



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:36 AM GMT

PDB ID : 2HT2
Title : Structure of the Escherichia coli ClC chloride channel Y445H mutant and Fab complex
Authors : Accardi, A.; Lobet, S.; Williams, C.; Miller, C.; Dutzler, R.
Deposited on : 2006-07-25
Resolution : 3.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

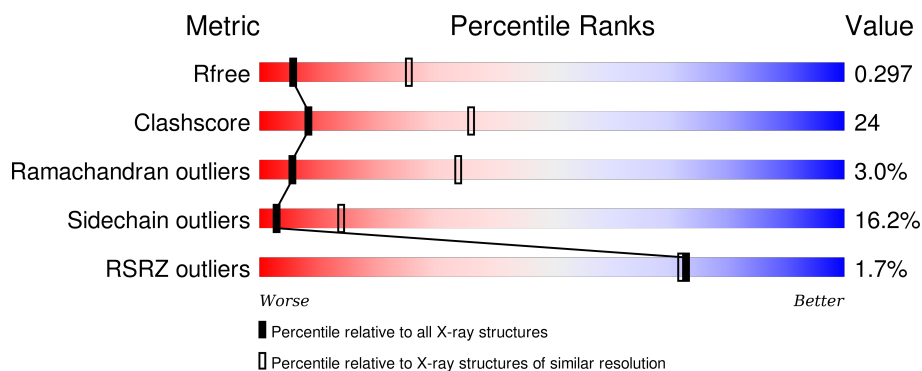
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	473	
1	B	473	
2	C	221	
2	E	221	
3	D	211	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	474	-	-	-	X
4	BR	B	474	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13221 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3331	2187	562	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3302	2171	555	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	HIS	TYR	ENGINEERED	UNP P37019
B	445	HIS	TYR	ENGINEERED	UNP P37019

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

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

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

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

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Br	0	0
			1	1		

Continued on next page...

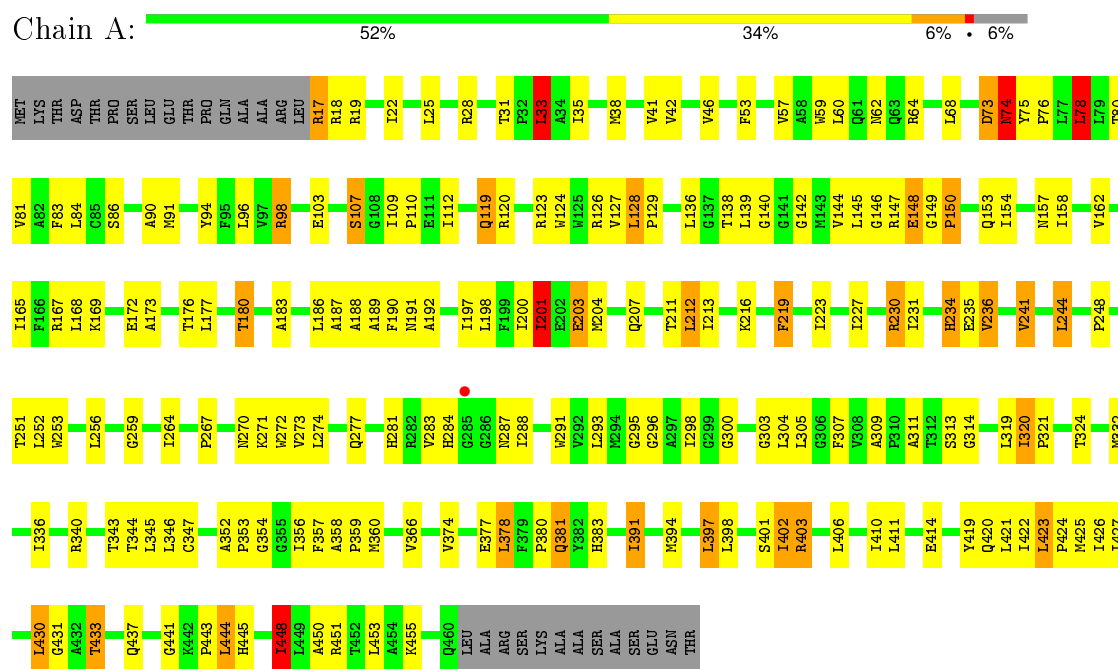
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		

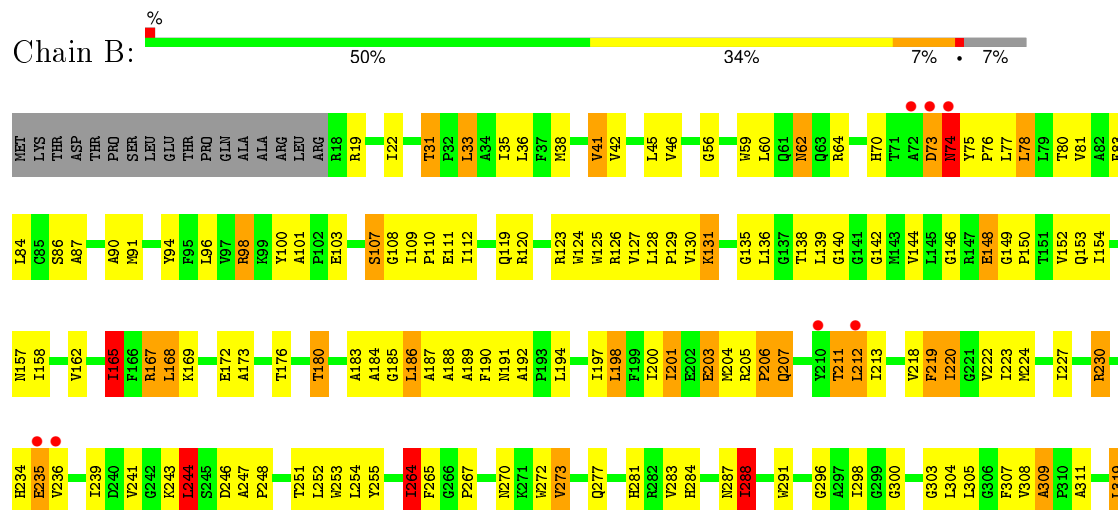
3 Residue-property plots

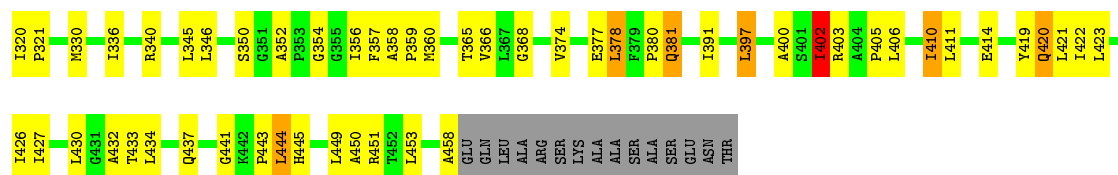
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: H(+)/Cl(-) exchange transporter clcA

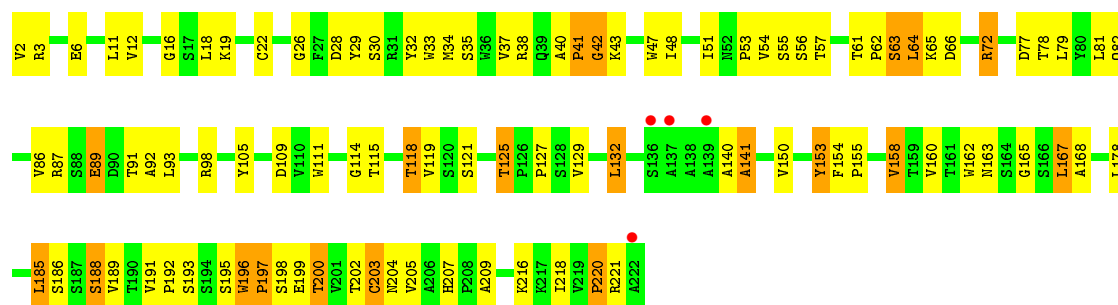


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

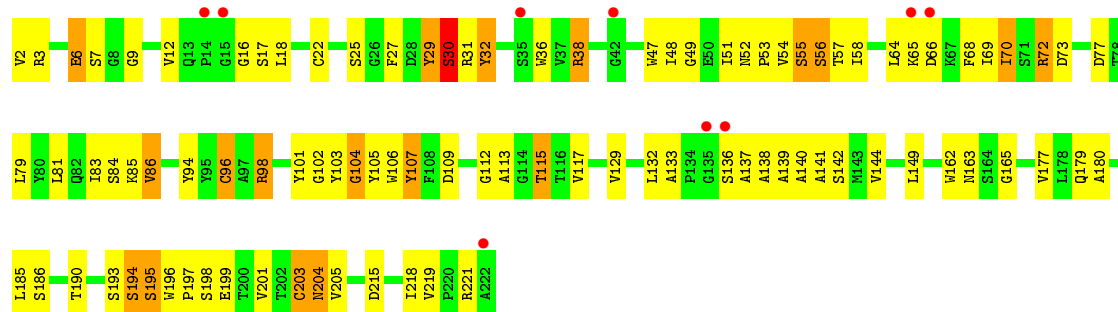




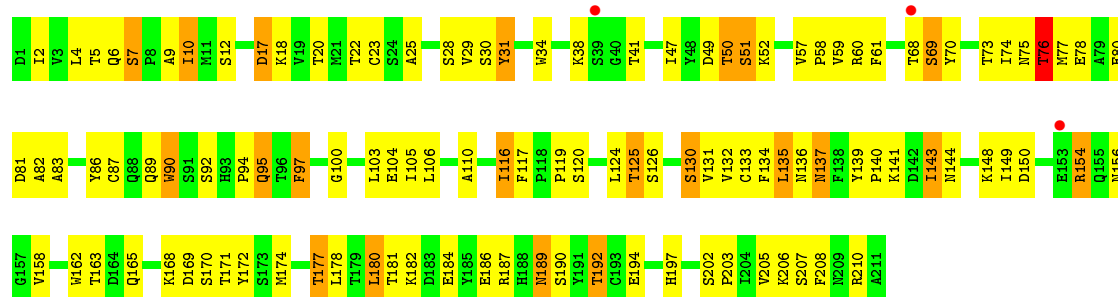
• Molecule 2: Fab fragment, heavy chain



• Molecule 2: Fab fragment, heavy chain

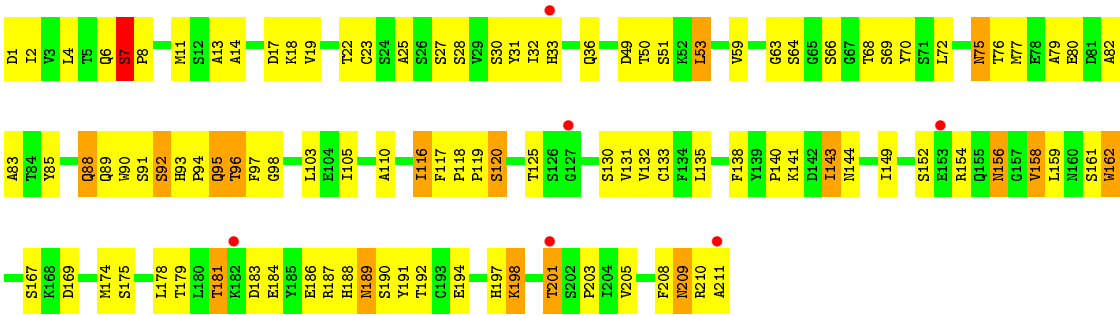


• Molecule 3: Fab fragment, light chain



• Molecule 3: Fab fragment, light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	232.29 Å 96.58 Å 170.56 Å 90.00° 131.43° 90.00°	Depositor
Resolution (Å)	40.00 – 3.32 20.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.00-3.32) 93.3 (20.04-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.29 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.270 , 0.305 0.254 , 0.297	Depositor DCC
R_{free} test set	2046 reflections (5.47%)	DCC
Wilson B-factor (Å ²)	104.8	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 56.1	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 42057 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13221	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.95	6/3403 (0.2%)	1.06	10/4618 (0.2%)
1	B	0.92	7/3374 (0.2%)	1.11	13/4580 (0.3%)
2	C	0.90	0/1721	0.86	0/2355
2	E	0.86	0/1721	0.81	0/2355
3	D	0.85	1/1660 (0.1%)	0.81	0/2257
3	F	0.81	0/1660	0.84	0/2257
All	All	0.90	14/13539 (0.1%)	0.97	23/18422 (0.1%)

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
2	C	0	1
2	E	0	2
3	F	0	1
All	All	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	VAL	CB-CG1	-14.24	1.23	1.52
1	A	41	VAL	CB-CG2	-9.85	1.32	1.52
1	B	41	VAL	CB-CG1	-9.28	1.33	1.52
1	B	41	VAL	CB-CG2	-8.78	1.34	1.52
1	B	458	ALA	C-O	7.20	1.37	1.23
1	B	235	GLU	CD-OE1	7.15	1.33	1.25
1	A	78	LEU	CG-CD1	-5.95	1.29	1.51
1	A	201	ILE	CB-CG2	-5.63	1.35	1.52
1	B	330	MET	SD-CE	-5.62	1.46	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	ILE	CG1-CD1	-5.62	1.11	1.50
3	D	130	SER	CB-OG	5.60	1.49	1.42
1	A	394	MET	SD-CE	-5.48	1.47	1.77
1	B	78	LEU	CG-CD1	-5.46	1.31	1.51
1	A	78	LEU	CG-CD2	-5.17	1.32	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	ILE	CG1-CB-CG2	-15.19	77.97	111.40
1	B	41	VAL	CG1-CB-CG2	-14.21	88.16	110.90
1	A	41	VAL	CG1-CB-CG2	-12.76	90.49	110.90
1	A	201	ILE	CG1-CB-CG2	-8.82	91.98	111.40
1	B	288	ILE	CG1-CB-CG2	-8.80	92.05	111.40
1	B	169	LYS	CD-CE-NZ	-8.64	91.82	111.70
1	A	78	LEU	CD1-CG-CD2	-8.52	84.94	110.50
1	B	78	LEU	CD1-CG-CD2	-8.43	85.20	110.50
1	A	169	LYS	CD-CE-NZ	-8.34	92.53	111.70
1	A	320	ILE	CG1-CB-CG2	-8.29	93.17	111.40
1	A	448	ILE	CG1-CB-CG2	-7.00	96.00	111.40
1	A	264	ILE	CG1-CB-CG2	-6.56	96.97	111.40
1	B	165	ILE	CG1-CB-CG2	-5.99	98.23	111.40
1	B	78	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	402	ILE	CA-CB-CG1	5.37	121.21	111.00
1	A	244	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	271	LYS	CD-CE-NZ	-5.30	99.50	111.70
1	B	458	ALA	CA-C-O	-5.29	109.00	120.10
1	A	391	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	B	131	LYS	CD-CE-NZ	5.22	123.70	111.70
1	B	264	ILE	CG1-CB-CG2	5.21	122.86	111.40
1	B	244	LEU	CB-CG-CD1	-5.06	102.39	111.00
1	B	205	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	196	TRP	Peptide
2	E	29	TYR	Peptide
2	E	32	TYR	Peptide
3	F	75	ASN	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	3331	0	3482	162	0
1	B	3302	0	3455	193	0
2	C	1672	0	1654	73	0
2	E	1672	0	1654	66	0
3	D	1621	0	1546	99	0
3	F	1621	0	1546	96	0
4	A	1	0	0	1	0
4	B	1	0	0	3	0
All	All	13221	0	13337	643	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 24.

All (643) 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:B:112:ILE:HD11	1:B:153:GLN:HA	1.25	1.18
3:D:95:GLN:H	3:D:95:GLN:CD	1.48	1.12
1:A:398:LEU:O	1:A:402:ILE:HG22	1.48	1.10
2:C:163:ASN:HD22	2:C:167:LEU:HD23	1.14	1.10
3:F:7:SER:HB3	3:F:8:PRO:CD	1.78	1.09
1:A:112:ILE:HD11	1:A:153:GLN:HA	1.10	1.06
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.39	1.03
1:A:22:ILE:HD11	1:B:453:LEU:HB3	1.39	1.02
3:F:95:GLN:H	3:F:95:GLN:NE2	1.58	1.01
2:E:36:TRP:CD1	2:E:70:ILE:HD11	1.99	0.96
2:E:51:ILE:HD13	2:E:58:ILE:HG12	1.45	0.95
2:E:70:ILE:HD11	2:E:81:LEU:HD13	1.44	0.95
3:D:95:GLN:N	3:D:95:GLN:OE1	2.00	0.94
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.47	0.94
1:A:381:GLN:HE21	1:A:381:GLN:H	0.98	0.93
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.51	0.92
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.52	0.91
1:A:112:ILE:CD1	1:A:153:GLN:HA	1.99	0.90
1:A:453:LEU:HB3	1:B:22:ILE:HD11	1.53	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLN:N	1:B:381:GLN:HE21	1.70	0.89
1:B:381:GLN:NE2	1:B:381:GLN:H	1.71	0.89
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.56	0.88
2:E:36:TRP:CD1	2:E:70:ILE:CD1	2.57	0.88
2:E:70:ILE:CD1	2:E:81:LEU:HD13	2.02	0.88
3:D:95:GLN:N	3:D:95:GLN:CD	2.24	0.88
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.56	0.88
1:B:112:ILE:CD1	1:B:153:GLN:HA	2.06	0.86
2:C:196:TRP:CE3	2:C:197:PRO:HD3	2.09	0.86
1:A:148:GLU:CD	1:A:357:PHE:HB2	1.97	0.85
1:A:410:ILE:HD11	1:B:194:LEU:HD13	1.58	0.84
1:A:410:ILE:HD11	1:B:194:LEU:CD1	2.07	0.84
2:C:196:TRP:CD2	2:C:197:PRO:HD3	2.12	0.84
1:B:110:PRO:HG3	4:B:474:BR:BR	2.32	0.84
1:A:86:SER:OG	1:A:303:GLY:HA3	1.78	0.83
3:F:77:MET:CE	3:F:103:LEU:HD21	2.08	0.82
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.59	0.82
3:D:76:THR:HG23	3:D:76:THR:O	1.79	0.82
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.62	0.81
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.46	0.81
3:F:116:ILE:HD13	3:F:117:PHE:N	1.96	0.81
2:C:163:ASN:ND2	2:C:167:LEU:HD23	1.93	0.81
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.46	0.80
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.47	0.80
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.64	0.80
1:A:381:GLN:N	1:A:381:GLN:HE21	1.79	0.79
3:F:90:TRP:CE2	3:F:95:GLN:NE2	2.51	0.78
2:C:196:TRP:CG	2:C:197:PRO:N	2.51	0.78
1:B:183:ALA:HB2	1:B:200:ILE:HD13	1.64	0.78
1:A:46:VAL:HG22	1:A:158:ILE:HD12	1.66	0.78
3:F:95:GLN:H	3:F:95:GLN:CD	1.87	0.77
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.49	0.77
2:E:51:ILE:HD11	2:E:55:SER:HA	1.65	0.77
1:A:192:ALA:HB1	1:A:414:GLU:OE2	1.84	0.77
3:D:12:SER:HA	3:D:104:GLU:O	1.84	0.77
2:C:202:THR:HG22	2:C:204:ASN:HD21	1.49	0.77
1:B:73:ASP:OD1	1:B:73:ASP:N	2.18	0.77
1:A:22:ILE:HD12	1:B:450:ALA:HA	1.67	0.77
3:D:17:ASP:OD1	3:D:18:LYS:N	2.18	0.76
3:D:116:ILE:HD13	3:D:117:PHE:N	2.01	0.76
1:B:200:ILE:HA	1:B:204:MET:HB2	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:O	1:B:180:THR:HG23	1.86	0.75
3:D:105:ILE:H	3:D:105:ILE:HD12	1.51	0.75
1:A:17:ARG:N	1:A:19:ARG:HH22	1.84	0.75
1:B:107:SER:HB3	4:B:474:BR:BR	2.40	0.75
1:A:235:GLU:O	1:A:236:VAL:HG23	1.88	0.74
1:A:223:ILE:CD1	1:B:426:ILE:HG21	2.17	0.74
1:A:42:VAL:HG22	1:A:162:VAL:HG21	1.69	0.74
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.70	0.74
3:F:143:ILE:HD13	3:F:144:ASN:N	2.03	0.73
1:A:381:GLN:NE2	1:A:381:GLN:H	1.81	0.73
1:A:422:ILE:HA	1:A:425:MET:HE3	1.70	0.73
3:D:29:VAL:HG23	3:D:70:TYR:CE1	2.23	0.73
1:A:444:LEU:HD22	1:A:444:LEU:O	1.89	0.73
1:B:90:ALA:HB3	1:B:296:GLY:HA2	1.70	0.73
3:D:2:ILE:HD12	3:D:2:ILE:H	1.54	0.73
1:B:191:ASN:HD21	1:B:230:ARG:HD3	1.54	0.72
1:A:223:ILE:HD11	1:B:426:ILE:HG21	1.71	0.72
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.23	0.72
1:B:154:ILE:O	1:B:158:ILE:HG13	1.90	0.72
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.72	0.72
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.19	0.72
3:D:29:VAL:HG23	3:D:70:TYR:HE1	1.53	0.72
1:B:109:ILE:N	1:B:110:PRO:HD2	2.05	0.72
1:A:200:ILE:HG22	1:A:201:ILE:N	2.04	0.71
3:D:189:ASN:C	3:D:189:ASN:HD22	1.92	0.71
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.71	0.70
3:F:149:ILE:HD12	3:F:191:TYR:CE2	2.26	0.70
1:B:241:VAL:O	1:B:241:VAL:HG12	1.89	0.70
2:C:200:THR:HG22	2:C:200:THR:O	1.90	0.70
1:A:274:LEU:HD21	1:A:448:ILE:CD1	2.21	0.70
3:D:76:THR:CG2	3:D:76:THR:O	2.40	0.69
3:F:7:SER:CB	3:F:8:PRO:CD	2.64	0.69
1:A:200:ILE:HA	1:A:204:MET:HB2	1.74	0.69
3:D:22:THR:HG22	3:D:23:CYS:H	1.57	0.69
1:A:274:LEU:HD21	1:A:448:ILE:HD12	1.74	0.69
1:B:381:GLN:HE21	1:B:381:GLN:H	0.85	0.69
1:B:243:LYS:HD2	1:B:420:GLN:OE1	1.94	0.69
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.26	0.69
2:C:207:HIS:NE2	2:C:209:ALA:HB3	2.09	0.69
3:D:68:THR:O	3:D:68:THR:HG23	1.92	0.69
1:B:86:SER:OG	1:B:303:GLY:HA3	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:143:ILE:HD13	3:D:144:ASN:O	1.94	0.68
2:E:6:GLU:OE1	2:E:112:GLY:HA3	1.93	0.68
1:A:380:PRO:HD2	1:A:381:GLN:NE2	2.08	0.67
1:B:422:ILE:HG12	1:B:426:ILE:HD12	1.77	0.67
1:A:398:LEU:O	1:A:402:ILE:CG2	2.35	0.66
1:A:73:ASP:OD1	1:A:73:ASP:N	2.28	0.66
1:A:356:ILE:HG23	1:A:360:MET:CE	2.25	0.66
3:D:50:THR:O	3:D:51:SER:HB3	1.94	0.66
1:A:154:ILE:O	1:A:158:ILE:HG13	1.97	0.66
1:A:59:TRP:O	1:A:62:ASN:HB3	1.96	0.66
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.78	0.65
1:B:148:GLU:CD	1:B:357:PHE:HB2	2.16	0.65
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.31	0.65
1:A:183:ALA:HB2	1:A:200:ILE:HD13	1.78	0.65
3:F:95:GLN:N	3:F:95:GLN:CD	2.48	0.65
3:F:7:SER:HB3	3:F:8:PRO:HD2	1.74	0.64
3:F:154:ARG:HH21	3:F:156:ASN:HB2	1.62	0.64
1:A:86:SER:HB2	1:A:300:GLY:HA2	1.79	0.64
1:A:17:ARG:N	1:A:19:ARG:NH2	2.46	0.64
3:D:143:ILE:HD13	3:D:144:ASN:N	2.12	0.64
1:A:176:THR:O	1:A:180:THR:HG23	1.97	0.64
1:B:150:PRO:O	1:B:154:ILE:HG13	1.97	0.64
3:D:149:ILE:HD13	3:D:154:ARG:HB3	1.79	0.64
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.63	0.64
2:C:40:ALA:O	2:C:43:LYS:HB2	1.97	0.64
1:B:59:TRP:O	1:B:62:ASN:HB2	1.98	0.64
3:D:75:ASN:O	3:D:76:THR:HG22	1.97	0.64
1:B:234:HIS:ND1	1:B:235:GLU:HG2	2.13	0.63
1:A:150:PRO:O	1:A:154:ILE:CG1	2.46	0.63
2:C:202:THR:CG2	2:C:204:ASN:HD21	2.11	0.63
1:A:421:LEU:O	1:A:425:MET:HG3	1.97	0.63
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.80	0.63
1:A:145:LEU:HD21	1:A:347:CYS:HB3	1.80	0.63
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.81	0.63
2:C:196:TRP:O	2:C:198:SER:N	2.30	0.63
1:B:144:VAL:O	1:B:144:VAL:HG12	1.99	0.63
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.14	0.62
3:D:74:ILE:HG21	3:D:81:ASP:OD2	1.98	0.62
1:B:356:ILE:HG23	1:B:360:MET:CE	2.28	0.62
2:E:6:GLU:OE1	2:E:113:ALA:N	2.31	0.62
3:F:82:ALA:HB2	3:F:105:ILE:CD1	2.27	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:22:THR:HG22	3:D:23:CYS:N	2.14	0.62
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.82	0.62
2:C:22:CYS:O	2:C:78:THR:HG23	1.99	0.62
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.18	0.62
1:B:187:ALA:O	1:B:189:ALA:N	2.33	0.62
3:F:83:ALA:HB3	3:F:85:TYR:CE1	2.35	0.62
3:D:189:ASN:ND2	3:D:210:ARG:H	1.97	0.62
1:B:223:ILE:HD13	1:B:223:ILE:N	2.14	0.62
3:F:7:SER:CB	3:F:8:PRO:HD3	2.21	0.61
1:A:90:ALA:HB3	1:A:296:GLY:HA2	1.82	0.61
2:E:204:ASN:HB3	2:E:215:ASP:OD1	1.99	0.61
1:A:172:GLU:HA	1:A:212:LEU:HD13	1.81	0.61
3:D:132:VAL:HG22	3:D:177:THR:HG23	1.81	0.61
1:A:426:ILE:HG21	1:B:223:ILE:CD1	2.30	0.61
1:A:227:ILE:HD11	1:B:427:ILE:HD11	1.83	0.61
2:C:196:TRP:CD2	2:C:197:PRO:CD	2.84	0.60
1:B:239:ILE:CD1	1:B:320:ILE:HD12	2.32	0.60
2:E:38:ARG:NH1	2:E:94:TYR:OH	2.33	0.60
2:E:6:GLU:OE2	2:E:96:CYS:N	2.22	0.60
1:A:410:ILE:HD11	1:B:194:LEU:HD11	1.82	0.60
2:C:42:GLY:O	2:C:43:LYS:HG3	2.02	0.60
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.83	0.60
2:E:103:TYR:HD2	3:F:31:TYR:CE2	2.20	0.60
1:B:172:GLU:HA	1:B:212:LEU:HD13	1.83	0.60
1:A:332:MET:O	1:A:336:ILE:HG12	2.02	0.60
1:B:109:ILE:N	1:B:110:PRO:CD	2.64	0.60
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.82	0.60
3:D:6:GLN:NE2	3:D:87:CYS:H	1.99	0.59
1:A:450:ALA:HA	1:B:22:ILE:HD12	1.84	0.59
2:E:70:ILE:CD1	2:E:81:LEU:CD1	2.77	0.59
1:B:239:ILE:HD11	1:B:320:ILE:HD12	1.84	0.59
1:B:200:ILE:HG22	1:B:201:ILE:N	2.17	0.59
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.84	0.59
1:A:18:ARG:HG3	1:B:119:GLN:OE1	2.02	0.59
1:B:197:ILE:O	1:B:201:ILE:HD13	2.01	0.59
3:D:10:ILE:H	3:D:10:ILE:HD12	1.67	0.59
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.82	0.59
3:D:49:ASP:O	3:D:51:SER:N	2.35	0.59
1:A:38:MET:O	1:A:42:VAL:HG23	2.03	0.59
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.84	0.59
3:F:158:VAL:HG23	3:F:178:LEU:HD13	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.18	0.59
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.85	0.59
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.68	0.58
1:B:46:VAL:HG22	1:B:158:ILE:HD12	1.84	0.58
1:B:319:LEU:HD11	1:B:366:VAL:CG2	2.32	0.58
2:C:158:VAL:HG12	2:C:207:HIS:HB2	1.86	0.58
1:B:444:LEU:O	1:B:444:LEU:HD22	2.03	0.58
1:A:406:LEU:HD13	1:B:219:PHE:CZ	2.38	0.58
3:F:4:LEU:HD23	3:F:25:ALA:HB2	1.85	0.58
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.28	0.58
2:C:11:LEU:HD11	2:C:154:PHE:HE2	1.69	0.58
1:B:35:ILE:HD11	1:B:173:ALA:HB2	1.84	0.58
1:B:98:ARG:HB2	1:B:288:ILE:CD1	2.34	0.58
2:E:51:ILE:HD12	2:E:57:THR:O	2.04	0.58
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.39	0.58
2:E:52:ASN:HB2	2:E:53:PRO:HD3	1.84	0.57
2:E:52:ASN:ND2	2:E:57:THR:HB	2.18	0.57
3:F:79:ALA:O	3:F:105:ILE:HD11	2.05	0.57
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.19	0.57
3:F:33:HIS:CE1	3:F:49:ASP:H	2.23	0.57
3:F:187:ARG:O	3:F:187:ARG:HG3	2.04	0.57
2:E:36:TRP:CD1	2:E:70:ILE:HD12	2.39	0.57
2:C:200:THR:O	2:C:200:THR:CG2	2.52	0.57
1:A:311:ALA:HB3	1:A:336:ILE:CD1	2.35	0.57
2:C:188:SER:HB2	3:D:134:PHE:CE2	2.40	0.56
3:F:95:GLN:N	3:F:95:GLN:NE2	2.42	0.56
2:E:6:GLU:HA	2:E:22:CYS:HA	1.85	0.56
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.87	0.56
1:A:203:GLU:OE2	1:A:445:HIS:HB2	2.05	0.56
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.40	0.56
3:F:116:ILE:HD11	3:F:208:PHE:CD2	2.40	0.56
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.87	0.56
3:D:2:ILE:HD11	3:D:92:SER:HB2	1.87	0.56
1:A:227:ILE:O	1:A:231:ILE:HG12	2.06	0.56
3:F:2:ILE:H	3:F:2:ILE:HD12	1.71	0.56
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.05	0.56
3:D:29:VAL:CG2	3:D:70:TYR:HE1	2.18	0.56
1:A:148:GLU:O	1:A:149:GLY:C	2.44	0.56
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.87	0.56
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.39	0.56
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HB2	1:B:288:ILE:HD11	1.87	0.56
1:B:405:PRO:HG2	1:B:406:LEU:H	1.71	0.55
1:A:283:VAL:O	1:A:283:VAL:HG12	2.06	0.55
1:A:187:ALA:O	1:A:189:ALA:N	2.40	0.55
3:F:143:ILE:HD13	3:F:144:ASN:H	1.72	0.55
2:E:30:SER:O	2:E:32:TYR:N	2.39	0.55
1:B:38:MET:O	1:B:42:VAL:HG23	2.06	0.55
2:C:196:TRP:C	2:C:198:SER:N	2.60	0.55
1:A:22:ILE:CD1	1:B:450:ALA:HA	2.35	0.55
3:D:150:ASP:OD2	3:D:189:ASN:N	2.36	0.55
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.71	0.55
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.89	0.55
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.33	0.55
1:A:360:MET:HG2	1:A:397:LEU:HD12	1.89	0.55
1:B:60:LEU:O	1:B:64:ARG:HG3	2.07	0.55
3:F:89:GLN:NE2	3:F:89:GLN:O	2.40	0.54
3:D:34:TRP:HB2	3:D:47:ILE:HB	1.89	0.54
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.42	0.54
1:A:311:ALA:HB1	1:A:336:ILE:HD12	1.89	0.54
3:D:134:PHE:HB3	3:D:136:ASN:ND2	2.22	0.54
2:C:202:THR:HG22	2:C:204:ASN:ND2	2.21	0.54
3:D:10:ILE:N	3:D:10:ILE:HD12	2.22	0.54
3:D:134:PHE:HB3	3:D:136:ASN:HD21	1.71	0.54
1:A:80:THR:HG22	1:A:84:LEU:HD12	1.90	0.54
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.89	0.54
1:B:108:GLY:HA3	1:B:153:GLN:NE2	2.23	0.54
3:D:189:ASN:C	3:D:189:ASN:ND2	2.61	0.54
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.89	0.54
2:E:68:PHE:C	2:E:69:ILE:HD12	2.28	0.54
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.23	0.54
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.43	0.54
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.43	0.53
1:B:86:SER:HB2	1:B:300:GLY:HA2	1.90	0.53
1:A:311:ALA:CB	1:A:336:ILE:HD12	2.37	0.53
2:C:61:THR:HG23	2:C:63:SER:HB3	1.89	0.53
1:A:427:ILE:HD11	1:B:227:ILE:HD11	1.90	0.53
1:B:267:PRO:O	1:B:270:ASN:HB2	2.09	0.53
3:D:82:ALA:O	3:D:83:ALA:HB2	2.09	0.53
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.91	0.53
2:E:196:TRP:HD1	2:E:201:VAL:HG23	1.74	0.53
2:E:132:LEU:HD11	2:E:149:LEU:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HD11	1:B:453:LEU:CB	2.27	0.53
3:D:50:THR:O	3:D:51:SER:CB	2.56	0.53
1:A:109:ILE:N	1:A:110:PRO:CD	2.71	0.53
3:F:132:VAL:HG12	3:F:133:CYS:N	2.22	0.53
2:C:111:TRP:N	2:C:111:TRP:CD1	2.77	0.53
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.27	0.52
1:B:374:VAL:HG12	1:B:378:LEU:HD12	1.92	0.52
2:C:195:SER:HA	2:C:199:GLU:OE2	2.10	0.52
2:E:30:SER:C	2:E:32:TYR:H	2.11	0.52
1:B:374:VAL:O	1:B:378:LEU:HB2	2.09	0.52
1:B:186:LEU:HG	1:B:186:LEU:O	2.10	0.52
2:C:43:LYS:HB3	2:C:43:LYS:NZ	2.24	0.52
3:D:165:GLN:HG2	3:D:170:SER:HA	1.90	0.52
3:F:4:LEU:HD22	3:F:23:CYS:SG	2.49	0.52
2:C:167:LEU:HD11	2:C:191:VAL:HG12	1.90	0.52
3:D:60:ARG:HD2	3:D:76:THR:O	2.10	0.52
1:B:241:VAL:O	1:B:241:VAL:CG1	2.56	0.52
2:E:31:ARG:HH11	2:E:31:ARG:HA	1.74	0.52
1:A:144:VAL:HG12	1:A:144:VAL:O	2.10	0.52
2:E:36:TRP:NE1	2:E:70:ILE:HD12	2.24	0.52
2:E:36:TRP:NE1	2:E:70:ILE:CD1	2.72	0.51
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.92	0.51
2:C:53:PRO:HA	2:C:72:ARG:CZ	2.40	0.51
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.92	0.51
1:B:56:GLY:HA3	1:B:136:LEU:HD11	1.92	0.51
1:A:150:PRO:O	1:A:154:ILE:HG12	2.09	0.51
3:F:116:ILE:C	3:F:116:ILE:HD13	2.30	0.51
1:B:235:GLU:O	1:B:236:VAL:HG23	2.10	0.51
1:A:283:VAL:O	1:A:283:VAL:CG1	2.58	0.51
3:F:132:VAL:CG1	3:F:133:CYS:N	2.73	0.51
2:C:127:PRO:HB2	2:C:150:VAL:HG13	1.93	0.51
1:A:426:ILE:HG22	1:A:427:ILE:N	2.24	0.51
2:E:51:ILE:CD1	2:E:58:ILE:HG12	2.30	0.51
3:F:31:TYR:HA	3:F:50:THR:OG1	2.11	0.51
1:B:135:GLY:O	1:B:136:LEU:C	2.49	0.51
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.46	0.51
1:A:35:ILE:HD11	1:A:173:ALA:HB2	1.92	0.51
3:F:156:ASN:OD1	3:F:156:ASN:N	2.44	0.51
1:A:216:LYS:HZ3	1:B:433:THR:HG22	1.75	0.51
2:C:129:VAL:O	2:C:216:LYS:HE3	2.11	0.51
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:HG12	1:B:265:PHE:N	2.23	0.50
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.93	0.50
2:E:70:ILE:HD13	2:E:81:LEU:CD1	2.41	0.50
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.11	0.50
3:D:2:ILE:HD13	3:D:89:GLN:NE2	2.26	0.50
1:A:403:ARG:HD2	1:A:433:THR:HG23	1.93	0.50
3:D:139:TYR:CD1	3:D:140:PRO:HA	2.46	0.50
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.42	0.50
1:A:33:LEU:HD23	1:A:33:LEU:O	2.12	0.50
1:A:216:LYS:NZ	1:B:437:GLN:HE21	2.10	0.50
3:D:189:ASN:HD21	3:D:210:ARG:N	2.10	0.50
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.94	0.50
3:D:2:ILE:HD12	3:D:2:ILE:N	2.25	0.50
3:D:68:THR:O	3:D:69:SER:HB2	2.12	0.50
3:D:38:LYS:O	3:D:41:THR:HG22	2.12	0.50
3:D:189:ASN:HD21	3:D:210:ARG:H	1.59	0.49
1:B:60:LEU:HD11	1:B:136:LEU:HG	1.93	0.49
3:F:18:LYS:HD2	3:F:75:ASN:OD1	2.12	0.49
1:B:98:ARG:HA	1:B:98:ARG:HE	1.77	0.49
3:F:191:TYR:HB2	3:F:208:PHE:CE2	2.48	0.49
3:F:149:ILE:HD12	3:F:191:TYR:CD2	2.47	0.49
1:A:272:TRP:HE3	1:A:345:LEU:HD11	1.78	0.49
1:B:203:GLU:OE2	1:B:445:HIS:HB2	2.12	0.49
3:D:149:ILE:N	3:D:149:ILE:HD12	2.28	0.49
3:D:181:THR:OG1	3:D:184:GLU:HB3	2.13	0.49
2:C:16:GLY:O	2:C:86:VAL:HG23	2.13	0.49
3:D:4:LEU:HD23	3:D:25:ALA:HB2	1.95	0.49
1:B:110:PRO:CG	4:B:474:BR:BR	3.11	0.49
1:A:267:PRO:O	1:A:270:ASN:HB2	2.13	0.49
3:F:2:ILE:N	3:F:2:ILE:HD12	2.27	0.49
3:F:72:LEU:HD23	3:F:72:LEU:C	2.33	0.49
3:F:14:ALA:O	3:F:17:ASP:HB2	2.13	0.49
3:F:7:SER:HB2	3:F:22:THR:HB	1.95	0.49
3:D:31:TYR:HA	3:D:50:THR:OG1	2.12	0.49
2:C:51:ILE:HG23	2:C:51:ILE:O	2.13	0.49
3:F:30:SER:HA	3:F:70:TYR:OH	2.13	0.49
3:D:17:ASP:OD1	3:D:17:ASP:C	2.50	0.49
3:D:124:LEU:C	3:D:126:SER:H	2.16	0.49
1:A:248:PRO:O	1:A:251:THR:HB	2.12	0.49
1:A:223:ILE:N	1:A:223:ILE:HD13	2.27	0.49
2:C:197:PRO:O	2:C:199:GLU:O	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ILE:HG12	1:B:426:ILE:CD1	2.43	0.48
1:A:267:PRO:HB3	1:A:441:GLY:HA3	1.96	0.48
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.93	0.48
1:B:107:SER:OG	1:B:108:GLY:N	2.45	0.48
1:A:73:ASP:O	1:A:74:ASN:C	2.52	0.48
2:C:105:TYR:CE1	3:D:31:TYR:HD1	2.30	0.48
1:B:212:LEU:HD12	1:B:212:LEU:H	1.77	0.48
2:C:11:LEU:CD1	2:C:154:PHE:HE2	2.25	0.48
1:A:60:LEU:O	1:A:64:ARG:HG3	2.13	0.48
2:C:185:LEU:C	2:C:185:LEU:HD12	2.33	0.48
3:D:7:SER:HB2	3:D:22:THR:HB	1.95	0.48
2:E:32:TYR:O	2:E:72:ARG:NH2	2.42	0.48
3:D:124:LEU:HD22	3:D:182:LYS:HG3	1.95	0.48
2:C:91:THR:HG23	2:C:118:THR:HA	1.95	0.48
2:E:36:TRP:HD1	2:E:70:ILE:CD1	2.19	0.48
3:F:13:ALA:HB3	3:F:77:MET:CE	2.44	0.48
3:F:130:SER:HA	3:F:178:LEU:O	2.14	0.48
2:C:87:ARG:HE	2:C:89:GLU:HB2	1.79	0.48
3:D:74:ILE:HD12	3:D:77:MET:HG3	1.96	0.48
1:B:197:ILE:O	1:B:201:ILE:CD1	2.62	0.48
3:D:22:THR:CG2	3:D:23:CYS:H	2.23	0.48
3:D:182:LYS:HE2	3:D:186:GLU:OE1	2.13	0.48
2:C:2:VAL:HG12	2:C:26:GLY:HA3	1.95	0.48
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.94	0.48
3:F:2:ILE:HD13	3:F:92:SER:HB2	1.95	0.48
1:B:283:VAL:O	1:B:283:VAL:HG12	2.13	0.48
1:B:190:PHE:CD1	1:B:411:LEU:HD11	2.49	0.48
3:D:29:VAL:CG2	3:D:70:TYR:CE1	2.94	0.47
1:A:176:THR:HG22	1:A:177:LEU:N	2.29	0.47
1:B:60:LEU:CD1	1:B:136:LEU:HG	2.44	0.47
2:C:64:LEU:HG	2:C:64:LEU:H	1.52	0.47
1:B:33:LEU:HD23	1:B:33:LEU:O	2.14	0.47
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.13	0.47
3:F:90:TRP:CD1	3:F:90:TRP:O	2.67	0.47
1:B:241:VAL:CG1	1:B:244:LEU:HD21	2.44	0.47
1:B:220:ILE:O	1:B:224:MET:HG2	2.14	0.47
1:A:119:GLN:HA	1:A:119:GLN:HE21	1.80	0.47
3:F:187:ARG:O	3:F:188:HIS:CG	2.67	0.47
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.29	0.47
1:A:187:ALA:C	1:A:189:ALA:H	2.18	0.47
1:B:140:GLY:C	1:B:142:GLY:H	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:O	1:A:253:TRP:C	2.53	0.47
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.82	0.47
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.29	0.47
1:B:198:LEU:HD12	1:B:406:LEU:HG	1.97	0.47
2:C:150:VAL:CG2	2:C:205:VAL:HG21	2.45	0.47
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.82	0.47
2:C:54:VAL:HG23	2:C:56:SER:OG	2.14	0.47
2:E:47:TRP:CD2	3:F:95:GLN:OE1	2.68	0.47
1:B:180:THR:HG22	1:B:218:VAL:HA	1.96	0.47
3:F:143:ILE:HG12	3:F:197:HIS:HB2	1.96	0.47
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.96	0.47
2:E:9:GLY:H	2:E:115:THR:HG21	1.79	0.47
1:A:190:PHE:CD1	1:A:411:LEU:HD11	2.49	0.47
3:F:51:SER:HB3	3:F:63:GLY:O	2.15	0.47
3:F:201:THR:O	3:F:203:PRO:HD3	2.15	0.47
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.50	0.47
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.97	0.47
3:F:11:MET:CE	3:F:19:VAL:HG13	2.45	0.47
2:E:197:PRO:O	2:E:199:GLU:N	2.48	0.47
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.36	0.47
3:F:66:SER:HA	3:F:70:TYR:CZ	2.50	0.47
2:C:30:SER:C	2:C:32:TYR:H	2.17	0.47
1:B:108:GLY:HA3	1:B:153:GLN:HE21	1.80	0.47
3:D:210:ARG:HH11	3:D:210:ARG:HG2	1.80	0.47
1:B:252:LEU:O	1:B:253:TRP:C	2.53	0.47
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.97	0.47
2:E:47:TRP:CE3	3:F:95:GLN:OE1	2.68	0.46
3:D:49:ASP:C	3:D:51:SER:H	2.19	0.46
1:B:73:ASP:O	1:B:74:ASN:C	2.54	0.46
2:C:158:VAL:CG1	2:C:207:HIS:HB2	2.45	0.46
1:B:270:ASN:O	1:B:273:VAL:HG12	2.15	0.46
2:C:12:VAL:HG23	2:C:119:VAL:HG13	1.96	0.46
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.51	0.46
3:D:105:ILE:N	3:D:105:ILE:HD12	2.24	0.46
3:D:2:ILE:CD1	3:D:92:SER:HB2	2.44	0.46
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.51	0.46
3:D:143:ILE:CD1	3:D:144:ASN:O	2.64	0.46
2:E:105:TYR:CD2	3:F:91:SER:HA	2.50	0.46
2:C:41:PRO:HD2	2:C:92:ALA:HA	1.98	0.46
2:E:129:VAL:HG21	2:E:205:VAL:HG21	1.96	0.46
2:E:221:ARG:NH2	3:F:120:SER:HA	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ALA:CB	1:A:336:ILE:CD1	2.93	0.46
2:E:136:SER:C	2:E:138:ALA:H	2.18	0.46
3:D:135:LEU:HD23	3:D:135:LEU:N	2.30	0.46
3:F:116:ILE:CD1	3:F:208:PHE:CD2	2.98	0.46
3:D:105:ILE:H	3:D:105:ILE:CD1	2.24	0.46
1:A:203:GLU:HG3	1:A:203:GLU:O	2.15	0.46
2:E:48:ILE:HD12	2:E:68:PHE:CZ	2.50	0.46
1:B:83:PHE:CD1	1:B:83:PHE:C	2.88	0.46
3:F:140:PRO:CD	3:F:198:LYS:HD2	2.46	0.46
1:B:305:LEU:C	1:B:307:PHE:H	2.19	0.46
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.50	0.46
1:B:90:ALA:O	1:B:94:TYR:HD1	1.99	0.46
1:A:234:HIS:C	1:A:234:HIS:HD1	2.19	0.46
1:B:192:ALA:HB1	1:B:414:GLU:OE2	2.16	0.46
2:C:197:PRO:O	2:C:198:SER:C	2.54	0.46
1:A:201:ILE:HG23	1:A:201:ILE:HD12	1.44	0.46
1:A:241:VAL:CG1	1:A:324:THR:HG21	2.46	0.46
2:C:165:GLY:O	2:C:168:ALA:HB2	2.16	0.46
1:B:402:ILE:HD13	1:B:402:ILE:HG21	1.06	0.46
1:B:183:ALA:O	1:B:184:ALA:C	2.53	0.46
1:A:17:ARG:HA	1:A:19:ARG:NH2	2.31	0.46
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.51	0.46
1:B:365:THR:O	1:B:368:GLY:N	2.49	0.46
1:A:25:LEU:HD11	1:B:449:LEU:HD23	1.98	0.45
1:A:272:TRP:CD1	1:A:272:TRP:N	2.83	0.45
1:A:219:PHE:CZ	1:B:406:LEU:HD13	2.51	0.45
1:B:187:ALA:C	1:B:189:ALA:H	2.19	0.45
1:B:283:VAL:CG1	1:B:283:VAL:O	2.63	0.45
1:B:311:ALA:HB1	1:B:336:ILE:HD13	1.97	0.45
1:A:147:ARG:O	1:A:148:GLU:C	2.54	0.45
1:B:198:LEU:HG	1:B:410:ILE:HD13	1.98	0.45
3:D:68:THR:CG2	3:D:68:THR:O	2.63	0.45
1:A:235:GLU:OE2	2:E:101:TYR:O	2.34	0.45
3:F:32:ILE:HD11	3:F:70:TYR:HB3	1.99	0.45
1:B:140:GLY:C	1:B:142:GLY:N	2.70	0.45
1:A:419:TYR:CE1	1:A:422:ILE:HD13	2.51	0.45
3:F:110:ALA:O	3:F:138:PHE:HA	2.16	0.45
1:A:140:GLY:C	1:A:142:GLY:H	2.19	0.45
1:A:291:TRP:O	1:A:295:GLY:N	2.49	0.45
1:A:305:LEU:C	1:A:307:PHE:H	2.20	0.45
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.88	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD12	1:A:212:LEU:H	1.82	0.45
1:B:346:LEU:O	1:B:350:SER:HB3	2.17	0.45
1:B:419:TYR:CE1	1:B:422:ILE:HD12	2.52	0.44
2:C:29:TYR:OH	2:C:79:LEU:HB2	2.17	0.44
1:B:360:MET:HG2	1:B:397:LEU:CD1	2.48	0.44
1:B:403:ARG:HD2	1:B:433:THR:HG23	1.99	0.44
1:B:80:THR:HG22	1:B:84:LEU:HD12	1.98	0.44
2:C:86:VAL:HG12	2:C:119:VAL:HG11	1.99	0.44
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.99	0.44
1:A:53:PHE:O	1:A:57:VAL:HG23	2.17	0.44
3:F:181:THR:OG1	3:F:184:GLU:HB3	2.16	0.44
1:B:108:GLY:CA	1:B:153:GLN:NE2	2.80	0.44
3:F:6:GLN:HE21	3:F:98:GLY:CA	2.24	0.44
1:A:360:MET:HG2	1:A:397:LEU:CD1	2.47	0.44
1:B:420:GLN:HB2	1:B:420:GLN:HE21	1.60	0.44
2:E:133:ALA:HB2	2:E:218:ILE:CG2	2.47	0.44
1:B:246:ASP:OD1	1:B:246:ASP:N	2.50	0.44
3:F:90:TRP:O	3:F:90:TRP:HD1	2.01	0.44
1:B:218:VAL:O	1:B:222:VAL:HG23	2.17	0.44
3:F:169:ASP:C	3:F:169:ASP:OD1	2.56	0.44
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.47	0.44
3:F:88:GLN:HE21	3:F:88:GLN:C	2.21	0.44
3:D:6:GLN:NE2	3:D:86:TYR:HA	2.26	0.44
1:B:31:THR:HB	1:B:36:LEU:HD21	2.00	0.44
1:B:206:PRO:HG2	1:B:211:THR:HG21	2.00	0.44
3:F:11:MET:HE1	3:F:19:VAL:HG13	2.00	0.44
3:D:57:VAL:HA	3:D:58:PRO:HD2	1.81	0.44
1:B:123:ARG:O	1:B:127:VAL:HG23	2.16	0.44
2:C:93:LEU:HD11	2:C:114:GLY:HA3	1.99	0.44
2:E:17:SER:HB2	2:E:83:ILE:O	2.18	0.44
1:B:111:GLU:OE2	1:B:120:ARG:NE	2.48	0.44
1:A:198:LEU:HA	1:A:201:ILE:CD1	2.48	0.43
1:A:406:LEU:HD13	1:B:219:PHE:CE1	2.53	0.43
3:D:77:MET:SD	3:D:103:LEU:HD21	2.58	0.43
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.53	0.43
1:B:421:LEU:O	1:B:422:ILE:C	2.55	0.43
3:D:189:ASN:HA	3:D:210:ARG:HD3	2.00	0.43
1:A:187:ALA:C	1:A:189:ALA:N	2.70	0.43
2:C:141:ALA:O	2:C:193:SER:CB	2.66	0.43
1:A:423:LEU:HB3	1:A:424:PRO:HD3	2.00	0.43
1:B:100:TYR:N	1:B:100:TYR:CD1	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:O	1:B:309:ALA:HB2	2.19	0.43
2:C:132:LEU:HD21	3:D:132:VAL:HG21	2.00	0.43
3:F:53:LEU:N	3:F:53:LEU:HD23	2.33	0.43
2:E:36:TRP:HE1	2:E:70:ILE:HD12	1.82	0.43
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.53	0.43
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.18	0.43
1:A:216:LYS:HZ1	1:B:437:GLN:HE21	1.65	0.43
3:D:182:LYS:O	3:D:186:GLU:HG3	2.18	0.43
3:F:77:MET:SD	3:F:103:LEU:HD21	2.59	0.43
1:B:197:ILE:HG13	1:B:197:ILE:H	1.65	0.43
1:A:198:LEU:HD21	1:B:198:LEU:HD11	2.01	0.43
1:B:241:VAL:HG11	1:B:391:ILE:HD11	2.00	0.43
1:B:356:ILE:HG23	1:B:360:MET:HE1	1.98	0.43
1:A:17:ARG:CA	1:A:19:ARG:NH2	2.82	0.43
1:A:107:SER:N	4:A:474:BR:BR	3.02	0.43
1:A:83:PHE:C	1:A:83:PHE:CD1	2.91	0.43
1:B:108:GLY:H	1:B:110:PRO:HD2	1.84	0.43
3:D:192:THR:HA	3:D:207:SER:HB2	2.00	0.43
3:D:97:PHE:CD2	3:D:97:PHE:N	2.87	0.43
1:A:78:LEU:HA	1:A:81:VAL:HG22	2.01	0.43
1:A:298:ILE:HD12	1:A:346:LEU:CD2	2.49	0.43
1:B:87:ALA:O	1:B:91:MET:HG3	2.19	0.43
3:D:89:GLN:OE1	3:D:90:TRP:N	2.52	0.43
2:E:221:ARG:HH21	3:F:120:SER:HA	1.83	0.43
1:B:207:GLN:HE21	1:B:207:GLN:CA	2.32	0.43
1:B:148:GLU:O	1:B:152:VAL:HG23	2.19	0.43
1:A:140:GLY:C	1:A:142:GLY:N	2.73	0.43
1:B:272:TRP:HE3	1:B:345:LEU:HD11	1.83	0.43
1:A:197:ILE:H	1:A:197:ILE:HG13	1.65	0.43
2:C:98:ARG:O	2:C:109:ASP:HB3	2.19	0.43
2:E:70:ILE:HA	2:E:70:ILE:HD13	1.66	0.42
1:A:75:TYR:HB3	1:A:76:PRO:CD	2.39	0.42
3:D:22:THR:CG2	3:D:23:CYS:N	2.80	0.42
1:A:313:SER:OG	1:A:314:GLY:N	2.52	0.42
1:B:183:ALA:O	1:B:186:LEU:N	2.53	0.42
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.49	0.42
1:B:42:VAL:O	1:B:46:VAL:HG23	2.19	0.42
2:C:51:ILE:HD13	2:C:72:ARG:HG2	2.01	0.42
3:F:27:SER:O	3:F:68:THR:HG22	2.19	0.42
2:E:129:VAL:CG2	2:E:205:VAL:HG21	2.50	0.42
1:A:374:VAL:O	1:A:378:LEU:HB2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:36:GLN:HG2	3:F:36:GLN:O	2.20	0.42
3:D:2:ILE:HD13	3:D:89:GLN:HE22	1.85	0.42
1:B:420:GLN:HG3	1:B:420:GLN:H	1.48	0.42
3:F:189:ASN:ND2	3:F:211:ALA:H	2.16	0.42
2:C:191:VAL:HB	2:C:192:PRO:HD2	2.01	0.42
1:B:357:PHE:CZ	1:B:402:ILE:HD11	2.54	0.42
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.55	0.42
3:D:77:MET:HG2	3:D:78:GLU:N	2.33	0.42
2:C:220:PRO:O	2:C:221:ARG:HG3	2.19	0.42
3:D:95:GLN:H	3:D:95:GLN:NE2	2.09	0.42
1:B:148:GLU:O	1:B:149:GLY:C	2.58	0.42
3:D:77:MET:HG2	3:D:78:GLU:H	1.85	0.42
1:B:98:ARG:CB	1:B:288:ILE:HD13	2.50	0.42
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.55	0.42
3:D:6:GLN:NE2	3:D:100:GLY:HA2	2.35	0.42
1:A:272:TRP:O	1:A:273:VAL:C	2.55	0.42
1:B:298:ILE:HD12	1:B:346:LEU:HD23	2.02	0.42
3:F:189:ASN:C	3:F:189:ASN:HD22	2.23	0.42
2:E:104:GLY:O	2:E:106:TRP:CD1	2.73	0.42
3:D:119:PRO:HD3	3:D:131:VAL:HG22	2.01	0.42
3:F:141:LYS:HB2	3:F:141:LYS:HE3	1.63	0.42
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.85	0.41
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.55	0.41
3:D:154:ARG:NH2	3:D:180:LEU:HD23	2.35	0.41
1:A:191:ASN:HD21	1:A:230:ARG:NH1	2.18	0.41
1:B:165:ILE:O	1:B:165:ILE:CG2	2.69	0.41
1:B:230:ARG:O	1:B:234:HIS:HB3	2.21	0.41
1:B:187:ALA:C	1:B:189:ALA:N	2.73	0.41
3:F:189:ASN:ND2	3:F:209:ASN:ND2	2.68	0.41
1:A:319:LEU:HD11	1:A:366:VAL:CG2	2.50	0.41
1:A:144:VAL:HG21	1:A:343:THR:HB	2.02	0.41
2:E:16:GLY:O	2:E:86:VAL:HG23	2.19	0.41
1:A:256:LEU:O	1:A:259:GLY:N	2.53	0.41
1:A:284:HIS:O	1:A:287:ASN:HB3	2.20	0.41
3:F:95:GLN:O	3:F:96:THR:HG23	2.21	0.41
1:B:183:ALA:C	1:B:185:GLY:N	2.73	0.41
1:A:344:THR:HG22	1:A:356:ILE:HD11	2.02	0.41
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.76	0.41
3:D:139:TYR:HA	3:D:140:PRO:O	2.21	0.41
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.50	0.41
1:B:356:ILE:HG13	1:B:356:ILE:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD13	1:A:307:PHE:HD1	1.85	0.41
1:B:251:THR:O	1:B:254:LEU:HB2	2.21	0.41
3:D:110:ALA:O	3:D:197:HIS:CE1	2.73	0.41
3:F:2:ILE:H	3:F:2:ILE:CD1	2.32	0.41
2:E:51:ILE:HB	2:E:58:ILE:HG23	2.02	0.41
1:A:270:ASN:O	1:A:273:VAL:HG12	2.21	0.41
2:C:153:TYR:H	2:C:153:TYR:HD2	1.67	0.41
1:B:247:ALA:HA	1:B:248:PRO:HD3	1.85	0.41
3:D:137:ASN:HA	3:D:171:THR:HB	2.03	0.41
2:E:144:VAL:O	2:E:144:VAL:HG13	2.20	0.41
2:E:179:GLN:HG2	3:F:159:LEU:HD11	2.02	0.41
3:D:61:PHE:HA	3:D:73:THR:O	2.20	0.41
3:D:202:SER:HA	3:D:203:PRO:HD2	1.80	0.41
3:D:94:PRO:HB2	3:D:95:GLN:OE1	2.21	0.41
1:B:124:TRP:C	1:B:126:ARG:N	2.75	0.41
2:C:160:VAL:HG22	2:C:205:VAL:HG22	2.03	0.41
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.89	0.41
2:C:185:LEU:HD12	2:C:185:LEU:O	2.20	0.41
1:A:119:GLN:O	1:A:120:ARG:HD2	2.21	0.41
1:B:400:ALA:HB2	1:B:432:ALA:HB1	2.03	0.41
3:F:210:ARG:HB3	3:F:210:ARG:CZ	2.51	0.41
2:C:196:TRP:CD1	2:C:197:PRO:N	2.87	0.41
1:B:234:HIS:HE2	3:D:52:LYS:NZ	2.18	0.41
2:C:6:GLU:HA	2:C:22:CYS:HA	2.03	0.41
2:E:133:ALA:HB2	2:E:218:ILE:HG22	2.03	0.41
2:E:163:ASN:C	2:E:165:GLY:N	2.74	0.41
1:B:149:GLY:O	1:B:150:PRO:C	2.60	0.40
2:E:196:TRP:CD1	2:E:201:VAL:HG23	2.54	0.40
3:F:93:HIS:CG	3:F:94:PRO:HA	2.56	0.40
3:F:33:HIS:HD2	3:F:88:GLN:HE22	1.69	0.40
1:B:241:VAL:HG12	1:B:244:LEU:CD2	2.52	0.40
2:E:98:ARG:O	2:E:109:ASP:HB3	2.21	0.40
1:A:437:GLN:HE22	1:B:31:THR:H	1.69	0.40
3:F:1:ASP:HB3	3:F:94:PRO:HD2	2.03	0.40
1:B:284:HIS:O	1:B:287:ASN:HB3	2.21	0.40
1:B:78:LEU:C	1:B:80:THR:N	2.73	0.40
2:C:19:LYS:HD3	2:C:82:GLN:HE21	1.85	0.40
1:B:131:LYS:HE2	1:B:153:GLN:NE2	2.37	0.40
3:F:116:ILE:CD1	3:F:116:ILE:C	2.90	0.40
2:E:22:CYS:HB3	2:E:79:LEU:HB3	2.03	0.40
1:B:356:ILE:O	1:B:359:PRO:HD2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:O	1:B:255:TYR:N	2.55	0.40
2:C:41:PRO:CD	2:C:92:ALA:HA	2.51	0.40
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.56	0.40
2:E:102:GLY:HA3	3:F:49:ASP:OD2	2.22	0.40
2:C:125:THR:HG22	2:C:153:TYR:HA	2.03	0.40
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.57	0.40
2:E:69:ILE:HD12	2:E:69:ILE:N	2.35	0.40
2:C:86:VAL:HG12	2:C:119:VAL:HG21	2.03	0.40
1:A:430:LEU:O	1:A:431:GLY:C	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/473 (93%)	391 (88%)	42 (10%)	9 (2%)	9	43
1	B	439/473 (93%)	379 (86%)	52 (12%)	8 (2%)	11	46
2	C	219/221 (99%)	191 (87%)	18 (8%)	10 (5%)	3	22
2	E	219/221 (99%)	182 (83%)	25 (11%)	12 (6%)	2	17
3	D	209/211 (99%)	173 (83%)	26 (12%)	10 (5%)	3	21
3	F	209/211 (99%)	181 (87%)	25 (12%)	3 (1%)	14	50
All	All	1737/1810 (96%)	1497 (86%)	188 (11%)	52 (3%)	5	34

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	B	188	ALA
1	B	309	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	62	PRO
2	C	65	LYS
2	C	197	PRO
3	D	31	TYR
3	D	50	THR
3	D	51	SER
3	D	69	SER
2	E	30	SER
2	E	65	LYS
2	E	140	ALA
3	F	198	LYS
1	B	107	SER
1	B	167	ARG
2	C	41	PRO
2	C	141	ALA
2	C	220	PRO
3	D	9	ALA
3	D	125	THR
2	E	137	ALA
2	E	141	ALA
2	E	194	SER
2	E	198	SER
1	A	107	SER
1	B	74	ASN
3	D	169	ASP
2	E	139	ALA
2	E	180	ALA
2	E	195	SER
3	F	7	SER
3	F	76	THR
1	A	74	ASN
1	A	188	ALA
2	C	55	SER
3	D	76	THR
3	D	90	TRP
1	A	33	LEU
2	C	140	ALA
1	B	33	LEU
3	D	137	ASN
2	E	25	SER
2	E	104	GLY
1	B	443	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	201	ILE
1	A	236	VAL
2	C	42	GLY
1	A	309	ALA
1	A	443	PRO
1	B	220	ILE
2	C	155	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/358 (94%)	284 (85%)	51 (15%)	3	16
1	B	332/358 (93%)	284 (86%)	48 (14%)	4	18
2	C	181/181 (100%)	153 (84%)	28 (16%)	3	15
2	E	181/181 (100%)	148 (82%)	33 (18%)	2	9
3	D	185/185 (100%)	151 (82%)	34 (18%)	2	9
3	F	185/185 (100%)	153 (83%)	32 (17%)	2	11
All	All	1399/1448 (97%)	1173 (84%)	226 (16%)	3	14

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	31	THR
1	A	33	LEU
1	A	73	ASP
1	A	74	ASN
1	A	78	LEU
1	A	96	LEU
1	A	98	ARG
1	A	103	GLU
1	A	119	GLN
1	A	128	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	136	LEU
1	A	139	LEU
1	A	148	GLU
1	A	150	PRO
1	A	165	ILE
1	A	168	LEU
1	A	180	THR
1	A	186	LEU
1	A	201	ILE
1	A	203	GLU
1	A	207	GLN
1	A	211	THR
1	A	212	LEU
1	A	213	ILE
1	A	219	PHE
1	A	230	ARG
1	A	234	HIS
1	A	241	VAL
1	A	244	LEU
1	A	277	GLN
1	A	288	ILE
1	A	293	LEU
1	A	304	LEU
1	A	340	ARG
1	A	377	GLU
1	A	378	LEU
1	A	381	GLN
1	A	391	ILE
1	A	397	LEU
1	A	401	SER
1	A	402	ILE
1	A	403	ARG
1	A	420	GLN
1	A	423	LEU
1	A	430	LEU
1	A	433	THR
1	A	444	LEU
1	A	448	ILE
1	A	451	ARG
1	A	455	LYS
1	B	19	ARG
1	B	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	41	VAL
1	B	45	LEU
1	B	62	ASN
1	B	70	HIS
1	B	73	ASP
1	B	74	ASN
1	B	77	LEU
1	B	96	LEU
1	B	98	ARG
1	B	103	GLU
1	B	139	LEU
1	B	148	GLU
1	B	165	ILE
1	B	167	ARG
1	B	168	LEU
1	B	180	THR
1	B	186	LEU
1	B	198	LEU
1	B	201	ILE
1	B	203	GLU
1	B	206	PRO
1	B	207	GLN
1	B	211	THR
1	B	212	LEU
1	B	213	ILE
1	B	219	PHE
1	B	230	ARG
1	B	244	LEU
1	B	264	ILE
1	B	273	VAL
1	B	277	GLN
1	B	288	ILE
1	B	304	LEU
1	B	319	LEU
1	B	340	ARG
1	B	377	GLU
1	B	378	LEU
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	410	ILE
1	B	420	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	423	LEU
1	B	430	LEU
1	B	444	LEU
1	B	451	ARG
2	C	3	ARG
2	C	18	LEU
2	C	28	ASP
2	C	35	SER
2	C	57	THR
2	C	63	SER
2	C	64	LEU
2	C	66	ASP
2	C	72	ARG
2	C	77	ASP
2	C	81	LEU
2	C	89	GLU
2	C	115	THR
2	C	118	THR
2	C	121	SER
2	C	125	THR
2	C	132	LEU
2	C	153	TYR
2	C	158	VAL
2	C	167	LEU
2	C	178	LEU
2	C	185	LEU
2	C	186	SER
2	C	188	SER
2	C	189	VAL
2	C	200	THR
2	C	203	CYS
2	C	218	ILE
3	D	5	THR
3	D	7	SER
3	D	10	ILE
3	D	17	ASP
3	D	20	THR
3	D	28	SER
3	D	30	SER
3	D	59	VAL
3	D	76	THR
3	D	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	95	GLN
3	D	97	PHE
3	D	106	LEU
3	D	116	ILE
3	D	120	SER
3	D	125	THR
3	D	130	SER
3	D	133	CYS
3	D	135	LEU
3	D	143	ILE
3	D	154	ARG
3	D	156	ASN
3	D	158	VAL
3	D	163	THR
3	D	168	LYS
3	D	177	THR
3	D	178	LEU
3	D	180	LEU
3	D	187	ARG
3	D	189	ASN
3	D	190	SER
3	D	192	THR
3	D	206	LYS
3	D	208	PHE
2	E	2	VAL
2	E	3	ARG
2	E	6	GLU
2	E	7	SER
2	E	12	VAL
2	E	27	PHE
2	E	30	SER
2	E	38	ARG
2	E	55	SER
2	E	56	SER
2	E	64	LEU
2	E	66	ASP
2	E	70	ILE
2	E	72	ARG
2	E	73	ASP
2	E	84	SER
2	E	85	LYS
2	E	86	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	96	CYS
2	E	98	ARG
2	E	107	TYR
2	E	115	THR
2	E	142	SER
2	E	177	VAL
2	E	185	LEU
2	E	186	SER
2	E	190	THR
2	E	193	SER
2	E	194	SER
2	E	195	SER
2	E	203	CYS
2	E	204	ASN
2	E	219	VAL
3	F	7	SER
3	F	28	SER
3	F	53	LEU
3	F	59	VAL
3	F	64	SER
3	F	69	SER
3	F	80	GLU
3	F	88	GLN
3	F	92	SER
3	F	95	GLN
3	F	96	THR
3	F	116	ILE
3	F	120	SER
3	F	125	THR
3	F	135	LEU
3	F	143	ILE
3	F	152	SER
3	F	156	ASN
3	F	158	VAL
3	F	161	SER
3	F	162	TRP
3	F	167	SER
3	F	175	SER
3	F	179	THR
3	F	181	THR
3	F	183	ASP
3	F	186	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	189	ASN
3	F	190	SER
3	F	192	THR
3	F	201	THR
3	F	209	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	74	ASN
1	A	119	GLN
1	A	153	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	A	277	GLN
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN
1	A	420	GLN
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
1	B	270	ASN
1	B	277	GLN
1	B	284	HIS
1	B	327	ASN
1	B	381	GLN
1	B	420	GLN
1	B	437	GLN
2	C	82	GLN
2	C	163	ASN
2	C	204	ASN
3	D	6	GLN
3	D	93	HIS
3	D	136	ASN
3	D	144	ASN
3	D	189	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	172	HIS
3	F	6	GLN
3	F	36	GLN
3	F	88	GLN
3	F	95	GLN
3	F	136	ASN
3	F	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/473 (93%)	-0.32	1 (0%) 95 96	37, 84, 144, 185	0
1	B	441/473 (93%)	-0.27	7 (1%) 74 73	35, 82, 139, 194	0
2	C	221/221 (100%)	-0.15	4 (1%) 71 70	38, 77, 144, 191	0
2	E	221/221 (100%)	-0.12	9 (4%) 41 39	32, 81, 137, 193	0
3	D	211/211 (100%)	-0.09	3 (1%) 78 78	44, 93, 133, 149	0
3	F	211/211 (100%)	0.05	6 (2%) 56 56	26, 76, 133, 199	0
All	All	1749/1810 (96%)	-0.19	30 (1%) 73 72	26, 83, 139, 199	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	136	SER	5.2
3	F	127	GLY	5.1
3	F	153	GLU	4.9
2	C	136	SER	4.6
3	F	211	ALA	3.7
2	C	137	ALA	3.6
1	B	74	ASN	3.6
2	E	35	SER	3.5
2	E	222	ALA	3.1
2	E	65	LYS	3.0
2	E	14	PRO	3.0
1	B	72	ALA	3.0
3	D	68	THR	2.8
1	B	73	ASP	2.8
2	C	139	ALA	2.8
2	C	222	ALA	2.6
3	D	39	SER	2.3
1	A	285	GLY	2.3
2	E	42	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	135	GLY	2.3
3	F	201	THR	2.2
1	B	236	VAL	2.2
3	F	33	HIS	2.2
1	B	212	LEU	2.2
3	F	182	LYS	2.2
1	B	210	TYR	2.1
1	B	235	GLU	2.1
2	E	15	GLY	2.1
2	E	66	ASP	2.1
3	D	153	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	BR	A	474	1/1	0.85	0.47	6.45	88,88,88,88	0
4	BR	B	474	1/1	0.93	0.54	6.22	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.