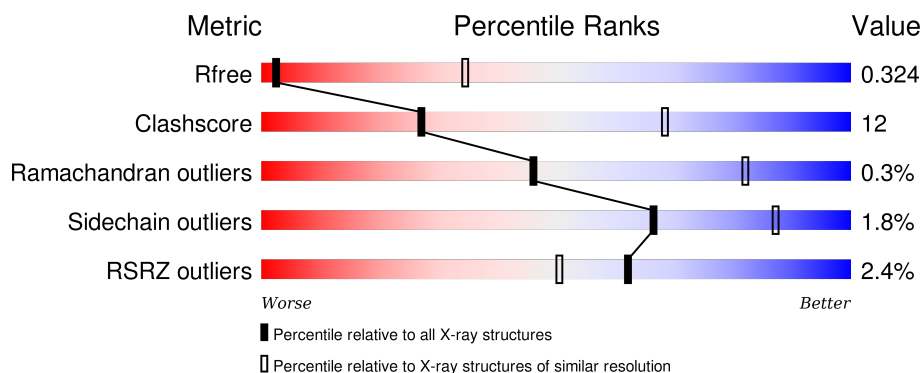
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	709	<div> <div>2%</div> <div>67%</div> <div>30%</div> <div>..</div> </div>
1	D	709	<div> <div>%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
2	B	754	<div> <div>2%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>
2	E	754	<div> <div>3%</div> <div>73%</div> <div>20%</div> <div>6%</div> </div>
3	C	782	<div> <div>3%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	782	<div><div></div><div>3%</div><div>67%</div><div>29%</div><div>..</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34720 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	D	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	E	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	F	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	775	ALA	-	expression tag	UNP Q9IMP3
C	776	ARG	-	expression tag	UNP Q9IMP3
C	777	GLU	-	expression tag	UNP Q9IMP3
C	778	ASN	-	expression tag	UNP Q9IMP3
C	779	LEU	-	expression tag	UNP Q9IMP3
C	780	TYR	-	expression tag	UNP Q9IMP3
C	781	PHE	-	expression tag	UNP Q9IMP3
C	782	GLN	-	expression tag	UNP Q9IMP3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	775	ALA	-	expression tag	UNP Q9IMP3
F	776	ARG	-	expression tag	UNP Q9IMP3
F	777	GLU	-	expression tag	UNP Q9IMP3
F	778	ASN	-	expression tag	UNP Q9IMP3
F	779	LEU	-	expression tag	UNP Q9IMP3
F	780	TYR	-	expression tag	UNP Q9IMP3
F	781	PHE	-	expression tag	UNP Q9IMP3
F	782	GLN	-	expression tag	UNP Q9IMP3

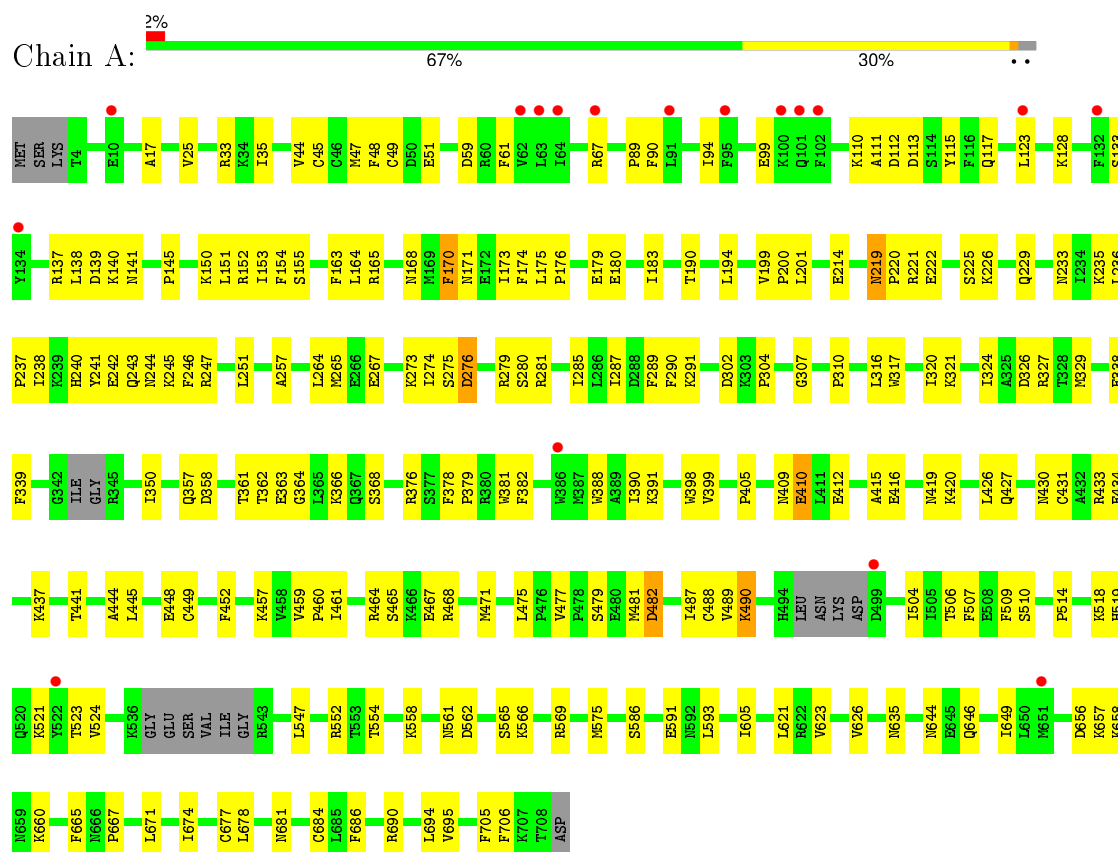
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

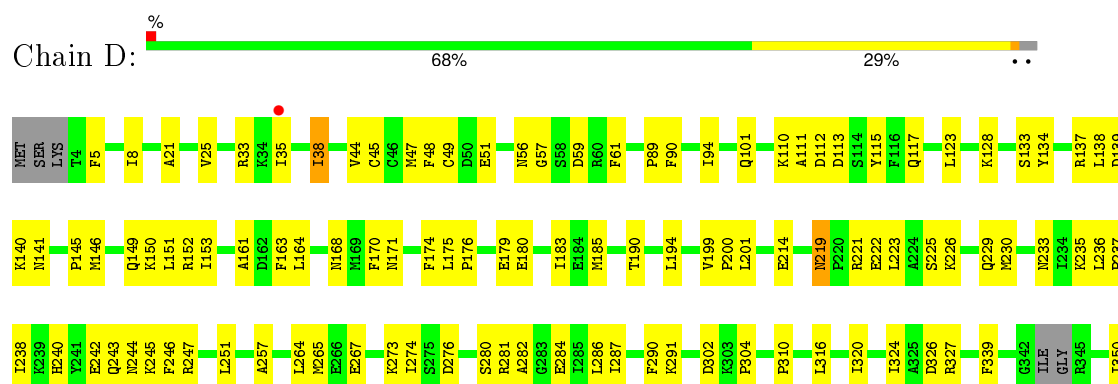
### 3 Residue-property plots

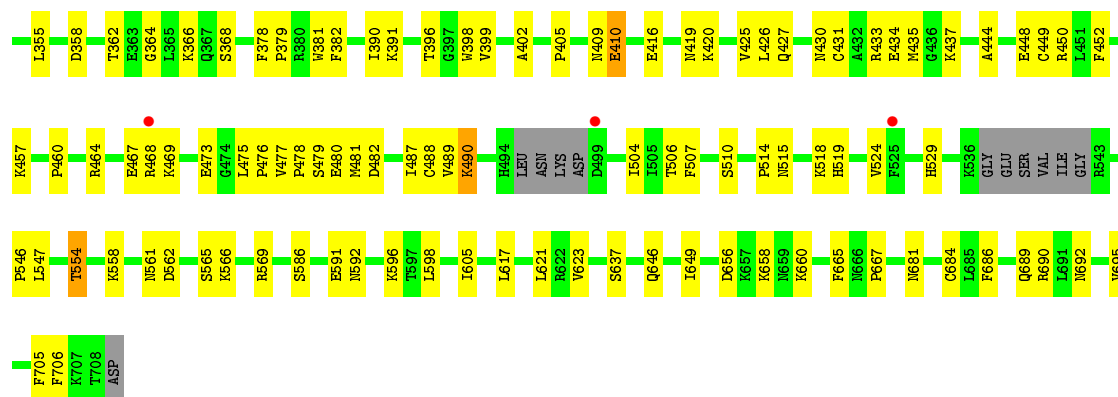
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Polymerase acidic protein



#### • Molecule 1: Polymerase acidic protein



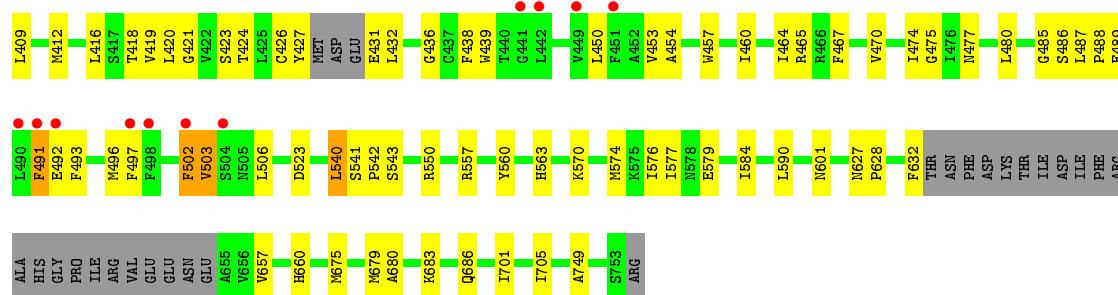


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

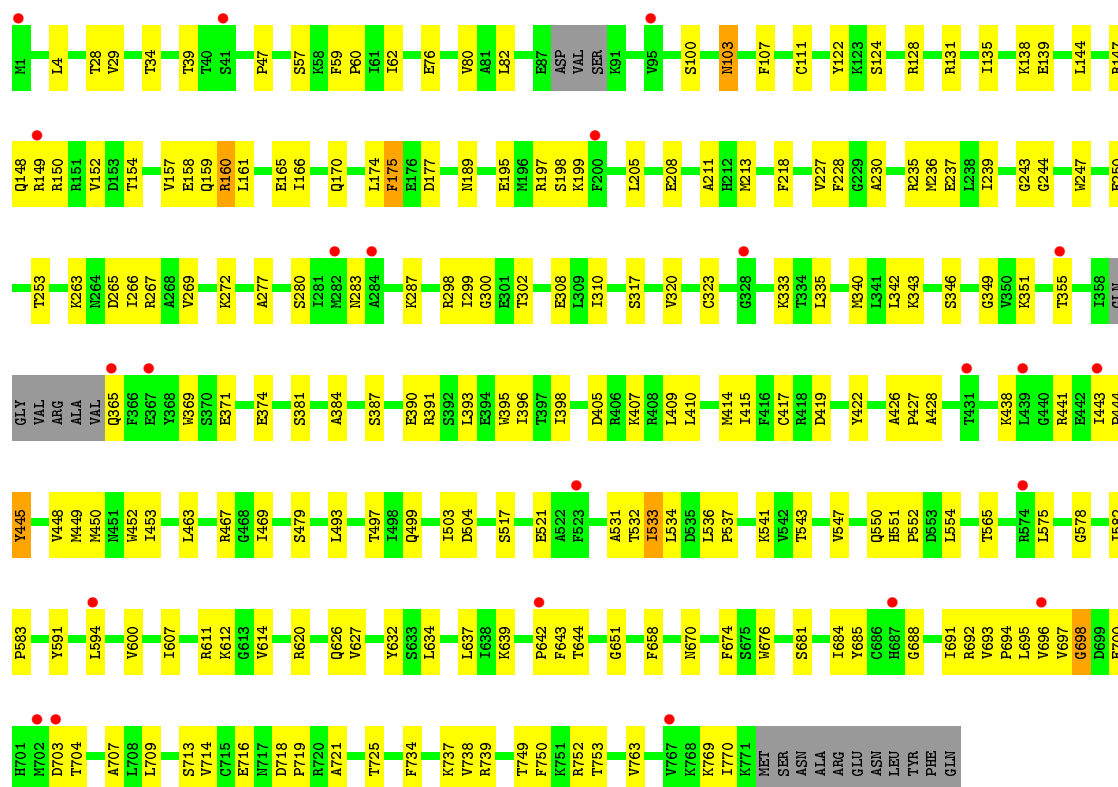


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

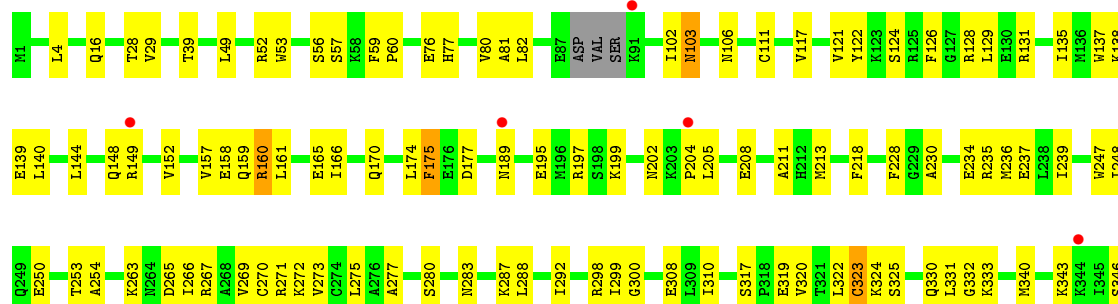




• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.66Å 185.66Å 598.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.90 100.57 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-3.90) 98.8 (100.57-3.90)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.286 , 0.326 0.286 , 0.324	Depositor DCC
$R_{free}$ test set	4770 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	161.2	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 132.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 95152 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	34720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.41	0/5746	0.57	1/7717 (0.0%)
1	D	0.43	0/5746	0.57	1/7717 (0.0%)
2	B	0.40	0/5749	0.56	0/7723
2	E	0.41	0/5749	0.57	0/7723
3	C	0.41	0/6185	0.59	0/8322
3	F	0.42	0/6185	0.59	0/8322
All	All	0.41	0/35360	0.58	2/47524 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASN	C-N-CD	5.11	139.14	128.40
1	D	219	ASN	C-N-CD	5.11	139.12	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5630	0	5632	147	0
1	D	5630	0	5632	167	0
2	B	5652	0	5749	127	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5652	0	5749	126	0
3	C	6076	0	6183	182	0
3	F	6076	0	6183	198	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
All	All	34720	0	35128	840	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (840) 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)
3:F:138:LYS:HE2	3:F:250:GLU:CG	1.22	1.59
3:F:138:LYS:CE	3:F:250:GLU:HG2	1.34	1.48
3:F:138:LYS:CE	3:F:250:GLU:CG	1.83	1.46
3:F:138:LYS:CE	3:F:250:GLU:CD	1.86	1.41
3:F:138:LYS:NZ	3:F:250:GLU:HG2	1.33	1.36
3:F:138:LYS:HE3	3:F:250:GLU:CD	1.42	1.33
3:C:718:ASP:CG	3:C:719:PRO:HD3	1.59	1.23
3:F:718:ASP:CG	3:F:719:PRO:HD3	1.60	1.21
1:D:396:THR:HG21	1:D:468:ARG:CD	1.70	1.20
2:E:18:ILE:HD12	2:E:497:PHE:CD1	1.76	1.20
1:D:396:THR:HG21	1:D:468:ARG:HD2	1.22	1.09
3:F:138:LYS:HE2	3:F:250:GLU:CB	1.83	1.09
2:B:724:MET:CG	3:C:725:THR:HG21	1.84	1.07
2:E:18:ILE:CD1	2:E:497:PHE:CD1	2.38	1.06
2:B:724:MET:HG2	3:C:725:THR:HG21	1.37	1.02
2:E:487:LEU:HG	2:E:488:PRO:HD2	1.43	0.98
3:F:138:LYS:HE2	3:F:250:GLU:CD	1.67	0.97
3:C:583:PRO:HG3	3:C:695:LEU:HD12	1.47	0.96
3:F:138:LYS:NZ	3:F:250:GLU:CG	2.15	0.95
1:D:396:THR:CG2	1:D:468:ARG:HD2	1.97	0.94
2:B:487:LEU:HG	2:B:488:PRO:HD2	1.50	0.93
3:F:138:LYS:HB3	3:F:250:GLU:HB2	1.50	0.93
3:F:138:LYS:HZ3	3:F:250:GLU:HG2	1.17	0.92
1:D:469:LYS:HD3	1:D:475:LEU:HD13	1.51	0.91
3:C:583:PRO:CG	3:C:695:LEU:HD12	2.04	0.87
3:C:694:PRO:C	3:C:695:LEU:HD23	1.94	0.87
1:A:176:PRO:HA	1:A:180:GLU:HB3	1.58	0.85
3:C:583:PRO:HB3	3:C:695:LEU:CD1	2.07	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:694:PRO:O	3:C:695:LEU:HD23	1.78	0.83
3:F:230:ALA:HB1	3:F:235:ARG:HD2	1.61	0.83
2:B:724:MET:HG3	3:C:725:THR:HG21	1.60	0.83
2:B:686:GLN:NE2	3:C:39:THR:OG1	2.11	0.82
2:E:18:ILE:HD12	2:E:497:PHE:CE1	2.15	0.82
2:E:487:LEU:HG	2:E:488:PRO:CD	2.09	0.82
3:C:583:PRO:CB	3:C:695:LEU:HD12	2.10	0.81
3:F:138:LYS:HE3	3:F:250:GLU:OE2	1.79	0.81
1:A:368:SER:HB2	2:B:359:LEU:HD23	1.60	0.81
3:C:583:PRO:CB	3:C:695:LEU:CD1	2.58	0.81
1:D:44:VAL:HG13	1:D:153:ILE:HD11	1.63	0.80
1:D:176:PRO:HA	1:D:180:GLU:HB3	1.62	0.80
1:D:477:VAL:HG12	1:D:478:PRO:O	1.82	0.79
3:C:583:PRO:HB3	3:C:695:LEU:HD12	1.62	0.79
3:F:138:LYS:CE	3:F:250:GLU:OE2	2.30	0.79
3:F:718:ASP:OD2	3:F:719:PRO:HD3	1.82	0.78
1:D:304:PRO:HG3	1:D:310:PRO:HB3	1.65	0.78
3:C:692:ARG:HG3	3:C:694:PRO:HD2	1.64	0.78
1:A:44:VAL:HG13	1:A:153:ILE:HD11	1.63	0.78
2:E:627:ASN:ND2	3:F:111:CYS:SG	2.57	0.77
2:E:68:PHE:HE1	2:E:406:GLY:HA3	1.48	0.77
1:D:151:LEU:HD13	3:F:753:THR:HG23	1.67	0.77
2:B:68:PHE:HE1	2:B:406:GLY:HA3	1.50	0.77
3:C:583:PRO:HG3	3:C:695:LEU:CD1	2.15	0.77
2:B:363:ARG:HD3	3:F:139:GLU:OE2	1.85	0.77
1:A:464:ARG:HG2	1:A:482:ASP:HB3	1.67	0.76
3:F:721:ALA:HB1	3:F:738:VAL:HA	1.65	0.76
1:D:138:LEU:HD11	1:D:140:LYS:HE3	1.66	0.76
2:B:487:LEU:HG	2:B:488:PRO:CD	2.14	0.76
3:C:533:ILE:HG22	3:C:534:LEU:H	1.49	0.75
1:A:304:PRO:HG3	1:A:310:PRO:HB3	1.69	0.75
2:E:686:GLN:NE2	3:F:39:THR:OG1	2.19	0.75
1:A:138:LEU:HD11	1:A:140:LYS:HE3	1.68	0.75
1:D:171:ASN:ND2	2:E:167:GLU:OE2	2.20	0.75
2:B:363:ARG:CD	3:F:139:GLU:OE2	2.35	0.74
1:A:264:LEU:HD21	1:A:267:GLU:HB2	1.67	0.74
2:E:68:PHE:CE1	2:E:406:GLY:HA3	2.23	0.74
3:F:533:ILE:HG22	3:F:534:LEU:H	1.51	0.74
3:C:230:ALA:HB1	3:C:235:ARG:HD2	1.68	0.74
3:C:533:ILE:HG22	3:C:534:LEU:N	2.02	0.73
1:A:25:VAL:HG21	1:A:35:ILE:HG22	1.71	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LYS:HB2	1:D:475:LEU:HD12	1.71	0.73
1:A:200:PRO:HG3	2:B:318:GLU:HB3	1.69	0.73
2:E:487:LEU:CG	2:E:488:PRO:HD2	2.19	0.72
1:D:25:VAL:HG21	1:D:35:ILE:HG22	1.71	0.72
2:E:349:LYS:NZ	2:E:407:GLY:O	2.21	0.72
3:C:531:ALA:O	3:C:532:THR:HG22	1.89	0.72
3:F:531:ALA:O	3:F:532:THR:HG22	1.90	0.72
3:C:721:ALA:HB1	3:C:738:VAL:HA	1.72	0.72
3:F:533:ILE:HG22	3:F:534:LEU:N	2.04	0.71
3:F:57:SER:HB2	3:F:60:PRO:HG3	1.72	0.71
2:E:350:PHE:HB3	2:E:401:VAL:HG21	1.71	0.71
3:C:718:ASP:OD1	3:C:719:PRO:HD3	1.89	0.71
1:A:171:ASN:ND2	2:B:167:GLU:OE2	2.24	0.70
3:C:57:SER:HB2	3:C:60:PRO:HG3	1.73	0.70
1:D:477:VAL:HG13	1:D:478:PRO:HD2	1.73	0.70
1:D:476:PRO:O	1:D:477:VAL:HG23	1.91	0.70
2:B:496:MET:HA	2:B:503:VAL:HG21	1.73	0.70
2:B:68:PHE:CE1	2:B:406:GLY:HA3	2.25	0.70
1:D:21:ALA:HA	1:D:38:ILE:HD11	1.73	0.70
2:B:147:GLN:NE2	2:B:685:TYR:CE2	2.60	0.70
2:B:349:LYS:NZ	2:B:407:GLY:O	2.20	0.70
3:C:718:ASP:OD2	3:C:719:PRO:HD3	1.90	0.70
1:D:469:LYS:CD	1:D:475:LEU:HD13	2.21	0.69
1:D:240:HIS:NE2	1:D:656:ASP:OD2	2.26	0.69
2:B:576:ILE:HD11	3:C:100:SER:HB2	1.75	0.69
1:D:477:VAL:HG11	1:D:480:GLU:OE2	1.91	0.69
1:A:151:LEU:HD13	3:C:753:THR:HG23	1.73	0.69
3:F:718:ASP:CG	3:F:719:PRO:CD	2.52	0.69
2:B:350:PHE:HB3	2:B:401:VAL:HG21	1.73	0.69
2:E:131:THR:HG21	2:E:251:ARG:HD2	1.74	0.69
3:C:718:ASP:CG	3:C:719:PRO:CD	2.51	0.68
1:D:419:ASN:ND2	2:E:543:SER:OG	2.26	0.68
1:D:396:THR:HG21	1:D:468:ARG:CG	2.23	0.68
2:B:487:LEU:CG	2:B:488:PRO:HD2	2.22	0.68
2:E:421:GLY:O	2:E:424:THR:OG1	2.11	0.68
1:D:350:ILE:HB	2:E:368:VAL:HG22	1.75	0.67
1:A:399:VAL:HB	1:A:427:GLN:HE22	1.58	0.67
1:D:222:GLU:HA	1:D:225:SER:HB3	1.75	0.67
3:F:138:LYS:HE2	3:F:250:GLU:HB2	1.75	0.67
2:B:431:GLU:HG3	2:B:432:LEU:H	1.59	0.67
3:C:174:LEU:C	3:C:174:LEU:HD23	2.15	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:701:ILE:HD11	3:F:208:GLU:HA	1.75	0.67
2:E:431:GLU:HG3	2:E:432:LEU:H	1.59	0.67
2:B:90:LEU:HA	2:B:93:LEU:HD12	1.77	0.67
3:F:235:ARG:NH2	3:F:253:THR:OG1	2.28	0.67
3:F:174:LEU:C	3:F:174:LEU:HD23	2.15	0.67
2:B:147:GLN:NE2	2:B:685:TYR:CD2	2.63	0.66
1:D:243:GLN:HG2	1:D:667:PRO:HG2	1.77	0.66
3:C:415:ILE:HD11	3:C:453:ILE:HD13	1.77	0.66
1:D:242:GLU:N	1:D:242:GLU:OE1	2.29	0.66
1:D:264:LEU:HD21	1:D:267:GLU:HB2	1.78	0.66
2:B:147:GLN:HE21	2:B:685:TYR:HE2	1.42	0.66
3:F:138:LYS:HE3	3:F:250:GLU:OE1	1.92	0.66
1:A:240:HIS:NE2	1:A:656:ASP:OD2	2.28	0.65
1:D:200:PRO:HG3	2:E:318:GLU:HB3	1.78	0.65
2:E:14:VAL:O	2:E:18:ILE:HG23	1.96	0.65
3:F:415:ILE:HD11	3:F:453:ILE:HD13	1.77	0.65
1:D:449:CYS:SG	1:D:490:LYS:NZ	2.68	0.65
2:E:420:LEU:O	2:E:423:SER:OG	2.10	0.65
2:E:496:MET:HA	2:E:503:VAL:HG21	1.78	0.65
2:B:265:CYS:HB3	2:B:274:PRO:HG3	1.79	0.65
1:D:473:GLU:OE2	1:D:475:LEU:HD21	1.97	0.64
3:C:694:PRO:O	3:C:709:LEU:O	2.15	0.64
2:B:421:GLY:O	2:B:424:THR:OG1	2.15	0.64
2:E:409:LEU:HD11	2:E:412:MET:HG2	1.79	0.64
3:C:175:PHE:CE1	3:C:177:ASP:HB2	2.33	0.64
3:C:670:ASN:HB3	3:C:676:TRP:H	1.62	0.64
3:C:583:PRO:CG	3:C:695:LEU:CD1	2.74	0.64
1:D:514:PRO:HG3	1:D:524:VAL:HG11	1.79	0.64
2:B:724:MET:HG3	3:C:725:THR:CG2	2.28	0.64
3:F:393:LEU:N	3:F:417:CYS:SG	2.71	0.63
1:D:410:GLU:HG2	3:F:137:TRP:HB3	1.80	0.63
1:D:637:SER:HB2	2:E:238:LEU:HA	1.79	0.63
2:B:724:MET:CG	3:C:725:THR:CG2	2.70	0.63
3:C:583:PRO:CB	3:C:695:LEU:HD13	2.27	0.63
3:C:693:VAL:N	3:C:694:PRO:CD	2.62	0.63
3:F:533:ILE:CG2	3:F:534:LEU:H	2.08	0.63
1:D:399:VAL:HB	1:D:427:GLN:HE22	1.63	0.63
2:B:282:ALA:HB2	3:C:148:GLN:HG2	1.80	0.63
1:A:291:LYS:HD3	1:A:324:ILE:HG22	1.81	0.63
3:C:583:PRO:HB3	3:C:695:LEU:HD13	1.80	0.63
1:A:449:CYS:SG	1:A:490:LYS:NZ	2.72	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:282:ALA:HB3	3:F:149:ARG:HD3	1.80	0.63
3:C:533:ILE:CG2	3:C:534:LEU:H	2.07	0.63
1:D:286:LEU:HD21	1:D:482:ASP:OD2	1.99	0.63
3:F:283:ASN:O	3:F:287:LYS:NZ	2.30	0.63
2:B:627:ASN:ND2	3:C:111:CYS:SG	2.72	0.62
1:D:396:THR:HG21	1:D:468:ARG:NE	2.14	0.62
1:D:219:ASN:HB2	1:D:221:ARG:HH11	1.63	0.62
2:E:18:ILE:CD1	2:E:497:PHE:HD1	2.11	0.62
2:E:303:ASN:ND2	2:E:488:PRO:O	2.33	0.62
1:D:477:VAL:CG1	1:D:478:PRO:HD2	2.29	0.62
3:F:271:ARG:HG2	3:F:319:GLU:HG2	1.81	0.62
1:A:222:GLU:HA	1:A:225:SER:HB3	1.82	0.62
3:C:235:ARG:NH2	3:C:253:THR:OG1	2.32	0.62
3:F:438:LYS:HG3	3:F:441:ARG:HB2	1.80	0.62
1:A:514:PRO:HG3	1:A:524:VAL:HG11	1.82	0.62
3:C:695:LEU:CD1	3:C:734:PHE:HZ	2.11	0.62
1:D:690:ARG:HH12	2:E:2:GLU:HB3	1.63	0.61
1:D:175:LEU:HB3	1:D:176:PRO:HD2	1.83	0.61
2:B:281:LYS:HB3	2:B:502:PHE:HE2	1.63	0.61
2:B:131:THR:HG21	2:B:251:ARG:HD2	1.82	0.61
3:F:189:ASN:ND2	3:F:308:GLU:OE1	2.34	0.61
1:A:405:PRO:HG2	2:B:601:ASN:ND2	2.16	0.61
3:C:438:LYS:HG3	3:C:441:ARG:HB2	1.82	0.61
1:A:233:ASN:HA	2:B:78:LEU:HD12	1.82	0.61
1:A:175:LEU:HB3	1:A:176:PRO:HD2	1.82	0.61
3:F:280:SER:HB3	3:F:287:LYS:HE2	1.83	0.61
1:A:575:MET:HG2	2:B:544:THR:HA	1.81	0.61
1:D:223:LEU:HD22	2:E:432:LEU:HD23	1.83	0.60
1:D:200:PRO:HB3	2:E:69:CYS:HB2	1.83	0.60
3:C:697:VAL:O	3:C:698:GLY:C	2.37	0.60
2:B:357:ILE:O	2:B:370:ILE:HG22	2.01	0.60
1:D:291:LYS:HD3	1:D:324:ILE:HG22	1.82	0.60
2:B:438:PHE:HB2	2:B:453:VAL:HB	1.83	0.60
2:E:51:ARG:NH2	2:E:77:GLU:O	2.34	0.60
1:A:242:GLU:N	1:A:242:GLU:OE1	2.34	0.60
1:A:243:GLN:HG2	1:A:667:PRO:HG2	1.82	0.60
3:C:280:SER:HB3	3:C:287:LYS:HE2	1.83	0.60
1:A:174:PHE:HB2	1:A:179:GLU:HB2	1.83	0.60
3:C:189:ASN:ND2	3:C:308:GLU:OE1	2.35	0.60
1:D:476:PRO:O	1:D:477:VAL:CG2	2.50	0.60
3:C:607:ILE:HB	3:C:612:LYS:HE3	1.82	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:138:LYS:CB	3:F:250:GLU:HB2	2.28	0.59
3:C:695:LEU:HD11	3:C:734:PHE:HZ	1.66	0.59
3:F:53:TRP:O	3:F:56:SER:OG	2.15	0.59
3:C:138:LYS:HB3	3:C:250:GLU:HB2	1.85	0.59
3:F:166:ILE:HD12	3:F:218:PHE:HB2	1.84	0.59
3:C:175:PHE:HD1	3:C:177:ASP:H	1.51	0.59
1:D:469:LYS:HD3	1:D:475:LEU:CD1	2.27	0.59
3:F:716:GLU:O	3:F:749:THR:OG1	2.14	0.58
1:D:402:ALA:HB3	2:E:550:ARG:HG2	1.85	0.58
3:C:150:ARG:HB3	3:C:152:VAL:HG23	1.83	0.58
3:C:716:GLU:O	3:C:749:THR:OG1	2.14	0.58
3:F:575:LEU:HD13	3:F:582:ILE:HG13	1.85	0.58
3:F:355:THR:HG22	3:F:365:GLN:HA	1.85	0.58
2:E:496:MET:HG2	2:E:503:VAL:HG11	1.84	0.58
1:A:214:GLU:OE1	2:B:336:LYS:NZ	2.35	0.58
2:E:439:TRP:HB2	2:E:450:LEU:HD11	1.86	0.58
2:E:154:LYS:HG2	2:E:159:PRO:HA	1.85	0.58
2:B:363:ARG:HD2	3:F:139:GLU:OE2	2.03	0.58
1:D:245:LYS:HA	1:D:706:PHE:HB2	1.84	0.58
2:B:106:PHE:HB3	2:B:327:ILE:HG23	1.84	0.57
1:A:245:LYS:HA	1:A:706:PHE:HB2	1.86	0.57
3:C:283:ASN:O	3:C:287:LYS:NZ	2.31	0.57
1:A:558:LYS:HA	1:A:561:ASN:HD22	1.69	0.57
1:D:558:LYS:HA	1:D:561:ASN:HD22	1.69	0.57
3:C:634:LEU:CD2	3:C:696:VAL:HA	2.34	0.57
2:E:265:CYS:HB3	2:E:274:PRO:HG3	1.87	0.57
2:E:134:TRP:HZ3	2:E:183:PHE:CE1	2.22	0.57
3:C:393:LEU:HD22	3:C:396:ILE:HD11	1.86	0.57
3:F:265:ASP:O	3:F:269:VAL:HG23	2.04	0.57
1:A:47:MET:O	1:A:152:ARG:NH1	2.38	0.57
2:B:710:ILE:HG13	3:C:29:VAL:HA	1.86	0.57
1:A:467:GLU:HB3	1:A:479:SER:HB2	1.86	0.57
1:D:274:ILE:HA	1:D:481:MET:HB3	1.86	0.57
2:B:398:GLN:HG3	2:B:399:LYS:H	1.70	0.57
2:B:675:MET:O	2:B:679:MET:HG2	2.05	0.56
2:E:359:LEU:HB2	2:E:368:VAL:HB	1.87	0.56
3:C:393:LEU:N	3:C:417:CYS:SG	2.78	0.56
2:B:134:TRP:HZ3	2:B:183:PHE:CE1	2.24	0.56
2:E:237:LYS:HE2	2:E:241:ARG:HE	1.70	0.56
3:C:277:ALA:HA	3:C:287:LYS:HD3	1.88	0.56
2:E:398:GLN:HG3	2:E:399:LYS:H	1.71	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:357:ILE:O	2:E:370:ILE:HG22	2.04	0.56
2:E:52:THR:HG22	2:E:54:VAL:H	1.70	0.56
1:D:174:PHE:HB2	1:D:179:GLU:HB2	1.86	0.56
2:B:52:THR:HG22	2:B:54:VAL:H	1.69	0.56
3:F:174:LEU:O	3:F:174:LEU:HD23	2.06	0.56
2:B:51:ARG:NH2	2:B:77:GLU:O	2.39	0.56
3:F:387:SER:HG	3:F:395:TRP:HE3	1.54	0.56
1:D:426:LEU:HD21	1:D:621:LEU:HD22	1.88	0.56
1:D:281:ARG:HD3	2:E:570:LYS:HB3	1.87	0.56
3:F:552:PRO:HB2	3:F:554:LEU:HG	1.87	0.56
2:E:90:LEU:HA	2:E:93:LEU:HD12	1.87	0.56
3:F:634:LEU:HA	3:F:637:LEU:HD12	1.87	0.56
1:D:47:MET:O	1:D:152:ARG:NH1	2.39	0.56
2:B:154:LYS:HG2	2:B:159:PRO:HA	1.86	0.56
1:D:51:GLU:OE1	1:D:51:GLU:N	2.38	0.56
1:D:59:ASP:OD2	3:F:769:LYS:NZ	2.38	0.56
1:D:230:MET:SD	2:E:465:ARG:HB3	2.46	0.55
2:E:574:MET:HA	2:E:577:ILE:HD12	1.88	0.55
2:E:281:LYS:HB3	2:E:502:PHE:HE2	1.71	0.55
1:A:566:LYS:HE3	1:A:569:ARG:HH21	1.71	0.55
2:B:496:MET:HG2	2:B:503:VAL:HG11	1.88	0.55
2:E:53:SER:H	2:E:73:GLU:HG3	1.71	0.55
3:C:148:GLN:HB3	3:C:504:ASP:OD2	2.07	0.55
1:D:286:LEU:HD11	1:D:482:ASP:OD2	2.07	0.55
1:A:338:GLU:HG2	3:F:254:ALA:HB1	1.88	0.55
3:F:681:SER:HB3	3:F:691:ILE:HD11	1.89	0.55
1:A:690:ARG:HH12	2:B:2:GLU:HB3	1.72	0.55
3:C:697:VAL:O	3:C:698:GLY:O	2.25	0.55
3:C:355:THR:HG22	3:C:365:GLN:HA	1.89	0.55
3:C:174:LEU:O	3:C:174:LEU:HD23	2.06	0.55
1:A:281:ARG:HD3	2:B:570:LYS:HB3	1.89	0.55
1:D:112:ASP:HB2	1:D:139:ASP:HB2	1.88	0.55
3:F:175:PHE:HD1	3:F:177:ASP:H	1.55	0.54
3:C:310:ILE:HD13	3:C:323:CYS:HB3	1.89	0.54
3:F:643:PHE:CZ	3:F:658:PHE:HB3	2.42	0.54
2:B:439:TRP:HB2	2:B:450:LEU:HD11	1.89	0.54
3:F:670:ASN:HB3	3:F:676:TRP:H	1.71	0.54
1:A:238:ILE:HG21	1:A:665:PHE:HA	1.89	0.54
3:F:565:THR:HG22	3:F:685:TYR:HB3	1.88	0.54
1:A:287:ILE:HA	1:A:290:PHE:HB2	1.89	0.54
1:A:382:PHE:HB3	1:A:686:PHE:CE1	2.42	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ALA:HB3	2:B:409:LEU:HD13	1.90	0.54
1:D:477:VAL:HG12	1:D:478:PRO:N	2.23	0.54
3:F:591:TYR:CD2	3:F:627:VAL:HG21	2.42	0.54
3:F:267:ARG:O	3:F:271:ARG:HG3	2.07	0.54
1:A:33:ARG:HH11	1:A:183:ILE:HG21	1.73	0.54
1:A:694:LEU:HD22	2:B:6:TYR:HB3	1.89	0.54
1:D:49:CYS:HB2	1:D:61:PHE:HB2	1.90	0.54
2:B:314:CYS:SG	2:B:477:ASN:ND2	2.81	0.54
1:D:409:ASN:OD1	1:D:409:ASN:N	2.40	0.54
3:F:536:LEU:HD12	3:F:537:PRO:HD2	1.89	0.54
2:E:438:PHE:HB2	2:E:453:VAL:HB	1.89	0.53
3:C:272:LYS:HZ2	3:C:543:THR:HG23	1.72	0.53
3:F:317:SER:HB3	3:F:320:VAL:HG23	1.91	0.53
3:C:333:LYS:HE3	3:C:343:LYS:HD3	1.90	0.53
3:C:444:PRO:HG2	3:C:533:ILE:HD11	1.91	0.53
1:A:274:ILE:HA	1:A:481:MET:HB3	1.90	0.53
1:A:409:ASN:N	1:A:409:ASN:OD1	2.41	0.53
3:C:387:SER:HG	3:C:395:TRP:HE3	1.55	0.53
3:C:721:ALA:CB	3:C:738:VAL:HA	2.37	0.53
3:F:271:ARG:O	3:F:275:LEU:HG	2.09	0.53
2:E:294:ARG:HG3	3:F:395:TRP:CH2	2.43	0.53
3:C:536:LEU:HD12	3:C:537:PRO:HD2	1.91	0.53
3:C:575:LEU:HD13	3:C:582:ILE:HG13	1.91	0.53
1:D:382:PHE:HB3	1:D:686:PHE:CE1	2.42	0.53
1:D:33:ARG:HH11	1:D:183:ILE:HG21	1.73	0.53
3:C:565:THR:HG22	3:C:685:TYR:HB3	1.90	0.53
2:E:51:ARG:HH12	2:E:78:LEU:HA	1.74	0.53
1:A:390:ILE:HD11	1:A:623:VAL:HA	1.91	0.53
1:D:265:MET:HG2	1:D:434:GLU:HG2	1.91	0.53
3:F:517:SER:N	3:F:521:GLU:O	2.34	0.53
3:C:693:VAL:N	3:C:694:PRO:HD2	2.23	0.53
3:F:277:ALA:HA	3:F:287:LYS:HD3	1.91	0.53
2:E:382:MET:SD	2:E:386:TYR:HB3	2.49	0.53
2:E:314:CYS:SG	2:E:477:ASN:ND2	2.82	0.53
1:D:56:ASN:OD1	1:D:57:GLY:N	2.40	0.52
2:E:628:PRO:HG3	3:F:205:LEU:HD13	1.91	0.52
3:F:718:ASP:OD1	3:F:719:PRO:HD3	2.07	0.52
1:A:398:TRP:CE3	1:A:465:SER:HB2	2.44	0.52
2:B:147:GLN:NE2	2:B:685:TYR:HE2	2.04	0.52
3:F:607:ILE:HB	3:F:612:LYS:HE3	1.90	0.52
1:A:59:ASP:OD2	3:C:769:LYS:NZ	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:PHE:HE1	3:C:177:ASP:HB2	1.72	0.52
2:E:542:PRO:HD3	3:F:247:TRP:CZ2	2.44	0.52
2:B:237:LYS:HE2	2:B:241:ARG:HE	1.74	0.52
3:C:620:ARG:NH2	3:C:644:THR:O	2.42	0.52
1:D:287:ILE:HA	1:D:290:PHE:HB2	1.90	0.52
1:D:390:ILE:HD11	1:D:623:VAL:HA	1.92	0.52
3:F:626:GLN:O	3:F:632:TYR:HB3	2.10	0.52
1:D:201:LEU:HD21	2:E:87:ILE:HD11	1.92	0.52
2:B:382:MET:SD	2:B:386:TYR:HB3	2.50	0.52
3:C:453:ILE:HG12	3:C:463:LEU:HD22	1.91	0.52
1:D:110:LYS:HG2	1:D:111:ALA:H	1.74	0.52
1:A:426:LEU:HD21	1:A:621:LEU:HD22	1.92	0.52
3:F:124:SER:HB2	3:F:128:ARG:HH21	1.73	0.52
3:F:346:SER:HB2	3:F:374:GLU:H	1.76	0.52
3:F:138:LYS:HB3	3:F:250:GLU:OE2	2.10	0.51
3:C:346:SER:HB2	3:C:374:GLU:H	1.74	0.51
3:F:393:LEU:HD22	3:F:396:ILE:HD11	1.92	0.51
2:B:51:ARG:HH12	2:B:78:LEU:HA	1.74	0.51
3:C:551:HIS:ND1	3:C:551:HIS:O	2.43	0.51
3:F:230:ALA:CB	3:F:235:ARG:HD2	2.37	0.51
2:B:359:LEU:HB2	2:B:368:VAL:HB	1.92	0.51
2:B:361:ASN:C	2:B:363:ARG:H	2.14	0.51
3:F:175:PHE:CE1	3:F:177:ASP:HB2	2.44	0.51
2:E:244:ALA:HB3	2:E:409:LEU:HD13	1.91	0.51
2:E:79:VAL:HB	2:E:480:LEU:HD11	1.92	0.51
3:C:681:SER:HB3	3:C:691:ILE:HD11	1.92	0.51
3:F:718:ASP:CB	3:F:719:PRO:HD3	2.36	0.51
1:A:657:LYS:HE3	2:B:9:PHE:O	2.10	0.51
1:A:155:SER:HB3	3:C:713:SER:OG	2.11	0.51
1:A:398:TRP:CG	1:A:433:ARG:HA	2.45	0.51
2:B:574:MET:HA	2:B:577:ILE:HD12	1.93	0.51
1:A:112:ASP:HB2	1:A:139:ASP:HB2	1.93	0.51
2:B:18:ILE:HG12	2:B:497:PHE:CE1	2.46	0.51
1:A:379:PRO:HB3	1:A:381:TRP:NE1	2.26	0.51
1:A:358:ASP:O	1:A:362:THR:HA	2.11	0.51
2:E:675:MET:O	2:E:679:MET:HG2	2.11	0.51
1:D:690:ARG:NH2	2:E:2:GLU:OE1	2.40	0.51
2:B:701:ILE:HD11	3:C:208:GLU:HA	1.92	0.51
1:A:51:GLU:N	1:A:51:GLU:OE1	2.43	0.51
3:F:734:PHE:HA	3:F:752:ARG:HG3	1.94	0.50
3:C:349:GLY:HA3	3:C:371:GLU:HG2	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:547:VAL:HG13	3:F:688:GLY:HA2	1.92	0.50
1:A:49:CYS:HB2	1:A:61:PHE:HB2	1.93	0.50
1:D:185:MET:HE2	2:E:337:ASP:HB3	1.93	0.50
3:C:578:GLY:HA2	3:C:734:PHE:CD2	2.47	0.50
3:C:547:VAL:HG13	3:C:688:GLY:HA2	1.93	0.50
3:C:591:TYR:CD2	3:C:627:VAL:HG21	2.45	0.50
3:F:333:LYS:HE3	3:F:343:LYS:HD3	1.92	0.50
1:D:467:GLU:HB3	1:D:479:SER:HB2	1.92	0.50
2:B:282:ALA:HB3	3:C:149:ARG:HD3	1.92	0.50
2:E:370:ILE:HD11	2:E:374:LYS:HB2	1.93	0.50
1:A:695:VAL:HG13	1:A:705:PHE:CD1	2.45	0.50
1:D:45:CYS:HB3	1:D:94:ILE:HD11	1.94	0.50
2:B:487:LEU:CD2	2:B:488:PRO:HD2	2.41	0.50
3:C:531:ALA:O	3:C:532:THR:CG2	2.60	0.50
2:B:517:GLY:N	2:B:523:ASP:OD1	2.26	0.50
1:A:677:CYS:HA	2:B:238:LEU:HD22	1.94	0.50
2:E:389:LEU:O	2:E:393:LEU:HD23	2.12	0.50
1:A:235:LYS:HZ3	2:B:464:ILE:HG22	1.75	0.50
2:E:542:PRO:HD3	3:F:247:TRP:CE2	2.46	0.50
1:A:90:PHE:HB2	1:A:123:LEU:HD21	1.94	0.50
1:D:238:ILE:HG21	1:D:665:PHE:HA	1.94	0.50
2:B:363:ARG:HD3	3:F:139:GLU:CD	2.32	0.49
1:D:368:SER:HB2	2:E:359:LEU:HD23	1.93	0.49
1:D:244:ASN:O	1:D:705:PHE:HA	2.12	0.49
3:C:230:ALA:CB	3:C:235:ARG:HD2	2.41	0.49
1:D:464:ARG:HG2	1:D:482:ASP:HB3	1.95	0.49
2:B:79:VAL:HB	2:B:480:LEU:HD11	1.94	0.49
1:D:405:PRO:HG2	2:E:601:ASN:ND2	2.27	0.49
1:A:674:ILE:O	1:A:678:LEU:HD13	2.11	0.49
3:F:158:GLU:HG3	3:F:159:GLN:HG3	1.94	0.49
3:F:148:GLN:HB3	3:F:504:ASP:OD2	2.11	0.49
1:A:287:ILE:CG2	1:A:460:PRO:HB3	2.43	0.49
3:C:317:SER:HB3	3:C:320:VAL:HG23	1.93	0.49
3:C:144:LEU:HD21	3:C:228:PHE:HB3	1.95	0.49
1:A:488:CYS:SG	1:A:504:ILE:HD11	2.51	0.49
1:A:416:GLU:HG2	1:A:420:LYS:HE2	1.94	0.49
1:D:469:LYS:CE	1:D:475:LEU:HD13	2.43	0.49
3:C:158:GLU:HG3	3:C:159:GLN:HG3	1.94	0.49
1:A:110:LYS:HG2	1:A:111:ALA:H	1.76	0.49
1:D:469:LYS:HB2	1:D:475:LEU:CD1	2.40	0.49
3:F:140:LEU:O	3:F:248:ILE:HG22	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:298:ARG:NH1	3:C:684:ILE:HD11	2.28	0.49
2:B:389:LEU:O	2:B:393:LEU:HD23	2.12	0.49
2:E:416:LEU:O	2:E:419:VAL:HB	2.13	0.49
1:D:358:ASP:O	1:D:362:THR:HA	2.13	0.49
1:D:398:TRP:CG	1:D:433:ARG:HA	2.47	0.49
2:B:697:GLU:OE1	3:C:175:PHE:CE2	2.66	0.49
1:A:586:SER:HA	1:A:593:LEU:HD12	1.95	0.49
3:C:552:PRO:HB2	3:C:554:LEU:HG	1.93	0.49
3:C:531:ALA:C	3:C:532:THR:HG22	2.33	0.49
2:E:282:ALA:HB2	3:F:148:GLN:HG2	1.94	0.49
2:E:49:TYR:CE1	2:E:81:PRO:HB2	2.48	0.49
3:F:139:GLU:O	3:F:140:LEU:HD23	2.13	0.49
2:B:53:SER:H	2:B:73:GLU:HG3	1.77	0.49
2:E:294:ARG:HA	3:F:395:TRP:CE2	2.47	0.49
1:D:287:ILE:CG2	1:D:460:PRO:HB3	2.42	0.49
1:A:128:LYS:HA	1:A:141:ASN:HD22	1.77	0.49
3:C:195:GLU:O	3:C:198:SER:OG	2.25	0.48
3:F:741:PHE:HA	3:F:747:VAL:HG22	1.94	0.48
3:F:197:ARG:NH1	3:F:703:ASP:O	2.46	0.48
1:A:222:GLU:O	1:A:226:LYS:HB2	2.12	0.48
3:C:28:THR:OG1	3:C:29:VAL:N	2.46	0.48
3:C:634:LEU:HA	3:C:637:LEU:HD12	1.95	0.48
2:E:467:PHE:O	2:E:470:VAL:HG12	2.13	0.48
1:A:361:THR:HG21	1:D:596:LYS:HE2	1.94	0.48
1:D:164:LEU:O	1:D:168:ASN:N	2.46	0.48
2:E:22:TYR:HB3	2:E:24:TYR:CD1	2.48	0.48
3:F:753:THR:HG22	3:F:754:ALA:O	2.14	0.48
1:D:558:LYS:HE3	3:F:49:LEU:HD11	1.95	0.48
3:C:131:ARG:NH1	3:C:237:GLU:OE1	2.47	0.48
2:B:467:PHE:O	2:B:470:VAL:HG12	2.14	0.48
1:D:364:GLY:O	2:E:361:ASN:HB3	2.13	0.48
1:A:363:GLU:OE1	1:D:592:ASN:O	2.31	0.48
2:B:123:SER:HB3	3:C:34:THR:HG22	1.96	0.48
3:F:620:ARG:NH2	3:F:644:THR:O	2.46	0.48
2:E:106:PHE:HB3	2:E:327:ILE:HG23	1.95	0.48
1:D:90:PHE:HB2	1:D:123:LEU:HD21	1.95	0.48
3:F:535:ASP:OD1	3:F:536:LEU:N	2.46	0.48
1:D:434:GLU:HA	1:D:437:LYS:HG2	1.96	0.48
1:D:518:LYS:HG3	1:D:519:HIS:CD2	2.49	0.48
1:A:113:ASP:O	1:A:117:GLN:HG2	2.14	0.48
3:F:713:SER:HB3	3:F:753:THR:HG21	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:393:LEU:HD21	3:F:467:ARG:CZ	2.44	0.48
1:A:635:ASN:ND2	2:B:27:PRO:O	2.45	0.48
1:D:469:LYS:CB	1:D:475:LEU:CD1	2.91	0.48
1:D:304:PRO:CG	1:D:310:PRO:HB3	2.41	0.48
3:C:422:TYR:OH	3:C:445:TYR:O	2.32	0.48
2:E:487:LEU:CD2	2:E:488:PRO:HD2	2.44	0.48
3:F:283:ASN:OD1	3:F:287:LYS:NZ	2.46	0.48
2:B:409:LEU:HD11	2:B:412:MET:HG2	1.96	0.48
1:D:431:CYS:O	1:D:435:MET:HG3	2.14	0.48
3:F:531:ALA:C	3:F:532:THR:HG22	2.34	0.47
2:B:370:ILE:HD11	2:B:374:LYS:HB2	1.96	0.47
3:C:469:ILE:HG22	3:C:493:LEU:HD13	1.96	0.47
3:F:737:LYS:HA	3:F:750:PHE:O	2.14	0.47
1:A:45:CYS:HB3	1:A:94:ILE:HD11	1.96	0.47
1:D:695:VAL:HG13	1:D:705:PHE:CD1	2.49	0.47
1:D:515:ASN:H	1:D:519:HIS:CD2	2.32	0.47
1:D:586:SER:HB2	1:D:591:GLU:O	2.14	0.47
3:F:476:LYS:O	3:F:480:SER:OG	2.19	0.47
3:F:397:THR:HA	3:F:497:THR:O	2.15	0.47
3:C:614:VAL:HG13	3:C:651:GLY:HA3	1.96	0.47
3:F:551:HIS:O	3:F:551:HIS:ND1	2.47	0.47
1:A:219:ASN:HB2	1:A:221:ARG:HH11	1.79	0.47
1:A:151:LEU:O	3:C:713:SER:OG	2.31	0.47
1:A:265:MET:HG2	1:A:434:GLU:HG2	1.95	0.47
3:C:422:TYR:CZ	3:C:449:MET:HG3	2.49	0.47
2:E:660:HIS:CE1	3:F:106:ASN:HD21	2.33	0.47
2:E:18:ILE:HD13	2:E:497:PHE:CD1	2.43	0.47
3:F:349:GLY:HA3	3:F:371:GLU:HG2	1.96	0.47
1:A:562:ASP:O	1:A:565:SER:OG	2.25	0.47
3:F:531:ALA:O	3:F:532:THR:CG2	2.60	0.47
2:B:491:PHE:CE1	2:B:493:PHE:HB2	2.50	0.47
1:D:391:LYS:O	1:D:430:ASN:ND2	2.43	0.47
3:F:131:ARG:NH1	3:F:237:GLU:OE1	2.48	0.47
1:D:128:LYS:HA	1:D:141:ASN:HD22	1.79	0.47
2:B:628:PRO:HG3	3:C:205:LEU:HD13	1.97	0.47
3:F:422:TYR:OH	3:F:445:TYR:O	2.32	0.47
3:C:340:MET:HE2	3:C:409:LEU:HD23	1.96	0.47
2:B:365:THR:HG22	2:B:366:LYS:HG3	1.97	0.47
1:D:416:GLU:HG2	1:D:420:LYS:HE2	1.97	0.47
3:F:381:SER:HB2	3:F:405:ASP:OD2	2.15	0.47
2:E:361:ASN:C	2:E:363:ARG:H	2.16	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ASP:O	1:D:117:GLN:HG2	2.14	0.47
3:F:139:GLU:O	3:F:140:LEU:HG	2.15	0.47
1:A:316:LEU:HD21	1:A:489:VAL:HG21	1.95	0.47
2:B:497:PHE:O	2:B:503:VAL:HB	2.15	0.47
2:B:147:GLN:NE2	2:B:685:TYR:HD2	2.10	0.47
1:D:222:GLU:O	1:D:226:LYS:HB2	2.15	0.47
2:E:52:THR:HA	2:E:73:GLU:HG2	1.96	0.47
3:F:422:TYR:CZ	3:F:449:MET:HG3	2.50	0.47
1:A:518:LYS:HG3	1:A:519:HIS:CD2	2.50	0.47
2:E:497:PHE:O	2:E:503:VAL:HB	2.15	0.46
1:A:115:TYR:CZ	1:A:175:LEU:HD12	2.50	0.46
1:D:477:VAL:CG1	1:D:478:PRO:CD	2.91	0.46
3:C:393:LEU:HD21	3:C:467:ARG:CZ	2.45	0.46
3:C:272:LYS:HE2	3:C:541:LYS:HA	1.97	0.46
3:F:351:LYS:HG2	3:F:369:TRP:NE1	2.30	0.46
1:A:165:ARG:HE	1:A:170:PHE:HZ	1.62	0.46
2:B:22:TYR:HB3	2:B:24:TYR:CD1	2.50	0.46
2:E:342:ALA:HB3	2:E:343:PRO:HD3	1.97	0.46
3:F:76:GLU:OE2	3:F:80:VAL:HB	2.15	0.46
1:D:222:GLU:N	1:D:222:GLU:OE1	2.49	0.46
2:E:523:ASP:OD2	2:E:560:TYR:OH	2.24	0.46
2:B:532:LYS:O	2:B:535:MET:N	2.48	0.46
1:D:273:LYS:O	1:D:481:MET:HB2	2.16	0.46
3:F:103:ASN:N	3:F:103:ASN:OD1	2.48	0.46
1:D:190:THR:O	1:D:194:LEU:HD13	2.16	0.46
3:C:713:SER:HB3	3:C:753:THR:HG21	1.96	0.46
1:A:388:TRP:CH2	1:A:430:ASN:HB3	2.50	0.46
3:F:157:VAL:O	3:F:160:ARG:HG3	2.15	0.46
3:F:170:GLN:HE21	3:F:211:ALA:HB1	1.80	0.46
3:F:340:MET:HE2	3:F:409:LEU:HD23	1.97	0.46
3:C:718:ASP:OD1	3:C:719:PRO:CD	2.63	0.46
2:E:487:LEU:HD23	2:E:489:GLU:H	1.81	0.46
3:F:533:ILE:HG22	3:F:534:LEU:HG	1.96	0.46
1:A:199:VAL:HA	1:A:200:PRO:HD3	1.78	0.46
1:D:89:PRO:HG2	1:D:90:PHE:HD1	1.81	0.46
1:A:445:LEU:HD12	1:A:459:VAL:HG11	1.98	0.46
1:D:229:GLN:O	1:D:233:ASN:HB2	2.15	0.46
1:A:165:ARG:NH2	2:B:707:ALA:HB2	2.30	0.46
1:D:562:ASP:OD1	3:F:52:ARG:NH1	2.49	0.46
1:A:251:LEU:HD21	1:A:378:PHE:HB2	1.97	0.46
1:A:644:ASN:ND2	2:B:236:GLY:HA3	2.31	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:VAL:O	3:C:160:ARG:HG3	2.16	0.46
3:F:692:ARG:HG3	3:F:694:PRO:HD2	1.96	0.46
3:C:138:LYS:HG2	3:C:139:GLU:N	2.31	0.46
1:A:382:PHE:HB3	1:A:686:PHE:CD1	2.51	0.46
2:B:436:GLY:HA3	2:B:454:ALA:HA	1.98	0.46
2:E:303:ASN:ND2	2:E:488:PRO:HA	2.30	0.46
2:B:303:ASN:ND2	2:B:488:PRO:O	2.49	0.46
2:E:350:PHE:HB3	2:E:401:VAL:CG2	2.44	0.46
1:D:280:SER:OG	1:D:464:ARG:NH2	2.49	0.46
3:C:381:SER:HB2	3:C:405:ASP:OD2	2.16	0.46
2:E:253:PHE:HA	2:E:256:ILE:HD12	1.98	0.46
2:E:18:ILE:CD1	2:E:497:PHE:CG	2.97	0.46
3:C:283:ASN:OD1	3:C:287:LYS:NZ	2.47	0.46
1:D:185:MET:CE	2:E:337:ASP:HB3	2.46	0.46
3:C:340:MET:CE	3:C:409:LEU:HD23	2.45	0.46
3:C:600:VAL:HG13	3:C:642:PRO:HA	1.97	0.46
2:B:363:ARG:O	1:D:409:ASN:ND2	2.48	0.46
3:F:453:ILE:HG12	3:F:463:LEU:HD22	1.98	0.46
1:D:183:ILE:HD13	2:E:334:LEU:HD13	1.98	0.46
1:D:658:LYS:HB2	1:D:660:LYS:HE3	1.98	0.46
1:D:316:LEU:HD22	1:D:339:PHE:CE2	2.51	0.46
2:E:475:GLY:O	2:E:477:ASN:ND2	2.49	0.45
3:F:310:ILE:HD13	3:F:323:CYS:HB3	1.98	0.45
3:C:122:TYR:CD1	3:C:213:MET:HG2	2.51	0.45
1:A:646:GLN:HA	1:A:649:ILE:HD12	1.98	0.45
3:F:298:ARG:NH1	3:F:684:ILE:HD11	2.31	0.45
1:D:214:GLU:OE1	2:E:336:LYS:NZ	2.48	0.45
1:D:382:PHE:HB3	1:D:686:PHE:CD1	2.51	0.45
1:A:241:TYR:O	1:A:244:ASN:ND2	2.49	0.45
3:C:265:ASP:O	3:C:269:VAL:HG23	2.16	0.45
3:C:444:PRO:O	3:C:448:VAL:HG23	2.16	0.45
1:A:145:PRO:O	1:A:150:LYS:HE3	2.17	0.45
3:F:419:ASP:OD2	3:F:467:ARG:NH1	2.49	0.45
1:D:566:LYS:HE3	1:D:569:ARG:HH21	1.81	0.45
3:C:76:GLU:OE2	3:C:80:VAL:HB	2.17	0.45
3:C:170:GLN:HE21	3:C:211:ALA:HB1	1.80	0.45
3:F:272:LYS:HZ2	3:F:543:THR:HG23	1.81	0.45
1:D:444:ALA:O	1:D:448:GLU:HG2	2.17	0.45
2:E:705:ILE:H	3:F:744:GLN:HB2	1.80	0.45
1:A:510:SER:O	1:A:547:LEU:HD12	2.17	0.45
2:B:491:PHE:HE1	2:B:493:PHE:HB2	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ALA:O	1:A:448:GLU:HG2	2.16	0.45
3:C:236:MET:SD	3:C:239:ILE:HD11	2.56	0.45
1:D:251:LEU:HD21	1:D:378:PHE:HB2	1.99	0.45
3:F:144:LEU:HD21	3:F:228:PHE:HB3	1.97	0.45
3:C:643:PHE:CZ	3:C:658:PHE:HB3	2.52	0.45
3:F:444:PRO:O	3:F:448:VAL:HG23	2.17	0.45
3:F:444:PRO:HG2	3:F:533:ILE:HD11	1.99	0.45
1:A:412:GLU:HG2	2:B:601:ASN:ND2	2.32	0.45
1:D:605:ILE:HG13	1:D:623:VAL:HG21	1.99	0.45
3:F:583:PRO:HD3	3:F:695:LEU:HD11	1.99	0.45
2:E:60:VAL:HG23	2:E:61:PHE:CD2	2.52	0.45
3:C:263:LYS:HA	3:C:266:ILE:HD12	1.98	0.45
3:C:59:PHE:N	3:C:60:PRO:HD3	2.32	0.45
3:C:272:LYS:NZ	3:C:543:THR:HG23	2.32	0.45
1:A:316:LEU:HD22	1:A:339:PHE:CE2	2.52	0.45
3:C:174:LEU:HD23	3:C:175:PHE:HB2	1.99	0.45
1:D:199:VAL:HA	1:D:200:PRO:HD3	1.75	0.45
3:F:384:ALA:HA	3:F:503:ILE:HD12	1.97	0.45
3:F:469:ILE:HG22	3:F:493:LEU:HD13	1.98	0.45
2:B:55:GLU:HG3	2:B:66:ARG:HG3	1.98	0.45
3:C:351:LYS:HG2	3:C:369:TRP:NE1	2.30	0.45
1:A:140:LYS:NZ	1:A:150:LYS:HE2	2.32	0.45
2:B:416:LEU:O	2:B:419:VAL:HB	2.17	0.45
2:E:584:ILE:HG21	2:E:590:LEU:HD21	1.99	0.45
1:D:133:SER:HB2	1:D:137:ARG:HB2	1.97	0.45
3:F:600:VAL:HG13	3:F:642:PRO:HA	1.99	0.45
3:C:139:GLU:N	3:C:139:GLU:OE1	2.50	0.45
3:F:197:ARG:HD3	3:F:704:THR:HG22	1.97	0.45
1:A:419:ASN:ND2	2:B:543:SER:OG	2.50	0.45
2:E:749:ALA:HB1	3:F:16:GLN:HA	1.99	0.45
1:A:67:ARG:NH1	3:C:770:ILE:HA	2.32	0.45
3:F:330:GLN:HG3	3:F:513:HIS:HB2	1.99	0.45
1:A:405:PRO:HB3	2:B:598:LEU:HG	1.98	0.44
1:A:665:PHE:HB2	2:B:480:LEU:O	2.17	0.44
3:C:166:ILE:HD12	3:C:218:PHE:HB2	1.98	0.44
1:A:190:THR:O	1:A:194:LEU:HD13	2.17	0.44
2:E:18:ILE:HD13	2:E:497:PHE:CG	2.52	0.44
3:F:174:LEU:HD23	3:F:175:PHE:HB2	1.99	0.44
2:E:557:ARG:HD3	2:E:563:HIS:HA	1.99	0.44
1:A:658:LYS:HB2	1:A:660:LYS:HE3	1.99	0.44
2:E:420:LEU:HD11	2:E:474:ILE:HD12	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:THR:HA	2:B:73:GLU:HG2	1.99	0.44
3:C:407:LYS:HA	3:C:410:LEU:HD12	2.00	0.44
3:C:517:SER:N	3:C:521:GLU:O	2.41	0.44
1:D:140:LYS:NZ	1:D:150:LYS:HE2	2.32	0.44
3:C:384:ALA:HA	3:C:503:ILE:HD12	1.99	0.44
1:D:326:ASP:OD1	1:D:327:ARG:N	2.50	0.44
1:D:282:ALA:C	1:D:284:GLU:H	2.21	0.44
1:A:275:SER:HB3	1:A:482:ASP:OD2	2.17	0.44
3:F:236:MET:HA	3:F:239:ILE:HG13	1.99	0.44
2:B:350:PHE:HB3	2:B:401:VAL:CG2	2.45	0.44
3:C:452:TRP:CE3	3:C:453:ILE:HG13	2.53	0.44
1:A:431:CYS:SG	1:A:626:VAL:HA	2.58	0.44
3:F:614:VAL:HG13	3:F:651:GLY:HA3	2.00	0.44
3:C:175:PHE:CD1	3:C:177:ASP:HB2	2.52	0.44
3:F:174:LEU:CD2	3:F:175:PHE:HB2	2.48	0.44
3:F:407:LYS:HA	3:F:410:LEU:HD12	1.98	0.44
3:F:28:THR:OG1	3:F:29:VAL:N	2.51	0.44
1:D:146:MET:N	1:D:149:GLN:OE1	2.49	0.44
3:C:414:MET:HE2	3:C:463:LEU:HD12	2.00	0.44
3:C:634:LEU:HD23	3:C:696:VAL:HA	1.99	0.44
1:A:586:SER:HB3	1:A:593:LEU:HB2	1.99	0.44
1:D:194:LEU:HG	2:E:348:ASN:HD22	1.82	0.44
3:F:139:GLU:OE1	3:F:139:GLU:N	2.51	0.44
3:C:533:ILE:HG22	3:C:534:LEU:HG	2.00	0.44
3:C:393:LEU:HD12	3:C:393:LEU:O	2.18	0.44
1:D:425:VAL:HG12	1:D:426:LEU:HD23	1.99	0.44
1:A:326:ASP:OD1	1:A:327:ARG:N	2.50	0.44
2:E:506:LEU:HD12	2:E:540:LEU:HD22	1.99	0.44
2:B:221:ILE:O	2:B:225:THR:OG1	2.32	0.44
3:C:704:THR:HB	3:C:707:ALA:HB3	2.00	0.44
1:A:681:ASN:HB3	1:A:684:CYS:HB3	2.00	0.44
1:A:320:ILE:HG21	1:A:487:ILE:HG21	2.00	0.44
3:F:463:LEU:HA	3:F:466:SER:HB3	2.00	0.43
1:A:257:ALA:HA	1:A:376:ARG:HG2	1.99	0.43
3:F:161:LEU:HD12	3:F:165:GLU:HG3	1.99	0.43
3:C:124:SER:HB2	3:C:128:ARG:HH21	1.83	0.43
2:B:273:LEU:HB2	2:B:418:THR:HG21	1.99	0.43
1:D:689:GLN:O	1:D:692:ASN:HB2	2.18	0.43
3:C:174:LEU:CD2	3:C:175:PHE:HB2	2.48	0.43
2:B:475:GLY:O	2:B:477:ASN:ND2	2.51	0.43
1:A:434:GLU:HA	1:A:437:LYS:HG2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TYR:CD1	2:B:507:ALA:HB1	2.54	0.43
1:D:378:PHE:HA	1:D:379:PRO:HD3	1.83	0.43
3:C:197:ARG:HD3	3:C:704:THR:HG22	2.00	0.43
2:B:534:ASN:ND2	2:B:538:ASN:OD1	2.48	0.43
3:F:126:PHE:O	3:F:129:LEU:HB3	2.19	0.43
3:C:103:ASN:OD1	3:C:103:ASN:N	2.51	0.43
1:D:410:GLU:HA	3:F:139:GLU:HB3	2.00	0.43
1:A:605:ILE:HG13	1:A:623:VAL:HG21	2.00	0.43
1:D:430:ASN:O	1:D:433:ARG:HB3	2.18	0.43
1:A:276:ASP:HB2	1:A:279:ARG:HB2	1.99	0.43
1:A:257:ALA:HB3	1:A:379:PRO:HG3	1.98	0.43
1:A:316:LEU:HD23	1:A:507:PHE:CZ	2.52	0.43
1:A:509:PHE:HB3	1:A:547:LEU:HD11	2.01	0.43
1:D:488:CYS:SG	1:D:504:ILE:HD11	2.57	0.43
2:B:506:LEU:HD12	2:B:540:LEU:HD22	2.00	0.43
1:D:450:ARG:HG2	3:F:56:SER:OG	2.19	0.43
1:A:273:LYS:O	1:A:481:MET:HB2	2.18	0.43
1:D:562:ASP:O	1:D:565:SER:OG	2.25	0.43
2:E:436:GLY:HA3	2:E:454:ALA:HA	2.00	0.43
2:B:457:TRP:HA	2:B:460:ILE:HD12	2.01	0.43
1:D:115:TYR:CZ	1:D:175:LEU:HD12	2.53	0.43
1:D:410:GLU:HG3	1:D:410:GLU:H	1.53	0.43
3:F:174:LEU:CD2	3:F:174:LEU:C	2.86	0.43
3:F:124:SER:O	3:F:128:ARG:HG3	2.18	0.43
1:D:257:ALA:HB3	1:D:379:PRO:HG3	2.00	0.43
1:A:236:LEU:HD12	1:A:237:PRO:HD2	2.00	0.43
3:C:299:ILE:HG22	3:C:300:GLY:N	2.33	0.43
3:C:335:LEU:HB3	3:C:342:LEU:O	2.19	0.43
2:B:493:PHE:O	2:B:496:MET:HB2	2.19	0.43
1:D:402:ALA:O	2:E:550:ARG:HD3	2.18	0.43
3:C:236:MET:HA	3:C:239:ILE:HG13	2.01	0.43
3:C:426:ALA:N	3:C:427:PRO:HD3	2.34	0.43
3:C:700:GLU:N	3:C:700:GLU:OE1	2.51	0.43
1:A:317:TRP:NE1	1:A:321:LYS:HD2	2.32	0.43
2:E:541:SER:HA	3:F:247:TRP:CZ2	2.54	0.43
1:A:415:ALA:HB1	2:B:546:LEU:HD22	2.00	0.43
1:D:246:PHE:O	1:D:247:ARG:HG2	2.19	0.43
1:D:243:GLN:O	1:D:243:GLN:HG3	2.19	0.43
3:F:393:LEU:O	3:F:393:LEU:HD12	2.19	0.43
3:C:419:ASP:OD2	3:C:467:ARG:NH1	2.52	0.43
1:D:316:LEU:HD21	1:D:489:VAL:HG21	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:THR:HG22	3:C:236:MET:HB3	2.01	0.43
3:C:161:LEU:HD12	3:C:165:GLU:HG3	2.00	0.43
1:A:133:SER:HB2	1:A:137:ARG:HB2	2.01	0.43
3:C:374:GLU:HG3	3:C:387:SER:HB3	2.01	0.42
3:C:144:LEU:HD23	3:C:244:GLY:O	2.19	0.42
3:F:131:ARG:NH1	3:F:234:GLU:OE1	2.46	0.42
1:D:379:PRO:HB3	1:D:381:TRP:NE1	2.34	0.42
3:F:426:ALA:N	3:F:427:PRO:HD3	2.34	0.42
3:C:390:GLU:O	3:C:391:ARG:HG2	2.19	0.42
2:E:340:SER:O	2:E:343:PRO:HD2	2.18	0.42
3:C:197:ARG:NH1	3:C:703:ASP:O	2.52	0.42
1:A:307:GLY:HA2	1:A:523:THR:HG23	2.01	0.42
2:E:680:ALA:HA	2:E:683:LYS:HE3	2.02	0.42
1:D:529:HIS:HA	1:D:546:PRO:HA	2.00	0.42
3:C:443:ILE:HD11	3:C:533:ILE:HG21	2.00	0.42
1:D:236:LEU:HD23	1:D:665:PHE:O	2.18	0.42
2:B:342:ALA:HB3	2:B:343:PRO:HD3	2.01	0.42
1:A:285:ILE:HG22	1:A:289:PHE:CD2	2.54	0.42
3:F:472:THR:HG23	3:F:492:SER:HB3	2.00	0.42
2:E:97:MET:HA	2:E:426:CYS:SG	2.58	0.42
3:F:59:PHE:N	3:F:60:PRO:HD3	2.33	0.42
3:F:414:MET:HE2	3:F:463:LEU:HD12	2.01	0.42
1:A:338:GLU:HG2	3:F:254:ALA:CB	2.49	0.42
2:E:457:TRP:HA	2:E:460:ILE:HD12	2.01	0.42
1:A:164:LEU:O	1:A:168:ASN:N	2.52	0.42
1:D:452:PHE:CD1	1:D:457:LYS:HD2	2.54	0.42
2:E:427:TYR:CD2	2:E:431:GLU:HB2	2.54	0.42
3:F:269:VAL:O	3:F:273:VAL:HG23	2.19	0.42
3:F:122:TYR:CD1	3:F:213:MET:HG2	2.55	0.42
2:E:273:LEU:HB2	2:E:418:THR:HG21	2.01	0.42
1:A:410:GLU:H	1:A:410:GLU:HG3	1.58	0.42
2:B:720:GLU:HG2	3:C:725:THR:HG22	2.02	0.42
1:A:350:ILE:HB	2:B:368:VAL:HG22	2.01	0.42
2:E:251:ARG:N	2:E:252:PRO:HD2	2.35	0.42
3:C:150:ARG:CB	3:C:152:VAL:HG23	2.48	0.42
2:B:584:ILE:HG21	2:B:590:LEU:HD21	2.01	0.42
3:F:138:LYS:HE2	3:F:250:GLU:HG2	1.10	0.42
1:D:477:VAL:CG1	1:D:478:PRO:N	2.83	0.42
1:A:244:ASN:O	1:A:705:PHE:HA	2.20	0.42
3:F:340:MET:CE	3:F:409:LEU:HD23	2.49	0.42
1:A:327:ARG:NE	1:A:329:MET:SD	2.93	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ASN:HB3	2:B:7:LEU:HG	2.01	0.42
2:E:487:LEU:CG	2:E:488:PRO:CD	2.87	0.42
1:D:145:PRO:O	1:D:150:LYS:HE3	2.20	0.42
1:D:112:ASP:OD1	1:D:112:ASP:N	2.53	0.42
1:D:236:LEU:HD12	1:D:237:PRO:HD2	2.02	0.42
1:A:357:GLN:O	1:A:361:THR:N	2.46	0.42
3:F:714:VAL:HG22	3:F:750:PHE:CE2	2.55	0.42
3:C:147:ARG:N	3:C:227:VAL:O	2.39	0.42
2:E:576:ILE:O	2:E:579:GLU:HG2	2.19	0.42
3:F:412:MET:HE3	3:F:412:MET:HB3	1.92	0.42
3:C:695:LEU:HD11	3:C:734:PHE:CZ	2.51	0.42
2:B:359:LEU:HD11	2:B:378:TYR:CE2	2.55	0.42
2:B:363:ARG:HA	1:D:409:ASN:CB	2.50	0.42
2:E:150:VAL:HG12	2:E:154:LYS:HE3	2.02	0.42
3:C:195:GLU:O	3:C:199:LYS:HG2	2.20	0.42
1:A:246:PHE:O	1:A:247:ARG:HG2	2.20	0.42
1:D:681:ASN:HB3	1:D:684:CYS:HB3	2.02	0.42
2:E:304:ILE:HG22	2:E:485:GLY:HA3	2.02	0.42
3:F:81:ALA:O	3:F:82:LEU:HD23	2.20	0.42
3:F:138:LYS:HZ1	3:F:250:GLU:CG	2.25	0.41
1:A:569:ARG:NH2	2:B:514:THR:HG21	2.35	0.41
1:A:430:ASN:O	1:A:433:ARG:HB3	2.20	0.41
2:E:660:HIS:HE1	3:F:106:ASN:HD21	1.66	0.41
1:A:170:PHE:O	1:A:173:ILE:HG22	2.20	0.41
3:F:693:VAL:HG23	3:F:694:PRO:HD3	2.01	0.41
2:E:302:VAL:HG22	2:E:486:SER:O	2.20	0.41
3:F:299:ILE:HG22	3:F:300:GLY:N	2.35	0.41
3:C:626:GLN:O	3:C:632:TYR:HB3	2.19	0.41
3:F:138:LYS:HE2	3:F:250:GLU:OE2	2.04	0.41
3:F:739:ARG:HA	3:F:749:THR:HG22	2.01	0.41
1:D:598:LEU:HD23	1:D:617:LEU:HD23	2.02	0.41
3:C:734:PHE:HA	3:C:752:ARG:HG3	2.02	0.41
2:B:491:PHE:CE2	2:B:498:PHE:CD2	3.08	0.41
3:C:739:ARG:HA	3:C:749:THR:HG22	2.01	0.41
1:A:671:LEU:HA	1:A:674:ILE:HD12	2.02	0.41
1:A:521:LYS:HD2	1:A:552:ARG:NH1	2.35	0.41
3:F:117:VAL:O	3:F:121:VAL:HG23	2.20	0.41
3:C:737:LYS:HA	3:C:750:PHE:O	2.20	0.41
3:F:138:LYS:HZ3	3:F:250:GLU:CG	2.04	0.41
2:E:493:PHE:O	2:E:496:MET:HB2	2.20	0.41
2:B:364:LYS:HA	2:B:364:LYS:HD3	1.95	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:646:GLN:HA	1:D:649:ILE:HD12	2.03	0.41
1:D:302:ASP:O	1:D:304:PRO:HD3	2.21	0.41
1:A:280:SER:OG	1:A:464:ARG:NH2	2.53	0.41
3:F:467:ARG:HD3	3:F:467:ARG:HA	1.93	0.41
1:D:504:ILE:HG22	1:D:554:THR:O	2.20	0.41
1:D:5:PHE:HA	1:D:8:ILE:HD12	2.02	0.41
1:A:452:PHE:CD1	1:A:457:LYS:HD2	2.55	0.41
1:D:510:SER:O	1:D:547:LEU:HD12	2.20	0.41
1:D:469:LYS:CD	1:D:475:LEU:CD1	2.95	0.41
1:A:364:GLY:O	2:B:361:ASN:HB3	2.21	0.41
3:F:139:GLU:O	3:F:139:GLU:HG2	2.20	0.41
3:F:452:TRP:CE3	3:F:453:ILE:HG13	2.55	0.41
3:F:76:GLU:HG2	3:F:77:HIS:H	1.86	0.41
1:D:316:LEU:HD23	1:D:507:PHE:CZ	2.55	0.41
3:F:322:LEU:O	3:F:325:SER:OG	2.29	0.41
3:F:758:ALA:O	3:F:762:ASP:HB2	2.20	0.41
3:F:324:LYS:NZ	3:F:331:LEU:HD22	2.35	0.41
3:C:398:ILE:O	3:C:499:GLN:N	2.45	0.41
1:A:201:LEU:HD21	2:B:87:ILE:HD11	2.03	0.41
3:F:195:GLU:O	3:F:199:LYS:HG2	2.20	0.41
2:B:150:VAL:HG12	2:B:154:LYS:HE3	2.03	0.41
1:A:89:PRO:HG2	1:A:90:PHE:HD1	1.86	0.41
1:A:99:GLU:OE2	1:A:128:LYS:NZ	2.50	0.41
3:C:76:GLU:HG3	3:C:82:LEU:HD11	2.01	0.41
3:F:272:LYS:NZ	3:F:543:THR:HG23	2.36	0.41
2:B:663:ARG:O	3:C:62:ILE:HD12	2.20	0.41
1:D:134:TYR:HB3	1:D:161:ALA:HB2	2.02	0.41
3:F:753:THR:HG22	3:F:754:ALA:N	2.36	0.41
2:B:304:ILE:HG13	2:B:450:LEU:HB3	2.02	0.41
3:F:595:TYR:CZ	3:F:620:ARG:HG3	2.56	0.41
1:A:431:CYS:SG	1:A:626:VAL:HG22	2.60	0.41
3:C:124:SER:O	3:C:128:ARG:HG3	2.21	0.41
2:E:55:GLU:HG3	2:E:66:ARG:HG3	2.02	0.41
2:E:491:PHE:CD1	2:E:492:GLU:N	2.89	0.41
1:A:229:GLN:O	1:A:233:ASN:HB2	2.21	0.41
1:A:245:LYS:HA	1:A:706:PHE:CB	2.51	0.41
1:A:287:ILE:HG21	1:A:460:PRO:HB3	2.03	0.41
3:F:236:MET:SD	3:F:239:ILE:HD11	2.61	0.41
2:E:632:PHE:CE1	3:F:102:ILE:HG23	2.56	0.41
1:A:441:THR:HG21	1:A:461:ILE:HA	2.03	0.41
3:F:202:ASN:O	3:F:204:PRO:HD3	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:332:GLY:HA3	3:F:512:ILE:HG22	2.02	0.41
1:D:355:LEU:HG	2:E:368:VAL:HG11	2.03	0.40
1:A:391:LYS:O	1:A:430:ASN:ND2	2.49	0.40
3:C:479:SER:HB2	3:C:497:THR:HB	2.02	0.40
3:C:582:ILE:N	3:C:583:PRO:HD2	2.36	0.40
1:D:101:GLN:NE2	1:D:128:LYS:HE3	2.36	0.40
1:D:320:ILE:HG21	1:D:487:ILE:HG21	2.03	0.40
3:F:288:LEU:O	3:F:292:ILE:HG12	2.21	0.40
1:D:396:THR:HG21	1:D:468:ARG:HG3	2.01	0.40
1:A:302:ASP:O	1:A:304:PRO:HD3	2.20	0.40
3:F:578:GLY:HA2	3:F:734:PHE:CD2	2.57	0.40
1:A:586:SER:HB2	1:A:591:GLU:O	2.21	0.40
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.94	0.40
3:C:299:ILE:N	3:C:302:THR:O	2.52	0.40
3:F:390:GLU:O	3:F:391:ARG:HG2	2.21	0.40
3:F:398:ILE:O	3:F:499:GLN:N	2.45	0.40
2:E:404:LEU:HA	2:E:405:PRO:HD3	1.79	0.40
1:A:154:PHE:HB3	3:C:714:VAL:HB	2.03	0.40
2:B:346:PHE:HA	2:B:349:LYS:HB3	2.04	0.40
3:F:175:PHE:HE1	3:F:177:ASP:HB2	1.86	0.40
3:C:639:LYS:HD3	3:C:674:PHE:CD1	2.56	0.40
3:F:263:LYS:HA	3:F:266:ILE:HD12	2.04	0.40
2:E:4:ASN:HB3	2:E:7:LEU:HG	2.03	0.40
1:D:235:LYS:NZ	2:E:464:ILE:HG22	2.36	0.40
2:B:580:PHE:HD1	3:C:107:PHE:HB2	1.86	0.40
1:D:140:LYS:HZ1	1:D:150:LYS:HE2	1.86	0.40
3:C:697:VAL:C	3:C:698:GLY:O	2.59	0.40
3:C:267:ARG:CZ	3:C:317:SER:HB2	2.52	0.40
3:F:479:SER:HB2	3:F:497:THR:HB	2.03	0.40
1:A:17:ALA:HB2	3:C:763:VAL:HG11	2.02	0.40
2:B:420:LEU:HD11	2:B:474:ILE:HD12	2.04	0.40
3:C:243:GLY:HA2	3:C:247:TRP:HB2	2.02	0.40
2:E:105:PHE:HE2	2:E:264:ILE:HG23	1.85	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	685/709 (97%)	643 (94%)	42 (6%)	0	100	100
1	D	685/709 (97%)	645 (94%)	40 (6%)	0	100	100
2	B	703/754 (93%)	666 (95%)	35 (5%)	2 (0%)	46	82
2	E	703/754 (93%)	673 (96%)	27 (4%)	3 (0%)	39	79
3	C	756/782 (97%)	688 (91%)	63 (8%)	5 (1%)	26	70
3	F	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	39	79
All	All	4288/4490 (96%)	4001 (93%)	274 (6%)	13 (0%)	46	82

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	405	PRO
3	C	698	GLY
2	E	405	PRO
2	B	503	VAL
2	E	503	VAL
3	F	550	GLN
3	C	428	ALA
3	C	533	ILE
3	C	550	GLN
3	F	428	ALA
3	F	533	ILE
2	E	23	PRO
3	C	47	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	618/631 (98%)	603 (98%)	15 (2%)	57	82
1	D	618/631 (98%)	608 (98%)	10 (2%)	70	88
2	B	629/669 (94%)	620 (99%)	9 (1%)	74	89
2	E	629/669 (94%)	618 (98%)	11 (2%)	68	88
3	C	669/686 (98%)	660 (99%)	9 (1%)	76	89
3	F	669/686 (98%)	655 (98%)	14 (2%)	61	85
All	All	3832/3972 (96%)	3764 (98%)	68 (2%)	66	87

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	163	PHE
1	A	170	PHE
1	A	220	PRO
1	A	276	ASP
1	A	366	LYS
1	A	410	GLU
1	A	468	ARG
1	A	471	MET
1	A	475	LEU
1	A	477	VAL
1	A	482	ASP
1	A	490	LYS
1	A	506	THR
1	A	554	THR
2	B	68	PHE
2	B	166	LEU
2	B	273	LEU
2	B	279	GLU
2	B	302	VAL
2	B	362	LYS
2	B	491	PHE
2	B	502	PHE
2	B	540	LEU
3	C	4	LEU
3	C	103	ASN
3	C	135	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	160	ARG
3	C	175	PHE
3	C	445	TYR
3	C	450	MET
3	C	594	LEU
3	C	611	ARG
1	D	38	ILE
1	D	48	PHE
1	D	163	PHE
1	D	170	PHE
1	D	276	ASP
1	D	366	LYS
1	D	410	GLU
1	D	490	LYS
1	D	506	THR
1	D	554	THR
2	E	68	PHE
2	E	89	SER
2	E	166	LEU
2	E	273	LEU
2	E	279	GLU
2	E	302	VAL
2	E	362	LYS
2	E	491	PHE
2	E	502	PHE
2	E	540	LEU
2	E	657	VAL
3	F	4	LEU
3	F	103	ASN
3	F	135	ILE
3	F	152	VAL
3	F	160	ARG
3	F	175	PHE
3	F	270	CYS
3	F	323	CYS
3	F	445	TYR
3	F	450	MET
3	F	594	LEU
3	F	611	ARG
3	F	695	LEU
3	F	725	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	101	GLN
1	A	141	ASN
1	A	494	HIS
1	A	519	HIS
1	A	561	ASN
1	A	635	ASN
1	A	644	ASN
1	A	680	ASN
2	B	147	GLN
2	B	303	ASN
2	B	461	HIS
2	B	537	ASN
2	B	627	ASN
2	B	660	HIS
2	B	686	GLN
3	C	148	GLN
3	C	550	GLN
3	C	717	ASN
1	D	31	HIS
1	D	101	GLN
1	D	141	ASN
1	D	494	HIS
1	D	519	HIS
1	D	561	ASN
1	D	680	ASN
2	E	303	ASN
2	E	315	GLN
2	E	316	GLN
2	E	477	ASN
2	E	537	ASN
2	E	627	ASN
2	E	660	HIS
2	E	686	GLN
3	F	148	GLN
3	F	550	GLN
3	F	717	ASN
3	F	744	GLN
3	F	756	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	693/709 (97%)	-0.05	17 (2%) 61 48	132, 195, 269, 299	0
1	D	693/709 (97%)	-0.11	4 (0%) 90 86	129, 191, 258, 295	0
2	B	711/754 (94%)	-0.03	13 (1%) 71 61	131, 192, 256, 317	0
2	E	711/754 (94%)	0.06	23 (3%) 51 38	130, 184, 266, 315	0
3	C	762/782 (97%)	0.02	23 (3%) 54 40	149, 222, 285, 358	0
3	F	762/782 (97%)	0.13	26 (3%) 49 37	134, 224, 287, 343	0
All	All	4332/4490 (96%)	0.00	106 (2%) 62 50	129, 202, 275, 358	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	242	ALA	6.1
3	F	631	HIS	5.3
2	E	237	LYS	5.1
3	C	1	MET	4.8
3	C	696	VAL	4.7
3	C	703	ASP	4.6
3	F	630	GLY	4.6
1	A	499	ASP	4.5
1	D	499	ASP	4.5
2	E	497	PHE	4.4
2	E	241	ARG	4.2
2	B	441	GLY	4.1
3	C	282	MET	4.0
3	F	695	LEU	3.8
2	E	25	THR	3.8
3	C	365	GLN	3.8
3	F	687	HIS	3.8
2	B	237	LYS	3.7
1	A	95	PHE	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	502	PHE	3.6
3	F	696	VAL	3.6
2	B	25	THR	3.5
2	B	504	SER	3.5
2	E	441	GLY	3.5
2	E	498	PHE	3.3
2	B	443	GLN	3.2
3	F	703	ASP	3.2
2	B	502	PHE	3.1
2	E	231	LYS	3.1
1	A	63	LEU	3.1
3	F	629	THR	3.1
3	F	149	ARG	3.1
1	A	102	PHE	3.0
3	F	586	ILE	3.0
3	C	439	LEU	3.0
3	C	574	ARG	3.0
3	C	149	ARG	3.0
2	E	230	ALA	3.0
3	F	594	LEU	2.9
3	C	767	VAL	2.9
1	A	386	TRP	2.8
2	E	449	VAL	2.8
3	F	431	THR	2.8
2	E	504	SER	2.7
3	C	200	PHE	2.7
2	B	490	LEU	2.7
2	B	236	GLY	2.7
2	E	492	GLU	2.7
2	E	491	PHE	2.7
3	C	284	ALA	2.6
2	E	32	HIS	2.6
3	F	357	TYR	2.6
3	F	571	LEU	2.6
2	E	490	LEU	2.6
1	A	132	PHE	2.5
3	C	594	LEU	2.5
3	C	702	MET	2.5
3	C	443	ILE	2.5
1	D	35	ILE	2.5
3	C	355	THR	2.4
2	E	442	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	239	GLN	2.4
3	C	328	GLY	2.4
1	A	62	VAL	2.4
2	B	442	LEU	2.4
3	C	687	HIS	2.4
3	F	204	PRO	2.4
1	A	64	ILE	2.4
2	B	23	PRO	2.3
3	C	367	GLU	2.3
3	F	700	GLU	2.3
1	A	100	LYS	2.3
3	F	91	LYS	2.3
1	A	123	LEU	2.3
3	C	95	VAL	2.3
2	B	22	TYR	2.3
2	B	497	PHE	2.3
3	F	689	ILE	2.3
1	A	522	TYR	2.3
2	E	238	LEU	2.3
3	C	523	PHE	2.3
2	E	29	PRO	2.3
2	E	451	PHE	2.3
3	F	652	MET	2.2
2	E	232	ASP	2.2
1	A	91	LEU	2.2
2	E	236	GLY	2.2
2	B	231	LYS	2.2
1	A	101	GLN	2.2
3	F	488	ARG	2.2
1	D	525	PHE	2.2
3	F	685	TYR	2.1
1	D	468	ARG	2.1
3	F	665	VAL	2.1
1	A	651	MET	2.1
3	C	41	SER	2.1
3	C	642	PRO	2.1
3	F	344	LYS	2.0
3	F	702	MET	2.0
3	C	431	THR	2.0
1	A	134	TYR	2.0
3	F	653	PHE	2.0
1	A	67	ARG	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	625	THR	2.0
3	F	189	ASN	2.0
1	A	10	GLU	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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	801	1/1	0.93	0.10	-1.07	185,185,185,185	0
4	MG	D	800	1/1	0.94	0.09	-1.28	200,200,200,200	0
4	MG	A	800	1/1	0.89	0.07	-1.43	204,204,204,204	0
4	MG	D	801	1/1	0.90	0.16	-	182,182,182,182	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.