



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:00 AM GMT

PDB ID : 3GR9
Title : Crystal structure of ColD H188K S187N
Authors : Holden, H.M.; Cook, P.D.; Kubiak, R.L.; Toomey, D.P.
Deposited on : 2009-03-25
Resolution : 2.20 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

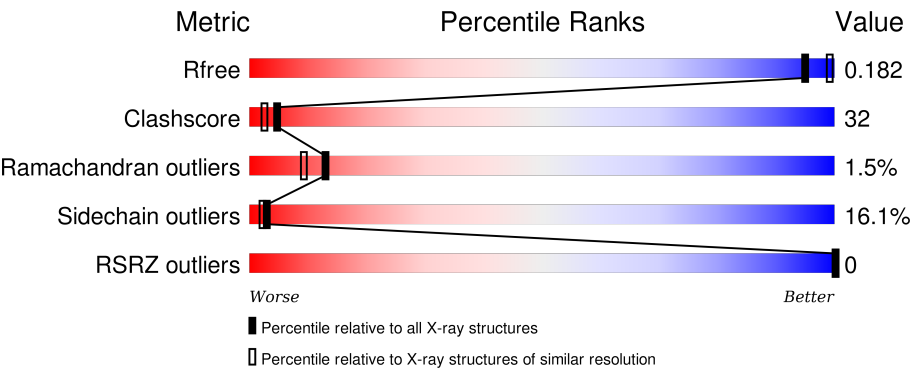
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.




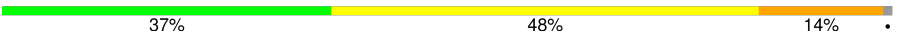

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	390	<div><div>48%</div><div>42%</div><div>8%</div><div>..</div></div>
1	B	390	<div><div>42%</div><div>44%</div><div>13%</div><div>.</div></div>
1	C	390	<div><div>45%</div><div>45%</div><div>8%</div><div>..</div></div>
1	D	390	<div><div>51%</div><div>42%</div><div>5%</div><div>.</div></div>
1	E	390	<div><div>47%</div><div>41%</div><div>11%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	390	
1	G	390	
1	H	390	

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
1	IT1	F	188	-	-	X	-
2	AKG	A	401	-	-	-	X
2	AKG	B	402	-	-	X	-
2	AKG	F	405	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25205 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 ColD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	1	0
			3092	1983	505	589	1	14			
1	B	385	Total	C	N	O	P	S	0	1	0
			3104	1992	506	591	1	14			
1	C	388	Total	C	N	O	P	S	0	1	0
			3128	2007	510	595	1	15			
1	D	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			
1	E	383	Total	C	N	O	P	S	0	1	0
			3082	1977	503	587	1	14			
1	F	386	Total	C	N	O	P	S	0	1	0
			3112	1996	508	593	1	14			
1	G	387	Total	C	N	O	P	S	0	1	0
			3120	2002	509	594	1	14			
1	H	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			

There are 32 discrepancies between the modelled and reference sequences:

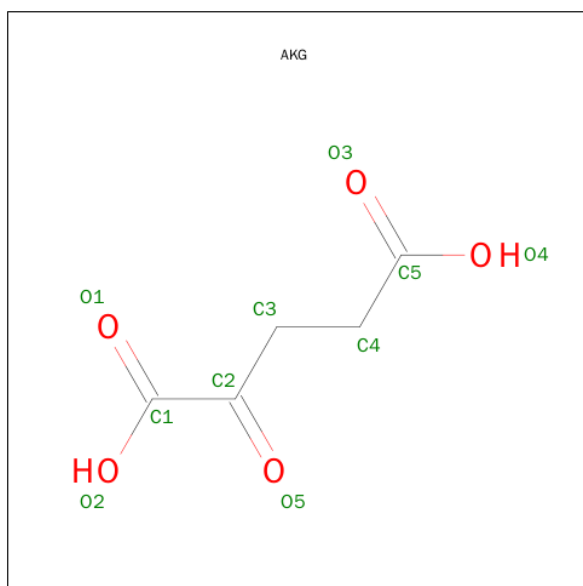
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
A	0	HIS	-	EXPRESSION TAG	UNP Q9F118
A	187	ASN	SER	ENGINEERED	UNP Q9F118
A	188	IT1	HIS	ENGINEERED	UNP Q9F118
B	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
B	0	HIS	-	EXPRESSION TAG	UNP Q9F118
B	187	ASN	SER	ENGINEERED	UNP Q9F118
B	188	IT1	HIS	ENGINEERED	UNP Q9F118
C	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
C	0	HIS	-	EXPRESSION TAG	UNP Q9F118
C	187	ASN	SER	ENGINEERED	UNP Q9F118
C	188	IT1	HIS	ENGINEERED	UNP Q9F118
D	-1	GLY	-	EXPRESSION TAG	UNP Q9F118

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP Q9F118
D	187	ASN	SER	ENGINEERED	UNP Q9F118
D	188	IT1	HIS	ENGINEERED	UNP Q9F118
E	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
E	0	HIS	-	EXPRESSION TAG	UNP Q9F118
E	187	ASN	SER	ENGINEERED	UNP Q9F118
E	188	IT1	HIS	ENGINEERED	UNP Q9F118
F	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
F	0	HIS	-	EXPRESSION TAG	UNP Q9F118
F	187	ASN	SER	ENGINEERED	UNP Q9F118
F	188	IT1	HIS	ENGINEERED	UNP Q9F118
G	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
G	0	HIS	-	EXPRESSION TAG	UNP Q9F118
G	187	ASN	SER	ENGINEERED	UNP Q9F118
G	188	IT1	HIS	ENGINEERED	UNP Q9F118
H	-1	GLY	-	EXPRESSION TAG	UNP Q9F118
H	0	HIS	-	EXPRESSION TAG	UNP Q9F118
H	187	ASN	SER	ENGINEERED	UNP Q9F118
H	188	IT1	HIS	ENGINEERED	UNP Q9F118

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		
2	H	1	Total	C	O	0	0
			10	5	5		

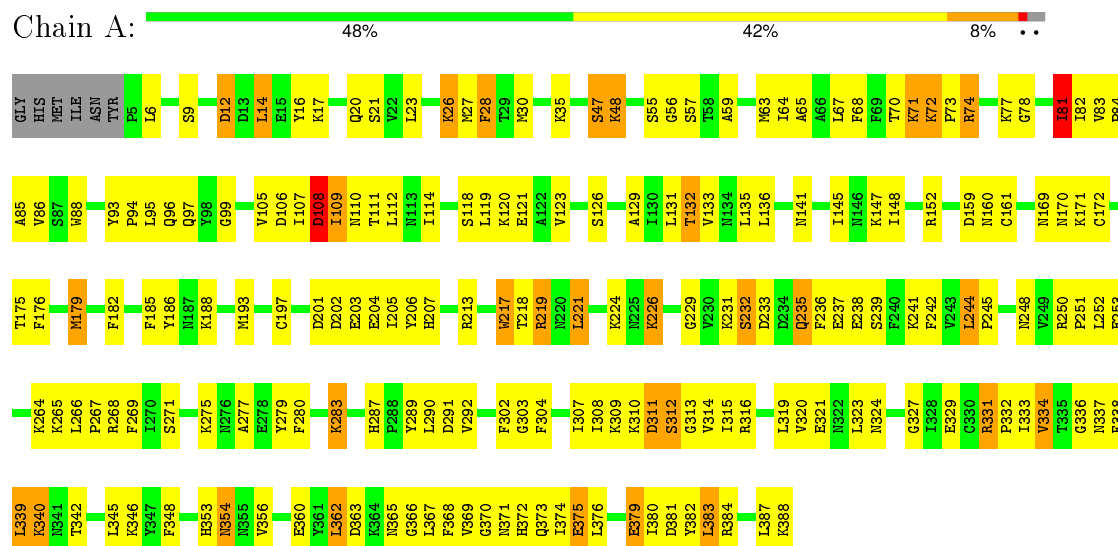
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	52	Total	O	0	0
			52	52		
3	C	50	Total	O	0	0
			50	50		
3	D	55	Total	O	0	0
			55	55		
3	E	37	Total	O	0	0
			37	37		
3	F	43	Total	O	0	0
			43	43		
3	G	41	Total	O	0	0
			41	41		
3	H	43	Total	O	0	0
			43	43		

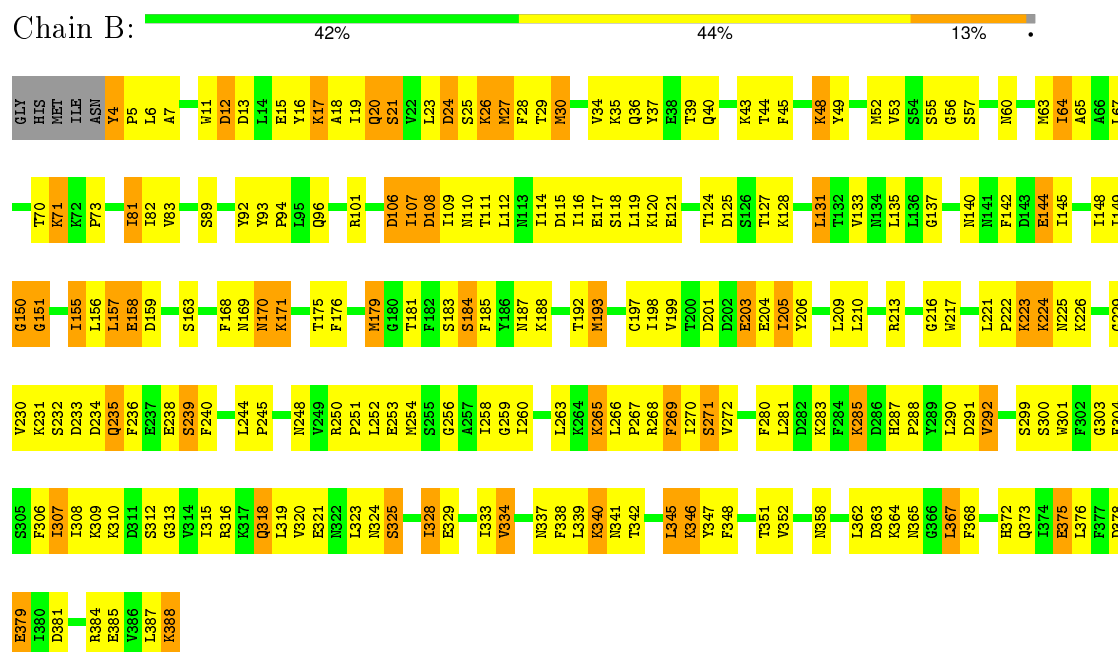
3 Residue-property plots

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.

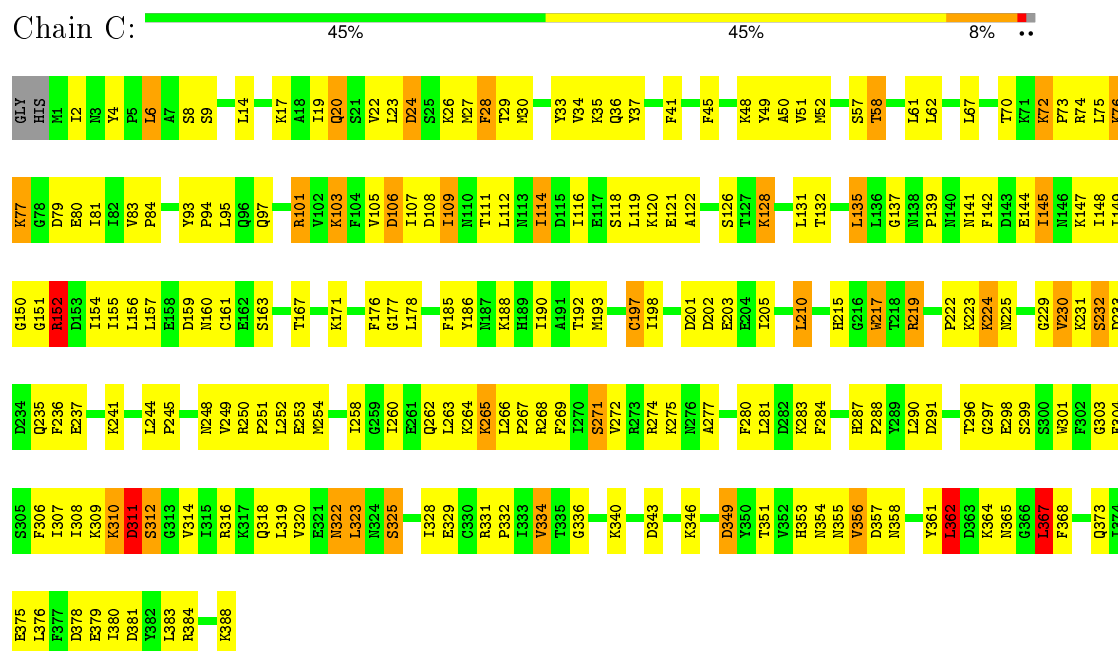
• Molecule 1: Cold

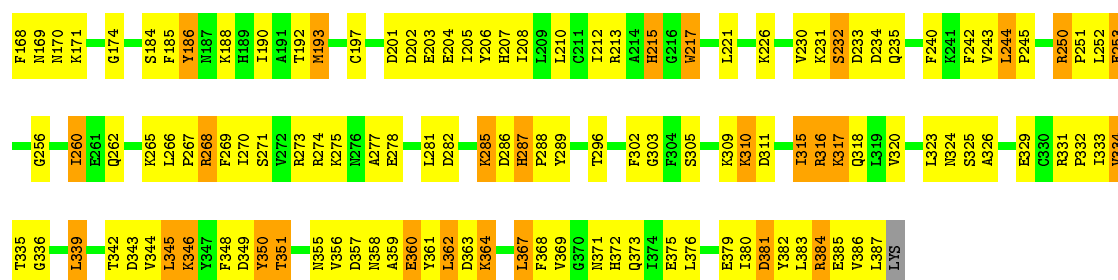


• Molecule 1: Cold

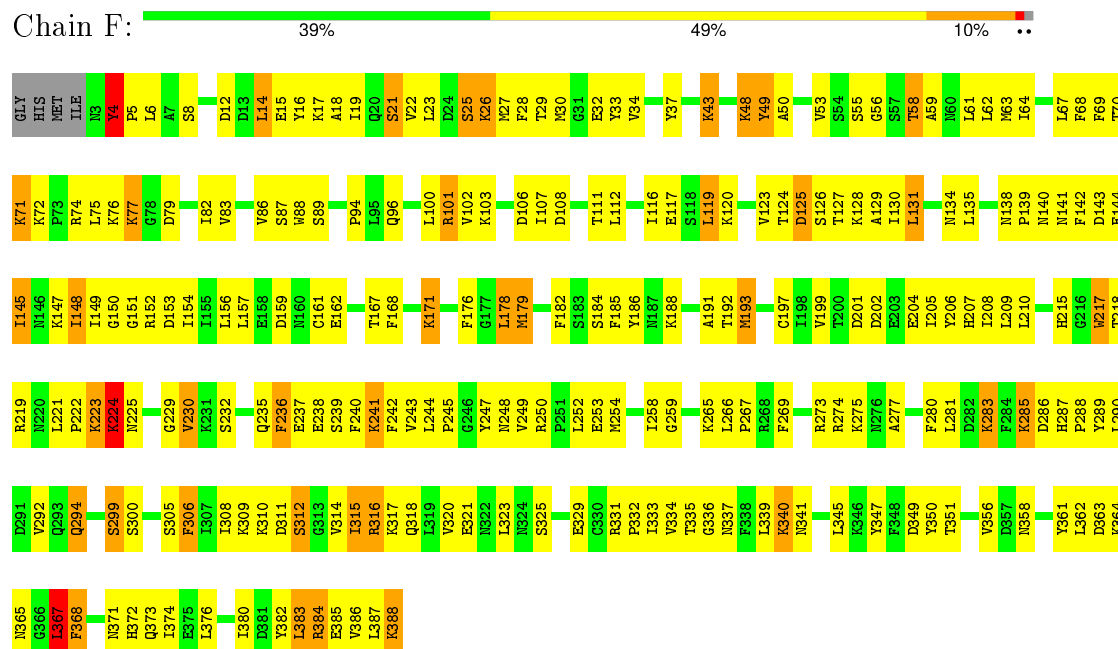


- Molecule 1: Cold

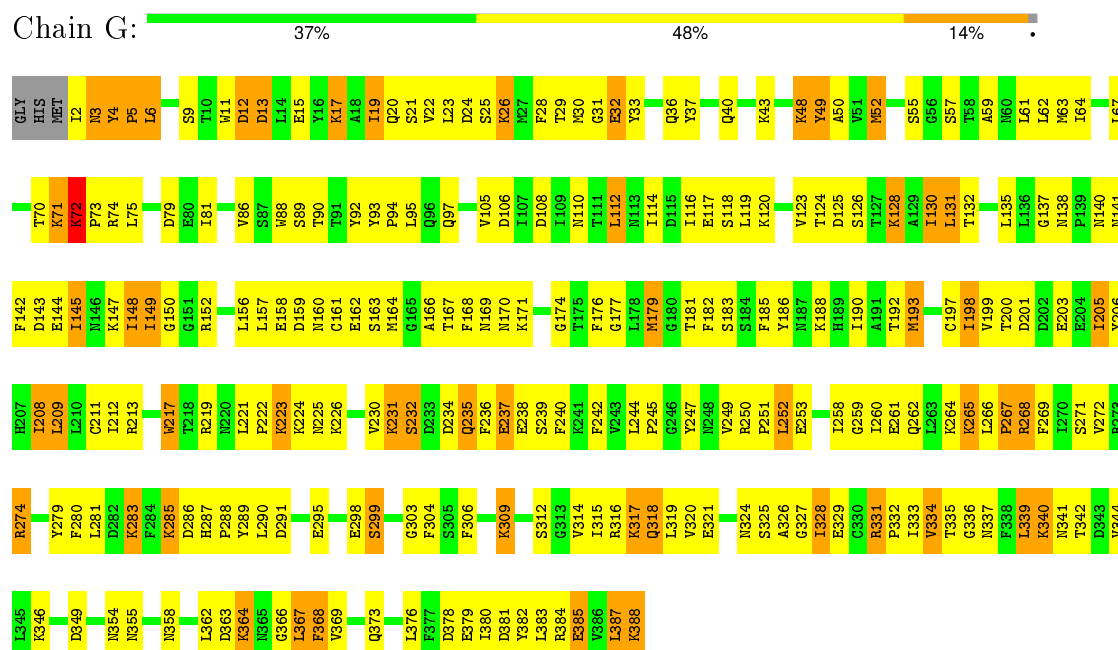




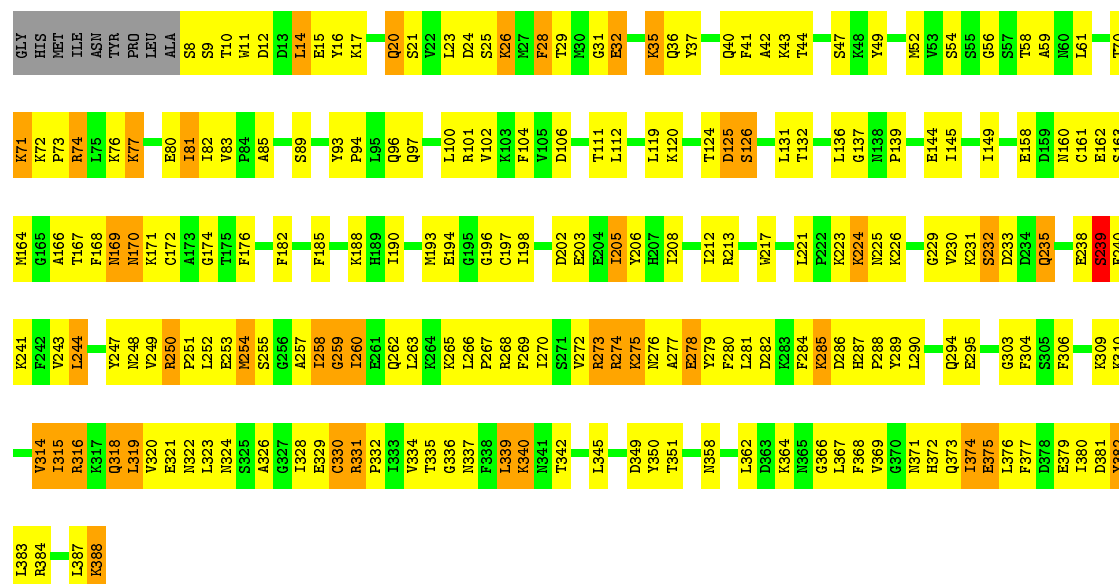
• Molecule 1: Cold



• Molecule 1: Cold



Chain H: 42% 44% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.73Å 114.66Å 114.57Å 78.98° 76.23° 76.33°	Depositor
Resolution (Å)	50.00 – 2.20 49.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.20) 86.9 (49.10-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.177 , 0.272 0.182 , 0.182	Depositor DCC
R_{free} test set	15293 reflections (11.13%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.8	EDS
Estimated twinning fraction	0.289 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 152769 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25205	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, IT1

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	0.73	0/3134	1.10	7/4230 (0.2%)
1	B	0.74	0/3147	1.09	6/4249 (0.1%)
1	C	0.72	0/3171	1.08	7/4281 (0.2%)
1	D	0.74	0/3113	1.09	6/4201 (0.1%)
1	E	0.70	0/3124	1.06	7/4219 (0.2%)
1	F	0.70	0/3155	1.07	6/4260 (0.1%)
1	G	0.70	1/3163 (0.0%)	1.07	6/4271 (0.1%)
1	H	0.68	0/3113	1.07	6/4201 (0.1%)
All	All	0.71	1/25120 (0.0%)	1.08	51/33912 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	231	LYS	CB-CG	6.07	1.69	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	G	339	LEU	CA-CB-CG	-7.37	98.35	115.30
1	C	323	LEU	CA-CB-CG	-7.13	98.90	115.30
1	A	213	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	E	381	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	D	290	LEU	CB-CG-CD1	-6.97	99.16	111.00
1	D	213	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	E	100	LEU	CA-CB-CG	-6.72	99.85	115.30
1	B	106	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	219	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	F	339	LEU	CA-CB-CG	-6.55	100.23	115.30
1	C	101	ARG	NE-CZ-NH1	-6.52	117.04	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	100	LEU	CB-CG-CD2	6.43	121.93	111.00
1	F	62	LEU	CB-CG-CD1	6.21	121.56	111.00
1	D	100	LEU	CA-CB-CG	-6.20	101.03	115.30
1	B	151	GLY	N-CA-C	-6.12	97.81	113.10
1	E	74	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	F	367	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	367	LEU	CA-CB-CG	6.06	129.24	115.30
1	C	290	LEU	CA-CB-CG	5.94	128.97	115.30
1	B	12	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	213	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	H	205	ILE	CB-CA-C	-5.77	100.06	111.60
1	E	250	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	62	LEU	CB-CG-CD1	5.69	120.67	111.00
1	B	157	LEU	CB-CG-CD1	-5.67	101.37	111.00
1	H	194	GLU	N-CA-C	-5.63	95.81	111.00
1	A	108	ASP	N-CA-C	-5.60	95.89	111.00
1	G	349	ASP	N-CA-C	-5.60	95.89	111.00
1	G	198	ILE	N-CA-C	-5.56	95.99	111.00
1	A	339	LEU	CA-CB-CG	5.55	128.07	115.30
1	H	213	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	H	14	LEU	CA-CB-CG	-5.47	102.72	115.30
1	E	371	ASN	N-CA-C	-5.45	96.29	111.00
1	G	72	LYS	C-N-CD	-5.42	108.68	120.60
1	B	339	LEU	CA-CB-CG	-5.36	102.97	115.30
1	F	224	LYS	N-CA-C	-5.35	96.55	111.00
1	G	387	LEU	CA-CB-CG	-5.34	103.02	115.30
1	B	171	LYS	N-CA-C	-5.34	96.59	111.00
1	A	81	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	D	75	LEU	CB-CG-CD2	5.28	119.97	111.00
1	H	258	ILE	CB-CA-C	-5.27	101.06	111.60
1	E	349	ASP	N-CA-C	-5.24	96.85	111.00
1	C	349	ASP	N-CA-C	-5.23	96.89	111.00
1	D	198	ILE	CB-CA-C	-5.18	101.23	111.60
1	H	198	ILE	CB-CA-C	-5.18	101.25	111.60
1	F	306	PHE	CB-CA-C	-5.11	100.17	110.40
1	A	72	LYS	N-CA-C	-5.04	97.39	111.00
1	G	252	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	E	29	THR	CB-CA-C	-5.01	98.08	111.60
1	C	362	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3092	0	3062	171	0
1	B	3104	0	3070	201	0
1	C	3128	0	3099	196	0
1	D	3072	0	3038	141	0
1	E	3082	0	3050	185	0
1	F	3112	0	3076	252	0
1	G	3120	0	3088	256	0
1	H	3072	0	3039	205	0
2	A	10	0	4	1	0
2	B	10	0	4	5	0
2	C	10	0	4	1	0
2	D	10	0	4	2	0
2	F	10	0	4	3	0
2	H	10	0	4	0	0
3	A	42	0	0	4	0
3	B	52	0	0	4	0
3	C	50	0	0	4	0
3	D	55	0	0	7	0
3	E	37	0	0	4	0
3	F	43	0	0	4	0
3	G	41	0	0	6	0
3	H	43	0	0	6	0
All	All	25205	0	24546	1569	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 32.

All (1569) 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:C:52:MET:SD	1:C:52:MET:CE	2.03	1.46
1:F:188:IT1:H4A	2:F:405:AKG:O5	1.36	1.25
1:B:124:THR:HG22	1:B:125:ASP:H	1.11	1.15
1:C:152:ARG:HH21	1:C:152:ARG:CG	1.59	1.12
1:F:222:PRO:HG2	1:F:225:ASN:HB3	1.26	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:ARG:NH2	1:E:364:LYS:HA	1.70	1.06
1:H:124:THR:HG22	1:H:126:SER:H	1.18	1.05
1:G:222:PRO:HD2	1:G:225:ASN:HB3	1.40	1.04
1:G:6:LEU:HD12	1:G:329:GLU:HG2	1.36	1.02
1:C:128:LYS:HB3	1:C:128:LYS:NZ	1.74	1.01
1:F:315:ILE:HD13	1:F:315:ILE:H	1.24	1.01
1:E:6:LEU:HD13	1:E:329:GLU:HG2	1.41	1.00
1:H:335:THR:HB	3:H:400:HOH:O	1.64	0.97
1:H:266:LEU:HB3	1:H:267:PRO:HD3	1.46	0.97
1:F:383:LEU:HD11	1:F:387:LEU:HD12	1.47	0.97
1:G:314:VAL:HG11	1:G:319:LEU:HD11	1.47	0.96
1:C:152:ARG:HH21	1:C:152:ARG:HG3	1.29	0.95
1:H:288:PRO:HG2	1:H:289:TYR:CD1	2.01	0.95
1:G:266:LEU:HB3	1:G:267:PRO:HD3	1.49	0.94
1:G:142:PHE:HA	1:G:145:ILE:HG13	1.50	0.94
1:C:67:LEU:HD13	1:C:75:LEU:HD12	1.49	0.94
1:G:274:ARG:HH11	1:G:274:ARG:HG2	1.33	0.94
1:E:384:ARG:HG3	1:E:384:ARG:HH11	1.30	0.93
1:H:12:ASP:HB3	1:H:14:LEU:HD12	1.47	0.92
1:B:36:GLN:HE21	1:B:40:GLN:HG2	1.30	0.92
1:A:310:LYS:O	1:A:311:ASP:HB2	1.65	0.92
1:H:288:PRO:HG2	1:H:289:TYR:HD1	1.34	0.91
1:C:310:LYS:O	1:C:311:ASP:HB2	1.69	0.91
1:A:93:TYR:HB2	1:A:94:PRO:HD3	1.53	0.90
1:B:133:VAL:HG22	1:B:159:ASP:HB3	1.52	0.90
1:B:333:ILE:HG22	1:B:334:VAL:HG23	1.54	0.90
1:E:117:GLU:OE2	1:E:120:LYS:NZ	2.05	0.90
1:C:274:ARG:HH11	1:C:274:ARG:HG2	1.36	0.90
1:C:128:LYS:HZ3	1:C:128:LYS:HB3	1.33	0.88
1:E:303:GLY:HA3	1:E:368:PHE:CZ	2.08	0.88
1:G:317:LYS:O	1:G:321:GLU:HG3	1.74	0.88
1:D:156:LEU:HD12	1:D:157:LEU:H	1.39	0.88
1:G:287:HIS:CG	1:G:288:PRO:HD2	2.09	0.88
1:C:67:LEU:CD1	1:C:75:LEU:HD12	2.04	0.87
1:H:14:LEU:HD12	1:H:14:LEU:H	1.40	0.87
1:B:48:LYS:HB2	1:B:201:ASP:HA	1.56	0.87
1:C:152:ARG:HH21	1:C:152:ARG:HG2	1.36	0.87
1:E:315:ILE:HD11	1:E:318:GLN:HB2	1.57	0.87
1:D:124:THR:HG22	1:D:125:ASP:H	1.37	0.86
1:D:306:PHE:HB2	1:D:367:LEU:HD13	1.57	0.86
1:F:384:ARG:HH11	1:F:384:ARG:HG3	1.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:HIS:CD2	1:G:288:PRO:HD2	2.10	0.85
1:B:269:PHE:CE1	1:B:373:GLN:HG3	2.11	0.85
1:H:303:GLY:HA3	1:H:368:PHE:CZ	2.11	0.85
1:B:124:THR:HG22	1:B:125:ASP:N	1.92	0.85
1:H:278:GLU:HA	1:H:281:LEU:HD12	1.57	0.84
1:F:289:TYR:O	1:F:290:LEU:HD23	1.75	0.84
1:F:111:THR:HG22	1:F:294:GLN:HE21	1.41	0.84
1:G:124:THR:HG22	1:G:125:ASP:N	1.91	0.84
1:E:382:TYR:O	1:E:386:VAL:HG23	1.77	0.83
1:E:336:GLY:HA2	1:E:362:LEU:HD21	1.61	0.83
1:B:287:HIS:CG	1:B:288:PRO:HD2	2.13	0.83
1:E:253:GLU:HA	1:E:253:GLU:OE1	1.76	0.83
1:G:209:LEU:HA	1:G:212:ILE:HG12	1.60	0.83
1:C:144:GLU:HA	1:C:147:LYS:HD3	1.61	0.82
1:C:6:LEU:CD1	1:C:329:GLU:HB3	2.10	0.82
1:G:285:LYS:HD2	1:G:286:ASP:OD2	1.79	0.82
1:F:48:LYS:HE2	1:F:201:ASP:HB3	1.61	0.82
1:A:332:PRO:HG2	1:B:240:PHE:CD1	2.15	0.82
1:A:6:LEU:HG	1:A:329:GLU:HG2	1.61	0.82
1:H:208:ILE:O	1:H:212:ILE:HG12	1.80	0.81
1:B:36:GLN:NE2	1:B:40:GLN:HG2	1.95	0.81
1:F:26:LYS:HB3	1:F:27:MET:CE	2.08	0.81
1:H:255:SER:HA	1:H:258:ILE:HD12	1.60	0.81
1:D:156:LEU:HD12	1:D:157:LEU:N	1.95	0.81
1:G:62:LEU:HD11	1:G:249:VAL:HG21	1.63	0.81
1:F:25:SER:O	1:F:27:MET:HE2	1.80	0.81
1:B:124:THR:CG2	1:B:125:ASP:H	1.92	0.81
1:C:254:MET:O	1:C:258:ILE:HD12	1.80	0.81
1:B:187:ASN:OD1	1:B:188:IT1:HGA	1.81	0.81
1:F:309:LYS:O	1:F:312:SER:HB3	1.78	0.81
1:C:322:ASN:HD22	1:C:322:ASN:N	1.77	0.81
1:H:31:GLY:N	1:H:253:GLU:OE1	2.12	0.81
1:D:331:ARG:HB2	1:D:332:PRO:HD2	1.61	0.80
1:C:152:ARG:NH2	1:C:152:ARG:HG3	1.91	0.80
1:H:26:LYS:HA	1:H:28:PHE:CZ	2.16	0.80
1:G:63:MET:HE3	1:G:157:LEU:HB3	1.63	0.80
1:G:120:LYS:HA	1:G:148:ILE:HD13	1.64	0.80
1:A:71:LYS:CE	1:A:71:LYS:HA	2.12	0.80
1:B:340:LYS:HE3	1:B:363:ASP:OD1	1.81	0.79
1:E:265:LYS:HG3	1:E:268:ARG:NH1	1.97	0.79
1:C:254:MET:HB2	3:C:419:HOH:O	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:SER:OG	1:C:314:VAL:HG13	1.82	0.79
1:H:81:ILE:HG13	1:H:82:ILE:N	1.95	0.79
1:G:287:HIS:CE1	1:G:288:PRO:HG2	2.18	0.79
1:C:328:ILE:HD13	1:C:383:LEU:HD12	1.64	0.79
1:D:124:THR:HG22	1:D:125:ASP:N	1.96	0.79
1:F:238:GLU:HA	1:F:241:LYS:HE2	1.65	0.79
1:H:284:PHE:HZ	1:H:387:LEU:HD12	1.45	0.79
1:G:236:PHE:CE1	1:H:332:PRO:HD3	2.18	0.78
1:B:341:ASN:O	1:B:345:LEU:HD22	1.82	0.78
1:A:119:LEU:O	1:A:123:VAL:HG23	1.84	0.78
1:B:303:GLY:HA3	1:B:368:PHE:CE2	2.19	0.78
1:E:268:ARG:HH21	1:E:268:ARG:HG2	1.47	0.78
1:B:269:PHE:CD1	1:B:373:GLN:HG3	2.19	0.77
1:B:30:MET:HE3	1:B:34:VAL:HG11	1.66	0.77
1:G:135:LEU:HD11	1:G:334:VAL:HG21	1.67	0.77
1:C:139:PRO:HD2	1:C:296:THR:O	1.85	0.77
1:E:265:LYS:HG3	1:E:268:ARG:HH11	1.49	0.77
1:H:168:PHE:CD2	1:H:169:ASN:ND2	2.53	0.77
1:F:266:LEU:HB3	1:F:267:PRO:HD3	1.66	0.77
1:B:268:ARG:O	1:B:272:VAL:HG23	1.83	0.77
1:C:120:LYS:HA	1:C:148:ILE:HD13	1.67	0.77
1:F:111:THR:HG22	1:F:294:GLN:NE2	1.99	0.77
1:D:271:SER:O	1:D:275:LYS:HD3	1.84	0.77
1:H:81:ILE:HD11	1:H:131:LEU:HB2	1.67	0.76
1:C:149:ILE:CG2	1:C:149:ILE:O	2.33	0.76
1:C:188:IT1:OP3	2:C:403:AKG:O3	2.03	0.76
1:A:332:PRO:HG2	1:B:240:PHE:CE1	2.20	0.76
1:E:168:PHE:CE2	1:E:169:ASN:ND2	2.54	0.76
1:G:112:LEU:N	1:G:112:LEU:HD23	2.01	0.76
1:F:161:CYS:HB2	1:F:188:IT1:C2	2.16	0.76
1:D:281:LEU:O	1:D:285:LYS:HB3	1.86	0.76
1:F:82:ILE:HD12	1:F:127:THR:HG21	1.68	0.75
1:B:337:ASN:O	1:B:340:LYS:HG2	1.86	0.75
1:H:83:VAL:HG12	1:H:131:LEU:HB3	1.66	0.75
1:G:289:TYR:CD2	1:G:314:VAL:HG21	2.22	0.75
1:B:319:LEU:O	1:B:323:LEU:HG	1.85	0.75
1:F:48:LYS:HB2	1:F:201:ASP:HA	1.69	0.75
1:H:315:ILE:HD13	1:H:315:ILE:H	1.50	0.75
1:E:265:LYS:C	1:E:267:PRO:HD2	2.06	0.75
1:B:316:ARG:O	1:B:320:VAL:HG23	1.87	0.75
1:C:152:ARG:HB2	1:C:154:ILE:HG13	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:ARG:NH1	1:E:384:ARG:HG3	1.95	0.75
1:G:274:ARG:NH1	1:G:274:ARG:HG2	1.94	0.74
1:G:203:GLU:HG2	1:G:226:LYS:HG3	1.67	0.74
1:D:70:THR:OG1	1:D:73:PRO:HA	1.87	0.74
1:C:210:LEU:HD23	1:C:210:LEU:N	2.02	0.74
1:E:332:PRO:HG3	1:F:236:PHE:CE2	2.23	0.74
1:B:188:IT1:OP3	2:B:402:AKG:H41	1.87	0.74
1:A:376:LEU:O	1:A:380:ILE:HD12	1.85	0.74
1:H:247:TYR:HB3	3:H:394:HOH:O	1.87	0.74
1:G:124:THR:HG22	1:G:125:ASP:H	1.52	0.74
1:B:30:MET:HG2	1:B:250:ARG:HD2	1.69	0.74
1:F:315:ILE:HD13	1:F:315:ILE:N	2.02	0.74
1:B:119:LEU:HD23	1:B:148:ILE:HD12	1.70	0.74
1:F:162:GLU:HG3	1:F:188:IT1:O3	1.88	0.73
1:C:152:ARG:HB2	1:C:154:ILE:CD1	2.18	0.73
1:B:256:GLY:O	1:B:260:ILE:HD12	1.87	0.73
1:G:314:VAL:CG1	1:G:319:LEU:HD11	2.16	0.73
1:F:111:THR:CG2	1:F:294:GLN:NE2	2.51	0.73
1:D:322:ASN:HD22	1:D:322:ASN:N	1.87	0.73
1:F:222:PRO:HG2	1:F:225:ASN:CB	2.12	0.73
1:F:207:HIS:CE1	1:F:222:PRO:HG3	2.23	0.73
1:E:265:LYS:HG2	1:E:269:PHE:CE1	2.24	0.73
1:G:376:LEU:O	1:G:380:ILE:HG13	1.89	0.73
1:B:268:ARG:HA	1:B:271:SER:OG	1.88	0.73
1:C:149:ILE:HG22	1:C:149:ILE:O	1.89	0.73
1:F:383:LEU:HD11	1:F:387:LEU:CD1	2.19	0.72
1:A:16:TYR:HE1	1:B:23:LEU:HD22	1.53	0.72
1:B:70:THR:OG1	1:B:73:PRO:HA	1.89	0.72
1:C:152:ARG:NH2	1:C:152:ARG:CG	2.32	0.72
1:G:161:CYS:HB2	1:G:188:IT1:C3	2.19	0.72
1:H:145:ILE:O	1:H:149:ILE:HD12	1.89	0.72
1:H:20:GLN:NE2	1:H:24:ASP:OD2	2.22	0.72
1:H:387:LEU:O	1:H:388:LYS:HD2	1.90	0.72
1:F:287:HIS:HE1	1:F:289:TYR:CZ	2.08	0.72
1:G:266:LEU:HB3	1:G:267:PRO:CD	2.19	0.72
1:H:32:GLU:H	1:H:32:GLU:CD	1.93	0.72
1:H:266:LEU:HB3	1:H:267:PRO:CD	2.20	0.72
1:B:81:ILE:HD11	1:B:131:LEU:HB2	1.72	0.71
1:D:106:ASP:HB2	1:D:356:VAL:HA	1.72	0.71
1:F:362:LEU:O	1:F:362:LEU:HD23	1.89	0.71
1:C:84:PRO:CA	1:C:114:ILE:HD12	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:HIS:CG	1:H:288:PRO:HD2	2.26	0.71
1:G:149:ILE:O	1:G:152:ARG:HG3	1.89	0.71
1:E:266:LEU:N	1:E:267:PRO:HD2	2.05	0.71
1:A:308:ILE:HB	1:A:365:ASN:HB3	1.71	0.71
1:F:224:LYS:HA	1:F:229:GLY:O	1.91	0.71
1:F:340:LYS:NZ	3:F:396:HOH:O	2.22	0.71
1:B:115:ASP:HB3	1:B:118:SER:HB2	1.73	0.71
1:H:287:HIS:NE2	1:H:290:LEU:HD12	2.05	0.71
1:A:289:TYR:HA	1:A:309:LYS:HD2	1.73	0.71
1:E:30:MET:HG3	1:E:34:VAL:HG11	1.72	0.71
1:C:280:PHE:CZ	1:C:304:PHE:HB3	2.26	0.71
1:D:54:SER:OG	1:D:58:THR:HG21	1.91	0.71
1:B:235:GLN:O	1:B:239:SER:HB2	1.91	0.71
1:F:101:ARG:NH1	1:F:349:ASP:OD1	2.22	0.71
1:B:53:VAL:CA	1:B:251:PRO:HG3	2.20	0.71
1:G:222:PRO:CD	1:G:225:ASN:HB3	2.18	0.70
1:H:326:ALA:HB1	1:H:382:TYR:OH	1.91	0.70
1:B:376:LEU:HB3	1:B:379:GLU:HG3	1.71	0.70
1:G:213:ARG:HD2	1:G:251:PRO:HD2	1.73	0.70
1:A:384:ARG:NH1	1:A:384:ARG:O	2.23	0.70
1:D:331:ARG:HB2	1:D:332:PRO:CD	2.21	0.70
1:E:385:GLU:HA	1:E:385:GLU:OE1	1.91	0.70
1:F:384:ARG:O	1:F:384:ARG:HG3	1.92	0.70
1:B:48:LYS:N	1:B:201:ASP:OD1	2.24	0.70
1:F:26:LYS:HB3	1:F:27:MET:HE1	1.73	0.70
1:F:116:ILE:HG22	1:F:117:GLU:N	2.05	0.70
1:H:266:LEU:O	1:H:270:ILE:HD12	1.92	0.70
1:F:82:ILE:HD12	1:F:127:THR:CG2	2.22	0.70
1:E:221:LEU:O	1:E:231:LYS:HE2	1.92	0.70
1:F:83:VAL:HG12	1:F:131:LEU:HB3	1.74	0.70
1:B:303:GLY:HA3	1:B:368:PHE:CZ	2.27	0.70
1:F:383:LEU:CD1	1:F:387:LEU:HD12	2.22	0.69
1:E:48:LYS:HB2	1:E:201:ASP:HA	1.72	0.69
1:F:6:LEU:HD12	1:F:329:GLU:HG2	1.74	0.69
1:H:70:THR:HG21	1:H:74:ARG:HE	1.56	0.69
1:C:274:ARG:HG2	1:C:274:ARG:NH1	2.06	0.69
1:C:6:LEU:HD12	1:C:329:GLU:HB3	1.73	0.69
1:G:281:LEU:O	1:G:285:LYS:HB3	1.92	0.69
1:E:34:VAL:O	1:E:38:GLU:HG3	1.93	0.69
1:D:306:PHE:HB2	1:D:367:LEU:CD1	2.21	0.69
1:E:278:GLU:HA	1:E:281:LEU:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LYS:N	1:C:201:ASP:OD1	2.23	0.69
1:D:284:PHE:CZ	1:D:384:ARG:HA	2.28	0.69
1:D:363:ASP:OD2	1:D:364:LYS:HE3	1.92	0.69
1:H:81:ILE:HD11	1:H:131:LEU:CB	2.23	0.69
1:H:318:GLN:O	1:H:322:ASN:ND2	2.26	0.69
1:C:41:PHE:O	1:C:45:PHE:HD1	1.76	0.69
1:G:33:TYR:HB2	1:G:253:GLU:OE2	1.91	0.69
1:E:331:ARG:HG3	1:E:332:PRO:O	1.92	0.69
1:H:272:VAL:HG11	1:H:373:GLN:O	1.92	0.69
1:B:83:VAL:HG12	1:B:131:LEU:HB3	1.75	0.69
1:C:277:ALA:O	1:C:280:PHE:HB3	1.93	0.69
1:C:80:GLU:HB3	1:C:126:SER:O	1.93	0.69
1:F:140:ASN:HB2	1:F:142:PHE:CE2	2.27	0.69
1:C:6:LEU:HD12	1:C:329:GLU:CG	2.23	0.69
1:E:269:PHE:O	1:E:273:ARG:HG3	1.93	0.69
1:F:383:LEU:O	1:F:383:LEU:HD12	1.93	0.68
1:A:362:LEU:HD23	1:A:363:ASP:N	2.08	0.68
1:H:285:LYS:NZ	1:H:285:LYS:HB2	1.99	0.68
1:F:384:ARG:HG3	1:F:384:ARG:NH1	2.05	0.68
1:F:142:PHE:HA	1:F:145:ILE:HG13	1.75	0.68
1:G:62:LEU:HD11	1:G:249:VAL:CG2	2.23	0.68
1:C:266:LEU:HB3	1:C:267:PRO:HD3	1.74	0.68
1:E:28:PHE:HB2	1:F:193:MET:HG2	1.76	0.68
1:B:5:PRO:HA	1:B:329:GLU:OE1	1.93	0.68
1:C:48:LYS:HB2	1:C:201:ASP:HA	1.76	0.68
1:B:108:ASP:C	1:B:108:ASP:OD1	2.30	0.68
1:E:12:ASP:OD1	1:E:13:ASP:N	2.27	0.68
1:A:207:HIS:ND1	1:A:226:LYS:HB2	2.09	0.68
1:D:334:VAL:HG12	1:D:335:THR:HG23	1.75	0.68
1:F:26:LYS:HB3	1:F:27:MET:HE2	1.75	0.67
1:B:108:ASP:OD1	1:B:110:ASN:N	2.25	0.67
1:D:40:GLN:OE1	1:D:260:ILE:HG23	1.93	0.67
1:E:117:GLU:O	1:E:120:LYS:HB3	1.93	0.67
1:E:310:LYS:O	1:E:311:ASP:HB2	1.94	0.67
1:H:170:ASN:N	1:H:170:ASN:HD22	1.93	0.67
1:G:5:PRO:HA	1:G:329:GLU:HB2	1.76	0.67
1:A:16:TYR:CE1	1:B:23:LEU:HD22	2.29	0.67
1:F:315:ILE:CD1	1:F:315:ILE:H	2.05	0.67
1:F:119:LEU:HD12	1:F:123:VAL:HG23	1.77	0.67
1:D:124:THR:CG2	1:D:125:ASP:H	2.07	0.67
1:D:276:ASN:ND2	1:D:376:LEU:HD12	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:PRO:HD2	1:G:225:ASN:CB	2.20	0.67
1:G:6:LEU:HD12	1:G:329:GLU:CG	2.19	0.67
1:E:315:ILE:HD11	1:E:318:GLN:CB	2.25	0.67
1:C:322:ASN:ND2	1:C:322:ASN:N	2.43	0.67
1:A:204:GLU:HB2	1:A:226:LYS:HG3	1.77	0.67
1:H:124:THR:HG22	1:H:126:SER:N	2.02	0.66
1:G:124:THR:CG2	1:G:125:ASP:H	2.08	0.66
1:H:254:MET:O	1:H:257:ALA:N	2.25	0.66
1:C:303:GLY:HA3	1:C:368:PHE:CE2	2.30	0.66
1:F:18:ALA:O	1:F:22:VAL:HG23	1.95	0.66
1:B:291:ASP:HB2	1:B:307:ILE:HG22	1.77	0.66
1:E:23:LEU:HD21	1:F:19:ILE:HD12	1.76	0.66
1:G:274:ARG:HH11	1:G:274:ARG:CG	2.07	0.66
1:G:138:ASN:HA	1:G:299:SER:HB2	1.77	0.66
1:C:57:SER:HB2	1:D:248:ASN:HB3	1.78	0.66
1:E:12:ASP:OD1	1:E:12:ASP:C	2.34	0.66
1:F:310:LYS:O	1:F:311:ASP:HB2	1.96	0.66
1:E:303:GLY:HA3	1:E:368:PHE:CE1	2.30	0.66
1:G:124:THR:CG2	1:G:125:ASP:N	2.57	0.66
1:E:360:GLU:HA	1:E:363:ASP:HB2	1.78	0.66
1:G:380:ILE:O	1:G:383:LEU:HB3	1.96	0.66
1:E:108:ASP:OD1	1:E:110:ASN:N	2.28	0.66
1:F:124:THR:HG22	1:F:125:ASP:N	2.11	0.66
1:H:284:PHE:CZ	1:H:387:LEU:HD12	2.29	0.66
1:F:287:HIS:CD2	1:F:288:PRO:HD2	2.31	0.66
1:B:209:LEU:HD23	1:B:209:LEU:N	2.09	0.66
1:F:25:SER:O	1:F:27:MET:HG2	1.96	0.65
1:H:320:VAL:HG13	1:H:330:CYS:SG	2.36	0.65
1:A:148:ILE:O	1:A:152:ARG:NH2	2.29	0.65
1:D:202:ASP:OD1	1:D:205:ILE:HG12	1.96	0.65
1:H:145:ILE:HG22	1:H:149:ILE:HD13	1.79	0.65
1:C:331:ARG:HD3	1:C:368:PHE:CD1	2.31	0.65
1:F:23:LEU:HD23	1:F:28:PHE:HE1	1.61	0.65
1:A:71:LYS:HE3	1:A:71:LYS:HA	1.77	0.65
1:B:280:PHE:HD2	1:B:281:LEU:HD23	1.61	0.65
1:F:129:ALA:HA	1:F:154:ILE:HG22	1.79	0.65
1:D:42:ALA:HB3	3:D:439:HOH:O	1.97	0.65
1:B:376:LEU:O	1:B:379:GLU:HG2	1.95	0.65
1:H:287:HIS:ND1	1:H:288:PRO:HD2	2.12	0.65
1:D:217:TRP:HB2	3:D:427:HOH:O	1.97	0.65
1:C:67:LEU:HD13	1:C:75:LEU:CD1	2.24	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:ILE:O	1:F:152:ARG:HB2	1.97	0.64
1:B:375:GLU:O	1:B:376:LEU:HD23	1.97	0.64
1:A:171:LYS:HD3	1:A:175:THR:OG1	1.97	0.64
1:G:192:THR:O	1:G:193:MET:HB2	1.97	0.64
1:D:289:TYR:CG	1:D:314:VAL:HG21	2.32	0.64
1:C:70:THR:HG21	1:C:74:ARG:HE	1.62	0.64
1:F:285:LYS:HG3	1:F:286:ASP:N	2.12	0.64
1:B:82:ILE:HD12	1:B:127:THR:HG23	1.78	0.64
1:A:319:LEU:O	1:A:323:LEU:HG	1.98	0.64
1:E:106:ASP:OD1	1:E:358:ASN:HB2	1.97	0.64
1:C:308:ILE:HD12	1:C:365:ASN:O	1.97	0.64
1:E:242:PHE:HE2	1:F:335:THR:HG21	1.63	0.64
1:H:224:LYS:HA	1:H:229:GLY:O	1.98	0.64
1:F:281:LEU:CD2	1:F:292:VAL:HG21	2.28	0.64
1:G:266:LEU:O	1:G:269:PHE:HB2	1.96	0.64
1:H:255:SER:CA	1:H:258:ILE:HD12	2.26	0.64
1:H:20:GLN:HE22	1:H:24:ASP:CG	2.01	0.64
1:G:55:SER:HB2	3:G:420:HOH:O	1.98	0.64
1:C:152:ARG:HB2	1:C:154:ILE:CG1	2.27	0.64
1:E:333:ILE:HG21	1:E:362:LEU:HD11	1.79	0.64
1:B:24:ASP:N	1:B:24:ASP:OD1	2.28	0.64
1:F:130:ILE:HG13	1:F:154:ILE:HG21	1.79	0.64
1:F:76:LYS:N	1:F:79:ASP:OD2	2.27	0.64
1:B:378:ASP:O	1:B:381:ASP:HB2	1.98	0.64
1:H:12:ASP:HB3	1:H:14:LEU:CD1	2.24	0.64
1:D:355:ASN:HD22	1:D:355:ASN:C	2.01	0.64
1:C:152:ARG:HG3	1:C:154:ILE:HD11	1.80	0.63
1:B:320:VAL:O	1:B:324:ASN:ND2	2.32	0.63
1:E:44:THR:HB	1:E:45:PHE:CD1	2.32	0.63
1:H:384:ARG:O	1:H:384:ARG:NH1	2.31	0.63
1:B:64:ILE:HG22	1:B:65:ALA:N	2.12	0.63
1:E:36:GLN:CG	1:E:260:ILE:HD11	2.28	0.63
1:A:105:VAL:HB	1:A:114:ILE:HD11	1.80	0.63
1:D:15:GLU:O	1:D:18:ALA:HB3	1.99	0.63
1:G:274:ARG:NH2	1:G:298:GLU:HG2	2.12	0.63
1:G:161:CYS:HB2	1:G:188:IT1:C2	2.28	0.63
1:F:266:LEU:HB3	1:F:267:PRO:CD	2.29	0.63
1:B:20:GLN:O	1:B:23:LEU:HB2	1.98	0.63
1:E:28:PHE:CB	1:F:193:MET:HG2	2.29	0.63
1:E:286:ASP:O	1:E:288:PRO:HD3	1.98	0.63
1:F:129:ALA:HA	1:F:154:ILE:CG2	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HD2	1:A:176:PHE:CE2	2.34	0.63
1:F:254:MET:O	1:F:258:ILE:HG13	1.98	0.63
1:A:63:MET:HG3	1:A:179:MET:HE3	1.80	0.63
1:G:72:LYS:HD2	1:G:73:PRO:HD2	1.80	0.63
1:A:96:GLN:HB2	1:A:348:PHE:CE2	2.34	0.63
1:B:205:ILE:O	1:B:209:LEU:HG	1.99	0.63
1:D:287:HIS:HE1	1:D:289:TYR:CE1	2.16	0.63
1:H:41:PHE:O	1:H:44:THR:HB	1.98	0.63
1:D:193:MET:HA	3:D:444:HOH:O	1.99	0.62
1:C:144:GLU:O	1:C:145:ILE:C	2.37	0.62
1:H:145:ILE:HG22	1:H:149:ILE:CD1	2.29	0.62
1:A:57:SER:HB2	1:B:248:ASN:HB3	1.81	0.62
1:H:203:GLU:OE1	1:H:226:LYS:HE2	1.98	0.62
1:G:52:MET:HG2	1:G:251:PRO:HG3	1.81	0.62
1:G:143:ASP:OD2	1:G:168:PHE:HE2	1.83	0.62
1:H:11:TRP:HA	1:H:15:GLU:OE1	1.99	0.62
1:C:135:LEU:HD11	1:C:334:VAL:HG21	1.80	0.62
1:G:376:LEU:HA	1:G:379:GLU:OE1	2.00	0.62
1:F:106:ASP:OD2	1:F:358:ASN:HB2	1.99	0.62
1:G:50:ALA:CB	1:G:199:VAL:HG12	2.29	0.62
1:E:93:TYR:HB2	1:E:94:PRO:HD3	1.81	0.62
1:G:48:LYS:HB2	1:G:201:ASP:HA	1.82	0.62
1:D:34:VAL:HG23	1:D:253:GLU:OE1	2.00	0.62
1:H:124:THR:CG2	1:H:126:SER:H	2.04	0.62
1:H:287:HIS:CE1	1:H:290:LEU:HD12	2.34	0.62
1:E:332:PRO:HG3	1:F:236:PHE:CD2	2.34	0.62
1:C:379:GLU:CD	1:C:379:GLU:H	2.02	0.62
1:E:360:GLU:O	1:E:363:ASP:HB3	2.00	0.62
1:D:70:THR:HG21	1:D:74:ARG:NE	2.15	0.62
1:D:14:LEU:HD12	1:D:265:LYS:HZ1	1.64	0.62
1:D:266:LEU:HB3	1:D:267:PRO:HD3	1.81	0.62
1:G:158:GLU:OE2	1:G:174:GLY:N	2.32	0.62
1:G:179:MET:HG2	1:G:198:ILE:CG2	2.29	0.62
1:G:334:VAL:HG12	1:G:335:THR:HG23	1.81	0.62
1:F:192:THR:O	1:F:193:MET:HB2	1.99	0.62
1:A:161:CYS:HB2	1:A:188:IT1:C2	2.30	0.62
1:F:289:TYR:C	1:F:309:LYS:HG3	2.20	0.62
1:F:285:LYS:HA	3:F:430:HOH:O	2.00	0.62
1:G:363:ASP:OD2	1:G:364:LYS:HE2	2.00	0.61
1:D:305:SER:HB2	1:D:333:ILE:HD11	1.82	0.61
1:E:242:PHE:CE2	1:F:335:THR:HG21	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:PHE:HE2	1:H:335:THR:HG21	1.64	0.61
1:G:279:TYR:CZ	1:G:283:LYS:HE2	2.35	0.61
1:F:34:VAL:HG23	1:F:253:GLU:OE1	2.01	0.61
1:G:266:LEU:O	1:G:269:PHE:N	2.34	0.61
1:C:83:VAL:HG12	1:C:131:LEU:HB3	1.82	0.61
1:H:171:LYS:HG2	1:H:176:PHE:CE1	2.36	0.61
1:C:20:GLN:HA	1:C:23:LEU:HD12	1.83	0.61
1:A:106:ASP:OD2	1:A:356:VAL:HA	2.00	0.61
1:G:162:GLU:HG3	1:G:188:IT1:O3	2.00	0.61
1:F:223:LYS:O	1:F:230:VAL:HA	2.01	0.61
1:G:116:ILE:O	1:G:120:LYS:HG3	2.01	0.61
1:F:70:THR:HG21	1:F:74:ARG:HE	1.66	0.61
1:A:71:LYS:HE2	1:A:71:LYS:HA	1.82	0.61
1:G:33:TYR:N	1:G:253:GLU:OE2	2.33	0.61
1:G:168:PHE:O	1:G:171:LYS:N	2.34	0.61
1:C:81:ILE:HD11	1:C:131:LEU:HB2	1.82	0.61
1:E:230:VAL:HG13	1:E:230:VAL:O	2.01	0.61
1:A:67:LEU:HD22	1:A:74:ARG:HG3	1.83	0.61
1:B:119:LEU:HD23	1:B:148:ILE:CD1	2.30	0.61
1:C:202:ASP:HB3	1:C:205:ILE:HG13	1.82	0.61
1:A:253:GLU:OE1	1:A:253:GLU:HA	2.01	0.61
1:F:23:LEU:O	1:F:26:LYS:NZ	2.31	0.60
1:B:265:LYS:O	1:B:268:ARG:HG3	2.01	0.60
1:F:222:PRO:CG	1:F:225:ASN:HB3	2.18	0.60
1:A:331:ARG:HD3	1:A:368:PHE:CD1	2.36	0.60
1:E:204:GLU:O	1:E:208:ILE:HG13	1.99	0.60
1:B:287:HIS:ND1	1:B:288:PRO:HD2	2.16	0.60
1:B:20:GLN:HA	1:B:20:GLN:OE1	2.01	0.60
1:F:138:ASN:HA	1:F:299:SER:HB2	1.84	0.60
1:C:34:VAL:O	1:C:37:TYR:HB3	2.02	0.60
1:H:303:GLY:HA3	1:H:368:PHE:CE2	2.36	0.60
1:G:149:ILE:HG22	1:G:150:GLY:N	2.15	0.60
1:C:328:ILE:HD13	1:C:383:LEU:CD1	2.31	0.60
1:A:218:THR:O	1:A:221:LEU:HB2	2.01	0.60
1:H:287:HIS:CE1	1:H:290:LEU:HG	2.36	0.60
1:H:20:GLN:NE2	1:H:24:ASP:CG	2.55	0.60
1:D:204:GLU:HG3	1:D:226:LYS:HB3	1.82	0.60
1:B:372:HIS:HD2	1:B:376:LEU:HD11	1.66	0.60
1:H:278:GLU:HA	1:H:281:LEU:CD1	2.29	0.60
1:G:208:ILE:O	1:G:211:CYS:HB3	2.02	0.60
1:F:383:LEU:C	1:F:383:LEU:HD12	2.21	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HA	1:B:28:PHE:CZ	2.37	0.60
1:E:281:LEU:O	1:E:282:ASP:C	2.40	0.60
1:D:218:THR:O	1:D:221:LEU:HB2	2.02	0.60
1:A:6:LEU:HD21	1:A:329:GLU:O	2.03	0.59
1:H:93:TYR:O	1:H:96:GLN:N	2.35	0.59
1:G:12:ASP:HB2	1:G:265:LYS:NZ	2.17	0.59
1:B:266:LEU:O	1:B:269:PHE:HB2	2.03	0.59
1:H:203:GLU:O	1:H:206:TYR:HB3	2.01	0.59
1:A:376:LEU:C	1:A:380:ILE:HD12	2.22	0.59
1:D:382:TYR:O	1:D:385:GLU:HB2	2.02	0.59
1:C:24:ASP:N	1:C:24:ASP:OD1	2.33	0.59
1:F:204:GLU:O	1:F:208:ILE:HG13	2.03	0.59
1:H:287:HIS:CE1	1:H:289:TYR:CE1	2.90	0.59
1:G:156:LEU:HD23	1:G:177:GLY:HA2	1.83	0.59
1:D:333:ILE:HG21	1:D:362:LEU:HD11	1.84	0.59
1:B:140:ASN:HB2	1:B:142:PHE:CZ	2.37	0.59
1:B:158:GLU:OE2	1:B:176:PHE:HB2	2.01	0.59
1:F:315:ILE:HG12	1:F:315:ILE:O	2.02	0.59
1:D:283:LYS:O	1:D:384:ARG:HD3	2.02	0.59
1:F:156:LEU:HD12	1:F:157:LEU:H	1.67	0.59
1:A:319:LEU:HD23	1:A:319:LEU:N	2.17	0.59
1:G:159:ASP:O	3:G:392:HOH:O	2.17	0.59
1:D:124:THR:CG2	1:D:125:ASP:N	2.64	0.59
1:G:20:GLN:O	1:G:23:LEU:HB2	2.03	0.59
1:D:184:SER:HB3	1:D:190:ILE:HG13	1.85	0.59
1:H:266:LEU:O	1:H:269:PHE:HB2	2.01	0.59
1:D:70:THR:HG21	1:D:74:ARG:HE	1.68	0.59
1:H:272:VAL:O	1:H:276:ASN:ND2	2.36	0.59
1:B:248:ASN:OD1	1:B:248:ASN:C	2.42	0.59
1:G:144:GLU:OE1	1:G:144:GLU:HA	2.03	0.59
1:G:37:TYR:CE1	1:G:259:GLY:HA3	2.38	0.59
1:G:140:ASN:HB3	1:G:145:ILE:HD11	1.85	0.59
1:H:279:TYR:CD2	1:H:380:ILE:HG21	2.38	0.59
1:A:6:LEU:O	1:A:372:HIS:NE2	2.36	0.58
1:C:19:ILE:O	1:C:23:LEU:HG	2.03	0.58
1:F:337:ASN:O	1:F:340:LYS:HG2	2.02	0.58
1:G:168:PHE:O	1:G:169:ASN:C	2.40	0.58
1:B:145:ILE:O	1:B:149:ILE:HD12	2.02	0.58
1:D:88:TRP:CZ2	2:D:404:AKG:H41	2.38	0.58
1:B:280:PHE:CD2	1:B:281:LEU:HD23	2.38	0.58
1:H:168:PHE:CE2	1:H:169:ASN:ND2	2.65	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ARG:HB3	1:D:155:ILE:HD11	1.84	0.58
1:F:362:LEU:C	1:F:362:LEU:HD23	2.23	0.58
1:E:36:GLN:HG3	1:E:260:ILE:HD11	1.84	0.58
1:F:331:ARG:HB2	1:F:332:PRO:HD2	1.83	0.58
1:D:206:TYR:CZ	1:D:210:LEU:HD11	2.38	0.58
1:H:124:THR:CG2	1:H:125:ASP:N	2.65	0.58
1:A:289:TYR:CA	1:A:309:LYS:HD2	2.33	0.58
1:E:268:ARG:HH21	1:E:268:ARG:CG	2.17	0.58
1:E:40:GLN:O	1:E:44:THR:OG1	2.21	0.58
1:F:185:PHE:O	1:F:186:TYR:C	2.41	0.58
1:H:287:HIS:CE1	1:H:288:PRO:HD2	2.39	0.58
1:A:217:TRP:NE1	1:A:219:ARG:HB2	2.19	0.58
1:F:161:CYS:HB2	1:F:188:IT1:C2A	2.34	0.57
1:F:156:LEU:HD12	1:F:157:LEU:N	2.18	0.57
1:B:82:ILE:HD12	1:B:127:THR:CG2	2.33	0.57
1:C:215:HIS:HD1	1:D:88:TRP:HE1	1.51	0.57
1:G:2:ILE:HD13	1:G:329:GLU:OE2	2.05	0.57
1:A:6:LEU:HG	1:A:329:GLU:CG	2.30	0.57
1:H:170:ASN:N	1:H:170:ASN:ND2	2.52	0.57
1:H:243:VAL:O	1:H:244:LEU:HD13	2.05	0.57
1:D:92:TYR:O	1:D:95:LEU:HB2	2.04	0.57
1:B:224:LYS:HA	1:B:229:GLY:O	2.03	0.57
1:C:6:LEU:HD12	1:C:329:GLU:CB	2.34	0.57
1:F:53:VAL:HG23	1:F:55:SER:O	2.03	0.57
1:B:287:HIS:CD2	1:B:288:PRO:HD2	2.39	0.57
1:F:23:LEU:HD23	1:F:28:PHE:CE1	2.38	0.57
1:A:204:GLU:HB2	1:A:226:LYS:CG	2.33	0.57
1:G:11:TRP:HA	1:G:15:GLU:OE1	2.04	0.57
1:B:109:ILE:O	1:B:109:ILE:HG13	2.04	0.57
1:A:84:PRO:HA	1:A:105:VAL:O	2.04	0.57
1:E:372:HIS:H	1:E:376:LEU:HD11	1.68	0.57
1:C:76:LYS:O	1:C:79:ASP:HB2	2.04	0.57
1:C:308:ILE:HG21	1:C:314:VAL:HG22	1.86	0.57
1:F:337:ASN:HB2	1:F:363:ASP:HB2	1.87	0.57
1:F:106:ASP:CG	1:F:358:ASN:HB2	2.25	0.57
1:H:56:GLY:O	1:H:59:ALA:HB3	2.03	0.57
1:G:160:ASN:HA	3:G:392:HOH:O	2.04	0.57
1:G:160:ASN:HB3	1:G:181:THR:O	2.05	0.57
1:G:261:GLU:O	1:G:264:LYS:HB2	2.05	0.57
1:B:17:LYS:O	1:B:21:SER:OG	2.23	0.57
1:F:382:TYR:O	1:F:386:VAL:HG23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:316:ARG:NH1	1:H:366:GLY:O	2.34	0.57
1:H:111:THR:O	1:H:112:LEU:HB2	2.05	0.57
1:C:192:THR:O	1:C:193:MET:HB2	2.05	0.57
1:H:315:ILE:HD13	1:H:315:ILE:N	2.20	0.57
1:H:279:TYR:CE2	1:H:380:ILE:HG21	2.40	0.57
1:H:36:GLN:HB3	1:H:260:ILE:HD11	1.87	0.57
1:A:265:LYS:C	1:A:267:PRO:HD2	2.25	0.57
1:A:111:THR:O	1:A:112:LEU:HB2	2.05	0.57
1:E:350:TYR:H	1:E:350:TYR:HD1	1.52	0.57
1:F:336:GLY:HA3	1:F:363:ASP:OD1	2.05	0.56
1:G:50:ALA:HB2	1:G:199:VAL:HG12	1.86	0.56
1:F:96:GLN:HE21	1:F:347:TYR:HB3	1.70	0.56
1:G:32:GLU:O	1:G:36:GLN:N	2.34	0.56
1:D:120:LYS:CA	1:D:148:ILE:HD13	2.34	0.56
1:F:188:IT1:OP3	2:F:405:AKG:O3	2.23	0.56
1:D:292:VAL:HB	3:D:407:HOH:O	2.04	0.56
1:E:289:TYR:HA	1:E:309:LYS:HD2	1.87	0.56
1:A:332:PRO:HD3	1:B:236:PHE:CE1	2.41	0.56
1:H:23:LEU:HA	1:H:28:PHE:HE1	1.70	0.56
1:E:274:ARG:O	1:E:277:ALA:HB3	2.06	0.56
1:H:235:GLN:HG3	1:H:239:SER:OG	2.06	0.56
1:C:222:PRO:HD2	1:C:225:ASN:HB3	1.87	0.56
1:E:207:HIS:O	1:E:210:LEU:HB2	2.06	0.56
1:F:161:CYS:HB2	1:F:188:IT1:H2AB	1.86	0.56
1:H:284:PHE:CZ	1:H:384:ARG:HD2	2.40	0.56
1:C:36:GLN:HG2	1:C:260:ILE:HD11	1.86	0.56
1:D:322:ASN:ND2	1:D:322:ASN:N	2.50	0.56
1:H:119:LEU:HD21	1:H:145:ILE:HD13	1.87	0.56
1:H:190:ILE:HG22	1:H:262:GLN:HB3	1.87	0.56
1:H:288:PRO:HG2	1:H:289:TYR:CE1	2.39	0.56
1:D:280:PHE:HD2	1:D:281:LEU:HD12	1.70	0.56
1:G:268:ARG:O	1:G:272:VAL:HG23	2.06	0.56
1:H:331:ARG:HD3	1:H:368:PHE:CD1	2.40	0.56
1:A:70:THR:HG21	1:A:74:ARG:HE	1.71	0.56
1:H:145:ILE:CG2	1:H:149:ILE:CD1	2.84	0.56
1:B:131:LEU:HD12	1:B:131:LEU:C	2.26	0.56
1:B:93:TYR:HB2	1:B:94:PRO:HD3	1.86	0.56
1:G:88:TRP:HD1	1:G:90:THR:HG1	1.52	0.56
1:B:188:IT1:OP3	2:B:402:AKG:O3	2.24	0.56
1:G:235:GLN:O	1:G:236:PHE:C	2.44	0.56
1:B:309:LYS:O	1:B:312:SER:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:VAL:HG23	1:F:244:LEU:HD12	1.88	0.56
1:B:232:SER:HB3	1:B:238:GLU:OE1	2.05	0.56
1:B:96:GLN:HB2	1:B:348:PHE:CE2	2.41	0.56
1:G:2:ILE:HG23	1:G:327:GLY:O	2.07	0.55
1:E:326:ALA:HB1	1:E:382:TYR:OH	2.06	0.55
1:A:331:ARG:HD3	1:A:368:PHE:CE1	2.42	0.55
1:E:215:HIS:O	1:E:242:PHE:HD1	1.89	0.55
1:H:284:PHE:HE1	1:H:287:HIS:CD2	2.24	0.55
1:C:322:ASN:H	1:C:322:ASN:ND2	2.03	0.55
1:C:223:LYS:O	1:C:230:VAL:HA	2.06	0.55
1:H:202:ASP:HB3	1:H:205:ILE:HG12	1.87	0.55
1:F:217:TRP:C	1:F:217:TRP:CD1	2.79	0.55
1:C:161:CYS:HB2	1:C:188:IT1:C2	2.36	0.55
1:A:337:ASN:O	1:A:340:LYS:HG2	2.06	0.55
1:A:65:ALA:O	1:A:68:PHE:HB2	2.06	0.55
1:G:289:TYR:HA	1:G:309:LYS:HD3	1.89	0.55
1:B:36:GLN:HE22	1:B:40:GLN:HE21	1.53	0.55
1:E:34:VAL:HG12	1:E:35:LYS:N	2.22	0.55
1:F:373:GLN:OE1	1:F:373:GLN:N	2.30	0.55
1:F:316:ARG:O	1:F:320:VAL:HG23	2.06	0.55
1:E:360:GLU:O	1:E:361:TYR:C	2.42	0.55
1:C:57:SER:OG	1:C:188:IT1:OP2	2.16	0.55
1:G:382:TYR:O	1:G:385:GLU:N	2.40	0.55
1:A:141:ASN:O	1:A:145:ILE:HG13	2.07	0.55
1:A:367:LEU:C	1:A:367:LEU:HD12	2.26	0.55
1:C:79:ASP:HB3	1:C:128:LYS:HG3	1.88	0.55
1:A:242:PHE:CE1	1:B:89:SER:HB3	2.42	0.55
1:B:155:ILE:HG22	1:B:156:LEU:N	2.22	0.55
1:G:288:PRO:HG2	1:G:289:TYR:H	1.70	0.55
1:G:108:ASP:OD1	1:G:110:ASN:N	2.36	0.55
1:G:324:ASN:C	1:G:326:ALA:H	2.10	0.55
1:C:103:LYS:HG3	1:C:351:THR:HG23	1.89	0.55
1:B:117:GLU:OE1	1:B:117:GLU:HA	2.07	0.55
1:F:6:LEU:CD1	1:F:329:GLU:HG2	2.37	0.55
1:C:217:TRP:CD2	1:C:219:ARG:HG3	2.42	0.55
1:F:204:GLU:O	1:F:205:ILE:C	2.43	0.54
1:F:82:ILE:CD1	1:F:127:THR:HG21	2.34	0.54
1:E:278:GLU:CA	1:E:281:LEU:HD12	2.36	0.54
1:B:37:TYR:CE1	1:B:263:LEU:HD11	2.42	0.54
1:B:45:PHE:O	1:B:175:THR:HG21	2.06	0.54
1:F:48:LYS:HB3	1:F:49:TYR:CD1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:CA	1:A:71:LYS:CE	2.86	0.54
1:D:284:PHE:CE1	1:D:384:ARG:HB2	2.42	0.54
1:G:262:GLN:NE2	1:G:262:GLN:HA	2.22	0.54
1:A:217:TRP:C	1:A:217:TRP:CD1	2.80	0.54
1:F:218:THR:O	1:F:221:LEU:HB2	2.08	0.54
1:H:266:LEU:C	1:H:270:ILE:HD12	2.27	0.54
1:A:303:GLY:HA3	1:A:368:PHE:CE2	2.43	0.54
1:A:331:ARG:HG3	1:A:368:PHE:HD1	1.72	0.54
1:C:120:LYS:CA	1:C:148:ILE:HD13	2.38	0.54
1:G:379:GLU:H	1:G:379:GLU:CD	2.11	0.54
1:A:235:GLN:O	1:A:236:PHE:C	2.44	0.54
1:B:11:TRP:HE3	1:B:16:TYR:CE1	2.25	0.54
1:A:48:LYS:HB2	1:A:201:ASP:HA	1.89	0.54
1:A:289:TYR:CD1	1:A:290:LEU:HG	2.43	0.54
1:H:32:GLU:OE2	1:H:253:GLU:OE2	2.25	0.54
1:B:379:GLU:CD	1:B:379:GLU:H	2.05	0.54
1:E:192:THR:O	1:E:193:MET:HB2	2.06	0.54
1:B:254:MET:O	1:B:258:ILE:HG13	2.07	0.54
1:D:129:ALA:HA	1:D:155:ILE:O	2.08	0.54
1:G:362:LEU:HD23	1:G:362:LEU:C	2.27	0.54
1:A:338:PHE:HB2	3:A:424:HOH:O	2.07	0.54
1:G:288:PRO:HB2	1:G:289:TYR:HD1	1.72	0.54
1:D:253:GLU:OE1	1:D:253:GLU:HA	2.07	0.54
1:C:167:THR:HA	1:C:171:LYS:O	2.07	0.54
1:C:250:ARG:NH2	1:D:185:PHE:CE1	2.75	0.54
1:D:35:LYS:CB	1:D:35:LYS:NZ	2.70	0.54
1:F:205:ILE:HG22	1:F:209:LEU:CD1	2.38	0.54
1:B:30:MET:HB3	1:B:251:PRO:O	2.07	0.54
1:H:70:THR:OG1	1:H:73:PRO:HA	2.08	0.54
1:F:96:GLN:NE2	1:F:347:TYR:HB3	2.22	0.54
1:C:132:THR:HB	3:C:410:HOH:O	2.07	0.54
1:H:106:ASP:OD1	1:H:358:ASN:HB2	2.08	0.54
1:F:58:THR:HG21	1:F:249:VAL:CG1	2.38	0.54
1:A:47:SER:HB2	3:A:400:HOH:O	2.08	0.54
1:D:56:GLY:HA3	1:D:183:SER:HB2	1.90	0.54
1:C:303:GLY:HA3	1:C:368:PHE:CZ	2.42	0.54
1:C:58:THR:HG21	1:C:249:VAL:CG1	2.38	0.54
1:B:111:THR:O	1:B:112:LEU:HB2	2.08	0.54
1:G:28:PHE:O	1:G:253:GLU:HB2	2.08	0.54
1:E:108:ASP:OD1	1:E:108:ASP:C	2.45	0.54
1:G:59:ALA:HA	1:G:198:ILE:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:CG	1:A:356:VAL:HA	2.29	0.54
1:F:37:TYR:CE1	1:F:259:GLY:HA3	2.43	0.54
1:H:101:ARG:NH2	1:H:351:THR:HB	2.23	0.54
1:F:103:LYS:HA	1:F:351:THR:O	2.07	0.54
1:F:219:ARG:NH2	1:F:240:PHE:CE1	2.76	0.54
1:E:360:GLU:HA	1:E:363:ASP:CB	2.38	0.53
1:F:124:THR:HG22	1:F:125:ASP:H	1.72	0.53
1:F:306:PHE:HB2	1:F:367:LEU:HD13	1.89	0.53
1:F:277:ALA:O	1:F:280:PHE:HB3	2.08	0.53
1:G:287:HIS:CG	1:G:288:PRO:CD	2.90	0.53
1:A:93:TYR:CB	1:A:94:PRO:HD3	2.31	0.53
1:B:188:IT1:C4A	2:B:402:AKG:O5	2.56	0.53
1:F:305:SER:HB2	1:F:333:ILE:HD13	1.90	0.53
1:G:331:ARG:CB	1:G:332:PRO:CD	2.86	0.53
1:F:363:ASP:C	1:F:364:LYS:HD3	2.28	0.53
1:G:144:GLU:HA	1:G:147:LYS:HD3	1.91	0.53
1:A:136:LEU:O	1:A:302:PHE:N	2.36	0.53
1:F:315:ILE:CD1	1:F:315:ILE:N	2.69	0.53
1:C:67:LEU:HD12	1:C:75:LEU:HD12	1.90	0.53
1:E:303:GLY:CA	1:E:368:PHE:CE1	2.92	0.53
1:G:285:LYS:HG3	1:G:286:ASP:N	2.23	0.53
1:H:119:LEU:CD2	1:H:145:ILE:HD13	2.37	0.53
1:E:32:GLU:O	1:E:36:GLN:HB3	2.08	0.53
1:G:217:TRP:HD1	1:G:217:TRP:O	1.91	0.53
1:H:337:ASN:O	1:H:340:LYS:HD3	2.09	0.53
1:G:222:PRO:HG2	1:G:224:LYS:O	2.08	0.53
1:H:277:ALA:O	1:H:281:LEU:HD12	2.08	0.53
1:F:289:TYR:HA	1:F:309:LYS:HD2	1.91	0.53
1:H:25:SER:O	1:H:26:LYS:HB2	2.09	0.53
1:F:305:SER:HB2	1:F:333:ILE:CD1	2.38	0.53
1:B:375:GLU:C	1:B:376:LEU:HD23	2.29	0.53
1:E:383:LEU:HG	1:E:387:LEU:HD12	1.90	0.53
1:F:388:LYS:HE3	1:F:388:LYS:HA	1.91	0.53
1:H:93:TYR:N	1:H:94:PRO:CD	2.71	0.53
1:F:331:ARG:HB2	1:F:332:PRO:CD	2.38	0.53
1:B:315:ILE:O	1:B:318:GLN:HB2	2.08	0.53
1:F:308:ILE:HB	1:F:365:ASN:HB3	1.90	0.53
1:F:202:ASP:OD1	1:F:205:ILE:HG12	2.08	0.53
1:H:287:HIS:ND1	1:H:290:LEU:HB2	2.23	0.53
3:G:395:HOH:O	1:H:93:TYR:HB2	2.09	0.53
1:E:96:GLN:HB2	1:E:348:PHE:CE2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:VAL:HG23	1:E:356:VAL:O	2.09	0.53
1:C:50:ALA:HA	1:C:198:ILE:O	2.09	0.53
1:C:152:ARG:NH2	1:C:152:ARG:HG2	2.14	0.53
1:D:333:ILE:O	1:D:333:ILE:HG22	2.06	0.53
1:D:188:IT1:OP3	2:D:404:AKG:O3	2.27	0.53
1:A:78:GLY:N	1:A:99:GLY:O	2.38	0.53
1:C:67:LEU:CD1	1:C:75:LEU:CD1	2.83	0.53
1:F:32:GLU:N	1:F:253:GLU:OE2	2.42	0.53
1:F:167:THR:HG23	1:F:171:LYS:O	2.09	0.53
1:A:315:ILE:HD12	1:A:315:ILE:H	1.73	0.53
1:C:297:GLY:C	1:C:298:GLU:HG3	2.29	0.53
1:G:266:LEU:HA	1:G:269:PHE:HB2	1.91	0.52
1:C:308:ILE:CG2	1:C:314:VAL:HG22	2.39	0.52
1:F:5:PRO:HA	1:F:329:GLU:HB2	1.91	0.52
1:F:167:THR:HG22	1:F:168:PHE:N	2.23	0.52
1:G:22:VAL:O	1:G:25:SER:OG	2.20	0.52
1:D:273:ARG:NH1	1:D:301:TRP:O	2.42	0.52
1:D:161:CYS:HB3	1:D:183:SER:HB3	1.92	0.52
1:C:122:ALA:HB2	1:C:353:HIS:CD2	2.44	0.52
1:G:120:LYS:HA	1:G:148:ILE:CD1	2.37	0.52
1:H:131:LEU:C	1:H:131:LEU:HD12	2.30	0.52
1:A:171:LYS:HG2	1:A:172:CYS:N	2.25	0.52
1:E:36:GLN:HG2	1:E:260:ILE:HD11	1.90	0.52
1:B:168:PHE:O	1:B:169:ASN:HB2	2.08	0.52
1:C:141:ASN:O	1:C:145:ILE:HG12	2.10	0.52
1:A:171:LYS:HB3	1:A:176:PHE:CZ	2.45	0.52
1:A:93:TYR:N	1:A:94:PRO:CD	2.73	0.52
1:F:111:THR:O	1:F:112:LEU:HB2	2.09	0.52
1:G:63:MET:CE	1:G:157:LEU:HD13	2.40	0.52
1:G:26:LYS:HE2	1:H:16:TYR:OH	2.09	0.52
1:H:287:HIS:CE1	1:H:290:LEU:CG	2.92	0.52
1:H:254:MET:N	3:H:423:HOH:O	2.30	0.52
1:G:235:GLN:O	1:G:239:SER:HB2	2.10	0.52
1:C:224:LYS:HA	1:C:229:GLY:O	2.09	0.52
1:C:107:ILE:C	1:C:107:ILE:HD12	2.30	0.52
1:H:284:PHE:CE1	1:H:287:HIS:CD2	2.97	0.52
1:B:53:VAL:HA	1:B:251:PRO:HG3	1.90	0.52
1:G:217:TRP:CE2	1:G:219:ARG:HB2	2.45	0.52
1:C:49:TYR:OH	1:C:203:GLU:HG3	2.10	0.52
1:H:158:GLU:OE2	1:H:174:GLY:N	2.30	0.52
1:A:26:LYS:HA	1:A:28:PHE:CZ	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASN:OD1	1:B:181:THR:HG21	2.10	0.52
1:F:108:ASP:C	1:F:108:ASP:OD1	2.48	0.52
1:B:337:ASN:HB2	1:B:363:ASP:HB2	1.92	0.52
1:E:111:THR:O	1:E:112:LEU:HB2	2.10	0.52
1:A:55:SER:HB3	3:B:396:HOH:O	2.08	0.52
1:E:384:ARG:CG	1:E:384:ARG:HH11	2.11	0.52
1:A:289:TYR:HD1	1:A:290:LEU:CD2	2.23	0.52
1:E:324:ASN:ND2	3:E:407:HOH:O	2.43	0.52
1:E:252:LEU:HB3	3:E:389:HOH:O	2.09	0.52
1:C:111:THR:O	1:C:112:LEU:HB2	2.10	0.52
1:B:287:HIS:CG	1:B:288:PRO:CD	2.91	0.52
1:G:200:THR:HG21	1:G:205:ILE:HG22	1.92	0.52
1:H:255:SER:HA	1:H:258:ILE:CD1	2.37	0.52
1:E:203:GLU:OE1	1:E:226:LYS:HE3	2.10	0.52
1:A:248:ASN:HB3	1:B:57:SER:HB2	1.92	0.52
1:B:216:GLY:HA3	1:B:244:LEU:O	2.10	0.51
1:G:106:ASP:OD2	1:G:358:ASN:HB2	2.10	0.51
1:G:221:LEU:HB2	1:G:231:LYS:HD2	1.91	0.51
1:D:362:LEU:HD23	1:D:363:ASP:N	2.25	0.51
1:A:362:LEU:HD23	1:A:363:ASP:CA	2.40	0.51
1:D:259:GLY:O	1:D:260:ILE:C	2.45	0.51
1:H:279:TYR:HE2	1:H:380:ILE:CG2	2.22	0.51
1:G:303:GLY:HA3	1:G:368:PHE:CE2	2.44	0.51
1:C:107:ILE:HD12	1:C:107:ILE:O	2.10	0.51
1:A:56:GLY:O	1:A:59:ALA:HB3	2.10	0.51
1:G:141:ASN:C	1:G:141:ASN:OD1	2.48	0.51
1:H:253:GLU:N	3:H:423:HOH:O	2.43	0.51
1:D:266:LEU:N	1:D:267:PRO:HD2	2.25	0.51
1:F:171:LYS:HB3	1:F:176:PHE:CZ	2.46	0.51
1:A:193:MET:CE	1:B:252:LEU:HD13	2.40	0.51
1:G:130:ILE:HG22	1:G:132:THR:HG23	1.91	0.51
1:C:152:ARG:CB	1:C:154:ILE:CD1	2.88	0.51
1:F:205:ILE:O	1:F:208:ILE:HB	2.10	0.51
1:F:224:LYS:HG3	1:F:225:ASN:N	2.25	0.51
1:H:284:PHE:CE1	1:H:384:ARG:HD2	2.45	0.51
1:C:380:ILE:O	1:C:383:LEU:N	2.44	0.51
1:F:119:LEU:HG	1:F:148:ILE:HD12	1.92	0.51
1:D:119:LEU:O	1:D:123:VAL:HG23	2.11	0.51
1:F:205:ILE:HA	1:F:208:ILE:HD12	1.93	0.51
1:A:93:TYR:O	1:A:97:GLN:HG3	2.10	0.51
1:H:331:ARG:CD	1:H:368:PHE:CD1	2.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:HIS:CE1	1:F:289:TYR:CZ	2.96	0.51
1:C:106:ASP:OD2	1:C:358:ASN:HB2	2.11	0.51
1:G:63:MET:HE2	1:G:157:LEU:HD13	1.93	0.51
1:E:266:LEU:O	1:E:269:PHE:HB2	2.11	0.51
1:F:178:LEU:HD23	1:F:179:MET:HE2	1.93	0.51
1:A:169:ASN:O	1:A:170:ASN:HB2	2.09	0.51
1:C:232:SER:OG	1:C:233:ASP:N	2.43	0.51
1:H:167:THR:O	1:H:167:THR:HG22	2.10	0.51
1:H:274:ARG:NH1	1:H:295:GLU:OE2	2.39	0.51
1:B:188:IT1:OP3	2:B:402:AKG:C4	2.57	0.51
1:F:141:ASN:O	1:F:145:ILE:HG12	2.09	0.51
1:A:221:LEU:O	1:A:231:LYS:NZ	2.31	0.51
1:G:12:ASP:N	1:G:15:GLU:OE1	2.39	0.51
1:F:29:THR:O	1:F:30:MET:C	2.48	0.51
1:D:231:LYS:HB3	1:D:238:GLU:OE2	2.10	0.51
1:H:384:ARG:O	1:H:387:LEU:O	2.28	0.51
1:G:135:LEU:HD12	1:G:162:GLU:OE1	2.10	0.51
1:C:84:PRO:N	1:C:114:ILE:HD12	2.25	0.51
1:E:221:LEU:HG	3:E:398:HOH:O	2.11	0.51
1:F:58:THR:HG21	1:F:249:VAL:HG12	1.93	0.51
1:G:235:GLN:HG2	1:G:236:PHE:N	2.26	0.51
1:G:19:ILE:O	1:G:20:GLN:C	2.49	0.51
1:A:353:HIS:O	1:A:354:ASN:HB3	2.11	0.51
1:C:343:ASP:O	1:C:346:LYS:HB2	2.11	0.51
1:H:278:GLU:CA	1:H:281:LEU:HD12	2.35	0.50
1:A:324:ASN:O	1:A:327:GLY:N	2.40	0.50
1:E:82:ILE:HD13	1:E:127:THR:HG23	1.93	0.50
1:H:287:HIS:ND1	1:H:290:LEU:N	2.60	0.50
1:G:385:GLU:O	1:G:388:LYS:HD2	2.12	0.50
1:B:25:SER:O	1:B:26:LYS:HB2	2.11	0.50
1:C:45:PHE:CD1	1:C:45:PHE:N	2.79	0.50
1:A:86:VAL:HG22	1:A:336:GLY:O	2.10	0.50
1:C:70:THR:OG1	1:C:73:PRO:HA	2.11	0.50
1:H:160:ASN:HA	3:H:391:HOH:O	2.11	0.50
1:A:277:ALA:O	1:A:280:PHE:HB3	2.11	0.50
1:E:262:GLN:HA	1:E:262:GLN:NE2	2.26	0.50
1:F:111:THR:HG23	1:F:294:GLN:NE2	2.26	0.50
1:E:362:LEU:HD23	1:E:363:ASP:N	2.27	0.50
1:H:37:TYR:HB2	1:H:260:ILE:CG1	2.41	0.50
1:E:320:VAL:HG22	1:E:367:LEU:HD12	1.94	0.50
1:C:147:LYS:O	1:C:150:GLY:N	2.33	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:TYR:CE1	1:A:290:LEU:HG	2.46	0.50
1:E:315:ILE:H	1:E:315:ILE:HD13	1.76	0.50
1:D:40:GLN:O	1:D:44:THR:N	2.39	0.50
1:G:331:ARG:HB2	1:G:332:PRO:HD2	1.94	0.50
1:G:331:ARG:HD3	1:G:368:PHE:CD1	2.46	0.50
1:F:376:LEU:HB2	1:F:380:ILE:HD12	1.91	0.50
1:E:355:ASN:C	1:E:355:ASN:OD1	2.49	0.50
1:G:49:TYR:CD2	1:G:206:TYR:CD2	3.00	0.50
1:A:171:LYS:HD2	1:A:176:PHE:CZ	2.46	0.50
1:G:217:TRP:NE1	1:G:219:ARG:HB2	2.26	0.50
1:B:192:THR:O	1:B:193:MET:HB2	2.11	0.50
1:B:135:LEU:HD21	1:B:334:VAL:HG21	1.92	0.50
1:C:6:LEU:HD12	1:C:329:GLU:HG2	1.94	0.50
1:D:106:ASP:CB	1:D:356:VAL:HA	2.41	0.50
1:E:277:ALA:O	1:E:281:LEU:HG	2.12	0.50
1:G:179:MET:HG2	1:G:198:ILE:HG23	1.94	0.50
1:F:253:GLU:OE1	1:F:253:GLU:HA	2.12	0.50
1:B:37:TYR:CE1	1:B:263:LEU:CD1	2.95	0.50
1:E:103:LYS:HA	1:E:351:THR:HG23	1.92	0.50
1:G:304:PHE:HB2	1:G:369:VAL:HG23	1.92	0.50
1:G:355:ASN:OD1	1:G:355:ASN:C	2.50	0.50
1:G:235:GLN:CG	1:G:236:PHE:N	2.75	0.50
1:B:320:VAL:HG12	1:B:324:ASN:HD21	1.75	0.50
1:A:171:LYS:HG2	1:A:172:CYS:H	1.76	0.50
1:E:118:SER:O	1:E:121:GLU:N	2.38	0.50
1:D:149:ILE:HG23	1:D:154:ILE:HB	1.93	0.50
1:H:287:HIS:CE1	1:H:289:TYR:CD1	2.99	0.50
1:A:362:LEU:HD23	1:A:362:LEU:C	2.32	0.50
1:F:269:PHE:O	1:F:273:ARG:HG3	2.12	0.50
1:F:341:ASN:O	1:F:345:LEU:HD12	2.12	0.50
1:D:109:ILE:HG13	1:D:109:ILE:O	2.11	0.50
1:B:304:PHE:HA	3:B:424:HOH:O	2.11	0.50
1:G:213:ARG:HG2	1:G:213:ARG:O	2.12	0.50
1:C:161:CYS:HB2	1:C:188:IT1:C3	2.42	0.50
1:G:331:ARG:HB2	1:G:332:PRO:CD	2.42	0.50
1:F:15:GLU:O	1:F:16:TYR:C	2.49	0.50
1:E:10:THR:HG22	1:E:373:GLN:NE2	2.27	0.50
1:E:343:ASP:O	1:E:346:LYS:HB2	2.12	0.50
1:H:331:ARG:CD	1:H:368:PHE:HD1	2.25	0.49
1:F:111:THR:CG2	1:F:294:GLN:HE22	2.25	0.49
1:G:171:LYS:HB3	1:G:176:PHE:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ASN:OD1	1:C:163:SER:HB2	2.11	0.49
1:G:225:ASN:ND2	1:G:231:LYS:HG3	2.27	0.49
1:F:287:HIS:HE1	1:F:289:TYR:CE1	2.30	0.49
1:E:333:ILE:HG22	1:E:333:ILE:O	2.12	0.49
1:C:265:LYS:HB2	1:C:269:PHE:CZ	2.47	0.49
1:B:281:LEU:HD23	1:B:281:LEU:N	2.26	0.49
1:F:33:TYR:HB2	1:F:253:GLU:HG3	1.93	0.49
1:G:333:ILE:HD13	1:G:366:GLY:HA3	1.94	0.49
1:F:235:GLN:O	1:F:237:GLU:N	2.45	0.49
1:G:30:MET:CE	1:G:213:ARG:NH2	2.75	0.49
1:H:320:VAL:O	1:H:321:GLU:C	2.49	0.49
1:D:249:VAL:HG23	1:D:249:VAL:O	2.12	0.49
1:D:265:LYS:C	1:D:267:PRO:HD2	2.32	0.49
1:A:136:LEU:C	1:A:302:PHE:HB3	2.32	0.49
1:G:13:ASP:O	1:G:17:LYS:HB2	2.12	0.49
1:D:208:ILE:O	1:D:212:ILE:HG23	2.12	0.49
1:A:82:ILE:CG2	1:A:83:VAL:N	2.75	0.49
1:G:288:PRO:HG2	1:G:289:TYR:CD1	2.47	0.49
1:B:206:TYR:O	1:B:209:LEU:HB2	2.13	0.49
1:G:182:PHE:CD1	1:G:182:PHE:N	2.80	0.49
1:C:119:LEU:O	1:C:120:LYS:C	2.50	0.49
1:E:29:THR:O	1:E:30:MET:C	2.51	0.49
1:D:355:ASN:ND2	1:D:355:ASN:C	2.65	0.49
1:C:297:GLY:O	1:C:298:GLU:HG3	2.13	0.49
1:D:224:LYS:HA	1:D:229:GLY:O	2.13	0.49
1:F:56:GLY:O	1:F:59:ALA:HB3	2.13	0.49
1:E:135:LEU:HD11	1:E:334:VAL:HG21	1.95	0.49
1:C:142:PHE:HA	1:C:145:ILE:HG13	1.94	0.49
1:B:266:LEU:N	1:B:267:PRO:HD2	2.28	0.49
1:F:111:THR:HG23	1:F:294:GLN:HE22	1.77	0.49
1:A:71:LYS:CA	1:A:71:LYS:HE3	2.42	0.49
1:C:190:ILE:HB	1:C:262:GLN:HB3	1.95	0.49
1:F:43:LYS:HA	3:F:424:HOH:O	2.11	0.49
1:E:62:LEU:HG	1:E:212:ILE:HG13	1.95	0.49
1:G:340:LYS:O	1:G:342:THR:N	2.43	0.49
1:H:388:LYS:CE	1:H:388:LYS:HA	2.42	0.49
1:B:269:PHE:HA	1:B:373:GLN:HB2	1.95	0.49
1:H:303:GLY:HA3	1:H:368:PHE:HZ	1.74	0.49
1:B:188:IT1:H4A	2:B:402:AKG:H41	1.95	0.49
1:B:34:VAL:O	1:B:35:LYS:C	2.51	0.49
1:D:289:TYR:CD2	1:D:314:VAL:HG21	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ASP:OD2	1:E:357:ASP:N	2.46	0.49
1:G:217:TRP:C	1:G:217:TRP:CD1	2.86	0.49
1:D:176:PHE:N	1:D:176:PHE:CD1	2.80	0.49
1:H:275:LYS:HE2	1:H:275:LYS:HB3	1.36	0.49
1:C:151:GLY:O	1:C:152:ARG:O	2.30	0.49
1:H:266:LEU:HG	1:H:270:ILE:HD11	1.95	0.49
1:A:287:HIS:HE1	1:A:289:TYR:CE1	2.31	0.49
1:E:282:ASP:O	1:E:285:LYS:HB2	2.12	0.49
1:E:93:TYR:N	1:E:94:PRO:CD	2.76	0.49
1:C:106:ASP:CG	1:C:358:ASN:HB2	2.33	0.49
1:B:362:LEU:C	1:B:362:LEU:HD23	2.33	0.49
1:C:322:ASN:O	1:C:325:SER:OG	2.28	0.48
1:G:303:GLY:HA3	1:G:368:PHE:CZ	2.48	0.48
1:F:67:LEU:HD12	1:F:75:LEU:HD12	1.94	0.48
1:D:168:PHE:O	1:D:169:ASN:HB2	2.11	0.48
1:D:267:PRO:O	1:D:270:ILE:HB	2.13	0.48
1:A:320:VAL:O	1:A:321:GLU:C	2.49	0.48
1:H:289:TYR:HA	1:H:309:LYS:HD2	1.96	0.48
1:H:279:TYR:CE2	1:H:380:ILE:CG2	2.96	0.48
1:C:215:HIS:NE2	1:C:250:ARG:NH1	2.61	0.48
1:A:291:ASP:HB2	1:A:307:ILE:O	2.13	0.48
1:F:315:ILE:HD11	1:F:318:GLN:HG2	1.94	0.48
1:H:315:ILE:O	1:H:319:LEU:HD12	2.13	0.48
1:H:221:LEU:O	1:H:231:LYS:NZ	2.39	0.48
1:E:50:ALA:HB1	1:E:197[A]:CYS:SG	2.54	0.48
1:C:94:PRO:O	1:C:95:LEU:C	2.49	0.48
1:F:356:VAL:HG23	1:F:356:VAL:O	2.13	0.48
1:H:284:PHE:CZ	1:H:387:LEU:CD1	2.96	0.48
1:A:6:LEU:HD22	1:A:370:GLY:H	1.79	0.48
1:B:320:VAL:O	1:B:321:GLU:C	2.52	0.48
1:B:4:TYR:O	1:B:329:GLU:HB2	2.12	0.48
1:E:289:TYR:HA	1:E:309:LYS:CD	2.43	0.48
1:C:58:THR:O	1:C:61:LEU:HB3	2.13	0.48
1:G:21:SER:O	1:G:22:VAL:C	2.51	0.48
1:H:182:PHE:O	1:H:196:GLY:HA2	2.13	0.48
1:G:287:HIS:ND1	1:G:290:LEU:HB2	2.28	0.48
1:G:316:ARG:O	1:G:320:VAL:HG23	2.14	0.48
1:H:131:LEU:HD12	1:H:132:THR:N	2.29	0.48
1:C:202:ASP:OD1	1:C:205:ILE:HG12	2.13	0.48
1:G:15:GLU:HG2	1:G:258:ILE:HG23	1.95	0.48
1:A:383:LEU:HD22	1:A:387:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:TYR:N	1:G:94:PRO:CD	2.75	0.48
1:B:6:LEU:HG	1:B:329:GLU:HB3	1.96	0.48
1:B:280:PHE:HD2	1:B:281:LEU:CD2	2.25	0.48
1:E:215:HIS:O	1:E:242:PHE:CD1	2.67	0.48
1:D:15:GLU:OE2	1:D:261:GLU:HB3	2.13	0.48
1:F:385:GLU:O	1:F:388:LYS:HG2	2.13	0.48
1:C:241:LYS:HB2	1:C:241:LYS:HE2	1.44	0.48
1:F:318:GLN:HA	1:F:318:GLN:OE1	2.12	0.48
1:A:287:HIS:CE1	1:A:290:LEU:HG	2.49	0.48
1:D:354:ASN:CG	1:D:355:ASN:N	2.66	0.48
1:G:337:ASN:HB2	1:G:363:ASP:HB2	1.96	0.48
1:D:204:GLU:HA	1:D:226:LYS:HG3	1.96	0.48
1:E:161:CYS:HB2	1:E:188:IT1:C2	2.44	0.48
1:D:242:PHE:N	1:D:242:PHE:CD1	2.81	0.48
1:E:25:SER:O	1:E:26:LYS:HB2	2.14	0.48
1:A:311:ASP:O	1:A:313:GLY:N	2.47	0.48
1:B:321:GLU:O	1:B:325:SER:OG	2.32	0.48
1:F:243:VAL:HG23	1:F:244:LEU:CD1	2.44	0.48
1:D:82:ILE:HD12	1:D:127:THR:CG2	2.44	0.48
1:A:108:ASP:OD1	1:A:110:ASN:N	2.40	0.48
1:F:68:PHE:N	1:F:68:PHE:CD1	2.82	0.48
1:E:362:LEU:HD23	1:E:362:LEU:C	2.34	0.48
1:B:24:ASP:HA	1:B:26:LYS:NZ	2.29	0.48
1:D:38:GLU:HB2	3:D:443:HOH:O	2.13	0.48
1:H:377:PHE:O	1:H:380:ILE:HB	2.14	0.48
1:G:306:PHE:O	1:G:366:GLY:HA2	2.14	0.48
1:F:86:VAL:O	1:F:87:SER:HB2	2.13	0.48
1:A:132:THR:HA	3:A:411:HOH:O	2.14	0.48
1:A:224:LYS:HA	1:A:229:GLY:O	2.14	0.48
1:C:9:SER:O	1:C:373:GLN:NE2	2.47	0.48
1:C:79:ASP:CB	1:C:128:LYS:HG3	2.44	0.47
1:G:52:MET:O	1:G:251:PRO:HG3	2.13	0.47
1:D:106:ASP:OD2	1:D:358:ASN:HB2	2.12	0.47
1:D:120:LYS:HA	1:D:148:ILE:HD13	1.96	0.47
1:F:269:PHE:HA	1:F:373:GLN:HB2	1.96	0.47
1:E:115:ASP:OD2	1:E:118:SER:HB2	2.14	0.47
1:D:23:LEU:HA	1:D:28:PHE:HE1	1.79	0.47
1:G:3:ASN:N	1:G:3:ASN:OD1	2.47	0.47
1:A:6:LEU:CG	1:A:329:GLU:HG2	2.40	0.47
1:G:280:PHE:HB2	1:G:380:ILE:HD13	1.95	0.47
1:G:382:TYR:O	1:G:383:LEU:C	2.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PRO:HA	1:C:114:ILE:HD12	1.95	0.47
1:C:34:VAL:HG23	1:C:253:GLU:OE1	2.14	0.47
1:G:12:ASP:HB2	1:G:265:LYS:HZ1	1.79	0.47
1:G:15:GLU:OE2	1:G:262:GLN:NE2	2.47	0.47
1:E:184:SER:HG	1:E:192:THR:HG1	1.49	0.47
1:C:137:GLY:O	1:C:299:SER:HA	2.14	0.47
1:B:292:VAL:HG12	3:B:399:HOH:O	2.12	0.47
1:G:71:LYS:HA	1:G:71:LYS:HD3	1.43	0.47
1:H:331:ARG:CG	1:H:368:PHE:HD1	2.27	0.47
1:E:168:PHE:CD2	1:E:169:ASN:ND2	2.81	0.47
1:G:112:LEU:CD2	1:G:112:LEU:N	2.76	0.47
1:D:266:LEU:N	1:D:267:PRO:CD	2.77	0.47
1:E:102:VAL:O	1:E:350:TYR:HA	2.14	0.47
1:F:58:THR:CG2	1:F:249:VAL:HG11	2.45	0.47
1:G:141:ASN:O	1:G:145:ILE:HG12	2.14	0.47
1:B:376:LEU:HB3	1:B:379:GLU:CG	2.43	0.47
1:G:171:LYS:HB3	1:G:176:PHE:HZ	1.79	0.47
1:F:218:THR:HB	1:F:221:LEU:HD12	1.96	0.47
1:G:333:ILE:CD1	1:G:366:GLY:HA3	2.44	0.47
1:D:344:VAL:CG1	1:D:345:LEU:N	2.77	0.47
1:G:138:ASN:OD1	1:G:295:GLU:HA	2.14	0.47
1:C:252:LEU:HD12	1:D:252:LEU:HD12	1.97	0.47
1:H:71:LYS:HA	1:H:71:LYS:HD3	1.51	0.47
1:A:289:TYR:CD1	1:A:290:LEU:CD2	2.97	0.47
1:E:265:LYS:HG2	1:E:269:PHE:CZ	2.48	0.47
1:E:10:THR:CG2	1:E:373:GLN:NE2	2.78	0.47
1:F:144:GLU:OE1	1:F:144:GLU:HA	2.14	0.47
1:E:331:ARG:O	1:E:368:PHE:N	2.41	0.47
1:E:324:ASN:C	1:E:326:ALA:H	2.18	0.47
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.54	0.47
1:F:124:THR:CG2	1:F:125:ASP:N	2.78	0.47
1:E:358:ASN:O	1:E:359:ALA:C	2.52	0.47
1:G:167:THR:HA	1:G:171:LYS:O	2.14	0.47
1:H:35:LYS:O	1:H:36:GLN:C	2.51	0.47
1:F:217:TRP:O	1:F:217:TRP:HD1	1.98	0.47
1:F:273:ARG:NH1	1:F:371:ASN:O	2.48	0.47
1:G:217:TRP:CD1	1:G:219:ARG:HB2	2.50	0.47
1:D:273:ARG:HB3	1:D:371:ASN:HD21	1.79	0.47
1:E:373:GLN:OE1	1:E:373:GLN:N	2.43	0.47
1:G:70:THR:O	1:G:71:LYS:C	2.53	0.47
1:B:342:THR:O	1:B:346:LYS:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:PHE:CG	1:D:373:GLN:HG3	2.50	0.47
1:H:345:LEU:HD23	1:H:345:LEU:HA	1.77	0.47
1:A:289:TYR:HD1	1:A:290:LEU:HD23	1.79	0.47
1:G:205:ILE:O	1:G:206:TYR:C	2.51	0.47
1:G:203:GLU:HA	1:G:206:TYR:HB3	1.97	0.47
1:B:376:LEU:C	1:B:379:GLU:HG2	2.35	0.47
1:H:320:VAL:HA	1:H:323:LEU:HD12	1.96	0.47
1:D:273:ARG:CB	1:D:371:ASN:HD21	2.27	0.47
1:C:118:SER:O	1:C:122:ALA:N	2.37	0.47
1:B:184:SER:HB2	1:B:192:THR:OG1	2.14	0.47
1:D:269:PHE:HA	1:D:373:GLN:HB2	1.97	0.47
1:D:232:SER:OG	1:D:233:ASP:N	2.48	0.47
1:F:374:ILE:O	1:F:374:ILE:HG13	2.14	0.47
1:H:304:PHE:HB2	1:H:369:VAL:HG22	1.97	0.47
1:E:303:GLY:HA3	1:E:368:PHE:HZ	1.75	0.47
1:D:367:LEU:N	1:D:367:LEU:CD1	2.78	0.47
1:A:85:ALA:N	1:A:105:VAL:O	2.47	0.47
1:F:373:GLN:H	1:F:373:GLN:CD	2.17	0.47
1:B:222:PRO:HG2	1:B:225:ASN:HB3	1.96	0.47
1:A:185:PHE:CG	1:A:186:TYR:N	2.83	0.47
1:C:101:ARG:NH1	1:C:349:ASP:OD1	2.42	0.47
1:H:185:PHE:HB3	1:H:188:IT1:HG	1.97	0.47
1:G:315:ILE:HB	1:G:318:GLN:HB2	1.96	0.47
1:G:206:TYR:O	1:G:209:LEU:HD12	2.14	0.47
1:G:235:GLN:O	1:G:237:GLU:N	2.48	0.47
1:B:53:VAL:N	1:B:251:PRO:HG3	2.30	0.47
1:F:150:GLY:C	1:F:152:ARG:H	2.18	0.47
1:D:231:LYS:HB3	1:D:238:GLU:CD	2.35	0.47
1:A:81:ILE:HG13	1:A:82:ILE:N	2.29	0.47
1:F:67:LEU:HD12	1:F:75:LEU:CD1	2.45	0.47
1:H:372:HIS:H	1:H:376:LEU:HD11	1.79	0.47
1:E:243:VAL:O	1:E:244:LEU:HD13	2.15	0.47
1:C:145:ILE:H	1:C:145:ILE:HG12	1.49	0.46
1:F:206:TYR:CD2	1:F:207:HIS:HD2	2.32	0.46
1:H:318:GLN:O	1:H:321:GLU:HB3	2.15	0.46
1:G:333:ILE:HD11	1:G:367:LEU:N	2.30	0.46
1:C:70:THR:HG21	1:C:74:ARG:NE	2.30	0.46
1:C:355:ASN:OD1	3:C:423:HOH:O	2.19	0.46
1:F:88:TRP:O	1:F:89:SER:C	2.52	0.46
1:C:152:ARG:CG	1:C:154:ILE:HD11	2.45	0.46
1:G:309:LYS:O	1:G:312:SER:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:HIS:CD2	1:H:288:PRO:HD2	2.51	0.46
1:H:268:ARG:O	1:H:272:VAL:HB	2.15	0.46
1:F:134:ASN:OD1	1:F:140:ASN:ND2	2.32	0.46
1:A:193:MET:HE3	1:B:252:LEU:HD13	1.97	0.46
1:G:182:PHE:HB3	3:G:409:HOH:O	2.15	0.46
1:G:61:LEU:HD21	1:G:247:TYR:CE1	2.49	0.46
1:E:120:LYS:HB2	1:E:120:LYS:HE3	1.37	0.46
1:G:316:ARG:O	1:G:317:LYS:C	2.54	0.46
1:C:202:ASP:HB3	1:C:205:ILE:CG1	2.44	0.46
1:F:6:LEU:HD12	1:F:329:GLU:CG	2.43	0.46
1:A:148:ILE:O	1:A:148:ILE:HG22	2.15	0.46
1:A:356:VAL:HG23	1:A:356:VAL:O	2.16	0.46
1:A:217:TRP:CE2	1:A:219:ARG:HB2	2.51	0.46
1:E:135:LEU:HG	1:E:136:LEU:HG	1.96	0.46
1:C:310:LYS:O	1:C:311:ASP:CB	2.50	0.46
1:E:253:GLU:O	1:E:256:GLY:N	2.49	0.46
1:C:6:LEU:HD12	1:C:329:GLU:OE2	2.16	0.46
1:A:136:LEU:HA	1:A:302:PHE:HB3	1.97	0.46
1:F:167:THR:HG23	1:F:171:LYS:C	2.36	0.46
1:D:337:ASN:HB2	1:D:359:ALA:O	2.16	0.46
1:E:147:LYS:HB2	1:E:147:LYS:HE2	1.66	0.46
1:G:37:TYR:CE1	1:G:259:GLY:C	2.89	0.46
1:G:119:LEU:O	1:G:123:VAL:HG23	2.16	0.46
1:C:137:GLY:HA2	1:C:163:SER:HA	1.97	0.46
1:A:82:ILE:HG22	1:A:83:VAL:N	2.30	0.46
1:D:41:PHE:O	1:D:45:PHE:HD1	1.98	0.46
1:B:67:LEU:HD21	1:B:179:MET:HE1	1.97	0.46
1:H:336:GLY:HA2	1:H:362:LEU:CD2	2.46	0.46
1:C:77:LYS:HG2	1:C:77:LYS:H	1.52	0.46
1:B:287:HIS:CE1	1:B:288:PRO:HD2	2.50	0.46
1:C:380:ILE:HG22	1:C:381:ASP:N	2.30	0.46
1:G:31:GLY:N	1:G:253:GLU:OE1	2.41	0.46
1:F:217:TRP:C	1:F:217:TRP:HD1	2.18	0.46
1:H:102:VAL:HG12	1:H:104:PHE:CE1	2.51	0.46
1:E:287:HIS:CD2	1:E:384:ARG:NE	2.83	0.46
1:E:336:GLY:HA2	1:E:362:LEU:CD2	2.40	0.46
1:A:362:LEU:HD23	1:A:363:ASP:HA	1.97	0.46
1:H:380:ILE:O	1:H:383:LEU:HB3	2.16	0.46
1:C:36:GLN:HG2	1:C:260:ILE:CD1	2.45	0.46
1:F:235:GLN:C	1:F:237:GLU:N	2.68	0.46
1:B:150:GLY:HA2	1:B:151:GLY:HA2	1.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:SER:OG	1:H:58:THR:HG21	2.16	0.46
1:H:287:HIS:CE1	1:H:290:LEU:CD1	2.98	0.46
1:F:26:LYS:CB	1:F:27:MET:HE2	2.44	0.46
1:C:149:ILE:O	1:C:149:ILE:HG23	2.16	0.46
1:B:120:LYS:HA	1:B:148:ILE:CG2	2.45	0.46
1:C:84:PRO:CB	1:C:114:ILE:HD12	2.46	0.46
1:G:253:GLU:OE1	1:G:253:GLU:HA	2.15	0.46
1:A:266:LEU:O	1:A:267:PRO:C	2.55	0.46
1:F:235:GLN:C	1:F:237:GLU:H	2.18	0.46
1:G:93:TYR:HB2	1:G:94:PRO:HD3	1.97	0.46
1:H:161:CYS:HB2	1:H:188:IT1:C2	2.46	0.46
1:H:137:GLY:HA2	1:H:163:SER:HA	1.97	0.46
1:H:42:ALA:HB1	1:H:47:SER:O	2.16	0.46
1:A:238:GLU:HA	1:A:238:GLU:OE1	2.16	0.46
1:H:124:THR:HG23	1:H:125:ASP:N	2.31	0.45
1:G:209:LEU:HA	1:G:212:ILE:CG1	2.39	0.45
1:B:29:THR:O	1:B:30:MET:C	2.54	0.45
1:H:314:VAL:CG1	1:H:319:LEU:HD21	2.46	0.45
1:G:70:THR:HG21	1:G:74:ARG:HE	1.82	0.45
1:A:232:SER:OG	1:A:233:ASP:N	2.49	0.45
1:H:52:MET:O	1:H:251:PRO:HG3	2.15	0.45
1:H:249:VAL:HG23	1:H:249:VAL:O	2.15	0.45
1:D:33:TYR:CG	1:D:257:ALA:HB2	2.51	0.45
1:A:266:LEU:N	1:A:267:PRO:HD2	2.31	0.45
1:A:12:ASP:C	1:A:12:ASP:OD1	2.54	0.45
1:F:120:LYS:HB2	1:F:120:LYS:HE2	1.44	0.45
1:F:159:ASP:CG	1:F:188:IT1:H2A	2.37	0.45
1:F:48:LYS:HE3	1:F:201:ASP:O	2.17	0.45
1:F:26:LYS:HZ2	1:F:26:LYS:HA	1.81	0.45
1:H:379:GLU:O	1:H:382:TYR:HB3	2.16	0.45
1:D:362:LEU:HD23	1:D:362:LEU:C	2.37	0.45
1:H:37:TYR:HB2	1:H:260:ILE:HG12	1.98	0.45
1:E:203:GLU:O	1:E:206:TYR:HB3	2.16	0.45
1:D:69:PHE:CZ	1:D:245:PRO:HD2	2.50	0.45
1:C:156:LEU:O	1:C:177:GLY:CA	2.64	0.45
1:B:234:ASP:C	1:B:234:ASP:OD1	2.52	0.45
1:D:346:LYS:HE2	1:D:346:LYS:HB2	1.54	0.45
1:D:185:PHE:HB2	3:D:400:HOH:O	2.15	0.45
1:E:86:VAL:O	1:E:87:SER:HB2	2.16	0.45
1:A:203:GLU:O	1:A:206:TYR:HB3	2.16	0.45
1:C:72:LYS:HA	1:C:72:LYS:HD2	1.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:TYR:O	1:F:209:LEU:HB2	2.16	0.45
1:E:266:LEU:N	1:E:267:PRO:CD	2.77	0.45
1:B:53:VAL:C	1:B:251:PRO:HG3	2.37	0.45
1:F:154:ILE:H	1:F:154:ILE:HD12	1.81	0.45
1:G:57:SER:HB2	1:H:248:ASN:HB3	1.98	0.45
1:C:26:LYS:HA	1:C:28:PHE:CZ	2.51	0.45
1:B:221:LEU:O	1:B:231:LYS:NZ	2.47	0.45
1:C:245:PRO:HA	1:D:93:TYR:CD1	2.52	0.45
1:G:64:ILE:O	1:G:67:LEU:HB2	2.17	0.45
1:H:331:ARG:O	1:H:368:PHE:N	2.43	0.45
1:A:331:ARG:CB	1:A:332:PRO:HD2	2.46	0.45
1:A:57:SER:OG	1:A:188:IT1:OP2	2.25	0.45
1:G:36:GLN:HB3	1:G:260:ILE:HD11	1.98	0.45
1:C:384:ARG:HG3	1:C:384:ARG:O	2.15	0.45
1:G:137:GLY:HA2	1:G:163:SER:HA	1.99	0.45
1:D:76:LYS:O	1:D:79:ASP:HB2	2.17	0.45
1:C:323:LEU:HA	1:C:323:LEU:HD23	1.62	0.45
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.65	0.45
1:C:361:TYR:CD1	1:C:361:TYR:C	2.91	0.45
1:C:159:ASP:OD2	1:C:188:IT1:H2A	2.16	0.45
1:G:108:ASP:OD1	1:G:108:ASP:C	2.56	0.45
1:G:88:TRP:HD1	1:G:90:THR:OG1	1.99	0.45
1:H:304:PHE:CE2	1:H:371:ASN:HB2	2.52	0.45
1:G:4:TYR:HB3	1:G:328:ILE:HA	1.99	0.45
1:F:102:VAL:O	1:F:350:TYR:HA	2.17	0.45
1:H:381:ASP:N	1:H:381:ASP:OD1	2.50	0.45
1:A:244:LEU:HA	1:A:245:PRO:HD3	1.67	0.45
1:D:273:ARG:HG2	1:D:371:ASN:ND2	2.32	0.45
1:F:182:PHE:HE1	1:F:199:VAL:HG22	1.82	0.45
1:H:375:GLU:O	1:H:375:GLU:HG2	2.17	0.45
1:A:311:ASP:O	1:A:312:SER:C	2.55	0.45
1:G:30:MET:HE3	1:G:213:ARG:NH2	2.32	0.45
1:G:37:TYR:CE1	1:G:259:GLY:CA	3.00	0.45
1:A:265:LYS:O	1:A:266:LEU:C	2.54	0.45
1:H:139:PRO:HG3	1:H:166:ALA:HB1	1.99	0.45
1:A:316:ARG:NH1	1:A:366:GLY:O	2.48	0.45
1:C:97:GLN:HB3	3:C:439:HOH:O	2.17	0.45
1:A:289:TYR:HB2	1:A:312:SER:HB2	1.99	0.44
1:B:12:ASP:N	1:B:15:GLU:OE1	2.36	0.44
1:G:67:LEU:HD13	1:G:75:LEU:HD12	1.98	0.44
1:E:217:TRP:CD1	1:E:217:TRP:C	2.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLN:O	1:B:373:GLN:HG2	2.16	0.44
1:F:289:TYR:CD1	1:F:290:LEU:CD2	3.00	0.44
1:C:280:PHE:CZ	1:C:304:PHE:CB	2.98	0.44
1:D:137:GLY:HA2	1:D:163:SER:CB	2.47	0.44
1:E:190:ILE:CG2	1:E:266:LEU:HD13	2.47	0.44
1:B:30:MET:CE	1:B:34:VAL:HG11	2.40	0.44
1:E:35:LYS:HB2	1:E:35:LYS:HE2	1.74	0.44
1:H:10:THR:HG22	1:H:373:GLN:NE2	2.32	0.44
1:A:161:CYS:HB2	1:A:188:IT1:C3	2.47	0.44
1:F:106:ASP:OD1	1:F:358:ASN:HB2	2.18	0.44
1:B:15:GLU:O	1:B:18:ALA:HB3	2.18	0.44
1:F:385:GLU:O	1:F:388:LYS:HD2	2.18	0.44
1:G:94:PRO:HA	1:G:97:GLN:HE21	1.82	0.44
1:H:248:ASN:OD1	1:H:250:ARG:HB2	2.18	0.44
1:D:81:ILE:HD11	1:D:131:LEU:HB2	1.98	0.44
1:E:67:LEU:CD2	1:E:74:ARG:HD3	2.48	0.44
1:C:263:LEU:HA	1:C:263:LEU:HD23	1.58	0.44
1:G:234:ASP:O	1:G:237:GLU:N	2.51	0.44
1:D:277:ALA:O	1:D:280:PHE:HB3	2.17	0.44
1:H:315:ILE:CD1	1:H:315:ILE:N	2.80	0.44
1:H:61:LEU:HD12	1:H:94:PRO:HB3	2.00	0.44
1:E:118:SER:O	1:E:119:LEU:C	2.55	0.44
1:C:287:HIS:CG	1:C:288:PRO:HD2	2.52	0.44
1:E:130:ILE:HG22	1:E:132:THR:HG23	1.98	0.44
1:E:130:ILE:HG22	1:E:132:THR:CG2	2.48	0.44
1:H:258:ILE:O	1:H:259:GLY:C	2.55	0.44
1:B:71:LYS:O	1:B:73:PRO:HD3	2.17	0.44
1:B:155:ILE:CG2	1:B:156:LEU:N	2.80	0.44
1:D:83:VAL:HG12	1:D:131:LEU:HD23	1.99	0.44
1:G:222:PRO:O	1:G:231:LYS:HD3	2.18	0.44
1:A:336:GLY:HA2	1:A:362:LEU:HD21	2.00	0.44
1:H:273:ARG:NH1	1:H:371:ASN:O	2.51	0.44
1:A:271:SER:O	1:A:275:LYS:HB2	2.17	0.44
1:C:22:VAL:HG22	1:C:33:TYR:CE2	2.52	0.44
1:C:51:VAL:O	1:C:197[B]:CYS:HA	2.17	0.44
1:G:141:ASN:O	1:G:141:ASN:OD1	2.36	0.44
1:E:323:LEU:HD23	1:E:386:VAL:HG11	1.99	0.44
1:G:213:ARG:HG3	1:G:249:VAL:HG23	1.99	0.44
1:B:323:LEU:O	1:B:328:ILE:HB	2.18	0.44
1:E:385:GLU:CA	1:E:385:GLU:OE1	2.64	0.44
1:D:300:SER:O	1:D:301:TRP:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:LEU:HA	1:E:302:PHE:HB3	1.98	0.44
1:E:380:ILE:O	1:E:381:ASP:C	2.55	0.44
1:A:382:TYR:HH	1:C:271:SER:HG	1.65	0.44
1:B:24:ASP:HA	1:B:26:LYS:HZ2	1.81	0.44
1:B:23:LEU:HD23	1:B:28:PHE:HE1	1.83	0.44
1:H:326:ALA:HB1	1:H:382:TYR:CZ	2.52	0.44
1:B:137:GLY:HA2	1:B:163:SER:HA	2.00	0.44
1:F:287:HIS:CG	1:F:288:PRO:HD2	2.52	0.44
1:B:340:LYS:NZ	3:B:409:HOH:O	2.50	0.44
1:G:161:CYS:HB3	1:G:183:SER:HB3	2.00	0.44
1:G:334:VAL:HG12	1:G:335:THR:N	2.33	0.44
1:E:169:ASN:C	1:E:171:LYS:N	2.71	0.44
1:E:30:MET:CG	1:E:34:VAL:HG11	2.44	0.44
1:C:58:THR:CG2	1:C:249:VAL:HG11	2.48	0.44
1:F:14:LEU:HA	1:F:14:LEU:HD12	1.73	0.44
1:D:225:ASN:OD1	1:D:228:THR:OG1	2.31	0.44
1:B:55:SER:O	1:B:56:GLY:C	2.54	0.44
1:D:263:LEU:HA	1:D:263:LEU:HD23	1.78	0.44
1:B:283:LYS:HA	1:B:283:LYS:HD2	1.75	0.44
1:G:225:ASN:HD21	1:G:231:LYS:HG3	1.83	0.43
1:E:5:PRO:HA	1:E:329:GLU:HB3	1.98	0.43
1:F:23:LEU:HA	1:F:23:LEU:HD23	1.76	0.43
1:C:318:GLN:O	1:C:322:ASN:ND2	2.51	0.43
1:E:268:ARG:O	1:E:269:PHE:C	2.55	0.43
1:H:315:ILE:CD1	1:H:315:ILE:H	2.25	0.43
1:F:141:ASN:C	1:F:141:ASN:OD1	2.55	0.43
1:D:37:TYR:CE1	1:D:259:GLY:HA3	2.52	0.43
1:F:76:LYS:HG2	1:F:79:ASP:OD2	2.18	0.43
1:A:217:TRP:HD1	1:A:217:TRP:C	2.21	0.43
1:E:289:TYR:CD1	1:E:289:TYR:N	2.86	0.43
1:D:35:LYS:HB2	1:D:35:LYS:NZ	2.32	0.43
1:G:119:LEU:HD11	1:G:130:ILE:CD1	2.48	0.43
1:D:82:ILE:HD12	1:D:127:THR:HG23	2.00	0.43
1:E:270:ILE:O	1:E:271:SER:C	2.55	0.43
1:G:244:LEU:HA	1:G:245:PRO:HD3	1.81	0.43
1:H:232:SER:OG	1:H:233:ASP:N	2.49	0.43
1:C:93:TYR:HB2	3:D:416:HOH:O	2.17	0.43
1:D:310:LYS:HB2	1:D:310:LYS:HE2	1.65	0.43
1:E:169:ASN:O	1:E:171:LYS:N	2.51	0.43
1:A:245:PRO:HA	1:B:93:TYR:CE1	2.54	0.43
1:E:193:MET:HB3	1:F:252:LEU:HD22	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:HG21	1:C:249:VAL:HG12	2.00	0.43
1:G:331:ARG:HB2	1:G:331:ARG:HE	1.71	0.43
1:G:92:TYR:O	1:G:95:LEU:HG	2.18	0.43
1:H:336:GLY:HA2	1:H:362:LEU:HD21	2.00	0.43
1:D:22:VAL:O	1:D:25:SER:OG	2.34	0.43
1:F:215:HIS:NE2	1:F:250:ARG:NH1	2.59	0.43
1:H:85:ALA:HB1	1:H:339:LEU:HD12	2.00	0.43
1:B:63:MET:HB3	1:B:63:MET:HE3	1.61	0.43
1:D:388:LYS:HA	1:D:388:LYS:HD2	1.51	0.43
1:F:224:LYS:HB2	1:F:224:LYS:HE3	1.37	0.43
1:F:333:ILE:HB	1:F:362:LEU:HD21	2.00	0.43
1:H:164:MET:HE3	1:H:190:ILE:HG12	1.99	0.43
1:C:217:TRP:C	1:C:217:TRP:CD1	2.92	0.43
1:G:333:ILE:CD1	1:G:367:LEU:N	2.81	0.43
1:A:186:TYR:C	1:A:186:TYR:CD2	2.92	0.43
1:E:69:PHE:CZ	1:E:245:PRO:HG2	2.53	0.43
1:H:77:LYS:HG2	1:H:77:LYS:H	1.64	0.43
1:A:64:ILE:N	1:A:64:ILE:HD13	2.29	0.43
1:F:289:TYR:HD1	1:F:290:LEU:CD2	2.31	0.43
1:G:209:LEU:O	1:G:213:ARG:N	2.48	0.43
1:F:21:SER:O	1:F:25:SER:HB3	2.18	0.43
1:A:283:LYS:O	1:A:384:ARG:HD3	2.17	0.43
1:F:145:ILE:HG12	1:F:145:ILE:H	1.24	0.43
1:D:354:ASN:CG	1:D:355:ASN:H	2.22	0.43
1:F:63:MET:HG3	1:F:179:MET:HE3	2.00	0.43
1:G:384:ARG:HH11	1:G:384:ARG:HG3	1.82	0.43
1:G:114:ILE:HG23	1:G:114:ILE:O	2.17	0.43
1:E:155:ILE:HG13	1:E:155:ILE:H	1.50	0.43
1:H:289:TYR:N	1:H:289:TYR:CD1	2.85	0.43
1:F:289:TYR:C	1:F:290:LEU:HD23	2.38	0.43
1:F:150:GLY:O	1:F:152:ARG:N	2.52	0.43
1:B:13:ASP:O	1:B:17:LYS:HG2	2.18	0.43
1:F:50:ALA:HB2	1:F:199:VAL:HG12	2.00	0.43
1:A:160:ASN:ND2	1:A:182:PHE:CE2	2.78	0.43
1:E:92:TYR:O	1:E:95:LEU:HG	2.18	0.43
1:A:202:ASP:HB3	1:A:205:ILE:HD12	2.01	0.43
1:H:20:GLN:OE1	1:H:23:LEU:HD12	2.18	0.43
1:G:148:ILE:O	1:G:149:ILE:C	2.55	0.43
1:B:71:LYS:HB2	1:B:71:LYS:HE3	1.08	0.43
1:H:182:PHE:N	1:H:182:PHE:CD1	2.86	0.43
1:G:89:SER:HB2	1:G:93:TYR:CZ	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ARG:CB	1:C:154:ILE:HD11	2.49	0.43
1:H:287:HIS:CG	1:H:290:LEU:HB2	2.53	0.43
1:F:142:PHE:HA	1:F:145:ILE:CG1	2.46	0.43
1:B:64:ILE:O	1:B:65:ALA:C	2.56	0.43
1:F:223:LYS:HD2	3:F:429:HOH:O	2.19	0.43
1:F:70:THR:O	1:F:71:LYS:C	2.57	0.43
1:B:145:ILE:HG22	1:B:149:ILE:CD1	2.49	0.43
1:G:331:ARG:HD3	1:G:368:PHE:HD1	1.84	0.43
1:G:368:PHE:C	1:G:368:PHE:CD1	2.92	0.43
1:G:137:GLY:O	1:G:166:ALA:HB2	2.19	0.43
1:G:86:VAL:HG22	1:G:336:GLY:O	2.18	0.43
1:A:379:GLU:HG3	1:A:379:GLU:O	2.18	0.43
1:G:387:LEU:HA	1:G:387:LEU:HD23	1.75	0.43
1:E:57:SER:HB2	1:F:248:ASN:HB3	2.00	0.43
1:G:223:LYS:HD3	1:G:231:LYS:HB2	2.00	0.43
1:B:56:GLY:HA3	1:B:183:SER:HB2	2.01	0.43
1:G:252:LEU:HD12	1:H:252:LEU:HD12	2.01	0.43
1:H:238:GLU:O	1:H:240:PHE:N	2.52	0.43
1:H:8:SER:OG	1:H:9:SER:N	2.52	0.43
1:H:263:LEU:HA	1:H:263:LEU:HD23	1.86	0.43
1:B:266:LEU:HB3	1:B:267:PRO:CD	2.48	0.43
1:F:310:LYS:O	1:F:311:ASP:CB	2.63	0.43
1:A:120:LYS:HG3	1:A:148:ILE:HD11	2.00	0.43
1:G:331:ARG:CB	1:G:332:PRO:HD2	2.49	0.43
1:C:155:ILE:HG22	1:C:156:LEU:N	2.34	0.43
1:G:75:LEU:HA	1:G:79:ASP:OD2	2.18	0.43
1:B:308:ILE:HB	1:B:365:ASN:HB3	2.01	0.43
1:C:109:ILE:HD12	1:C:307:ILE:CD1	2.49	0.43
1:C:356:VAL:O	1:C:357:ASP:C	2.56	0.43
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.80	0.43
1:F:314:VAL:CG1	1:F:315:ILE:N	2.81	0.43
1:F:148:ILE:O	1:F:152:ARG:NH2	2.51	0.43
1:B:137:GLY:HA2	1:B:163:SER:CB	2.49	0.43
1:A:250:ARG:NH2	1:B:185:PHE:CE1	2.87	0.43
1:A:292:VAL:HB	3:A:412:HOH:O	2.18	0.43
1:E:232:SER:OG	1:E:233:ASP:N	2.52	0.43
1:F:77:LYS:H	1:F:77:LYS:HG2	1.63	0.43
1:F:161:CYS:CB	1:F:188:IT1:C2	2.94	0.42
1:H:266:LEU:N	1:H:267:PRO:CD	2.82	0.42
1:H:266:LEU:CB	1:H:267:PRO:HD3	2.31	0.42
1:E:303:GLY:C	1:E:368:PHE:CE1	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:HE1	1:F:201:ASP:O	2.01	0.42
1:C:322:ASN:HA	1:C:325:SER:OG	2.19	0.42
1:F:266:LEU:CB	1:F:267:PRO:CD	2.95	0.42
1:G:362:LEU:HD23	1:G:363:ASP:N	2.34	0.42
1:H:372:HIS:HB2	1:H:374:ILE:HG13	1.99	0.42
1:F:248:ASN:OD1	1:F:248:ASN:C	2.58	0.42
1:C:291:ASP:OD2	1:C:309:LYS:HG2	2.18	0.42
1:E:52:MET:HG2	1:E:251:PRO:HG3	1.99	0.42
1:E:65:ALA:O	1:E:68:PHE:HB2	2.19	0.42
1:G:373:GLN:H	1:G:373:GLN:CD	2.22	0.42
1:B:124:THR:CG2	1:B:125:ASP:N	2.62	0.42
1:G:287:HIS:CE1	1:G:290:LEU:HD12	2.55	0.42
1:F:130:ILE:O	1:F:156:LEU:HD12	2.19	0.42
1:D:34:VAL:O	1:D:38:GLU:HG3	2.19	0.42
1:E:185:PHE:CE1	1:F:250:ARG:NH2	2.87	0.42
1:C:248:ASN:HB3	1:D:57:SER:HB2	2.00	0.42
1:G:105:VAL:CG1	1:G:118:SER:HB2	2.50	0.42
1:B:299:SER:HB3	1:B:301:TRP:NE1	2.34	0.42
1:B:116:ILE:HG21	1:B:144:GLU:HG2	2.01	0.42
1:F:129:ALA:HA	1:F:154:ILE:HG23	2.01	0.42
1:D:86:VAL:HG21	1:D:107:ILE:HD13	2.01	0.42
1:C:319:LEU:O	1:C:320:VAL:C	2.57	0.42
1:B:250:ARG:HA	1:B:251:PRO:HD3	1.85	0.42
1:A:63:MET:CG	1:A:179:MET:HE3	2.48	0.42
1:A:264:LYS:O	1:A:267:PRO:HD2	2.20	0.42
1:D:120:LYS:CB	1:D:148:ILE:CD1	2.96	0.42
1:F:4:TYR:C	1:F:4:TYR:CD1	2.93	0.42
1:A:371:ASN:C	1:A:372:HIS:HD2	2.22	0.42
1:B:119:LEU:O	1:B:120:LYS:C	2.57	0.42
1:C:331:ARG:HB2	1:C:332:PRO:CD	2.50	0.42
1:G:337:ASN:O	1:G:340:LYS:HD3	2.19	0.42
1:H:111:THR:HG22	1:H:294:GLN:HB3	2.01	0.42
1:G:232:SER:HB3	1:G:238:GLU:OE1	2.19	0.42
1:C:185:PHE:CG	1:C:186:TYR:N	2.87	0.42
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.83	0.42
1:A:375:GLU:O	1:A:375:GLU:HG2	2.18	0.42
1:E:317:LYS:HB3	1:E:317:LYS:HE3	1.70	0.42
1:E:158:GLU:CD	1:E:174:GLY:H	2.20	0.42
1:E:303:GLY:C	1:E:368:PHE:HE1	2.23	0.42
1:H:225:ASN:N	1:H:229:GLY:O	2.45	0.42
1:A:266:LEU:N	1:A:267:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:LEU:O	1:E:63:MET:C	2.58	0.42
1:H:137:GLY:HA2	1:H:163:SER:CB	2.50	0.42
1:A:250:ARG:HA	1:A:251:PRO:HD3	1.93	0.42
1:F:287:HIS:CE1	1:F:289:TYR:CE2	3.07	0.42
1:G:117:GLU:O	1:G:120:LYS:HB2	2.20	0.42
1:B:341:ASN:C	1:B:345:LEU:HD22	2.40	0.42
1:D:287:HIS:HE1	1:D:289:TYR:CZ	2.37	0.42
1:G:37:TYR:HE1	1:G:259:GLY:C	2.23	0.42
1:H:190:ILE:CG2	1:H:262:GLN:HB3	2.49	0.42
1:A:136:LEU:CA	1:A:302:PHE:HB3	2.49	0.42
1:A:12:ASP:OD1	1:A:14:LEU:HG	2.20	0.42
1:C:284:PHE:CE1	1:C:384:ARG:HD2	2.55	0.42
1:B:351:THR:OG1	1:B:352:VAL:N	2.52	0.42
1:E:339:LEU:HA	1:E:339:LEU:HD13	1.53	0.42
1:F:26:LYS:CA	1:F:26:LYS:HZ2	2.32	0.42
1:G:239:SER:HB3	1:G:240:PHE:CD2	2.55	0.42
1:F:119:LEU:HD12	1:F:119:LEU:O	2.20	0.42
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.87	0.42
1:E:106:ASP:OD2	1:E:356:VAL:HA	2.19	0.42
1:E:184:SER:OG	1:E:192:THR:OG1	2.27	0.42
1:H:80:GLU:HA	1:H:101:ARG:O	2.19	0.42
1:F:388:LYS:HE3	1:F:388:LYS:CA	2.47	0.42
1:E:47:SER:OG	1:E:49:TYR:O	2.37	0.42
1:G:128:LYS:HA	1:G:128:LYS:HD2	1.33	0.42
1:H:303:GLY:CA	1:H:368:PHE:CE2	3.01	0.42
1:E:268:ARG:NH2	1:E:268:ARG:CG	2.79	0.42
1:E:269:PHE:N	1:E:269:PHE:CD1	2.87	0.42
1:B:7:ALA:HA	1:B:372:HIS:HE1	1.84	0.42
1:C:376:LEU:HA	1:C:379:GLU:OE1	2.20	0.42
1:E:348:PHE:N	1:E:348:PHE:CD1	2.88	0.42
1:H:162:GLU:HG3	1:H:188:IT1:O3	2.20	0.42
1:A:14:LEU:H	1:A:14:LEU:HG	1.74	0.42
1:F:184:SER:O	1:F:191:ALA:HA	2.20	0.42
1:G:81:ILE:HD11	1:G:131:LEU:HB2	2.02	0.42
1:A:279:TYR:CE2	1:A:381:ASP:OD1	2.72	0.42
1:G:314:VAL:HG12	1:G:315:ILE:N	2.33	0.42
1:C:310:LYS:HG3	1:C:361:TYR:CE2	2.55	0.42
1:F:111:THR:O	1:F:112:LEU:CB	2.68	0.42
1:B:287:HIS:HA	1:B:288:PRO:HD3	1.77	0.42
1:E:207:HIS:CE1	1:E:226:LYS:H	2.37	0.42
1:A:269:PHE:CE1	1:A:373:GLN:HG3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:LEU:HD23	1:F:323:LEU:HA	1.65	0.42
1:H:266:LEU:CB	1:H:267:PRO:CD	2.91	0.41
1:G:287:HIS:ND1	1:G:288:PRO:HG2	2.33	0.41
1:D:331:ARG:O	1:D:368:PHE:N	2.51	0.41
1:H:272:VAL:HG11	1:H:373:GLN:C	2.40	0.41
1:C:265:LYS:O	1:C:266:LEU:C	2.58	0.41
1:G:59:ALA:HB1	1:G:198:ILE:HG13	2.01	0.41
1:D:145:ILE:O	1:D:149:ILE:HG13	2.19	0.41
1:G:384:ARG:NH1	1:G:384:ARG:HG3	2.35	0.41
1:G:341:ASN:O	1:G:344:VAL:HG12	2.19	0.41
1:A:20:GLN:HA	1:A:23:LEU:HD12	2.02	0.41
1:G:378:ASP:O	1:G:381:ASP:HB2	2.20	0.41
1:B:49:TYR:O	1:B:199:VAL:HA	2.20	0.41
1:F:289:TYR:HA	1:F:309:LYS:CD	2.49	0.41
1:G:124:THR:HG22	1:G:126:SER:H	1.85	0.41
1:A:70:THR:O	1:A:71:LYS:C	2.58	0.41
1:F:6:LEU:O	1:F:372:HIS:CE1	2.73	0.41
1:C:265:LYS:HD3	1:C:269:PHE:CZ	2.55	0.41
1:E:44:THR:HG1	1:E:44:THR:H	1.43	0.41
1:G:364:LYS:H	1:G:364:LYS:HG2	1.65	0.41
1:G:324:ASN:C	1:G:326:ALA:N	2.73	0.41
1:B:12:ASP:O	1:B:16:TYR:HD1	2.03	0.41
1:C:171:LYS:HB3	1:C:176:PHE:CZ	2.54	0.41
1:F:58:THR:CG2	1:F:249:VAL:CG1	2.98	0.41
1:B:168:PHE:C	1:B:170:ASN:N	2.73	0.41
1:G:92:TYR:C	1:G:94:PRO:HD2	2.41	0.41
1:A:333:ILE:HD12	1:A:366:GLY:HA3	2.02	0.41
1:B:306:PHE:HB2	1:B:367:LEU:HD12	2.02	0.41
1:E:88:TRP:CG	1:E:89:SER:N	2.88	0.41
1:F:61:LEU:HD21	1:F:247:TYR:CZ	2.55	0.41
1:B:36:GLN:O	1:B:39:THR:N	2.53	0.41
1:A:70:THR:O	1:A:73:PRO:HD3	2.20	0.41
1:G:72:LYS:HA	1:G:73:PRO:HD3	1.81	0.41
1:F:138:ASN:OD1	1:F:139:PRO:HD2	2.21	0.41
1:C:250:ARG:HA	1:C:251:PRO:HD3	1.84	0.41
1:B:156:LEU:HD12	1:B:157:LEU:H	1.86	0.41
1:B:37:TYR:CE1	1:B:259:GLY:HA3	2.55	0.41
1:A:81:ILE:HD11	1:A:131:LEU:HB2	2.02	0.41
1:A:279:TYR:HE2	1:A:381:ASP:OD1	2.02	0.41
1:E:202:ASP:OD2	1:E:205:ILE:HG12	2.19	0.41
1:B:71:LYS:HE2	1:B:204:GLU:CD	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ALA:HA	1:B:372:HIS:CE1	2.55	0.41
1:G:33:TYR:HB2	1:G:253:GLU:CD	2.39	0.41
1:F:316:ARG:HE	1:F:316:ARG:HB3	1.64	0.41
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.35	0.41
1:D:176:PHE:H	1:D:176:PHE:HD1	1.69	0.41
1:D:316:ARG:NH1	1:D:366:GLY:O	2.53	0.41
1:B:385:GLU:HA	1:B:388:LYS:HE2	2.01	0.41
1:B:107:ILE:HA	1:B:114:ILE:HA	2.02	0.41
1:B:27:MET:SD	1:B:27:MET:C	2.98	0.41
1:A:70:THR:HG21	1:A:74:ARG:NE	2.35	0.41
1:G:185:PHE:HB2	3:G:420:HOH:O	2.20	0.41
1:E:41:PHE:O	1:E:45:PHE:HD1	2.04	0.41
1:G:61:LEU:HD21	1:G:247:TYR:CZ	2.56	0.41
1:B:223:LYS:O	1:B:230:VAL:HA	2.21	0.41
1:F:143:ASP:O	1:F:147:LYS:HG3	2.20	0.41
1:E:335:THR:HG21	1:F:242:PHE:CZ	2.56	0.41
1:F:159:ASP:OD2	1:F:188:IT1:H2A	2.20	0.41
1:H:290:LEU:HD22	1:H:306:PHE:HB3	2.02	0.41
1:G:298:GLU:O	1:G:299:SER:C	2.57	0.41
1:G:250:ARG:HA	1:G:251:PRO:HD2	1.91	0.41
1:G:149:ILE:N	1:G:149:ILE:CD1	2.81	0.41
1:D:334:VAL:HG12	1:D:335:THR:N	2.36	0.41
1:D:202:ASP:CG	1:D:205:ILE:HG12	2.41	0.41
1:C:122:ALA:HB2	1:C:353:HIS:CG	2.56	0.41
1:E:67:LEU:HD22	1:E:74:ARG:HD3	2.03	0.41
1:A:382:TYR:OH	1:C:271:SER:OG	2.38	0.41
1:C:319:LEU:HD23	1:C:319:LEU:HA	1.73	0.41
1:E:305:SER:N	3:E:408:HOH:O	2.53	0.41
1:C:29:THR:CG2	1:C:30:MET:N	2.81	0.41
1:E:250:ARG:NH2	2:F:405:AKG:O3	2.43	0.41
1:H:277:ALA:O	1:H:280:PHE:HB3	2.21	0.41
1:G:156:LEU:HG	1:G:157:LEU:N	2.34	0.41
1:G:108:ASP:O	1:G:112:LEU:N	2.52	0.41
1:G:379:GLU:N	1:G:379:GLU:CD	2.73	0.41
1:B:252:LEU:O	1:B:253:GLU:C	2.59	0.41
1:A:81:ILE:HD12	1:A:129:ALA:HB3	2.03	0.41
1:F:12:ASP:OD1	1:F:14:LEU:HB2	2.20	0.41
1:C:268:ARG:O	1:C:272:VAL:HG23	2.20	0.41
1:F:274:ARG:HG2	1:F:274:ARG:NH1	2.35	0.41
1:E:331:ARG:HB2	1:E:332:PRO:HD2	2.02	0.41
1:B:345:LEU:C	1:B:347:TYR:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:O	1:B:20:GLN:C	2.57	0.41
1:C:105:VAL:HB	1:C:114:ILE:HD11	2.03	0.41
1:H:337:ASN:HB3	1:H:340:LYS:HD3	2.02	0.41
1:E:82:ILE:HG23	1:E:83:VAL:N	2.35	0.41
1:D:22:VAL:HG22	1:D:33:TYR:CD2	2.55	0.41
1:D:137:GLY:HA2	1:D:163:SER:HA	2.03	0.41
1:B:92:TYR:CE2	1:B:338:PHE:CG	3.09	0.41
1:E:77:LYS:HB3	1:E:77:LYS:HE2	1.15	0.41
1:C:178:LEU:HG	1:C:178:LEU:O	2.21	0.41
1:F:314:VAL:HG12	1:F:315:ILE:N	2.35	0.41
1:C:310:LYS:HE2	1:C:310:LYS:HB3	1.45	0.41
1:D:156:LEU:CD1	1:D:157:LEU:N	2.78	0.41
1:G:49:TYR:OH	1:G:203:GLU:HB2	2.21	0.41
1:G:285:LYS:HD2	1:G:286:ASP:CG	2.39	0.41
1:A:304:PHE:O	1:A:368:PHE:HA	2.21	0.41
1:F:361:TYR:O	1:F:362:LEU:C	2.59	0.41
1:C:84:PRO:HA	1:C:114:ILE:CD1	2.51	0.41
1:C:280:PHE:O	1:C:281:LEU:C	2.57	0.41
1:F:140:ASN:HB2	1:F:142:PHE:CZ	2.56	0.41
1:E:240:PHE:CD2	1:F:332:PRO:HG2	2.56	0.41
1:B:156:LEU:HD12	1:B:157:LEU:N	2.36	0.41
1:D:35:LYS:HZ1	1:D:35:LYS:HB2	1.86	0.41
1:A:136:LEU:C	1:A:302:PHE:CB	2.89	0.41
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.65	0.41
1:A:88:TRP:CZ2	2:A:401:AKG:H41	2.56	0.41
1:B:40:GLN:O	1:B:44:THR:OG1	2.30	0.41
1:C:192:THR:HA	1:C:258:ILE:HG21	2.02	0.41
1:H:168:PHE:O	1:H:169:ASN:C	2.59	0.41
1:E:345:LEU:O	1:E:346:LYS:C	2.57	0.41
1:C:244:LEU:HA	1:C:245:PRO:HD3	1.91	0.41
1:D:228:THR:HG1	1:D:228:THR:H	1.56	0.41
1:F:61:LEU:HA	1:F:94:PRO:HB3	2.02	0.41
1:B:106:ASP:OD2	1:B:358:ASN:HB2	2.21	0.41
1:C:150:GLY:HA3	1:C:151:GLY:HA3	1.39	0.40
1:E:316:ARG:HH22	1:E:364:LYS:HA	1.73	0.40
1:G:235:GLN:C	1:G:237:GLU:N	2.73	0.40
1:A:384:ARG:HD2	1:A:384:ARG:HA	1.76	0.40
1:A:188:IT1:C4A	1:A:188:IT1:OP4	2.68	0.40
1:H:279:TYR:HD2	1:H:380:ILE:HG21	1.85	0.40
1:F:376:LEU:HB2	1:F:380:ILE:CD1	2.51	0.40
1:F:50:ALA:CB	1:F:199:VAL:HG12	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:ILE:HD12	1:F:64:ILE:HG23	1.83	0.40
1:G:287:HIS:ND1	1:G:290:LEU:N	2.69	0.40
1:G:319:LEU:HG	1:G:319:LEU:H	1.76	0.40
1:G:192:THR:O	1:G:193:MET:CB	2.67	0.40
1:C:108:ASP:O	1:C:112:LEU:N	2.48	0.40
1:C:101:ARG:HE	1:C:349:ASP:CG	2.24	0.40
1:E:95:LEU:N	1:E:95:LEU:HD23	2.36	0.40
1:B:49:TYR:OH	1:B:203:GLU:HG3	2.21	0.40
1:C:336:GLY:HA2	1:C:362:LEU:HD21	2.03	0.40
1:F:283:LYS:HA	1:F:283:LYS:HD3	1.30	0.40
1:E:269:PHE:H	1:E:269:PHE:HD1	1.70	0.40
1:B:376:LEU:HA	1:B:379:GLU:OE2	2.21	0.40
1:E:192:THR:O	1:E:193:MET:CB	2.69	0.40
1:B:346:LYS:H	1:B:346:LYS:HG2	1.52	0.40
1:H:304:PHE:CZ	1:H:371:ASN:HB2	2.55	0.40
1:F:69:PHE:CZ	1:F:245:PRO:HG2	2.56	0.40
1:B:52:MET:O	1:B:213:ARG:NH1	2.42	0.40
1:A:95:LEU:HG	1:A:95:LEU:H	1.57	0.40
1:E:186:TYR:CD1	1:E:186:TYR:C	2.93	0.40
1:C:128:LYS:HB3	1:C:128:LYS:HZ2	1.77	0.40
1:B:120:LYS:HA	1:B:148:ILE:HG23	2.02	0.40
1:D:34:VAL:HG23	1:D:253:GLU:HA	2.03	0.40
1:F:223:LYS:HE2	1:F:223:LYS:HB3	2.00	0.40
1:C:253:GLU:OE1	1:C:253:GLU:HA	2.21	0.40
1:G:144:GLU:OE1	1:G:147:LYS:HD3	2.22	0.40
1:D:185:PHE:CD1	1:D:194:GLU:OE1	2.74	0.40
1:H:101:ARG:NH1	1:H:349:ASP:OD1	2.53	0.40
1:B:244:LEU:HA	1:B:245:PRO:HD3	1.83	0.40
1:G:130:ILE:HG21	1:G:130:ILE:HD12	1.83	0.40
1:B:221:LEU:O	1:B:231:LYS:HE2	2.22	0.40
1:E:335:THR:HG21	1:F:242:PHE:CE2	2.57	0.40
1:B:52:MET:HG3	1:B:197[B]:CYS:HG	1.86	0.40
1:A:133:VAL:HG22	1:A:159:ASP:HB3	2.03	0.40
1:E:139:PRO:O	1:E:296:THR:HB	2.21	0.40
1:F:368:PHE:CD1	1:F:368:PHE:C	2.94	0.40
1:A:109:ILE:HA	1:A:109:ILE:HD12	1.88	0.40
1:A:135:LEU:HD21	1:A:334:VAL:HG21	2.03	0.40
1:F:287:HIS:HE1	1:F:289:TYR:CE2	2.37	0.40
1:C:119:LEU:HD12	1:C:119:LEU:HA	1.76	0.40
1:H:70:THR:HG1	1:H:74:ARG:HD3	1.87	0.40
1:H:225:ASN:O	1:H:229:GLY:HA2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:PHE:HA	3:H:402:HOH:O	2.22	0.40
1:C:306:PHE:HB2	1:C:367:LEU:HD13	2.03	0.40
1:C:235:GLN:O	1:C:237:GLU:N	2.55	0.40
1:G:164:MET:CE	1:G:190:ILE:HG12	2.51	0.40
1:E:234:ASP:OD1	1:E:234:ASP:C	2.58	0.40
1:D:167:THR:HG22	1:D:172:CYS:HA	2.03	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	382/390 (98%)	352 (92%)	25 (6%)	5 (1%)	15	11
1	B	383/390 (98%)	342 (89%)	35 (9%)	6 (2%)	12	8
1	C	386/390 (99%)	336 (87%)	43 (11%)	7 (2%)	11	7
1	D	379/390 (97%)	354 (93%)	22 (6%)	3 (1%)	24	22
1	E	381/390 (98%)	337 (88%)	37 (10%)	7 (2%)	11	7
1	F	384/390 (98%)	338 (88%)	41 (11%)	5 (1%)	15	11
1	G	385/390 (99%)	339 (88%)	40 (10%)	6 (2%)	12	8
1	H	379/390 (97%)	327 (86%)	46 (12%)	6 (2%)	12	8
All	All	3059/3120 (98%)	2725 (89%)	289 (9%)	45 (2%)	13	9

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	C	152	ARG
1	G	354	ASN
1	A	311	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	150	GLY
1	C	301	TRP
1	C	311	ASP
1	D	186	TYR
1	E	186	TYR
1	E	193	MET
1	E	325	SER
1	G	186	TYR
1	G	193	MET
1	G	299	SER
1	H	193	MET
1	H	314	VAL
1	A	334	VAL
1	C	236	PHE
1	E	30	MET
1	E	334	VAL
1	F	151	GLY
1	F	193	MET
1	F	236	PHE
1	G	325	SER
1	G	334	VAL
1	H	239	SER
1	H	334	VAL
1	A	354	ASN
1	B	193	MET
1	B	235	GLN
1	B	285	LYS
1	B	334	VAL
1	C	334	VAL
1	C	354	ASN
1	D	334	VAL
1	F	334	VAL
1	A	30	MET
1	C	106	ASP
1	D	301	TRP
1	H	259	GLY
1	B	313	GLY
1	E	215	HIS
1	H	260	ILE
1	E	116	ILE
1	F	4	TYR

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	340/344 (99%)	287 (84%)	53 (16%)	3	2
1	B	341/344 (99%)	284 (83%)	57 (17%)	3	2
1	C	344/344 (100%)	291 (85%)	53 (15%)	3	2
1	D	338/344 (98%)	293 (87%)	45 (13%)	5	4
1	E	339/344 (98%)	292 (86%)	47 (14%)	4	3
1	F	342/344 (99%)	285 (83%)	57 (17%)	3	2
1	G	343/344 (100%)	282 (82%)	61 (18%)	2	1
1	H	338/344 (98%)	269 (80%)	69 (20%)	1	1
All	All	2725/2752 (99%)	2283 (84%)	442 (16%)	3	2

All (442) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	12	ASP
1	A	14	LEU
1	A	17	LYS
1	A	21	SER
1	A	26	LYS
1	A	27	MET
1	A	28	PHE
1	A	35	LYS
1	A	47	SER
1	A	48	LYS
1	A	71	LYS
1	A	72	LYS
1	A	74	ARG
1	A	77	LYS
1	A	81	ILE
1	A	107	ILE
1	A	108	ASP
1	A	109	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	118	SER
1	A	121	GLU
1	A	126	SER
1	A	132	THR
1	A	147	LYS
1	A	179	MET
1	A	197[A]	CYS
1	A	197[B]	CYS
1	A	217	TRP
1	A	221	LEU
1	A	226	LYS
1	A	232	SER
1	A	235	GLN
1	A	237	GLU
1	A	239	SER
1	A	241	LYS
1	A	244	LEU
1	A	252	LEU
1	A	268	ARG
1	A	283	LYS
1	A	314	VAL
1	A	331	ARG
1	A	339	LEU
1	A	340	LYS
1	A	342	THR
1	A	346	LYS
1	A	360	GLU
1	A	362	LEU
1	A	369	VAL
1	A	374	ILE
1	A	375	GLU
1	A	379	GLU
1	A	383	LEU
1	A	388	LYS
1	B	4	TYR
1	B	17	LYS
1	B	20	GLN
1	B	21	SER
1	B	24	ASP
1	B	26	LYS
1	B	27	MET
1	B	30	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	LYS
1	B	48	LYS
1	B	64	ILE
1	B	71	LYS
1	B	81	ILE
1	B	101	ARG
1	B	107	ILE
1	B	108	ASP
1	B	121	GLU
1	B	128	LYS
1	B	131	LEU
1	B	144	GLU
1	B	155	ILE
1	B	158	GLU
1	B	170	ASN
1	B	171	LYS
1	B	179	MET
1	B	184	SER
1	B	198	ILE
1	B	203	GLU
1	B	205	ILE
1	B	217	TRP
1	B	223	LYS
1	B	224	LYS
1	B	226	LYS
1	B	233	ASP
1	B	239	SER
1	B	265	LYS
1	B	269	PHE
1	B	270	ILE
1	B	271	SER
1	B	285	LYS
1	B	290	LEU
1	B	292	VAL
1	B	300	SER
1	B	307	ILE
1	B	310	LYS
1	B	318	GLN
1	B	325	SER
1	B	328	ILE
1	B	340	LYS
1	B	345	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	346	LYS
1	B	364	LYS
1	B	367	LEU
1	B	375	GLU
1	B	379	GLU
1	B	384	ARG
1	B	388	LYS
1	C	2	ILE
1	C	4	TYR
1	C	6	LEU
1	C	8	SER
1	C	14	LEU
1	C	17	LYS
1	C	20	GLN
1	C	24	ASP
1	C	27	MET
1	C	28	PHE
1	C	35	LYS
1	C	58	THR
1	C	72	LYS
1	C	76	LYS
1	C	77	LYS
1	C	103	LYS
1	C	109	ILE
1	C	114	ILE
1	C	116	ILE
1	C	121	GLU
1	C	128	LYS
1	C	135	LEU
1	C	145	ILE
1	C	152	ARG
1	C	157	LEU
1	C	197[A]	CYS
1	C	197[B]	CYS
1	C	210	LEU
1	C	217	TRP
1	C	219	ARG
1	C	224	LYS
1	C	230	VAL
1	C	231	LYS
1	C	232	SER
1	C	264	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	265	LYS
1	C	271	SER
1	C	275	LYS
1	C	283	LYS
1	C	310	LYS
1	C	311	ASP
1	C	312	SER
1	C	316	ARG
1	C	322	ASN
1	C	325	SER
1	C	340	LYS
1	C	356	VAL
1	C	362	LEU
1	C	364	LYS
1	C	367	LEU
1	C	375	GLU
1	C	378	ASP
1	C	388	LYS
1	D	10	THR
1	D	13	ASP
1	D	26	LYS
1	D	29	THR
1	D	48	LYS
1	D	62	LEU
1	D	72	LYS
1	D	87	SER
1	D	108	ASP
1	D	120	LYS
1	D	135	LEU
1	D	145	ILE
1	D	147	LYS
1	D	171	LYS
1	D	178	LEU
1	D	184	SER
1	D	217	TRP
1	D	220	ASN
1	D	228	THR
1	D	232	SER
1	D	235	GLN
1	D	237	GLU
1	D	245	PRO
1	D	268	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	271	SER
1	D	275	LYS
1	D	278	GLU
1	D	285	LYS
1	D	316	ARG
1	D	317	LYS
1	D	318	GLN
1	D	321	GLU
1	D	331	ARG
1	D	333	ILE
1	D	340	LYS
1	D	343	ASP
1	D	355	ASN
1	D	367	LEU
1	D	368	PHE
1	D	369	VAL
1	D	373	GLN
1	D	374	ILE
1	D	378	ASP
1	D	384	ARG
1	D	388	LYS
1	E	6	LEU
1	E	13	ASP
1	E	27	MET
1	E	36	GLN
1	E	40	GLN
1	E	43	LYS
1	E	47	SER
1	E	72	LYS
1	E	77	LYS
1	E	97	GLN
1	E	118	SER
1	E	120	LYS
1	E	121	GLU
1	E	128	LYS
1	E	144	GLU
1	E	155	ILE
1	E	170	ASN
1	E	213	ARG
1	E	217	TRP
1	E	232	SER
1	E	235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	244	LEU
1	E	253	GLU
1	E	260	ILE
1	E	268	ARG
1	E	275	LYS
1	E	285	LYS
1	E	287	HIS
1	E	310	LYS
1	E	315	ILE
1	E	316	ARG
1	E	317	LYS
1	E	339	LEU
1	E	342	THR
1	E	344	VAL
1	E	345	LEU
1	E	346	LYS
1	E	350	TYR
1	E	351	THR
1	E	360	GLU
1	E	362	LEU
1	E	364	LYS
1	E	367	LEU
1	E	369	VAL
1	E	375	GLU
1	E	379	GLU
1	E	384	ARG
1	F	4	TYR
1	F	8	SER
1	F	14	LEU
1	F	17	LYS
1	F	21	SER
1	F	25	SER
1	F	26	LYS
1	F	43	LYS
1	F	48	LYS
1	F	49	TYR
1	F	58	THR
1	F	71	LYS
1	F	72	LYS
1	F	77	LYS
1	F	101	ARG
1	F	107	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	119	LEU
1	F	125	ASP
1	F	126	SER
1	F	128	LYS
1	F	131	LEU
1	F	135	LEU
1	F	145	ILE
1	F	148	ILE
1	F	153	ASP
1	F	171	LYS
1	F	178	LEU
1	F	179	MET
1	F	197[A]	CYS
1	F	197[B]	CYS
1	F	210	LEU
1	F	217	TRP
1	F	223	LYS
1	F	224	LYS
1	F	230	VAL
1	F	232	SER
1	F	239	SER
1	F	241	LYS
1	F	265	LYS
1	F	275	LYS
1	F	283	LYS
1	F	285	LYS
1	F	294	GLN
1	F	299	SER
1	F	300	SER
1	F	312	SER
1	F	315	ILE
1	F	316	ARG
1	F	317	LYS
1	F	321	GLU
1	F	325	SER
1	F	340	LYS
1	F	367	LEU
1	F	368	PHE
1	F	383	LEU
1	F	384	ARG
1	F	388	LYS
1	G	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	4	TYR
1	G	5	PRO
1	G	6	LEU
1	G	9	SER
1	G	12	ASP
1	G	13	ASP
1	G	17	LYS
1	G	19	ILE
1	G	24	ASP
1	G	26	LYS
1	G	29	THR
1	G	32	GLU
1	G	40	GLN
1	G	43	LYS
1	G	48	LYS
1	G	49	TYR
1	G	52	MET
1	G	71	LYS
1	G	72	LYS
1	G	112	LEU
1	G	128	LYS
1	G	130	ILE
1	G	131	LEU
1	G	145	ILE
1	G	148	ILE
1	G	149	ILE
1	G	170	ASN
1	G	179	MET
1	G	197[A]	CYS
1	G	197[B]	CYS
1	G	205	ILE
1	G	208	ILE
1	G	209	LEU
1	G	217	TRP
1	G	223	LYS
1	G	230	VAL
1	G	232	SER
1	G	235	GLN
1	G	237	GLU
1	G	265	LYS
1	G	267	PRO
1	G	268	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	271	SER
1	G	274	ARG
1	G	283	LYS
1	G	285	LYS
1	G	291	ASP
1	G	309	LYS
1	G	317	LYS
1	G	318	GLN
1	G	328	ILE
1	G	331	ARG
1	G	339	LEU
1	G	340	LYS
1	G	346	LYS
1	G	364	LYS
1	G	367	LEU
1	G	368	PHE
1	G	385	GLU
1	G	388	LYS
1	H	17	LYS
1	H	20	GLN
1	H	21	SER
1	H	26	LYS
1	H	28	PHE
1	H	29	THR
1	H	32	GLU
1	H	35	LYS
1	H	40	GLN
1	H	43	LYS
1	H	49	TYR
1	H	71	LYS
1	H	72	LYS
1	H	74	ARG
1	H	76	LYS
1	H	77	LYS
1	H	81	ILE
1	H	89	SER
1	H	97	GLN
1	H	100	LEU
1	H	120	LYS
1	H	125	ASP
1	H	126	SER
1	H	136	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	144	GLU
1	H	169	ASN
1	H	170	ASN
1	H	172	CYS
1	H	197[A]	CYS
1	H	197[B]	CYS
1	H	217	TRP
1	H	223	LYS
1	H	224	LYS
1	H	230	VAL
1	H	232	SER
1	H	235	GLN
1	H	239	SER
1	H	241	LYS
1	H	244	LEU
1	H	250	ARG
1	H	254	MET
1	H	265	LYS
1	H	273	ARG
1	H	274	ARG
1	H	275	LYS
1	H	278	GLU
1	H	282	ASP
1	H	285	LYS
1	H	286	ASP
1	H	310	LYS
1	H	315	ILE
1	H	316	ARG
1	H	318	GLN
1	H	319	LEU
1	H	324	ASN
1	H	328	ILE
1	H	329	GLU
1	H	330	CYS
1	H	331	ARG
1	H	339	LEU
1	H	340	LYS
1	H	342	THR
1	H	350	TYR
1	H	364	LYS
1	H	367	LEU
1	H	374	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	375	GLU
1	H	382	TYR
1	H	388	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	322	ASN
1	A	324	ASN
1	A	353	HIS
1	B	36	GLN
1	B	318	GLN
1	B	322	ASN
1	B	324	ASN
1	B	372	HIS
1	C	322	ASN
1	D	20	GLN
1	D	235	GLN
1	D	322	ASN
1	D	353	HIS
1	E	97	GLN
1	E	322	ASN
1	F	3	ASN
1	F	170	ASN
1	F	207	HIS
1	F	287	HIS
1	F	294	GLN
1	G	97	GLN
1	G	322	ASN
1	G	365	ASN
1	G	372	HIS
1	H	20	GLN
1	H	36	GLN
1	H	97	GLN
1	H	170	ASN
1	H	322	ASN
1	H	324	ASN
1	H	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	IT1	A	188	1	23,24,25	1.52	4 (17%)	28,32,34	1.43	5 (17%)
1	IT1	B	188	1	23,24,25	1.09	2 (8%)	28,32,34	1.22	4 (14%)
1	IT1	C	188	1	23,24,25	1.11	1 (4%)	28,32,34	1.04	1 (3%)
1	IT1	D	188	1	23,24,25	1.20	2 (8%)	28,32,34	1.08	2 (7%)
1	IT1	E	188	1	23,24,25	1.31	3 (13%)	28,32,34	1.13	0
1	IT1	F	188	1	23,24,25	1.11	1 (4%)	28,32,34	1.14	1 (3%)
1	IT1	G	188	1	23,24,25	1.18	2 (8%)	28,32,34	1.02	1 (3%)
1	IT1	H	188	1	23,24,25	1.41	4 (17%)	28,32,34	1.00	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IT1	A	188	1	-	0/15/17/19	0/1/1/1
1	IT1	B	188	1	-	0/15/17/19	0/1/1/1
1	IT1	C	188	1	-	0/15/17/19	0/1/1/1
1	IT1	D	188	1	-	0/15/17/19	0/1/1/1
1	IT1	E	188	1	-	0/15/17/19	0/1/1/1
1	IT1	F	188	1	-	0/15/17/19	0/1/1/1
1	IT1	G	188	1	-	0/15/17/19	0/1/1/1
1	IT1	H	188	1	-	0/15/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	IT1	C3-C2	-3.50	1.38	1.40
1	F	188	IT1	C3-C2	-2.98	1.38	1.40
1	H	188	IT1	C3-C2	-2.28	1.39	1.40
1	A	188	IT1	P-OP3	2.10	1.62	1.54
1	E	188	IT1	P-OP2	2.31	1.63	1.54
1	E	188	IT1	P-OP3	2.35	1.63	1.54
1	D	188	IT1	P-OP2	2.47	1.63	1.54
1	H	188	IT1	P-OP3	2.47	1.63	1.54
1	B	188	IT1	P-OP2	2.49	1.63	1.54
1	G	188	IT1	P-OP3	2.66	1.64	1.54
1	A	188	IT1	P-OP2	2.69	1.64	1.54
1	H	188	IT1	P-OP2	2.78	1.64	1.54
1	B	188	IT1	P-OP1	2.92	1.60	1.51
1	G	188	IT1	P-OP1	2.97	1.60	1.51
1	C	188	IT1	P-OP1	3.08	1.61	1.51
1	A	188	IT1	P-OP1	3.94	1.64	1.51
1	E	188	IT1	P-OP1	3.98	1.64	1.51
1	D	188	IT1	P-OP1	4.01	1.64	1.51
1	H	188	IT1	P-OP1	4.06	1.64	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	IT1	OP4-C5A-C5	-3.12	103.84	108.99
1	G	188	IT1	CD-CE-NZ	-2.90	106.22	110.98
1	B	188	IT1	CD-CE-NZ	-2.82	106.35	110.98
1	A	188	IT1	CD-CE-NZ	-2.76	106.45	110.98
1	C	188	IT1	OP4-C5A-C5	-2.51	104.85	108.99
1	F	188	IT1	C5-C6-N1	-2.37	119.74	123.86
1	B	188	IT1	C2A-C2-C3	-2.17	118.42	121.04
1	A	188	IT1	C2A-C2-C3	-2.14	118.46	121.04
1	H	188	IT1	O-C-CA	-2.11	119.98	125.49
1	B	188	IT1	O-C-CA	-2.07	120.09	125.49
1	D	188	IT1	CE-NZ-C4A	2.15	125.17	118.97
1	A	188	IT1	CE-NZ-C4A	2.18	125.26	118.97
1	A	188	IT1	CB-CA-N	2.38	117.30	110.52
1	D	188	IT1	O3-C3-C2	2.50	122.01	117.66
1	B	188	IT1	OP2-P-OP4	2.83	114.72	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	188	IT1	4	0
1	B	188	IT1	6	0
1	C	188	IT1	5	0
1	D	188	IT1	1	0
1	E	188	IT1	1	0
1	F	188	IT1	9	0
1	G	188	IT1	3	0
1	H	188	IT1	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AKG	A	401	-	3,9,9	0.35	0	4,11,11	1.08	0
2	AKG	B	402	-	3,9,9	1.08	0	4,11,11	1.98	2 (50%)
2	AKG	C	403	-	3,9,9	0.44	0	4,11,11	1.17	0
2	AKG	D	404	-	3,9,9	0.32	0	4,11,11	2.13	1 (25%)
2	AKG	F	405	-	3,9,9	0.25	0	4,11,11	1.54	1 (25%)
2	AKG	H	406	-	3,9,9	1.00	0	4,11,11	2.59	3 (75%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AKG	A	401	-	-	0/3/9/9	0/0/0/0
2	AKG	B	402	-	-	0/3/9/9	0/0/0/0
2	AKG	C	403	-	-	0/3/9/9	0/0/0/0
2	AKG	D	404	-	-	0/3/9/9	0/0/0/0
2	AKG	F	405	-	-	0/3/9/9	0/0/0/0
2	AKG	H	406	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	404	AKG	C3-C4-C5	-3.57	106.20	112.75
2	H	406	AKG	C4-C3-C2	-3.34	104.53	112.98
2	H	406	AKG	C3-C4-C5	-3.29	106.72	112.75
2	B	402	AKG	C3-C4-C5	-3.00	107.24	112.75
2	F	405	AKG	C4-C3-C2	-2.82	105.86	112.98
2	B	402	AKG	C4-C3-C2	-2.40	106.92	112.98
2	H	406	AKG	O5-C2-C3	-2.16	116.19	120.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AKG	1	0
2	B	402	AKG	5	0
2	C	403	AKG	1	0
2	D	404	AKG	2	0
2	F	405	AKG	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	383/390 (98%)	-1.57	0 100 100	11, 37, 67, 96	0
1	B	384/390 (98%)	-1.57	0 100 100	14, 36, 70, 88	0
1	C	387/390 (99%)	-1.56	0 100 100	10, 38, 73, 89	0
1	D	380/390 (97%)	-1.58	0 100 100	11, 37, 66, 94	0
1	E	382/390 (97%)	-1.54	0 100 100	13, 42, 72, 94	0
1	F	385/390 (98%)	-1.55	0 100 100	13, 40, 73, 92	0
1	G	386/390 (98%)	-1.53	0 100 100	15, 45, 74, 98	0
1	H	380/390 (97%)	-1.52	0 100 100	14, 45, 77, 100	0
All	All	3067/3120 (98%)	-1.55	0 100 100	10, 40, 73, 100	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	IT1	D	188	24/25	1.00	0.05	-	14,36,61,69	0
1	IT1	E	188	24/25	1.00	0.05	-	5,40,99,99	0
1	IT1	F	188	24/25	0.99	0.06	-	32,59,99,99	0
1	IT1	G	188	24/25	1.00	0.05	-	13,26,57,66	0
1	IT1	A	188	24/25	1.00	0.05	-	7,34,55,78	0
1	IT1	B	188	24/25	1.00	0.05	-	11,28,86,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	IT1	C	188	24/25	1.00	0.05	-	10,26,55,83	0
1	IT1	H	188	24/25	1.00	0.05	-	13,39,98,99	0

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(\AA^2)	Q<0.9
2	AKG	A	401	10/10	0.99	0.07	5.98	34,66,99,99	0
2	AKG	F	405	10/10	0.99	0.06	2.95	43,62,99,99	0
2	AKG	B	402	10/10	0.99	0.05	0.61	16,32,70,79	0
2	AKG	D	404	10/10	0.99	0.05	0.40	23,42,99,99	0
2	AKG	C	403	10/10	0.99	0.04	-1.26	16,32,99,99	0
2	AKG	H	406	10/10	0.99	0.04	-1.60	15,37,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.