



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 10:56 PM EDT

PDB ID : 1SZP  
Title : A Crystal Structure of the Rad51 Filament  
Authors : Conway, A.B.; Lynch, T.W.; Zhang, Y.; Fortin, G.S.; Symington, L.S.; Rice, P.A.  
Deposited on : 2004-04-06  
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

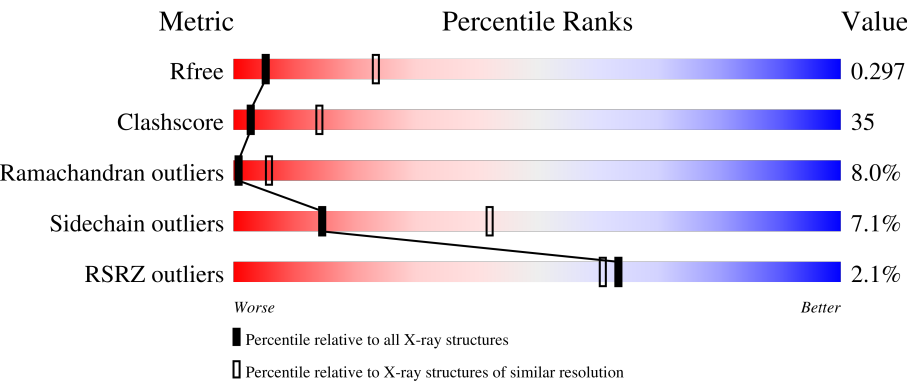
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 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 3.25 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))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	321	<div><div>0%</div><div>33%40%18%•8%</div></div>
1	B	321	<div><div>4%</div><div>32%43%10%•15%</div></div>
1	C	321	<div><div>3%</div><div>33%40%11%•15%</div></div>
1	D	321	<div><div>2%</div><div>36%40%13%•9%</div></div>
1	E	321	<div><div>2%</div><div>39%40%10%•8%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	321	

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
2	SO4	B	502	-	-	X	-
2	SO4	C	503	-	-	X	-
2	SO4	D	504	-	-	X	-
2	SO4	E	505	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12583 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 DNA repair protein RAD51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2148	1349	376	408	15			
1	B	274	Total	C	N	O	S	0	0	0
			1985	1245	351	376	13			
1	C	274	Total	C	N	O	S	0	0	0
			1995	1249	354	378	14			
1	D	293	Total	C	N	O	S	0	0	0
			2143	1344	377	406	16			
1	E	294	Total	C	N	O	S	0	0	0
			2147	1346	378	407	16			
1	F	294	Total	C	N	O	S	0	0	0
			2135	1341	372	407	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	MET	-	initiating methionine	UNP P25454
A	345	THR	ILE	engineered mutation	UNP P25454
B	80	MET	-	initiating methionine	UNP P25454
B	345	THR	ILE	engineered mutation	UNP P25454
C	80	MET	-	initiating methionine	UNP P25454
C	345	THR	ILE	engineered mutation	UNP P25454
D	80	MET	-	initiating methionine	UNP P25454
D	345	THR	ILE	engineered mutation	UNP P25454
E	80	MET	-	initiating methionine	UNP P25454
E	345	THR	ILE	engineered mutation	UNP P25454
F	80	MET	-	initiating methionine	UNP P25454
F	345	THR	ILE	engineered mutation	UNP P25454

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

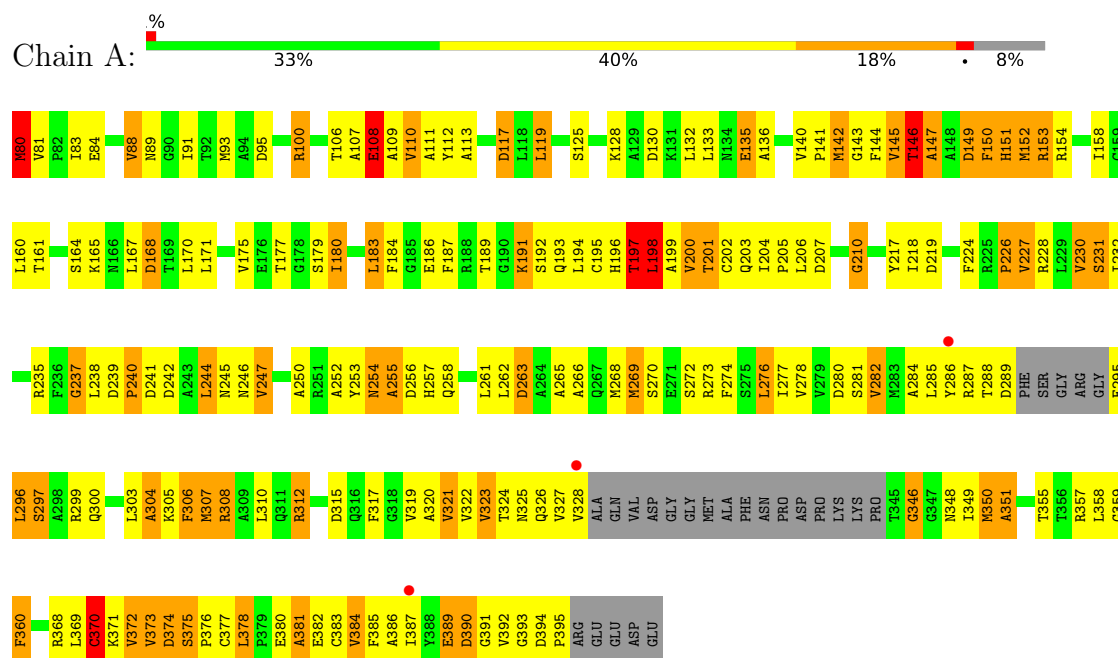


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

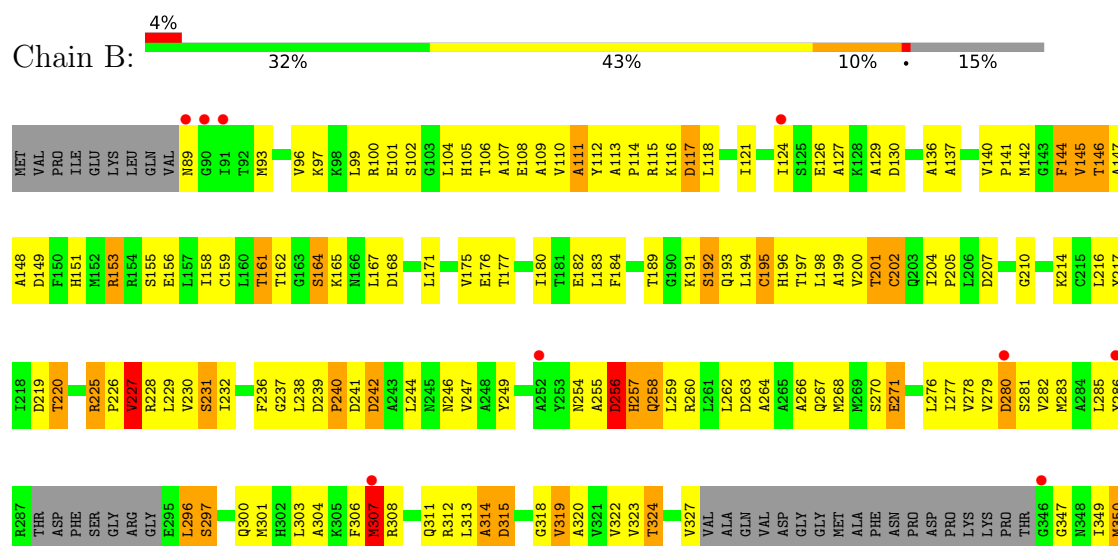
### 3 Residue-property plots

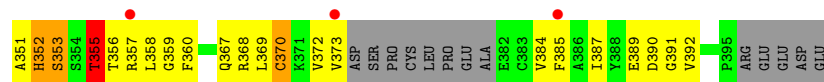
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: DNA repair protein RAD51

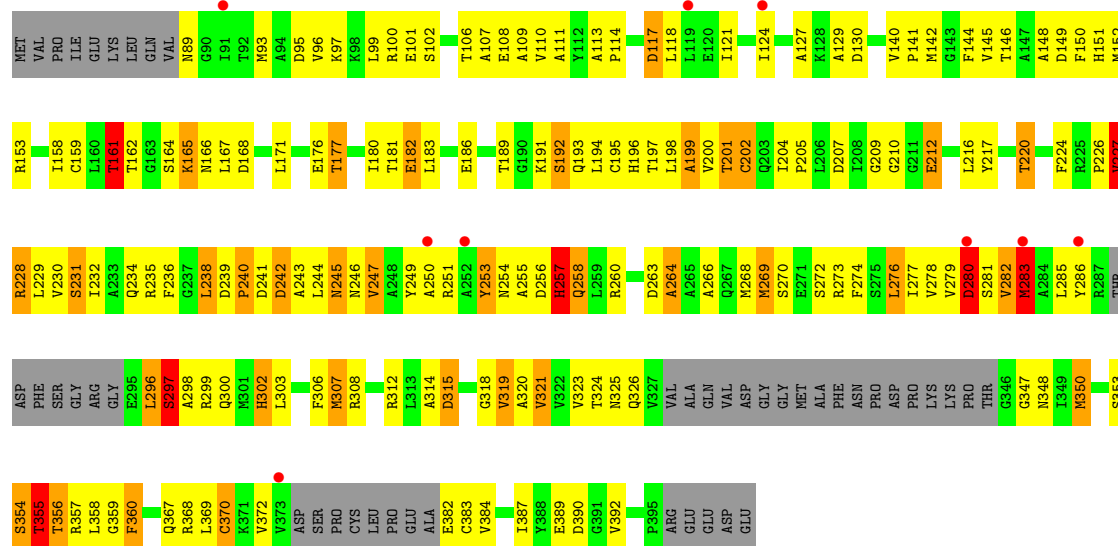


#### • Molecule 1: DNA repair protein RAD51

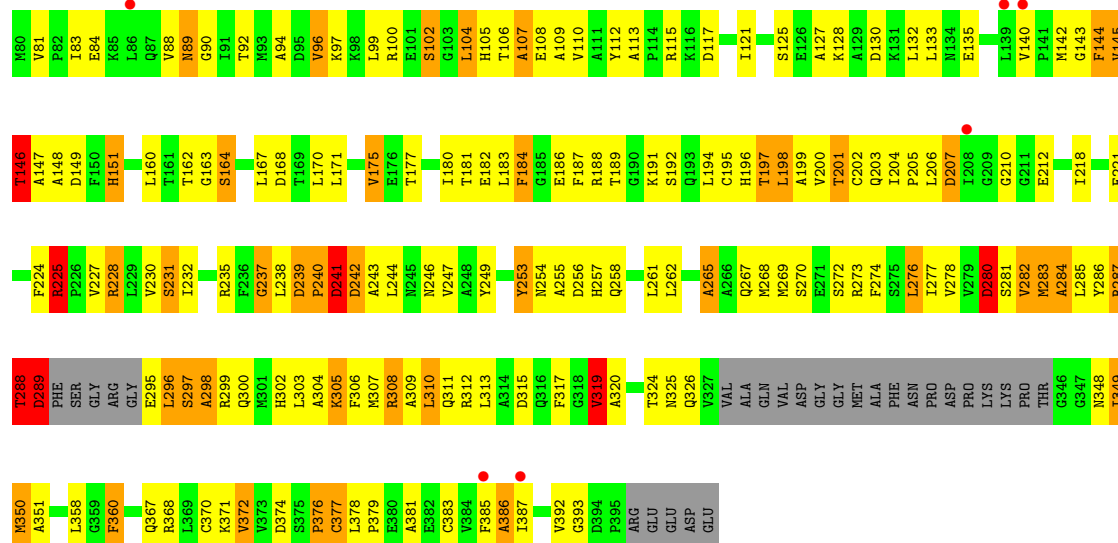




• Molecule 1: DNA repair protein RAD51

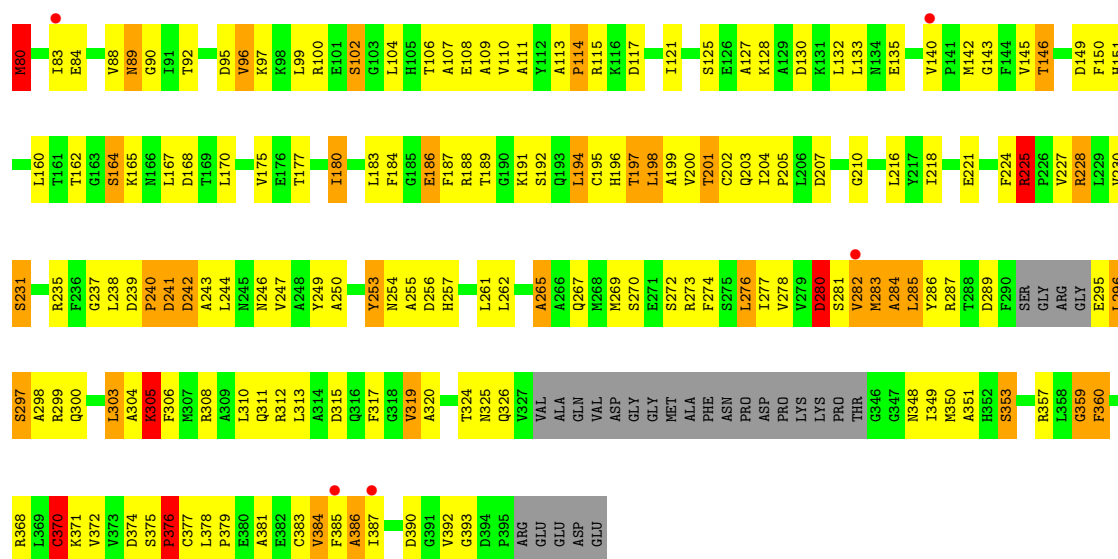


• Molecule 1: DNA repair protein RAD51

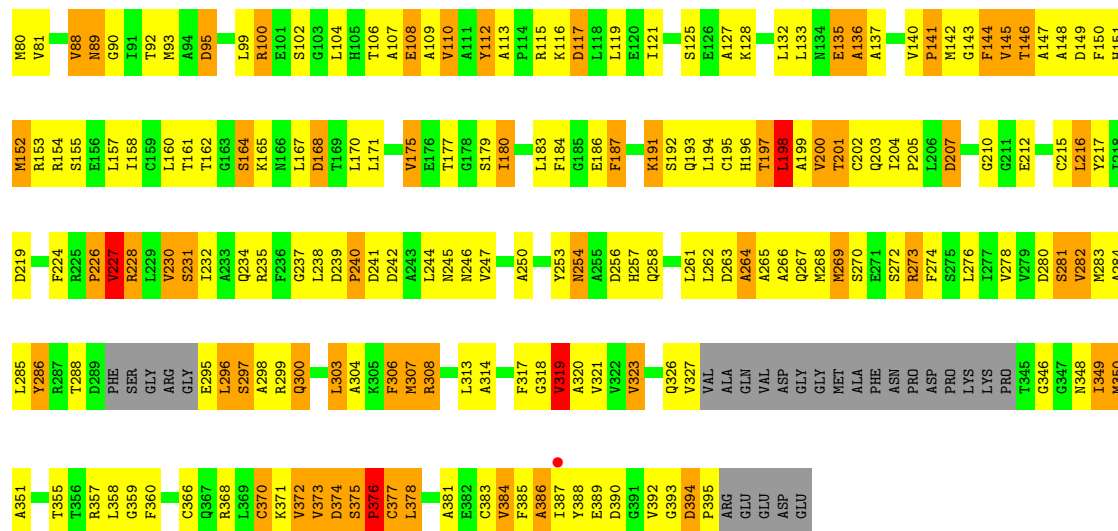


• Molecule 1: DNA repair protein RAD51





Chain F: 32% 40% 18% 8%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.26Å 135.26Å 128.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.25 36.26 – 3.25	Depositor EDS
% Data completeness (in resolution range)	88.4 (40.00-3.25) 99.1 (36.26-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.268 , 0.320 0.250 , 0.297	Depositor DCC
$R_{free}$ test set	4063 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.408 for -h,-k,l 0.046 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	2.15	72/2177 (3.3%)	1.55	23/2951 (0.8%)
1	B	1.81	25/2009 (1.2%)	1.48	23/2719 (0.8%)
1	C	1.85	38/2019 (1.9%)	1.45	23/2730 (0.8%)
1	D	1.90	43/2172 (2.0%)	1.50	23/2942 (0.8%)
1	E	1.87	40/2176 (1.8%)	1.49	20/2947 (0.7%)
1	F	2.14	72/2164 (3.3%)	1.55	22/2934 (0.7%)
All	All	1.96	290/12717 (2.3%)	1.50	134/17223 (0.8%)

All (290) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	308	ARG	CG-CD	12.86	1.84	1.51
1	F	386	ALA	CA-CB	-11.61	1.28	1.52
1	B	227	VAL	CB-CG2	10.88	1.75	1.52
1	C	227	VAL	CB-CG2	10.04	1.74	1.52
1	C	202	CYS	CB-SG	-9.82	1.65	1.82
1	A	308	ARG	CG-CD	9.80	1.76	1.51
1	A	360	PHE	CD2-CE2	-9.69	1.19	1.39
1	A	386	ALA	CA-CB	-9.63	1.32	1.52
1	F	200	VAL	CB-CG1	-9.31	1.33	1.52
1	B	315	ASP	CB-CG	8.94	1.70	1.51
1	F	314	ALA	CA-CB	-8.85	1.33	1.52
1	F	306	PHE	CE1-CZ	-8.68	1.20	1.37
1	B	217	TYR	CE2-CZ	-8.61	1.27	1.38
1	C	217	TYR	CE1-CZ	-8.57	1.27	1.38
1	A	278	VAL	CB-CG2	-8.50	1.35	1.52
1	F	360	PHE	CD2-CE2	-8.49	1.22	1.39
1	A	217	TYR	CD1-CE1	-8.35	1.26	1.39
1	E	145	VAL	CB-CG2	-8.32	1.35	1.52
1	D	255	ALA	CA-CB	-8.30	1.35	1.52
1	C	217	TYR	CG-CD1	-8.23	1.28	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	187	PHE	CE2-CZ	8.23	1.52	1.37
1	D	282	VAL	CA-CB	-8.10	1.37	1.54
1	D	317	PHE	CG-CD1	-8.05	1.26	1.38
1	A	200	VAL	CB-CG1	-7.97	1.36	1.52
1	F	135	GLU	CD-OE1	7.86	1.34	1.25
1	A	360	PHE	CE1-CZ	-7.86	1.22	1.37
1	A	306	PHE	CE1-CZ	-7.74	1.22	1.37
1	D	84	GLU	CD-OE1	7.73	1.34	1.25
1	F	247	VAL	CB-CG2	-7.69	1.36	1.52
1	C	315	ASP	CB-CG	7.67	1.67	1.51
1	A	187	PHE	CE1-CZ	7.64	1.51	1.37
1	A	323	VAL	CB-CG2	-7.60	1.36	1.52
1	D	319	VAL	CB-CG1	-7.59	1.36	1.52
1	A	217	TYR	CG-CD1	-7.56	1.29	1.39
1	A	375	SER	C-O	-7.54	1.09	1.23
1	F	217	TYR	CD1-CE1	-7.54	1.28	1.39
1	C	217	TYR	CD2-CE2	-7.53	1.28	1.39
1	E	306	PHE	CE1-CZ	-7.49	1.23	1.37
1	F	360	PHE	CD1-CE1	-7.47	1.24	1.39
1	E	100	ARG	CG-CD	7.47	1.70	1.51
1	C	217	TYR	CE2-CZ	-7.47	1.28	1.38
1	F	321	VAL	CB-CG2	-7.47	1.37	1.52
1	C	217	TYR	CD1-CE1	-7.46	1.28	1.39
1	F	253	TYR	CG-CD2	-7.34	1.29	1.39
1	B	279	VAL	CA-CB	-7.33	1.39	1.54
1	A	253	TYR	CG-CD2	-7.32	1.29	1.39
1	A	304	ALA	CA-CB	-7.31	1.37	1.52
1	D	317	PHE	CE2-CZ	-7.29	1.23	1.37
1	A	147	ALA	C-O	-7.27	1.09	1.23
1	A	187	PHE	CD2-CE2	7.25	1.53	1.39
1	C	253	TYR	CE2-CZ	-7.24	1.29	1.38
1	D	113	ALA	CA-CB	-7.23	1.37	1.52
1	A	247	VAL	CB-CG2	-7.21	1.37	1.52
1	F	323	VAL	CB-CG2	-7.20	1.37	1.52
1	F	308	ARG	CD-NE	7.17	1.58	1.46
1	D	144	PHE	CG-CD1	-7.11	1.28	1.38
1	B	236	PHE	CE1-CZ	-7.07	1.24	1.37
1	E	282	VAL	CA-CB	-7.04	1.40	1.54
1	A	145	VAL	CB-CG2	-7.00	1.38	1.52
1	E	110	VAL	CA-CB	-7.00	1.40	1.54
1	D	305	LYS	CD-CE	6.99	1.68	1.51
1	F	303	LEU	CG-CD1	-6.91	1.26	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	219	ASP	C-O	-6.89	1.10	1.23
1	D	310	LEU	C-O	-6.86	1.10	1.23
1	D	283	MET	SD-CE	6.85	2.16	1.77
1	C	236	PHE	CD2-CE2	-6.85	1.25	1.39
1	C	236	PHE	CE1-CZ	-6.81	1.24	1.37
1	C	274	PHE	CB-CG	-6.80	1.39	1.51
1	A	143	GLY	C-O	-6.79	1.12	1.23
1	D	96	VAL	C-O	-6.79	1.10	1.23
1	B	217	TYR	CE1-CZ	-6.78	1.29	1.38
1	A	108	GLU	CD-OE2	-6.75	1.18	1.25
1	E	228	ARG	NE-CZ	6.74	1.41	1.33
1	F	375	SER	C-O	-6.74	1.10	1.23
1	E	184	PHE	CD1-CE1	-6.71	1.25	1.39
1	F	286	TYR	CZ-OH	6.71	1.49	1.37
1	A	308	ARG	CB-CG	6.71	1.70	1.52
1	B	202	CYS	CB-SG	-6.68	1.70	1.82
1	D	184	PHE	CD1-CE1	-6.67	1.25	1.39
1	B	279	VAL	CA-C	-6.67	1.35	1.52
1	D	115	ARG	C-O	-6.65	1.10	1.23
1	E	353	SER	CB-OG	-6.64	1.33	1.42
1	F	137	ALA	CA-CB	6.61	1.66	1.52
1	A	391	GLY	C-O	-6.60	1.13	1.23
1	D	100	ARG	CG-CD	6.58	1.68	1.51
1	C	144	PHE	CD1-CE1	-6.56	1.26	1.39
1	D	360	PHE	CB-CG	-6.55	1.40	1.51
1	D	225	ARG	NE-CZ	-6.54	1.24	1.33
1	F	247	VAL	CB-CG1	-6.54	1.39	1.52
1	C	279	VAL	CA-C	-6.51	1.36	1.52
1	D	145	VAL	CB-CG2	-6.50	1.39	1.52
1	A	219	ASP	C-O	-6.50	1.11	1.23
1	E	115	ARG	C-O	-6.46	1.11	1.23
1	F	191	LYS	C-O	-6.45	1.11	1.23
1	A	88	VAL	CB-CG1	-6.44	1.39	1.52
1	A	198	LEU	CG-CD1	-6.44	1.28	1.51
1	F	373	VAL	CA-CB	-6.44	1.41	1.54
1	F	184	PHE	C-O	-6.43	1.11	1.23
1	D	107	ALA	CA-CB	-6.41	1.39	1.52
1	A	359	GLY	C-O	-6.40	1.13	1.23
1	A	360	PHE	CG-CD2	-6.40	1.29	1.38
1	F	278	VAL	CB-CG2	-6.40	1.39	1.52
1	E	84	GLU	CD-OE1	6.38	1.32	1.25
1	F	143	GLY	C-O	-6.37	1.13	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	TYR	CZ-OH	6.31	1.48	1.37
1	A	382	GLU	C-O	-6.31	1.11	1.23
1	D	350	MET	CG-SD	-6.30	1.64	1.81
1	F	300	GLN	C-O	-6.29	1.11	1.23
1	A	110	VAL	CA-CB	-6.25	1.41	1.54
1	D	282	VAL	CB-CG1	-6.24	1.39	1.52
1	E	283	MET	CG-SD	-6.24	1.65	1.81
1	F	198	LEU	CG-CD1	-6.23	1.28	1.51
1	C	320	ALA	CA-CB	-6.23	1.39	1.52
1	F	224	PHE	CB-CG	-6.23	1.40	1.51
1	F	307	MET	SD-CE	-6.21	1.43	1.77
1	F	274	PHE	CE2-CZ	-6.21	1.25	1.37
1	D	187	PHE	CE2-CZ	6.20	1.49	1.37
1	E	96	VAL	C-O	-6.20	1.11	1.23
1	C	278	VAL	CB-CG2	-6.20	1.39	1.52
1	B	320	ALA	CA-CB	-6.18	1.39	1.52
1	C	231	SER	CB-OG	6.18	1.50	1.42
1	A	226	PRO	CA-C	-6.17	1.40	1.52
1	F	217	TYR	CG-CD1	-6.16	1.31	1.39
1	F	317	PHE	CG-CD2	-6.15	1.29	1.38
1	E	317	PHE	CE2-CZ	-6.15	1.25	1.37
1	A	321	VAL	CB-CG1	-6.14	1.40	1.52
1	C	256	ASP	CB-CG	6.13	1.64	1.51
1	A	274	PHE	CG-CD1	-6.10	1.29	1.38
1	E	319	VAL	CB-CG1	-6.10	1.40	1.52
1	C	247	VAL	CB-CG1	-6.09	1.40	1.52
1	E	180	ILE	C-O	-6.04	1.11	1.23
1	B	322	VAL	CB-CG1	-6.02	1.40	1.52
1	A	112	TYR	CD2-CE2	-6.00	1.30	1.39
1	A	360	PHE	CD1-CE1	-6.00	1.27	1.39
1	F	326	GLN	CG-CD	5.97	1.64	1.51
1	E	386	ALA	CA-CB	-5.96	1.40	1.52
1	A	253	TYR	CG-CD1	-5.93	1.31	1.39
1	C	192	SER	CB-OG	-5.89	1.34	1.42
1	A	224	PHE	CD1-CE1	-5.87	1.27	1.39
1	C	274	PHE	CG-CD2	-5.86	1.29	1.38
1	A	317	PHE	CG-CD2	-5.85	1.29	1.38
1	F	303	LEU	C-O	-5.84	1.12	1.23
1	E	114	PRO	CG-CD	-5.83	1.31	1.50
1	E	80	MET	C-O	-5.82	1.12	1.23
1	C	279	VAL	CA-CB	-5.81	1.42	1.54
1	F	253	TYR	CZ-OH	5.80	1.47	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	GLU	CD-OE1	5.79	1.32	1.25
1	D	372	VAL	CB-CG2	-5.79	1.40	1.52
1	B	327	VAL	CB-CG1	5.79	1.65	1.52
1	A	112	TYR	CD1-CE1	-5.78	1.30	1.39
1	B	231	SER	CB-OG	5.75	1.49	1.42
1	F	187	PHE	CE1-CZ	5.74	1.48	1.37
1	B	391	GLY	C-O	-5.74	1.14	1.23
1	F	360	PHE	CG-CD2	-5.74	1.30	1.38
1	E	253	TYR	CE2-CZ	-5.73	1.31	1.38
1	A	135	GLU	CD-OE1	5.73	1.31	1.25
1	E	310	LEU	C-O	-5.73	1.12	1.23
1	F	224	PHE	CD1-CE1	-5.72	1.27	1.39
1	A	191	LYS	C-O	-5.71	1.12	1.23
1	A	372	VAL	CB-CG1	-5.71	1.40	1.52
1	D	268	MET	CG-SD	5.71	1.96	1.81
1	A	324	THR	CB-CG2	-5.70	1.33	1.52
1	C	321	VAL	CA-CB	-5.70	1.42	1.54
1	A	278	VAL	C-O	-5.69	1.12	1.23
1	C	209	GLY	C-O	-5.69	1.14	1.23
1	C	249	TYR	CZ-OH	5.67	1.47	1.37
1	D	218	ILE	C-O	-5.67	1.12	1.23
1	A	375	SER	CB-OG	5.67	1.49	1.42
1	A	373	VAL	CA-CB	-5.66	1.42	1.54
1	B	249	TYR	CE1-CZ	5.65	1.45	1.38
1	C	350	MET	CG-SD	-5.64	1.66	1.81
1	D	184	PHE	CB-CG	-5.62	1.41	1.51
1	C	283	MET	SD-CE	5.61	2.09	1.77
1	A	100	ARG	NE-CZ	-5.61	1.25	1.33
1	C	212	GLU	CD-OE2	-5.59	1.19	1.25
1	D	143	GLY	C-O	-5.59	1.14	1.23
1	F	359	GLY	C-O	-5.58	1.14	1.23
1	A	253	TYR	CD2-CE2	-5.58	1.30	1.39
1	B	320	ALA	C-O	-5.57	1.12	1.23
1	F	274	PHE	CG-CD1	-5.57	1.30	1.38
1	F	162	THR	C-O	-5.56	1.12	1.23
1	E	256	ASP	CB-CG	5.56	1.63	1.51
1	A	218	ILE	C-O	-5.56	1.12	1.23
1	F	100	ARG	NE-CZ	-5.56	1.25	1.33
1	E	286	TYR	CG-CD2	-5.55	1.31	1.39
1	C	269	MET	C-O	-5.54	1.12	1.23
1	F	187	PHE	CD2-CE2	5.53	1.50	1.39
1	B	352	HIS	C-O	5.53	1.33	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	221	GLU	CD-OE2	5.53	1.31	1.25
1	D	242	ASP	CB-CG	5.53	1.63	1.51
1	C	314	ALA	CA-CB	-5.52	1.40	1.52
1	C	220	THR	CA-CB	5.52	1.67	1.53
1	F	145	VAL	CB-CG2	-5.52	1.41	1.52
1	D	349	ILE	CA-CB	-5.50	1.42	1.54
1	F	373	VAL	C-O	-5.50	1.12	1.23
1	F	112	TYR	CD1-CE1	-5.49	1.31	1.39
1	A	326	GLN	CG-CD	5.48	1.63	1.51
1	D	253	TYR	CE2-CZ	-5.48	1.31	1.38
1	F	226	PRO	CA-C	-5.48	1.41	1.52
1	A	224	PHE	CB-CG	-5.48	1.42	1.51
1	A	247	VAL	CB-CG1	-5.45	1.41	1.52
1	A	263	ASP	CA-CB	-5.45	1.42	1.53
1	E	317	PHE	CG-CD1	-5.45	1.30	1.38
1	C	236	PHE	CD1-CE1	-5.45	1.28	1.39
1	F	152	MET	C-O	-5.44	1.13	1.23
1	B	256	ASP	CB-CG	5.43	1.63	1.51
1	F	372	VAL	CB-CG1	-5.43	1.41	1.52
1	A	110	VAL	N-CA	-5.43	1.35	1.46
1	D	253	TYR	CD1-CE1	-5.43	1.31	1.39
1	A	389	GLU	CD-OE1	5.42	1.31	1.25
1	F	110	VAL	N-CA	-5.42	1.35	1.46
1	A	83	ILE	CA-CB	-5.40	1.42	1.54
1	E	265	ALA	C-O	-5.40	1.13	1.23
1	E	303	LEU	C-O	-5.40	1.13	1.23
1	A	146	THR	CB-CG2	5.39	1.70	1.52
1	F	228	ARG	NE-CZ	5.39	1.40	1.33
1	F	321	VAL	CB-CG1	-5.39	1.41	1.52
1	E	194	LEU	C-O	-5.39	1.13	1.23
1	A	276	LEU	C-O	-5.38	1.13	1.23
1	E	359	GLY	C-O	-5.37	1.15	1.23
1	D	386	ALA	CA-CB	-5.37	1.41	1.52
1	C	360	PHE	CE2-CZ	-5.37	1.27	1.37
1	C	232	ILE	CA-CB	-5.35	1.42	1.54
1	E	360	PHE	CB-CG	-5.35	1.42	1.51
1	A	197	THR	C-O	-5.35	1.13	1.23
1	A	112	TYR	CG-CD2	-5.33	1.32	1.39
1	C	199	ALA	CA-CB	-5.33	1.41	1.52
1	A	252	ALA	C-O	-5.33	1.13	1.23
1	F	234	GLN	C-O	-5.32	1.13	1.23
1	B	307	MET	CG-SD	-5.32	1.67	1.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	278	VAL	CB-CG2	-5.31	1.41	1.52
1	F	81	VAL	CB-CG1	-5.30	1.41	1.52
1	A	322	VAL	C-O	-5.30	1.13	1.23
1	D	110	VAL	CA-CB	-5.30	1.43	1.54
1	D	287	ARG	CG-CD	5.30	1.65	1.51
1	B	144	PHE	CD2-CE2	-5.29	1.28	1.39
1	C	150	PHE	C-O	-5.25	1.13	1.23
1	F	88	VAL	CB-CG2	5.25	1.63	1.52
1	E	221	GLU	CD-OE2	5.24	1.31	1.25
1	A	303	LEU	C-O	-5.22	1.13	1.23
1	E	218	ILE	C-O	-5.22	1.13	1.23
1	A	152	MET	C-O	-5.22	1.13	1.23
1	A	150	PHE	C-O	-5.21	1.13	1.23
1	F	136	ALA	C-O	-5.21	1.13	1.23
1	D	298	ALA	CA-CB	5.21	1.63	1.52
1	D	228	ARG	NE-CZ	5.20	1.39	1.33
1	F	321	VAL	CA-CB	-5.20	1.43	1.54
1	F	384	VAL	CA-CB	-5.20	1.43	1.54
1	F	360	PHE	CE1-CZ	-5.19	1.27	1.37
1	A	108	GLU	CA-C	-5.18	1.39	1.52
1	B	355	THR	C-O	-5.18	1.13	1.23
1	F	144	PHE	CB-CG	-5.16	1.42	1.51
1	F	227	VAL	CB-CG2	5.16	1.63	1.52
1	F	327	VAL	CB-CG1	5.15	1.63	1.52
1	F	215	CYS	CA-CB	-5.15	1.42	1.53
1	C	165	LYS	CD-CE	5.14	1.64	1.51
1	D	175	VAL	CB-CG2	-5.14	1.42	1.52
1	F	253	TYR	CG-CD1	-5.13	1.32	1.39
1	E	143	GLY	C-O	-5.13	1.15	1.23
1	B	314	ALA	CA-CB	-5.13	1.41	1.52
1	E	184	PHE	CD2-CE2	-5.12	1.29	1.39
1	D	182	GLU	CD-OE1	-5.12	1.20	1.25
1	F	135	GLU	CG-CD	5.12	1.59	1.51
1	A	184	PHE	C-O	-5.11	1.13	1.23
1	A	244	LEU	C-O	-5.11	1.13	1.23
1	E	186	GLU	C-O	-5.11	1.13	1.23
1	B	192	SER	CB-OG	-5.10	1.35	1.42
1	F	359	GLY	N-CA	-5.10	1.38	1.46
1	A	359	GLY	N-CA	-5.08	1.38	1.46
1	F	273	ARG	C-O	-5.08	1.13	1.23
1	F	175	VAL	CB-CG2	-5.08	1.42	1.52
1	B	145	VAL	CA-CB	-5.08	1.44	1.54

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	TYR	CD1-CE1	-5.07	1.31	1.39
1	E	150	PHE	CE1-CZ	-5.07	1.27	1.37
1	D	115	ARG	CA-C	-5.07	1.39	1.52
1	E	349	ILE	CA-CB	-5.06	1.43	1.54
1	E	284	ALA	CA-CB	-5.06	1.41	1.52
1	A	230	VAL	CB-CG2	-5.06	1.42	1.52
1	A	274	PHE	CE2-CZ	-5.05	1.27	1.37
1	F	264	ALA	C-O	-5.05	1.13	1.23
1	F	357	ARG	CG-CD	-5.04	1.39	1.51
1	D	286	TYR	CD2-CE2	5.04	1.47	1.39
1	F	230	VAL	CB-CG2	-5.04	1.42	1.52
1	D	265	ALA	CA-C	-5.04	1.39	1.52
1	C	182	GLU	CD-OE1	5.04	1.31	1.25
1	F	282	VAL	C-O	5.02	1.32	1.23
1	E	80	MET	SD-CE	5.02	2.06	1.77
1	E	305	LYS	CD-CE	5.02	1.63	1.51
1	B	355	THR	CA-C	-5.01	1.40	1.52
1	D	278	VAL	CB-CG2	-5.01	1.42	1.52

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	D	225	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	E	225	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	F	308	ARG	NE-CZ-NH1	-11.07	114.77	120.30
1	E	117	ASP	CB-CG-OD2	10.90	128.11	118.30
1	F	390	ASP	CB-CG-OD2	10.76	127.98	118.30
1	B	390	ASP	CB-CG-OD2	10.44	127.70	118.30
1	C	390	ASP	CB-CG-OD2	10.36	127.62	118.30
1	D	117	ASP	CB-CG-OD2	9.77	127.09	118.30
1	C	263	ASP	CB-CG-OD2	9.71	127.04	118.30
1	A	95	ASP	CB-CG-OD2	9.65	126.99	118.30
1	D	289	ASP	CB-CG-OD2	9.39	126.75	118.30
1	B	225	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	F	95	ASP	CB-CG-OD2	9.26	126.63	118.30
1	F	263	ASP	CB-CG-OD2	9.26	126.63	118.30
1	A	117	ASP	CB-CG-OD2	9.22	126.59	118.30
1	A	100	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	D	256	ASP	CB-CG-OD2	8.94	126.34	118.30
1	A	390	ASP	CB-CG-OD2	8.93	126.34	118.30
1	E	225	ARG	NE-CZ-NH2	-8.56	116.02	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ASP	CB-CG-OD2	8.38	125.84	118.30
1	F	263	ASP	CB-CG-OD1	-8.37	110.77	118.30
1	B	280	ASP	CB-CG-OD2	8.35	125.81	118.30
1	E	168	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	80	MET	CG-SD-CE	8.28	113.44	100.20
1	F	308	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	C	207	ASP	CB-CG-OD2	8.08	125.57	118.30
1	D	168	ASP	CB-CG-OD2	7.86	125.38	118.30
1	C	315	ASP	CB-CG-OD2	7.63	125.17	118.30
1	B	256	ASP	CB-CG-OD2	7.62	125.16	118.30
1	D	376	PRO	N-CD-CG	-7.61	91.79	103.20
1	B	263	ASP	CB-CG-OD2	7.57	125.11	118.30
1	C	263	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	E	235	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	219	ASP	CB-CG-OD1	7.40	124.96	118.30
1	F	100	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	E	280	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	219	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	168	ASP	CB-CG-OD2	7.11	124.70	118.30
1	F	376	PRO	N-CD-CG	-7.09	92.56	103.20
1	E	308	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	E	376	PRO	N-CD-CG	-6.85	92.93	103.20
1	F	119	LEU	CB-CG-CD2	-6.80	99.44	111.00
1	D	280	ASP	CB-CG-OD2	6.79	124.41	118.30
1	C	117	ASP	CB-CG-OD2	6.77	124.39	118.30
1	E	287	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	F	117	ASP	CB-CG-OD2	6.63	124.27	118.30
1	E	284	ALA	N-CA-C	6.55	128.70	111.00
1	F	384	VAL	CB-CA-C	-6.45	99.14	111.40
1	C	257	HIS	CB-CA-C	-6.44	97.52	110.40
1	B	117	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	207	ASP	CB-CG-OD2	6.43	124.08	118.30
1	B	247	VAL	CB-CA-C	-6.42	99.19	111.40
1	B	262	LEU	CB-CG-CD2	6.39	121.86	111.00
1	C	256	ASP	CB-CG-OD2	6.33	124.00	118.30
1	E	357	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	F	394	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	B	315	ASP	CB-CG-OD1	6.29	123.96	118.30
1	F	168	ASP	CB-CG-OD2	6.26	123.93	118.30
1	B	279	VAL	CB-CA-C	-6.23	99.56	111.40
1	A	149	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	370	CYS	CA-CB-SG	-6.21	102.82	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	E	242	ASP	CB-CG-OD2	6.16	123.84	118.30
1	E	102	SER	CB-CA-C	-6.13	98.46	110.10
1	A	378	LEU	CB-CG-CD2	6.08	121.33	111.00
1	C	228	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	299	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	263	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	B	315	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	308	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	130	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	263	ASP	CB-CG-OD1	-5.87	113.01	118.30
1	A	357	ARG	CG-CD-NE	-5.86	99.50	111.80
1	A	384	VAL	CB-CA-C	-5.82	100.33	111.40
1	C	370	CYS	CA-CB-SG	-5.80	103.56	114.00
1	B	315	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	A	108	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	D	280	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	E	390	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	83	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	F	319	VAL	CB-CA-C	-5.72	100.53	111.40
1	F	216	LEU	CB-CG-CD1	-5.65	101.40	111.00
1	C	279	VAL	N-CA-C	-5.63	95.81	111.00
1	C	251	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	D	284	ALA	N-CA-C	5.56	126.02	111.00
1	E	256	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	153	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	161	THR	OG1-CB-CG2	-5.51	97.32	110.00
1	D	130	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	251	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	235	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	177	THR	OG1-CB-CG2	-5.48	97.40	110.00
1	C	315	ASP	OD1-CG-OD2	-5.46	112.93	123.30
1	E	130	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	152	MET	N-CA-C	-5.45	96.29	111.00
1	E	241	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	130	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	119	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	B	324	THR	CB-CA-C	-5.40	97.01	111.60
1	F	216	LEU	CA-CB-CG	-5.40	102.89	115.30
1	F	180	ILE	CG1-CB-CG2	-5.40	99.53	111.40
1	D	235	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	212	GLU	OE1-CD-OE2	-5.30	116.93	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	378	LEU	N-CA-C	5.27	125.23	111.00
1	D	225	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	F	186	GLU	N-CA-CB	5.26	120.07	110.60
1	D	100	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	210	GLY	N-CA-C	5.25	126.22	113.10
1	D	239	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	241	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	238	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	A	183	LEU	CB-CA-C	-5.22	100.29	110.20
1	C	210	GLY	N-CA-C	5.21	126.11	113.10
1	D	277	ILE	CG1-CB-CG2	-5.20	99.97	111.40
1	D	102	SER	CB-CA-C	-5.19	100.24	110.10
1	B	390	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	B	219	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	224	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	F	183	LEU	CB-CA-C	-5.15	100.41	110.20
1	A	117	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	153	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	221	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	180	ILE	CG1-CB-CG2	-5.10	100.18	111.40
1	B	220	THR	OG1-CB-CG2	-5.10	98.28	110.00
1	D	146	THR	N-CA-C	-5.09	97.26	111.00
1	D	113	ALA	CB-CA-C	-5.09	102.47	110.10
1	E	384	VAL	CB-CA-C	-5.07	101.78	111.40
1	E	96	VAL	CB-CA-C	-5.02	101.86	111.40
1	B	195	CYS	CA-CB-SG	-5.02	104.96	114.00
1	D	115	ARG	N-CA-C	-5.02	97.45	111.00
1	D	104	LEU	CA-CB-CG	-5.01	103.77	115.30
1	A	100	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	F	207	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2148	0	2095	152	0
1	B	1985	0	1931	162	0
1	C	1995	0	1944	152	0
1	D	2143	0	2094	144	0
1	E	2147	0	2095	131	1
1	F	2135	0	2075	163	1
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
2	E	5	0	0	2	0
2	F	5	0	0	0	0
All	All	12583	0	12234	876	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (876) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:CB	1:B:227:VAL:CG2	1.75	1.62
1:F:308:ARG:CD	1:F:308:ARG:CG	1.84	1.55
1:A:308:ARG:CD	1:A:308:ARG:CG	1.76	1.52
1:A:93:MET:CE	1:A:93:MET:SD	2.02	1.45
1:F:93:MET:CE	1:F:93:MET:SD	2.05	1.44
1:E:80:MET:SD	1:E:80:MET:CE	2.06	1.42
1:C:283:MET:SD	1:C:283:MET:CE	2.09	1.40
1:D:283:MET:SD	1:D:283:MET:CE	2.16	1.33
1:C:158:ILE:O	1:C:177:THR:HG23	1.49	1.12
1:A:230:VAL:HG23	1:A:231:SER:H	1.18	1.08
1:A:230:VAL:HG23	1:A:231:SER:N	1.68	1.07
1:B:158:ILE:O	1:B:177:THR:HG23	1.56	1.05
1:F:230:VAL:HG23	1:F:231:SER:H	1.14	1.02
1:C:355:THR:O	1:C:356:THR:OG1	1.77	1.00
1:B:360:PHE:CE2	1:B:370:CYS:SG	2.55	0.99
1:A:327:VAL:O	1:A:328:VAL:HB	1.62	0.99
1:A:230:VAL:CG2	1:A:231:SER:H	1.76	0.96
1:B:367:GLN:O	1:B:368:ARG:HG2	1.66	0.96
1:B:281:SER:OG	1:B:324:THR:O	1.83	0.95
1:F:230:VAL:CG2	1:F:231:SER:H	1.80	0.95
1:F:230:VAL:HG23	1:F:231:SER:N	1.74	0.94
1:C:367:GLN:O	1:C:368:ARG:HG2	1.69	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:O	1:C:177:THR:CG2	2.15	0.93
1:C:281:SER:OG	1:C:324:THR:O	1.86	0.93
1:B:355:THR:OG1	1:B:356:THR:N	1.99	0.91
1:C:191:LYS:HB2	2:C:503:SO4:O2	1.71	0.91
1:F:286:TYR:OH	1:F:346:GLY:HA2	1.70	0.91
1:B:230:VAL:HG23	1:B:231:SER:N	1.84	0.91
1:A:146:THR:HG23	1:A:149:ASP:HB2	1.52	0.90
1:C:171:LEU:HD21	1:C:358:LEU:HD11	1.52	0.90
1:B:230:VAL:HG23	1:B:231:SER:H	1.37	0.89
1:B:191:LYS:HB2	2:B:502:SO4:O3	1.73	0.88
1:D:240:PRO:O	1:D:242:ASP:N	2.06	0.88
1:F:296:LEU:O	1:F:297:SER:C	2.09	0.88
1:C:230:VAL:HG23	1:C:231:SER:N	1.89	0.87
1:A:296:LEU:O	1:A:297:SER:C	2.11	0.86
1:A:286:TYR:OH	1:A:346:GLY:HA2	1.75	0.86
1:F:196:HIS:O	1:F:199:ALA:HB3	1.76	0.85
1:C:159:CYS:SG	1:C:176:GLU:HA	2.16	0.85
1:A:374:ASP:O	1:A:375:SER:OG	1.94	0.85
1:E:240:PRO:O	1:E:242:ASP:N	2.10	0.84
1:A:196:HIS:O	1:A:199:ALA:HB3	1.77	0.84
1:C:193:GLN:HG3	1:C:387:ILE:HD13	1.57	0.84
1:A:288:THR:HG23	1:D:305:LYS:NZ	1.94	0.82
1:D:177:THR:HG22	1:D:320:ALA:HB2	1.61	0.82
1:A:160:LEU:HD22	1:A:202:CYS:HA	1.61	0.81
1:C:182:GLU:OE2	1:C:350:MET:HE2	1.81	0.81
1:A:288:THR:HG23	1:D:305:LYS:HZ1	1.45	0.80
1:B:193:GLN:HG3	1:B:387:ILE:HD13	1.64	0.80
1:C:244:LEU:O	1:C:246:ASN:N	2.15	0.80
1:F:146:THR:HG23	1:F:149:ASP:HB2	1.62	0.80
1:A:125:SER:OG	1:A:128:LYS:HB2	1.82	0.79
1:B:110:VAL:O	1:B:113:ALA:HB3	1.83	0.79
1:D:238:LEU:O	1:D:240:PRO:HD3	1.84	0.78
1:B:360:PHE:CD2	1:B:370:CYS:SG	2.77	0.78
1:C:110:VAL:O	1:C:113:ALA:HB3	1.84	0.78
1:F:125:SER:OG	1:F:128:LYS:HB2	1.84	0.78
1:B:158:ILE:O	1:B:177:THR:CG2	2.31	0.78
1:B:159:CYS:SG	1:B:176:GLU:HA	2.24	0.78
1:B:240:PRO:O	1:B:242:ASP:N	2.17	0.78
1:C:240:PRO:O	1:C:242:ASP:N	2.16	0.77
1:A:141:PRO:O	1:A:142:MET:HG3	1.84	0.77
1:C:244:LEU:C	1:C:246:ASN:H	1.85	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:VAL:CG2	1:B:231:SER:H	1.98	0.76
1:B:184:PHE:O	1:B:359:GLY:HA2	1.84	0.76
1:C:230:VAL:HG23	1:C:231:SER:H	1.50	0.76
1:A:327:VAL:O	1:A:328:VAL:CB	2.34	0.76
1:E:238:LEU:O	1:E:240:PRO:HD3	1.85	0.76
1:E:140:VAL:O	1:E:142:MET:HG2	1.86	0.75
1:B:244:LEU:C	1:B:246:ASN:H	1.89	0.75
1:F:384:VAL:HG12	1:F:385:PHE:N	2.00	0.75
1:C:355:THR:C	1:C:356:THR:HG1	1.89	0.75
1:F:175:VAL:HG11	1:F:198:LEU:HD11	1.69	0.75
1:B:201:THR:HA	1:B:204:ILE:HG12	1.68	0.74
1:E:283:MET:CE	1:E:303:LEU:HD22	2.18	0.74
1:A:239:ASP:O	1:A:242:ASP:HB3	1.87	0.74
1:F:348:ASN:O	1:F:349:ILE:C	2.25	0.74
1:F:374:ASP:O	1:F:375:SER:OG	2.06	0.74
1:B:230:VAL:CG2	1:B:231:SER:N	2.51	0.73
1:D:201:THR:HA	1:D:204:ILE:HG12	1.71	0.73
1:F:201:THR:HA	1:F:204:ILE:HG12	1.71	0.72
1:C:158:ILE:O	1:C:177:THR:OG1	2.07	0.72
1:D:224:PHE:C	1:D:225:ARG:HD3	2.10	0.72
1:C:189:THR:O	1:C:368:ARG:HD2	1.90	0.71
1:F:239:ASP:O	1:F:242:ASP:HB3	1.90	0.71
1:A:110:VAL:O	1:A:113:ALA:HB3	1.90	0.71
1:B:171:LEU:HD21	1:B:358:LEU:HD11	1.72	0.71
1:E:296:LEU:O	1:E:297:SER:C	2.26	0.71
1:C:183:LEU:O	1:C:324:THR:HA	1.91	0.71
1:F:244:LEU:C	1:F:246:ASN:H	1.94	0.71
1:C:99:LEU:O	1:C:102:SER:HB3	1.90	0.71
1:F:99:LEU:O	1:F:102:SER:HB3	1.91	0.71
1:C:194:LEU:O	1:C:195:CYS:C	2.27	0.71
1:D:230:VAL:HG23	1:D:231:SER:N	2.06	0.71
1:E:230:VAL:HG23	1:E:231:SER:N	2.05	0.70
1:B:349:ILE:O	1:B:353:SER:OG	2.09	0.70
1:E:170:LEU:HD21	1:E:381:ALA:O	1.91	0.70
1:A:235:ARG:NH1	1:A:392:VAL:O	2.25	0.70
1:E:201:THR:HA	1:E:204:ILE:HG12	1.74	0.70
1:C:164:SER:OG	1:C:167:LEU:HB2	1.92	0.69
1:E:283:MET:O	1:E:285:LEU:N	2.24	0.69
1:F:177:THR:HG22	1:F:320:ALA:HB2	1.73	0.69
1:A:258:GLN:NE2	1:A:306:PHE:CZ	2.58	0.69
1:C:230:VAL:CG2	1:C:231:SER:N	2.54	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:SER:OG	1:B:167:LEU:HB2	1.92	0.69
1:A:80:MET:HE3	1:A:270:SER:HA	1.73	0.69
1:D:140:VAL:O	1:D:142:MET:HG2	1.93	0.69
1:D:239:ASP:HB2	1:D:242:ASP:HB3	1.74	0.69
1:B:191:LYS:HG2	1:B:360:PHE:HD1	1.58	0.69
1:C:194:LEU:C	1:C:194:LEU:HD23	2.14	0.68
1:E:191:LYS:N	2:E:505:SO4:O3	2.24	0.68
1:E:96:VAL:HG12	1:E:97:LYS:N	2.09	0.68
1:E:175:VAL:HG11	1:E:198:LEU:HD11	1.76	0.68
1:C:106:THR:HG22	1:C:107:ALA:N	2.09	0.67
1:A:175:VAL:HG11	1:A:198:LEU:HD11	1.75	0.67
1:C:191:LYS:O	1:C:192:SER:C	2.31	0.67
1:C:230:VAL:CG2	1:C:231:SER:H	2.06	0.67
1:C:239:ASP:HB2	1:C:242:ASP:HB3	1.77	0.67
1:F:235:ARG:NH1	1:F:392:VAL:O	2.26	0.67
1:E:239:ASP:HB2	1:E:242:ASP:HB3	1.77	0.67
1:A:244:LEU:HB2	1:D:148:ALA:HB2	1.75	0.67
1:B:99:LEU:O	1:B:102:SER:HB3	1.95	0.67
1:A:80:MET:CE	1:A:270:SER:HA	2.24	0.67
1:E:283:MET:HE3	1:E:303:LEU:HD22	1.75	0.67
1:A:254:ASN:HB3	1:D:112:TYR:O	1.96	0.66
1:C:360:PHE:CE2	1:C:370:CYS:SG	2.89	0.66
1:D:238:LEU:O	1:D:240:PRO:CD	2.43	0.66
1:E:191:LYS:O	1:E:192:SER:C	2.33	0.66
1:E:224:PHE:CD2	1:E:249:TYR:CE1	2.84	0.66
1:A:239:ASP:HB2	1:A:242:ASP:HB3	1.78	0.66
1:B:106:THR:O	1:B:109:ALA:HB3	1.95	0.66
1:B:189:THR:O	1:B:368:ARG:HD2	1.96	0.66
1:C:196:HIS:O	1:C:199:ALA:HB3	1.95	0.66
1:D:191:LYS:O	1:D:192:SER:C	2.32	0.66
1:D:258:GLN:NE2	1:D:306:PHE:CZ	2.64	0.66
1:F:171:LEU:HD21	1:F:358:LEU:HD11	1.78	0.65
1:E:230:VAL:HG23	1:E:231:SER:H	1.60	0.65
1:D:106:THR:O	1:D:109:ALA:N	2.30	0.65
1:F:303:LEU:HG	1:F:303:LEU:O	1.97	0.65
1:B:191:LYS:O	1:B:192:SER:C	2.31	0.65
1:B:240:PRO:C	1:B:242:ASP:H	2.00	0.65
1:B:159:CYS:SG	1:B:176:GLU:HG3	2.37	0.65
1:C:255:ALA:HA	1:C:285:LEU:HD23	1.78	0.64
1:A:204:ILE:O	1:A:210:GLY:HA3	1.97	0.64
1:C:350:MET:O	1:C:354:SER:N	2.22	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:HG22	1:A:306:PHE:CE2	2.33	0.64
1:E:240:PRO:C	1:E:242:ASP:H	1.99	0.64
1:F:204:ILE:O	1:F:210:GLY:HA3	1.97	0.64
1:A:146:THR:HG23	1:A:149:ASP:CB	2.26	0.64
1:A:295:GLU:O	1:A:296:LEU:C	2.36	0.64
1:C:159:CYS:SG	1:C:176:GLU:HG3	2.37	0.64
1:D:296:LEU:O	1:D:297:SER:C	2.36	0.64
1:C:240:PRO:C	1:C:242:ASP:H	2.00	0.64
1:B:106:THR:HG22	1:B:107:ALA:N	2.13	0.63
1:C:114:PRO:O	1:C:118:LEU:HG	1.98	0.63
1:E:253:TYR:CE2	1:F:112:TYR:CE1	2.86	0.63
1:E:297:SER:O	1:E:300:GLN:N	2.31	0.63
1:B:183:LEU:O	1:B:324:THR:HA	1.98	0.63
1:F:146:THR:HG23	1:F:149:ASP:CB	2.29	0.63
1:B:93:MET:O	1:B:97:LYS:HG3	1.98	0.63
1:F:296:LEU:O	1:F:297:SER:O	2.17	0.63
1:A:193:GLN:HG3	1:A:387:ILE:HG21	1.79	0.63
1:F:286:TYR:HH	1:F:346:GLY:HA2	1.60	0.63
1:A:384:VAL:HG12	1:A:385:PHE:N	2.14	0.63
1:F:384:VAL:CG1	1:F:385:PHE:N	2.61	0.63
1:D:312:ARG:O	1:D:315:ASP:N	2.32	0.63
1:B:194:LEU:O	1:B:195:CYS:C	2.34	0.62
1:D:83:ILE:HG21	1:D:96:VAL:HG13	1.81	0.62
1:D:196:HIS:O	1:D:199:ALA:HB3	1.99	0.62
1:D:283:MET:O	1:D:285:LEU:N	2.32	0.62
1:E:164:SER:OG	1:E:167:LEU:HB2	2.00	0.62
1:F:370:CYS:O	1:F:370:CYS:SG	2.56	0.62
1:C:93:MET:O	1:C:97:LYS:HG3	2.00	0.62
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.15	0.61
1:D:240:PRO:C	1:D:242:ASP:H	2.03	0.61
1:A:244:LEU:C	1:A:246:ASN:H	2.04	0.61
1:A:286:TYR:CZ	1:A:346:GLY:HA2	2.35	0.61
1:B:194:LEU:HA	1:B:392:VAL:CG2	2.30	0.61
1:F:197:THR:OG1	1:F:392:VAL:HG23	1.99	0.61
1:A:171:LEU:HD21	1:A:358:LEU:HD11	1.83	0.61
1:C:350:MET:O	1:C:353:SER:N	2.34	0.61
1:D:170:LEU:HD21	1:D:381:ALA:O	1.98	0.61
1:E:238:LEU:O	1:E:240:PRO:CD	2.48	0.61
1:C:226:PRO:O	1:C:228:ARG:N	2.33	0.60
1:C:306:PHE:O	1:C:308:ARG:N	2.34	0.60
1:F:106:THR:O	1:F:107:ALA:C	2.32	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD23	1:B:194:LEU:C	2.21	0.60
1:E:106:THR:O	1:E:109:ALA:N	2.34	0.60
1:C:140:VAL:O	1:C:142:MET:HG2	2.02	0.60
1:C:201:THR:HA	1:C:204:ILE:HG12	1.83	0.60
1:C:318:GLY:O	1:C:319:VAL:O	2.19	0.60
1:D:230:VAL:HG23	1:D:231:SER:H	1.64	0.60
1:D:204:ILE:HB	1:D:210:GLY:HA3	1.84	0.60
1:A:240:PRO:O	1:A:242:ASP:N	2.35	0.60
1:C:191:LYS:HG2	1:C:360:PHE:CD1	2.37	0.60
1:C:347:GLY:CA	1:C:357:ARG:HH22	2.14	0.60
1:E:272:SER:OG	1:E:273:ARG:N	2.33	0.60
1:B:350:MET:O	1:B:352:HIS:N	2.33	0.60
1:A:201:THR:HA	1:A:204:ILE:HG12	1.83	0.60
1:B:191:LYS:HG2	1:B:360:PHE:CD1	2.36	0.60
1:B:244:LEU:O	1:B:246:ASN:N	2.35	0.59
1:C:347:GLY:CA	1:C:357:ARG:NH2	2.65	0.59
1:D:194:LEU:O	1:D:195:CYS:C	2.34	0.59
1:E:253:TYR:CD2	1:F:112:TYR:CD1	2.90	0.59
1:D:146:THR:HG23	1:D:149:ASP:HB2	1.84	0.59
1:A:177:THR:HG22	1:A:320:ALA:HB2	1.84	0.59
1:F:265:ALA:O	1:F:269:MET:HG3	2.03	0.59
1:A:300:GLN:O	1:A:349:ILE:HD13	2.02	0.59
1:B:244:LEU:C	1:B:246:ASN:N	2.55	0.59
1:D:350:MET:O	1:D:351:ALA:C	2.37	0.59
1:D:360:PHE:N	1:D:360:PHE:CD1	2.68	0.59
1:B:194:LEU:HG	1:B:392:VAL:HG21	1.85	0.59
1:D:175:VAL:HG11	1:D:198:LEU:HD11	1.84	0.59
1:F:348:ASN:O	1:F:350:MET:N	2.35	0.59
1:F:110:VAL:O	1:F:113:ALA:HB3	2.01	0.59
1:F:240:PRO:O	1:F:242:ASP:N	2.35	0.59
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.68	0.59
1:E:125:SER:OG	1:E:128:LYS:HB2	2.02	0.59
1:D:104:LEU:CD2	1:D:109:ALA:HB1	2.33	0.58
1:E:224:PHE:CD2	1:E:249:TYR:CD1	2.91	0.58
1:C:347:GLY:HA3	1:C:357:ARG:HH22	1.67	0.58
1:A:272:SER:OG	1:A:273:ARG:N	2.34	0.58
1:D:287:ARG:O	1:D:288:THR:C	2.40	0.58
1:F:244:LEU:O	1:F:246:ASN:N	2.36	0.58
1:C:95:ASP:O	1:C:96:VAL:C	2.40	0.58
1:E:261:LEU:O	1:E:262:LEU:C	2.40	0.58
1:C:148:ALA:O	1:C:149:ASP:C	2.40	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:PHE:CD2	1:D:249:TYR:CE1	2.92	0.58
1:E:200:VAL:C	1:E:202:CYS:H	2.06	0.58
1:B:99:LEU:HD23	1:B:121:ILE:HD13	1.85	0.58
1:B:144:PHE:CE2	1:C:250:ALA:HB2	2.39	0.58
1:C:99:LEU:HD23	1:C:121:ILE:HD13	1.84	0.58
1:C:200:VAL:C	1:C:202:CYS:H	2.07	0.58
1:D:265:ALA:O	1:D:269:MET:HG3	2.03	0.58
1:B:227:VAL:CG2	1:B:227:VAL:CG1	2.73	0.57
1:E:250:ALA:HB2	1:F:144:PHE:CE2	2.38	0.57
1:F:272:SER:OG	1:F:273:ARG:N	2.37	0.57
1:B:114:PRO:O	1:B:118:LEU:HG	2.04	0.57
1:C:182:GLU:OE2	1:C:350:MET:CE	2.51	0.57
1:A:106:THR:HG22	1:A:108:GLU:H	1.69	0.57
1:C:354:SER:C	1:C:356:THR:H	2.07	0.57
1:C:360:PHE:CD2	1:C:370:CYS:SG	2.97	0.57
1:E:83:ILE:HG21	1:E:96:VAL:HG13	1.86	0.57
1:A:179:SER:HB2	1:A:355:THR:HG21	1.86	0.57
1:F:106:THR:HG22	1:F:108:GLU:H	1.69	0.57
1:F:194:LEU:C	1:F:194:LEU:HD23	2.25	0.57
1:A:374:ASP:C	1:A:375:SER:HG	2.01	0.57
1:B:281:SER:HB2	1:B:324:THR:OG1	2.04	0.57
1:C:367:GLN:C	1:C:368:ARG:HG2	2.24	0.57
1:D:186:GLU:O	1:D:189:THR:HG23	2.04	0.57
1:D:311:GLN:NE2	1:D:311:GLN:O	2.37	0.57
1:E:250:ALA:HB2	1:F:144:PHE:CD2	2.39	0.57
1:A:151:HIS:CG	1:A:151:HIS:O	2.57	0.57
1:A:152:MET:O	1:A:154:ARG:N	2.37	0.57
1:C:226:PRO:O	1:C:227:VAL:C	2.39	0.57
1:C:296:LEU:O	1:C:297:SER:C	2.43	0.57
1:C:297:SER:O	1:C:300:GLN:N	2.38	0.57
1:D:238:LEU:O	1:D:240:PRO:N	2.37	0.57
1:E:146:THR:HG23	1:E:149:ASP:HB2	1.87	0.57
1:E:194:LEU:O	1:E:195:CYS:C	2.41	0.57
1:A:288:THR:CG2	1:D:305:LYS:NZ	2.67	0.57
1:E:283:MET:HE1	1:E:303:LEU:HD22	1.86	0.57
1:D:297:SER:O	1:D:300:GLN:N	2.39	0.56
1:E:276:LEU:O	1:E:276:LEU:HD23	2.05	0.56
1:B:258:GLN:NE2	1:B:306:PHE:CE1	2.65	0.56
1:B:306:PHE:O	1:B:308:ARG:N	2.38	0.56
1:C:100:ARG:C	1:C:102:SER:H	2.09	0.56
1:C:350:MET:HA	1:C:353:SER:OG	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:MET:O	1:E:351:ALA:C	2.44	0.56
1:B:124:ILE:HG22	1:B:129:ALA:HB2	1.87	0.56
1:B:312:ARG:O	1:B:315:ASP:N	2.38	0.56
1:E:186:GLU:O	1:E:189:THR:HG23	2.06	0.56
1:B:126:GLU:O	1:B:130:ASP:OD2	2.24	0.56
1:A:197:THR:OG1	1:A:392:VAL:HG23	2.06	0.56
1:B:180:ILE:HB	1:B:355:THR:HG23	1.88	0.56
1:D:191:LYS:NZ	1:D:326:GLN:HG2	2.21	0.56
1:E:244:LEU:HB2	1:F:148:ALA:HB2	1.87	0.56
1:F:244:LEU:C	1:F:246:ASN:N	2.58	0.56
1:A:373:VAL:O	1:A:374:ASP:O	2.23	0.55
1:B:100:ARG:C	1:B:102:SER:H	2.10	0.55
1:C:124:ILE:HG22	1:C:129:ALA:HB2	1.88	0.55
1:B:350:MET:O	1:B:351:ALA:C	2.43	0.55
1:C:240:PRO:C	1:C:242:ASP:N	2.57	0.55
1:E:230:VAL:CG2	1:E:231:SER:H	2.18	0.55
1:E:239:ASP:O	1:E:242:ASP:HB3	2.06	0.55
1:B:96:VAL:HG12	1:B:100:ARG:HE	1.71	0.55
1:B:168:ASP:O	1:B:171:LEU:N	2.39	0.55
1:B:258:GLN:HB2	1:B:285:LEU:CD2	2.36	0.55
1:C:200:VAL:O	1:C:202:CYS:N	2.40	0.55
1:D:225:ARG:HD3	1:D:225:ARG:N	2.22	0.55
1:A:175:VAL:HG23	1:A:175:VAL:O	2.06	0.55
1:A:245:ASN:HA	1:D:146:THR:OG1	2.05	0.55
1:B:360:PHE:CE2	1:B:370:CYS:HB2	2.40	0.55
1:D:104:LEU:HD23	1:D:109:ALA:HB1	1.89	0.55
1:D:272:SER:OG	1:D:273:ARG:N	2.39	0.55
1:D:296:LEU:O	1:D:299:ARG:N	2.39	0.55
1:A:196:HIS:O	1:A:199:ALA:CB	2.53	0.55
1:E:230:VAL:CG2	1:E:231:SER:N	2.69	0.55
1:A:305:LYS:O	1:A:308:ARG:HG2	2.06	0.55
1:B:360:PHE:CE2	1:B:370:CYS:CB	2.89	0.55
1:A:227:VAL:HG11	1:D:377:CYS:HB3	1.89	0.55
1:D:261:LEU:O	1:D:262:LEU:C	2.44	0.55
1:D:348:ASN:O	1:D:349:ILE:C	2.43	0.55
1:F:135:GLU:O	1:F:136:ALA:C	2.43	0.55
1:F:170:LEU:HG	1:F:372:VAL:HG21	1.89	0.55
1:B:227:VAL:CG2	1:B:227:VAL:CA	2.77	0.55
1:C:194:LEU:HG	1:C:392:VAL:HG21	1.89	0.55
1:D:88:VAL:O	1:D:90:GLY:N	2.40	0.55
1:E:253:TYR:CD2	1:F:112:TYR:CE1	2.95	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLN:O	1:B:349:ILE:HG21	2.06	0.55
1:C:264:ALA:O	1:C:268:MET:HG3	2.07	0.55
1:D:239:ASP:O	1:D:242:ASP:HB3	2.07	0.55
1:A:348:ASN:O	1:A:349:ILE:C	2.42	0.54
1:D:88:VAL:O	1:D:89:ASN:C	2.45	0.54
1:E:162:THR:HG21	1:E:167:LEU:HD23	1.89	0.54
1:C:145:VAL:HG23	1:C:145:VAL:O	2.07	0.54
1:C:350:MET:O	1:C:354:SER:OG	2.25	0.54
1:A:106:THR:O	1:A:107:ALA:C	2.41	0.54
1:C:118:LEU:HB3	1:C:129:ALA:HB1	1.89	0.54
1:F:392:VAL:HG12	1:F:393:GLY:N	2.22	0.54
1:A:304:ALA:C	1:A:306:PHE:N	2.60	0.54
1:F:300:GLN:O	1:F:349:ILE:HD13	2.07	0.54
1:B:258:GLN:HB2	1:B:285:LEU:HD23	1.90	0.54
1:D:105:HIS:O	1:D:106:THR:OG1	2.23	0.54
1:D:132:LEU:O	1:D:135:GLU:N	2.41	0.54
1:E:132:LEU:O	1:E:135:GLU:N	2.41	0.54
1:E:196:HIS:O	1:E:199:ALA:HB3	2.08	0.54
1:B:192:SER:N	2:B:502:SO4:O3	2.26	0.54
1:D:171:LEU:HD21	1:D:358:LEU:HD21	1.89	0.54
1:D:289:ASP:OD1	1:D:289:ASP:C	2.46	0.54
1:F:193:GLN:HG3	1:F:387:ILE:HD13	1.89	0.54
1:D:203:GLN:OE1	1:D:246:ASN:HB3	2.08	0.53
1:F:140:VAL:HG12	1:F:141:PRO:HD2	1.91	0.53
1:F:261:LEU:O	1:F:262:LEU:C	2.45	0.53
1:A:282:VAL:HG22	1:A:306:PHE:HE2	1.73	0.53
1:B:239:ASP:HB2	1:B:242:ASP:HB3	1.90	0.53
1:C:191:LYS:N	2:C:503:SO4:O4	2.41	0.53
1:D:106:THR:O	1:D:107:ALA:C	2.47	0.53
1:D:358:LEU:HB3	1:D:360:PHE:HE1	1.72	0.53
1:D:385:PHE:CD1	1:D:386:ALA:N	2.76	0.53
1:E:359:GLY:O	1:E:370:CYS:HA	2.09	0.53
1:B:227:VAL:CG2	1:B:227:VAL:HB	2.19	0.53
1:F:161:THR:HG23	1:F:161:THR:O	2.08	0.53
1:F:394:ASP:HB3	1:F:395:PRO:HD2	1.90	0.53
1:A:125:SER:OG	1:A:128:LYS:CB	2.54	0.53
1:A:287:ARG:C	1:A:289:ASP:H	2.12	0.53
1:B:267:GLN:O	1:B:271:GLU:HG2	2.08	0.53
1:E:276:LEU:HD23	1:E:276:LEU:C	2.28	0.53
1:F:151:HIS:O	1:F:151:HIS:CG	2.62	0.53
1:A:237:GLY:O	1:A:238:LEU:HG	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:HB	1:A:323:VAL:CG1	2.39	0.53
1:F:179:SER:HB2	1:F:355:THR:HG21	1.89	0.53
1:B:197:THR:O	1:B:198:LEU:C	2.43	0.53
1:C:359:GLY:O	1:C:370:CYS:HA	2.09	0.53
1:D:244:LEU:C	1:D:246:ASN:H	2.12	0.53
1:F:240:PRO:C	1:F:242:ASP:H	2.12	0.53
1:B:112:TYR:CD1	1:C:253:TYR:CG	2.97	0.53
1:E:348:ASN:O	1:E:351:ALA:N	2.42	0.53
1:B:140:VAL:O	1:B:142:MET:HG2	2.08	0.53
1:C:194:LEU:HA	1:C:392:VAL:CG2	2.39	0.53
1:C:238:LEU:O	1:C:240:PRO:HD3	2.09	0.53
1:D:303:LEU:O	1:D:304:ALA:C	2.45	0.53
1:E:106:THR:O	1:E:107:ALA:C	2.48	0.53
1:E:244:LEU:C	1:E:246:ASN:H	2.12	0.53
1:A:200:VAL:O	1:A:202:CYS:N	2.42	0.52
1:C:168:ASP:O	1:C:171:LEU:N	2.42	0.52
1:D:200:VAL:C	1:D:202:CYS:H	2.12	0.52
1:F:284:ALA:C	1:F:286:TYR:N	2.60	0.52
1:F:286:TYR:CZ	1:F:346:GLY:HA2	2.45	0.52
1:A:193:GLN:HG3	1:A:387:ILE:CG2	2.39	0.52
1:B:158:ILE:O	1:B:177:THR:OG1	2.20	0.52
1:D:254:ASN:OD1	1:D:254:ASN:C	2.48	0.52
1:C:244:LEU:C	1:C:246:ASN:N	2.51	0.52
1:F:299:ARG:HG3	1:F:299:ARG:HH11	1.74	0.52
1:A:240:PRO:C	1:A:242:ASP:N	2.63	0.52
1:D:276:LEU:HD23	1:D:276:LEU:O	2.09	0.52
1:E:200:VAL:O	1:E:202:CYS:N	2.42	0.52
1:F:237:GLY:O	1:F:238:LEU:HG	2.10	0.52
1:A:306:PHE:O	1:A:307:MET:C	2.44	0.52
1:A:132:LEU:O	1:A:133:LEU:C	2.48	0.52
1:A:288:THR:CG2	1:D:305:LYS:HZ3	2.23	0.52
1:B:118:LEU:HB3	1:B:129:ALA:HB1	1.89	0.52
1:F:194:LEU:O	1:F:195:CYS:C	2.46	0.52
1:B:277:ILE:HG22	1:B:278:VAL:N	2.24	0.52
1:E:238:LEU:O	1:E:240:PRO:N	2.42	0.52
1:C:350:MET:C	1:C:354:SER:OG	2.49	0.52
1:B:359:GLY:O	1:B:370:CYS:HA	2.10	0.52
1:D:385:PHE:HD1	1:D:386:ALA:N	2.08	0.52
1:F:282:VAL:HB	1:F:323:VAL:CG1	2.39	0.52
1:F:297:SER:O	1:F:298:ALA:C	2.49	0.52
1:C:238:LEU:O	1:C:240:PRO:N	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASN:OD1	1:D:254:ASN:O	2.28	0.51
1:B:196:HIS:O	1:B:199:ALA:HB3	2.10	0.51
1:D:230:VAL:CG2	1:D:231:SER:H	2.22	0.51
1:E:240:PRO:C	1:E:242:ASP:N	2.54	0.51
1:B:201:THR:HA	1:B:204:ILE:CG1	2.38	0.51
1:D:201:THR:O	1:D:210:GLY:HA2	2.10	0.51
1:F:160:LEU:HD22	1:F:202:CYS:HA	1.92	0.51
1:F:299:ARG:HG3	1:F:299:ARG:NH1	2.25	0.51
1:B:200:VAL:C	1:B:202:CYS:N	2.64	0.51
1:F:141:PRO:HG2	1:F:142:MET:H	1.75	0.51
1:A:240:PRO:C	1:A:242:ASP:H	2.14	0.51
1:B:204:ILE:HB	1:B:210:GLY:HA3	1.93	0.51
1:C:99:LEU:O	1:C:102:SER:CB	2.59	0.51
1:F:152:MET:O	1:F:154:ARG:N	2.42	0.51
1:A:235:ARG:HD2	1:A:390:ASP:OD1	2.10	0.51
1:C:106:THR:CG2	1:C:107:ALA:N	2.74	0.51
1:D:180:ILE:HG22	1:D:181:THR:N	2.26	0.51
1:B:296:LEU:O	1:B:297:SER:C	2.49	0.51
1:C:220:THR:HG21	1:C:281:SER:O	2.10	0.51
1:D:367:GLN:O	1:D:368:ARG:HG2	2.10	0.51
1:E:104:LEU:CD2	1:E:109:ALA:HB1	2.41	0.51
1:E:312:ARG:O	1:E:315:ASP:N	2.43	0.51
1:F:106:THR:O	1:F:109:ALA:HB3	2.10	0.51
1:F:175:VAL:HG23	1:F:175:VAL:O	2.10	0.51
1:F:200:VAL:O	1:F:202:CYS:N	2.43	0.51
1:C:389:GLU:HG2	1:C:389:GLU:O	2.11	0.51
1:E:253:TYR:CG	1:F:112:TYR:CD1	2.98	0.51
1:A:200:VAL:C	1:A:202:CYS:H	2.14	0.51
1:C:200:VAL:C	1:C:202:CYS:N	2.63	0.51
1:E:384:VAL:HG12	1:E:385:PHE:N	2.26	0.51
1:C:306:PHE:O	1:C:307:MET:C	2.46	0.51
1:E:274:PHE:CD1	1:E:274:PHE:N	2.78	0.51
1:F:240:PRO:C	1:F:242:ASP:N	2.63	0.51
1:B:360:PHE:CD2	1:B:370:CYS:HB2	2.46	0.50
1:D:276:LEU:HD23	1:D:276:LEU:C	2.32	0.50
1:F:295:GLU:O	1:F:296:LEU:C	2.49	0.50
1:B:286:TYR:CD2	1:B:303:LEU:HD13	2.46	0.50
1:C:254:ASN:OD1	1:C:254:ASN:O	2.29	0.50
1:D:230:VAL:CG2	1:D:231:SER:N	2.71	0.50
1:D:258:GLN:NE2	1:D:306:PHE:CE1	2.75	0.50
1:E:160:LEU:HD22	1:E:202:CYS:HA	1.92	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:SER:O	1:A:165:LYS:C	2.48	0.50
1:A:277:ILE:HB	1:A:321:VAL:HG22	1.94	0.50
1:B:164:SER:O	1:B:165:LYS:C	2.50	0.50
1:B:352:HIS:NE2	1:C:326:GLN:OE1	2.44	0.50
1:C:238:LEU:O	1:C:240:PRO:CD	2.60	0.50
1:E:162:THR:CB	1:E:167:LEU:HD23	2.41	0.50
1:F:100:ARG:NH1	1:F:100:ARG:HG2	2.27	0.50
1:F:304:ALA:C	1:F:306:PHE:N	2.63	0.50
1:B:200:VAL:C	1:B:202:CYS:H	2.13	0.50
1:D:240:PRO:O	1:D:243:ALA:N	2.45	0.50
1:E:283:MET:CE	1:E:303:LEU:CD2	2.90	0.50
1:E:296:LEU:O	1:E:299:ARG:N	2.44	0.50
1:B:148:ALA:O	1:B:149:ASP:C	2.48	0.50
1:E:177:THR:HG22	1:E:320:ALA:HB2	1.94	0.50
1:E:247:VAL:O	1:F:147:ALA:N	2.44	0.50
1:B:147:ALA:HB2	1:C:247:VAL:HB	1.93	0.50
1:C:282:VAL:HB	1:C:323:VAL:CG1	2.42	0.50
1:E:204:ILE:HB	1:E:210:GLY:HA3	1.94	0.50
1:A:370:CYS:O	1:A:370:CYS:SG	2.68	0.50
1:B:286:TYR:HE2	1:B:303:LEU:N	2.10	0.50
1:C:106:THR:HG22	1:C:108:GLU:H	1.77	0.50
1:C:196:HIS:O	1:C:197:THR:C	2.48	0.50
1:F:282:VAL:CG2	1:F:323:VAL:HG13	2.41	0.50
1:F:385:PHE:HD1	1:F:386:ALA:N	2.10	0.50
1:A:239:ASP:HB2	1:A:242:ASP:CB	2.42	0.50
1:B:155:SER:O	1:B:156:GLU:C	2.47	0.50
1:B:306:PHE:O	1:B:307:MET:C	2.48	0.50
1:D:96:VAL:HG12	1:D:97:LYS:N	2.22	0.50
1:D:295:GLU:O	1:D:296:LEU:C	2.50	0.49
1:E:99:LEU:HD23	1:E:121:ILE:HD13	1.93	0.49
1:F:144:PHE:O	1:F:145:VAL:HG13	2.12	0.49
1:A:244:LEU:CB	1:D:148:ALA:HB2	2.40	0.49
1:C:164:SER:O	1:C:165:LYS:C	2.46	0.49
1:C:266:ALA:C	1:C:268:MET:N	2.64	0.49
1:C:347:GLY:O	1:C:348:ASN:C	2.50	0.49
1:F:125:SER:OG	1:F:128:LYS:CB	2.57	0.49
1:B:283:MET:O	1:B:286:TYR:HB2	2.12	0.49
1:C:238:LEU:O	1:C:239:ASP:C	2.49	0.49
1:D:348:ASN:O	1:D:350:MET:N	2.45	0.49
1:E:200:VAL:C	1:E:202:CYS:N	2.64	0.49
1:E:240:PRO:O	1:E:243:ALA:N	2.46	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ASP:HB2	1:F:242:ASP:HB3	1.95	0.49
1:A:180:ILE:HG12	1:A:321:VAL:CG1	2.42	0.49
1:B:318:GLY:O	1:B:319:VAL:O	2.30	0.49
1:E:201:THR:O	1:E:210:GLY:HA2	2.12	0.49
1:F:194:LEU:HD21	1:F:198:LEU:HD12	1.94	0.49
1:F:232:ILE:O	1:F:235:ARG:HB3	2.12	0.49
1:A:384:VAL:CG1	1:A:385:PHE:N	2.75	0.49
1:B:200:VAL:O	1:B:202:CYS:N	2.46	0.49
1:C:268:MET:C	1:C:270:SER:H	2.16	0.49
1:D:175:VAL:CG1	1:D:198:LEU:HD11	2.43	0.49
1:F:366:CYS:HA	1:F:368:ARG:HH12	1.78	0.49
1:C:106:THR:O	1:C:109:ALA:HB3	2.12	0.49
1:E:265:ALA:O	1:E:269:MET:HG3	2.13	0.49
1:A:368:ARG:HG3	1:A:387:ILE:HD11	1.95	0.49
1:D:108:GLU:OE1	1:D:108:GLU:N	2.45	0.49
1:F:348:ASN:C	1:F:350:MET:N	2.64	0.49
1:F:371:LYS:HG2	1:F:372:VAL:N	2.28	0.49
1:B:360:PHE:CD2	1:B:370:CYS:CB	2.95	0.49
1:D:83:ILE:HG21	1:D:96:VAL:CG1	2.42	0.49
1:F:155:SER:C	1:F:157:LEU:H	2.16	0.49
1:F:196:HIS:O	1:F:199:ALA:CB	2.55	0.49
1:F:250:ALA:HB1	1:F:261:LEU:HD13	1.94	0.49
1:A:175:VAL:O	1:A:175:VAL:CG2	2.61	0.48
1:B:151:HIS:CG	1:B:151:HIS:O	2.66	0.48
1:B:226:PRO:O	1:B:228:ARG:N	2.46	0.48
1:D:162:THR:O	1:D:197:THR:HG21	2.13	0.48
1:D:360:PHE:N	1:D:360:PHE:HD1	2.07	0.48
1:E:106:THR:O	1:E:109:ALA:HB3	2.13	0.48
1:E:283:MET:HE1	1:E:303:LEU:CD2	2.43	0.48
1:F:266:ALA:C	1:F:268:MET:N	2.64	0.48
1:B:161:THR:OG1	1:B:162:THR:N	2.44	0.48
1:C:161:THR:OG1	1:C:162:THR:N	2.44	0.48
1:D:371:LYS:HG2	1:D:372:VAL:N	2.28	0.48
1:F:306:PHE:O	1:F:307:MET:C	2.46	0.48
1:A:258:GLN:NE2	1:A:306:PHE:CE1	2.71	0.48
1:E:311:GLN:O	1:E:311:GLN:NE2	2.45	0.48
1:D:160:LEU:HD22	1:D:202:CYS:HA	1.95	0.48
1:A:100:ARG:NH1	1:A:100:ARG:CG	2.68	0.48
1:E:203:GLN:OE1	1:E:246:ASN:HB3	2.12	0.48
1:F:385:PHE:CD1	1:F:385:PHE:C	2.86	0.48
1:B:226:PRO:O	1:B:227:VAL:C	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:O	1:A:195:CYS:C	2.51	0.48
1:C:306:PHE:C	1:C:308:ARG:N	2.67	0.48
1:D:247:VAL:O	1:D:247:VAL:HG12	2.09	0.48
1:C:355:THR:O	1:C:356:THR:CB	2.62	0.48
1:B:194:LEU:CD2	1:B:198:LEU:HD12	2.44	0.47
1:D:164:SER:O	1:D:164:SER:OG	2.30	0.47
1:C:196:HIS:O	1:C:199:ALA:N	2.47	0.47
1:D:200:VAL:O	1:D:202:CYS:N	2.47	0.47
1:F:372:VAL:HG12	1:F:372:VAL:O	2.14	0.47
1:A:348:ASN:C	1:A:350:MET:N	2.66	0.47
1:B:164:SER:OG	1:B:167:LEU:CB	2.60	0.47
1:C:255:ALA:HB1	1:C:286:TYR:CE2	2.49	0.47
1:D:224:PHE:CD2	1:D:249:TYR:CD1	3.02	0.47
1:E:162:THR:CG2	1:E:167:LEU:HD23	2.44	0.47
1:A:196:HIS:O	1:A:197:THR:C	2.50	0.47
1:B:145:VAL:HG23	1:B:145:VAL:O	2.14	0.47
1:A:144:PHE:O	1:A:145:VAL:HG13	2.14	0.47
1:D:238:LEU:O	1:D:239:ASP:C	2.53	0.47
1:D:267:GLN:O	1:D:270:SER:HB3	2.15	0.47
1:A:167:LEU:O	1:A:168:ASP:C	2.52	0.47
1:A:175:VAL:CG1	1:A:198:LEU:HD11	2.42	0.47
1:A:304:ALA:O	1:A:306:PHE:N	2.47	0.47
1:B:230:VAL:O	1:B:231:SER:C	2.50	0.47
1:A:244:LEU:O	1:A:246:ASN:N	2.47	0.47
1:B:255:ALA:HA	1:B:285:LEU:CD2	2.44	0.47
1:B:355:THR:HG1	1:B:356:THR:H	1.58	0.47
1:D:280:ASP:HA	1:D:281:SER:HA	1.68	0.47
1:E:295:GLU:O	1:E:296:LEU:C	2.52	0.47
1:A:348:ASN:O	1:A:350:MET:N	2.48	0.47
1:B:106:THR:HG22	1:B:108:GLU:H	1.79	0.47
1:D:191:LYS:HB2	2:D:504:SO4:O3	2.14	0.47
1:B:306:PHE:C	1:B:308:ARG:N	2.67	0.47
1:F:296:LEU:O	1:F:299:ARG:N	2.47	0.47
1:B:117:ASP:O	1:B:121:ILE:HD11	2.15	0.47
1:C:280:ASP:HA	1:C:281:SER:HA	1.77	0.47
1:C:312:ARG:O	1:C:315:ASP:N	2.47	0.47
1:E:88:VAL:O	1:E:89:ASN:C	2.53	0.47
1:A:237:GLY:C	1:A:238:LEU:HG	2.35	0.46
1:B:182:GLU:OE1	1:B:357:ARG:HG2	2.14	0.46
1:B:196:HIS:O	1:B:197:THR:C	2.51	0.46
1:B:238:LEU:O	1:B:239:ASP:C	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ALA:C	1:B:268:MET:N	2.66	0.46
1:D:303:LEU:C	1:D:303:LEU:HD12	2.36	0.46
1:E:253:TYR:CZ	1:F:112:TYR:CE1	3.03	0.46
1:B:350:MET:O	1:B:353:SER:N	2.49	0.46
1:F:104:LEU:H	1:F:104:LEU:HG	1.40	0.46
1:A:280:ASP:HA	1:A:281:SER:HA	1.69	0.46
1:F:164:SER:O	1:F:165:LYS:C	2.49	0.46
1:F:230:VAL:O	1:F:231:SER:C	2.52	0.46
1:C:255:ALA:HA	1:C:285:LEU:CD2	2.45	0.46
1:D:200:VAL:C	1:D:202:CYS:N	2.69	0.46
1:D:310:LEU:O	1:D:311:GLN:C	2.47	0.46
1:E:371:LYS:HG2	1:E:372:VAL:N	2.31	0.46
1:C:117:ASP:O	1:C:121:ILE:HD11	2.16	0.46
1:E:296:LEU:O	1:E:298:ALA:N	2.49	0.46
1:F:286:TYR:CE1	1:F:303:LEU:HD22	2.50	0.46
1:A:200:VAL:C	1:A:202:CYS:N	2.67	0.46
1:A:227:VAL:HG22	1:D:151:HIS:CE1	2.51	0.46
1:B:144:PHE:O	1:B:145:VAL:HG13	2.16	0.46
1:C:230:VAL:O	1:C:231:SER:C	2.53	0.46
1:E:197:THR:OG1	1:E:392:VAL:HG23	2.15	0.46
1:E:303:LEU:O	1:E:304:ALA:C	2.52	0.46
1:F:203:GLN:OE1	1:F:246:ASN:HB3	2.16	0.46
1:A:180:ILE:HD11	1:A:310:LEU:HB3	1.98	0.46
1:E:281:SER:C	1:E:283:MET:N	2.67	0.46
1:A:244:LEU:C	1:A:246:ASN:N	2.65	0.46
1:C:234:GLN:O	1:C:235:ARG:C	2.52	0.46
1:D:237:GLY:O	1:D:238:LEU:HG	2.16	0.46
1:A:247:VAL:O	1:D:147:ALA:N	2.49	0.46
1:B:112:TYR:O	1:C:254:ASN:HB3	2.16	0.46
1:C:195:CYS:O	1:C:196:HIS:C	2.54	0.46
1:C:276:LEU:HG	1:C:277:ILE:N	2.31	0.46
1:F:200:VAL:C	1:F:202:CYS:H	2.20	0.45
1:A:392:VAL:HG12	1:A:393:GLY:N	2.31	0.45
1:E:125:SER:O	1:E:127:ALA:N	2.48	0.45
1:E:160:LEU:HB2	1:E:175:VAL:HG22	1.97	0.45
1:C:204:ILE:HG23	1:C:205:PRO:HD2	1.97	0.45
1:D:206:LEU:HG	1:D:212:GLU:OE2	2.17	0.45
1:F:285:LEU:HA	1:F:285:LEU:HD23	1.60	0.45
1:A:111:ALA:HB1	1:A:142:MET:SD	2.57	0.45
1:B:204:ILE:HA	1:B:205:PRO:HD3	1.79	0.45
1:C:194:LEU:O	1:C:194:LEU:HD23	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ILE:CG2	1:D:181:THR:N	2.80	0.45
1:D:274:PHE:CD1	1:D:274:PHE:N	2.84	0.45
1:F:384:VAL:CG1	1:F:385:PHE:H	2.30	0.45
1:D:184:PHE:CD1	1:D:184:PHE:C	2.90	0.45
1:F:88:VAL:O	1:F:90:GLY:N	2.49	0.45
1:F:230:VAL:CG2	1:F:231:SER:N	2.43	0.45
1:F:238:LEU:O	1:F:240:PRO:HD3	2.16	0.45
1:A:232:ILE:O	1:A:235:ARG:HB3	2.17	0.45
1:C:197:THR:O	1:C:198:LEU:C	2.53	0.45
1:D:392:VAL:HG12	1:D:393:GLY:N	2.32	0.45
1:F:237:GLY:C	1:F:238:LEU:HG	2.37	0.45
1:F:284:ALA:C	1:F:286:TYR:H	2.18	0.45
1:A:140:VAL:C	1:A:141:PRO:O	2.51	0.45
1:A:170:LEU:HD11	1:A:381:ALA:O	2.17	0.45
1:A:286:TYR:CE1	1:A:346:GLY:HA2	2.51	0.45
1:B:183:LEU:HD22	1:B:360:PHE:CE1	2.52	0.45
1:B:255:ALA:HB1	1:B:286:TYR:CE1	2.52	0.45
1:A:282:VAL:CG2	1:A:306:PHE:HE2	2.29	0.45
1:D:240:PRO:C	1:D:242:ASP:N	2.57	0.45
1:F:140:VAL:CG1	1:F:141:PRO:HD2	2.47	0.45
1:E:108:GLU:O	1:E:111:ALA:HB3	2.17	0.45
1:A:93:MET:O	1:A:93:MET:HG2	2.16	0.44
1:C:164:SER:OG	1:C:167:LEU:CB	2.63	0.44
1:E:162:THR:O	1:E:197:THR:HG21	2.17	0.44
1:E:371:LYS:CG	1:E:372:VAL:N	2.80	0.44
1:F:226:PRO:O	1:F:227:VAL:C	2.54	0.44
1:F:262:LEU:HD11	1:F:306:PHE:CE1	2.52	0.44
1:F:373:VAL:O	1:F:373:VAL:HG13	2.17	0.44
1:A:183:LEU:HD23	1:A:358:LEU:HB2	1.99	0.44
1:C:255:ALA:HB1	1:C:286:TYR:HE2	1.82	0.44
1:D:125:SER:OG	1:D:128:LYS:HB2	2.18	0.44
1:F:389:GLU:O	1:F:389:GLU:HG2	2.16	0.44
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.88	0.44
1:B:303:LEU:O	1:B:303:LEU:HG	2.17	0.44
1:F:167:LEU:O	1:F:168:ASP:C	2.54	0.44
1:B:311:GLN:O	1:B:312:ARG:C	2.53	0.44
1:C:100:ARG:C	1:C:102:SER:N	2.71	0.44
1:C:258:GLN:HB2	1:C:285:LEU:CD2	2.47	0.44
1:C:283:MET:CE	1:C:283:MET:CG	2.94	0.44
1:E:92:THR:OG1	1:E:95:ASP:OD2	2.31	0.44
1:E:375:SER:O	1:E:376:PRO:C	2.54	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:LEU:HD23	1:F:121:ILE:HD13	2.00	0.44
1:F:194:LEU:C	1:F:194:LEU:CD2	2.86	0.44
1:A:152:MET:O	1:A:153:ARG:C	2.56	0.44
1:B:106:THR:CG2	1:B:107:ALA:N	2.79	0.44
1:B:216:LEU:HD23	1:B:277:ILE:HG23	1.99	0.44
1:C:191:LYS:HG2	1:C:360:PHE:HD1	1.80	0.44
1:D:99:LEU:HD23	1:D:121:ILE:HD13	1.99	0.44
1:F:318:GLY:O	1:F:319:VAL:O	2.36	0.44
1:A:255:ALA:HB2	1:A:289:ASP:O	2.17	0.44
1:A:296:LEU:O	1:A:297:SER:O	2.33	0.44
1:B:239:ASP:O	1:B:242:ASP:HB3	2.18	0.44
1:B:255:ALA:HA	1:B:285:LEU:HD23	2.00	0.44
1:D:239:ASP:HB2	1:D:242:ASP:CB	2.47	0.44
1:E:164:SER:O	1:E:165:LYS:C	2.56	0.44
1:E:204:ILE:HG22	1:E:205:PRO:N	2.31	0.44
1:B:198:LEU:C	1:B:200:VAL:N	2.71	0.44
1:B:282:VAL:HB	1:B:323:VAL:CG1	2.48	0.44
1:D:170:LEU:HD11	1:D:381:ALA:HB3	1.99	0.44
1:E:281:SER:O	1:E:283:MET:N	2.51	0.44
1:E:285:LEU:HD13	1:E:285:LEU:HA	1.78	0.44
1:A:371:LYS:HG2	1:A:372:VAL:N	2.33	0.44
1:B:194:LEU:O	1:B:194:LEU:HD23	2.18	0.44
1:F:254:ASN:OD1	1:F:254:ASN:C	2.56	0.44
1:A:203:GLN:OE1	1:A:246:ASN:HB3	2.18	0.44
1:D:162:THR:HB	1:D:167:LEU:HD23	1.98	0.44
1:D:297:SER:OG	1:D:298:ALA:N	2.47	0.44
1:E:162:THR:HB	1:E:167:LEU:HD23	2.00	0.44
1:E:244:LEU:CB	1:F:148:ALA:HB2	2.48	0.44
1:F:144:PHE:C	1:F:145:VAL:HG13	2.39	0.44
1:F:148:ALA:O	1:F:149:ASP:C	2.55	0.44
1:F:375:SER:HA	1:F:376:PRO:HD2	1.62	0.44
1:D:205:PRO:O	1:D:207:ASP:N	2.51	0.43
1:E:88:VAL:O	1:E:90:GLY:N	2.51	0.43
1:E:162:THR:HG21	1:E:167:LEU:CD2	2.48	0.43
1:F:158:ILE:HG21	1:F:158:ILE:HD13	1.70	0.43
1:B:124:ILE:CG2	1:B:129:ALA:HB2	2.47	0.43
1:B:197:THR:O	1:B:199:ALA:N	2.51	0.43
1:B:198:LEU:C	1:B:200:VAL:H	2.20	0.43
1:C:151:HIS:O	1:C:151:HIS:CG	2.70	0.43
1:C:272:SER:OG	1:C:273:ARG:N	2.51	0.43
1:E:350:MET:O	1:E:353:SER:N	2.50	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:PHE:CD1	1:E:386:ALA:N	2.86	0.43
1:F:191:LYS:O	1:F:192:SER:C	2.54	0.43
1:F:194:LEU:CD2	1:F:198:LEU:HD12	2.48	0.43
1:A:106:THR:O	1:A:109:ALA:HB3	2.18	0.43
1:A:304:ALA:C	1:A:306:PHE:H	2.21	0.43
1:D:81:VAL:O	1:D:106:THR:HG23	2.19	0.43
1:D:125:SER:O	1:D:127:ALA:N	2.51	0.43
1:E:132:LEU:O	1:E:133:LEU:C	2.57	0.43
1:F:180:ILE:HD13	1:F:180:ILE:HG21	1.77	0.43
1:F:196:HIS:O	1:F:197:THR:C	2.54	0.43
1:C:124:ILE:CG2	1:C:129:ALA:HB2	2.47	0.43
1:E:277:ILE:HG21	1:E:277:ILE:HD13	1.75	0.43
1:E:392:VAL:HG12	1:E:393:GLY:N	2.34	0.43
1:F:100:ARG:HG2	1:F:100:ARG:HH11	1.83	0.43
1:B:140:VAL:O	1:B:141:PRO:C	2.56	0.43
1:D:104:LEU:HD22	1:D:109:ALA:HB1	2.00	0.43
1:D:183:LEU:O	1:D:324:THR:HA	2.19	0.43
1:E:125:SER:OG	1:E:128:LYS:CB	2.65	0.43
1:E:167:LEU:HD12	1:E:167:LEU:HA	1.84	0.43
1:F:374:ASP:C	1:F:375:SER:HG	2.13	0.43
1:A:250:ALA:HB2	1:D:144:PHE:CE2	2.53	0.43
1:C:106:THR:O	1:C:107:ALA:C	2.55	0.43
1:C:110:VAL:O	1:C:113:ALA:CB	2.61	0.43
1:C:194:LEU:C	1:C:194:LEU:CD2	2.86	0.43
1:E:164:SER:OG	1:E:167:LEU:CB	2.66	0.43
1:B:110:VAL:O	1:B:113:ALA:CB	2.62	0.43
1:B:384:VAL:CG1	1:B:385:PHE:N	2.78	0.43
1:A:205:PRO:O	1:A:206:LEU:C	2.56	0.43
1:B:254:ASN:OD1	1:B:254:ASN:O	2.36	0.43
1:B:268:MET:C	1:B:270:SER:H	2.21	0.43
1:C:204:ILE:HA	1:C:205:PRO:HD3	1.72	0.43
1:F:200:VAL:C	1:F:202:CYS:N	2.72	0.43
1:B:226:PRO:O	1:B:229:LEU:N	2.50	0.43
1:C:354:SER:C	1:C:356:THR:N	2.72	0.43
1:D:92:THR:C	1:D:94:ALA:N	2.70	0.43
1:E:183:LEU:O	1:E:324:THR:HA	2.19	0.43
1:F:164:SER:OG	1:F:167:LEU:HB2	2.19	0.43
1:F:170:LEU:HG	1:F:372:VAL:CG2	2.48	0.43
1:F:205:PRO:HA	1:F:212:GLU:HG3	2.00	0.43
1:A:226:PRO:O	1:A:227:VAL:C	2.56	0.43
1:E:170:LEU:HD12	1:E:170:LEU:HA	1.80	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:PHE:N	1:E:274:PHE:HD1	2.17	0.43
1:F:194:LEU:HD23	1:F:194:LEU:O	2.19	0.43
1:F:269:MET:HE1	1:F:313:LEU:HD22	2.01	0.43
1:F:385:PHE:CD1	1:F:386:ALA:N	2.86	0.43
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.70	0.42
1:A:226:PRO:O	1:A:228:ARG:N	2.51	0.42
1:B:112:TYR:HB3	1:C:253:TYR:HB3	2.00	0.42
1:B:259:LEU:O	1:B:260:ARG:C	2.56	0.42
1:C:347:GLY:HA2	1:C:357:ARG:NH2	2.34	0.42
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.83	0.42
1:A:296:LEU:HG	1:A:297:SER:N	2.34	0.42
1:C:180:ILE:HG22	1:C:181:THR:N	2.33	0.42
1:A:88:VAL:O	1:A:91:ILE:HD12	2.19	0.42
1:C:186:GLU:O	1:C:189:THR:HG23	2.18	0.42
1:C:298:ALA:O	1:C:299:ARG:C	2.55	0.42
1:D:253:TYR:N	1:D:253:TYR:CD1	2.87	0.42
1:E:198:LEU:HD23	1:E:198:LEU:HA	1.65	0.42
1:F:125:SER:O	1:F:127:ALA:N	2.51	0.42
1:B:100:ARG:C	1:B:102:SER:N	2.71	0.42
1:D:204:ILE:HG22	1:D:205:PRO:N	2.35	0.42
1:A:175:VAL:HG11	1:A:198:LEU:CD1	2.46	0.42
1:A:186:GLU:O	1:A:189:THR:HG23	2.19	0.42
1:A:312:ARG:O	1:A:315:ASP:N	2.52	0.42
1:B:301:MET:O	1:B:304:ALA:HB3	2.20	0.42
1:C:226:PRO:O	1:C:229:LEU:N	2.53	0.42
1:F:88:VAL:O	1:F:89:ASN:C	2.57	0.42
1:F:132:LEU:O	1:F:133:LEU:C	2.56	0.42
1:A:312:ARG:O	1:A:315:ASP:HB2	2.20	0.42
1:B:303:LEU:O	1:B:307:MET:HG2	2.19	0.42
1:D:244:LEU:C	1:D:246:ASN:N	2.72	0.42
1:E:108:GLU:OE1	1:E:108:GLU:N	2.48	0.42
1:C:257:HIS:HA	1:C:260:ARG:HE	1.85	0.42
1:D:367:GLN:C	1:D:368:ARG:HG2	2.40	0.42
1:E:254:ASN:OD1	1:E:254:ASN:O	2.38	0.42
1:F:115:ARG:O	1:F:116:LYS:C	2.58	0.42
1:F:266:ALA:O	1:F:267:GLN:C	2.58	0.42
1:B:369:LEU:HD23	1:B:370:CYS:N	2.35	0.42
1:C:205:PRO:HA	1:C:212:GLU:HG3	2.02	0.42
1:C:302:HIS:O	1:C:303:LEU:C	2.57	0.42
1:D:106:THR:O	1:D:109:ALA:HB3	2.20	0.42
1:F:392:VAL:HG12	1:F:393:GLY:H	1.83	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:O	1:A:161:THR:HG23	2.19	0.42
1:A:374:ASP:C	1:A:375:SER:OG	2.54	0.42
1:B:110:VAL:O	1:B:111:ALA:C	2.58	0.42
1:B:198:LEU:HA	1:B:198:LEU:HD23	1.82	0.42
1:C:277:ILE:HB	1:C:321:VAL:HG22	2.01	0.42
1:C:281:SER:HB2	1:C:324:THR:OG1	2.20	0.42
1:D:240:PRO:O	1:D:241:ASP:C	2.52	0.42
1:E:80:MET:CE	1:E:80:MET:CG	2.94	0.42
1:F:280:ASP:HA	1:F:281:SER:HA	1.77	0.42
1:F:303:LEU:O	1:F:303:LEU:CG	2.64	0.42
1:A:266:ALA:C	1:A:268:MET:N	2.72	0.42
1:A:191:LYS:O	1:A:192:SER:C	2.57	0.41
1:A:389:GLU:O	1:A:389:GLU:HG2	2.19	0.41
1:A:394:ASP:HB3	1:A:395:PRO:HD2	2.01	0.41
1:B:220:THR:HG21	1:B:281:SER:O	2.20	0.41
1:B:360:PHE:HA	1:B:369:LEU:O	2.20	0.41
1:C:254:ASN:OD1	1:C:254:ASN:C	2.57	0.41
1:E:104:LEU:H	1:E:104:LEU:HG	1.58	0.41
1:E:238:LEU:O	1:E:239:ASP:C	2.58	0.41
1:F:288:THR:HA	1:F:299:ARG:NH2	2.35	0.41
1:B:146:THR:HG23	1:B:149:ASP:HB2	2.01	0.41
1:B:196:HIS:O	1:B:199:ALA:N	2.52	0.41
1:B:230:VAL:O	1:B:232:ILE:N	2.54	0.41
1:C:240:PRO:O	1:C:243:ALA:N	2.53	0.41
1:D:162:THR:CB	1:D:167:LEU:HD23	2.50	0.41
1:E:280:ASP:HA	1:E:281:SER:HA	1.74	0.41
1:F:268:MET:O	1:F:270:SER:N	2.53	0.41
1:F:376:PRO:HB2	1:F:377:CYS:H	1.64	0.41
1:B:256:ASP:O	1:B:258:GLN:N	2.53	0.41
1:E:244:LEU:C	1:E:246:ASN:N	2.72	0.41
1:A:135:GLU:O	1:A:136:ALA:C	2.58	0.41
1:A:350:MET:O	1:A:351:ALA:C	2.59	0.41
1:B:347:GLY:O	1:B:350:MET:HB2	2.20	0.41
1:B:389:GLU:O	1:B:389:GLU:HG2	2.21	0.41
1:E:113:ALA:HA	1:E:114:PRO:HD3	1.66	0.41
1:E:281:SER:O	1:E:282:VAL:C	2.58	0.41
1:F:92:THR:O	1:F:95:ASP:N	2.51	0.41
1:B:104:LEU:O	1:B:105:HIS:CG	2.73	0.41
1:B:182:GLU:OE1	1:B:357:ARG:CG	2.69	0.41
1:B:240:PRO:C	1:B:242:ASP:N	2.57	0.41
1:D:132:LEU:O	1:D:133:LEU:C	2.58	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:VAL:O	1:D:146:THR:C	2.57	0.41
1:F:100:ARG:NH1	1:F:100:ARG:CG	2.77	0.41
1:F:226:PRO:O	1:F:228:ARG:N	2.53	0.41
1:A:265:ALA:O	1:A:269:MET:HG3	2.20	0.41
1:A:304:ALA:O	1:A:305:LYS:C	2.59	0.41
1:A:369:LEU:O	1:A:370:CYS:CB	2.68	0.41
1:C:369:LEU:HD21	1:C:382:GLU:HB2	2.03	0.41
1:D:92:THR:C	1:D:94:ALA:H	2.24	0.41
1:D:230:VAL:O	1:D:232:ILE:N	2.54	0.41
1:D:296:LEU:O	1:D:298:ALA:N	2.53	0.41
1:F:164:SER:O	1:F:164:SER:OG	2.34	0.41
1:A:360:PHE:CD1	1:A:360:PHE:N	2.88	0.41
1:B:115:ARG:O	1:B:116:LYS:C	2.58	0.41
1:C:194:LEU:HA	1:C:392:VAL:HG21	2.02	0.41
1:C:384:VAL:O	1:C:384:VAL:HG12	2.13	0.41
1:D:144:PHE:O	1:D:145:VAL:HG13	2.20	0.41
1:F:175:VAL:O	1:F:175:VAL:CG2	2.68	0.41
1:F:204:ILE:HB	1:F:210:GLY:HA3	2.02	0.41
1:A:158:ILE:HG21	1:A:158:ILE:HD13	1.77	0.41
1:A:261:LEU:O	1:A:262:LEU:C	2.58	0.41
1:B:175:VAL:O	1:B:175:VAL:HG23	2.19	0.41
1:C:166:ASN:HB3	1:C:383:CYS:SG	2.61	0.41
1:D:188:ARG:HA	2:D:504:SO4:O4	2.20	0.41
1:E:125:SER:O	1:E:128:LYS:N	2.54	0.41
1:E:170:LEU:HG	1:E:372:VAL:HG21	2.02	0.41
1:E:254:ASN:OD1	1:E:254:ASN:C	2.59	0.41
1:E:265:ALA:O	1:E:269:MET:HE3	2.21	0.41
1:E:368:ARG:HG3	1:E:387:ILE:HD11	2.03	0.41
1:F:306:PHE:O	1:F:308:ARG:N	2.53	0.41
1:A:81:VAL:HB	1:A:107:ALA:HB3	2.02	0.41
1:A:141:PRO:O	1:A:142:MET:CG	2.63	0.41
1:A:147:ALA:O	1:A:150:PHE:HB3	2.21	0.41
1:A:230:VAL:O	1:A:231:SER:C	2.60	0.41
1:B:96:VAL:CG1	1:B:100:ARG:HE	2.34	0.41
1:B:136:ALA:O	1:B:137:ALA:C	2.59	0.41
1:B:311:GLN:O	1:B:314:ALA:HB3	2.21	0.41
1:C:196:HIS:O	1:C:199:ALA:CB	2.66	0.41
1:D:170:LEU:O	1:D:378:LEU:HD22	2.20	0.41
1:D:281:SER:O	1:D:282:VAL:C	2.59	0.41
1:D:319:VAL:HB	1:D:320:ALA:H	1.76	0.41
1:F:147:ALA:O	1:F:150:PHE:HB3	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD23	1:B:358:LEU:HB2	2.03	0.41
1:B:256:ASP:O	1:B:257:HIS:C	2.58	0.41
1:C:325:ASN:HD22	1:C:326:GLN:N	2.19	0.41
1:D:224:PHE:O	1:D:225:ARG:HD3	2.21	0.41
1:E:180:ILE:HG21	1:E:180:ILE:HD13	1.81	0.41
1:E:224:PHE:C	1:E:225:ARG:HD3	2.42	0.41
1:A:284:ALA:C	1:A:286:TYR:N	2.74	0.40
1:A:300:GLN:CB	1:A:349:ILE:HD11	2.51	0.40
1:A:306:PHE:O	1:A:308:ARG:N	2.55	0.40
1:D:96:VAL:O	1:D:97:LYS:C	2.59	0.40
1:D:163:GLY:O	1:D:393:GLY:HA2	2.21	0.40
1:D:368:ARG:HG3	1:D:387:ILE:HD11	2.02	0.40
1:E:267:GLN:O	1:E:270:SER:HB3	2.21	0.40
1:F:268:MET:C	1:F:270:SER:H	2.24	0.40
1:F:282:VAL:HG22	1:F:306:PHE:CE2	2.56	0.40
1:C:216:LEU:HB3	1:C:277:ILE:HG12	2.03	0.40
1:C:244:LEU:O	1:C:245:ASN:C	2.56	0.40
1:D:107:ALA:O	1:D:108:GLU:C	2.58	0.40
1:E:188:ARG:HA	2:E:505:SO4:O2	2.21	0.40
1:E:360:PHE:N	1:E:360:PHE:CD1	2.88	0.40
1:F:282:VAL:HG23	1:F:323:VAL:HG13	2.01	0.40
1:B:184:PHE:CD2	1:B:358:LEU:O	2.74	0.40
1:C:193:GLN:CG	1:C:387:ILE:HD13	2.41	0.40
1:F:170:LEU:HD21	1:F:372:VAL:HG23	2.04	0.40
1:A:119:LEU:HA	1:A:119:LEU:HD23	1.84	0.40
1:A:380:GLU:O	1:A:381:ALA:HB2	2.22	0.40
1:B:184:PHE:HZ	1:B:373:VAL:CG1	2.34	0.40
1:B:350:MET:C	1:B:352:HIS:N	2.72	0.40
1:C:268:MET:O	1:C:270:SER:N	2.54	0.40
1:D:308:ARG:O	1:D:309:ALA:C	2.58	0.40
1:F:373:VAL:O	1:F:374:ASP:O	2.39	0.40
1:F:388:TYR:CD1	1:F:388:TYR:N	2.88	0.40
1:A:192:SER:HB2	2:A:501:SO4:S	2.60	0.40
1:F:170:LEU:HD11	1:F:381:ALA:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:LYS:NZ	1:F:288:THR:OG1[2_545]	2.07	0.13

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/321 (90%)	206 (71%)	55 (19%)	28 (10%)	0	4
1	B	266/321 (83%)	187 (70%)	58 (22%)	21 (8%)	1	6
1	C	266/321 (83%)	189 (71%)	57 (21%)	20 (8%)	1	7
1	D	287/321 (89%)	195 (68%)	73 (25%)	19 (7%)	1	9
1	E	288/321 (90%)	200 (69%)	66 (23%)	22 (8%)	1	6
1	F	288/321 (90%)	206 (72%)	57 (20%)	25 (9%)	1	5
All	All	1684/1926 (87%)	1183 (70%)	366 (22%)	135 (8%)	1	6

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	MET
1	A	153	ARG
1	A	257	HIS
1	A	296	LEU
1	A	297	SER
1	A	319	VAL
1	A	351	ALA
1	A	376	PRO
1	B	227	VAL
1	B	297	SER
1	B	319	VAL
1	C	227	VAL
1	C	297	SER
1	C	319	VAL
1	D	151	HIS
1	D	241	ASP
1	D	284	ALA
1	D	288	THR
1	D	296	LEU
1	D	297	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	319	VAL
1	D	374	ASP
1	D	376	PRO
1	E	151	HIS
1	E	241	ASP
1	E	284	ALA
1	E	296	LEU
1	E	297	SER
1	E	319	VAL
1	E	376	PRO
1	F	227	VAL
1	F	257	HIS
1	F	296	LEU
1	F	319	VAL
1	F	351	ALA
1	F	374	ASP
1	F	376	PRO
1	A	151	HIS
1	A	227	VAL
1	A	241	ASP
1	A	255	ALA
1	A	350	MET
1	A	374	ASP
1	B	241	ASP
1	B	257	HIS
1	C	153	ARG
1	C	241	ASP
1	C	296	LEU
1	C	307	MET
1	C	356	THR
1	D	201	THR
1	D	227	VAL
1	D	240	PRO
1	D	257	HIS
1	D	313	LEU
1	E	201	THR
1	E	227	VAL
1	E	240	PRO
1	E	257	HIS
1	E	289	ASP
1	E	313	LEU
1	E	370	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	374	ASP
1	F	153	ARG
1	F	201	THR
1	F	241	ASP
1	F	297	SER
1	A	198	LEU
1	A	201	THR
1	A	269	MET
1	A	307	MET
1	B	127	ALA
1	B	264	ALA
1	B	307	MET
1	C	127	ALA
1	C	201	THR
1	C	245	ASN
1	C	257	HIS
1	C	258	GLN
1	C	264	ALA
1	C	269	MET
1	C	372	VAL
1	D	197	THR
1	D	198	LEU
1	E	237	GLY
1	E	255	ALA
1	F	117	ASP
1	F	141	PRO
1	F	198	LEU
1	F	264	ALA
1	F	269	MET
1	F	350	MET
1	A	197	THR
1	A	381	ALA
1	B	101	GLU
1	B	111	ALA
1	B	153	ARG
1	B	256	ASP
1	B	258	GLN
1	B	296	LEU
1	C	101	GLU
1	C	111	ALA
1	C	240	PRO
1	D	237	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	197	THR
1	E	379	PRO
1	F	197	THR
1	F	256	ASP
1	F	283	MET
1	F	349	ILE
1	A	84	GLU
1	A	117	ASP
1	A	240	PRO
1	A	256	ASP
1	A	370	CYS
1	B	201	THR
1	B	214	LYS
1	B	240	PRO
1	C	355	THR
1	D	307	MET
1	D	379	PRO
1	E	198	LEU
1	F	240	PRO
1	F	245	ASN
1	F	258	GLN
1	F	378	LEU
1	A	346	GLY
1	A	378	LEU
1	B	313	LEU
1	B	350	MET
1	B	372	VAL
1	E	305	LYS
1	A	237	GLY
1	B	237	GLY
1	E	378	LEU

### 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.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/260 (84%)	202 (93%)	15 (7%)	15	43
1	B	197/260 (76%)	186 (94%)	11 (6%)	21	52
1	C	199/260 (76%)	186 (94%)	13 (6%)	17	46
1	D	217/260 (84%)	200 (92%)	17 (8%)	12	38
1	E	217/260 (84%)	198 (91%)	19 (9%)	10	33
1	F	215/260 (83%)	200 (93%)	15 (7%)	15	43
All	All	1262/1560 (81%)	1172 (93%)	90 (7%)	14	42

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	MET
1	A	89	ASN
1	A	108	GLU
1	A	146	THR
1	A	207	ASP
1	A	231	SER
1	A	254	ASN
1	A	263	ASP
1	A	276	LEU
1	A	282	VAL
1	A	285	LEU
1	A	325	ASN
1	A	370	CYS
1	A	377	CYS
1	A	383	CYS
1	B	89	ASN
1	B	146	THR
1	B	161	THR
1	B	164	SER
1	B	225	ARG
1	B	242	ASP
1	B	271	GLU
1	B	276	LEU
1	B	280	ASP
1	B	353	SER
1	B	355	THR
1	C	89	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	141	PRO
1	C	146	THR
1	C	161	THR
1	C	242	ASP
1	C	276	LEU
1	C	280	ASP
1	C	282	VAL
1	C	283	MET
1	C	297	SER
1	C	302	HIS
1	C	354	SER
1	C	355	THR
1	D	89	ASN
1	D	102	SER
1	D	146	THR
1	D	164	SER
1	D	207	ASP
1	D	225	ARG
1	D	228	ARG
1	D	231	SER
1	D	276	LEU
1	D	280	ASP
1	D	288	THR
1	D	289	ASP
1	D	302	HIS
1	D	325	ASN
1	D	370	CYS
1	D	377	CYS
1	D	383	CYS
1	E	80	MET
1	E	89	ASN
1	E	102	SER
1	E	146	THR
1	E	164	SER
1	E	207	ASP
1	E	216	LEU
1	E	225	ARG
1	E	228	ARG
1	E	231	SER
1	E	276	LEU
1	E	280	ASP
1	E	285	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	325	ASN
1	E	326	GLN
1	E	370	CYS
1	E	376	PRO
1	E	377	CYS
1	E	383	CYS
1	F	80	MET
1	F	89	ASN
1	F	108	GLU
1	F	146	THR
1	F	164	SER
1	F	187	PHE
1	F	207	ASP
1	F	216	LEU
1	F	231	SER
1	F	254	ASN
1	F	276	LEU
1	F	281	SER
1	F	370	CYS
1	F	377	CYS
1	F	383	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	166	ASN
1	A	267	GLN
1	A	325	ASN
1	B	89	ASN
1	B	105	HIS
1	B	325	ASN
1	C	89	ASN
1	C	105	HIS
1	C	267	GLN
1	C	325	ASN
1	D	89	ASN
1	D	151	HIS
1	D	325	ASN
1	E	87	GLN
1	E	89	ASN
1	E	325	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	89	ASN
1	F	166	ASN
1	F	311	GLN
1	F	325	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	SO4	E	505	-	4,4,4	1.40	1 (25%)	6,6,6	1.65	1 (16%)
2	SO4	D	504	-	4,4,4	0.97	0	6,6,6	2.14	3 (50%)
2	SO4	C	503	-	4,4,4	0.58	0	6,6,6	1.81	2 (33%)
2	SO4	F	506	-	4,4,4	0.42	0	6,6,6	0.97	0
2	SO4	B	502	-	4,4,4	0.59	0	6,6,6	1.84	2 (33%)
2	SO4	A	501	-	4,4,4	0.97	0	6,6,6	1.24	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	505	SO4	O1-S	-2.45	1.32	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	SO4	O4-S-O3	3.34	123.31	109.06
2	D	504	SO4	O3-S-O2	3.31	126.57	109.31
2	B	502	SO4	O4-S-O1	3.00	124.97	109.31
2	D	504	SO4	O2-S-O1	-2.93	87.78	109.43
2	E	505	SO4	O4-S-O3	2.87	121.30	109.06
2	C	503	SO4	O4-S-O1	-2.69	95.29	109.31
2	B	502	SO4	O2-S-O1	-2.45	91.34	109.43
2	A	501	SO4	O3-S-O1	-2.08	98.45	109.31
2	D	504	SO4	O4-S-O2	-2.02	98.76	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	505	SO4	2	0
2	D	504	SO4	2	0
2	C	503	SO4	2	0
2	B	502	SO4	2	0
2	A	501	SO4	1	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	295/321 (91%)	-0.01	3 (1%) 82 82	6, 36, 69, 98	0
1	B	274/321 (85%)	0.22	12 (4%) 34 32	23, 64, 98, 128	0
1	C	274/321 (85%)	0.21	9 (3%) 46 43	22, 63, 99, 121	0
1	D	293/321 (91%)	0.04	6 (2%) 65 63	12, 51, 81, 112	0
1	E	294/321 (91%)	0.05	5 (1%) 70 67	15, 53, 82, 112	0
1	F	294/321 (91%)	-0.01	1 (0%) 94 94	5, 35, 72, 93	0
All	All	1724/1926 (89%)	0.08	36 (2%) 63 61	5, 49, 93, 128	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	346	GLY	5.8
1	C	286	TYR	4.7
1	C	373	VAL	4.3
1	B	90	GLY	3.9
1	B	124	ILE	3.7
1	E	387	ILE	3.7
1	B	91	ILE	3.3
1	B	373	VAL	3.2
1	A	328	VAL	3.1
1	C	91	ILE	2.9
1	E	140	VAL	2.8
1	B	280	ASP	2.6
1	C	280	ASP	2.6
1	B	286	TYR	2.6
1	C	250	ALA	2.5
1	D	139	LEU	2.4
1	D	387	ILE	2.4
1	C	124	ILE	2.4
1	E	83	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	252	ALA	2.4
1	C	119	LEU	2.4
1	B	357	ARG	2.3
1	C	283	MET	2.3
1	A	286	TYR	2.2
1	D	140	VAL	2.2
1	A	387	ILE	2.1
1	B	89	ASN	2.1
1	B	252	ALA	2.1
1	B	385	PHE	2.1
1	B	307	MET	2.1
1	D	86	LEU	2.1
1	D	208	ILE	2.1
1	E	282	VAL	2.1
1	F	387	ILE	2.1
1	D	385	PHE	2.0
1	E	385	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	502	5/5	0.92	0.13	55,58,62,69	0
2	SO4	C	503	5/5	0.92	0.13	49,52,62,65	0
2	SO4	D	504	5/5	0.96	0.14	33,36,42,43	0
2	SO4	E	505	5/5	0.97	0.16	32,35,35,39	0
2	SO4	A	501	5/5	0.98	0.14	37,40,47,48	0
2	SO4	F	506	5/5	0.98	0.12	36,41,44,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.