



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:19 AM GMT

PDB ID : 3OGM
Title : Structure of COI1-ASK1 in complex with coronatine and the JAZ1 degron
Authors : Sheard, L.B.; Tan, X.; Mao, H.; Withers, J.; Ben-Nissan, G.; Hinds, T.R.;
Hsu, F.; Sharon, M.; Browse, J.; He, S.Y.; Rizo, J.; Howe, G.A.; Zheng, N.
Deposited on : 2010-08-17
Resolution : 3.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

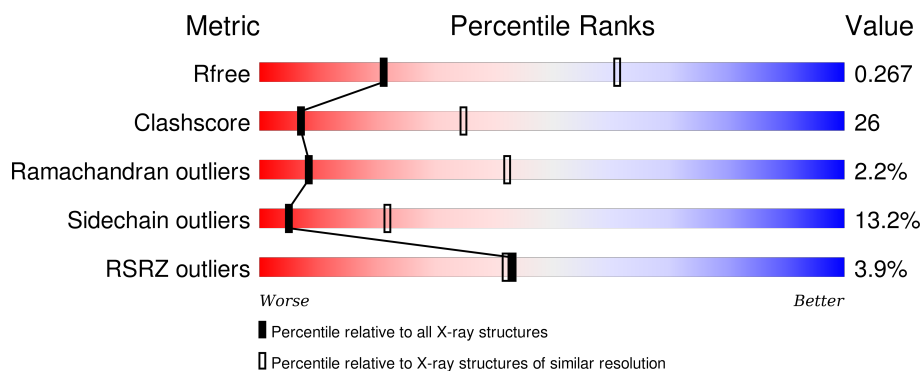
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)

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	160	<div> <div>4%</div> <div>49% 36% 6% 10%</div> </div>
1	C	160	<div> <div>6%</div> <div>52% 33% 6% 10%</div> </div>
1	E	160	<div> <div>4%</div> <div>51% 34% 5% 10%</div> </div>
1	G	160	<div> <div>3%</div> <div>48% 38% • • 10%</div> </div>
1	I	160	<div> <div>5%</div> <div>46% 39% 6% 10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	160	
1	M	160	
1	O	160	
2	B	592	
2	D	592	
2	F	592	
2	H	592	
2	J	592	
2	L	592	
2	N	592	
2	P	592	
3	Q	21	
3	R	21	
3	S	21	
3	U	21	
3	V	21	
3	W	21	
3	X	21	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OGK	H	4100	X	-	X	-
5	PO4	B	1101	-	X	-	-
5	PO4	B	1103	-	X	-	X
5	PO4	B	1104	-	X	-	X
5	PO4	D	1101	-	X	-	X
5	PO4	D	1102	-	X	-	X
5	PO4	D	1103	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	F	1101	-	X	-	X
5	PO4	F	1102	-	X	-	X
5	PO4	H	1101	-	X	-	-
5	PO4	H	1103	-	X	-	-
5	PO4	H	1104	-	-	-	X
5	PO4	J	1101	-	-	-	X
5	PO4	J	1102	-	-	-	X
5	PO4	J	1104	-	-	-	X
5	PO4	L	1101	-	X	-	X
5	PO4	L	1102	-	X	-	X
5	PO4	L	1103	-	X	-	X
5	PO4	L	1104	-	-	-	X
5	PO4	N	1102	-	-	-	X
5	PO4	N	1103	-	-	-	X
5	PO4	N	1104	-	-	-	X
5	PO4	P	1101	-	-	-	X
5	PO4	P	1103	-	-	X	-
5	PO4	P	1104	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46877 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 SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	C	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	E	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	G	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	I	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	K	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	M	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			
1	O	144	Total	C	N	O	S	0	0	0
			1146	720	185	235	6			

- Molecule 2 is a protein called Coronatine-insensitive protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	D	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	F	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	H	562	Total	C	N	O	S	0	0	0
			4486	2840	779	831	36			
2	J	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	L	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

Continued on next page...

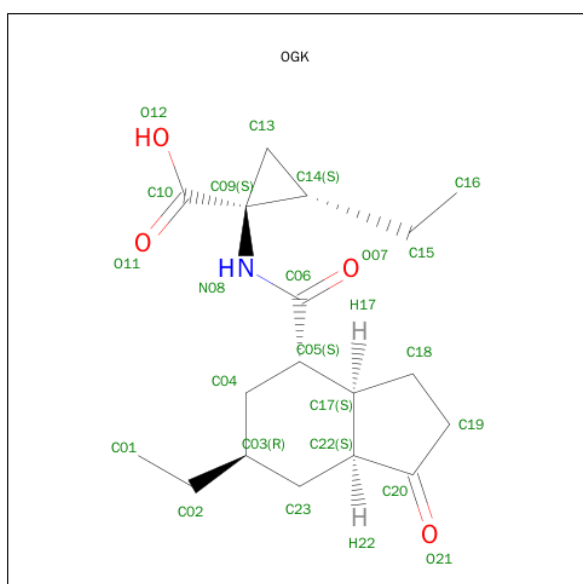
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			
2	P	568	Total	C	N	O	S	0	0	0
			4541	2873	790	842	36			

- Molecule 3 is a protein called JAZ1 degron peptide.

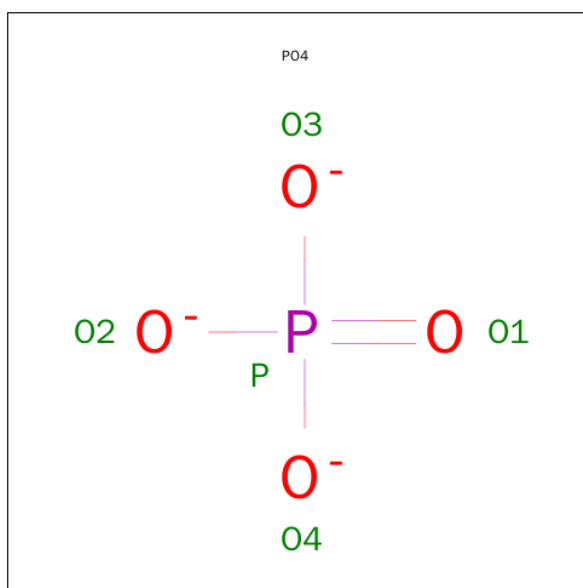
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	R	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	S	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	U	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	V	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	W	18	Total	C	N	O	0	0	0
			156	99	34	23			
3	X	18	Total	C	N	O	0	0	0
			156	99	34	23			

- Molecule 4 is (1S,2S)-2-ETHYL-1-({[(3AS,4S,6R,7AS)-6-ETHYL-1-OXOOCTAHYDR O-1H-INDEN-4-YL]CARBONYL}AMINO)CYCLOPROPANECARBOXYLIC ACID (three-letter code: OGK) (formula: C₁₈H₂₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			23	18	1	4		
4	D	1	Total	C	N	O	0	0
			23	18	1	4		
4	F	1	Total	C	N	O	0	0
			23	18	1	4		
4	H	1	Total	C	N	O	0	0
			23	18	1	4		
4	J	1	Total	C	N	O	0	0
			23	18	1	4		
4	L	1	Total	C	N	O	0	0
			23	18	1	4		
4	N	1	Total	C	N	O	0	0
			23	18	1	4		
4	P	1	Total	C	N	O	0	0
			23	18	1	4		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	L	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

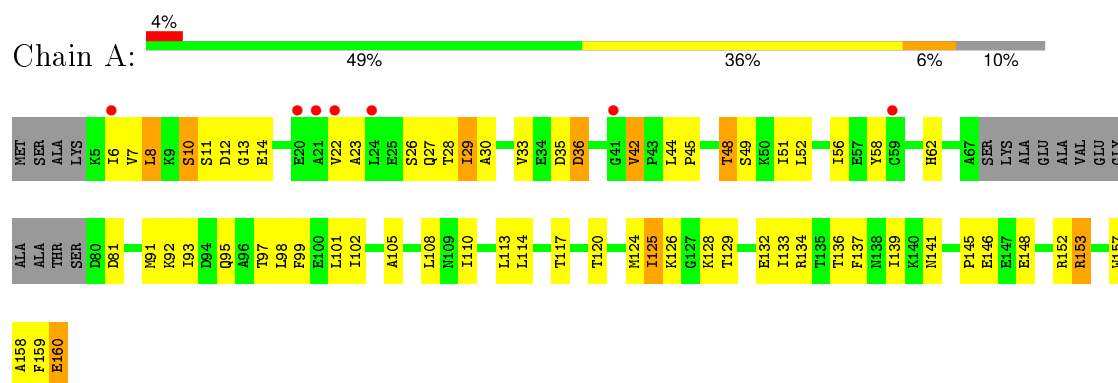
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	N	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		
5	P	1	Total	O	P	0	0
			5	4	1		

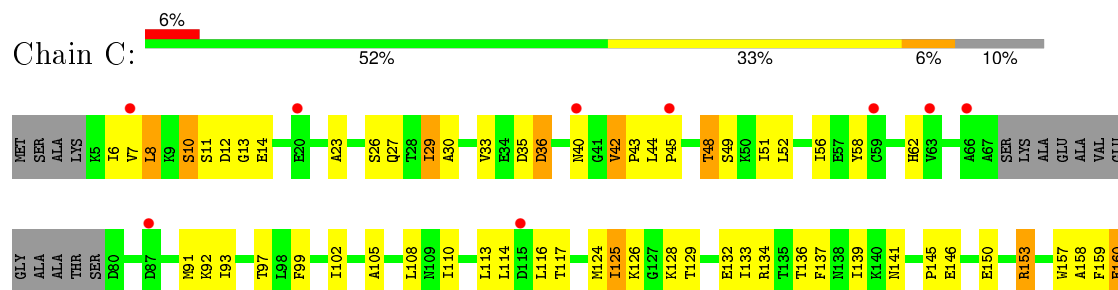
3 Residue-property plots [i](#)

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.

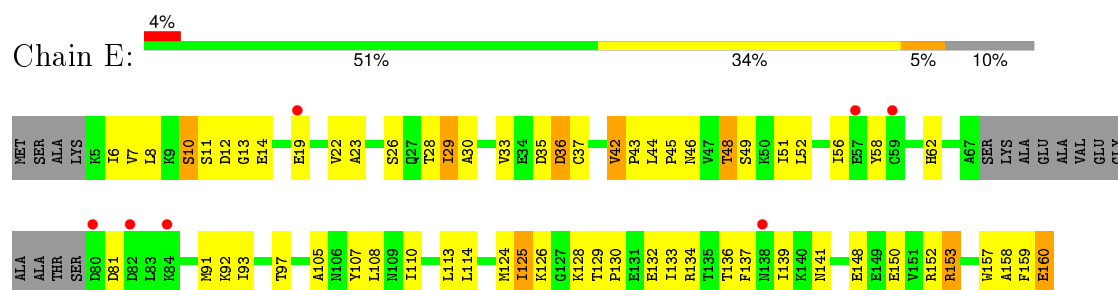
• Molecule 1: SKP1-like protein 1A



• Molecule 1: SKP1-like protein 1A

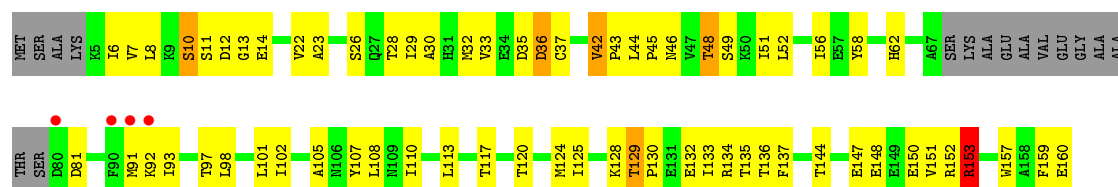


• Molecule 1: SKP1-like protein 1A

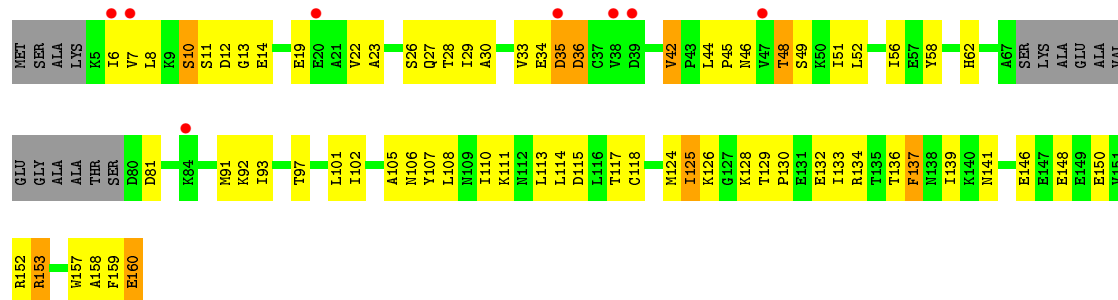


• Molecule 1: SKP1-like protein 1A

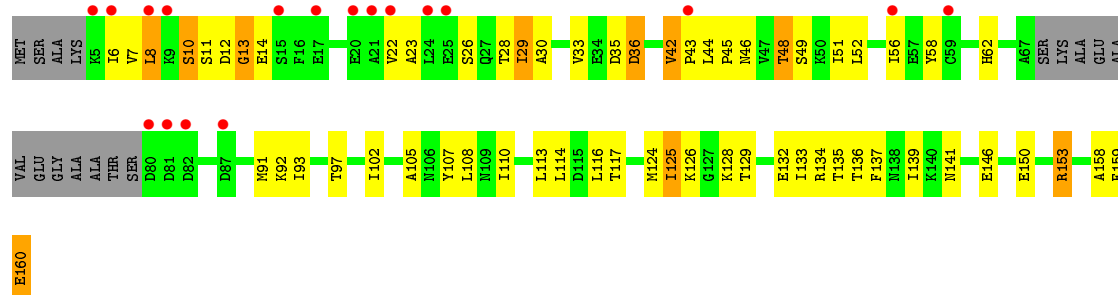




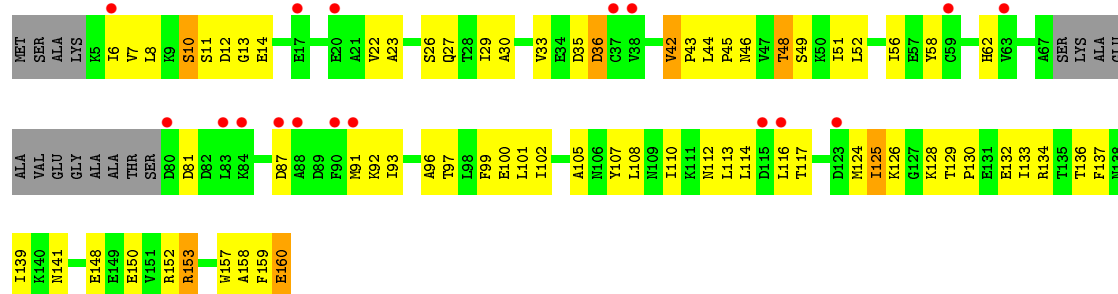
• Molecule 1: SKP1-like protein 1A



• Molecule 1: SKP1-like protein 1A

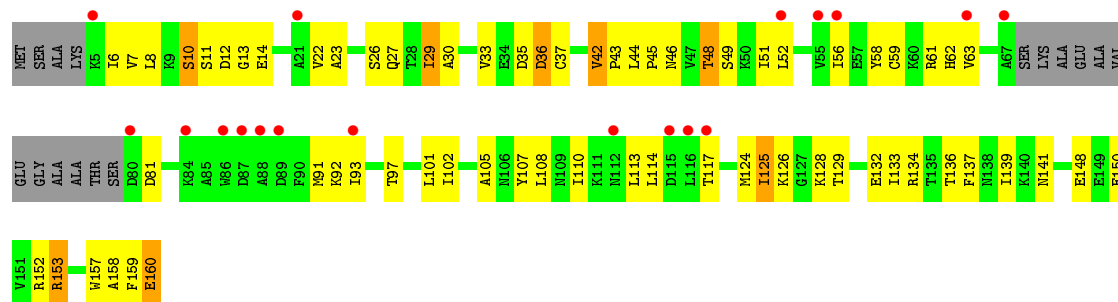


• Molecule 1: SKP1-like protein 1A

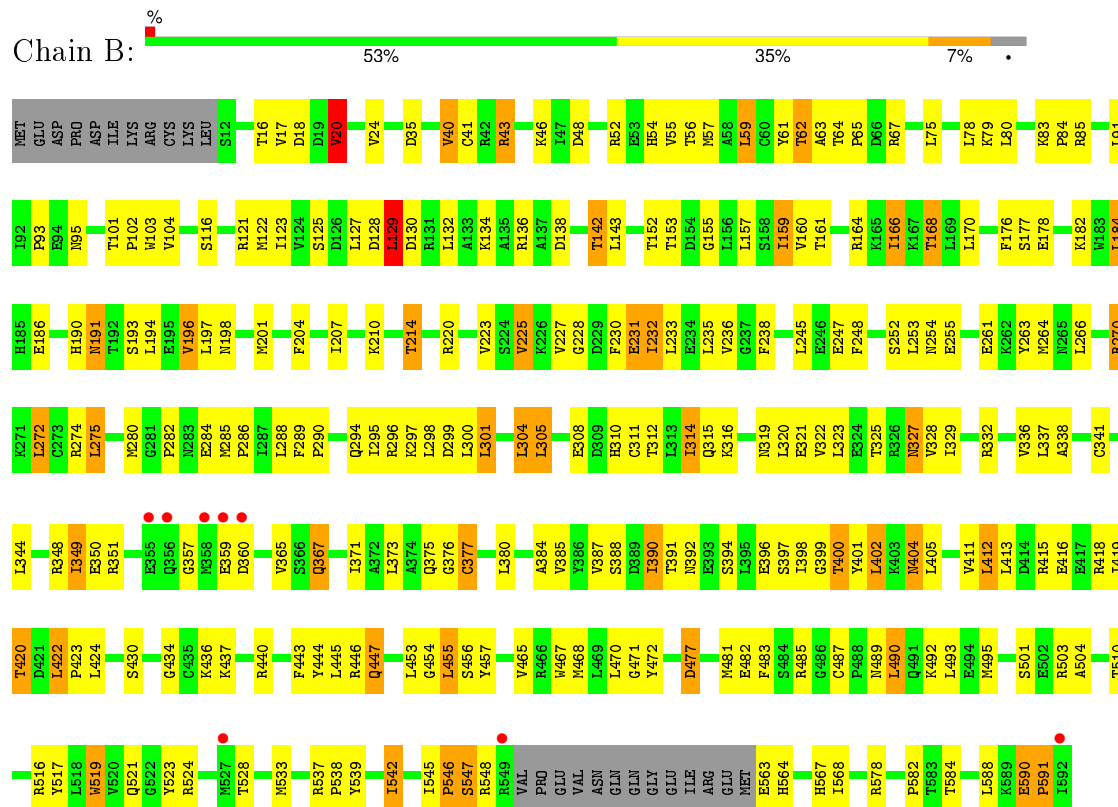


• Molecule 1: SKP1-like protein 1A

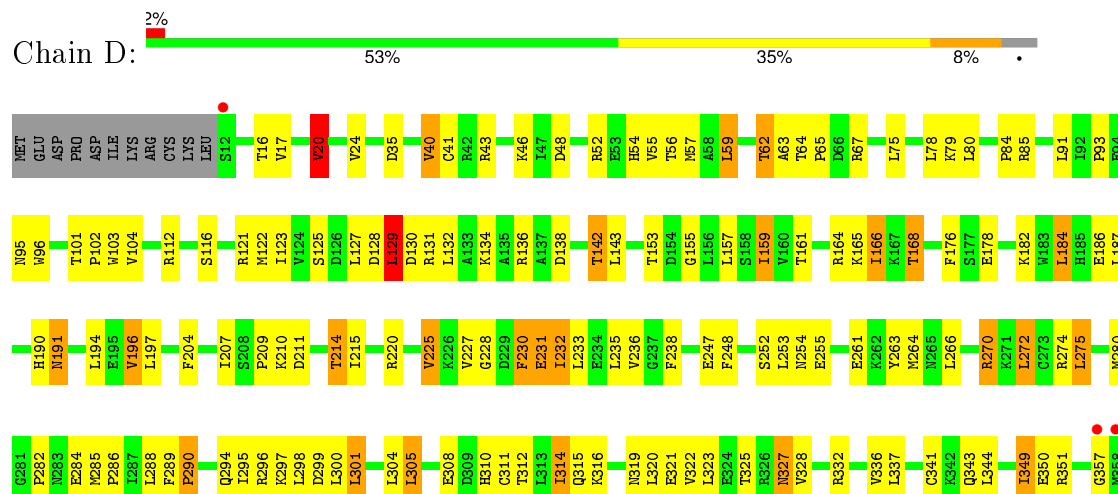


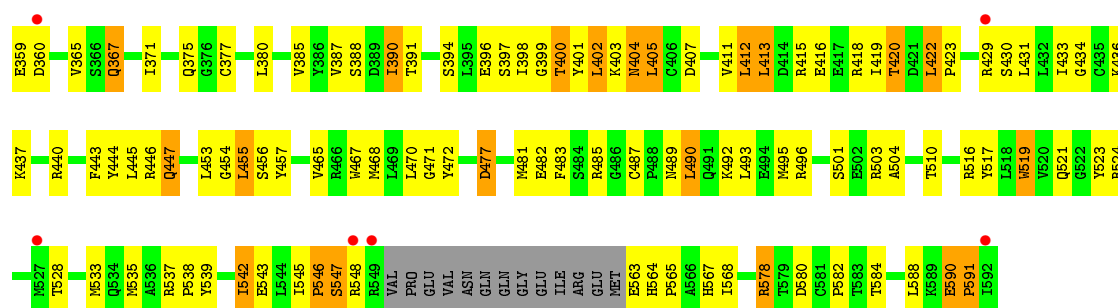


• Molecule 2: Coronatine-insensitive protein 1



• Molecule 2: Coronatine-insensitive protein 1

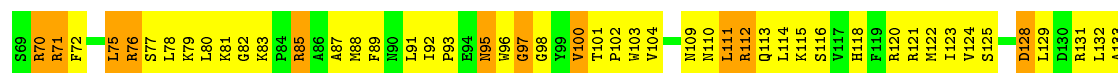


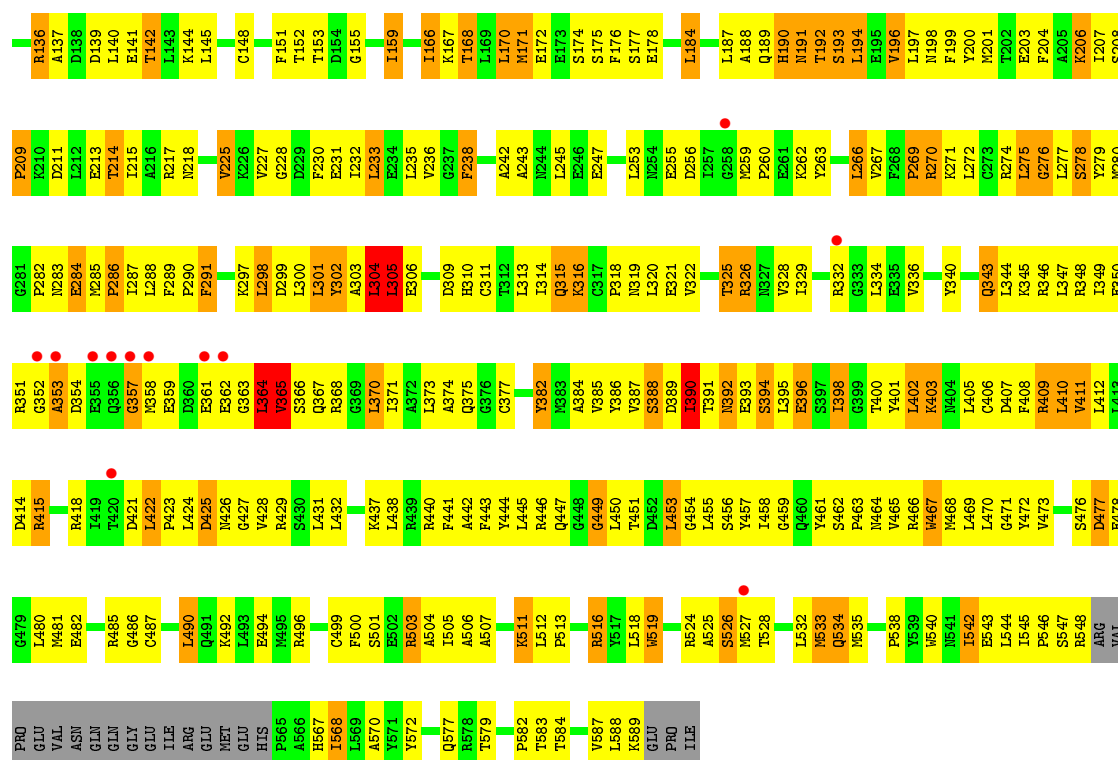


• Molecule 2: Coronatine-insensitive protein 1

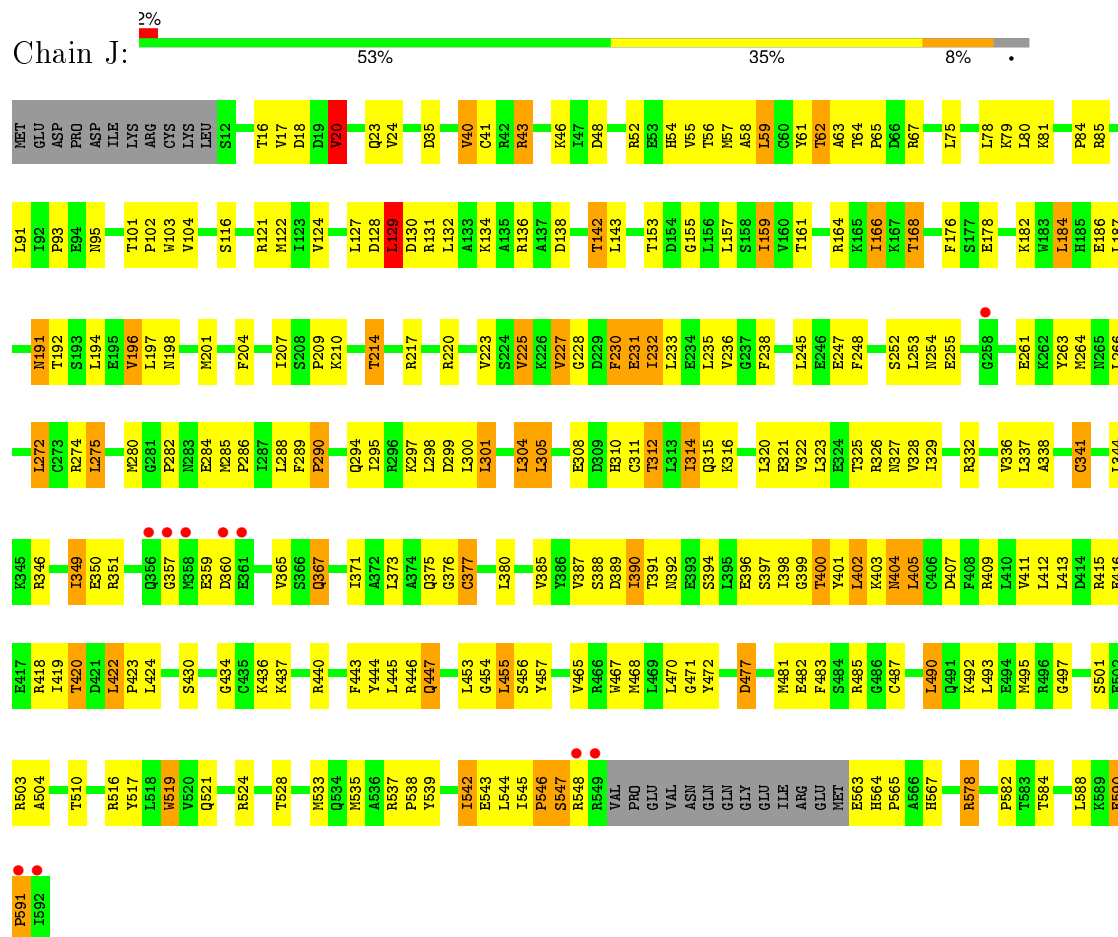


• Molecule 2: Coronatine-insensitive protein 1

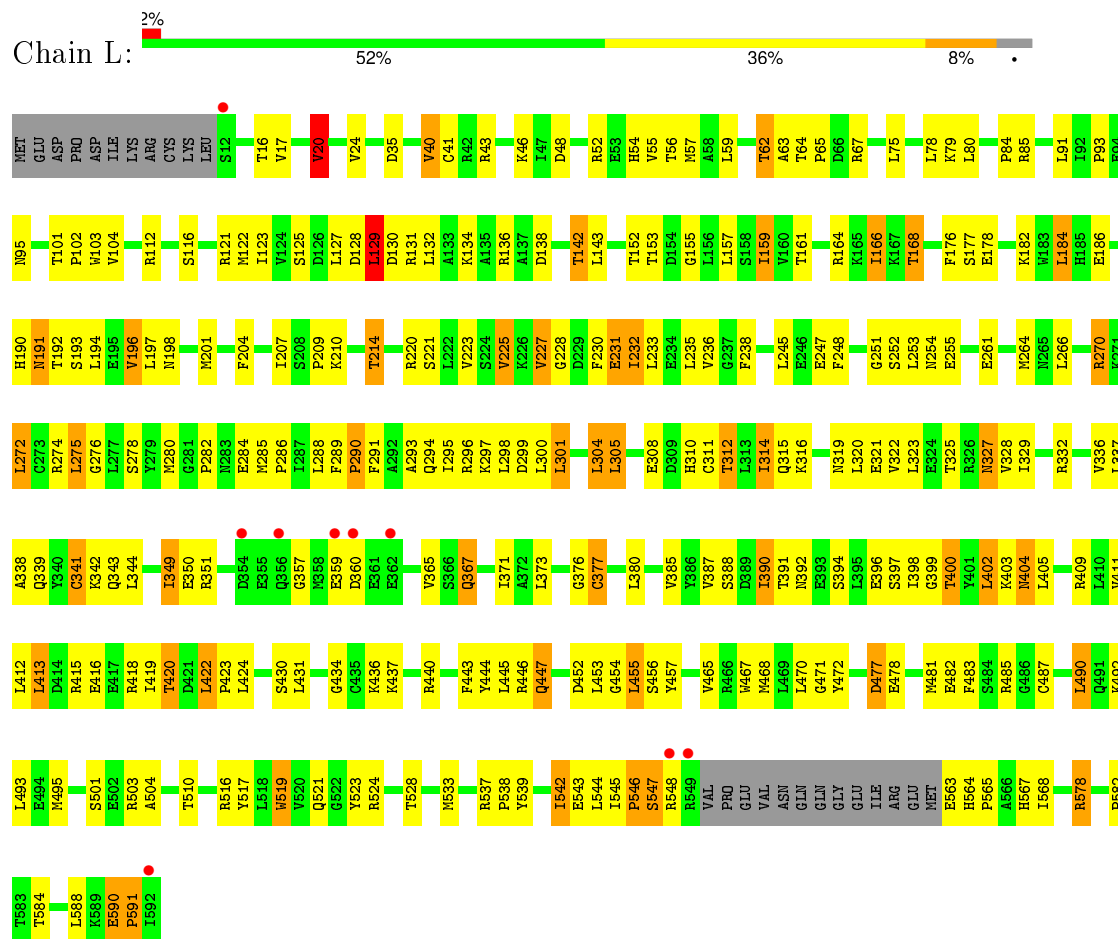




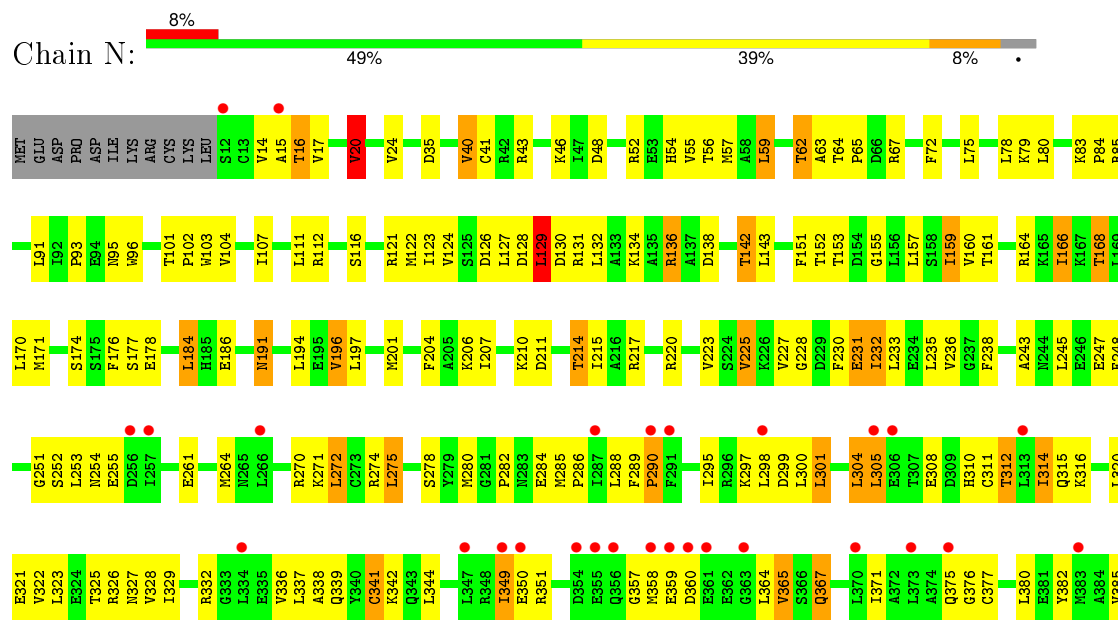
• Molecule 2: Coronatine-insensitive protein 1

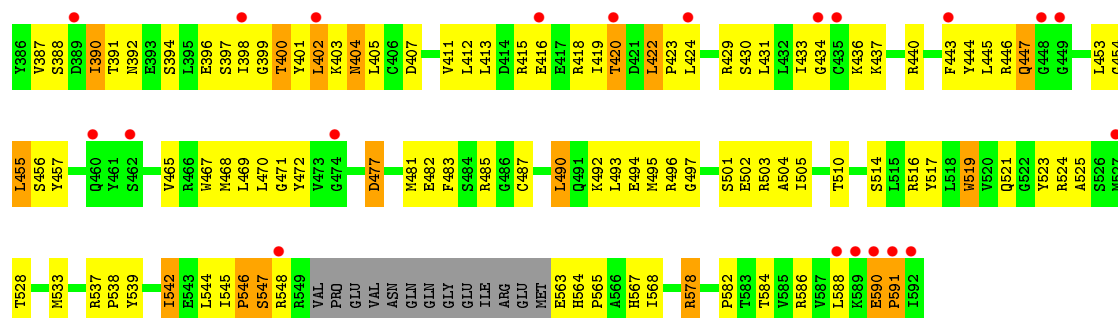


• Molecule 2: Coronatine-insensitive protein 1

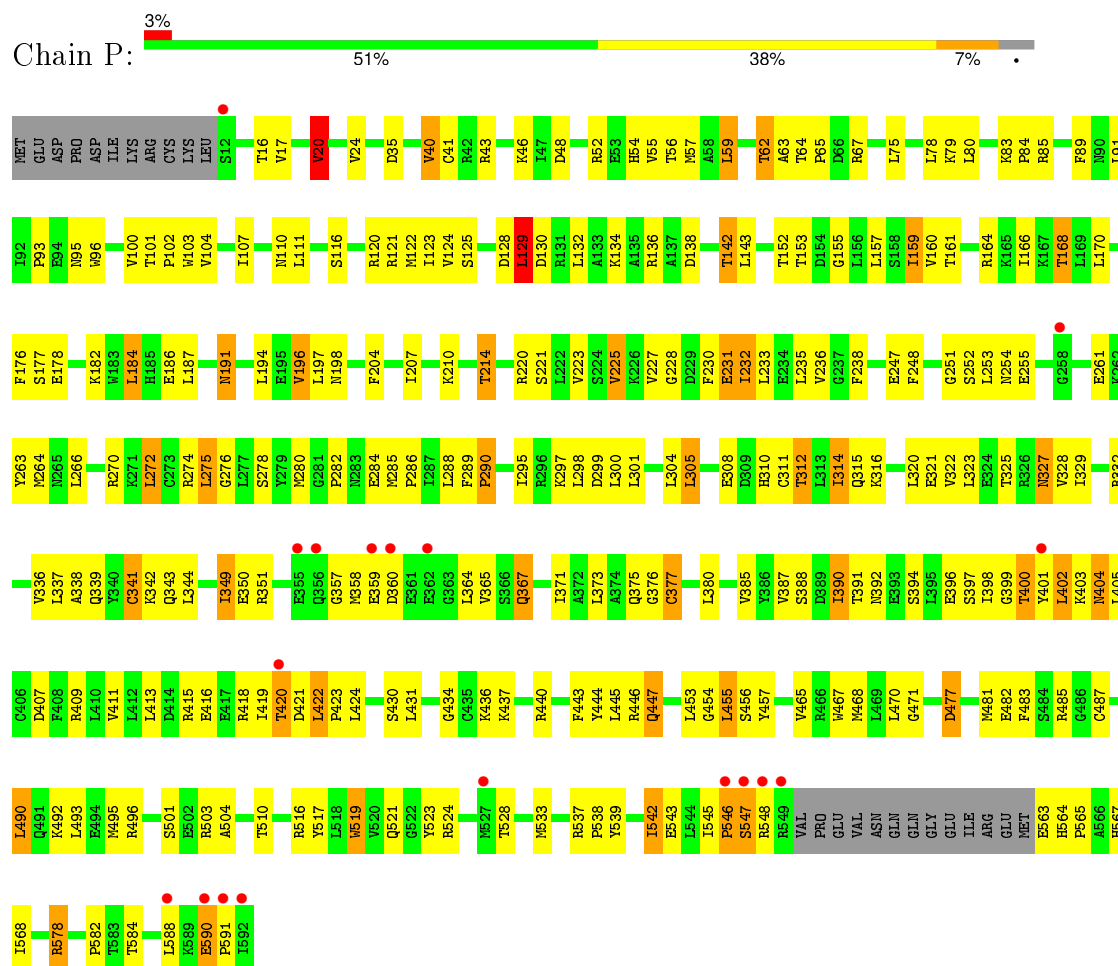


• Molecule 2: Coronatine-insensitive protein 1

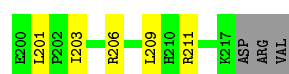




• Molecule 2: Coronatine-insensitive protein 1



• Molecule 3: JAZ1 degron peptide



• Molecule 3: JAZ1 degron peptide





- Molecule 3: JAZ1 degron peptide

Chain S: 



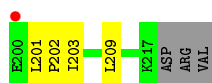
- Molecule 3: JAZ1 degron peptide

Chain U: 



- Molecule 3: JAZ1 degron peptide

Chain V: 



- Molecule 3: JAZ1 degron peptide

Chain W: 



- Molecule 3: JAZ1 degron peptide

Chain X: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.17Å 220.76Å 149.54Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	49.94 – 3.34 49.94 – 3.34	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.94-3.34) 85.8 (49.94-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.226 , 0.270 0.224 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (2.12%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 103078 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46877	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, OGK

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	0.44	0/1162	0.56	0/1571
1	C	0.45	0/1162	0.58	0/1571
1	E	0.45	0/1162	0.59	0/1571
1	G	0.52	0/1162	0.63	0/1571
1	I	0.44	0/1162	0.57	0/1571
1	K	0.43	0/1162	0.57	0/1571
1	M	0.50	0/1162	0.59	0/1571
1	O	0.45	0/1162	0.56	0/1571
2	B	0.49	0/4623	0.63	1/6238 (0.0%)
2	D	0.50	0/4623	0.64	1/6238 (0.0%)
2	F	0.46	0/4623	0.64	1/6238 (0.0%)
2	H	0.58	0/4566	0.83	2/6161 (0.0%)
2	J	0.49	0/4623	0.64	1/6238 (0.0%)
2	L	0.45	0/4623	0.63	1/6238 (0.0%)
2	N	0.58	0/4623	0.67	1/6238 (0.0%)
2	P	0.47	0/4623	0.63	1/6238 (0.0%)
3	Q	0.42	0/158	0.53	0/208
3	R	0.39	0/158	0.52	0/208
3	S	0.38	0/158	0.55	0/208
3	U	0.46	0/158	0.55	0/208
3	V	0.41	0/158	0.54	0/208
3	W	0.43	0/158	0.57	0/208
3	X	0.40	0/158	0.53	0/208
All	All	0.50	0/47329	0.65	9/63851 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	LEU	CA-CB-CG	7.63	132.84	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	129	LEU	CA-CB-CG	7.51	132.58	115.30
2	L	129	LEU	CA-CB-CG	7.50	132.54	115.30
2	B	129	LEU	CA-CB-CG	7.40	132.32	115.30
2	N	129	LEU	CA-CB-CG	7.21	131.87	115.30
2	D	129	LEU	CA-CB-CG	7.03	131.47	115.30
2	P	129	LEU	CA-CB-CG	6.39	130.00	115.30
2	H	304	LEU	CA-CB-CG	-5.41	102.86	115.30
2	H	390	ILE	CB-CA-C	-5.06	101.47	111.60

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	1146	0	1117	63	0
1	C	1146	0	1117	57	0
1	E	1146	0	1117	69	0
1	G	1146	0	1117	65	0
1	I	1146	0	1117	69	0
1	K	1146	0	1117	55	0
1	M	1146	0	1117	86	0
1	O	1146	0	1117	69	0
2	B	4541	0	4583	222	0
2	D	4541	0	4583	225	0
2	F	4541	0	4583	219	0
2	H	4486	0	4534	431	0
2	J	4541	0	4583	226	0
2	L	4541	0	4583	233	0
2	N	4541	0	4583	271	0
2	P	4541	0	4583	224	0
3	Q	156	0	171	7	0
3	R	156	0	171	5	0
3	S	156	0	171	5	0
3	U	156	0	171	6	0
3	V	156	0	171	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	156	0	171	7	0
3	X	156	0	171	5	0
4	B	23	0	27	7	0
4	D	23	0	27	7	0
4	F	23	0	27	7	0
4	H	23	0	27	16	0
4	J	23	0	27	7	0
4	L	23	0	27	7	0
4	N	23	0	27	6	0
4	P	23	0	27	8	0
5	B	20	0	0	3	0
5	D	20	0	0	2	0
5	F	20	0	0	2	0
5	H	20	0	0	3	0
5	J	20	0	0	2	0
5	L	20	0	0	2	0
5	N	20	0	0	3	0
5	P	20	0	0	3	0
All	All	46877	0	46964	2465	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 26.

All (2465) 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)
2:H:116:SER:HB2	2:H:142:THR:HG23	1.35	1.09
2:P:168:THR:HB	2:P:196:VAL:HG13	1.35	1.08
2:D:168:THR:HB	2:D:196:VAL:HG13	1.35	1.08
2:L:168:THR:HB	2:L:196:VAL:HG13	1.35	1.06
2:J:168:THR:HB	2:J:196:VAL:HG13	1.35	1.06
2:L:542:ILE:HD11	2:L:588:LEU:HD12	1.35	1.06
2:N:168:THR:HB	2:N:196:VAL:HG13	1.38	1.05
2:B:168:THR:HB	2:B:196:VAL:HG13	1.37	1.05
2:N:142:THR:HB	2:N:168:THR:HG23	1.38	1.05
1:M:93:ILE:HD12	1:M:97:THR:HG22	1.40	1.04
2:H:78:LEU:HD12	2:H:79:LYS:H	1.22	1.04
2:H:311:CYS:HB3	2:H:336:VAL:HG21	1.34	1.04
2:F:142:THR:HB	2:F:168:THR:HG23	1.40	1.04
2:J:542:ILE:HD11	2:J:588:LEU:HD12	1.40	1.04
2:D:542:ILE:HD11	2:D:588:LEU:HD12	1.40	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD12	1:A:97:THR:HG22	1.40	1.02
2:F:168:THR:HB	2:F:196:VAL:HG13	1.39	1.01
2:F:542:ILE:HD11	2:F:588:LEU:HD12	1.43	1.01
2:H:310:HIS:O	2:H:314:ILE:HG12	1.61	1.00
2:P:142:THR:HB	2:P:168:THR:HG23	1.43	1.00
2:N:542:ILE:HD11	2:N:588:LEU:HD12	1.40	0.99
2:P:542:ILE:HD11	2:P:588:LEU:HD12	1.45	0.98
2:F:93:PRO:HA	2:F:548:ARG:HB2	1.44	0.98
2:L:142:THR:HB	2:L:168:THR:HG23	1.46	0.98
2:P:357:GLY:HA2	2:P:415:ARG:HH22	1.29	0.97
2:L:93:PRO:HA	2:L:548:ARG:HB2	1.42	0.97
2:P:93:PRO:HA	2:P:548:ARG:HB2	1.44	0.97
1:M:159:PHE:O	1:M:160:GLU:HB2	1.63	0.96
2:F:357:GLY:HA2	2:F:415:ARG:HH22	1.30	0.96
2:H:392:ASN:O	2:H:396:GLU:HG2	1.66	0.96
2:B:357:GLY:HA2	2:B:415:ARG:HH22	1.31	0.96
1:K:93:ILE:HD12	1:K:97:THR:HG22	1.45	0.95
1:O:93:ILE:HD12	1:O:97:THR:HG22	1.49	0.95
2:H:152:THR:HG22	2:H:177:SER:HB2	1.47	0.95
2:D:93:PRO:HA	2:D:548:ARG:HB2	1.48	0.95
2:B:93:PRO:HA	2:B:548:ARG:HB2	1.48	0.94
2:J:93:PRO:HA	2:J:548:ARG:HB2	1.48	0.94
2:L:357:GLY:HA2	2:L:415:ARG:HH22	1.29	0.94
2:N:93:PRO:HA	2:N:548:ARG:HB2	1.50	0.94
1:K:159:PHE:O	1:K:160:GLU:HB2	1.66	0.94
2:J:357:GLY:HA2	2:J:415:ARG:HH22	1.30	0.94
1:E:93:ILE:HD12	1:E:97:THR:HG22	1.46	0.94
2:J:142:THR:HB	2:J:168:THR:HG23	1.49	0.93
2:H:95:ASN:H	2:H:95:ASN:HD22	1.09	0.93
2:B:142:THR:HB	2:B:168:THR:HG23	1.51	0.93
1:C:93:ILE:HD12	1:C:97:THR:HG22	1.49	0.93
1:I:93:ILE:HD12	1:I:97:THR:HG22	1.47	0.93
2:B:542:ILE:HD11	2:B:588:LEU:HD12	1.50	0.93
1:A:159:PHE:O	1:A:160:GLU:HB2	1.69	0.93
1:E:159:PHE:O	1:E:160:GLU:HB2	1.67	0.92
1:O:159:PHE:O	1:O:160:GLU:HB2	1.67	0.92
2:D:357:GLY:HA2	2:D:415:ARG:HH22	1.32	0.92
1:G:160:GLU:HG3	2:H:52:ARG:HH21	1.35	0.92
2:N:357:GLY:HA2	2:N:415:ARG:HH22	1.32	0.91
1:I:159:PHE:O	1:I:160:GLU:HB2	1.67	0.91
1:G:93:ILE:HD12	1:G:97:THR:HG22	1.52	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:286:PRO:HA	2:H:289:PHE:CE2	2.06	0.91
2:H:415:ARG:HH12	2:H:472:TYR:HE1	1.08	0.91
1:C:159:PHE:O	1:C:160:GLU:HB2	1.69	0.90
2:J:590:GLU:HB3	2:J:591:PRO:HD2	1.54	0.90
2:B:444:TYR:HA	2:B:471:GLY:HA3	1.54	0.90
2:B:210:LYS:O	2:B:214:THR:HG22	1.72	0.90
2:D:444:TYR:HA	2:D:471:GLY:HA3	1.53	0.89
2:F:590:GLU:HB3	2:F:591:PRO:HD2	1.54	0.89
2:L:590:GLU:HB3	2:L:591:PRO:HD2	1.54	0.89
2:D:590:GLU:HB3	2:D:591:PRO:HD2	1.55	0.89
2:J:419:ILE:HD13	2:J:446:ARG:HH12	1.38	0.88
2:N:444:TYR:HA	2:N:471:GLY:HA3	1.55	0.88
2:H:322:VAL:HG22	2:H:346:ARG:HB2	1.54	0.88
1:E:107:TYR:OH	2:L:294:GLN:NE2	2.07	0.88
2:P:590:GLU:HB3	2:P:591:PRO:HD2	1.53	0.88
2:N:590:GLU:HB3	2:N:591:PRO:HD2	1.54	0.87
2:B:590:GLU:HB3	2:B:591:PRO:HD2	1.54	0.87
2:F:444:TYR:HA	2:F:471:GLY:HA3	1.55	0.87
2:J:367:GLN:HB3	2:J:391:THR:HG22	1.58	0.86
2:L:444:TYR:HA	2:L:471:GLY:HA3	1.57	0.86
1:E:105:ALA:HB3	1:E:114:LEU:HD13	1.56	0.86
1:K:108:LEU:HD12	1:K:110:ILE:HD11	1.58	0.86
2:B:419:ILE:HD13	2:B:446:ARG:HH12	1.40	0.86
2:H:365:VAL:HG11	2:H:387:VAL:HG22	1.55	0.85
2:H:519:TRP:NE1	4:H:4100:OGK:H01	1.90	0.85
1:M:125:ILE:HG23	1:M:133:ILE:HD12	1.58	0.85
2:N:367:GLN:HB3	2:N:391:THR:HG22	1.57	0.85
2:J:444:TYR:HA	2:J:471:GLY:HA3	1.56	0.85
2:J:210:LYS:O	2:J:214:THR:HG22	1.77	0.85
2:L:349:ILE:HG13	2:L:385:VAL:HG22	1.57	0.85
2:P:286:PRO:HA	2:P:289:PHE:CE2	2.12	0.85
1:E:43:PRO:HG2	2:L:319:ASN:ND2	1.92	0.85
2:H:152:THR:CG2	2:H:177:SER:HB2	2.07	0.85
1:M:102:ILE:HD12	2:N:20:VAL:HG21	1.58	0.84
2:H:40:VAL:O	2:H:41:CYS:HB3	1.78	0.84
2:H:285:MET:HG2	2:H:286:PRO:HD3	1.57	0.84
2:H:415:ARG:NH1	2:H:472:TYR:CE1	2.46	0.84
2:H:440:ARG:HB3	2:H:467:TRP:HD1	1.43	0.84
1:G:153:ARG:HG3	1:G:157:TRP:CZ3	2.13	0.84
2:H:95:ASN:ND2	2:H:95:ASN:H	1.75	0.83
2:D:142:THR:HB	2:D:168:THR:HG23	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:SER:HB2	2:B:142:THR:HG23	1.59	0.83
2:H:199:PHE:CZ	2:H:227:VAL:HG23	2.13	0.83
1:I:125:ILE:HG23	1:I:133:ILE:HD12	1.58	0.83
2:N:328:VAL:HG22	2:N:359:GLU:HB2	1.61	0.82
2:D:210:LYS:O	2:D:214:THR:HG22	1.77	0.82
2:L:210:LYS:O	2:L:214:THR:HG22	1.80	0.82
2:F:210:LYS:O	2:F:214:THR:HG22	1.79	0.82
2:F:367:GLN:HB3	2:F:391:THR:HG22	1.61	0.82
2:L:367:GLN:HB3	2:L:391:THR:HG22	1.60	0.82
2:P:444:TYR:HA	2:P:471:GLY:HA3	1.61	0.82
2:D:116:SER:HB2	2:D:142:THR:HG23	1.62	0.82
1:I:108:LEU:HD12	1:I:110:ILE:HD11	1.62	0.81
1:M:108:LEU:HD12	1:M:110:ILE:HD11	1.62	0.81
2:H:387:VAL:HG11	2:H:390:ILE:HD13	1.60	0.81
1:A:108:LEU:HD12	1:A:110:ILE:HD11	1.61	0.81
2:D:367:GLN:HB3	2:D:391:THR:HG22	1.60	0.81
2:P:419:ILE:HD13	2:P:446:ARG:HH12	1.44	0.81
2:H:256:ASP:OD2	2:H:259:MET:HG2	1.80	0.81
2:J:286:PRO:HA	2:J:289:PHE:CE2	2.16	0.81
2:N:419:ILE:HD13	2:N:446:ARG:HH12	1.44	0.81
2:H:253:LEU:HD11	2:H:277:LEU:HD13	1.62	0.81
2:N:116:SER:HB2	2:N:142:THR:HG23	1.60	0.81
1:M:102:ILE:HG21	2:N:20:VAL:HG22	1.62	0.81
2:J:164:ARG:HE	2:N:112:ARG:CG	1.94	0.81
4:N:7100:OGK:H18A	4:N:7100:OGK:HN08	1.45	0.81
2:P:328:VAL:HG22	2:P:359:GLU:HB2	1.62	0.81
2:N:210:LYS:O	2:N:214:THR:HG22	1.81	0.80
2:D:419:ILE:HD13	2:D:446:ARG:HH12	1.44	0.80
2:P:210:LYS:O	2:P:214:THR:HG22	1.79	0.80
2:H:286:PRO:HA	2:H:289:PHE:CD2	2.15	0.80
2:L:286:PRO:HA	2:L:289:PHE:CE2	2.15	0.80
2:P:367:GLN:HB3	2:P:391:THR:HG22	1.63	0.80
2:H:361:GLU:HA	2:H:388:SER:OG	1.81	0.80
2:B:328:VAL:HG22	2:B:359:GLU:HB2	1.64	0.80
2:F:419:ILE:HD13	2:F:446:ARG:HH12	1.47	0.79
2:N:349:ILE:HG13	2:N:385:VAL:HG22	1.62	0.79
1:O:125:ILE:HG23	1:O:133:ILE:HD12	1.63	0.79
2:H:441:PHE:O	2:H:468:MET:HA	1.82	0.79
1:A:125:ILE:HG23	1:A:133:ILE:HD12	1.65	0.79
2:L:289:PHE:CD1	2:L:316:LYS:HD2	2.18	0.79
2:D:328:VAL:HG22	2:D:359:GLU:HB2	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:328:VAL:HG22	2:F:359:GLU:HB2	1.63	0.79
2:F:112:ARG:HG2	2:L:164:ARG:HD2	1.65	0.79
2:H:364:LEU:HD13	2:H:388:SER:OG	1.81	0.79
2:B:367:GLN:HB3	2:B:391:THR:HG22	1.63	0.79
2:F:116:SER:HB2	2:F:142:THR:HG23	1.65	0.78
4:B:1100:OGK:HN08	4:B:1100:OGK:H18A	1.48	0.78
2:B:286:PRO:HA	2:B:289:PHE:CE2	2.18	0.78
2:P:116:SER:HB2	2:P:142:THR:HG23	1.65	0.78
2:B:289:PHE:CD1	2:B:316:LYS:HD2	2.18	0.78
2:L:161:THR:HG22	2:L:186:GLU:HG2	1.65	0.78
2:J:328:VAL:HG22	2:J:359:GLU:HB2	1.66	0.78
2:J:349:ILE:HG13	2:J:385:VAL:HG22	1.64	0.78
2:H:283:ASN:O	2:H:286:PRO:HD2	1.83	0.78
1:M:96:ALA:HB1	2:N:14:VAL:HG12	1.65	0.78
2:L:419:ILE:HD13	2:L:446:ARG:HH12	1.49	0.78
2:H:411:VAL:HG13	2:H:444:TYR:HB3	1.66	0.77
2:D:349:ILE:HG13	2:D:385:VAL:HG22	1.63	0.77
2:L:116:SER:HB2	2:L:142:THR:HG23	1.64	0.77
2:H:519:TRP:HE1	4:H:4100:OGK:H01	1.46	0.77
2:D:289:PHE:CD1	2:D:316:LYS:HD2	2.19	0.77
2:F:286:PRO:HA	2:F:289:PHE:CE2	2.19	0.77
2:H:533:MET:CE	2:H:588:LEU:HD13	2.14	0.77
2:H:387:VAL:CG1	2:H:390:ILE:HD13	2.14	0.77
1:M:102:ILE:HG21	2:N:20:VAL:CG2	2.14	0.77
4:H:4100:OGK:H18A	4:H:4100:OGK:HN08	1.50	0.77
4:P:8100:OGK:HN08	4:P:8100:OGK:H18A	1.49	0.77
1:K:125:ILE:HG23	1:K:133:ILE:HD12	1.67	0.77
2:H:459:GLY:O	2:H:486:GLY:HA3	1.84	0.77
1:I:105:ALA:HB3	1:I:114:LEU:HD13	1.66	0.77
2:L:328:VAL:HG22	2:L:359:GLU:HB2	1.65	0.77
2:D:286:PRO:HA	2:D:289:PHE:CE2	2.20	0.77
2:N:492:LYS:HE3	2:N:517:TYR:CE2	2.20	0.77
2:N:286:PRO:HA	2:N:289:PHE:CE2	2.19	0.77
2:H:450:LEU:HD11	2:H:454:GLY:HA3	1.65	0.76
2:N:289:PHE:CD1	2:N:316:LYS:HD2	2.19	0.76
1:C:125:ILE:HG23	1:C:133:ILE:HD12	1.65	0.76
2:H:542:ILE:HD11	2:H:588:LEU:HB2	1.67	0.76
2:P:286:PRO:HA	2:P:289:PHE:CD2	2.20	0.76
4:D:2100:OGK:HN08	4:D:2100:OGK:H18A	1.49	0.76
2:J:164:ARG:HE	2:N:112:ARG:HG3	1.51	0.76
2:P:168:THR:HB	2:P:196:VAL:CG1	2.13	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:289:PHE:CD1	2:P:316:LYS:HD2	2.20	0.75
4:F:3100:OGK:HN08	4:F:3100:OGK:H18A	1.49	0.75
2:J:116:SER:HB2	2:J:142:THR:HG23	1.65	0.75
2:N:168:THR:HB	2:N:196:VAL:CG1	2.16	0.75
2:J:308:GLU:HG3	2:J:332:ARG:HH22	1.52	0.75
1:C:108:LEU:HD12	1:C:110:ILE:HD11	1.69	0.75
1:E:125:ILE:HG23	1:E:133:ILE:HD12	1.69	0.75
1:E:108:LEU:HD12	1:E:110:ILE:HD11	1.68	0.75
2:H:321:GLU:HA	2:H:344:LEU:HA	1.69	0.75
2:H:365:VAL:HG21	2:H:387:VAL:HG13	1.68	0.75
2:H:467:TRP:HH2	2:H:494:GLU:OE1	1.70	0.75
2:N:391:THR:HG23	2:N:394:SER:H	1.52	0.75
2:F:289:PHE:CD1	2:F:316:LYS:HD2	2.22	0.74
2:L:308:GLU:HG3	2:L:332:ARG:HH22	1.51	0.74
2:H:170:LEU:HD23	2:H:170:LEU:O	1.86	0.74
2:H:415:ARG:NH1	2:H:472:TYR:HE1	1.84	0.74
1:K:124:MET:O	1:K:128:LYS:HE2	1.87	0.74
2:B:270:ARG:HB3	1:O:107:TYR:CD1	2.22	0.74
1:O:108:LEU:HD12	1:O:110:ILE:HD11	1.70	0.74
2:H:298:LEU:HD22	2:H:300:LEU:HG	1.70	0.74
2:J:289:PHE:CD1	2:J:316:LYS:HD2	2.22	0.74
1:M:124:MET:O	1:M:128:LYS:HE2	1.88	0.74
3:S:203:ILE:HD12	3:S:203:ILE:H	1.53	0.74
1:E:43:PRO:CG	2:L:319:ASN:ND2	2.50	0.74
1:M:129:THR:O	1:M:133:ILE:HG12	1.86	0.74
2:N:84:PRO:HB3	2:N:517:TYR:OH	1.87	0.73
2:F:472:TYR:OH	3:S:201:LEU:HB2	1.88	0.73
2:B:161:THR:HG22	2:B:186:GLU:HG2	1.68	0.73
2:J:286:PRO:HA	2:J:289:PHE:CD2	2.24	0.73
4:L:6100:OGK:H18A	4:L:6100:OGK:HN08	1.52	0.73
2:L:168:THR:HB	2:L:196:VAL:CG1	2.16	0.73
2:J:164:ARG:HD2	2:N:112:ARG:HG2	1.70	0.73
2:B:391:THR:HG23	2:B:394:SER:H	1.53	0.73
2:F:308:GLU:HG3	2:F:332:ARG:HH22	1.53	0.73
1:E:124:MET:O	1:E:128:LYS:HE2	1.89	0.73
2:H:136:ARG:NE	2:H:136:ARG:HA	2.04	0.73
2:P:391:THR:HG23	2:P:394:SER:H	1.54	0.73
2:H:120:ARG:NH2	5:H:1102:PO4:O3	2.20	0.73
2:H:412:LEU:HD11	2:H:445:LEU:HD22	1.69	0.72
2:J:391:THR:HG23	2:J:394:SER:H	1.54	0.72
4:J:5100:OGK:HN08	4:J:5100:OGK:H18A	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:308:GLU:HG3	2:N:332:ARG:HH22	1.54	0.72
1:K:129:THR:O	1:K:133:ILE:HG12	1.89	0.72
2:B:253:LEU:HD12	2:B:280:MET:HB2	1.72	0.72
2:D:440:ARG:HB3	2:D:467:TRP:HE3	1.54	0.72
2:H:467:TRP:CH2	2:H:494:GLU:OE1	2.42	0.72
2:H:76:ARG:HG2	2:H:76:ARG:HH11	1.55	0.72
2:J:168:THR:HB	2:J:196:VAL:CG1	2.17	0.72
2:L:286:PRO:HA	2:L:289:PHE:CD2	2.24	0.72
1:I:124:MET:O	1:I:128:LYS:HE2	1.89	0.72
2:B:349:ILE:HG13	2:B:385:VAL:HG22	1.71	0.72
2:P:308:GLU:HG3	2:P:332:ARG:HH22	1.53	0.72
2:H:391:THR:OG1	2:H:393:GLU:HB2	1.90	0.72
2:D:319:ASN:ND2	1:G:43:PRO:HG2	2.03	0.72
3:W:203:ILE:HD12	3:W:203:ILE:H	1.55	0.72
2:H:78:LEU:HD12	2:H:79:LYS:N	2.01	0.71
1:G:108:LEU:HD12	1:G:110:ILE:HD11	1.72	0.71
2:D:308:GLU:HG3	2:D:332:ARG:HH22	1.55	0.71
2:P:161:THR:HG22	2:P:186:GLU:HG2	1.71	0.71
2:D:391:THR:HG23	2:D:394:SER:H	1.54	0.71
1:M:99:PHE:HD2	2:N:15:ALA:O	1.73	0.71
2:B:157:LEU:O	2:B:161:THR:HG23	1.91	0.71
2:H:334:LEU:CD2	2:H:373:LEU:HD22	2.21	0.71
2:F:286:PRO:HA	2:F:289:PHE:CD2	2.25	0.71
2:B:308:GLU:HG3	2:B:332:ARG:HH22	1.56	0.71
1:E:129:THR:O	1:E:133:ILE:HG12	1.89	0.71
2:P:349:ILE:HG13	2:P:385:VAL:HG22	1.72	0.71
3:V:203:ILE:HD12	3:V:203:ILE:H	1.55	0.71
2:H:540:TRP:CZ2	2:H:570:ALA:HB1	2.25	0.71
2:D:492:LYS:HE3	2:D:517:TYR:CE2	2.26	0.70
2:H:211:ASP:O	2:H:215:ILE:HG13	1.91	0.70
1:E:105:ALA:CB	1:E:114:LEU:HD13	2.21	0.70
2:N:55:VAL:HG23	2:N:75:LEU:HD21	1.72	0.70
1:M:112:ASN:C	1:M:114:LEU:H	1.95	0.70
2:J:161:THR:HG22	2:J:186:GLU:HG2	1.73	0.70
3:U:203:ILE:H	3:U:203:ILE:HD12	1.56	0.70
2:L:391:THR:HG23	2:L:394:SER:H	1.56	0.70
2:H:76:ARG:HH11	2:H:76:ARG:CG	2.04	0.70
2:F:161:THR:HG22	2:F:186:GLU:HG2	1.72	0.70
2:F:85:ARG:NH2	4:F:3100:OGK:O07	2.23	0.70
2:H:116:SER:CB	2:H:142:THR:HG23	2.16	0.70
2:B:492:LYS:HE3	2:B:517:TYR:CE2	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:LEU:HD22	2:H:61:TYR:HB2	1.73	0.70
2:H:311:CYS:CB	2:H:336:VAL:HG21	2.19	0.70
2:P:55:VAL:HG23	2:P:75:LEU:HD21	1.73	0.70
2:H:370:LEU:N	2:H:370:LEU:HD23	2.06	0.70
2:H:364:LEU:HD22	2:H:388:SER:H	1.54	0.70
2:H:191:ASN:HD21	2:H:194:LEU:H	1.37	0.70
2:H:118:HIS:CD2	2:H:144:LYS:HD3	2.26	0.70
1:C:124:MET:O	1:C:128:LYS:HE2	1.92	0.70
2:F:101:THR:HG22	2:F:128:ASP:OD1	1.91	0.70
2:H:450:LEU:CD1	2:H:454:GLY:HA3	2.22	0.69
2:J:419:ILE:HD13	2:J:446:ARG:NH1	2.07	0.69
2:H:325:THR:O	2:H:349:ILE:HA	1.91	0.69
2:D:286:PRO:HA	2:D:289:PHE:CD2	2.28	0.69
2:P:191:ASN:HD21	2:P:194:LEU:H	1.40	0.69
1:I:35:ASP:HB3	2:N:243:ALA:HB1	1.73	0.69
2:L:143:LEU:HD23	2:L:159:ILE:HD13	1.75	0.69
1:M:10:SER:HB2	1:M:52:LEU:HD23	1.74	0.69
2:B:101:THR:HG22	2:B:128:ASP:OD1	1.92	0.69
2:F:295:ILE:HG21	2:F:298:LEU:HD13	1.74	0.69
2:B:350:GLU:HB3	3:Q:209:LEU:HD21	1.74	0.69
2:N:521:GLN:HG3	2:N:567:HIS:HD2	1.55	0.69
2:D:161:THR:HG22	2:D:186:GLU:HG2	1.75	0.69
2:F:168:THR:HB	2:F:196:VAL:CG1	2.18	0.69
2:B:419:ILE:HD13	2:B:446:ARG:NH1	2.08	0.69
2:F:349:ILE:HG13	2:F:385:VAL:HG22	1.73	0.69
2:H:367:GLN:O	2:H:371:ILE:HG13	1.93	0.69
2:H:176:PHE:CZ	2:H:204:PHE:CZ	2.80	0.69
2:F:297:LYS:HG3	2:F:322:VAL:HB	1.75	0.69
2:B:286:PRO:HA	2:B:289:PHE:CD2	2.27	0.69
2:F:157:LEU:O	2:F:161:THR:HG23	1.92	0.69
2:H:116:SER:HB2	2:H:142:THR:CG2	2.18	0.69
1:M:93:ILE:HD12	1:M:97:THR:CG2	2.21	0.69
2:H:133:ALA:HB2	2:H:159:ILE:HG22	1.75	0.69
2:P:492:LYS:HE3	2:P:517:TYR:CE2	2.28	0.69
3:X:203:ILE:HD12	3:X:203:ILE:H	1.58	0.69
3:R:203:ILE:HD12	3:R:203:ILE:H	1.56	0.69
2:F:391:THR:HG23	2:F:394:SER:H	1.55	0.68
2:N:161:THR:HG22	2:N:186:GLU:HG2	1.76	0.68
2:H:414:ASP:HB3	2:H:446:ARG:NH2	2.08	0.68
2:N:286:PRO:HA	2:N:289:PHE:CD2	2.28	0.68
2:H:278:SER:O	2:H:280:MET:N	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:ARG:NE	2:N:112:ARG:CG	2.55	0.68
1:K:10:SER:HB2	1:K:52:LEU:HD23	1.76	0.68
3:Q:203:ILE:HD12	3:Q:203:ILE:H	1.57	0.68
2:H:519:TRP:HH2	2:H:567:HIS:CE1	2.10	0.68
1:A:124:MET:O	1:A:128:LYS:HE2	1.94	0.68
2:N:519:TRP:HE1	4:N:7100:OGK:H01	1.57	0.68
2:L:253:LEU:HD12	2:L:280:MET:HB2	1.74	0.68
2:P:101:THR:HG22	2:P:128:ASP:OD1	1.93	0.68
2:B:168:THR:HB	2:B:196:VAL:CG1	2.18	0.68
2:J:164:ARG:CD	2:N:112:ARG:HG2	2.24	0.68
4:N:7100:OGK:C18	4:N:7100:OGK:HN08	2.07	0.68
2:L:468:MET:HE3	2:L:470:LEU:HD21	1.76	0.68
1:M:100:GLU:HG2	2:N:15:ALA:HB2	1.76	0.68
2:J:297:LYS:HG3	2:J:322:VAL:HB	1.75	0.68
1:O:129:THR:O	1:O:133:ILE:HG12	1.94	0.68
2:D:57:MET:HE3	2:D:62:THR:HG22	1.76	0.68
2:P:547:SER:HB3	2:P:564:HIS:CB	2.24	0.67
2:B:143:LEU:HD23	2:B:159:ILE:HD13	1.75	0.67
2:H:444:TYR:HA	2:H:471:GLY:HA3	1.76	0.67
1:I:129:THR:O	1:I:133:ILE:HG12	1.94	0.67
2:B:547:SER:HB3	2:B:564:HIS:CB	2.25	0.67
2:J:295:ILE:HG21	2:J:298:LEU:HD13	1.76	0.67
2:J:101:THR:HG22	2:J:128:ASP:OD1	1.94	0.67
2:L:492:LYS:HE3	2:L:517:TYR:CE2	2.29	0.67
2:H:81:LYS:HG2	2:H:120:ARG:HD3	1.77	0.67
2:J:547:SER:HB3	2:J:564:HIS:CB	2.24	0.67
2:B:84:PRO:HB3	2:B:517:TYR:OH	1.94	0.67
2:N:282:PRO:HA	2:N:285:MET:HE2	1.77	0.67
2:P:295:ILE:HG21	2:P:298:LEU:HD13	1.75	0.67
1:C:40:ASN:HB3	1:K:13:GLY:O	1.94	0.67
2:J:337:LEU:HD12	2:J:341:CYS:SG	2.34	0.67
2:P:157:LEU:O	2:P:161:THR:HG23	1.93	0.67
2:L:487:CYS:HB3	2:L:490:LEU:HB2	1.76	0.67
2:J:350:GLU:HB3	3:U:209:LEU:HD21	1.77	0.67
2:N:388:SER:O	2:N:416:GLU:HG3	1.95	0.67
2:D:297:LYS:HG3	2:D:322:VAL:HB	1.77	0.67
2:H:52:ARG:NH1	2:H:72:PHE:CZ	2.63	0.67
2:L:547:SER:HB3	2:L:564:HIS:CB	2.25	0.67
2:H:85:ARG:NH2	4:H:4100:OGK:O07	2.29	0.66
2:D:547:SER:HB3	2:D:564:HIS:CB	2.25	0.66
1:O:105:ALA:HB3	1:O:114:LEU:HD13	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:157:LEU:O	2:N:161:THR:HG23	1.96	0.66
2:D:295:ILE:HG21	2:D:298:LEU:HD13	1.78	0.66
2:N:297:LYS:HG3	2:N:322:VAL:HB	1.78	0.66
2:H:533:MET:HE1	2:H:588:LEU:HD13	1.77	0.66
2:H:59:LEU:CD2	2:H:61:TYR:HB2	2.25	0.66
2:J:440:ARG:HB3	2:J:467:TRP:HE3	1.59	0.66
1:M:52:LEU:O	1:M:56:ILE:HG13	1.96	0.66
2:P:253:LEU:HD12	2:P:280:MET:HB2	1.77	0.66
2:H:398:ILE:HG23	2:H:402:LEU:HD11	1.76	0.66
2:N:295:ILE:HG21	2:N:298:LEU:HD13	1.78	0.66
1:A:93:ILE:HD12	1:A:97:THR:CG2	2.22	0.66
2:P:419:ILE:HD13	2:P:446:ARG:NH1	2.11	0.66
2:N:101:THR:HG22	2:N:128:ASP:OD1	1.96	0.66
2:J:492:LYS:HE3	2:J:517:TYR:CE2	2.30	0.66
2:F:455:LEU:HD22	2:F:483:PHE:HB2	1.78	0.66
2:J:157:LEU:O	2:J:161:THR:HG23	1.95	0.66
2:L:472:TYR:OH	3:V:201:LEU:HB2	1.96	0.66
1:G:10:SER:HB2	1:G:52:LEU:HD23	1.77	0.66
2:H:546:PRO:HD2	2:H:584:THR:O	1.96	0.65
2:P:282:PRO:HA	2:P:285:MET:HE2	1.78	0.65
2:J:487:CYS:HB3	2:J:490:LEU:HB2	1.79	0.65
2:D:472:TYR:OH	3:R:201:LEU:HB2	1.96	0.65
2:D:282:PRO:HA	2:D:285:MET:HE2	1.79	0.65
1:I:105:ALA:HB3	1:I:114:LEU:CD1	2.26	0.65
2:H:492:LYS:NZ	2:H:516:ARG:HH11	1.93	0.65
2:B:487:CYS:HB3	2:B:490:LEU:HB2	1.77	0.65
2:B:590:GLU:HB3	2:B:591:PRO:CD	2.27	0.65
2:H:40:VAL:O	2:H:41:CYS:CB	2.43	0.65
2:J:138:ASP:OD2	2:J:164:ARG:HG3	1.96	0.65
2:B:85:ARG:NH2	4:B:1100:OGK:O07	2.28	0.65
2:N:57:MET:HE3	2:N:62:THR:HG22	1.79	0.65
2:N:547:SER:HB3	2:N:564:HIS:CB	2.26	0.65
2:H:375:GLN:HG2	2:H:401:TYR:CD1	2.31	0.65
2:N:129:LEU:HD21	2:N:155:GLY:HA3	1.78	0.65
2:P:487:CYS:HB3	2:P:490:LEU:HB2	1.77	0.65
2:H:304:LEU:O	2:H:304:LEU:HD13	1.96	0.65
2:H:95:ASN:HD22	2:H:95:ASN:N	1.78	0.65
1:E:37:CYS:SG	2:L:296:ARG:NH2	2.69	0.65
2:J:164:ARG:NE	2:N:112:ARG:HG2	2.11	0.65
2:N:143:LEU:HD23	2:N:159:ILE:HD13	1.78	0.65
2:J:191:ASN:HD21	2:J:194:LEU:H	1.45	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:PRO:HB3	2:F:517:TYR:OH	1.96	0.65
1:C:10:SER:HB2	1:C:52:LEU:HD23	1.79	0.65
2:H:533:MET:HE3	2:H:588:LEU:HD13	1.78	0.65
2:N:487:CYS:HB3	2:N:490:LEU:HB2	1.77	0.65
2:F:350:GLU:HB3	3:S:209:LEU:HD21	1.77	0.65
2:H:545:ILE:HB	2:H:567:HIS:HB2	1.79	0.64
2:B:440:ARG:HB3	2:B:467:TRP:HE3	1.61	0.64
2:H:492:LYS:NZ	2:H:516:ARG:NH1	2.45	0.64
2:L:297:LYS:HG3	2:L:322:VAL:HB	1.80	0.64
2:N:399:GLY:O	2:N:434:GLY:HA3	1.97	0.64
2:H:52:ARG:NH1	2:H:72:PHE:CE2	2.66	0.64
2:H:442:ALA:HB1	2:H:469:LEU:HB3	1.78	0.64
2:P:440:ARG:HB3	2:P:467:TRP:HE3	1.62	0.64
1:C:113:LEU:O	1:C:117:THR:HG23	1.96	0.64
2:B:295:ILE:HG21	2:B:298:LEU:HD13	1.79	0.64
1:I:26:SER:OG	1:I:108:LEU:HB3	1.98	0.64
2:F:101:THR:OG1	2:F:102:PRO:HD3	1.96	0.64
2:D:101:THR:HG22	2:D:128:ASP:OD1	1.98	0.64
2:H:371:ILE:O	2:H:375:GLN:HG3	1.97	0.64
2:D:191:ASN:HD21	2:D:194:LEU:H	1.44	0.64
2:H:286:PRO:C	2:H:288:LEU:H	2.00	0.64
2:F:143:LEU:HD23	2:F:159:ILE:HD13	1.78	0.64
2:L:440:ARG:HB3	2:L:467:TRP:HE3	1.61	0.64
1:O:10:SER:HB2	1:O:52:LEU:HD23	1.79	0.64
2:J:253:LEU:HD12	2:J:280:MET:HB2	1.80	0.64
1:M:102:ILE:CD1	2:N:20:VAL:HG21	2.26	0.64
2:D:487:CYS:HB3	2:D:490:LEU:HB2	1.80	0.64
2:H:384:ALA:HB2	2:H:409:ARG:HG3	1.79	0.64
2:H:409:ARG:HB2	4:H:4100:OGK:H16B	1.79	0.64
2:P:85:ARG:NH2	4:P:8100:OGK:O07	2.29	0.64
2:F:40:VAL:O	2:F:41:CYS:HB3	1.96	0.64
2:H:104:VAL:HG21	2:H:128:ASP:HB2	1.80	0.64
2:F:253:LEU:HD12	2:F:280:MET:HB2	1.79	0.64
2:H:364:LEU:O	2:H:365:VAL:HG13	1.97	0.64
2:L:157:LEU:O	2:L:161:THR:HG23	1.98	0.64
1:A:10:SER:HB2	1:A:52:LEU:HD23	1.78	0.63
1:I:10:SER:HB2	1:I:52:LEU:HD23	1.78	0.63
2:B:521:GLN:HG3	2:B:567:HIS:HD2	1.63	0.63
1:A:12:ASP:OD2	1:A:49:SER:HB2	1.98	0.63
2:H:225:VAL:HG22	2:H:245:LEU:HD11	1.80	0.63
2:P:57:MET:HE3	2:P:62:THR:HG22	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:SER:O	2:D:416:GLU:HG3	1.99	0.63
2:N:521:GLN:HG3	2:N:567:HIS:CD2	2.33	0.63
2:N:298:LEU:HD23	2:N:300:LEU:HD11	1.81	0.63
2:F:57:MET:HE3	2:F:62:THR:HG22	1.80	0.63
1:O:124:MET:O	1:O:128:LYS:HE2	1.97	0.63
1:C:129:THR:O	1:C:133:ILE:HG12	1.99	0.63
2:L:191:ASN:HD21	2:L:194:LEU:H	1.46	0.63
1:A:129:THR:O	1:A:133:ILE:HG12	1.98	0.63
1:M:96:ALA:HB1	2:N:14:VAL:CG1	2.28	0.63
1:M:102:ILE:CG2	2:N:20:VAL:CG2	2.76	0.63
2:J:55:VAL:HG23	2:J:75:LEU:HD21	1.79	0.63
2:D:168:THR:HB	2:D:196:VAL:CG1	2.21	0.63
2:N:519:TRP:NE1	4:N:7100:OGK:H01	2.12	0.63
2:F:521:GLN:HG3	2:F:567:HIS:HD2	1.64	0.63
1:M:12:ASP:OD2	1:M:49:SER:HB2	1.99	0.63
2:P:311:CYS:HB3	2:P:336:VAL:HG21	1.80	0.63
1:K:102:ILE:HG12	1:K:117:THR:HB	1.80	0.63
2:H:357:GLY:C	2:H:359:GLU:H	2.02	0.63
2:N:419:ILE:HD13	2:N:446:ARG:NH1	2.13	0.63
2:D:294:GLN:NE2	1:G:107:TYR:OH	2.32	0.63
2:N:311:CYS:HB3	2:N:336:VAL:HG21	1.79	0.63
1:I:102:ILE:HG23	1:I:118:CYS:SG	2.39	0.63
2:J:590:GLU:HB3	2:J:591:PRO:CD	2.27	0.62
2:H:501:SER:HB3	2:H:524:ARG:NH1	2.14	0.62
2:H:230:PHE:HB3	2:H:235:LEU:HD21	1.81	0.62
2:F:547:SER:HB3	2:F:564:HIS:CB	2.28	0.62
2:B:191:ASN:HD21	2:B:194:LEU:H	1.47	0.62
2:D:590:GLU:HB3	2:D:591:PRO:CD	2.28	0.62
1:E:10:SER:HB2	1:E:52:LEU:HD23	1.79	0.62
1:E:45:PRO:HB2	2:L:291:PHE:HA	1.81	0.62
2:N:85:ARG:NH2	4:N:7100:OGK:O07	2.28	0.62
2:F:282:PRO:HA	2:F:285:MET:HE2	1.81	0.62
2:F:492:LYS:HE3	2:F:517:TYR:CE2	2.34	0.62
2:H:366:SER:OG	2:H:368:ARG:HG2	1.99	0.62
2:J:164:ARG:HE	2:N:112:ARG:HG2	1.64	0.62
2:D:190:HIS:CG	2:H:112:ARG:HH11	2.17	0.62
2:N:310:HIS:O	2:N:314:ILE:HG12	2.00	0.62
2:F:590:GLU:HB3	2:F:591:PRO:CD	2.28	0.62
2:L:138:ASP:OD2	2:L:164:ARG:HG3	1.98	0.62
2:L:84:PRO:HB3	2:L:517:TYR:OH	1.99	0.62
2:L:295:ILE:HG21	2:L:298:LEU:HD13	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:455:LEU:HD22	2:L:483:PHE:HB2	1.81	0.62
2:N:63:ALA:HB1	2:N:67:ARG:HD2	1.82	0.62
2:L:55:VAL:HG23	2:L:75:LEU:HD21	1.81	0.62
2:N:253:LEU:HD12	2:N:280:MET:HB2	1.81	0.62
2:J:521:GLN:HG3	2:J:567:HIS:HD2	1.65	0.62
2:H:544:LEU:O	2:H:546:PRO:HD3	2.00	0.62
2:F:468:MET:HE3	2:F:470:LEU:HD21	1.82	0.62
2:D:350:GLU:HB3	3:R:209:LEU:HD21	1.81	0.62
2:F:440:ARG:HB3	2:F:467:TRP:HE3	1.65	0.62
2:B:388:SER:O	2:B:416:GLU:HG3	2.00	0.62
2:F:487:CYS:HB3	2:F:490:LEU:HB2	1.80	0.62
2:D:419:ILE:HD13	2:D:446:ARG:NH1	2.13	0.62
2:P:129:LEU:HD21	2:P:155:GLY:HA3	1.82	0.61
2:H:101:THR:HG23	2:H:131:ARG:HH12	1.65	0.61
2:H:442:ALA:CB	2:H:469:LEU:HB3	2.30	0.61
2:P:184:LEU:HD12	2:P:207:ILE:HB	1.81	0.61
2:H:253:LEU:HD13	2:H:284:GLU:HG3	1.82	0.61
2:H:440:ARG:HB3	2:H:467:TRP:CD1	2.31	0.61
2:J:164:ARG:NE	2:N:112:ARG:HG3	2.15	0.61
2:N:455:LEU:HD22	2:N:483:PHE:HB2	1.82	0.61
2:F:399:GLY:O	2:F:434:GLY:HA3	2.00	0.61
2:F:365:VAL:HG23	2:F:387:VAL:HA	1.83	0.61
2:H:85:ARG:O	2:H:88:MET:HG2	2.01	0.61
2:B:282:PRO:HA	2:B:285:MET:HE2	1.82	0.61
1:K:52:LEU:O	1:K:56:ILE:HG13	2.01	0.61
2:N:101:THR:OG1	2:N:102:PRO:HD3	2.00	0.61
1:A:99:PHE:HZ	1:A:137:PHE:HE1	1.46	0.61
2:D:253:LEU:HD12	2:D:280:MET:HB2	1.81	0.61
2:H:89:PHE:CE1	4:H:4100:OGK:H17	2.35	0.61
2:L:419:ILE:HD13	2:L:446:ARG:NH1	2.15	0.61
1:M:137:PHE:CD1	2:N:17:VAL:HG21	2.36	0.61
2:J:57:MET:HE3	2:J:62:THR:HG22	1.82	0.61
2:L:184:LEU:HD12	2:L:207:ILE:HB	1.82	0.61
4:P:8100:OGK:C18	4:P:8100:OGK:HN08	2.13	0.61
1:E:48:THR:HG22	1:E:51:ILE:HB	1.82	0.61
2:P:310:HIS:O	2:P:314:ILE:HG12	2.00	0.61
2:H:461:TYR:C	2:H:463:PRO:HD3	2.20	0.61
1:O:137:PHE:CD1	2:P:17:VAL:HG21	2.35	0.61
2:P:533:MET:HE3	2:P:588:LEU:HD13	1.83	0.61
2:H:412:LEU:HD12	2:H:445:LEU:HA	1.83	0.61
1:M:26:SER:OG	1:M:108:LEU:HB3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:419:ILE:HD13	2:F:446:ARG:NH1	2.16	0.61
2:D:227:VAL:CG1	2:D:228:GLY:N	2.64	0.61
2:H:40:VAL:HG23	2:H:40:VAL:O	1.99	0.61
2:L:85:ARG:NH2	4:L:6100:OGK:O07	2.30	0.61
2:P:590:GLU:HB3	2:P:591:PRO:CD	2.26	0.61
2:P:455:LEU:HD22	2:P:483:PHE:HB2	1.81	0.61
1:E:12:ASP:OD2	1:E:49:SER:HB2	2.00	0.61
2:J:129:LEU:HD21	2:J:155:GLY:HA3	1.82	0.61
2:L:590:GLU:HB3	2:L:591:PRO:CD	2.27	0.60
2:N:311:CYS:O	2:N:315:GLN:HB2	2.00	0.60
1:A:137:PHE:CD1	2:B:17:VAL:HG21	2.36	0.60
2:L:388:SER:O	2:L:416:GLU:HG3	2.01	0.60
2:L:542:ILE:CD1	2:L:588:LEU:HD12	2.21	0.60
2:J:101:THR:OG1	2:J:102:PRO:HD3	2.00	0.60
2:H:428:VAL:HG11	2:H:443:PHE:CZ	2.36	0.60
2:N:272:LEU:HD21	2:N:275:LEU:HB3	1.82	0.60
2:H:392:ASN:HD22	2:H:422:LEU:HD13	1.66	0.60
2:B:533:MET:HE3	2:B:588:LEU:HD13	1.82	0.60
1:E:52:LEU:O	1:E:56:ILE:HG13	2.01	0.60
2:H:124:VAL:O	2:H:151:PHE:HB3	2.02	0.60
1:E:6:ILE:HD12	1:E:23:ALA:HB3	1.82	0.60
2:L:227:VAL:CG1	2:L:228:GLY:N	2.64	0.60
2:N:367:GLN:O	2:N:371:ILE:HG22	2.01	0.60
2:J:547:SER:HB3	2:J:564:HIS:HB3	1.83	0.60
2:H:109:ASN:C	2:H:110:ASN:HD22	2.05	0.60
2:H:233:LEU:HA	2:H:236:VAL:HG23	1.82	0.60
2:P:388:SER:O	2:P:416:GLU:HG3	2.00	0.60
2:P:565:PRO:HG2	3:X:201:LEU:HD21	1.83	0.60
2:L:521:GLN:HG3	2:L:567:HIS:HD2	1.64	0.60
2:J:519:TRP:HE1	4:J:5100:OGK:H01	1.66	0.60
1:G:52:LEU:O	1:G:56:ILE:HG13	2.02	0.60
1:I:52:LEU:O	1:I:56:ILE:HG13	2.01	0.60
2:F:130:ASP:OD1	2:F:134:LYS:HE3	2.00	0.60
2:H:396:GLU:O	2:H:400:THR:HG23	2.01	0.60
2:D:91:LEU:O	2:D:567:HIS:HE1	1.83	0.60
1:G:137:PHE:HB3	2:H:17:VAL:HG21	1.82	0.60
2:B:311:CYS:O	2:B:315:GLN:HB2	2.01	0.60
2:H:425:ASP:OD2	2:H:451:THR:HG23	2.02	0.60
2:L:101:THR:HG22	2:L:128:ASP:OD1	2.01	0.60
2:B:365:VAL:HG23	2:B:387:VAL:HA	1.84	0.60
4:F:3100:OGK:HN08	4:F:3100:OGK:C18	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:PRO:HB3	2:D:517:TYR:OH	2.02	0.60
2:L:227:VAL:HG13	2:L:228:GLY:N	2.16	0.60
2:F:310:HIS:O	2:F:314:ILE:HG12	2.02	0.60
1:A:58:TYR:CD2	1:A:113:LEU:HD13	2.37	0.60
2:H:87:ALA:HB2	2:H:92:ILE:HG13	1.83	0.60
1:M:100:GLU:HG2	2:N:15:ALA:CB	2.31	0.60
2:D:101:THR:HG22	2:D:128:ASP:HB3	1.83	0.60
2:B:443:PHE:CE2	2:B:445:LEU:HD11	2.37	0.60
2:H:445:LEU:HD12	2:H:473:VAL:HG12	1.83	0.60
2:H:469:LEU:HD12	2:H:494:GLU:O	2.01	0.60
2:D:367:GLN:HB3	2:D:391:THR:CG2	2.31	0.60
2:P:547:SER:HB3	2:P:564:HIS:HB3	1.84	0.60
2:J:519:TRP:NE1	4:J:5100:OGK:H01	2.17	0.60
2:B:298:LEU:HD23	2:B:300:LEU:HD11	1.84	0.60
2:H:47:ILE:O	2:H:51:THR:HG23	2.02	0.60
2:H:76:ARG:NH1	2:H:76:ARG:CG	2.65	0.60
2:B:101:THR:OG1	2:B:102:PRO:HD3	2.02	0.60
1:G:30:ALA:O	1:G:33:VAL:HG22	2.01	0.60
2:B:468:MET:HE3	2:B:470:LEU:HD21	1.82	0.60
2:J:367:GLN:HB3	2:J:391:THR:CG2	2.31	0.59
1:G:153:ARG:HG2	1:G:153:ARG:NH1	2.17	0.59
1:M:99:PHE:HB2	2:N:15:ALA:CB	2.32	0.59
2:D:157:LEU:O	2:D:161:THR:HG23	2.02	0.59
1:M:158:ALA:HA	2:N:62:THR:HG21	1.84	0.59
1:E:30:ALA:O	1:E:33:VAL:HG22	2.02	0.59
2:B:297:LYS:HG3	2:B:322:VAL:HB	1.83	0.59
2:L:365:VAL:HG23	2:L:387:VAL:HA	1.84	0.59
1:M:48:THR:HG22	1:M:51:ILE:HB	1.84	0.59
2:N:91:LEU:O	2:N:567:HIS:HE1	1.85	0.59
2:N:275:LEU:HD11	2:N:288:LEU:HD21	1.83	0.59
2:H:22:GLU:HG2	2:H:47:ILE:CD1	2.32	0.59
2:B:121:ARG:NH2	5:B:1103:PO4:O4	2.34	0.59
2:N:65:PRO:HB3	2:N:103:TRP:CE3	2.37	0.59
2:H:230:PHE:CD1	2:H:235:LEU:HD21	2.37	0.59
2:J:388:SER:O	2:J:416:GLU:HG3	2.03	0.59
2:P:298:LEU:HD23	2:P:300:LEU:HD11	1.84	0.59
2:D:184:LEU:HD12	2:D:207:ILE:HB	1.84	0.59
2:D:40:VAL:O	2:D:41:CYS:HB3	2.02	0.59
2:H:392:ASN:O	2:H:396:GLU:CG	2.45	0.59
1:O:93:ILE:HD12	1:O:97:THR:CG2	2.29	0.59
2:D:101:THR:OG1	2:D:102:PRO:HD3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:357:GLY:HA2	2:P:415:ARG:NH2	2.11	0.59
2:H:444:TYR:OH	2:H:496:ARG:HD3	2.01	0.59
2:N:367:GLN:HB3	2:N:391:THR:CG2	2.30	0.59
2:H:125:SER:HB2	2:H:128:ASP:H	1.67	0.59
2:L:129:LEU:HD21	2:L:155:GLY:HA3	1.85	0.59
1:G:130:PRO:HD3	2:H:36:SER:HB2	1.84	0.59
2:H:22:GLU:HG2	2:H:47:ILE:HD11	1.83	0.59
2:B:227:VAL:CG1	2:B:228:GLY:N	2.65	0.59
2:D:311:CYS:O	2:D:315:GLN:HB2	2.03	0.59
1:K:12:ASP:OD2	1:K:49:SER:HB2	2.01	0.59
1:A:52:LEU:O	1:A:56:ILE:HG13	2.01	0.59
1:E:158:ALA:HA	2:F:62:THR:HG21	1.84	0.59
2:J:351:ARG:O	2:J:351:ARG:HG3	2.03	0.59
2:P:468:MET:HE3	2:P:470:LEU:HD21	1.83	0.59
2:H:412:LEU:HD11	2:H:445:LEU:CD2	2.33	0.59
1:E:43:PRO:HG3	2:L:319:ASN:HD21	1.67	0.59
2:N:65:PRO:HA	2:N:103:TRP:CZ3	2.38	0.59
2:D:261:GLU:HG2	2:D:264:MET:HG3	1.85	0.59
2:L:197:LEU:O	2:L:225:VAL:HA	2.02	0.59
2:B:261:GLU:HG2	2:B:264:MET:HG3	1.85	0.59
2:P:91:LEU:O	2:P:567:HIS:HE1	1.86	0.58
2:J:357:GLY:HA2	2:J:415:ARG:NH2	2.12	0.58
1:I:93:ILE:HD12	1:I:97:THR:CG2	2.26	0.58
2:B:519:TRP:NE1	4:B:1100:OGK:H01	2.18	0.58
2:N:404:ASN:HA	2:N:437:LYS:HD2	1.85	0.58
1:C:12:ASP:OD2	1:C:49:SER:HB2	2.03	0.58
1:G:153:ARG:HG2	1:G:153:ARG:HH11	1.67	0.58
2:D:319:ASN:ND2	1:G:43:PRO:CG	2.65	0.58
2:L:547:SER:HB3	2:L:564:HIS:HB3	1.86	0.58
1:C:52:LEU:O	1:C:56:ILE:HG13	2.02	0.58
2:P:311:CYS:O	2:P:315:GLN:HB2	2.04	0.58
1:K:158:ALA:HA	2:L:62:THR:HG21	1.84	0.58
1:M:105:ALA:HB2	1:M:113:LEU:HD23	1.83	0.58
2:F:227:VAL:CG1	2:F:228:GLY:N	2.66	0.58
2:P:197:LEU:O	2:P:225:VAL:HA	2.03	0.58
1:E:137:PHE:CD1	2:F:17:VAL:HG21	2.39	0.58
2:B:57:MET:HE3	2:B:62:THR:HG22	1.85	0.58
2:J:233:LEU:O	2:J:236:VAL:HG23	2.04	0.58
2:P:337:LEU:HD12	2:P:341:CYS:SG	2.44	0.58
2:F:80:LEU:HB2	2:F:122:MET:CE	2.33	0.58
2:J:533:MET:HE3	2:J:588:LEU:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:GLY:HA2	2:F:415:ARG:NH2	2.12	0.58
2:L:357:GLY:HA2	2:L:415:ARG:NH2	2.11	0.58
2:P:84:PRO:HB3	2:P:517:TYR:OH	2.04	0.58
2:B:63:ALA:HB1	2:B:67:ARG:HD2	1.85	0.58
2:H:311:CYS:HB3	2:H:336:VAL:CG2	2.22	0.58
2:P:519:TRP:NE1	4:P:8100:OGK:H01	2.18	0.58
4:J:5100:OGK:HN08	4:J:5100:OGK:C18	2.16	0.58
2:J:91:LEU:O	2:J:567:HIS:HE1	1.87	0.58
2:B:227:VAL:HG13	2:B:228:GLY:N	2.19	0.58
1:G:98:LEU:HD21	1:G:120:THR:HG22	1.85	0.58
2:F:388:SER:O	2:F:416:GLU:HG3	2.03	0.58
2:H:390:ILE:HD11	2:H:410:LEU:HD11	1.83	0.58
2:N:80:LEU:HB2	2:N:122:MET:CE	2.34	0.58
1:O:12:ASP:OD2	1:O:49:SER:HB2	2.04	0.58
2:F:129:LEU:HD21	2:F:155:GLY:HA3	1.86	0.58
2:L:282:PRO:HA	2:L:285:MET:HE2	1.85	0.58
2:P:519:TRP:HE1	4:P:8100:OGK:H01	1.67	0.58
2:J:40:VAL:O	2:J:41:CYS:HB3	2.03	0.58
2:P:272:LEU:HD21	2:P:275:LEU:HB3	1.84	0.58
2:H:519:TRP:CH2	2:H:567:HIS:CE1	2.92	0.58
2:D:440:ARG:HB3	2:D:467:TRP:CE3	2.37	0.58
1:E:158:ALA:HA	2:F:62:THR:CG2	2.34	0.58
2:H:25:MET:HG2	2:H:47:ILE:HG22	1.86	0.58
1:G:12:ASP:OD2	1:G:49:SER:HB2	2.04	0.58
2:P:399:GLY:O	2:P:434:GLY:HA3	2.03	0.58
2:H:305:LEU:HD23	2:H:305:LEU:H	1.69	0.58
2:B:444:TYR:HA	2:B:471:GLY:CA	2.30	0.58
2:L:367:GLN:HB3	2:L:391:THR:CG2	2.32	0.58
2:D:547:SER:HB3	2:D:564:HIS:HB3	1.85	0.58
2:D:227:VAL:HG13	2:D:228:GLY:N	2.19	0.58
1:K:137:PHE:CD1	2:L:17:VAL:HG21	2.39	0.58
2:D:129:LEU:HD21	2:D:155:GLY:HA3	1.85	0.58
2:L:130:ASP:OD1	2:L:134:LYS:HE3	2.03	0.58
2:L:533:MET:HE3	2:L:588:LEU:HD13	1.85	0.57
2:F:446:ARG:HG2	2:F:447:GLN:H	1.69	0.57
1:I:134:ARG:HB2	1:I:139:ILE:O	2.04	0.57
2:B:129:LEU:HD21	2:B:155:GLY:HA3	1.85	0.57
2:B:477:ASP:OD2	2:B:504:ALA:HB2	2.04	0.57
2:H:38:SER:O	2:H:45:PHE:HB2	2.04	0.57
2:D:533:MET:HE3	2:D:588:LEU:HD13	1.87	0.57
2:P:101:THR:HG22	2:P:128:ASP:HB3	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:396:GLU:O	2:F:400:THR:HB	2.04	0.57
2:N:184:LEU:HD12	2:N:207:ILE:HB	1.86	0.57
1:O:91:MET:SD	1:O:117:THR:HG22	2.44	0.57
2:H:519:TRP:HE1	4:H:4100:OGK:C01	2.16	0.57
1:M:158:ALA:HA	2:N:62:THR:CG2	2.34	0.57
2:B:396:GLU:O	2:B:400:THR:HB	2.04	0.57
1:G:159:PHE:CE2	2:H:68:LEU:HD13	2.39	0.57
2:H:444:TYR:CD1	2:H:471:GLY:HA2	2.39	0.57
1:O:134:ARG:HB2	1:O:139:ILE:O	2.04	0.57
2:J:197:LEU:O	2:J:225:VAL:HA	2.04	0.57
2:B:91:LEU:O	2:B:567:HIS:HE1	1.87	0.57
2:J:184:LEU:HD12	2:J:207:ILE:HB	1.86	0.57
2:B:519:TRP:HE1	4:B:1100:OGK:H01	1.70	0.57
2:B:270:ARG:CB	1:O:107:TYR:CD1	2.88	0.57
2:B:101:THR:HG22	2:B:128:ASP:HB3	1.85	0.57
2:D:233:LEU:O	2:D:236:VAL:HG23	2.04	0.57
2:F:55:VAL:HG23	2:F:75:LEU:HD21	1.87	0.57
2:N:590:GLU:HB3	2:N:591:PRO:CD	2.27	0.57
1:I:105:ALA:CB	1:I:114:LEU:HD13	2.33	0.57
2:D:365:VAL:HG23	2:D:387:VAL:HA	1.85	0.57
2:P:297:LYS:HG3	2:P:322:VAL:HB	1.85	0.57
2:H:587:VAL:HG12	2:H:587:VAL:O	2.04	0.57
2:B:547:SER:HB3	2:B:564:HIS:HB3	1.86	0.57
1:M:134:ARG:HB2	1:M:139:ILE:O	2.04	0.57
2:H:395:LEU:HB3	2:H:427:GLY:O	2.04	0.57
2:L:93:PRO:HA	2:L:548:ARG:CB	2.26	0.57
2:J:101:THR:CG2	2:J:128:ASP:OD1	2.53	0.57
1:O:158:ALA:HA	2:P:62:THR:HG21	1.87	0.57
2:F:227:VAL:HG13	2:F:228:GLY:N	2.19	0.57
2:H:121:ARG:NH2	5:H:1103:PO4:O4	2.38	0.57
2:B:138:ASP:OD2	2:B:164:ARG:HG3	2.05	0.57
2:D:130:ASP:OD1	2:D:134:LYS:HE3	2.04	0.57
2:J:344:LEU:HD23	2:J:380:LEU:HD21	1.87	0.57
2:N:191:ASN:HD21	2:N:194:LEU:H	1.50	0.57
1:O:48:THR:HG22	1:O:51:ILE:HB	1.87	0.57
2:H:95:ASN:ND2	2:H:95:ASN:N	2.44	0.57
2:J:84:PRO:HB3	2:J:517:TYR:OH	2.05	0.57
2:P:40:VAL:O	2:P:41:CYS:HB3	2.02	0.57
2:N:261:GLU:HG2	2:N:264:MET:HG3	1.87	0.57
1:I:160:GLU:HA	1:I:160:GLU:OE2	2.05	0.56
2:H:407:ASP:OD1	2:H:440:ARG:HD2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:542:ILE:CD1	2:H:588:LEU:HB2	2.35	0.56
1:E:134:ARG:HB2	1:E:139:ILE:O	2.05	0.56
1:K:6:ILE:HD12	1:K:23:ALA:HB3	1.86	0.56
2:P:396:GLU:O	2:P:400:THR:HB	2.04	0.56
1:A:48:THR:HG22	1:A:51:ILE:HB	1.86	0.56
2:J:143:LEU:HD23	2:J:159:ILE:HD13	1.87	0.56
2:L:311:CYS:O	2:L:315:GLN:HB2	2.04	0.56
1:E:160:GLU:HA	1:E:160:GLU:OE2	2.05	0.56
1:M:102:ILE:HD12	2:N:20:VAL:CG2	2.31	0.56
2:F:91:LEU:O	2:F:567:HIS:HE1	1.88	0.56
2:J:101:THR:HG22	2:J:128:ASP:HB3	1.86	0.56
2:H:225:VAL:HG21	2:H:238:PHE:HZ	1.70	0.56
2:D:396:GLU:O	2:D:400:THR:HB	2.05	0.56
2:L:357:GLY:CA	2:L:415:ARG:HH22	2.13	0.56
2:H:365:VAL:CG2	2:H:387:VAL:HG13	2.34	0.56
1:G:130:PRO:O	1:G:134:ARG:HG3	2.05	0.56
2:P:521:GLN:HG3	2:P:567:HIS:HD2	1.69	0.56
2:D:519:TRP:HE1	4:D:2100:OGK:H01	1.69	0.56
2:L:519:TRP:NE1	4:L:6100:OGK:H01	2.20	0.56
2:N:547:SER:HB3	2:N:564:HIS:HB3	1.86	0.56
1:O:52:LEU:O	1:O:56:ILE:HG13	2.05	0.56
2:F:443:PHE:CE2	2:F:445:LEU:HD11	2.40	0.56
2:F:261:GLU:HG2	2:F:264:MET:HG3	1.87	0.56
2:B:233:LEU:O	2:B:236:VAL:HG23	2.04	0.56
2:N:223:VAL:O	2:N:245:LEU:HD12	2.06	0.56
2:F:311:CYS:O	2:F:315:GLN:HB2	2.06	0.56
1:K:30:ALA:O	1:K:33:VAL:HG22	2.05	0.56
2:J:565:PRO:HG2	3:U:201:LEU:HD21	1.86	0.56
2:P:350:GLU:HB3	3:X:209:LEU:HD21	1.86	0.56
2:J:272:LEU:HD21	2:J:275:LEU:HB3	1.88	0.56
1:M:58:TYR:CD2	1:M:113:LEU:HD13	2.40	0.56
2:P:54:HIS:HE1	2:P:56:THR:OG1	1.88	0.56
2:P:227:VAL:CG1	2:P:228:GLY:N	2.68	0.56
2:H:411:VAL:CG1	2:H:444:TYR:HB3	2.35	0.56
1:E:43:PRO:HG2	2:L:319:ASN:HD22	1.68	0.56
2:H:82:GLY:HA3	2:H:122:MET:HG2	1.88	0.56
2:F:101:THR:CG2	2:F:128:ASP:OD1	2.54	0.56
2:D:298:LEU:HD23	2:D:300:LEU:HD11	1.87	0.56
2:L:311:CYS:HB3	2:L:336:VAL:HG21	1.88	0.56
2:D:121:ARG:NH2	5:D:1103:PO4:O4	2.37	0.56
2:H:276:GLY:HA3	2:H:299:ASP:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:93:PRO:HA	2:P:548:ARG:CB	2.29	0.56
2:D:357:GLY:HA2	2:D:415:ARG:NH2	2.14	0.56
2:H:334:LEU:HD22	2:H:373:LEU:HD22	1.85	0.56
2:N:40:VAL:O	2:N:41:CYS:HB3	2.04	0.56
1:C:48:THR:HG22	1:C:51:ILE:HB	1.86	0.56
2:F:482:GLU:O	2:F:485:ARG:HG2	2.05	0.56
2:N:396:GLU:O	2:N:400:THR:HB	2.05	0.56
2:D:404:ASN:HA	2:D:437:LYS:HD2	1.86	0.56
1:I:30:ALA:O	1:I:33:VAL:HG22	2.06	0.56
2:P:404:ASN:HA	2:P:437:LYS:HD2	1.88	0.56
2:N:477:ASP:OD2	2:N:504:ALA:HB2	2.05	0.56
2:B:472:TYR:OH	3:Q:201:LEU:HB2	2.05	0.56
2:H:447:GLN:HG3	2:H:447:GLN:O	2.05	0.56
2:D:444:TYR:HA	2:D:471:GLY:CA	2.31	0.56
2:H:384:ALA:CB	2:H:409:ARG:HG3	2.35	0.56
2:H:199:PHE:CE1	2:H:227:VAL:HG23	2.41	0.56
2:L:519:TRP:HE1	4:L:6100:OGK:H01	1.71	0.56
2:L:337:LEU:HD12	2:L:341:CYS:SG	2.46	0.56
2:P:443:PHE:CE2	2:P:445:LEU:HD11	2.40	0.56
2:H:326:ARG:HA	2:H:350:GLU:O	2.05	0.56
1:C:158:ALA:HA	2:D:62:THR:CG2	2.36	0.56
2:J:365:VAL:HG23	2:J:387:VAL:HA	1.87	0.56
2:F:275:LEU:HD11	2:F:288:LEU:HD21	1.88	0.56
2:D:138:ASP:OD2	2:D:164:ARG:HG3	2.06	0.56
1:G:48:THR:HG22	1:G:51:ILE:HB	1.88	0.56
2:H:343:GLN:CD	2:H:343:GLN:H	2.09	0.56
2:H:285:MET:CG	2:H:286:PRO:HD3	2.34	0.56
2:H:469:LEU:HD21	4:H:4100:OGK:H05	1.88	0.56
2:P:367:GLN:O	2:P:371:ILE:HG22	2.05	0.56
2:N:321:GLU:HA	2:N:344:LEU:HA	1.87	0.56
2:N:344:LEU:HD23	2:N:380:LEU:HD21	1.86	0.56
2:F:191:ASN:HD21	2:F:194:LEU:H	1.53	0.56
2:N:468:MET:HE3	2:N:470:LEU:HD21	1.88	0.56
2:B:40:VAL:O	2:B:41:CYS:HB3	2.06	0.56
2:L:396:GLU:O	2:L:400:THR:HB	2.06	0.56
2:F:93:PRO:HA	2:F:548:ARG:CB	2.29	0.56
2:D:411:VAL:HG22	2:D:444:TYR:HB3	1.87	0.56
1:M:96:ALA:CB	2:N:14:VAL:HG12	2.34	0.56
2:F:519:TRP:NE1	4:F:3100:OGK:H01	2.21	0.56
1:A:95:GLN:HE21	1:A:124:MET:HE3	1.71	0.56
2:H:462:SER:N	2:H:463:PRO:HD3	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:ALA:HA	2:L:62:THR:CG2	2.35	0.56
1:A:134:ARG:HB2	1:A:139:ILE:O	2.06	0.56
2:B:310:HIS:O	2:B:314:ILE:HG12	2.05	0.56
1:I:12:ASP:OD2	1:I:49:SER:HB2	2.05	0.56
2:F:184:LEU:HD12	2:F:207:ILE:HB	1.88	0.56
2:H:291:PHE:H	2:H:291:PHE:HD2	1.53	0.56
2:H:390:ILE:HD12	2:H:410:LEU:HD21	1.88	0.55
2:N:546:PRO:HD3	2:N:584:THR:O	2.06	0.55
2:B:55:VAL:HG23	2:B:75:LEU:HD21	1.88	0.55
2:P:351:ARG:HG3	2:P:351:ARG:O	2.06	0.55
2:L:272:LEU:HD21	2:L:275:LEU:HB3	1.87	0.55
1:G:125:ILE:HD11	2:H:44:TRP:HH2	1.71	0.55
2:L:399:GLY:O	2:L:434:GLY:HA3	2.06	0.55
1:C:30:ALA:O	1:C:33:VAL:HG22	2.05	0.55
2:L:411:VAL:HG22	2:L:444:TYR:HB3	1.88	0.55
2:D:519:TRP:NE1	4:D:2100:OGK:H01	2.20	0.55
2:H:76:ARG:O	2:H:114:LEU:HD12	2.07	0.55
2:B:397:SER:O	2:B:400:THR:HG22	2.06	0.55
2:P:397:SER:O	2:P:400:THR:HG22	2.06	0.55
2:L:40:VAL:O	2:L:41:CYS:HB3	2.06	0.55
2:J:396:GLU:O	2:J:400:THR:HB	2.05	0.55
1:E:45:PRO:HG3	2:L:293:ALA:HB3	1.87	0.55
1:G:153:ARG:HH11	1:G:153:ARG:CG	2.19	0.55
2:J:282:PRO:HA	2:J:285:MET:HE2	1.88	0.55
4:N:7100:OGK:C18	4:N:7100:OGK:N08	2.69	0.55
4:L:6100:OGK:HN08	4:L:6100:OGK:C18	2.17	0.55
2:H:477:ASP:O	2:H:481:MET:HG2	2.06	0.55
2:H:366:SER:HB3	2:H:368:ARG:HG3	1.88	0.55
1:O:153:ARG:NH2	2:P:539:TYR:CE1	2.74	0.55
2:F:519:TRP:HE1	4:F:3100:OGK:H01	1.71	0.55
1:G:26:SER:OG	1:G:108:LEU:HB3	2.06	0.55
2:J:261:GLU:HG2	2:J:264:MET:HG3	1.89	0.55
1:E:45:PRO:CD	2:L:294:GLN:HB2	2.37	0.55
2:L:101:THR:HG22	2:L:128:ASP:HB3	1.88	0.55
1:A:158:ALA:HA	2:B:62:THR:HG21	1.88	0.55
2:L:398:ILE:HG23	2:L:402:LEU:HD11	1.89	0.55
1:I:6:ILE:HD12	1:I:23:ALA:HB3	1.88	0.55
2:J:446:ARG:HG2	2:J:447:GLN:H	1.71	0.55
4:D:2100:OGK:C18	4:D:2100:OGK:HN08	2.19	0.55
2:P:101:THR:CG2	2:P:128:ASP:OD1	2.54	0.55
2:F:310:HIS:O	2:F:314:ILE:CG1	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:THR:HG22	1:K:51:ILE:HB	1.88	0.55
2:J:95:ASN:O	2:J:582:PRO:HG3	2.06	0.55
2:D:143:LEU:HD23	2:D:159:ILE:HD13	1.89	0.55
1:A:6:ILE:HD12	1:A:23:ALA:HB3	1.87	0.55
2:B:296:ARG:NH2	1:O:37:CYS:SG	2.80	0.55
2:H:232:ILE:HG13	2:H:253:LEU:HD21	1.89	0.55
2:F:367:GLN:HB3	2:F:391:THR:CG2	2.34	0.55
1:O:105:ALA:CB	1:O:114:LEU:HD13	2.37	0.55
2:H:374:ALA:HB2	2:H:398:ILE:HD12	1.88	0.55
1:C:102:ILE:HG12	1:C:117:THR:HB	1.89	0.55
2:P:310:HIS:O	2:P:314:ILE:CG1	2.55	0.55
1:A:30:ALA:O	1:A:33:VAL:HG22	2.06	0.55
2:J:311:CYS:O	2:J:315:GLN:HB2	2.06	0.55
2:P:261:GLU:HG2	2:P:264:MET:HG3	1.89	0.55
2:H:382:TYR:C	2:H:382:TYR:CD1	2.79	0.55
1:M:102:ILE:HB	2:N:20:VAL:HG21	1.89	0.55
1:O:48:THR:HG22	1:O:51:ILE:CG1	2.37	0.55
2:D:80:LEU:HB2	2:D:122:MET:CE	2.37	0.55
1:M:30:ALA:O	1:M:33:VAL:HG22	2.07	0.55
1:G:6:ILE:HD12	1:G:23:ALA:HB3	1.89	0.55
2:B:197:LEU:O	2:B:225:VAL:HA	2.07	0.55
1:A:91:MET:O	1:A:93:ILE:N	2.40	0.55
2:J:444:TYR:HA	2:J:471:GLY:CA	2.32	0.55
2:B:547:SER:HB3	2:B:564:HIS:CG	2.42	0.55
2:J:130:ASP:OD1	2:J:134:LYS:HE3	2.06	0.55
2:N:440:ARG:HB3	2:N:467:TRP:HE3	1.72	0.55
2:N:365:VAL:HG23	2:N:387:VAL:HA	1.88	0.55
2:H:232:ILE:HG13	2:H:253:LEU:CD2	2.37	0.55
2:D:319:ASN:HD22	1:G:43:PRO:HG2	1.71	0.55
2:J:298:LEU:HD23	2:J:300:LEU:HD11	1.88	0.55
2:B:311:CYS:HB3	2:B:336:VAL:HG21	1.89	0.55
2:L:57:MET:HE2	2:L:62:THR:HG22	1.88	0.55
2:N:397:SER:O	2:N:400:THR:HG22	2.07	0.55
1:G:129:THR:HG23	1:G:132:GLU:CD	2.27	0.55
2:D:197:LEU:O	2:D:225:VAL:HA	2.06	0.55
2:B:20:VAL:O	2:B:24:VAL:HG23	2.07	0.55
1:O:30:ALA:O	1:O:33:VAL:HG22	2.06	0.55
2:L:444:TYR:HA	2:L:471:GLY:CA	2.34	0.54
2:P:547:SER:HB3	2:P:564:HIS:CG	2.42	0.54
2:B:101:THR:CG2	2:B:128:ASP:OD1	2.55	0.54
2:H:201:MET:HG3	2:H:302:TYR:CE1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:ALA:HB1	2:L:67:ARG:HD2	1.87	0.54
1:M:6:ILE:HD12	1:M:23:ALA:HB3	1.89	0.54
2:N:444:TYR:HA	2:N:471:GLY:CA	2.31	0.54
1:K:26:SER:OG	1:K:108:LEU:HB3	2.07	0.54
1:O:26:SER:OG	1:O:108:LEU:HB3	2.07	0.54
2:F:298:LEU:HD23	2:F:300:LEU:HD11	1.88	0.54
2:H:104:VAL:HG21	2:H:128:ASP:CB	2.37	0.54
2:P:365:VAL:HG23	2:P:387:VAL:HA	1.89	0.54
2:B:404:ASN:HA	2:B:437:LYS:HD2	1.89	0.54
2:F:357:GLY:CA	2:F:415:ARG:HH22	2.12	0.54
2:H:363:GLY:O	2:H:364:LEU:C	2.46	0.54
2:P:454:GLY:O	2:P:457:TYR:HB2	2.08	0.54
1:I:137:PHE:CD1	2:J:17:VAL:HG21	2.43	0.54
2:N:95:ASN:O	2:N:582:PRO:HG3	2.07	0.54
2:L:91:LEU:O	2:L:567:HIS:HE1	1.89	0.54
1:C:134:ARG:HB2	1:C:139:ILE:O	2.07	0.54
2:N:533:MET:HE3	2:N:588:LEU:HD13	1.89	0.54
1:E:52:LEU:HD12	1:E:52:LEU:O	2.06	0.54
2:H:375:GLN:HG2	2:H:401:TYR:CE1	2.42	0.54
2:N:314:ILE:HD11	2:N:329:ILE:HD11	1.90	0.54
1:A:158:ALA:HA	2:B:62:THR:CG2	2.37	0.54
2:N:465:VAL:HG11	2:N:468:MET:HG3	1.89	0.54
2:J:477:ASP:OD2	2:J:504:ALA:HB2	2.08	0.54
2:L:350:GLU:HB3	3:V:209:LEU:HD21	1.89	0.54
2:J:455:LEU:HD22	2:J:483:PHE:HB2	1.88	0.54
2:H:54:HIS:ND1	2:H:55:VAL:N	2.56	0.54
2:P:357:GLY:CA	2:P:415:ARG:HH22	2.12	0.54
2:J:367:GLN:HG3	2:J:390:ILE:HA	1.89	0.54
1:M:99:PHE:CD2	2:N:16:THR:C	2.81	0.54
2:L:547:SER:HB3	2:L:564:HIS:CG	2.43	0.54
2:F:547:SER:HB3	2:F:564:HIS:HB3	1.88	0.54
2:H:428:VAL:HG11	2:H:443:PHE:CE2	2.42	0.54
2:P:227:VAL:HG13	2:P:228:GLY:N	2.22	0.54
2:D:468:MET:HE3	2:D:470:LEU:HD21	1.90	0.54
1:A:145:PRO:HB2	2:D:539:TYR:CE2	2.42	0.54
1:M:159:PHE:O	1:M:160:GLU:CB	2.47	0.54
1:M:160:GLU:HA	1:M:160:GLU:OE2	2.08	0.54
2:N:446:ARG:HG2	2:N:447:GLN:H	1.73	0.54
2:P:367:GLN:HB3	2:P:391:THR:CG2	2.34	0.54
2:H:506:ALA:HB1	2:H:535:MET:HB2	1.88	0.54
2:F:519:TRP:CZ3	2:F:567:HIS:CG	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:440:ARG:HB3	2:J:467:TRP:CE3	2.43	0.54
1:A:58:TYR:CE1	1:A:62:HIS:CE1	2.96	0.54
2:N:211:ASP:O	2:N:215:ILE:HG13	2.08	0.54
2:P:344:LEU:HD23	2:P:380:LEU:HD21	1.90	0.54
2:P:121:ARG:NH2	5:P:1103:PO4:O4	2.40	0.54
2:P:152:THR:HG22	2:P:177:SER:HB2	1.90	0.54
2:H:153:THR:CG2	2:H:178:GLU:HA	2.38	0.54
1:A:137:PHE:HD1	2:B:17:VAL:HG21	1.72	0.54
2:N:78:LEU:HD12	2:N:79:LYS:H	1.72	0.54
2:H:266:LEU:HD13	2:H:267:VAL:N	2.22	0.54
2:J:357:GLY:CA	2:J:415:ARG:HH22	2.13	0.54
1:A:160:GLU:OE2	1:A:160:GLU:HA	2.08	0.54
2:N:55:VAL:CG2	2:N:75:LEU:HD21	2.37	0.54
2:L:153:THR:HG23	2:L:178:GLU:HA	1.90	0.54
2:H:478:GLU:O	2:H:482:GLU:HG2	2.06	0.54
1:C:93:ILE:HD12	1:C:97:THR:CG2	2.32	0.54
2:D:521:GLN:HG3	2:D:567:HIS:HD2	1.71	0.54
1:E:128:LYS:HB3	1:E:132:GLU:HB2	1.91	0.54
2:L:490:LEU:HD11	2:L:493:LEU:HD13	1.90	0.54
2:L:261:GLU:HG2	2:L:264:MET:HG3	1.90	0.54
2:N:54:HIS:HE1	2:N:56:THR:OG1	1.91	0.54
2:N:357:GLY:CA	2:N:415:ARG:HH22	2.14	0.53
2:N:320:LEU:HD21	2:N:323:LEU:HB2	1.90	0.53
2:L:54:HIS:HE1	2:L:56:THR:OG1	1.90	0.53
2:J:227:VAL:CG1	2:J:228:GLY:N	2.71	0.53
2:P:143:LEU:HD23	2:P:159:ILE:HD13	1.90	0.53
2:B:521:GLN:HG3	2:B:567:HIS:CD2	2.43	0.53
2:F:80:LEU:HB2	2:F:122:MET:HE1	1.90	0.53
1:I:48:THR:HG22	1:I:51:ILE:HB	1.91	0.53
1:C:6:ILE:HD12	1:C:23:ALA:HB3	1.90	0.53
2:P:221:SER:O	2:P:223:VAL:HG23	2.08	0.53
1:E:105:ALA:HB3	1:E:114:LEU:CD1	2.32	0.53
2:N:143:LEU:CD2	2:N:159:ILE:HD13	2.38	0.53
2:L:101:THR:OG1	2:L:102:PRO:HD3	2.08	0.53
1:K:134:ARG:HB2	1:K:139:ILE:O	2.09	0.53
2:J:201:MET:HB3	3:U:211:ARG:HH12	1.74	0.53
2:F:65:PRO:HA	2:F:103:TRP:CZ3	2.44	0.53
2:L:314:ILE:HD11	2:L:329:ILE:HD11	1.90	0.53
2:F:85:ARG:NH1	5:F:1101:PO4:O3	2.41	0.53
1:K:113:LEU:O	1:K:117:THR:HG23	2.08	0.53
2:D:270:ARG:HB3	1:G:107:TYR:CD1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:HG22	1:C:51:ILE:CG1	2.38	0.53
1:I:6:ILE:HG22	1:I:7:VAL:N	2.24	0.53
2:B:501:SER:HA	2:B:524:ARG:HB2	1.91	0.53
1:A:98:LEU:HD21	1:A:120:THR:HG22	1.90	0.53
1:M:91:MET:O	1:M:93:ILE:N	2.40	0.53
1:K:91:MET:O	1:K:93:ILE:N	2.40	0.53
2:N:367:GLN:HG3	2:N:390:ILE:HA	1.90	0.53
2:B:294:GLN:NE2	1:O:107:TYR:OH	2.42	0.53
2:H:98:GLY:O	2:H:122:MET:HE3	2.08	0.53
2:J:547:SER:HB3	2:J:564:HIS:CG	2.44	0.53
2:L:465:VAL:HG11	2:L:468:MET:HG3	1.91	0.53
2:B:298:LEU:HB2	2:B:320:LEU:HD11	1.90	0.53
2:H:43:ARG:HH21	2:H:47:ILE:HD11	1.73	0.53
2:J:399:GLY:O	2:J:434:GLY:HA3	2.08	0.53
2:D:55:VAL:HG23	2:D:75:LEU:HD21	1.91	0.53
2:N:454:GLY:O	2:N:457:TYR:HB2	2.09	0.53
2:F:404:ASN:HA	2:F:437:LYS:HD2	1.89	0.53
2:H:111:LEU:C	2:H:113:GLN:H	2.10	0.53
1:C:91:MET:O	1:C:93:ILE:N	2.41	0.53
2:F:444:TYR:HA	2:F:471:GLY:CA	2.32	0.53
2:B:367:GLN:HB3	2:B:391:THR:CG2	2.34	0.53
2:B:184:LEU:HD12	2:B:207:ILE:HB	1.90	0.53
2:J:468:MET:HE3	2:J:470:LEU:HD21	1.91	0.53
1:I:153:ARG:HG2	1:I:157:TRP:CZ3	2.44	0.53
2:L:121:ARG:NH2	5:L:1103:PO4:O4	2.42	0.53
1:M:87:ASP:OD2	1:M:116:LEU:HD22	2.09	0.53
2:H:364:LEU:HD22	2:H:388:SER:N	2.24	0.53
2:F:367:GLN:HG3	2:F:390:ILE:HA	1.91	0.53
2:L:367:GLN:HG3	2:L:390:ILE:HA	1.89	0.53
2:H:423:PRO:HB3	2:H:425:ASP:OD2	2.09	0.53
1:C:134:ARG:HH11	2:D:40:VAL:HA	1.74	0.53
2:F:397:SER:O	2:F:400:THR:HG22	2.08	0.53
2:B:80:LEU:HB2	2:B:122:MET:HE1	1.91	0.53
2:D:63:ALA:HB1	2:D:67:ARG:HD2	1.91	0.53
1:A:159:PHE:O	1:A:160:GLU:CB	2.52	0.53
2:H:286:PRO:C	2:H:288:LEU:N	2.62	0.53
2:H:362:GLU:C	2:H:364:LEU:N	2.61	0.53
2:P:325:THR:O	2:P:349:ILE:HA	2.09	0.53
2:D:101:THR:CG2	2:D:128:ASP:OD1	2.56	0.53
2:F:311:CYS:HB3	2:F:336:VAL:HG21	1.91	0.53
2:F:153:THR:HG23	2:F:178:GLU:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:GLU:OE2	1:K:160:GLU:HA	2.09	0.53
1:E:11:SER:HA	1:E:45:PRO:HA	1.90	0.53
4:H:4100:OGK:C18	4:H:4100:OGK:HN08	2.21	0.53
1:M:102:ILE:HB	2:N:20:VAL:CG2	2.39	0.53
2:N:519:TRP:CZ3	2:N:567:HIS:CG	2.97	0.53
1:E:26:SER:OG	1:E:108:LEU:HB3	2.09	0.53
2:L:440:ARG:HB3	2:L:467:TRP:CE3	2.43	0.53
2:F:547:SER:HB3	2:F:564:HIS:CG	2.44	0.53
1:A:48:THR:HG22	1:A:51:ILE:CG1	2.39	0.53
2:H:97:GLY:HA3	2:H:123:ILE:CD1	2.38	0.53
2:D:443:PHE:CE2	2:D:445:LEU:HD11	2.44	0.53
2:D:455:LEU:HD22	2:D:483:PHE:HB2	1.90	0.53
1:K:93:ILE:HD12	1:K:97:THR:CG2	2.28	0.53
2:N:93:PRO:HA	2:N:548:ARG:CB	2.33	0.53
2:B:419:ILE:HD11	2:B:446:ARG:HH22	1.74	0.53
2:B:367:GLN:HG3	2:B:390:ILE:HA	1.90	0.53
2:H:65:PRO:HG3	2:H:103:TRP:CD2	2.44	0.53
2:N:59:LEU:O	2:N:62:THR:HB	2.08	0.53
1:O:158:ALA:HA	2:P:62:THR:CG2	2.39	0.53
1:M:134:ARG:CZ	1:M:141:ASN:HD22	2.22	0.53
2:J:227:VAL:HG13	2:J:228:GLY:N	2.23	0.53
2:H:214:THR:HA	2:H:217:ARG:HG2	1.91	0.53
2:N:197:LEU:O	2:N:225:VAL:HA	2.09	0.53
2:L:80:LEU:HB2	2:L:122:MET:CE	2.39	0.53
2:B:93:PRO:HA	2:B:548:ARG:CB	2.32	0.52
1:G:160:GLU:HB3	2:H:31:PRO:HB3	1.90	0.52
2:H:187:LEU:HB3	2:H:215:ILE:HD11	1.90	0.52
2:H:111:LEU:O	2:H:113:GLN:N	2.42	0.52
1:I:58:TYR:CD2	1:I:113:LEU:HD13	2.44	0.52
2:B:275:LEU:HD11	2:B:288:LEU:HD21	1.89	0.52
2:J:422:LEU:HB3	2:J:423:PRO:HD3	1.90	0.52
2:H:184:LEU:HD12	2:H:207:ILE:HB	1.91	0.52
2:L:542:ILE:HD11	2:L:588:LEU:CD1	2.24	0.52
2:H:280:MET:HE1	2:H:285:MET:HA	1.90	0.52
2:H:535:MET:CE	2:H:542:ILE:HG21	2.39	0.52
1:O:58:TYR:CD2	1:O:113:LEU:HD13	2.44	0.52
1:O:6:ILE:HD12	1:O:23:ALA:HB3	1.90	0.52
2:B:399:GLY:O	2:B:434:GLY:HA3	2.09	0.52
2:H:494:GLU:HG2	2:H:519:TRP:HB3	1.91	0.52
2:P:411:VAL:HG22	2:P:444:TYR:HB3	1.91	0.52
1:M:52:LEU:HD12	1:M:52:LEU:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:101:THR:HG22	2:N:128:ASP:HB3	1.90	0.52
2:H:492:LYS:HZ3	2:H:516:ARG:HH11	1.57	0.52
1:I:134:ARG:CZ	1:I:141:ASN:HD22	2.23	0.52
2:L:397:SER:O	2:L:400:THR:HG22	2.08	0.52
2:F:454:GLY:O	2:F:457:TYR:HB2	2.09	0.52
2:N:138:ASP:OD2	2:N:164:ARG:HG3	2.09	0.52
1:I:159:PHE:O	1:I:160:GLU:CB	2.49	0.52
1:M:102:ILE:CD1	2:N:20:VAL:CG2	2.88	0.52
2:P:546:PRO:HD3	2:P:584:THR:O	2.08	0.52
1:M:99:PHE:HB2	2:N:15:ALA:HB3	1.90	0.52
1:C:11:SER:HA	1:C:45:PRO:HA	1.90	0.52
2:D:190:HIS:ND1	2:H:112:ARG:HD2	2.24	0.52
2:F:337:LEU:HD12	2:F:341:CYS:SG	2.49	0.52
2:H:192:THR:HG22	2:H:218:ASN:O	2.10	0.52
2:D:54:HIS:HE1	2:D:56:THR:OG1	1.92	0.52
2:N:233:LEU:O	2:N:236:VAL:HG23	2.08	0.52
2:L:344:LEU:HD23	2:L:380:LEU:HD21	1.91	0.52
2:D:235:LEU:O	2:D:238:PHE:HB3	2.10	0.52
2:J:456:SER:HB2	2:J:482:GLU:HB3	1.91	0.52
2:H:354:ASP:O	2:H:354:ASP:OD2	2.28	0.52
1:C:160:GLU:OE2	1:C:160:GLU:HA	2.09	0.52
2:H:365:VAL:HG21	2:H:387:VAL:CA	2.39	0.52
2:F:289:PHE:HB2	2:F:290:PRO:HD3	1.91	0.52
2:D:519:TRP:CZ3	2:D:567:HIS:CG	2.97	0.52
2:P:55:VAL:CG2	2:P:75:LEU:HD21	2.37	0.52
2:H:402:LEU:HD13	2:H:405:LEU:HG	1.92	0.52
1:G:48:THR:HG22	1:G:51:ILE:CG1	2.39	0.52
2:J:232:ILE:HD12	2:J:252:SER:H	1.74	0.52
1:O:160:GLU:HA	1:O:160:GLU:OE2	2.10	0.52
2:L:446:ARG:HG2	2:L:447:GLN:H	1.74	0.52
2:D:547:SER:HB3	2:D:564:HIS:CG	2.43	0.52
1:C:26:SER:OG	1:C:108:LEU:HB3	2.10	0.52
2:N:547:SER:HB3	2:N:564:HIS:CG	2.44	0.52
1:O:137:PHE:HD1	2:P:17:VAL:HG21	1.72	0.52
2:P:275:LEU:HD11	2:P:288:LEU:HD21	1.91	0.52
2:P:501:SER:HA	2:P:524:ARG:HB2	1.92	0.52
2:P:446:ARG:HG2	2:P:447:GLN:H	1.74	0.52
2:N:472:TYR:OH	3:W:201:LEU:HB2	2.10	0.52
2:D:446:ARG:HG2	2:D:447:GLN:H	1.74	0.52
2:N:325:THR:O	2:N:349:ILE:HA	2.09	0.52
2:H:170:LEU:HD23	2:H:170:LEU:C	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:545:ILE:HG22	2:L:546:PRO:CD	2.40	0.52
1:I:158:ALA:HA	2:J:62:THR:HG21	1.90	0.52
2:L:235:LEU:O	2:L:238:PHE:HB3	2.10	0.52
2:F:521:GLN:HG3	2:F:567:HIS:CD2	2.45	0.52
2:L:521:GLN:HG3	2:L:567:HIS:CD2	2.44	0.52
2:D:275:LEU:HD11	2:D:288:LEU:HD21	1.92	0.52
2:N:130:ASP:OD1	2:N:134:LYS:HE3	2.09	0.52
1:K:153:ARG:NH2	2:L:539:TYR:CE1	2.78	0.52
2:D:375:GLN:HG2	2:D:401:TYR:CE1	2.45	0.52
2:N:456:SER:HB2	2:N:482:GLU:HB3	1.92	0.52
2:B:454:GLY:O	2:B:457:TYR:HB2	2.10	0.52
2:F:533:MET:HE3	2:F:588:LEU:HD13	1.91	0.52
2:F:411:VAL:HG22	2:F:444:TYR:HB3	1.92	0.52
2:D:367:GLN:HG3	2:D:390:ILE:HA	1.92	0.52
2:P:419:ILE:CD1	2:P:446:ARG:HH22	2.23	0.52
2:D:85:ARG:NH2	4:D:2100:OGK:O07	2.35	0.52
2:J:521:GLN:HG3	2:J:567:HIS:CD2	2.45	0.52
2:H:225:VAL:CG2	2:H:245:LEU:HD11	2.40	0.52
2:D:311:CYS:HB3	2:D:336:VAL:HG21	1.91	0.52
2:J:275:LEU:HD11	2:J:288:LEU:HD21	1.90	0.52
2:J:465:VAL:HG11	2:J:468:MET:HG3	1.91	0.52
2:B:54:HIS:HE1	2:B:56:THR:OG1	1.92	0.52
2:J:305:LEU:HD23	2:J:305:LEU:O	2.10	0.52
2:H:306:GLU:O	2:H:310:HIS:HD2	1.92	0.52
2:J:93:PRO:HA	2:J:548:ARG:CB	2.33	0.52
4:B:1100:OGK:C18	4:B:1100:OGK:HN08	2.19	0.52
2:J:85:ARG:NH2	4:J:5100:OGK:O07	2.33	0.52
2:N:298:LEU:HB2	2:N:320:LEU:HD11	1.92	0.52
2:P:407:ASP:OD1	2:P:440:ARG:HD2	2.10	0.52
2:H:328:VAL:HG12	2:H:359:GLU:HG2	1.92	0.52
2:F:422:LEU:HB3	2:F:423:PRO:HD3	1.92	0.52
2:L:404:ASN:HA	2:L:437:LYS:HD2	1.92	0.52
2:B:337:LEU:HD12	2:B:341:CYS:SG	2.50	0.52
2:J:80:LEU:HB2	2:J:122:MET:CE	2.39	0.52
1:C:137:PHE:CD1	2:D:17:VAL:HG21	2.45	0.52
1:E:93:ILE:HD12	1:E:97:THR:CG2	2.29	0.51
1:G:151:VAL:CG1	2:H:39:LEU:HD21	2.40	0.51
2:P:367:GLN:HG3	2:P:390:ILE:HA	1.92	0.51
2:D:519:TRP:CZ3	2:D:567:HIS:ND1	2.79	0.51
1:M:137:PHE:HD1	2:N:17:VAL:HG21	1.74	0.51
2:N:101:THR:CG2	2:N:128:ASP:OD1	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:ASN:ND2	2:D:194:LEU:H	2.07	0.51
2:N:310:HIS:O	2:N:314:ILE:CG1	2.58	0.51
2:H:302:TYR:N	2:H:302:TYR:CD2	2.74	0.51
2:P:80:LEU:HB2	2:P:122:MET:CE	2.40	0.51
2:H:532:LEU:HD11	2:H:568:ILE:HD13	1.92	0.51
2:P:456:SER:HB2	2:P:482:GLU:HB3	1.92	0.51
2:F:235:LEU:O	2:F:238:PHE:HB3	2.10	0.51
2:H:411:VAL:CG2	4:H:4100:OGK:H16A	2.40	0.51
2:B:367:GLN:O	2:B:371:ILE:HG22	2.09	0.51
1:M:112:ASN:C	1:M:114:LEU:N	2.62	0.51
2:N:456:SER:CB	2:N:482:GLU:HB3	2.40	0.51
2:L:477:ASP:OD2	2:L:504:ALA:HB2	2.10	0.51
2:P:233:LEU:O	2:P:236:VAL:HG23	2.11	0.51
2:P:251:GLY:O	2:P:278:SER:HB2	2.10	0.51
2:B:446:ARG:HG2	2:B:447:GLN:H	1.75	0.51
2:P:101:THR:OG1	2:P:102:PRO:HD3	2.10	0.51
2:P:398:ILE:HG23	2:P:402:LEU:HD11	1.92	0.51
2:F:233:LEU:O	2:F:236:VAL:HG23	2.09	0.51
2:H:418:ARG:HG2	2:H:446:ARG:NH1	2.25	0.51
2:H:455:LEU:HD21	2:H:473:VAL:CG2	2.40	0.51
1:C:158:ALA:HA	2:D:62:THR:HG21	1.91	0.51
2:D:298:LEU:HB2	2:D:320:LEU:HD11	1.93	0.51
1:A:11:SER:HA	1:A:45:PRO:HA	1.92	0.51
1:M:87:ASP:HB3	1:M:116:LEU:HD21	1.92	0.51
2:H:406:CYS:HA	2:H:438:LEU:HA	1.92	0.51
2:J:235:LEU:O	2:J:238:PHE:HB3	2.10	0.51
2:F:63:ALA:HB1	2:F:67:ARG:HD2	1.91	0.51
2:B:455:LEU:HD22	2:B:483:PHE:HB2	1.91	0.51
2:D:93:PRO:HA	2:D:548:ARG:CB	2.32	0.51
2:H:65:PRO:HA	2:H:103:TRP:CZ3	2.44	0.51
2:B:143:LEU:CD2	2:B:159:ILE:HD13	2.40	0.51
1:E:48:THR:HG22	1:E:51:ILE:CG1	2.40	0.51
1:O:48:THR:CG2	1:O:51:ILE:HG12	2.41	0.51
2:N:153:THR:HG23	2:N:178:GLU:HA	1.93	0.51
2:H:424:LEU:O	2:H:426:ASN:N	2.43	0.51
2:N:337:LEU:HD12	2:N:341:CYS:SG	2.51	0.51
2:N:542:ILE:CD1	2:N:588:LEU:HD12	2.28	0.51
2:H:382:TYR:CD2	2:H:407:ASP:HB3	2.46	0.51
1:A:52:LEU:HD12	1:A:52:LEU:O	2.10	0.51
2:F:546:PRO:HD3	2:F:584:THR:O	2.08	0.51
1:A:105:ALA:HB2	1:A:113:LEU:HD23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:48:THR:HG22	1:M:51:ILE:CG1	2.40	0.51
2:J:311:CYS:HB3	2:J:336:VAL:HG21	1.91	0.51
1:I:48:THR:HG22	1:I:51:ILE:CG1	2.40	0.51
2:F:255:GLU:HG3	2:F:255:GLU:O	2.11	0.51
2:H:278:SER:C	2:H:280:MET:H	2.13	0.51
2:H:496:ARG:HD2	4:H:4100:OGK:H23A	1.92	0.51
1:A:134:ARG:HH11	2:B:40:VAL:HA	1.75	0.51
2:P:63:ALA:HB1	2:P:67:ARG:HD2	1.91	0.51
1:A:153:ARG:NH2	2:B:539:TYR:CE1	2.79	0.51
2:J:501:SER:HA	2:J:524:ARG:HB2	1.92	0.51
2:D:422:LEU:HB3	2:D:423:PRO:HD3	1.93	0.51
2:P:247:GLU:HA	2:P:274:ARG:O	2.11	0.51
2:H:306:GLU:OE2	2:H:306:GLU:HA	2.09	0.51
2:L:519:TRP:HH2	2:L:567:HIS:CE1	2.29	0.51
2:P:191:ASN:ND2	2:P:194:LEU:H	2.06	0.51
2:F:298:LEU:HB2	2:F:320:LEU:HD11	1.92	0.51
1:K:137:PHE:HD1	2:L:17:VAL:HG21	1.76	0.51
1:K:48:THR:HG22	1:K:51:ILE:CG1	2.41	0.51
2:P:232:ILE:HD12	2:P:252:SER:H	1.76	0.51
2:L:78:LEU:HD12	2:L:79:LYS:H	1.76	0.51
1:O:91:MET:CE	1:O:117:THR:HG22	2.41	0.51
2:F:367:GLN:O	2:F:371:ILE:HG22	2.10	0.51
2:P:78:LEU:HD12	2:P:79:LYS:H	1.74	0.51
2:D:310:HIS:O	2:D:314:ILE:HG12	2.11	0.51
1:O:91:MET:O	1:O:93:ILE:N	2.44	0.51
2:H:414:ASP:HB3	2:H:446:ARG:HH21	1.76	0.51
1:O:11:SER:HA	1:O:45:PRO:HA	1.92	0.51
2:F:272:LEU:HD21	2:F:275:LEU:HB3	1.92	0.51
2:B:272:LEU:HD21	2:B:275:LEU:HB3	1.93	0.51
2:N:422:LEU:HB3	2:N:423:PRO:HD3	1.93	0.51
2:F:501:SER:HA	2:F:524:ARG:HB2	1.93	0.51
2:F:305:LEU:HD23	2:F:305:LEU:O	2.11	0.51
2:H:365:VAL:HG21	2:H:387:VAL:CG1	2.39	0.50
2:H:390:ILE:HD11	2:H:412:LEU:CD2	2.41	0.50
2:H:409:ARG:HD2	4:H:4100:OGK:H13A	1.92	0.50
2:B:519:TRP:HH2	2:B:567:HIS:CE1	2.29	0.50
2:B:546:PRO:HD3	2:B:584:THR:O	2.11	0.50
2:B:320:LEU:HD21	2:B:323:LEU:HB2	1.93	0.50
2:D:272:LEU:HD21	2:D:275:LEU:HB3	1.92	0.50
1:M:153:ARG:HG2	1:M:157:TRP:CZ3	2.46	0.50
2:B:153:THR:HG23	2:B:178:GLU:HA	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:LEU:O	2:B:305:LEU:HD23	2.11	0.50
2:B:255:GLU:HG3	2:B:255:GLU:O	2.11	0.50
2:F:542:ILE:CD1	2:F:588:LEU:HD12	2.30	0.50
2:F:143:LEU:CD2	2:F:159:ILE:HD13	2.41	0.50
1:C:134:ARG:NH1	2:D:40:VAL:HA	2.26	0.50
2:B:482:GLU:O	2:B:485:ARG:HG2	2.11	0.50
2:B:357:GLY:CA	2:B:415:ARG:HH22	2.12	0.50
2:P:289:PHE:HB2	2:P:290:PRO:HD3	1.92	0.50
2:H:370:LEU:HB2	2:H:394:SER:HB3	1.93	0.50
2:F:398:ILE:O	2:F:402:LEU:HD12	2.12	0.50
2:H:291:PHE:N	2:H:291:PHE:CD2	2.79	0.50
2:P:65:PRO:HA	2:P:103:TRP:CZ3	2.46	0.50
2:L:482:GLU:O	2:L:485:ARG:HG2	2.11	0.50
2:F:110:ASN:HA	2:L:190:HIS:HE1	1.77	0.50
2:P:153:THR:HG23	2:P:178:GLU:HA	1.92	0.50
1:C:91:MET:O	1:C:93:ILE:HG12	2.12	0.50
2:H:87:ALA:HB2	2:H:92:ILE:HB	1.93	0.50
1:K:128:LYS:HB3	1:K:132:GLU:HB2	1.93	0.50
2:H:230:PHE:CB	2:H:235:LEU:HD21	2.41	0.50
1:I:158:ALA:HA	2:J:62:THR:CG2	2.41	0.50
2:P:159:ILE:HD12	2:P:166:ILE:HD11	1.93	0.50
2:F:95:ASN:O	2:F:582:PRO:HG3	2.12	0.50
2:D:456:SER:HB2	2:D:482:GLU:HB3	1.94	0.50
2:H:432:LEU:HD11	2:H:458:ILE:HD13	1.93	0.50
2:N:523:TYR:CE2	2:N:568:ILE:HD11	2.47	0.50
2:J:519:TRP:HH2	2:J:567:HIS:CE1	2.30	0.50
2:B:440:ARG:HB3	2:B:467:TRP:CE3	2.45	0.50
2:B:80:LEU:HB2	2:B:122:MET:CE	2.41	0.50
2:B:130:ASP:OD1	2:B:134:LYS:HE3	2.12	0.50
2:L:233:LEU:O	2:L:236:VAL:HG23	2.11	0.50
2:H:145:LEU:O	2:H:171:MET:HA	2.10	0.50
2:J:419:ILE:HD11	2:J:446:ARG:HH22	1.75	0.50
1:K:105:ALA:HB2	1:K:113:LEU:HD23	1.93	0.50
2:D:20:VAL:O	2:D:24:VAL:HG23	2.11	0.50
2:P:422:LEU:HB3	2:P:423:PRO:HD3	1.93	0.50
2:H:464:ASN:O	2:H:466:ARG:HD2	2.11	0.50
2:P:289:PHE:HD1	2:P:316:LYS:HD2	1.73	0.50
2:J:289:PHE:HB2	2:J:290:PRO:HD3	1.93	0.50
1:A:128:LYS:HB3	1:A:132:GLU:HB2	1.94	0.50
2:B:159:ILE:HD12	2:B:166:ILE:HD11	1.94	0.50
1:E:48:THR:HG22	1:E:51:ILE:CB	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:477:ASP:OD2	2:F:504:ALA:HB2	2.12	0.50
2:H:392:ASN:ND2	2:H:422:LEU:HD13	2.26	0.50
1:K:26:SER:HB3	1:K:29:ILE:HG13	1.93	0.50
1:I:128:LYS:HB3	1:I:132:GLU:HB2	1.94	0.50
2:F:465:VAL:HG11	2:F:468:MET:HG3	1.93	0.50
2:J:398:ILE:HG23	2:J:402:LEU:HD11	1.94	0.50
2:H:289:PHE:N	2:H:290:PRO:CD	2.74	0.50
2:H:282:PRO:HB3	2:H:309:ASP:OD2	2.11	0.50
2:H:496:ARG:HB2	4:H:4100:OGK:H01A	1.94	0.50
2:H:367:GLN:N	2:H:367:GLN:CD	2.65	0.50
2:L:320:LEU:HD21	2:L:323:LEU:HB2	1.93	0.50
1:M:130:PRO:O	1:M:134:ARG:HG2	2.12	0.50
2:P:482:GLU:O	2:P:485:ARG:HG2	2.12	0.50
2:N:227:VAL:CG1	2:N:228:GLY:N	2.74	0.50
2:F:197:LEU:O	2:F:225:VAL:HA	2.12	0.50
2:B:232:ILE:HD12	2:B:252:SER:H	1.76	0.50
2:F:232:ILE:HD12	2:F:252:SER:H	1.76	0.50
1:G:113:LEU:O	1:G:117:THR:HG23	2.11	0.50
1:K:91:MET:O	1:K:93:ILE:HG12	2.12	0.49
2:P:419:ILE:HD11	2:P:446:ARG:HH22	1.75	0.49
2:J:164:ARG:HH21	2:N:136:ARG:HH21	1.60	0.49
2:D:407:ASP:OD1	2:D:440:ARG:HD2	2.12	0.49
2:H:191:ASN:ND2	2:H:194:LEU:H	2.08	0.49
1:O:113:LEU:HG	1:O:113:LEU:O	2.12	0.49
1:G:11:SER:HA	1:G:45:PRO:HA	1.94	0.49
2:H:516:ARG:HA	2:H:572:TYR:HD1	1.75	0.49
2:P:465:VAL:HG11	2:P:468:MET:HG3	1.94	0.49
2:B:310:HIS:O	2:B:314:ILE:CG1	2.58	0.49
2:J:80:LEU:HB2	2:J:122:MET:HE1	1.94	0.49
2:P:80:LEU:HB2	2:P:122:MET:HE1	1.94	0.49
2:D:310:HIS:O	2:D:314:ILE:CG1	2.60	0.49
2:J:54:HIS:HE1	2:J:56:THR:OG1	1.95	0.49
2:H:289:PHE:N	2:H:290:PRO:HD2	2.27	0.49
1:M:102:ILE:CB	2:N:20:VAL:CG2	2.90	0.49
2:N:565:PRO:HG2	3:W:201:LEU:HD21	1.94	0.49
2:H:191:ASN:ND2	2:H:193:SER:H	2.10	0.49
1:O:134:ARG:CZ	1:O:141:ASN:HD22	2.25	0.49
2:D:398:ILE:HG23	2:D:402:LEU:HD11	1.94	0.49
2:L:310:HIS:O	2:L:314:ILE:HG12	2.12	0.49
2:H:97:GLY:CA	2:H:123:ILE:HD11	2.42	0.49
2:P:477:ASP:OD2	2:P:504:ALA:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:MET:O	1:E:93:ILE:N	2.45	0.49
2:H:387:VAL:HG11	2:H:390:ILE:CD1	2.39	0.49
1:K:132:GLU:O	1:K:136:THR:HG23	2.12	0.49
2:J:519:TRP:CZ3	2:J:567:HIS:CG	3.01	0.49
2:H:357:GLY:C	2:H:359:GLU:N	2.66	0.49
1:C:134:ARG:CZ	1:C:141:ASN:HD22	2.24	0.49
2:P:138:ASP:OD2	2:P:164:ARG:HG3	2.12	0.49
2:N:357:GLY:HA2	2:N:415:ARG:NH2	2.14	0.49
2:L:519:TRP:CZ3	2:L:567:HIS:CG	3.00	0.49
2:B:350:GLU:HB3	3:Q:209:LEU:CD2	2.40	0.49
1:C:58:TYR:CE1	1:C:62:HIS:CE1	3.00	0.49
2:P:468:MET:CE	2:P:470:LEU:HD11	2.42	0.49
1:A:134:ARG:NH1	2:B:40:VAL:HA	2.27	0.49
2:P:159:ILE:HG13	2:P:160:VAL:N	2.26	0.49
2:D:65:PRO:HA	2:D:103:TRP:CZ3	2.48	0.49
2:N:116:SER:CB	2:N:142:THR:HG23	2.36	0.49
1:A:91:MET:O	1:A:93:ILE:HG12	2.13	0.49
1:I:91:MET:O	1:I:93:ILE:N	2.42	0.49
2:H:487:CYS:HB3	2:H:490:LEU:HB2	1.95	0.49
2:B:519:TRP:CZ3	2:B:567:HIS:CG	3.00	0.49
2:H:492:LYS:HZ3	2:H:516:ARG:NH1	2.09	0.49
2:B:419:ILE:CD1	2:B:446:ARG:HH22	2.26	0.49
2:J:411:VAL:HG22	2:J:444:TYR:HB3	1.93	0.49
1:G:10:SER:OG	1:G:11:SER:N	2.46	0.49
2:N:159:ILE:HG13	2:N:160:VAL:N	2.27	0.49
2:H:428:VAL:CG1	2:H:443:PHE:CZ	2.96	0.49
1:M:48:THR:HG22	1:M:51:ILE:CB	2.42	0.49
2:J:159:ILE:HD12	2:J:166:ILE:HD11	1.94	0.49
1:K:134:ARG:HH11	2:L:40:VAL:HA	1.76	0.49
2:L:80:LEU:HB2	2:L:122:MET:HE1	1.95	0.49
2:N:375:GLN:HG2	2:N:401:TYR:CE1	2.48	0.49
2:D:211:ASP:O	2:D:215:ILE:HG13	2.12	0.49
2:J:404:ASN:HA	2:J:437:LYS:HD2	1.94	0.49
2:J:443:PHE:CE2	2:J:445:LEU:HD11	2.48	0.49
2:P:248:PHE:CD2	2:P:248:PHE:C	2.86	0.49
1:A:26:SER:OG	1:A:108:LEU:HB3	2.13	0.49
1:O:128:LYS:HB3	1:O:132:GLU:HB2	1.94	0.49
2:N:289:PHE:HB2	2:N:290:PRO:HD3	1.94	0.49
2:D:519:TRP:HH2	2:D:567:HIS:CE1	2.31	0.49
1:C:128:LYS:HB3	1:C:132:GLU:HB2	1.95	0.49
2:F:295:ILE:HG21	2:F:298:LEU:CD1	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:320:LEU:HD21	2:P:323:LEU:HB2	1.93	0.49
2:F:407:ASP:OD1	2:F:440:ARG:HD2	2.12	0.49
2:H:83:LYS:O	2:H:121:ARG:NH1	2.35	0.49
2:N:235:LEU:O	2:N:238:PHE:HB3	2.12	0.49
2:L:223:VAL:O	2:L:245:LEU:HD12	2.13	0.49
2:H:332:ARG:O	2:H:336:VAL:HG23	2.13	0.49
2:H:450:LEU:HD11	2:H:454:GLY:CA	2.39	0.49
2:H:450:LEU:CG	2:H:454:GLY:HA3	2.43	0.49
2:B:546:PRO:O	2:B:547:SER:HB2	2.13	0.49
2:J:490:LEU:HD11	2:J:493:LEU:HD13	1.94	0.49
1:O:10:SER:OG	1:O:11:SER:N	2.46	0.49
2:L:227:VAL:HG13	2:L:228:GLY:H	1.76	0.49
2:N:400:THR:O	2:N:403:LYS:HE2	2.12	0.49
1:O:153:ARG:HG2	1:O:157:TRP:CZ3	2.48	0.49
2:J:482:GLU:O	2:J:485:ARG:HG2	2.13	0.49
2:H:431:LEU:HD23	2:H:432:LEU:N	2.27	0.49
2:L:255:GLU:HG3	2:L:255:GLU:O	2.13	0.49
2:N:170:LEU:HD23	2:N:170:LEU:C	2.33	0.49
2:P:255:GLU:O	2:P:255:GLU:HG3	2.13	0.49
2:H:153:THR:HG23	2:H:178:GLU:HA	1.95	0.49
2:F:409:ARG:HD3	4:F:3100:OGK:H13A	1.93	0.49
1:I:134:ARG:HH11	2:J:40:VAL:HA	1.77	0.49
2:L:275:LEU:HD11	2:L:288:LEU:HD21	1.93	0.49
2:D:482:GLU:O	2:D:485:ARG:HG2	2.12	0.49
2:D:247:GLU:HA	2:D:274:ARG:O	2.12	0.49
2:P:130:ASP:OD1	2:P:134:LYS:HE3	2.12	0.49
2:N:469:LEU:HA	2:N:494:GLU:O	2.11	0.49
2:H:385:VAL:HG12	2:H:387:VAL:HG23	1.95	0.49
2:H:259:MET:N	2:H:260:PRO:HD3	2.28	0.49
2:H:57:MET:HB2	2:H:80:LEU:HD23	1.95	0.49
2:N:311:CYS:CB	2:N:336:VAL:HG21	2.43	0.49
2:L:298:LEU:HB2	2:L:320:LEU:HD11	1.94	0.49
2:F:490:LEU:HD11	2:F:493:LEU:HD13	1.95	0.49
2:J:153:THR:HG23	2:J:178:GLU:HA	1.94	0.49
1:K:159:PHE:O	1:K:160:GLU:CB	2.50	0.48
2:D:57:MET:CE	2:D:62:THR:HG22	2.43	0.48
2:N:546:PRO:O	2:N:547:SER:HB2	2.12	0.48
2:H:43:ARG:NH2	2:H:47:ILE:HD11	2.28	0.48
1:K:134:ARG:NH1	2:L:40:VAL:HA	2.28	0.48
2:J:397:SER:O	2:J:400:THR:HG22	2.13	0.48
2:L:538:PRO:O	2:L:539:TYR:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:96:TRP:O	2:N:578:ARG:NH2	2.41	0.48
2:D:153:THR:HG23	2:D:178:GLU:HA	1.95	0.48
2:N:152:THR:HG22	2:N:177:SER:HB2	1.95	0.48
2:F:538:PRO:O	2:F:539:TYR:HB2	2.13	0.48
2:B:321:GLU:HA	2:B:344:LEU:HA	1.94	0.48
2:L:546:PRO:HD3	2:L:584:THR:O	2.11	0.48
2:N:57:MET:CE	2:N:62:THR:HG22	2.43	0.48
1:K:58:TYR:CD2	1:K:113:LEU:HD13	2.47	0.48
2:J:400:THR:O	2:J:403:LYS:HE2	2.13	0.48
2:N:482:GLU:O	2:N:485:ARG:HG2	2.13	0.48
2:L:501:SER:HA	2:L:524:ARG:HB2	1.95	0.48
2:H:526:SER:O	2:H:527:MET:C	2.52	0.48
2:H:326:ARG:O	2:H:329:ILE:HG22	2.12	0.48
2:H:85:ARG:NH1	5:H:1101:PO4:O2	2.45	0.48
2:B:282:PRO:HA	2:B:285:MET:CE	2.44	0.48
2:L:419:ILE:CD1	2:L:446:ARG:HH22	2.27	0.48
2:P:519:TRP:CZ3	2:P:567:HIS:CG	3.01	0.48
2:F:519:TRP:CZ3	2:F:567:HIS:ND1	2.81	0.48
1:A:48:THR:CG2	1:A:51:ILE:HG12	2.43	0.48
2:B:176:PHE:CZ	2:B:204:PHE:CZ	3.01	0.48
2:F:247:GLU:HA	2:F:274:ARG:O	2.13	0.48
2:J:255:GLU:HG3	2:J:255:GLU:O	2.12	0.48
2:D:255:GLU:O	2:D:255:GLU:HG3	2.13	0.48
2:H:454:GLY:O	2:H:457:TYR:HB2	2.12	0.48
1:M:128:LYS:HB2	1:M:133:ILE:CD1	2.43	0.48
2:N:419:ILE:CD1	2:N:446:ARG:HH22	2.26	0.48
1:E:134:ARG:HH11	2:F:40:VAL:HA	1.78	0.48
2:L:519:TRP:CZ3	2:L:567:HIS:ND1	2.82	0.48
2:J:546:PRO:HD3	2:J:584:THR:O	2.14	0.48
1:O:48:THR:HG22	1:O:51:ILE:CB	2.43	0.48
2:D:397:SER:O	2:D:400:THR:HG22	2.13	0.48
2:P:456:SER:CB	2:P:482:GLU:HB3	2.43	0.48
2:F:231:GLU:HG2	2:F:254:ASN:HD22	1.78	0.48
2:F:152:THR:HG22	2:F:177:SER:HB2	1.95	0.48
2:L:578:ARG:HG3	2:L:578:ARG:H	1.44	0.48
2:B:247:GLU:HA	2:B:274:ARG:O	2.14	0.48
2:D:399:GLY:O	2:D:434:GLY:HA3	2.13	0.48
2:F:46:LYS:HE3	2:F:46:LYS:HB2	1.61	0.48
2:H:486:GLY:O	2:H:487:CYS:C	2.51	0.48
2:L:85:ARG:NH1	5:L:1101:PO4:O3	2.46	0.48
2:J:519:TRP:CZ3	2:J:567:HIS:ND1	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:159:ILE:HD12	2:N:166:ILE:HD11	1.95	0.48
1:C:153:ARG:NH2	2:D:539:TYR:CE1	2.81	0.48
2:H:476:SER:C	2:H:478:GLU:H	2.16	0.48
2:B:539:TYR:OH	1:C:146:GLU:HA	2.13	0.48
2:D:454:GLY:O	2:D:457:TYR:HB2	2.14	0.48
1:I:111:LYS:O	1:I:115:ASP:HB2	2.12	0.48
2:L:454:GLY:O	2:L:457:TYR:HB2	2.13	0.48
2:N:501:SER:HA	2:N:524:ARG:HB2	1.95	0.48
2:D:296:ARG:NH2	1:G:37:CYS:SG	2.87	0.48
2:D:305:LEU:HD23	2:D:305:LEU:O	2.13	0.48
2:J:454:GLY:O	2:J:457:TYR:HB2	2.14	0.48
2:H:364:LEU:HD21	2:H:386:TYR:O	2.13	0.48
2:J:546:PRO:O	2:J:547:SER:HB2	2.13	0.48
2:H:391:THR:C	2:H:393:GLU:N	2.67	0.48
2:J:295:ILE:HG21	2:J:298:LEU:CD1	2.43	0.48
1:G:137:PHE:HB3	2:H:17:VAL:CG2	2.43	0.48
2:N:80:LEU:HB2	2:N:122:MET:HE2	1.95	0.48
1:G:48:THR:CG2	1:G:51:ILE:HG12	2.44	0.48
2:L:398:ILE:O	2:L:402:LEU:HD12	2.12	0.48
2:H:316:LYS:O	2:H:318:PRO:HD3	2.14	0.48
2:F:446:ARG:HG2	2:F:447:GLN:N	2.28	0.48
2:D:546:PRO:HD3	2:D:584:THR:O	2.13	0.48
2:F:101:THR:HG22	2:F:128:ASP:HB3	1.95	0.48
2:B:477:ASP:N	2:B:477:ASP:OD1	2.46	0.48
2:J:456:SER:CB	2:J:482:GLU:HB3	2.43	0.48
2:H:431:LEU:CD2	2:H:432:LEU:HD23	2.43	0.48
1:E:153:ARG:HG2	1:E:157:TRP:CZ3	2.49	0.48
2:F:127:LEU:HD21	2:F:131:ARG:NH2	2.28	0.48
2:B:170:LEU:HD23	2:B:170:LEU:C	2.34	0.48
1:I:26:SER:HB3	1:I:29:ILE:HG13	1.96	0.48
2:N:419:ILE:HD11	2:N:446:ARG:HH22	1.79	0.48
2:L:289:PHE:HD1	2:L:316:LYS:HD2	1.73	0.48
2:H:542:ILE:HD11	2:H:588:LEU:HD12	1.96	0.48
2:H:57:MET:HE2	2:H:62:THR:HG22	1.95	0.48
1:M:11:SER:HA	1:M:45:PRO:HA	1.96	0.48
2:N:545:ILE:HG22	2:N:546:PRO:CD	2.44	0.48
1:A:105:ALA:HB3	1:A:114:LEU:HD13	1.94	0.48
2:D:465:VAL:HG11	2:D:468:MET:HG3	1.96	0.48
2:L:477:ASP:OD1	2:L:477:ASP:N	2.47	0.48
2:L:456:SER:HB2	2:L:482:GLU:HB3	1.94	0.48
2:J:121:ARG:NH2	5:J:1103:PO4:O4	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:176:PHE:CZ	2:P:204:PHE:CZ	3.02	0.48
2:H:21:ILE:HD12	2:H:24:VAL:HB	1.95	0.48
2:N:282:PRO:HA	2:N:285:MET:CE	2.43	0.48
1:E:134:ARG:CZ	1:E:141:ASN:HD22	2.26	0.48
2:H:492:LYS:HZ1	2:H:516:ARG:NH1	2.10	0.48
2:N:392:ASN:HD21	2:N:424:LEU:HA	1.77	0.48
2:L:251:GLY:O	2:L:278:SER:HB2	2.13	0.48
2:D:176:PHE:CZ	2:D:204:PHE:CZ	3.01	0.48
2:H:365:VAL:HG21	2:H:387:VAL:HA	1.95	0.48
2:L:419:ILE:HD11	2:L:446:ARG:HH22	1.79	0.48
2:P:521:GLN:HG3	2:P:567:HIS:CD2	2.48	0.48
2:H:170:LEU:HB2	2:H:198:ASN:HB3	1.95	0.48
2:H:477:ASP:OD2	2:H:501:SER:OG	2.23	0.48
1:A:48:THR:HG22	1:A:51:ILE:CB	2.43	0.48
1:G:6:ILE:HG22	1:G:7:VAL:N	2.28	0.48
2:N:387:VAL:O	2:N:413:LEU:HD22	2.14	0.48
2:F:523:TYR:CE2	2:F:568:ILE:HD11	2.49	0.48
1:K:11:SER:HA	1:K:45:PRO:HA	1.95	0.48
2:F:96:TRP:O	2:F:578:ARG:NH2	2.42	0.48
2:D:321:GLU:HA	2:D:344:LEU:HA	1.96	0.48
2:L:127:LEU:HD21	2:L:131:ARG:NH2	2.29	0.48
2:P:170:LEU:HD23	2:P:170:LEU:C	2.34	0.48
1:E:45:PRO:CB	2:L:291:PHE:HA	2.44	0.47
2:H:412:LEU:HD12	2:H:445:LEU:CA	2.44	0.47
2:L:367:GLN:O	2:L:371:ILE:HG22	2.14	0.47
2:D:367:GLN:O	2:D:371:ILE:HG22	2.14	0.47
2:B:519:TRP:CZ3	2:B:567:HIS:ND1	2.82	0.47
2:J:545:ILE:HG22	2:J:546:PRO:CD	2.43	0.47
2:L:298:LEU:HD23	2:L:300:LEU:HD11	1.95	0.47
1:E:48:THR:HG23	1:E:51:ILE:H	1.79	0.47
1:O:134:ARG:HH11	2:P:40:VAL:HA	1.78	0.47
2:N:191:ASN:ND2	2:N:194:LEU:H	2.12	0.47
2:N:443:PHE:CE2	2:N:445:LEU:HD11	2.48	0.47
2:H:364:LEU:HD22	2:H:365:VAL:HG22	1.96	0.47
2:J:164:ARG:HD2	2:N:112:ARG:CZ	2.45	0.47
2:N:519:TRP:CZ3	2:N:567:HIS:ND1	2.82	0.47
2:N:289:PHE:HD1	2:N:316:LYS:HD2	1.76	0.47
2:J:298:LEU:HB2	2:J:320:LEU:HD11	1.96	0.47
2:D:295:ILE:HG21	2:D:298:LEU:CD1	2.43	0.47
2:B:227:VAL:HG13	2:B:228:GLY:H	1.78	0.47
2:N:351:ARG:O	2:N:351:ARG:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:THR:CG2	1:I:51:ILE:HG12	2.43	0.47
2:L:456:SER:CB	2:L:482:GLU:HB3	2.44	0.47
2:H:247:GLU:HA	2:H:274:ARG:O	2.14	0.47
2:H:114:LEU:O	2:H:136:ARG:NH1	2.48	0.47
2:H:64:THR:O	2:H:65:PRO:C	2.51	0.47
2:H:204:PHE:O	2:H:206:LYS:N	2.47	0.47
2:N:490:LEU:HD11	2:N:493:LEU:HD13	1.96	0.47
1:M:48:THR:CG2	1:M:51:ILE:HG12	2.45	0.47
1:G:120:THR:O	1:G:124:MET:HG3	2.14	0.47
1:C:48:THR:CG2	1:C:51:ILE:HG12	2.44	0.47
2:D:477:ASP:OD2	2:D:504:ALA:HB2	2.12	0.47
2:J:63:ALA:HB1	2:J:67:ARG:HD2	1.96	0.47
2:N:171:MET:O	2:N:174:SER:HB2	2.14	0.47
2:J:247:GLU:HA	2:J:274:ARG:O	2.14	0.47
2:D:232:ILE:HD12	2:D:252:SER:H	1.79	0.47
2:N:176:PHE:CZ	2:N:204:PHE:CZ	3.02	0.47
2:D:412:LEU:HD12	2:D:412:LEU:C	2.35	0.47
2:H:280:MET:HG2	2:H:280:MET:O	2.14	0.47
2:J:446:ARG:HG2	2:J:447:GLN:N	2.29	0.47
2:F:297:LYS:HE3	2:F:297:LYS:HB2	1.65	0.47
2:L:545:ILE:HG22	2:L:546:PRO:N	2.30	0.47
2:N:297:LYS:HB2	2:N:297:LYS:HE3	1.62	0.47
2:D:565:PRO:HG2	3:R:201:LEU:HD21	1.97	0.47
2:P:440:ARG:HB3	2:P:467:TRP:CE3	2.45	0.47
1:I:11:SER:HA	1:I:45:PRO:HA	1.95	0.47
2:N:247:GLU:HA	2:N:274:ARG:O	2.14	0.47
2:D:501:SER:HA	2:D:524:ARG:HB2	1.96	0.47
2:N:248:PHE:CD2	2:N:248:PHE:C	2.87	0.47
2:B:248:PHE:CD2	2:B:248:PHE:C	2.87	0.47
1:E:105:ALA:HB2	1:E:113:LEU:HD23	1.96	0.47
2:H:89:PHE:CE2	4:H:4100:OGK:H04A	2.50	0.47
2:D:289:PHE:HD1	2:D:316:LYS:HD2	1.73	0.47
1:E:132:GLU:O	1:E:136:THR:HG23	2.15	0.47
2:B:465:VAL:HG11	2:B:468:MET:HG3	1.95	0.47
1:K:134:ARG:CZ	1:K:141:ASN:HD22	2.28	0.47
2:J:398:ILE:C	2:J:400:THR:H	2.17	0.47
2:F:138:ASP:OD2	2:F:164:ARG:HG3	2.14	0.47
2:B:422:LEU:HB3	2:B:423:PRO:HD3	1.96	0.47
2:H:315:GLN:HG3	2:H:340:TYR:CE1	2.50	0.47
1:I:52:LEU:HD12	1:I:52:LEU:O	2.14	0.47
2:H:262:LYS:HD2	2:H:263:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:LEU:HB2	2:D:122:MET:HE1	1.96	0.47
2:P:477:ASP:OD1	2:P:477:ASP:N	2.48	0.47
2:P:543:GLU:OE2	2:P:578:ARG:HD3	2.13	0.47
2:H:269:PRO:O	2:H:270:ARG:C	2.52	0.47
2:F:375:GLN:HG2	2:F:401:TYR:CE1	2.49	0.47
2:H:53:GLU:O	2:H:75:LEU:HD22	2.15	0.47
2:H:153:THR:HG23	2:H:177:SER:O	2.15	0.47
2:H:52:ARG:NH1	2:H:72:PHE:HZ	2.11	0.47
2:J:285:MET:N	2:J:286:PRO:CD	2.78	0.47
2:P:546:PRO:O	2:P:547:SER:HB2	2.15	0.47
1:C:26:SER:HB3	1:C:29:ILE:HG13	1.96	0.47
2:D:320:LEU:HD21	2:D:323:LEU:HB2	1.97	0.47
1:C:52:LEU:HD12	1:C:52:LEU:O	2.14	0.47
2:J:57:MET:CE	2:J:62:THR:HG22	2.43	0.47
2:P:398:ILE:O	2:P:402:LEU:HD12	2.14	0.47
2:H:532:LEU:O	2:H:534:GLN:N	2.48	0.47
2:L:543:GLU:OE2	2:L:578:ARG:HD3	2.15	0.47
2:L:339:GLN:HA	2:L:342:LYS:HE2	1.96	0.47
2:L:247:GLU:HA	2:L:274:ARG:O	2.13	0.47
2:D:95:ASN:O	2:D:582:PRO:HG3	2.15	0.47
2:P:444:TYR:HA	2:P:471:GLY:CA	2.37	0.47
1:E:26:SER:HB3	1:E:29:ILE:HG13	1.97	0.47
1:I:35:ASP:CB	2:N:243:ALA:HB1	2.42	0.47
2:H:367:GLN:CA	2:H:367:GLN:OE1	2.62	0.47
2:P:298:LEU:HB2	2:P:320:LEU:HD11	1.96	0.47
2:B:468:MET:CE	2:B:470:LEU:HD11	2.45	0.47
2:P:321:GLU:HA	2:P:344:LEU:HA	1.97	0.47
1:G:105:ALA:HB2	1:G:113:LEU:HD23	1.97	0.47
2:J:472:TYR:CD2	2:J:497:GLY:O	2.68	0.47
2:F:113:GLN:HE22	2:L:192:THR:HG21	1.80	0.47
2:H:352:GLY:O	2:H:353:ALA:HB2	2.15	0.47
2:J:223:VAL:O	2:J:245:LEU:HD12	2.14	0.47
1:M:132:GLU:O	1:M:136:THR:HG23	2.14	0.47
2:N:20:VAL:O	2:N:24:VAL:HG23	2.15	0.47
2:J:289:PHE:HD1	2:J:316:LYS:HD2	1.77	0.47
2:H:468:MET:HG3	2:H:490:LEU:HD21	1.96	0.47
2:J:325:THR:O	2:J:349:ILE:HA	2.15	0.47
2:D:289:PHE:HB2	2:D:290:PRO:HD3	1.97	0.47
2:H:187:LEU:HA	2:H:187:LEU:HD23	1.72	0.47
2:D:190:HIS:HE1	2:H:110:ASN:HA	1.80	0.47
2:F:400:THR:O	2:F:403:LYS:HE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:THR:HG22	1:C:51:ILE:CB	2.44	0.47
1:G:58:TYR:CE1	1:G:62:HIS:CE1	3.03	0.47
2:H:168:THR:HB	2:H:196:VAL:HG13	1.96	0.47
2:H:58:ALA:HA	2:H:81:LYS:HD2	1.97	0.47
2:L:297:LYS:HB2	2:L:297:LYS:HE3	1.64	0.47
2:F:440:ARG:HB3	2:F:467:TRP:CE3	2.48	0.47
1:I:134:ARG:NH1	2:J:40:VAL:HA	2.30	0.47
1:C:114:LEU:C	1:C:116:LEU:H	2.17	0.47
2:J:310:HIS:O	2:J:314:ILE:CG1	2.63	0.47
1:I:91:MET:O	1:I:93:ILE:HG12	2.14	0.46
2:H:284:GLU:O	2:H:287:ILE:HG23	2.15	0.46
1:G:134:ARG:HH11	2:H:40:VAL:HA	1.80	0.46
1:M:137:PHE:HD1	2:N:17:VAL:CG2	2.27	0.46
2:F:320:LEU:HD21	2:F:323:LEU:HB2	1.96	0.46
2:L:546:PRO:O	2:L:547:SER:HB2	2.15	0.46
2:J:191:ASN:ND2	2:J:194:LEU:H	2.11	0.46
2:H:197:LEU:O	2:H:225:VAL:HA	2.15	0.46
2:H:230:PHE:HD1	2:H:235:LEU:HD21	1.78	0.46
2:D:477:ASP:N	2:D:477:ASP:OD1	2.47	0.46
2:L:523:TYR:CE2	2:L:568:ILE:HD11	2.50	0.46
2:H:78:LEU:CD1	2:H:79:LYS:H	2.11	0.46
2:B:357:GLY:HA2	2:B:415:ARG:NH2	2.12	0.46
2:H:31:PRO:O	2:H:35:ASP:HB2	2.16	0.46
1:K:108:LEU:HD12	1:K:110:ILE:CD1	2.40	0.46
2:H:92:ILE:HG23	2:H:93:PRO:HD2	1.97	0.46
1:M:128:LYS:HB3	1:M:132:GLU:HB2	1.96	0.46
2:P:519:TRP:CZ3	2:P:567:HIS:ND1	2.83	0.46
2:P:519:TRP:HH2	2:P:567:HIS:CE1	2.32	0.46
2:F:159:ILE:HG13	2:F:160:VAL:N	2.29	0.46
2:B:590:GLU:O	2:B:591:PRO:C	2.54	0.46
2:P:85:ARG:NH1	5:P:1101:PO4:O3	2.48	0.46
2:P:311:CYS:CB	2:P:336:VAL:HG21	2.46	0.46
1:E:6:ILE:HG22	1:E:7:VAL:N	2.30	0.46
2:F:396:GLU:HG2	2:F:430:SER:OG	2.15	0.46
2:J:396:GLU:HG2	2:J:430:SER:OG	2.16	0.46
1:C:114:LEU:C	1:C:116:LEU:N	2.68	0.46
2:P:373:LEU:HD12	2:P:377:CYS:SG	2.54	0.46
2:L:65:PRO:HA	2:L:103:TRP:CZ3	2.50	0.46
1:G:91:MET:O	1:G:93:ILE:N	2.47	0.46
2:H:469:LEU:HA	2:H:494:GLU:O	2.14	0.46
2:P:285:MET:N	2:P:286:PRO:CD	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:ILE:HG22	2:B:546:PRO:CD	2.45	0.46
2:N:490:LEU:O	2:N:514:SER:HB2	2.14	0.46
1:M:58:TYR:CE1	1:M:62:HIS:CE1	3.04	0.46
1:E:137:PHE:HD1	2:F:17:VAL:HG21	1.79	0.46
2:B:456:SER:HB2	2:B:482:GLU:HB3	1.98	0.46
2:N:227:VAL:HG13	2:N:228:GLY:N	2.30	0.46
2:F:266:LEU:HD13	2:F:266:LEU:HA	1.81	0.46
2:N:338:ALA:O	2:N:376:GLY:HA3	2.15	0.46
2:H:148:CYS:O	2:H:174:SER:HA	2.16	0.46
1:C:159:PHE:O	1:C:160:GLU:CB	2.52	0.46
2:H:450:LEU:HD21	2:H:455:LEU:N	2.30	0.46
1:E:42:VAL:HG22	1:E:42:VAL:O	2.15	0.46
2:B:85:ARG:NH1	5:B:1101:PO4:O3	2.49	0.46
2:L:446:ARG:HG2	2:L:447:GLN:N	2.31	0.46
1:G:26:SER:C	1:G:28:THR:H	2.19	0.46
1:M:99:PHE:CB	2:N:15:ALA:HB1	2.45	0.46
2:L:143:LEU:CD2	2:L:159:ILE:HD13	2.43	0.46
2:N:398:ILE:O	2:N:402:LEU:HD12	2.16	0.46
1:G:48:THR:HG23	1:G:51:ILE:H	1.80	0.46
1:G:48:THR:HG22	1:G:51:ILE:CB	2.45	0.46
2:N:468:MET:CE	2:N:470:LEU:HD11	2.46	0.46
2:L:310:HIS:O	2:L:314:ILE:CG1	2.64	0.46
2:P:235:LEU:O	2:P:238:PHE:HB3	2.14	0.46
2:J:310:HIS:O	2:J:314:ILE:HG12	2.16	0.46
2:L:422:LEU:HB3	2:L:423:PRO:HD3	1.97	0.46
2:J:373:LEU:HD12	2:J:377:CYS:SG	2.55	0.46
2:L:232:ILE:HD12	2:L:252:SER:H	1.80	0.46
2:J:419:ILE:CD1	2:J:446:ARG:HH22	2.28	0.46
2:D:282:PRO:HA	2:D:285:MET:CE	2.45	0.46
2:D:285:MET:N	2:D:286:PRO:CD	2.79	0.46
1:I:106:ASN:ND2	2:J:23:GLN:NE2	2.63	0.46
4:F:3100:OGK:N08	4:F:3100:OGK:C18	2.77	0.46
2:B:270:ARG:O	1:O:107:TYR:HE1	1.98	0.46
2:H:298:LEU:HD13	2:H:300:LEU:HD11	1.96	0.46
2:F:191:ASN:ND2	2:F:194:LEU:H	2.13	0.46
1:G:125:ILE:HD11	2:H:44:TRP:CH2	2.51	0.46
1:C:153:ARG:HG2	1:C:157:TRP:CZ3	2.50	0.46
2:H:29:THR:HG23	2:H:30:ASP:N	2.31	0.46
2:L:46:LYS:HE3	2:L:46:LYS:HB2	1.60	0.46
1:G:160:GLU:HG3	2:H:52:ARG:NH2	2.18	0.46
2:L:367:GLN:CB	2:L:391:THR:HG22	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:57:MET:CE	2:P:62:THR:HG22	2.46	0.46
2:F:456:SER:CB	2:F:482:GLU:HB3	2.46	0.46
2:D:299:ASP:OD2	2:D:301:LEU:HB2	2.16	0.46
2:F:344:LEU:HD23	2:F:380:LEU:HD21	1.98	0.46
2:J:46:LYS:HE3	2:J:46:LYS:HB2	1.55	0.46
2:L:198:ASN:C	2:L:198:ASN:OD1	2.53	0.46
2:J:367:GLN:O	2:J:371:ILE:HG22	2.15	0.46
2:B:367:GLN:CB	2:B:391:THR:HG22	2.41	0.46
1:K:52:LEU:O	1:K:52:LEU:HD12	2.16	0.46
1:O:134:ARG:NH1	2:P:40:VAL:HA	2.31	0.46
2:B:539:TYR:CE2	1:C:145:PRO:HB2	2.51	0.46
2:J:294:GLN:NE2	1:M:107:TYR:OH	2.49	0.46
1:M:46:ASN:HB2	1:M:107:TYR:CZ	2.51	0.46
2:P:282:PRO:HA	2:P:285:MET:CE	2.43	0.46
2:D:419:ILE:HD11	2:D:446:ARG:HH22	1.81	0.46
2:B:289:PHE:N	2:B:290:PRO:CD	2.79	0.46
2:P:545:ILE:HG22	2:P:546:PRO:CD	2.45	0.46
2:B:253:LEU:CD1	2:B:280:MET:HB2	2.42	0.46
2:F:101:THR:N	2:F:102:PRO:CD	2.79	0.46
2:B:191:ASN:ND2	2:B:194:LEU:H	2.11	0.46
2:L:101:THR:CG2	2:L:128:ASP:OD1	2.63	0.46
2:B:398:ILE:O	2:B:402:LEU:HD12	2.16	0.46
2:H:291:PHE:N	2:H:291:PHE:HD2	2.11	0.46
1:C:137:PHE:HD1	2:D:17:VAL:HG21	1.79	0.46
2:F:121:ARG:NH2	5:F:1103:PO4:O4	2.48	0.46
1:O:159:PHE:O	1:O:160:GLU:CB	2.51	0.46
2:H:253:LEU:HD12	2:H:280:MET:HB2	1.97	0.46
2:H:285:MET:HE1	2:H:309:ASP:HB3	1.98	0.46
2:H:390:ILE:CD1	2:H:410:LEU:HD11	2.45	0.46
2:L:325:THR:O	2:L:349:ILE:HA	2.16	0.46
2:P:446:ARG:HG2	2:P:447:GLN:N	2.31	0.46
2:H:501:SER:HB2	2:H:503:ARG:NH2	2.31	0.46
2:J:538:PRO:O	2:J:539:TYR:HB2	2.16	0.46
2:F:392:ASN:HD21	2:F:424:LEU:HA	1.80	0.46
2:L:248:PHE:CD2	2:L:248:PHE:C	2.89	0.46
2:P:542:ILE:CD1	2:P:588:LEU:HD12	2.32	0.45
1:G:26:SER:HB3	1:G:29:ILE:HG13	1.97	0.45
2:H:80:LEU:HD11	2:H:103:TRP:CD2	2.51	0.45
2:N:545:ILE:HG22	2:N:546:PRO:HD2	1.98	0.45
2:N:546:PRO:HB2	2:N:547:SER:H	1.67	0.45
1:I:102:ILE:CG2	1:I:118:CYS:SG	3.03	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:468:MET:CE	2:F:470:LEU:HD11	2.46	0.45
2:H:129:LEU:HD23	2:H:155:GLY:HA3	1.98	0.45
2:H:233:LEU:HD21	2:H:262:LYS:HG2	1.97	0.45
2:D:412:LEU:O	2:D:412:LEU:HD12	2.15	0.45
2:J:20:VAL:O	2:J:24:VAL:HG23	2.16	0.45
2:N:339:GLN:HA	2:N:342:LYS:HE2	1.98	0.45
2:F:170:LEU:C	2:F:170:LEU:HD23	2.36	0.45
2:D:116:SER:CB	2:D:142:THR:HG23	2.40	0.45
2:H:365:VAL:CG2	2:H:388:SER:H	2.29	0.45
2:N:496:ARG:NH2	3:W:201:LEU:HD22	2.31	0.45
2:B:289:PHE:HD1	2:B:316:LYS:HD2	1.75	0.45
2:F:398:ILE:HG23	2:F:402:LEU:HD11	1.97	0.45
1:I:58:TYR:CE1	1:I:62:HIS:CE1	3.04	0.45
2:B:351:ARG:O	2:B:351:ARG:HG3	2.16	0.45
2:B:327:ASN:HD22	2:B:327:ASN:N	2.13	0.45
2:B:436:LYS:HB3	2:B:436:LYS:HE2	1.72	0.45
1:G:130:PRO:HG3	2:H:39:LEU:HB2	1.98	0.45
2:P:409:ARG:HD3	4:P:8100:OGK:H13A	1.98	0.45
1:G:52:LEU:O	1:G:52:LEU:HD12	2.16	0.45
2:F:387:VAL:O	2:F:413:LEU:HD22	2.17	0.45
2:D:468:MET:CE	2:D:470:LEU:HD11	2.46	0.45
2:J:176:PHE:CZ	2:J:204:PHE:CZ	3.04	0.45
5:N:1102:PO4:O3	3:W:206:ARG:NH2	2.45	0.45
2:F:436:LYS:HE2	2:F:436:LYS:HB3	1.72	0.45
1:E:159:PHE:O	1:E:160:GLU:CB	2.51	0.45
1:G:93:ILE:HD12	1:G:97:THR:CG2	2.36	0.45
4:L:6100:OGK:N08	4:L:6100:OGK:C18	2.79	0.45
2:B:101:THR:HG22	2:B:128:ASP:CB	2.46	0.45
2:F:490:LEU:HD23	2:F:490:LEU:HA	1.74	0.45
2:P:387:VAL:O	2:P:413:LEU:HD22	2.17	0.45
2:D:96:TRP:O	2:D:578:ARG:NH2	2.42	0.45
2:F:351:ARG:O	2:F:351:ARG:HG3	2.15	0.45
2:L:305:LEU:HD23	2:L:305:LEU:O	2.16	0.45
1:M:91:MET:SD	1:M:117:THR:HG22	2.55	0.45
2:H:418:ARG:HB3	2:H:421:ASP:HB2	1.99	0.45
2:F:367:GLN:CB	2:F:391:THR:HG22	2.41	0.45
2:H:487:CYS:HB2	2:H:512:LEU:CD2	2.46	0.45
2:F:472:TYR:CD2	2:F:497:GLY:O	2.70	0.45
2:J:546:PRO:O	2:J:547:SER:CB	2.65	0.45
1:M:137:PHE:CD1	2:N:17:VAL:CG2	2.99	0.45
2:H:243:ALA:C	2:H:245:LEU:H	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:503:ARG:HG2	2:H:504:ALA:N	2.31	0.45
1:M:6:ILE:HG22	1:M:7:VAL:N	2.31	0.45
2:D:456:SER:CB	2:D:482:GLU:HB3	2.47	0.45
2:P:523:TYR:CE2	2:P:568:ILE:HD11	2.52	0.45
2:B:65:PRO:HA	2:B:103:TRP:CZ3	2.52	0.45
1:E:58:TYR:CE1	1:E:62:HIS:CE1	3.04	0.45
2:B:338:ALA:O	2:B:376:GLY:HA3	2.17	0.45
1:E:19:GLU:N	1:E:19:GLU:OE1	2.47	0.45
2:N:255:GLU:O	2:N:255:GLU:HG3	2.16	0.45
1:M:91:MET:O	1:M:93:ILE:HG12	2.16	0.45
1:O:91:MET:O	1:O:93:ILE:HG12	2.17	0.45
1:E:10:SER:OG	1:E:11:SER:N	2.48	0.45
2:F:519:TRP:HH2	2:F:567:HIS:CE1	2.34	0.45
1:E:134:ARG:NH1	2:F:40:VAL:HA	2.32	0.45
2:L:159:ILE:HD12	2:L:166:ILE:HD11	1.98	0.45
1:E:48:THR:CG2	1:E:51:ILE:HG12	2.46	0.45
2:L:57:MET:CE	2:L:62:THR:HG22	2.47	0.45
1:O:48:THR:HG23	1:O:51:ILE:H	1.82	0.45
2:P:285:MET:N	2:P:286:PRO:HD2	2.32	0.45
1:I:125:ILE:HG23	1:I:133:ILE:CD1	2.39	0.45
2:N:446:ARG:HG2	2:N:447:GLN:N	2.32	0.45
2:D:446:ARG:HG2	2:D:447:GLN:N	2.32	0.45
2:H:351:ARG:HG3	2:H:359:GLU:OE2	2.16	0.45
2:F:456:SER:HB2	2:F:482:GLU:HB3	1.98	0.45
2:N:440:ARG:HB3	2:N:467:TRP:CE3	2.51	0.45
1:C:42:VAL:HA	1:C:43:PRO:HD3	1.79	0.45
2:D:127:LEU:HB2	2:N:126:ASP:HB3	1.99	0.45
2:J:127:LEU:HD21	2:J:131:ARG:NH2	2.32	0.45
2:L:563:GLU:O	2:L:563:GLU:HG3	2.17	0.45
2:D:327:ASN:HD22	2:D:327:ASN:N	2.15	0.45
2:D:357:GLY:CA	2:D:415:ARG:HH22	2.14	0.45
2:H:387:VAL:HG12	2:H:390:ILE:HD13	1.95	0.45
1:M:102:ILE:CB	2:N:20:VAL:HG21	2.47	0.45
2:L:282:PRO:HA	2:L:285:MET:CE	2.47	0.45
2:B:545:ILE:HB	2:B:567:HIS:HB2	1.98	0.45
2:B:289:PHE:HB2	2:B:290:PRO:HD3	1.97	0.45
2:L:419:ILE:O	2:L:420:THR:O	2.34	0.45
1:I:102:ILE:HG12	1:I:117:THR:CB	2.47	0.45
3:X:201:LEU:HD23	3:X:201:LEU:HA	1.80	0.45
1:K:6:ILE:HG22	1:K:7:VAL:N	2.32	0.45
2:D:400:THR:O	2:D:403:LYS:HE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:ARG:HD3	2:B:413:LEU:HD11	1.98	0.45
1:I:46:ASN:HB2	1:I:107:TYR:CZ	2.52	0.45
2:J:187:LEU:HD23	2:J:187:LEU:HA	1.82	0.45
2:D:248:PHE:CD2	2:D:248:PHE:C	2.90	0.45
2:H:91:LEU:O	2:H:567:HIS:HE1	2.00	0.45
2:D:289:PHE:N	2:D:290:PRO:CD	2.80	0.45
1:G:42:VAL:O	1:G:42:VAL:HG22	2.17	0.45
1:I:102:ILE:HG12	1:I:117:THR:HB	1.99	0.45
1:O:137:PHE:HD1	2:P:17:VAL:CG2	2.29	0.45
2:N:407:ASP:OD1	2:N:440:ARG:HD2	2.17	0.45
2:D:523:TYR:CE2	2:D:568:ILE:HD11	2.52	0.45
2:J:198:ASN:OD1	2:J:198:ASN:C	2.55	0.45
2:L:544:LEU:HD11	2:L:588:LEU:HD11	1.99	0.45
2:H:400:THR:C	2:H:403:LYS:HE2	2.37	0.45
1:G:42:VAL:HA	1:G:43:PRO:HD3	1.79	0.45
1:M:99:PHE:CZ	2:N:17:VAL:HG22	2.52	0.45
2:F:546:PRO:O	2:F:547:SER:HB2	2.17	0.45
2:L:55:VAL:CG2	2:L:75:LEU:HD21	2.44	0.45
2:D:159:ILE:HD12	2:D:166:ILE:HD11	1.99	0.45
1:C:6:ILE:HG22	1:C:7:VAL:N	2.32	0.45
2:H:96:TRP:HE3	2:H:97:GLY:N	2.15	0.45
1:O:6:ILE:HG22	1:O:7:VAL:N	2.32	0.45
2:H:53:GLU:O	2:H:75:LEU:CD2	2.65	0.45
2:D:351:ARG:O	2:D:351:ARG:HG3	2.16	0.45
2:N:429:ARG:O	2:N:433:ILE:HD12	2.17	0.45
2:F:89:PHE:CD1	3:S:206:ARG:HA	2.52	0.45
2:L:412:LEU:HD12	2:L:412:LEU:C	2.37	0.45
2:H:275:LEU:C	2:H:275:LEU:HD12	2.37	0.45
2:H:467:TRP:HZ3	2:H:494:GLU:HG3	1.82	0.44
2:N:367:GLN:CB	2:N:391:THR:HG22	2.37	0.44
2:J:285:MET:N	2:J:286:PRO:HD2	2.32	0.44
2:D:546:PRO:O	2:D:547:SER:HB2	2.16	0.44
2:J:490:LEU:HD23	2:J:490:LEU:HA	1.79	0.44
2:D:490:LEU:HD11	2:D:493:LEU:HD13	1.98	0.44
2:B:311:CYS:CB	2:B:336:VAL:HG21	2.47	0.44
2:N:398:ILE:HG23	2:N:402:LEU:HD11	1.99	0.44
1:K:48:THR:CG2	1:K:51:ILE:HG12	2.48	0.44
2:P:120:ARG:NH2	5:P:1103:PO4:O4	2.48	0.44
2:D:578:ARG:HG3	2:D:578:ARG:H	1.46	0.44
2:F:251:GLY:O	2:F:278:SER:HB2	2.17	0.44
2:F:20:VAL:O	2:F:24:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:VAL:HA	1:K:43:PRO:HD3	1.81	0.44
2:P:339:GLN:HA	2:P:342:LYS:HE2	1.99	0.44
2:B:412:LEU:HD12	2:B:412:LEU:C	2.37	0.44
2:F:544:LEU:HD11	2:F:588:LEU:HD11	2.00	0.44
2:J:419:ILE:O	2:J:420:THR:C	2.55	0.44
2:B:419:ILE:O	2:B:420:THR:O	2.35	0.44
3:W:201:LEU:HA	3:W:202:PRO:HD3	1.83	0.44
2:P:367:GLN:CB	2:P:391:THR:HG22	2.42	0.44
2:L:468:MET:CE	2:L:470:LEU:HD11	2.48	0.44
2:B:59:LEU:O	2:B:62:THR:HB	2.17	0.44
2:J:321:GLU:HA	2:J:344:LEU:HA	1.99	0.44
2:D:398:ILE:C	2:D:400:THR:H	2.20	0.44
2:H:97:GLY:HA3	2:H:123:ILE:HD11	1.98	0.44
1:E:153:ARG:NH2	2:F:539:TYR:CE1	2.85	0.44
2:L:443:PHE:CE2	2:L:445:LEU:HD11	2.52	0.44
2:L:373:LEU:HD12	2:L:377:CYS:SG	2.57	0.44
2:P:375:GLN:HG2	2:P:401:TYR:CE1	2.52	0.44
2:B:392:ASN:HD21	2:B:424:LEU:HA	1.82	0.44
2:N:46:LYS:HE3	2:N:46:LYS:HB2	1.54	0.44
1:O:91:MET:HE3	1:O:117:THR:HG22	1.98	0.44
2:H:409:ARG:HA	2:H:442:ALA:O	2.18	0.44
2:H:410:LEU:HD13	2:H:411:VAL:O	2.18	0.44
2:H:87:ALA:HB2	2:H:92:ILE:CG1	2.47	0.44
2:N:519:TRP:HH2	2:N:567:HIS:CE1	2.35	0.44
2:D:419:ILE:CD1	2:D:446:ARG:HH22	2.29	0.44
2:P:545:ILE:HG22	2:P:546:PRO:HD2	1.99	0.44
2:D:521:GLN:HG3	2:D:567:HIS:CD2	2.50	0.44
1:O:26:SER:HB3	1:O:29:ILE:HG13	1.98	0.44
1:O:58:TYR:CE1	1:O:62:HIS:CE1	3.05	0.44
2:F:545:ILE:HG22	2:F:546:PRO:CD	2.47	0.44
2:N:80:LEU:HB2	2:N:122:MET:HE1	1.97	0.44
2:P:96:TRP:O	2:P:578:ARG:NH2	2.44	0.44
2:P:168:THR:CB	2:P:196:VAL:HG13	2.26	0.44
1:E:107:TYR:CD1	2:L:270:ARG:HB3	2.52	0.44
2:F:419:ILE:CD1	2:F:446:ARG:HH22	2.31	0.44
2:B:546:PRO:HB2	2:B:547:SER:H	1.68	0.44
4:D:2100:OGK:N08	4:D:2100:OGK:H18A	2.26	0.44
2:D:545:ILE:HB	2:D:567:HIS:HB2	1.99	0.44
1:A:95:GLN:NE2	1:A:124:MET:HE3	2.32	0.44
2:P:101:THR:HG22	2:P:128:ASP:CB	2.47	0.44
2:L:191:ASN:ND2	2:L:194:LEU:H	2.12	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:423:PRO:HA	2:H:449:GLY:O	2.18	0.44
2:J:380:LEU:HD23	2:J:380:LEU:HA	1.79	0.44
2:P:396:GLU:HG2	2:P:430:SER:OG	2.16	0.44
2:L:400:THR:O	2:L:403:LYS:HE2	2.18	0.44
2:D:351:ARG:HD3	2:D:413:LEU:HD11	1.98	0.44
2:L:338:ALA:O	2:L:376:GLY:HA3	2.17	0.44
2:D:533:MET:CE	2:D:588:LEU:HD13	2.47	0.44
2:J:419:ILE:O	2:J:420:THR:O	2.36	0.44
2:H:208:SER:HA	2:H:209:PRO:HD2	1.82	0.44
2:H:101:THR:HB	2:H:102:PRO:HD3	1.98	0.44
1:O:137:PHE:CD1	2:P:17:VAL:CG2	3.01	0.44
2:J:539:TYR:OH	1:K:146:GLU:HA	2.18	0.44
2:H:97:GLY:CA	2:H:123:ILE:CD1	2.96	0.44
1:I:148:GLU:HG2	1:I:152:ARG:HH12	1.83	0.44
2:J:338:ALA:O	2:J:376:GLY:HA3	2.17	0.44
2:J:304:LEU:HA	2:J:304:LEU:HD12	1.71	0.44
2:P:419:ILE:O	2:P:420:THR:C	2.56	0.44
2:D:419:ILE:O	2:D:420:THR:C	2.56	0.44
2:H:535:MET:HG2	2:H:535:MET:O	2.17	0.44
4:J:5100:OGK:C18	4:J:5100:OGK:N08	2.79	0.44
2:J:85:ARG:NH1	5:J:1101:PO4:O3	2.50	0.44
2:D:297:LYS:HE3	2:D:297:LYS:HB2	1.68	0.44
2:P:314:ILE:HD11	2:P:329:ILE:HD11	1.99	0.44
2:P:538:PRO:O	2:P:539:TYR:HB2	2.18	0.44
2:P:65:PRO:HB3	2:P:103:TRP:CE3	2.52	0.44
2:D:344:LEU:HD23	2:D:380:LEU:HD21	1.98	0.44
2:J:299:ASP:OD2	2:J:301:LEU:HB2	2.18	0.44
2:J:392:ASN:HD21	2:J:424:LEU:HA	1.82	0.44
2:N:231:GLU:HG2	2:N:254:ASN:HD22	1.82	0.44
2:H:511:LYS:HB2	2:H:511:LYS:HE2	1.66	0.44
2:P:419:ILE:O	2:P:420:THR:O	2.36	0.44
2:N:419:ILE:O	2:N:420:THR:C	2.56	0.44
1:M:96:ALA:CB	2:N:14:VAL:CG1	2.95	0.44
4:P:8100:OGK:C18	4:P:8100:OGK:N08	2.75	0.44
1:M:99:PHE:HB2	2:N:15:ALA:HB1	2.00	0.44
2:L:545:ILE:HG22	2:L:546:PRO:HD2	1.98	0.44
2:H:225:VAL:HG21	2:H:238:PHE:CZ	2.53	0.44
1:A:137:PHE:HD1	2:B:17:VAL:CG2	2.31	0.44
2:H:423:PRO:CB	2:H:425:ASP:OD2	2.65	0.44
2:F:55:VAL:CG2	2:F:75:LEU:HD21	2.48	0.44
1:K:48:THR:HG22	1:K:51:ILE:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:382:TYR:CD2	2:N:407:ASP:HB3	2.53	0.44
2:D:75:LEU:HA	2:D:75:LEU:HD23	1.81	0.44
1:I:153:ARG:NH2	2:J:539:TYR:CE1	2.86	0.44
2:L:321:GLU:HA	2:L:344:LEU:HA	1.98	0.44
2:H:275:LEU:C	2:H:275:LEU:CD1	2.86	0.44
2:N:83:LYS:O	2:N:121:ARG:NH1	2.46	0.44
2:J:263:TYR:O	2:J:266:LEU:HD23	2.18	0.44
2:N:85:ARG:NH1	5:N:1101:PO4:O3	2.51	0.44
2:F:419:ILE:O	2:F:420:THR:C	2.56	0.44
2:B:545:ILE:HG22	2:B:546:PRO:HD2	2.00	0.44
1:E:129:THR:HB	1:E:130:PRO:HD2	2.00	0.44
2:D:319:ASN:HD21	1:G:43:PRO:HG3	1.82	0.44
2:N:101:THR:N	2:N:102:PRO:CD	2.81	0.44
2:F:230:PHE:O	2:F:252:SER:HB3	2.18	0.44
2:D:127:LEU:HD21	2:D:131:ARG:NH2	2.33	0.44
1:G:148:GLU:HG3	1:G:152:ARG:NH1	2.33	0.44
2:D:266:LEU:HD13	2:D:266:LEU:HA	1.80	0.44
2:J:78:LEU:HD12	2:J:79:LYS:H	1.83	0.44
2:L:276:GLY:HA3	2:L:299:ASP:HB3	2.00	0.44
2:J:543:GLU:OE2	2:J:578:ARG:HD3	2.16	0.44
2:D:46:LYS:HB2	2:D:46:LYS:HE3	1.55	0.44
2:H:289:PHE:CE1	2:H:316:LYS:HD3	2.53	0.44
2:H:519:TRP:CH2	2:H:567:HIS:ND1	2.86	0.44
1:C:58:TYR:CD2	1:C:113:LEU:HD13	2.52	0.44
1:O:52:LEU:O	1:O:52:LEU:HD12	2.17	0.44
2:L:75:LEU:HD23	2:L:75:LEU:HA	1.83	0.44
2:H:101:THR:N	2:H:102:PRO:CD	2.81	0.44
2:J:468:MET:CE	2:J:470:LEU:HD11	2.48	0.44
1:I:34:GLU:O	2:N:271:LYS:HE3	2.18	0.44
2:L:176:PHE:CZ	2:L:204:PHE:CZ	3.06	0.44
2:H:189:GLN:C	2:H:190:HIS:ND1	2.71	0.44
2:B:419:ILE:O	2:B:420:THR:C	2.56	0.43
2:B:446:ARG:HG2	2:B:447:GLN:N	2.33	0.43
2:H:390:ILE:HD11	2:H:412:LEU:HD21	2.00	0.43
2:H:411:VAL:HG13	2:H:444:TYR:CB	2.40	0.43
1:I:108:LEU:HD12	1:I:110:ILE:CD1	2.43	0.43
2:D:165:LYS:NZ	2:H:139:ASP:OD1	2.43	0.43
2:J:545:ILE:HG22	2:J:546:PRO:HD2	1.99	0.43
2:P:125:SER:O	2:P:129:LEU:HD22	2.18	0.43
2:N:184:LEU:HA	2:N:184:LEU:HD23	1.86	0.43
1:C:48:THR:HG23	1:C:51:ILE:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:398:ILE:C	2:N:400:THR:H	2.20	0.43
2:D:538:PRO:O	2:D:539:TYR:HB2	2.18	0.43
2:B:18:ASP:OD2	2:B:43:ARG:HD2	2.17	0.43
2:N:251:GLY:O	2:N:278:SER:HB2	2.18	0.43
2:N:305:LEU:HD23	2:N:305:LEU:O	2.18	0.43
2:N:436:LYS:HE2	2:N:436:LYS:HB3	1.75	0.43
2:F:590:GLU:O	2:F:591:PRO:C	2.57	0.43
2:F:419:ILE:O	2:F:420:THR:O	2.36	0.43
2:H:512:LEU:HA	2:H:513:PRO:HD3	1.71	0.43
2:J:320:LEU:HD21	2:J:323:LEU:HB2	1.99	0.43
1:I:10:SER:OG	1:I:11:SER:N	2.50	0.43
2:B:57:MET:CE	2:B:62:THR:HG22	2.48	0.43
2:D:233:LEU:HD23	2:D:233:LEU:HA	1.78	0.43
1:I:48:THR:HG22	1:I:51:ILE:CB	2.48	0.43
2:D:209:PRO:HD3	2:D:230:PHE:HE2	1.83	0.43
2:H:166:ILE:CG2	2:H:167:LYS:N	2.80	0.43
2:B:373:LEU:HD12	2:B:377:CYS:SG	2.58	0.43
2:L:116:SER:CB	2:L:142:THR:HG23	2.43	0.43
2:N:519:TRP:HA	2:N:568:ILE:O	2.18	0.43
1:K:137:PHE:HD1	2:L:17:VAL:CG2	2.31	0.43
1:A:27:GLN:HA	1:A:30:ALA:HB3	2.00	0.43
2:H:266:LEU:HD13	2:H:267:VAL:H	1.82	0.43
2:F:578:ARG:HG3	2:F:578:ARG:H	1.51	0.43
2:H:196:VAL:HG22	2:H:196:VAL:O	2.17	0.43
2:L:392:ASN:HD21	2:L:424:LEU:HA	1.84	0.43
2:H:318:PRO:C	2:H:320:LEU:H	2.22	0.43
1:M:26:SER:HB3	1:M:29:ILE:HG13	2.00	0.43
4:B:1100:OGK:C18	4:B:1100:OGK:N08	2.79	0.43
2:H:542:ILE:HD12	2:H:543:GLU:N	2.33	0.43
2:D:85:ARG:NH1	5:D:1101:PO4:O3	2.51	0.43
2:N:546:PRO:O	2:N:547:SER:CB	2.66	0.43
2:B:125:SER:O	2:B:129:LEU:HD22	2.19	0.43
2:P:398:ILE:C	2:P:400:THR:H	2.20	0.43
1:A:146:GLU:HA	2:D:539:TYR:OH	2.18	0.43
2:B:235:LEU:O	2:B:238:PHE:HB3	2.18	0.43
2:F:248:PHE:C	2:F:248:PHE:CD2	2.91	0.43
1:M:101:LEU:HD23	1:M:101:LEU:HA	1.80	0.43
2:P:289:PHE:N	2:P:290:PRO:CD	2.81	0.43
1:O:128:LYS:HB2	1:O:133:ILE:CD1	2.49	0.43
4:B:1100:OGK:N08	4:B:1100:OGK:H18A	2.24	0.43
2:B:519:TRP:C	2:B:519:TRP:CD1	2.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:289:PHE:N	2:N:290:PRO:CD	2.81	0.43
2:B:325:THR:O	2:B:349:ILE:HA	2.19	0.43
3:R:201:LEU:HD23	3:R:201:LEU:HA	1.85	0.43
1:C:113:LEU:O	1:C:117:THR:CG2	2.65	0.43
2:J:55:VAL:CG2	2:J:75:LEU:HD21	2.47	0.43
1:A:6:ILE:HG22	1:A:7:VAL:N	2.34	0.43
2:F:321:GLU:HA	2:F:344:LEU:HA	1.99	0.43
2:L:95:ASN:O	2:L:582:PRO:HG3	2.18	0.43
2:L:351:ARG:O	2:L:351:ARG:HG3	2.19	0.43
2:F:176:PHE:CZ	2:F:204:PHE:CZ	3.07	0.43
2:J:231:GLU:HG2	2:J:254:ASN:HD22	1.83	0.43
2:J:18:ASP:OD2	2:J:43:ARG:HD2	2.19	0.43
1:O:42:VAL:HG22	1:O:42:VAL:O	2.18	0.43
1:O:101:LEU:HD23	1:O:101:LEU:HA	1.88	0.43
2:P:343:GLN:NE2	2:P:343:GLN:HA	2.33	0.43
2:H:444:TYR:CD1	2:H:471:GLY:CA	3.01	0.43
2:J:308:GLU:O	2:J:312:THR:HG23	2.18	0.43
1:K:58:TYR:CE1	1:K:62:HIS:CE1	3.06	0.43
2:F:545:ILE:HG22	2:F:546:PRO:HD2	2.00	0.43
2:D:227:VAL:HG13	2:D:228:GLY:H	1.80	0.43
2:B:59:LEU:HD22	2:B:61:TYR:H	1.83	0.43
2:L:311:CYS:CB	2:L:336:VAL:HG21	2.48	0.43
2:L:398:ILE:C	2:L:400:THR:H	2.22	0.43
2:D:485:ARG:HE	2:D:485:ARG:HB3	1.69	0.43
2:L:152:THR:HG22	2:L:177:SER:HB2	2.01	0.43
2:N:304:LEU:HD12	2:N:304:LEU:HA	1.71	0.43
2:D:563:GLU:HG3	2:D:563:GLU:O	2.19	0.43
2:J:248:PHE:CD2	2:J:248:PHE:C	2.92	0.43
2:D:542:ILE:CD1	2:D:588:LEU:HD12	2.29	0.43
1:E:107:TYR:HE1	2:L:270:ARG:O	2.02	0.43
2:F:419:ILE:HD11	2:F:446:ARG:HH22	1.84	0.43
2:D:546:PRO:O	2:D:547:SER:CB	2.67	0.43
3:S:201:LEU:HD23	3:S:201:LEU:HA	1.79	0.43
2:B:157:LEU:HD12	2:B:157:LEU:O	2.19	0.43
2:H:367:GLN:HA	2:H:367:GLN:OE1	2.18	0.43
2:B:159:ILE:HG13	2:B:160:VAL:N	2.29	0.43
2:J:407:ASP:OD1	2:J:440:ARG:HD2	2.19	0.43
2:B:398:ILE:C	2:B:400:THR:H	2.22	0.43
2:H:301:LEU:HB3	2:H:302:TYR:CD2	2.53	0.43
2:H:207:ILE:H	2:H:207:ILE:HG12	1.59	0.43
1:C:8:LEU:HD23	1:C:42:VAL:CG1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:266:LEU:HA	2:J:266:LEU:HD13	1.79	0.43
2:L:351:ARG:HD3	2:L:413:LEU:HD11	2.00	0.43
2:F:502:GLU:HG3	2:F:525:ALA:HA	2.00	0.43
1:M:42:VAL:HA	1:M:43:PRO:HD3	1.79	0.43
2:L:304:LEU:HD12	2:L:304:LEU:HA	1.75	0.43
2:B:116:SER:CB	2:B:142:THR:HG23	2.40	0.43
2:N:411:VAL:HG22	2:N:444:TYR:HB3	1.99	0.43
2:H:444:TYR:CE1	2:H:471:GLY:HA2	2.54	0.43
2:L:419:ILE:O	2:L:420:THR:C	2.56	0.43
2:D:519:TRP:HZ3	2:D:567:HIS:ND1	2.15	0.43
2:F:125:SER:O	2:F:128:ASP:OD2	2.37	0.43
2:D:59:LEU:O	2:D:62:THR:HB	2.18	0.43
2:N:490:LEU:HD23	2:N:490:LEU:HA	1.82	0.43
1:A:10:SER:OG	1:A:11:SER:N	2.52	0.43
2:J:59:LEU:HD22	2:J:61:TYR:H	1.84	0.43
2:H:129:LEU:HA	2:H:129:LEU:HD12	1.69	0.43
1:A:48:THR:HG23	1:A:51:ILE:H	1.84	0.43
1:M:148:GLU:HG2	1:M:152:ARG:HH12	1.83	0.43
2:H:480:LEU:HD22	2:H:500:PHE:CD1	2.53	0.43
2:P:46:LYS:HE3	2:P:46:LYS:HB2	1.54	0.43
2:N:412:LEU:HD12	2:N:412:LEU:O	2.18	0.43
2:J:542:ILE:CD1	2:J:588:LEU:HD12	2.29	0.43
2:B:411:VAL:HG22	2:B:444:TYR:HB3	2.01	0.43
2:H:325:THR:OG1	2:H:326:ARG:N	2.51	0.43
2:H:385:VAL:CG1	2:H:387:VAL:HG23	2.48	0.43
2:H:412:LEU:CD1	2:H:445:LEU:CD2	2.97	0.43
1:I:132:GLU:O	1:I:136:THR:HG23	2.19	0.43
1:A:108:LEU:HD12	1:A:110:ILE:CD1	2.42	0.43
2:N:472:TYR:CD2	2:N:497:GLY:O	2.71	0.43
2:F:136:ARG:HH21	2:L:164:ARG:HH21	1.65	0.43
2:H:298:LEU:HD22	2:H:300:LEU:CG	2.45	0.43
2:D:190:HIS:CD2	2:H:112:ARG:NH1	2.86	0.43
2:J:233:LEU:HA	2:J:233:LEU:HD23	1.81	0.43
1:M:134:ARG:HH11	2:N:40:VAL:HA	1.82	0.43
2:B:233:LEU:HD23	2:B:233:LEU:HA	1.80	0.43
3:U:201:LEU:HA	3:U:201:LEU:HD23	1.85	0.43
2:P:227:VAL:HG13	2:P:228:GLY:H	1.82	0.43
2:N:396:GLU:HG2	2:N:430:SER:OG	2.18	0.43
2:N:380:LEU:HA	2:N:380:LEU:HD23	1.77	0.43
2:F:65:PRO:HB3	2:F:103:TRP:CE3	2.54	0.43
1:M:153:ARG:CG	1:M:157:TRP:CZ3	3.02	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:MET:HB3	3:Q:211:ARG:HH12	1.82	0.43
5:B:1102:PO4:O3	3:Q:206:ARG:NH2	2.49	0.43
2:B:190:HIS:HE1	2:P:110:ASN:HA	1.84	0.43
1:E:91:MET:O	1:E:93:ILE:HG12	2.18	0.43
2:D:590:GLU:O	2:D:591:PRO:C	2.56	0.43
2:H:362:GLU:O	2:H:364:LEU:N	2.52	0.43
1:E:42:VAL:HA	1:E:43:PRO:HD3	1.79	0.43
1:E:128:LYS:HB2	1:E:133:ILE:CD1	2.49	0.43
2:L:565:PRO:HG2	3:V:201:LEU:HD21	1.99	0.43
2:F:311:CYS:CB	2:F:336:VAL:HG21	2.49	0.43
2:B:55:VAL:CG2	2:B:75:LEU:HD21	2.49	0.43
2:N:351:ARG:HD3	2:N:413:LEU:HD11	2.00	0.43
2:H:97:GLY:HA3	2:H:123:ILE:HD12	1.99	0.43
2:B:538:PRO:O	2:B:539:TYR:HB2	2.19	0.43
1:G:58:TYR:CD2	1:G:113:LEU:HD13	2.54	0.43
1:M:42:VAL:O	1:M:42:VAL:HG22	2.18	0.43
2:B:375:GLN:HG2	2:B:401:TYR:CE1	2.53	0.43
2:J:58:ALA:O	2:J:81:LYS:HB2	2.19	0.43
2:D:580:ASP:HA	2:N:206:LYS:HE3	2.01	0.43
2:H:316:LYS:C	2:H:318:PRO:HD3	2.40	0.42
2:H:450:LEU:HG	2:H:454:GLY:HA3	2.01	0.42
2:D:546:PRO:HB2	2:D:547:SER:H	1.72	0.42
2:F:519:TRP:CH2	2:F:567:HIS:CG	3.07	0.42
2:J:308:GLU:HG3	2:J:332:ARG:NH2	2.28	0.42
2:J:545:ILE:HG22	2:J:546:PRO:N	2.34	0.42
1:A:95:GLN:NE2	1:A:124:MET:CE	2.82	0.42
1:I:27:GLN:HA	1:I:30:ALA:HB3	2.01	0.42
2:P:578:ARG:HG3	2:P:578:ARG:H	1.44	0.42
2:D:263:TYR:O	2:D:266:LEU:HD23	2.19	0.42
2:L:231:GLU:HG2	2:L:254:ASN:HD22	1.83	0.42
1:I:42:VAL:HG22	1:I:42:VAL:O	2.18	0.42
2:H:437:LYS:HB3	2:H:437:LYS:HE2	1.80	0.42
2:D:343:GLN:NE2	2:D:343:GLN:HA	2.34	0.42
2:J:544:LEU:HD11	2:J:588:LEU:HD11	2.01	0.42
2:H:310:HIS:O	2:H:314:ILE:CG1	2.49	0.42
1:E:45:PRO:HD2	2:L:294:GLN:HB2	2.01	0.42
1:K:26:SER:C	1:K:28:THR:H	2.21	0.42
2:H:303:ALA:O	2:H:326:ARG:NH2	2.52	0.42
1:A:26:SER:HB3	1:A:29:ILE:HG13	2.01	0.42
2:B:523:TYR:CE2	2:B:568:ILE:HD11	2.54	0.42
1:E:26:SER:C	1:E:28:THR:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:304:LEU:HD22	2:H:304:LEU:HA	1.48	0.42
2:D:311:CYS:CB	2:D:336:VAL:HG21	2.50	0.42
2:B:344:LEU:HD23	2:B:380:LEU:HD21	2.01	0.42
2:P:338:ALA:O	2:P:376:GLY:HA3	2.19	0.42
2:B:198:ASN:OD1	2:B:198:ASN:C	2.57	0.42
2:B:46:LYS:HB2	2:B:46:LYS:HE3	1.51	0.42
2:J:289:PHE:N	2:J:290:PRO:CD	2.82	0.42
2:H:542:ILE:HD12	2:H:542:ILE:C	2.39	0.42
2:J:297:LYS:HE3	2:J:297:LYS:HB2	1.62	0.42
2:J:101:THR:N	2:J:102:PRO:CD	2.82	0.42
1:G:46:ASN:HB2	1:G:107:TYR:CZ	2.54	0.42
2:B:396:GLU:HG2	2:B:430:SER:OG	2.19	0.42
2:N:465:VAL:CG1	2:N:468:MET:HG3	2.48	0.42
1:C:27:GLN:HA	1:C:30:ALA:HB3	2.00	0.42
1:G:102:ILE:HG12	1:G:117:THR:OG1	2.18	0.42
2:H:20:VAL:O	2:H:24:VAL:HG23	2.20	0.42
2:D:380:LEU:HD23	2:D:380:LEU:HA	1.71	0.42
2:H:168:THR:CG2	2:H:196:VAL:HG13	2.50	0.42
2:L:299:ASP:OD2	2:L:301:LEU:HB2	2.18	0.42
2:N:412:LEU:HD12	2:N:412:LEU:C	2.40	0.42
2:D:78:LEU:HD12	2:D:79:LYS:H	1.85	0.42
2:D:231:GLU:HG2	2:D:254:ASN:HD22	1.84	0.42
2:F:198:ASN:OD1	2:F:198:ASN:C	2.56	0.42
2:N:544:LEU:HD11	2:N:588:LEU:CD1	2.50	0.42
1:E:46:ASN:HB2	1:E:107:TYR:CZ	2.54	0.42
2:J:367:GLN:CB	2:J:391:THR:HG22	2.37	0.42
2:H:350:GLU:CB	2:H:386:TYR:CD1	3.02	0.42
2:B:519:TRP:CH2	2:B:567:HIS:CE1	3.07	0.42
2:P:546:PRO:O	2:P:547:SER:CB	2.67	0.42
4:P:8100:OGK:N08	4:P:8100:OGK:H18A	2.25	0.42
4:D:2100:OGK:N08	4:D:2100:OGK:C18	2.81	0.42
2:H:208:SER:O	2:H:211:ASP:N	2.50	0.42
3:V:201:LEU:HA	3:V:202:PRO:HD3	1.82	0.42
2:N:280:MET:HG2	2:N:280:MET:O	2.19	0.42
2:B:398:ILE:HG23	2:B:402:LEU:HD11	2.02	0.42
2:N:477:ASP:N	2:N:477:ASP:OD1	2.52	0.42
1:M:87:ASP:HB3	1:M:116:LEU:CD2	2.49	0.42
1:A:148:GLU:HG2	1:A:152:ARG:HH12	1.84	0.42
2:N:232:ILE:HD12	2:N:252:SER:H	1.83	0.42
2:H:505:ILE:C	2:H:507:ALA:N	2.73	0.42
2:F:452:ASP:OD1	2:F:478:GLU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:VAL:O	2:P:24:VAL:HG23	2.19	0.42
2:F:542:ILE:CG1	2:F:588:LEU:HB2	2.49	0.42
2:F:544:LEU:HD11	2:F:588:LEU:CD1	2.50	0.42
2:J:590:GLU:O	2:J:591:PRO:C	2.57	0.42
2:H:412:LEU:O	2:H:414:ASP:N	2.53	0.42
2:H:136:ARG:O	2:H:139:ASP:HB2	2.19	0.42
1:E:137:PHE:CD1	2:F:17:VAL:CG2	3.02	0.42
2:P:431:LEU:C	2:P:431:LEU:HD12	2.39	0.42
1:M:134:ARG:NE	1:M:141:ASN:HB2	2.34	0.42
1:K:48:THR:HG23	1:K:51:ILE:H	1.85	0.42
1:I:48:THR:HG23	1:I:51:ILE:H	1.85	0.42
2:L:221:SER:O	2:L:223:VAL:HG23	2.18	0.42
2:D:299:ASP:C	2:D:301:LEU:H	2.23	0.42
2:N:127:LEU:HD21	2:N:131:ARG:NH2	2.34	0.42
2:L:20:VAL:O	2:L:24:VAL:HG23	2.19	0.42
2:B:95:ASN:O	2:B:582:PRO:HG3	2.20	0.42
2:F:221:SER:O	2:F:223:VAL:HG23	2.20	0.42
2:J:563:GLU:O	2:J:563:GLU:HG3	2.19	0.42
2:H:362:GLU:HB3	2:H:363:GLY:H	1.52	0.42
2:L:519:TRP:C	2:L:519:TRP:CD1	2.90	0.42
2:H:518:LEU:HB3	2:H:570:ALA:HB3	2.02	0.42
2:H:194:LEU:HA	2:H:194:LEU:HD12	1.77	0.42
2:J:350:GLU:HB3	3:U:209:LEU:CD2	2.46	0.42
2:B:490:LEU:HD11	2:B:493:LEU:HD13	2.01	0.42
2:B:295:ILE:HG21	2:B:298:LEU:CD1	2.47	0.42
2:H:242:ALA:HB1	2:H:245:LEU:HB2	2.02	0.42
1:M:48:THR:HG23	1:M:51:ILE:H	1.84	0.42
2:F:227:VAL:HG13	2:F:228:GLY:H	1.84	0.42
2:D:125:SER:O	2:D:129:LEU:HD22	2.20	0.42
1:A:134:ARG:CZ	1:A:141:ASN:HD22	2.32	0.42
1:I:137:PHE:HD1	2:J:17:VAL:HG21	1.83	0.42
2:B:456:SER:CB	2:B:482:GLU:HB3	2.49	0.42
2:J:65:PRO:HA	2:J:103:TRP:CZ3	2.54	0.42
2:L:431:LEU:HD12	2:L:431:LEU:O	2.19	0.42
2:D:436:LYS:HE2	2:D:436:LYS:HB3	1.74	0.42
2:H:320:LEU:HD12	2:H:321:GLU:H	1.84	0.42
1:I:128:LYS:HB2	1:I:133:ILE:CD1	2.50	0.42
2:L:308:GLU:O	2:L:312:THR:HG23	2.20	0.42
1:C:132:GLU:O	1:C:136:THR:HG23	2.20	0.42
2:F:347:LEU:HD11	2:F:349:ILE:HD11	2.01	0.42
2:L:253:LEU:CD1	2:L:280:MET:HB2	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:101:THR:HG22	2:J:128:ASP:CB	2.48	0.42
2:P:59:LEU:O	2:P:62:THR:HB	2.19	0.42
1:I:101:LEU:HB3	1:I:117:THR:HG21	2.01	0.42
1:A:137:PHE:CD1	2:B:17:VAL:CG2	3.03	0.42
2:J:59:LEU:O	2:J:62:THR:HB	2.20	0.42
2:P:431:LEU:O	2:P:431:LEU:HD12	2.20	0.42
1:O:48:THR:HG22	1:O:51:ILE:HG12	2.01	0.42
1:A:98:LEU:CD2	1:A:120:THR:HG22	2.49	0.42
1:A:153:ARG:HG2	1:A:157:TRP:CZ3	2.54	0.42
2:H:115:LYS:O	2:H:141:GLU:N	2.51	0.42
2:F:339:GLN:HA	2:F:342:LYS:HE2	2.01	0.42
2:L:452:ASP:OD1	2:L:478:GLU:HB2	2.20	0.42
2:F:469:LEU:HA	2:F:494:GLU:O	2.19	0.42
2:P:231:GLU:HG2	2:P:254:ASN:HD22	1.84	0.42
2:N:299:ASP:OD2	2:N:301:LEU:HB2	2.19	0.42
2:B:299:ASP:OD2	2:B:301:LEU:HB2	2.19	0.42
2:F:563:GLU:HG3	2:F:563:GLU:O	2.20	0.42
1:G:91:MET:O	1:G:93:ILE:HG12	2.19	0.42
2:J:325:THR:OG1	2:J:326:ARG:N	2.53	0.42
2:H:535:MET:HE1	2:H:542:ILE:HG21	2.01	0.42
2:B:270:ARG:CB	1:O:107:TYR:HD1	2.31	0.42
1:M:10:SER:OG	1:M:11:SER:N	2.52	0.42
2:D:101:THR:HG22	2:D:128:ASP:CB	2.48	0.42
2:F:159:ILE:HD12	2:F:166:ILE:HD11	2.00	0.42
2:H:503:ARG:HE	2:H:503:ARG:H	1.66	0.42
2:F:78:LEU:HD12	2:F:79:LYS:H	1.84	0.42
2:F:211:ASP:O	2:F:215:ILE:HG13	2.19	0.42
1:G:101:LEU:HA	1:G:101:LEU:HD23	1.82	0.42
2:H:390:ILE:HG12	2:H:390:ILE:H	1.64	0.42
2:B:546:PRO:O	2:B:547:SER:CB	2.66	0.42
2:F:289:PHE:HD1	2:F:316:LYS:HD2	1.76	0.42
1:K:135:THR:HG22	1:K:136:THR:N	2.34	0.42
2:H:213:GLU:HA	2:H:238:PHE:HB2	2.01	0.42
2:J:477:ASP:N	2:J:477:ASP:OD1	2.53	0.42
2:N:429:ARG:HG2	2:N:433:ILE:HD12	2.02	0.42
2:L:412:LEU:HD12	2:L:412:LEU:O	2.19	0.42
1:O:59:CYS:O	1:O:63:VAL:HG23	2.19	0.42
1:A:8:LEU:HD23	1:A:42:VAL:CG1	2.50	0.42
2:P:563:GLU:HG3	2:P:563:GLU:O	2.20	0.42
2:H:285:MET:O	2:H:287:ILE:N	2.53	0.42
2:N:419:ILE:O	2:N:420:THR:O	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:99:PHE:CE2	2:N:17:VAL:N	2.88	0.42
2:H:462:SER:HB2	2:H:465:VAL:HB	2.02	0.42
2:F:380:LEU:HD23	2:F:380:LEU:HA	1.74	0.42
2:P:392:ASN:ND2	2:P:421:ASP:OD1	2.48	0.42
2:D:431:LEU:HD12	2:D:431:LEU:C	2.39	0.42
2:D:419:ILE:O	2:D:420:THR:O	2.38	0.41
2:L:546:PRO:O	2:L:547:SER:CB	2.67	0.41
2:B:300:LEU:HD12	2:B:323:LEU:HD11	2.02	0.41
2:F:314:ILE:HD11	2:F:329:ILE:HD11	2.01	0.41
1:M:134:ARG:NH1	2:N:40:VAL:HA	2.35	0.41
2:D:396:GLU:HG2	2:D:430:SER:OG	2.20	0.41
2:L:396:GLU:HG2	2:L:430:SER:OG	2.19	0.41
2:H:188:ALA:HB1	2:H:214:THR:OG1	2.20	0.41
2:B:272:LEU:C	2:B:272:LEU:CD2	2.88	0.41
2:D:296:ARG:HH12	1:G:32:MET:HG3	1.85	0.41
2:D:543:GLU:OE2	2:D:578:ARG:HD3	2.20	0.41
2:N:326:ARG:HA	2:N:350:GLU:O	2.20	0.41
1:A:102:ILE:HG12	1:A:117:THR:HB	2.02	0.41
2:H:100:VAL:O	2:H:100:VAL:HG13	2.19	0.41
2:L:285:MET:N	2:L:286:PRO:CD	2.83	0.41
2:F:282:PRO:HA	2:F:285:MET:CE	2.48	0.41
2:F:285:MET:N	2:F:286:PRO:CD	2.81	0.41
2:L:308:GLU:HG3	2:L:332:ARG:NH2	2.26	0.41
2:P:253:LEU:CD1	2:P:280:MET:HB2	2.49	0.41
1:I:101:LEU:HD23	1:I:101:LEU:HA	1.83	0.41
2:H:428:VAL:CG2	2:H:429:ARG:N	2.83	0.41
1:A:48:THR:HG22	1:A:51:ILE:HG12	2.03	0.41
2:J:143:LEU:CD2	2:J:159:ILE:HD13	2.50	0.41
3:Q:201:LEU:HA	3:Q:201:LEU:HD23	1.85	0.41
2:H:184:LEU:HD23	2:H:184:LEU:HA	1.69	0.41
2:J:314:ILE:HD11	2:J:329:ILE:HD11	2.01	0.41
2:B:223:VAL:O	2:B:245:LEU:HD12	2.20	0.41
2:D:337:LEU:HD12	2:D:341:CYS:SG	2.60	0.41
2:N:544:LEU:HD11	2:N:588:LEU:HD11	2.01	0.41
2:H:87:ALA:HB2	2:H:92:ILE:CB	2.50	0.41
1:I:129:THR:HB	1:I:130:PRO:HD2	2.03	0.41
1:O:125:ILE:HG23	1:O:133:ILE:CD1	2.44	0.41
1:I:106:ASN:HB2	1:I:114:LEU:HD11	2.02	0.41
1:E:134:ARG:NE	1:E:141:ASN:HB2	2.35	0.41
2:J:322:VAL:HG13	2:J:346:ARG:HB2	2.01	0.41
1:O:105:ALA:HB2	1:O:113:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:75:LEU:HD23	2:J:75:LEU:HA	1.83	0.41
1:M:27:GLN:HA	1:M:30:ALA:HB3	2.02	0.41
1:K:46:ASN:HB2	1:K:107:TYR:CZ	2.55	0.41
2:N:502:GLU:HG3	2:N:525:ALA:HA	2.03	0.41
2:N:358:MET:HG3	2:N:364:LEU:HG	2.01	0.41
2:L:209:PRO:HD3	2:L:230:PHE:HE2	1.84	0.41
2:B:348:ARG:HG3	2:B:384:ALA:HB3	2.02	0.41
2:N:107:ILE:HA	2:N:111:LEU:HB2	2.02	0.41
1:I:19:GLU:OE1	1:I:19:GLU:N	2.51	0.41
2:B:563:GLU:HG3	2:B:563:GLU:O	2.21	0.41
2:N:590:GLU:O	2:N:591:PRO:C	2.57	0.41
2:L:289:PHE:N	2:L:290:PRO:CD	2.82	0.41
2:D:325:THR:O	2:D:349:ILE:HA	2.20	0.41
2:H:347:LEU:CD2	2:H:373:LEU:HD21	2.50	0.41
2:P:83:LYS:HA	2:P:84:PRO:HD3	1.86	0.41
1:C:105:ALA:HB2	1:C:113:LEU:HD23	2.02	0.41
2:L:125:SER:O	2:L:129:LEU:HD22	2.20	0.41
2:H:395:LEU:HB3	2:H:427:GLY:C	2.40	0.41
2:F:343:GLN:NE2	2:F:343:GLN:HA	2.35	0.41
2:H:411:VAL:HG23	4:H:4100:OGK:H16A	2.02	0.41
1:M:125:ILE:HG23	1:M:133:ILE:CD1	2.39	0.41
2:N:519:TRP:HZ3	2:N:567:HIS:ND1	2.18	0.41
2:P:328:VAL:CG2	2:P:359:GLU:HB2	2.43	0.41
2:L:289:PHE:HB2	2:L:290:PRO:HD3	2.01	0.41
2:P:308:GLU:O	2:P:312:THR:HG23	2.21	0.41
1:A:132:GLU:O	1:A:136:THR:HG23	2.20	0.41
2:P:490:LEU:HD11	2:P:493:LEU:HD13	2.03	0.41
2:H:124:VAL:CG1	2:H:129:LEU:HD13	2.51	0.41
1:K:137:PHE:CD1	2:L:17:VAL:CG2	3.03	0.41
1:O:102:ILE:HD12	2:P:20:VAL:HG21	2.02	0.41
2:P:89:PHE:CD1	3:X:206:ARG:HA	2.56	0.41
2:F:54:HIS:HE1	2:F:56:THR:OG1	2.03	0.41
2:B:266:LEU:HD13	2:B:266:LEU:HA	1.83	0.41
2:D:187:LEU:HD23	2:D:187:LEU:HA	1.88	0.41
2:P:436:LYS:HB3	2:P:436:LYS:HE2	1.74	0.41
2:L:590:GLU:O	2:L:591:PRO:C	2.57	0.41
2:H:365:VAL:HG21	2:H:387:VAL:CB	2.50	0.41
2:D:285:MET:N	2:D:286:PRO:HD2	2.36	0.41
2:L:519:TRP:CH2	2:L:567:HIS:CE1	3.08	0.41
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.97	0.41
2:F:311:CYS:SG	2:F:333:GLY:HA2	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:153:ARG:NH2	2:P:539:TYR:HE1	2.19	0.41
2:H:54:HIS:O	2:H:55:VAL:HG23	2.20	0.41
2:H:111:LEU:C	2:H:113:GLN:N	2.74	0.41
1:A:101:LEU:HB3	1:A:117:THR:HG21	2.01	0.41
2:P:545:ILE:HB	2:P:567:HIS:HB2	2.01	0.41
2:J:409:ARG:HD3	4:J:5100:OGK:H13A	2.01	0.41
2:N:308:GLU:HG3	2:N:332:ARG:NH2	2.30	0.41
1:I:134:ARG:NE	1:I:141:ASN:HB2	2.36	0.41
2:H:315:GLN:HG3	2:H:340:TYR:CZ	2.55	0.41
1:K:8:LEU:HD23	1:K:42:VAL:CG1	2.50	0.41
2:L:431:LEU:HD12	2:L:431:LEU:C	2.41	0.41
2:B:231:GLU:HG2	2:B:254:ASN:HD22	1.86	0.41
2:J:209:PRO:HD3	2:J:230:PHE:HE2	1.85	0.41
2:N:586:ARG:NH2	2:N:588:LEU:HD21	2.35	0.41
2:H:52:ARG:HH11	2:H:72:PHE:HE2	1.69	0.41
2:P:590:GLU:O	2:P:591:PRO:C	2.58	0.41
2:H:408:PHE:C	2:H:409:ARG:HG2	2.41	0.41
2:N:496:ARG:HA	2:N:521:GLN:O	2.19	0.41
2:P:490:LEU:HA	2:P:490:LEU:HD23	1.72	0.41
2:J:124:VAL:CG1	2:J:129:LEU:HD13	2.50	0.41
2:L:101:THR:N	2:L:102:PRO:CD	2.84	0.41
1:C:137:PHE:HD1	2:D:17:VAL:CG2	2.34	0.41
2:H:168:THR:HG22	2:H:196:VAL:HG13	2.01	0.41
2:N:121:ARG:NH2	5:N:1103:PO4:O4	2.54	0.41
2:D:429:ARG:HG2	2:D:433:ILE:HD12	2.02	0.41
2:P:198:ASN:OD1	2:P:198:ASN:C	2.59	0.41
2:D:405:LEU:HA	2:D:405:LEU:HD23	1.88	0.41
2:L:533:MET:CE	2:L:588:LEU:HD13	2.51	0.41
2:H:455:LEU:HD21	2:H:473:VAL:HG21	2.03	0.41
2:H:92:ILE:HD11	2:H:519:TRP:CZ3	2.56	0.41
2:B:328:VAL:CG2	2:B:359:GLU:HB2	2.45	0.41
2:H:468:MET:HE2	2:H:470:LEU:HD21	2.02	0.41
2:B:519:TRP:HA	2:B:568:ILE:O	2.21	0.41
2:D:545:ILE:HG22	2:D:546:PRO:CD	2.51	0.41
2:H:170:LEU:HA	2:H:198:ASN:O	2.20	0.41
1:O:46:ASN:HB2	1:O:107:TYR:CZ	2.56	0.41
2:J:545:ILE:HB	2:J:567:HIS:HB2	2.03	0.41
2:N:308:GLU:O	2:N:312:THR:HG23	2.21	0.41
2:H:391:THR:O	2:H:393:GLU:N	2.54	0.41
2:H:59:LEU:O	2:H:62:THR:HB	2.21	0.41
2:L:490:LEU:HD23	2:L:490:LEU:HA	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:584:THR:HG22	2:H:584:THR:O	2.21	0.41
2:J:191:ASN:ND2	2:J:192:THR:N	2.68	0.41
2:N:398:ILE:HG22	2:N:431:LEU:HD13	2.02	0.41
2:B:314:ILE:HD11	2:B:329:ILE:HD11	2.03	0.41
1:G:129:THR:OG1	1:G:132:GLU:HG3	2.21	0.41
1:C:99:PHE:CE2	2:D:17:VAL:HG22	2.56	0.41
1:G:148:GLU:HG3	1:G:152:ARG:HH11	1.85	0.41
2:P:392:ASN:HD21	2:P:424:LEU:HA	1.85	0.41
2:B:78:LEU:HD12	2:B:79:LYS:H	1.86	0.41
2:J:405:LEU:HA	2:J:405:LEU:HD23	1.85	0.41
2:F:338:ALA:O	2:F:376:GLY:HA3	2.21	0.41
2:J:412:LEU:C	2:J:412:LEU:HD12	2.41	0.41
2:H:70:ARG:O	2:H:72:PHE:N	2.54	0.41
2:J:367:GLN:NE2	2:J:389:ASP:OD1	2.54	0.41
1:A:26:SER:C	1:A:28:THR:H	2.24	0.41
2:J:328:VAL:CG2	2:J:359:GLU:HB2	2.45	0.41
1:C:125:ILE:HG23	1:C:133:ILE:CD1	2.44	0.41
2:H:98:GLY:C	2:H:122:MET:HE3	2.41	0.41
2:J:519:TRP:C	2:J:519:TRP:CD1	2.92	0.41
1:O:114:LEU:HD12	1:O:114:LEU:HA	1.91	0.41
1:A:141:ASN:C	1:A:141:ASN:OD1	2.58	0.41
2:H:352:GLY:O	2:H:353:ALA:CB	2.69	0.41
2:F:480:LEU:HB2	2:F:500:PHE:CE2	2.56	0.41
2:L:436:LYS:HE2	2:L:436:LYS:HB3	1.70	0.41
1:G:147:GLU:HG3	1:G:147:GLU:H	1.60	0.41
2:D:489:ASN:HA	2:D:489:ASN:HD22	1.65	0.41
2:J:533:MET:C	2:J:535:MET:H	2.24	0.40
2:D:533:MET:C	2:D:535:MET:H	2.25	0.40
2:B:533:MET:CE	2:B:588:LEU:HD13	2.47	0.40
1:G:130:PRO:HD3	2:H:36:SER:CB	2.50	0.40
1:I:26:SER:C	1:I:28:THR:H	2.25	0.40
2:L:409:ARG:HD3	4:L:6100:OGK:H13A	2.03	0.40
2:H:120:ARG:O	2:H:122:MET:HG3	2.20	0.40
2:P:101:THR:N	2:P:102:PRO:CD	2.84	0.40
1:C:158:ALA:HA	2:D:62:THR:HG23	2.03	0.40
1:C:10:SER:OG	1:C:11:SER:N	2.54	0.40
2:P:399:GLY:HA3	2:P:431:LEU:HA	2.04	0.40
2:D:404:ASN:HB3	2:D:437:LYS:HD2	2.03	0.40
2:F:263:TYR:O	2:F:266:LEU:HD23	2.20	0.40
2:B:152:THR:HG22	2:B:177:SER:HB2	2.03	0.40
1:K:114:LEU:C	1:K:116:LEU:N	2.73	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:276:GLY:HA3	2:P:299:ASP:HB3	2.02	0.40
2:P:266:LEU:HA	2:P:266:LEU:HD13	1.86	0.40
2:L:327:ASN:HD22	2:L:327:ASN:N	2.18	0.40
2:L:266:LEU:HA	2:L:266:LEU:HD13	1.83	0.40
2:P:305:LEU:HD23	2:P:305:LEU:O	2.19	0.40
2:N:563:GLU:HG3	2:N:563:GLU:O	2.21	0.40
3:W:201:LEU:HD23	3:W:201:LEU:HA	1.81	0.40
2:N:285:MET:N	2:N:286:PRO:CD	2.85	0.40
1:E:130:PRO:O	1:E:134:ARG:HG2	2.20	0.40
2:N:55:VAL:HG21	2:N:72:PHE:CD1	2.56	0.40
2:N:545:ILE:HG22	2:N:546:PRO:N	2.36	0.40
2:D:490:LEU:HD23	2:D:490:LEU:HA	1.74	0.40
2:F:55:VAL:HG21	2:F:72:PHE:CD1	2.56	0.40
2:P:232:ILE:O	2:P:235:LEU:HB2	2.21	0.40
2:H:274:ARG:HA	2:H:297:LYS:HB3	2.03	0.40
2:F:392:ASN:ND2	2:F:421:ASP:OD1	2.54	0.40
2:F:429:ARG:HG2	2:F:433:ILE:HD12	2.04	0.40
2:B:127:LEU:HB2	2:F:126:ASP:HB3	2.03	0.40
2:P:95:ASN:O	2:P:582:PRO:HG3	2.21	0.40
2:B:489:ASN:HA	2:B:489:ASN:HD22	1.66	0.40
2:B:304:LEU:HD12	2:B:304:LEU:HA	1.72	0.40
2:H:32:LYS:HD3	2:H:32:LYS:HA	1.81	0.40
2:F:118:HIS:CD2	2:F:118:HIS:C	2.94	0.40
2:J:436:LYS:HE2	2:J:436:LYS:HB3	1.77	0.40
2:N:328:VAL:CG2	2:N:359:GLU:HB2	2.41	0.40
2:B:545:ILE:HG22	2:B:546:PRO:N	2.36	0.40
2:F:289:PHE:N	2:F:290:PRO:CD	2.84	0.40
2:P:519:TRP:HZ3	2:P:567:HIS:ND1	2.20	0.40
2:L:519:TRP:HZ3	2:L:567:HIS:ND1	2.20	0.40
2:B:83:LYS:HA	2:B:84:PRO:HD3	1.86	0.40
2:P:184:LEU:HA	2:P:184:LEU:HD23	1.85	0.40
2:F:398:ILE:C	2:F:400:THR:H	2.25	0.40
2:P:351:ARG:HD3	2:P:413:LEU:HD11	2.03	0.40
1:I:153:ARG:CG	1:I:157:TRP:CZ3	3.04	0.40
1:I:146:GLU:HA	2:L:539:TYR:OH	2.22	0.40
2:N:501:SER:O	2:N:505:ILE:HG12	2.21	0.40
2:B:263:TYR:O	2:B:266:LEU:HD23	2.21	0.40
2:P:107:ILE:HA	2:P:111:LEU:HB2	2.03	0.40
2:P:100:VAL:HG11	2:P:124:VAL:HG22	2.03	0.40
2:P:187:LEU:HA	2:P:187:LEU:HD23	1.85	0.40
2:P:327:ASN:N	2:P:327:ASN:HD22	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:SER:CB	1:K:29:ILE:HG13	2.50	0.40
4:H:4100:OGK:N08	4:H:4100:OGK:C18	2.84	0.40
1:O:132:GLU:O	1:O:136:THR:HG23	2.22	0.40
1:E:26:SER:CB	1:E:29:ILE:HG13	2.51	0.40
2:F:308:GLU:HG3	2:F:332:ARG:NH2	2.28	0.40
2:H:191:ASN:ND2	2:H:193:SER:N	2.70	0.40
1:K:114:LEU:C	1:K:116:LEU:H	2.25	0.40
2:P:263:TYR:O	2:P:266:LEU:HD23	2.21	0.40
1:G:135:THR:HG22	1:G:136:THR:HG23	2.04	0.40
2:N:124:VAL:O	2:N:151:PHE:HB3	2.20	0.40
2:B:319:ASN:ND2	1:O:43:PRO:HG2	2.36	0.40
1:O:148:GLU:HG2	1:O:152:ARG:HH12	1.85	0.40
2:N:538:PRO:O	2:N:539:TYR:HB2	2.21	0.40
2:L:343:GLN:NE2	2:L:343:GLN:HA	2.36	0.40
2:P:289:PHE:N	2:P:290:PRO:HD2	2.37	0.40
2:B:285:MET:N	2:B:286:PRO:CD	2.85	0.40
2:N:492:LYS:HG3	2:N:517:TYR:CD2	2.57	0.40
2:N:289:PHE:N	2:N:290:PRO:HD2	2.37	0.40
2:F:519:TRP:HZ3	2:F:567:HIS:ND1	2.17	0.40
2:H:80:LEU:CD1	2:H:103:TRP:CG	3.05	0.40
2:H:191:ASN:C	2:H:191:ASN:HD22	2.24	0.40
2:H:374:ALA:CB	2:H:398:ILE:HD12	2.49	0.40
2:J:253:LEU:CD1	2:J:280:MET:HB2	2.49	0.40
2:F:398:ILE:HG22	2:F:431:LEU:HD13	2.03	0.40
2:P:400:THR:O	2:P:403:LYS:HE2	2.22	0.40
2:N:398:ILE:CG2	2:N:431:LEU:HD13	2.52	0.40
2:J:375:GLN:HG2	2:J:401:TYR:CE1	2.56	0.40
2:H:453:LEU:O	2:H:456:SER:HB3	2.21	0.40
1:E:148:GLU:HG2	1:E:152:ARG:HH12	1.86	0.40
2:P:358:MET:HG3	2:P:364:LEU:HG	2.03	0.40
1:O:61:ARG:HA	1:O:61:ARG:HD2	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	4	31
1	C	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	4	31
1	E	140/160 (88%)	118 (84%)	17 (12%)	5 (4%)	4	31
1	G	140/160 (88%)	113 (81%)	21 (15%)	6 (4%)	3	25
1	I	140/160 (88%)	117 (84%)	17 (12%)	6 (4%)	3	25
1	K	140/160 (88%)	116 (83%)	19 (14%)	5 (4%)	4	31
1	M	140/160 (88%)	115 (82%)	20 (14%)	5 (4%)	4	31
1	O	140/160 (88%)	115 (82%)	19 (14%)	6 (4%)	3	25
2	B	564/592 (95%)	501 (89%)	57 (10%)	6 (1%)	17	57
2	D	564/592 (95%)	503 (89%)	53 (9%)	8 (1%)	14	51
2	F	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	16	55
2	H	558/592 (94%)	426 (76%)	95 (17%)	37 (7%)	1	13
2	J	564/592 (95%)	505 (90%)	52 (9%)	7 (1%)	16	55
2	L	564/592 (95%)	501 (89%)	55 (10%)	8 (1%)	14	51
2	N	564/592 (95%)	502 (89%)	55 (10%)	7 (1%)	16	55
2	P	564/592 (95%)	500 (89%)	58 (10%)	6 (1%)	17	57
3	Q	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	R	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	S	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	U	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	V	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
3	W	16/21 (76%)	15 (94%)	1 (6%)	0	100	100
3	X	16/21 (76%)	14 (88%)	2 (12%)	0	100	100
All	All	5738/6163 (93%)	4968 (87%)	641 (11%)	129 (2%)	8	42

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
2	B	420	THR
2	B	546	PRO
2	D	420	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	546	PRO
2	F	420	THR
2	F	546	PRO
2	H	41	CYS
2	H	71	ARG
2	H	172	GLU
2	H	200	TYR
2	H	270	ARG
2	H	278	SER
2	H	357	GLY
2	H	364	LEU
2	H	425	ASP
2	H	525	ALA
2	H	526	SER
2	J	420	THR
2	J	546	PRO
1	K	92	LYS
2	L	420	THR
2	L	546	PRO
2	N	420	THR
2	N	546	PRO
2	P	420	THR
2	P	546	PRO
1	A	10	SER
1	A	13	GLY
1	A	36	ASP
1	A	126	LYS
2	B	547	SER
1	C	10	SER
1	C	13	GLY
1	C	36	ASP
1	C	92	LYS
1	C	126	LYS
2	D	547	SER
1	E	10	SER
1	E	13	GLY
1	E	36	ASP
1	E	92	LYS
1	E	126	LYS
1	G	10	SER
1	G	13	GLY
1	G	36	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	92	LYS
1	G	128	LYS
2	H	97	GLY
2	H	228	GLY
2	H	271	LYS
2	H	279	TYR
2	H	353	ALA
2	H	365	VAL
2	H	392	ASN
2	H	449	GLY
2	H	528	THR
1	I	10	SER
1	I	13	GLY
1	I	36	ASP
1	I	92	LYS
1	I	126	LYS
2	J	547	SER
1	K	10	SER
1	K	36	ASP
1	K	126	LYS
2	L	547	SER
1	M	10	SER
1	M	13	GLY
1	M	36	ASP
1	M	92	LYS
1	M	126	LYS
1	O	10	SER
1	O	36	ASP
1	O	92	LYS
1	O	126	LYS
2	P	547	SER
2	B	590	GLU
2	D	590	GLU
2	F	20	VAL
2	F	547	SER
2	F	590	GLU
2	H	70	ARG
2	H	319	ASN
2	H	499	CYS
2	H	533	MET
2	H	577	GLN
2	H	582	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	590	GLU
1	K	13	GLY
2	L	590	GLU
2	N	547	SER
2	N	590	GLU
1	O	13	GLY
2	P	590	GLU
2	B	20	VAL
2	D	20	VAL
2	D	112	ARG
2	H	112	ARG
2	H	137	ALA
2	H	269	PRO
2	H	305	LEU
2	H	358	MET
2	H	538	PRO
2	L	112	ARG
2	N	290	PRO
2	P	20	VAL
2	D	290	PRO
2	H	206	LYS
1	I	137	PHE
2	J	20	VAL
2	J	290	PRO
2	L	20	VAL
2	L	290	PRO
2	N	20	VAL
1	O	27	GLN
2	P	290	PRO
2	F	290	PRO
1	G	153	ARG
2	H	209	PRO
2	H	276	GLY
2	H	20	VAL
2	H	286	PRO
2	B	591	PRO
2	D	591	PRO
2	N	591	PRO
2	F	591	PRO
2	J	591	PRO
2	L	591	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/137 (93%)	114 (90%)	13 (10%)	9	35
1	C	127/137 (93%)	115 (91%)	12 (9%)	11	39
1	E	127/137 (93%)	113 (89%)	14 (11%)	8	31
1	G	127/137 (93%)	113 (89%)	14 (11%)	8	31
1	I	127/137 (93%)	114 (90%)	13 (10%)	9	35
1	K	127/137 (93%)	114 (90%)	13 (10%)	9	35
1	M	127/137 (93%)	114 (90%)	13 (10%)	9	35
1	O	127/137 (93%)	113 (89%)	14 (11%)	8	31
2	B	500/523 (96%)	433 (87%)	67 (13%)	5	21
2	D	500/523 (96%)	432 (86%)	68 (14%)	5	21
2	F	500/523 (96%)	433 (87%)	67 (13%)	5	21
2	H	494/523 (94%)	397 (80%)	97 (20%)	1	7
2	J	500/523 (96%)	433 (87%)	67 (13%)	5	21
2	L	500/523 (96%)	431 (86%)	69 (14%)	4	20
2	N	500/523 (96%)	432 (86%)	68 (14%)	5	21
2	P	500/523 (96%)	434 (87%)	66 (13%)	5	22
3	Q	16/19 (84%)	16 (100%)	0	100	100
3	R	16/19 (84%)	16 (100%)	0	100	100
3	S	16/19 (84%)	16 (100%)	0	100	100
3	U	16/19 (84%)	16 (100%)	0	100	100
3	V	16/19 (84%)	16 (100%)	0	100	100
3	W	16/19 (84%)	16 (100%)	0	100	100
3	X	16/19 (84%)	16 (100%)	0	100	100
All	All	5122/5413 (95%)	4447 (87%)	675 (13%)	5	22

All (675) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	14	GLU
1	A	22	VAL
1	A	29	ILE
1	A	35	ASP
1	A	36	ASP
1	A	42	VAL
1	A	44	LEU
1	A	48	THR
1	A	81	ASP
1	A	125	ILE
1	A	153	ARG
1	A	160	GLU
2	B	16	THR
2	B	20	VAL
2	B	35	ASP
2	B	40	VAL
2	B	43	ARG
2	B	48	ASP
2	B	52	ARG
2	B	59	LEU
2	B	62	THR
2	B	64	THR
2	B	104	VAL
2	B	123	ILE
2	B	129	LEU
2	B	132	LEU
2	B	136	ARG
2	B	142	THR
2	B	159	ILE
2	B	166	ILE
2	B	168	THR
2	B	182	LYS
2	B	184	LEU
2	B	191	ASN
2	B	193	SER
2	B	196	VAL
2	B	214	THR
2	B	220	ARG
2	B	225	VAL
2	B	230	PHE
2	B	231	GLU
2	B	232	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	270	ARG
2	B	272	LEU
2	B	275	LEU
2	B	284	GLU
2	B	301	LEU
2	B	304	LEU
2	B	305	LEU
2	B	312	THR
2	B	314	ILE
2	B	327	ASN
2	B	349	ILE
2	B	360	ASP
2	B	367	GLN
2	B	377	CYS
2	B	390	ILE
2	B	400	THR
2	B	402	LEU
2	B	404	ASN
2	B	405	LEU
2	B	412	LEU
2	B	418	ARG
2	B	422	LEU
2	B	447	GLN
2	B	453	LEU
2	B	455	LEU
2	B	477	ASP
2	B	481	MET
2	B	490	LEU
2	B	495	MET
2	B	503	ARG
2	B	510	THR
2	B	516	ARG
2	B	519	TRP
2	B	528	THR
2	B	537	ARG
2	B	542	ILE
2	B	578	ARG
1	C	8	LEU
1	C	14	GLU
1	C	29	ILE
1	C	35	ASP
1	C	36	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	42	VAL
1	C	44	LEU
1	C	48	THR
1	C	125	ILE
1	C	150	GLU
1	C	153	ARG
1	C	160	GLU
2	D	16	THR
2	D	20	VAL
2	D	35	ASP
2	D	40	VAL
2	D	43	ARG
2	D	48	ASP
2	D	52	ARG
2	D	59	LEU
2	D	62	THR
2	D	64	THR
2	D	104	VAL
2	D	123	ILE
2	D	129	LEU
2	D	132	LEU
2	D	136	ARG
2	D	142	THR
2	D	159	ILE
2	D	166	ILE
2	D	168	THR
2	D	182	LYS
2	D	184	LEU
2	D	191	ASN
2	D	196	VAL
2	D	214	THR
2	D	220	ARG
2	D	225	VAL
2	D	230	PHE
2	D	231	GLU
2	D	232	ILE
2	D	270	ARG
2	D	272	LEU
2	D	275	LEU
2	D	284	GLU
2	D	301	LEU
2	D	304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	305	LEU
2	D	312	THR
2	D	314	ILE
2	D	327	ASN
2	D	349	ILE
2	D	360	ASP
2	D	367	GLN
2	D	377	CYS
2	D	390	ILE
2	D	400	THR
2	D	402	LEU
2	D	404	ASN
2	D	405	LEU
2	D	412	LEU
2	D	413	LEU
2	D	418	ARG
2	D	422	LEU
2	D	447	GLN
2	D	453	LEU
2	D	455	LEU
2	D	477	ASP
2	D	481	MET
2	D	490	LEU
2	D	495	MET
2	D	496	ARG
2	D	503	ARG
2	D	510	THR
2	D	516	ARG
2	D	519	TRP
2	D	528	THR
2	D	537	ARG
2	D	542	ILE
2	D	578	ARG
1	E	8	LEU
1	E	14	GLU
1	E	22	VAL
1	E	29	ILE
1	E	35	ASP
1	E	36	ASP
1	E	42	VAL
1	E	44	LEU
1	E	48	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	81	ASP
1	E	125	ILE
1	E	150	GLU
1	E	153	ARG
1	E	160	GLU
2	F	16	THR
2	F	20	VAL
2	F	35	ASP
2	F	40	VAL
2	F	43	ARG
2	F	48	ASP
2	F	52	ARG
2	F	59	LEU
2	F	62	THR
2	F	64	THR
2	F	104	VAL
2	F	123	ILE
2	F	129	LEU
2	F	132	LEU
2	F	136	ARG
2	F	142	THR
2	F	159	ILE
2	F	166	ILE
2	F	168	THR
2	F	182	LYS
2	F	184	LEU
2	F	191	ASN
2	F	196	VAL
2	F	201	MET
2	F	214	THR
2	F	220	ARG
2	F	225	VAL
2	F	231	GLU
2	F	232	ILE
2	F	270	ARG
2	F	272	LEU
2	F	275	LEU
2	F	284	GLU
2	F	301	LEU
2	F	304	LEU
2	F	305	LEU
2	F	312	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	314	ILE
2	F	327	ASN
2	F	349	ILE
2	F	360	ASP
2	F	367	GLN
2	F	377	CYS
2	F	390	ILE
2	F	400	THR
2	F	402	LEU
2	F	404	ASN
2	F	405	LEU
2	F	412	LEU
2	F	413	LEU
2	F	418	ARG
2	F	422	LEU
2	F	447	GLN
2	F	453	LEU
2	F	455	LEU
2	F	477	ASP
2	F	481	MET
2	F	490	LEU
2	F	495	MET
2	F	503	ARG
2	F	510	THR
2	F	516	ARG
2	F	519	TRP
2	F	528	THR
2	F	537	ARG
2	F	542	ILE
2	F	578	ARG
1	G	8	LEU
1	G	14	GLU
1	G	22	VAL
1	G	35	ASP
1	G	36	ASP
1	G	42	VAL
1	G	44	LEU
1	G	48	THR
1	G	81	ASP
1	G	129	THR
1	G	133	ILE
1	G	144	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	150	GLU
1	G	153	ARG
2	H	14	VAL
2	H	17	VAL
2	H	20	VAL
2	H	21	ILE
2	H	35	ASP
2	H	40	VAL
2	H	46	LYS
2	H	52	ARG
2	H	59	LEU
2	H	62	THR
2	H	64	THR
2	H	71	ARG
2	H	75	LEU
2	H	76	ARG
2	H	77	SER
2	H	85	ARG
2	H	95	ASN
2	H	100	VAL
2	H	111	LEU
2	H	128	ASP
2	H	132	LEU
2	H	136	ARG
2	H	140	LEU
2	H	142	THR
2	H	159	ILE
2	H	166	ILE
2	H	168	THR
2	H	170	LEU
2	H	171	MET
2	H	175	SER
2	H	184	LEU
2	H	190	HIS
2	H	191	ASN
2	H	192	THR
2	H	193	SER
2	H	194	LEU
2	H	196	VAL
2	H	203	GLU
2	H	214	THR
2	H	225	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	231	GLU
2	H	233	LEU
2	H	238	PHE
2	H	255	GLU
2	H	266	LEU
2	H	272	LEU
2	H	275	LEU
2	H	284	GLU
2	H	291	PHE
2	H	298	LEU
2	H	301	LEU
2	H	302	TYR
2	H	304	LEU
2	H	305	LEU
2	H	313	LEU
2	H	315	GLN
2	H	316	LYS
2	H	325	THR
2	H	326	ARG
2	H	343	GLN
2	H	345	LYS
2	H	348	ARG
2	H	364	LEU
2	H	365	VAL
2	H	370	LEU
2	H	377	CYS
2	H	382	TYR
2	H	388	SER
2	H	389	ASP
2	H	390	ILE
2	H	394	SER
2	H	396	GLU
2	H	398	ILE
2	H	402	LEU
2	H	403	LYS
2	H	409	ARG
2	H	410	LEU
2	H	411	VAL
2	H	415	ARG
2	H	422	LEU
2	H	453	LEU
2	H	467	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	477	ASP
2	H	485	ARG
2	H	490	LEU
2	H	503	ARG
2	H	511	LYS
2	H	516	ARG
2	H	519	TRP
2	H	534	GLN
2	H	542	ILE
2	H	547	SER
2	H	548	ARG
2	H	568	ILE
2	H	579	THR
2	H	583	THR
2	H	589	LYS
1	I	8	LEU
1	I	14	GLU
1	I	22	VAL
1	I	35	ASP
1	I	36	ASP
1	I	42	VAL
1	I	44	LEU
1	I	48	THR
1	I	81	ASP
1	I	125	ILE
1	I	150	GLU
1	I	153	ARG
1	I	160	GLU
2	J	16	THR
2	J	20	VAL
2	J	35	ASP
2	J	40	VAL
2	J	43	ARG
2	J	48	ASP
2	J	52	ARG
2	J	59	LEU
2	J	62	THR
2	J	64	THR
2	J	104	VAL
2	J	129	LEU
2	J	132	LEU
2	J	136	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	142	THR
2	J	159	ILE
2	J	166	ILE
2	J	168	THR
2	J	182	LYS
2	J	184	LEU
2	J	191	ASN
2	J	196	VAL
2	J	214	THR
2	J	217	ARG
2	J	220	ARG
2	J	225	VAL
2	J	227	VAL
2	J	230	PHE
2	J	231	GLU
2	J	232	ILE
2	J	272	LEU
2	J	275	LEU
2	J	284	GLU
2	J	301	LEU
2	J	304	LEU
2	J	305	LEU
2	J	312	THR
2	J	314	ILE
2	J	327	ASN
2	J	341	CYS
2	J	349	ILE
2	J	360	ASP
2	J	367	GLN
2	J	377	CYS
2	J	390	ILE
2	J	400	THR
2	J	402	LEU
2	J	404	ASN
2	J	405	LEU
2	J	413	LEU
2	J	418	ARG
2	J	422	LEU
2	J	447	GLN
2	J	453	LEU
2	J	455	LEU
2	J	477	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	481	MET
2	J	490	LEU
2	J	495	MET
2	J	503	ARG
2	J	510	THR
2	J	516	ARG
2	J	519	TRP
2	J	528	THR
2	J	537	ARG
2	J	542	ILE
2	J	578	ARG
1	K	8	LEU
1	K	14	GLU
1	K	22	VAL
1	K	29	ILE
1	K	35	ASP
1	K	36	ASP
1	K	42	VAL
1	K	44	LEU
1	K	48	THR
1	K	125	ILE
1	K	150	GLU
1	K	153	ARG
1	K	160	GLU
2	L	16	THR
2	L	20	VAL
2	L	35	ASP
2	L	40	VAL
2	L	43	ARG
2	L	48	ASP
2	L	52	ARG
2	L	59	LEU
2	L	62	THR
2	L	64	THR
2	L	104	VAL
2	L	123	ILE
2	L	129	LEU
2	L	132	LEU
2	L	136	ARG
2	L	142	THR
2	L	159	ILE
2	L	166	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	168	THR
2	L	182	LYS
2	L	184	LEU
2	L	191	ASN
2	L	193	SER
2	L	196	VAL
2	L	201	MET
2	L	214	THR
2	L	220	ARG
2	L	225	VAL
2	L	227	VAL
2	L	231	GLU
2	L	232	ILE
2	L	270	ARG
2	L	272	LEU
2	L	275	LEU
2	L	284	GLU
2	L	301	LEU
2	L	304	LEU
2	L	305	LEU
2	L	312	THR
2	L	314	ILE
2	L	327	ASN
2	L	341	CYS
2	L	349	ILE
2	L	360	ASP
2	L	367	GLN
2	L	377	CYS
2	L	390	ILE
2	L	400	THR
2	L	402	LEU
2	L	404	ASN
2	L	405	LEU
2	L	413	LEU
2	L	418	ARG
2	L	422	LEU
2	L	447	GLN
2	L	453	LEU
2	L	455	LEU
2	L	477	ASP
2	L	481	MET
2	L	490	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	495	MET
2	L	503	ARG
2	L	510	THR
2	L	516	ARG
2	L	519	TRP
2	L	528	THR
2	L	537	ARG
2	L	542	ILE
2	L	578	ARG
1	M	8	LEU
1	M	14	GLU
1	M	22	VAL
1	M	35	ASP
1	M	36	ASP
1	M	42	VAL
1	M	44	LEU
1	M	48	THR
1	M	81	ASP
1	M	125	ILE
1	M	150	GLU
1	M	153	ARG
1	M	160	GLU
2	N	16	THR
2	N	20	VAL
2	N	35	ASP
2	N	40	VAL
2	N	43	ARG
2	N	48	ASP
2	N	52	ARG
2	N	59	LEU
2	N	62	THR
2	N	64	THR
2	N	104	VAL
2	N	123	ILE
2	N	129	LEU
2	N	132	LEU
2	N	136	ARG
2	N	142	THR
2	N	159	ILE
2	N	166	ILE
2	N	168	THR
2	N	184	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	191	ASN
2	N	196	VAL
2	N	201	MET
2	N	214	THR
2	N	217	ARG
2	N	220	ARG
2	N	225	VAL
2	N	230	PHE
2	N	231	GLU
2	N	232	ILE
2	N	270	ARG
2	N	272	LEU
2	N	275	LEU
2	N	284	GLU
2	N	301	LEU
2	N	304	LEU
2	N	305	LEU
2	N	312	THR
2	N	314	ILE
2	N	327	ASN
2	N	341	CYS
2	N	349	ILE
2	N	360	ASP
2	N	365	VAL
2	N	367	GLN
2	N	377	CYS
2	N	390	ILE
2	N	400	THR
2	N	402	LEU
2	N	404	ASN
2	N	405	LEU
2	N	418	ARG
2	N	422	LEU
2	N	447	GLN
2	N	453	LEU
2	N	455	LEU
2	N	477	ASP
2	N	481	MET
2	N	490	LEU
2	N	495	MET
2	N	503	ARG
2	N	510	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	516	ARG
2	N	519	TRP
2	N	528	THR
2	N	537	ARG
2	N	542	ILE
2	N	578	ARG
1	O	8	LEU
1	O	14	GLU
1	O	22	VAL
1	O	29	ILE
1	O	35	ASP
1	O	36	ASP
1	O	42	VAL
1	O	44	LEU
1	O	48	THR
1	O	81	ASP
1	O	125	ILE
1	O	150	GLU
1	O	153	ARG
1	O	160	GLU
2	P	16	THR
2	P	20	VAL
2	P	35	ASP
2	P	40	VAL
2	P	43	ARG
2	P	48	ASP
2	P	52	ARG
2	P	59	LEU
2	P	62	THR
2	P	64	THR
2	P	104	VAL
2	P	123	ILE
2	P	129	LEU
2	P	132	LEU
2	P	136	ARG
2	P	142	THR
2	P	159	ILE
2	P	168	THR
2	P	182	LYS
2	P	184	LEU
2	P	191	ASN
2	P	196	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	214	THR
2	P	220	ARG
2	P	225	VAL
2	P	230	PHE
2	P	231	GLU
2	P	232	ILE
2	P	270	ARG
2	P	272	LEU
2	P	275	LEU
2	P	284	GLU
2	P	301	LEU
2	P	304	LEU
2	P	305	LEU
2	P	312	THR
2	P	314	ILE
2	P	327	ASN
2	P	341	CYS
2	P	349	ILE
2	P	360	ASP
2	P	367	GLN
2	P	377	CYS
2	P	390	ILE
2	P	400	THR
2	P	402	LEU
2	P	404	ASN
2	P	405	LEU
2	P	418	ARG
2	P	422	LEU
2	P	447	GLN
2	P	453	LEU
2	P	455	LEU
2	P	477	ASP
2	P	481	MET
2	P	490	LEU
2	P	495	MET
2	P	496	ARG
2	P	503	ARG
2	P	510	THR
2	P	516	ARG
2	P	519	TRP
2	P	528	THR
2	P	537	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	542	ILE
2	P	578	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	62	HIS
1	A	95	GLN
2	B	54	HIS
2	B	74	ASN
2	B	109	ASN
2	B	191	ASN
2	B	254	ASN
2	B	294	GLN
2	B	319	ASN
2	B	327	ASN
2	B	343	GLN
2	B	460	GLN
2	B	489	ASN
2	B	564	HIS
2	B	567	HIS
1	C	46	ASN
1	C	62	HIS
2	D	54	HIS
2	D	74	ASN
2	D	109	ASN
2	D	190	HIS
2	D	191	ASN
2	D	254	ASN
2	D	294	GLN
2	D	319	ASN
2	D	327	ASN
2	D	343	GLN
2	D	460	GLN
2	D	489	ASN
2	D	564	HIS
2	D	567	HIS
1	E	46	ASN
1	E	62	HIS
1	E	95	GLN
2	F	54	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	74	ASN
2	F	109	ASN
2	F	113	GLN
2	F	191	ASN
2	F	254	ASN
2	F	327	ASN
2	F	343	GLN
2	F	460	GLN
2	F	489	ASN
2	F	564	HIS
2	F	567	HIS
1	G	46	ASN
1	G	62	HIS
2	H	23	GLN
2	H	74	ASN
2	H	95	ASN
2	H	110	ASN
2	H	191	ASN
2	H	310	HIS
2	H	375	GLN
2	H	392	ASN
2	H	447	GLN
2	H	460	GLN
2	H	489	ASN
2	H	530	GLN
2	H	577	GLN
1	I	46	ASN
1	I	62	HIS
1	I	106	ASN
2	J	23	GLN
2	J	54	HIS
2	J	109	ASN
2	J	191	ASN
2	J	254	ASN
2	J	294	GLN
2	J	327	ASN
2	J	343	GLN
2	J	460	GLN
2	J	489	ASN
2	J	564	HIS
2	J	567	HIS
1	K	46	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	62	HIS
2	L	54	HIS
2	L	74	ASN
2	L	109	ASN
2	L	190	HIS
2	L	191	ASN
2	L	254	ASN
2	L	294	GLN
2	L	319	ASN
2	L	327	ASN
2	L	343	GLN
2	L	460	GLN
2	L	489	ASN
2	L	564	HIS
2	L	567	HIS
1	M	46	ASN
1	M	62	HIS
2	N	54	HIS
2	N	109	ASN
2	N	191	ASN
2	N	254	ASN
2	N	327	ASN
2	N	343	GLN
2	N	460	GLN
2	N	489	ASN
2	N	564	HIS
2	N	567	HIS
1	O	46	ASN
1	O	62	HIS
2	P	54	HIS
2	P	109	ASN
2	P	191	ASN
2	P	254	ASN
2	P	327	ASN
2	P	343	GLN
2	P	460	GLN
2	P	489	ASN
2	P	564	HIS
2	P	567	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

40 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$
4	OGK	B	1100	-	22,25,25	6.44	8 (36%)	25,38,38	2.68	12 (48%)
5	PO4	B	1101	-	4,4,4	2.84	4 (100%)	6,6,6	0.29	0
5	PO4	B	1102	-	4,4,4	2.90	3 (75%)	6,6,6	0.27	0
5	PO4	B	1103	-	4,4,4	2.91	4 (100%)	6,6,6	0.27	0
5	PO4	B	1104	-	4,4,4	2.88	4 (100%)	6,6,6	0.27	0
5	PO4	D	1101	-	4,4,4	2.79	4 (100%)	6,6,6	0.32	0
5	PO4	D	1102	-	4,4,4	2.87	4 (100%)	6,6,6	0.26	0
5	PO4	D	1103	-	4,4,4	2.97	4 (100%)	6,6,6	0.29	0
5	PO4	D	1104	-	4,4,4	2.94	3 (75%)	6,6,6	0.29	0
4	OGK	D	2100	-	22,25,25	6.55	8 (36%)	25,38,38	2.73	11 (44%)
5	PO4	F	1101	-	4,4,4	2.88	4 (100%)	6,6,6	0.33	0
5	PO4	F	1102	-	4,4,4	3.10	4 (100%)	6,6,6	0.27	0
5	PO4	F	1103	-	4,4,4	2.93	3 (75%)	6,6,6	0.29	0
5	PO4	F	1104	-	4,4,4	3.07	3 (75%)	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OGK	F	3100	-	22,25,25	6.45	9 (40%)	25,38,38	2.72	11 (44%)
5	PO4	H	1101	-	4,4,4	3.12	4 (100%)	6,6,6	0.27	0
5	PO4	H	1102	-	4,4,4	3.00	3 (75%)	6,6,6	0.29	0
5	PO4	H	1103	-	4,4,4	3.13	4 (100%)	6,6,6	0.28	0
5	PO4	H	1104	-	4,4,4	3.09	3 (75%)	6,6,6	0.32	0
4	OGK	H	4100	-	22,25,25	6.38	9 (40%)	25,38,38	2.78	13 (52%)
5	PO4	J	1101	-	4,4,4	2.89	3 (75%)	6,6,6	0.31	0
5	PO4	J	1102	-	4,4,4	2.97	3 (75%)	6,6,6	0.28	0
5	PO4	J	1103	-	4,4,4	2.81	3 (75%)	6,6,6	0.27	0
5	PO4	J	1104	-	4,4,4	2.83	3 (75%)	6,6,6	0.28	0
4	OGK	J	5100	-	22,25,25	6.53	9 (40%)	25,38,38	2.76	12 (48%)
5	PO4	L	1101	-	4,4,4	3.01	4 (100%)	6,6,6	0.30	0
5	PO4	L	1102	-	4,4,4	2.97	4 (100%)	6,6,6	0.26	0
5	PO4	L	1103	-	4,4,4	2.87	4 (100%)	6,6,6	0.29	0
5	PO4	L	1104	-	4,4,4	3.03	3 (75%)	6,6,6	0.27	0
4	OGK	L	6100	-	22,25,25	6.37	9 (40%)	25,38,38	2.68	12 (48%)
5	PO4	N	1101	-	4,4,4	3.23	3 (75%)	6,6,6	0.35	0
5	PO4	N	1102	-	4,4,4	3.00	3 (75%)	6,6,6	0.28	0
5	PO4	N	1103	-	4,4,4	2.87	3 (75%)	6,6,6	0.33	0
5	PO4	N	1104	-	4,4,4	3.03	3 (75%)	6,6,6	0.29	0
4	OGK	N	7100	-	22,25,25	6.15	9 (40%)	25,38,38	2.77	11 (44%)
5	PO4	P	1101	-	4,4,4	2.87	3 (75%)	6,6,6	0.29	0
5	PO4	P	1102	-	4,4,4	2.93	3 (75%)	6,6,6	0.28	0
5	PO4	P	1103	-	4,4,4	2.85	3 (75%)	6,6,6	0.28	0
5	PO4	P	1104	-	4,4,4	2.92	3 (75%)	6,6,6	0.28	0
4	OGK	P	8100	-	22,25,25	6.52	7 (31%)	25,38,38	2.75	11 (44%)

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
4	OGK	B	1100	-	-	0/13/52/52	0/2/3/3
5	PO4	B	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1103	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	B	1104	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	D	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	D	2100	-	-	0/13/52/52	0/2/3/3
5	PO4	F	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	F	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	F	3100	-	-	0/13/52/52	0/2/3/3
5	PO4	H	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	H	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	H	4100	-	1/1/9/10	0/13/52/52	0/2/3/3
5	PO4	J	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	J	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	J	5100	-	-	0/13/52/52	0/2/3/3
5	PO4	L	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	L	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	L	6100	-	-	0/13/52/52	0/2/3/3
5	PO4	N	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	N	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	N	7100	-	-	0/13/52/52	0/2/3/3
5	PO4	P	1101	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1102	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1103	-	-	0/0/0/0	0/0/0/0
5	PO4	P	1104	-	-	0/0/0/0	0/0/0/0
4	OGK	P	8100	-	-	0/13/52/52	0/2/3/3

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	5100	OGK	C13-C09	-22.40	1.27	1.51
4	D	2100	OGK	C13-C09	-22.30	1.27	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	8100	OGK	C13-C09	-22.04	1.28	1.51
4	F	3100	OGK	C13-C09	-21.99	1.28	1.51
4	B	1100	OGK	C13-C09	-21.74	1.28	1.51
4	L	6100	OGK	C13-C09	-21.73	1.28	1.51
4	H	4100	OGK	C13-C09	-21.51	1.28	1.51
4	N	7100	OGK	C13-C09	-20.73	1.29	1.51
4	P	8100	OGK	C09-C14	-17.83	1.33	1.52
4	D	2100	OGK	C09-C14	-17.64	1.33	1.52
4	J	5100	OGK	C09-C14	-17.42	1.34	1.52
4	F	3100	OGK	C09-C14	-17.33	1.34	1.52
4	B	1100	OGK	C09-C14	-17.24	1.34	1.52
4	L	6100	OGK	C09-C14	-17.10	1.34	1.52
4	H	4100	OGK	C09-C14	-17.08	1.34	1.52
4	N	7100	OGK	C09-C14	-16.35	1.35	1.52
4	B	1100	OGK	C13-C14	-7.01	1.31	1.50
4	D	2100	OGK	C13-C14	-6.86	1.32	1.50
4	H	4100	OGK	C13-C14	-6.75	1.32	1.50
4	J	5100	OGK	C13-C14	-6.69	1.32	1.50
4	L	6100	OGK	C13-C14	-6.64	1.32	1.50
4	F	3100	OGK	C13-C14	-6.57	1.33	1.50
4	P	8100	OGK	C13-C14	-6.47	1.33	1.50
4	N	7100	OGK	C13-C14	-6.22	1.33	1.50
4	F	3100	OGK	C18-C17	-3.32	1.44	1.54
4	B	1100	OGK	C18-C17	-3.26	1.44	1.54
4	P	8100	OGK	C18-C17	-3.18	1.45	1.54
4	J	5100	OGK	C18-C17	-3.15	1.45	1.54
4	D	2100	OGK	C18-C17	-3.05	1.45	1.54
4	H	4100	OGK	C18-C17	-3.03	1.45	1.54
4	N	7100	OGK	C18-C17	-3.02	1.45	1.54
4	L	6100	OGK	C18-C17	-2.82	1.46	1.54
4	J	5100	OGK	O07-C06	-2.54	1.18	1.23
4	D	2100	OGK	O07-C06	-2.49	1.18	1.23
4	H	4100	OGK	O07-C06	-2.41	1.18	1.23
5	D	1103	PO4	P-O2	-2.41	1.44	1.53
4	L	6100	OGK	O07-C06	-2.35	1.18	1.23
4	B	1100	OGK	O07-C06	-2.25	1.19	1.23
5	H	1101	PO4	P-O2	-2.14	1.45	1.53
5	B	1101	PO4	P-O2	-2.14	1.45	1.53
5	D	1102	PO4	P-O2	-2.14	1.45	1.53
5	L	1102	PO4	P-O2	-2.12	1.45	1.53
5	F	1101	PO4	P-O2	-2.12	1.45	1.53
5	H	1103	PO4	P-O2	-2.05	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1102	PO4	P-O2	-2.05	1.46	1.53
5	L	1101	PO4	P-O2	-2.04	1.46	1.53
5	B	1104	PO4	P-O2	-2.04	1.46	1.53
4	N	7100	OGK	O07-C06	-2.02	1.19	1.23
5	B	1103	PO4	P-O2	-2.02	1.46	1.53
4	F	3100	OGK	O07-C06	-2.02	1.19	1.23
5	L	1103	PO4	P-O2	-2.01	1.46	1.53
5	D	1101	PO4	P-O2	-2.01	1.46	1.53
4	N	7100	OGK	C05-C06	2.03	1.55	1.52
4	F	3100	OGK	C05-C06	2.19	1.55	1.52
4	H	4100	OGK	C09-N08	2.31	1.50	1.45
4	P	8100	OGK	C05-C06	2.44	1.56	1.52
4	J	5100	OGK	C09-N08	2.51	1.50	1.45
4	F	3100	OGK	C09-N08	2.54	1.50	1.45
4	H	4100	OGK	C05-C06	2.56	1.56	1.52
4	L	6100	OGK	C09-N08	2.62	1.50	1.45
4	L	6100	OGK	C05-C06	2.65	1.56	1.52
5	D	1101	PO4	P-O1	2.68	1.64	1.52
4	N	7100	OGK	C09-N08	2.71	1.50	1.45
4	B	1100	OGK	C09-N08	2.72	1.50	1.45
4	D	2100	OGK	C05-C06	2.74	1.56	1.52
4	J	5100	OGK	C05-C06	2.74	1.56	1.52
4	F	3100	OGK	C23-C22	2.77	1.58	1.53
5	L	1101	PO4	P-O1	2.78	1.64	1.52
5	J	1101	PO4	P-O1	2.80	1.64	1.52
5	B	1101	PO4	P-O4	2.82	1.63	1.53
5	B	1101	PO4	P-O1	2.85	1.64	1.52
5	B	1103	PO4	P-O4	2.89	1.63	1.53
5	D	1102	PO4	P-O3	2.90	1.63	1.53
5	J	1103	PO4	P-O4	2.92	1.63	1.53
5	L	1102	PO4	P-O1	2.92	1.65	1.52
5	L	1103	PO4	P-O4	2.92	1.63	1.53
5	P	1101	PO4	P-O1	2.94	1.65	1.52
5	B	1103	PO4	P-O1	2.94	1.65	1.52
5	H	1101	PO4	P-O1	2.94	1.65	1.52
5	H	1104	PO4	P-O1	2.94	1.65	1.52
5	P	1102	PO4	P-O1	2.94	1.65	1.52
5	B	1104	PO4	P-O1	2.95	1.65	1.52
5	D	1104	PO4	P-O1	2.96	1.65	1.52
5	F	1103	PO4	P-O1	2.97	1.65	1.52
5	F	1101	PO4	P-O1	2.97	1.65	1.52
5	J	1102	PO4	P-O1	2.97	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	1103	PO4	P-O1	2.97	1.65	1.52
5	N	1104	PO4	P-O1	2.98	1.65	1.52
5	H	1102	PO4	P-O1	2.98	1.65	1.52
5	N	1101	PO4	P-O1	2.99	1.65	1.52
5	J	1104	PO4	P-O4	2.99	1.64	1.53
5	D	1102	PO4	P-O1	2.99	1.65	1.52
5	P	1104	PO4	P-O1	3.02	1.65	1.52
5	D	1103	PO4	P-O1	3.02	1.65	1.52
5	L	1103	PO4	P-O1	3.03	1.65	1.52
5	J	1103	PO4	P-O1	3.04	1.65	1.52
5	N	1103	PO4	P-O1	3.04	1.65	1.52
5	N	1102	PO4	P-O1	3.04	1.65	1.52
5	B	1102	PO4	P-O1	3.06	1.65	1.52
5	D	1101	PO4	P-O3	3.06	1.64	1.53
5	H	1103	PO4	P-O1	3.11	1.66	1.52
5	F	1101	PO4	P-O4	3.13	1.64	1.53
5	P	1101	PO4	P-O4	3.13	1.64	1.53
5	B	1104	PO4	P-O4	3.14	1.64	1.53
5	D	1103	PO4	P-O4	3.15	1.64	1.53
5	L	1104	PO4	P-O1	3.16	1.66	1.52
5	F	1101	PO4	P-O3	3.16	1.64	1.53
5	J	1103	PO4	P-O3	3.16	1.64	1.53
4	J	5100	OGK	C23-C22	3.16	1.58	1.53
5	B	1102	PO4	P-O3	3.17	1.64	1.53
4	D	2100	OGK	C23-C22	3.18	1.58	1.53
5	D	1103	PO4	P-O3	3.22	1.65	1.53
5	J	1104	PO4	P-O1	3.23	1.66	1.52
5	L	1102	PO4	P-O4	3.23	1.65	1.53
5	F	1104	PO4	P-O1	3.23	1.66	1.52
5	D	1101	PO4	P-O4	3.23	1.65	1.53
5	N	1103	PO4	P-O4	3.23	1.65	1.53
5	B	1104	PO4	P-O3	3.24	1.65	1.53
5	P	1102	PO4	P-O4	3.24	1.65	1.53
5	H	1102	PO4	P-O3	3.25	1.65	1.53
5	J	1104	PO4	P-O3	3.26	1.65	1.53
5	P	1103	PO4	P-O3	3.26	1.65	1.53
5	P	1101	PO4	P-O3	3.27	1.65	1.53
5	P	1103	PO4	P-O4	3.27	1.65	1.53
4	B	1100	OGK	C23-C22	3.27	1.58	1.53
5	J	1102	PO4	P-O4	3.27	1.65	1.53
5	P	1104	PO4	P-O3	3.28	1.65	1.53
5	D	1104	PO4	P-O4	3.31	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1102	PO4	P-O4	3.32	1.65	1.53
5	F	1102	PO4	P-O1	3.32	1.66	1.52
5	F	1103	PO4	P-O3	3.32	1.65	1.53
5	D	1102	PO4	P-O4	3.32	1.65	1.53
5	L	1104	PO4	P-O3	3.33	1.65	1.53
5	F	1102	PO4	P-O4	3.33	1.65	1.53
5	L	1103	PO4	P-O3	3.35	1.65	1.53
5	J	1101	PO4	P-O3	3.35	1.65	1.53
5	P	1104	PO4	P-O4	3.36	1.65	1.53
5	N	1102	PO4	P-O3	3.37	1.65	1.53
4	L	6100	OGK	C23-C22	3.39	1.59	1.53
5	N	1103	PO4	P-O3	3.42	1.65	1.53
5	N	1104	PO4	P-O3	3.42	1.65	1.53
5	B	1101	PO4	P-O3	3.43	1.65	1.53
5	L	1102	PO4	P-O3	3.43	1.65	1.53
5	H	1103	PO4	P-O4	3.45	1.65	1.53
5	L	1101	PO4	P-O4	3.45	1.65	1.53
5	J	1101	PO4	P-O4	3.46	1.65	1.53
5	D	1104	PO4	P-O3	3.46	1.65	1.53
5	F	1104	PO4	P-O3	3.47	1.65	1.53
5	F	1104	PO4	P-O4	3.48	1.65	1.53
5	J	1102	PO4	P-O3	3.48	1.65	1.53
5	P	1102	PO4	P-O3	3.49	1.65	1.53
5	F	1102	PO4	P-O3	3.49	1.66	1.53
5	N	1102	PO4	P-O4	3.51	1.66	1.53
5	L	1101	PO4	P-O3	3.51	1.66	1.53
4	P	8100	OGK	C23-C22	3.52	1.59	1.53
5	F	1103	PO4	P-O4	3.52	1.66	1.53
5	H	1102	PO4	P-O4	3.54	1.66	1.53
5	H	1101	PO4	P-O4	3.56	1.66	1.53
5	H	1104	PO4	P-O4	3.56	1.66	1.53
5	B	1103	PO4	P-O3	3.58	1.66	1.53
5	L	1104	PO4	P-O4	3.61	1.66	1.53
5	H	1101	PO4	P-O3	3.63	1.66	1.53
5	H	1103	PO4	P-O3	3.65	1.66	1.53
5	N	1101	PO4	P-O4	3.71	1.66	1.53
5	N	1104	PO4	P-O4	3.71	1.66	1.53
5	H	1104	PO4	P-O3	3.79	1.67	1.53
5	N	1101	PO4	P-O3	4.24	1.68	1.53
4	N	7100	OGK	C23-C22	4.24	1.60	1.53
4	H	4100	OGK	C23-C22	4.84	1.61	1.53
4	H	4100	OGK	C06-N08	6.18	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	6100	OGK	C06-N08	6.20	1.47	1.34
4	J	5100	OGK	C06-N08	6.25	1.47	1.34
4	D	2100	OGK	C06-N08	6.58	1.48	1.34
4	N	7100	OGK	C06-N08	6.62	1.48	1.34
4	P	8100	OGK	C06-N08	6.86	1.49	1.34
4	F	3100	OGK	C06-N08	6.91	1.49	1.34
4	B	1100	OGK	C06-N08	7.04	1.49	1.34

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	5100	OGK	C13-C14-C09	-6.75	57.22	60.38
4	F	3100	OGK	C13-C14-C09	-6.51	57.33	60.38
4	P	8100	OGK	C13-C14-C09	-6.42	57.37	60.38
4	D	2100	OGK	C13-C14-C09	-6.30	57.43	60.38
4	L	6100	OGK	C13-C14-C09	-6.25	57.45	60.38
4	N	7100	OGK	C13-C14-C09	-6.13	57.51	60.38
4	H	4100	OGK	C13-C14-C09	-5.88	57.63	60.38
4	B	1100	OGK	C13-C14-C09	-5.71	57.70	60.38
4	B	1100	OGK	C18-C17-C05	-5.19	100.00	116.96
4	F	3100	OGK	C18-C17-C05	-5.04	100.47	116.96
4	P	8100	OGK	C18-C17-C05	-4.94	100.80	116.96
4	N	7100	OGK	C18-C17-C05	-4.82	101.19	116.96
4	D	2100	OGK	C18-C17-C05	-4.82	101.21	116.96
4	L	6100	OGK	C18-C17-C05	-4.52	102.19	116.96
4	J	5100	OGK	C18-C17-C05	-4.43	102.47	116.96
4	B	1100	OGK	O07-C06-C05	-4.24	116.69	121.56
4	H	4100	OGK	C19-C20-C22	-3.86	105.53	108.96
4	H	4100	OGK	C13-C09-N08	-3.58	112.35	117.71
4	D	2100	OGK	C04-C03-C02	-3.52	106.58	112.80
4	H	4100	OGK	C18-C17-C05	-3.50	105.53	116.96
4	J	5100	OGK	C04-C03-C02	-3.18	107.20	112.80
4	L	6100	OGK	C04-C03-C02	-3.16	107.22	112.80
4	D	2100	OGK	C13-C09-N08	-3.06	113.14	117.71
4	P	8100	OGK	C04-C03-C02	-2.91	107.67	112.80
4	B	1100	OGK	C04-C03-C02	-2.80	107.86	112.80
4	F	3100	OGK	C13-C09-N08	-2.79	113.54	117.71
4	N	7100	OGK	C19-C20-C22	-2.75	106.52	108.96
4	P	8100	OGK	O07-C06-C05	-2.66	118.50	121.56
4	P	8100	OGK	C13-C09-N08	-2.62	113.79	117.71
4	L	6100	OGK	C13-C09-N08	-2.62	113.80	117.71
4	N	7100	OGK	C13-C09-N08	-2.50	113.97	117.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3100	OGK	O07-C06-C05	-2.46	118.73	121.56
4	B	1100	OGK	C13-C09-N08	-2.46	114.03	117.71
4	J	5100	OGK	C13-C09-N08	-2.44	114.07	117.71
4	F	3100	OGK	C04-C03-C02	-2.43	108.52	112.80
4	J	5100	OGK	O07-C06-N08	-2.23	117.86	123.04
4	N	7100	OGK	C04-C03-C02	-2.10	109.10	112.80
4	L	6100	OGK	O07-C06-N08	-2.03	118.33	123.04
4	N	7100	OGK	O07-C06-C05	-2.03	119.23	121.56
4	F	3100	OGK	C05-C06-N08	2.02	118.97	116.30
4	L	6100	OGK	C09-C13-C14	2.10	61.90	60.89
4	P	8100	OGK	C05-C06-N08	2.13	119.12	116.30
4	D	2100	OGK	C09-C13-C14	2.14	61.92	60.89
4	H	4100	OGK	C09-C13-C14	2.17	61.93	60.89
4	J	5100	OGK	C09-C13-C14	2.19	61.94	60.89
4	B	1100	OGK	C13-C09-C14	2.27	60.20	59.04
4	H	4100	OGK	C05-C04-C03	2.33	114.82	109.91
4	B	1100	OGK	C18-C17-C22	2.34	106.57	103.87
4	L	6100	OGK	C05-C06-N08	2.38	119.44	116.30
4	B	1100	OGK	C09-C13-C14	2.52	62.10	60.89
4	D	2100	OGK	C05-C06-N08	2.56	119.69	116.30
4	J	5100	OGK	C05-C06-N08	2.67	119.82	116.30
4	H	4100	OGK	C13-C09-C14	2.74	60.44	59.04
4	F	3100	OGK	C04-C05-C06	2.83	117.76	111.16
4	N	7100	OGK	C04-C05-C06	2.85	117.80	111.16
4	B	1100	OGK	C04-C05-C06	2.91	117.95	111.16
4	B	1100	OGK	C05-C06-N08	2.95	120.19	116.30
4	L	6100	OGK	C18-C17-C22	2.96	107.28	103.87
4	J	5100	OGK	C04-C05-C06	3.08	118.33	111.16
4	H	4100	OGK	C22-C23-C03	3.08	116.40	109.91
4	P	8100	OGK	C04-C05-C06	3.15	118.50	111.16
4	P	8100	OGK	C18-C17-C22	3.15	107.50	103.87
4	L	6100	OGK	C13-C09-C14	3.15	60.65	59.04
4	D	2100	OGK	C13-C09-C14	3.15	60.65	59.04
4	D	2100	OGK	C04-C05-C06	3.25	118.74	111.16
4	H	4100	OGK	C18-C17-C22	3.30	107.68	103.87
4	L	6100	OGK	C04-C05-C06	3.35	118.97	111.16
4	N	7100	OGK	C13-C09-C14	3.36	60.76	59.04
4	D	2100	OGK	C18-C17-C22	3.47	107.87	103.87
4	J	5100	OGK	C13-C09-C14	3.52	60.84	59.04
4	H	4100	OGK	C04-C03-C23	3.56	115.98	109.70
4	H	4100	OGK	C04-C05-C17	3.60	117.52	110.04
4	F	3100	OGK	C13-C09-C14	3.61	60.89	59.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	7100	OGK	C05-C04-C03	3.88	118.08	109.91
4	H	4100	OGK	C04-C05-C06	3.92	120.30	111.16
4	J	5100	OGK	C18-C17-C22	3.93	108.41	103.87
4	F	3100	OGK	C18-C17-C22	3.98	108.46	103.87
4	F	3100	OGK	C05-C04-C03	4.10	118.55	109.91
4	P	8100	OGK	C13-C09-C14	4.17	61.17	59.04
4	B	1100	OGK	C05-C04-C03	4.19	118.74	109.91
4	J	5100	OGK	C05-C04-C03	4.24	118.84	109.91
4	D	2100	OGK	C05-C04-C03	4.52	119.42	109.91
4	P	8100	OGK	C05-C04-C03	4.61	119.63	109.91
4	N	7100	OGK	C18-C17-C22	4.63	109.22	103.87
4	L	6100	OGK	C05-C04-C03	4.75	119.91	109.91
4	H	4100	OGK	C23-C03-C02	4.90	121.43	112.80
4	D	2100	OGK	C04-C05-C17	4.97	120.35	110.04
4	L	6100	OGK	C04-C05-C17	5.08	120.58	110.04
4	F	3100	OGK	C04-C05-C17	5.09	120.60	110.04
4	J	5100	OGK	C04-C05-C17	5.19	120.82	110.04
4	P	8100	OGK	C04-C05-C17	5.26	120.95	110.04
4	B	1100	OGK	C04-C05-C17	5.28	121.01	110.04
4	N	7100	OGK	C04-C05-C17	5.67	121.81	110.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	4100	OGK	C03

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1100	OGK	7	0
5	B	1101	PO4	1	0
5	B	1102	PO4	1	0
5	B	1103	PO4	1	0
5	D	1101	PO4	1	0
5	D	1103	PO4	1	0
4	D	2100	OGK	7	0
5	F	1101	PO4	1	0
5	F	1103	PO4	1	0
4	F	3100	OGK	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1101	PO4	1	0
5	H	1102	PO4	1	0
5	H	1103	PO4	1	0
4	H	4100	OGK	16	0
5	J	1101	PO4	1	0
5	J	1103	PO4	1	0
4	J	5100	OGK	7	0
5	L	1101	PO4	1	0
5	L	1103	PO4	1	0
4	L	6100	OGK	7	0
5	N	1101	PO4	1	0
5	N	1102	PO4	1	0
5	N	1103	PO4	1	0
4	N	7100	OGK	6	0
5	P	1101	PO4	1	0
5	P	1103	PO4	2	0
4	P	8100	OGK	8	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, 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	144/160 (90%)	0.53	7 (4%) 33 32	50, 100, 151, 168	0
1	C	144/160 (90%)	0.59	9 (6%) 23 24	50, 102, 153, 170	0
1	E	144/160 (90%)	0.36	7 (4%) 33 32	54, 101, 151, 171	0
1	G	144/160 (90%)	0.16	4 (2%) 56 56	49, 96, 149, 170	0
1	I	144/160 (90%)	0.40	8 (5%) 28 27	50, 100, 150, 170	0
1	K	144/160 (90%)	0.67	18 (12%) 5 4	53, 102, 152, 170	0
1	M	144/160 (90%)	0.70	17 (11%) 6 5	55, 102, 152, 175	0
1	O	144/160 (90%)	0.67	18 (12%) 5 4	51, 101, 151, 173	0
2	B	568/592 (95%)	-0.13	8 (1%) 78 79	38, 76, 136, 201	0
2	D	568/592 (95%)	-0.01	9 (1%) 74 74	38, 75, 135, 200	0
2	F	568/592 (95%)	-0.06	18 (3%) 51 51	40, 79, 136, 202	0
2	H	562/592 (94%)	-0.21	13 (2%) 64 63	34, 73, 127, 191	0
2	J	568/592 (95%)	-0.12	10 (1%) 71 70	39, 77, 136, 204	0
2	L	568/592 (95%)	-0.12	9 (1%) 74 74	41, 79, 135, 202	0
2	N	568/592 (95%)	0.42	49 (8%) 13 12	41, 82, 137, 206	0
2	P	568/592 (95%)	-0.07	18 (3%) 51 51	40, 80, 138, 204	0
3	Q	18/21 (85%)	-0.11	0 100 100	72, 93, 116, 143	0
3	R	18/21 (85%)	-0.05	0 100 100	71, 88, 115, 145	0
3	S	18/21 (85%)	-0.32	0 100 100	73, 93, 117, 143	0
3	U	18/21 (85%)	-0.14	0 100 100	71, 88, 112, 143	0
3	V	18/21 (85%)	0.03	1 (5%) 28 27	75, 93, 115, 143	0
3	W	18/21 (85%)	0.29	1 (5%) 28 27	80, 96, 119, 143	0
3	X	18/21 (85%)	-0.08	1 (5%) 28 27	76, 91, 119, 143	0
All	All	5816/6163 (94%)	0.07	225 (3%) 43 42	34, 82, 141, 206	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	591	PRO	8.7
2	B	549	ARG	6.4
2	N	590	GLU	6.3
2	N	360	ASP	6.1
2	P	12	SER	6.0
2	P	592	ILE	6.0
2	N	592	ILE	6.0
2	J	360	ASP	6.0
2	F	547	SER	5.6
1	M	80	ASP	5.5
2	P	362	GLU	5.4
2	D	360	ASP	5.1
2	L	359	GLU	5.0
1	O	80	ASP	4.9
2	N	359	GLU	4.8
2	F	355	GLU	4.8
1	M	115	ASP	4.8
2	P	547	SER	4.5
1	A	24	LEU	4.5
2	N	355	GLU	4.5
2	H	356	GLN	4.4
2	P	591	PRO	4.4
2	J	592	ILE	4.2
2	L	592	ILE	4.2
2	H	355	GLU	4.2
2	D	12	SER	4.2
2	H	352	GLY	4.1
2	N	373	LEU	4.1
2	F	356	GLN	4.1
3	V	200	GLU	4.1
2	N	354	ASP	4.1
2	L	356	GLN	4.0
2	N	356	GLN	4.0
2	N	358	MET	3.9
2	J	549	ARG	3.9
2	F	546	PRO	3.9
2	P	356	GLN	3.7
2	F	592	ILE	3.7
2	L	360	ASP	3.7
2	P	548	ARG	3.6
2	F	12	SER	3.6
1	K	6	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	X	200	GLU	3.6
3	W	200	GLU	3.5
2	D	592	ILE	3.5
2	N	389	ASP	3.4
2	F	591	PRO	3.4
2	N	266	LEU	3.4
2	H	12	SER	3.4
1	O	116	LEU	3.4
2	B	356	GLN	3.3
2	J	548	ARG	3.3
1	A	59	CYS	3.3
2	F	360	ASP	3.3
1	M	87	ASP	3.3
1	M	63	VAL	3.2
1	M	116	LEU	3.2
1	I	38	VAL	3.2
2	L	12	SER	3.2
2	P	549	ARG	3.2
1	I	35	ASP	3.2
1	A	20	GLU	3.1
2	B	359	GLU	3.1
2	F	359	GLU	3.1
1	A	21	ALA	3.1
1	O	88	ALA	3.1
1	E	138	ASN	3.0
1	O	5	LYS	3.0
1	C	7	VAL	3.0
2	N	383	MET	3.0
2	H	420	THR	3.0
2	H	332	ARG	3.0
2	F	416	GLU	3.0
2	L	354	ASP	3.0
2	B	360	ASP	3.0
2	N	12	SER	2.9
1	O	55	VAL	2.9
2	J	361	GLU	2.9
2	N	15	ALA	2.9
1	E	80	ASP	2.9
2	H	358	MET	2.9
1	O	117	THR	2.9
2	P	420	THR	2.9
2	L	548	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	38	VAL	2.9
1	A	41	GLY	2.8
1	K	59	CYS	2.8
2	N	474	GLY	2.8
1	O	21	ALA	2.8
2	J	358	MET	2.8
2	H	357	GLY	2.8
2	F	590	GLU	2.8
1	O	56	ILE	2.8
1	A	6	ILE	2.8
2	B	592	ILE	2.8
2	N	424	LEU	2.8
1	M	84	LYS	2.7
2	B	358	MET	2.7
1	E	84	LYS	2.7
2	F	549	ARG	2.7
2	P	546	PRO	2.7
2	P	590	GLU	2.7
1	C	59	CYS	2.7
1	M	20	GLU	2.7
2	N	291	PHE	2.7
2	B	527	MET	2.7
1	K	25	GLU	2.6
1	M	6	ILE	2.6
2	D	548	ARG	2.6
1	C	115	ASP	2.6
2	J	356	GLN	2.6
1	M	37	CYS	2.6
2	H	353	ALA	2.6
1	K	22	VAL	2.6
1	K	8	LEU	2.6
1	C	45	PRO	2.6
1	C	40	ASN	2.6
1	K	87	ASP	2.6
2	F	358	MET	2.6
1	M	123	ASP	2.5
2	P	258	GLY	2.5
2	D	358	MET	2.5
1	K	24	LEU	2.5
1	C	66	ALA	2.5
1	K	20	GLU	2.5
1	K	21	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	370	LEU	2.5
1	I	47	VAL	2.5
2	N	306	GLU	2.5
1	I	39	ASP	2.5
1	K	82	ASP	2.5
1	O	89	ASP	2.5
1	O	52	LEU	2.5
1	E	82	ASP	2.5
1	K	80	ASP	2.5
1	M	17	GLU	2.5
2	F	361	GLU	2.5
1	O	87	ASP	2.4
2	N	588	LEU	2.4
2	J	591	PRO	2.4
2	B	355	GLU	2.4
2	D	527	MET	2.4
2	N	256	ASP	2.4
1	O	86	TRP	2.4
2	F	588	LEU	2.4
1	C	20	GLU	2.4
2	H	361	GLU	2.4
2	N	548	ARG	2.4
1	O	84	LYS	2.4
2	N	290	PRO	2.4
1	O	63	VAL	2.4
2	F	548	ARG	2.4
2	L	549	ARG	2.4
2	N	462	SER	2.4
2	N	416	GLU	2.4
2	N	298	LEU	2.4
1	K	43	PRO	2.4
1	O	112	ASN	2.3
2	N	334	LEU	2.3
2	P	359	GLU	2.3
1	E	19	GLU	2.3
2	N	527	MET	2.3
2	N	363	GLY	2.3
2	N	449	GLY	2.3
1	M	83	LEU	2.3
2	H	362	GLU	2.3
2	D	549	ARG	2.3
2	N	420	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	527	MET	2.3
1	K	15	SER	2.3
2	N	313	LEU	2.3
1	E	57	GLU	2.3
2	N	402	LEU	2.3
1	I	6	ILE	2.3
1	I	7	VAL	2.2
2	N	361	GLU	2.2
1	C	63	VAL	2.2
1	C	87	ASP	2.2
1	K	9	LYS	2.2
2	N	434	GLY	2.2
1	K	17	GLU	2.2
2	N	287	ILE	2.2
1	O	67	ALA	2.2
1	A	22	VAL	2.2
1	K	5	LYS	2.1
1	G	90	PHE	2.1
2	N	435	CYS	2.1
1	O	115	ASP	2.1
2	P	588	LEU	2.1
1	M	91	MET	2.1
2	D	429	ARG	2.1
2	N	349	ILE	2.1
2	J	258	GLY	2.1
2	N	398	ILE	2.1
2	P	401	TYR	2.1
1	K	81	ASP	2.1
2	P	360	ASP	2.1
1	M	88	ALA	2.1
2	L	362	GLU	2.1
2	N	589	LYS	2.1
2	N	305	LEU	2.1
2	P	527	MET	2.1
1	M	59	CYS	2.1
1	G	80	ASP	2.1
2	N	347	LEU	2.1
1	I	20	GLU	2.1
1	O	93	ILE	2.0
1	G	92	LYS	2.0
2	N	257	ILE	2.0
2	N	460	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	357	GLY	2.0
2	P	355	GLU	2.0
1	M	90	PHE	2.0
1	E	59	CYS	2.0
2	D	357	GLY	2.0
2	H	258	GLY	2.0
2	N	443	PHE	2.0
2	F	354	ASP	2.0
1	K	56	ILE	2.0
2	N	375	GLN	2.0
2	N	350	GLU	2.0
2	J	357	GLY	2.0
2	N	448	GLY	2.0
1	I	84	LYS	2.0
1	G	91	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	PO4	J	1102	5/5	0.95	0.39	12.94	67,86,95,104	0
5	PO4	H	1104	5/5	0.87	0.36	6.35	54,57,114,134	0
5	PO4	L	1102	5/5	0.96	0.36	5.86	73,82,96,100	0
5	PO4	P	1101	5/5	0.98	0.28	5.49	57,62,74,75	0
5	PO4	N	1102	5/5	0.92	0.35	5.17	78,90,92,113	0
5	PO4	L	1101	5/5	0.96	0.32	4.25	48,58,74,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PO4	F	1102	5/5	0.88	0.29	4.23	64,90,96,109	0
5	PO4	P	1104	5/5	0.92	0.26	4.16	73,75,110,121	0
5	PO4	J	1104	5/5	0.92	0.33	3.58	76,81,112,117	0
5	PO4	L	1103	5/5	0.94	0.32	3.31	52,56,69,89	0
5	PO4	J	1101	5/5	0.97	0.26	3.31	50,55,74,79	0
5	PO4	N	1104	5/5	0.90	0.35	2.63	82,83,118,122	0
5	PO4	N	1103	5/5	0.90	0.37	2.60	56,56,74,85	0
5	PO4	L	1104	5/5	0.89	0.27	2.55	76,78,119,123	0
5	PO4	B	1103	5/5	0.98	0.28	2.42	54,54,61,76	0
5	PO4	F	1101	5/5	0.96	0.24	2.33	52,58,68,88	0
5	PO4	B	1104	5/5	0.92	0.24	2.28	68,79,102,119	0
5	PO4	D	1102	5/5	0.97	0.24	2.21	66,79,93,93	0
5	PO4	D	1101	5/5	0.97	0.29	2.11	51,55,63,80	0
5	PO4	H	1101	5/5	0.98	0.21	1.93	36,45,63,88	0
5	PO4	B	1102	5/5	0.96	0.24	1.89	70,84,93,100	0
5	PO4	F	1103	5/5	0.96	0.28	1.83	53,57,73,86	0
5	PO4	B	1101	5/5	0.97	0.22	1.69	58,59,65,75	0
5	PO4	J	1103	5/5	0.97	0.26	1.54	53,53,64,77	0
5	PO4	D	1103	5/5	0.98	0.30	1.41	48,52,55,81	0
5	PO4	P	1103	5/5	0.97	0.24	1.08	50,58,73,85	0
4	OGK	P	8100	23/23	0.96	0.25	1.05	64,75,88,90	0
5	PO4	N	1101	5/5	0.87	0.31	0.99	51,59,80,82	0
5	PO4	D	1104	5/5	0.88	0.24	0.90	72,73,107,122	0
4	OGK	H	4100	23/23	0.93	0.25	0.90	44,71,85,98	0
5	PO4	P	1102	5/5	0.94	0.20	0.74	72,87,98,108	0
4	OGK	F	3100	23/23	0.95	0.24	0.56	64,72,91,94	0
4	OGK	D	2100	23/23	0.96	0.25	0.46	60,72,81,86	0
4	OGK	J	5100	23/23	0.96	0.24	0.44	59,67,88,93	0
4	OGK	L	6100	23/23	0.95	0.23	0.42	62,71,90,92	0
4	OGK	B	1100	23/23	0.95	0.23	0.33	62,73,87,93	0
4	OGK	N	7100	23/23	0.88	0.26	-0.13	65,79,100,104	0
5	PO4	F	1104	5/5	0.93	0.19	-0.14	72,81,117,120	0
5	PO4	H	1102	5/5	0.94	0.33	-	58,59,72,88	0
5	PO4	H	1103	5/5	0.97	0.20	-	38,47,52,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.