



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:23 am GMT

PDB ID : 3KDO
Title : Crystal structure of Type III Rubisco SP6 mutant complexed with 2-CABP
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2009-10-23
Resolution : 2.36 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

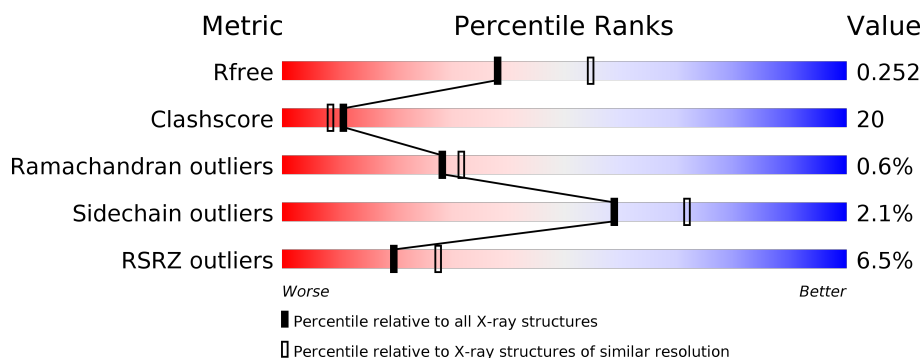
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	444	<div> <div>10%</div> <div>54%</div> <div>42%</div> <div>..</div> </div>
1	B	444	<div> <div>8%</div> <div>68%</div> <div>30%</div> <div>..</div> </div>
1	C	444	<div> <div>4%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
1	D	444	<div> <div>2%</div> <div>74%</div> <div>24%</div> <div>..</div> </div>
1	E	444	<div> <div>9%</div> <div>72%</div> <div>27%</div> <div>..</div> </div>
1	F	444	<div> <div>5%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	444	<div><div></div><div>2%70%27%<div><div></div><div></div></div></div></div>
1	H	444	<div><div></div><div>11%60%37%<div><div></div><div></div></div></div></div>
1	I	444	<div><div></div><div>5%70%28%<div><div></div><div></div></div></div></div>
1	J	444	<div><div></div><div>8%69%29%<div><div></div><div></div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36065 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3341	2146	569	616	10			
1	B	438	Total	C	N	O	S	0	0	0
			3391	2179	575	627	10			
1	C	440	Total	C	N	O	S	0	0	0
			3420	2196	580	634	10			
1	D	437	Total	C	N	O	S	0	0	0
			3419	2195	582	632	10			
1	E	440	Total	C	N	O	S	0	0	0
			3418	2198	582	628	10			
1	F	437	Total	C	N	O	S	0	0	0
			3415	2195	581	629	10			
1	G	437	Total	C	N	O	S	0	0	0
			3423	2200	582	631	10			
1	H	438	Total	C	N	O	S	0	0	0
			3382	2178	574	620	10			
1	I	438	Total	C	N	O	S	0	0	0
			3410	2190	582	628	10			
1	J	438	Total	C	N	O	S	0	0	0
			3415	2195	581	629	10			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	ENGINEERED	UNP O93627
A	327	ARG	LYS	ENGINEERED	UNP O93627
A	328	ASP	TRP	ENGINEERED	UNP O93627
A	329	ILE	ASP	ENGINEERED	UNP O93627
A	330	THR	VAL	ENGINEERED	UNP O93627
A	331	LEU	ILE	ENGINEERED	UNP O93627
A	332	GLY	GLN	ENGINEERED	UNP O93627
A	333	PHE	ASN	ENGINEERED	UNP O93627
A	334	VAL	ALA	ENGINEERED	UNP O93627

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	ASP	ARG	ENGINEERED	UNP O93627
A	336	LEU	ILE	ENGINEERED	UNP O93627
B	326	GLU	GLY	ENGINEERED	UNP O93627
B	327	ARG	LYS	ENGINEERED	UNP O93627
B	328	ASP	TRP	ENGINEERED	UNP O93627
B	329	ILE	ASP	ENGINEERED	UNP O93627
B	330	THR	VAL	ENGINEERED	UNP O93627
B	331	LEU	ILE	ENGINEERED	UNP O93627
B	332	GLY	GLN	ENGINEERED	UNP O93627
B	333	PHE	ASN	ENGINEERED	UNP O93627
B	334	VAL	ALA	ENGINEERED	UNP O93627
B	335	ASP	ARG	ENGINEERED	UNP O93627
B	336	LEU	ILE	ENGINEERED	UNP O93627
C	326	GLU	GLY	ENGINEERED	UNP O93627
C	327	ARG	LYS	ENGINEERED	UNP O93627
C	328	ASP	TRP	ENGINEERED	UNP O93627
C	329	ILE	ASP	ENGINEERED	UNP O93627
C	330	THR	VAL	ENGINEERED	UNP O93627
C	331	LEU	ILE	ENGINEERED	UNP O93627
C	332	GLY	GLN	ENGINEERED	UNP O93627
C	333	PHE	ASN	ENGINEERED	UNP O93627
C	334	VAL	ALA	ENGINEERED	UNP O93627
C	335	ASP	ARG	ENGINEERED	UNP O93627
C	336	LEU	ILE	ENGINEERED	UNP O93627
D	326	GLU	GLY	ENGINEERED	UNP O93627
D	327	ARG	LYS	ENGINEERED	UNP O93627
D	328	ASP	TRP	ENGINEERED	UNP O93627
D	329	ILE	ASP	ENGINEERED	UNP O93627
D	330	THR	VAL	ENGINEERED	UNP O93627
D	331	LEU	ILE	ENGINEERED	UNP O93627
D	332	GLY	GLN	ENGINEERED	UNP O93627
D	333	PHE	ASN	ENGINEERED	UNP O93627
D	334	VAL	ALA	ENGINEERED	UNP O93627
D	335	ASP	ARG	ENGINEERED	UNP O93627
D	336	LEU	ILE	ENGINEERED	UNP O93627
E	326	GLU	GLY	ENGINEERED	UNP O93627
E	327	ARG	LYS	ENGINEERED	UNP O93627
E	328	ASP	TRP	ENGINEERED	UNP O93627
E	329	ILE	ASP	ENGINEERED	UNP O93627
E	330	THR	VAL	ENGINEERED	UNP O93627
E	331	LEU	ILE	ENGINEERED	UNP O93627
E	332	GLY	GLN	ENGINEERED	UNP O93627

Continued on next page...

Continued from previous page...

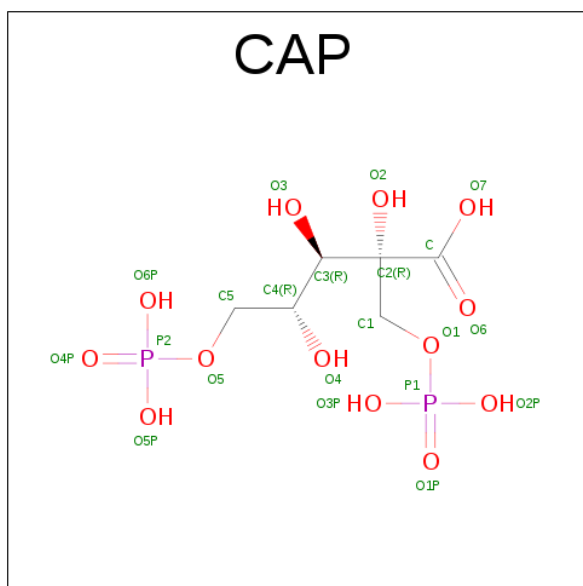
Chain	Residue	Modelled	Actual	Comment	Reference
E	333	PHE	ASN	ENGINEERED	UNP O93627
E	334	VAL	ALA	ENGINEERED	UNP O93627
E	335	ASP	ARG	ENGINEERED	UNP O93627
E	336	LEU	ILE	ENGINEERED	UNP O93627
F	326	GLU	GLY	ENGINEERED	UNP O93627
F	327	ARG	LYS	ENGINEERED	UNP O93627
F	328	ASP	TRP	ENGINEERED	UNP O93627
F	329	ILE	ASP	ENGINEERED	UNP O93627
F	330	THR	VAL	ENGINEERED	UNP O93627
F	331	LEU	ILE	ENGINEERED	UNP O93627
F	332	GLY	GLN	ENGINEERED	UNP O93627
F	333	PHE	ASN	ENGINEERED	UNP O93627
F	334	VAL	ALA	ENGINEERED	UNP O93627
F	335	ASP	ARG	ENGINEERED	UNP O93627
F	336	LEU	ILE	ENGINEERED	UNP O93627
G	326	GLU	GLY	ENGINEERED	UNP O93627
G	327	ARG	LYS	ENGINEERED	UNP O93627
G	328	ASP	TRP	ENGINEERED	UNP O93627
G	329	ILE	ASP	ENGINEERED	UNP O93627
G	330	THR	VAL	ENGINEERED	UNP O93627
G	331	LEU	ILE	ENGINEERED	UNP O93627
G	332	GLY	GLN	ENGINEERED	UNP O93627
G	333	PHE	ASN	ENGINEERED	UNP O93627
G	334	VAL	ALA	ENGINEERED	UNP O93627
G	335	ASP	ARG	ENGINEERED	UNP O93627
G	336	LEU	ILE	ENGINEERED	UNP O93627
H	326	GLU	GLY	ENGINEERED	UNP O93627
H	327	ARG	LYS	ENGINEERED	UNP O93627
H	328	ASP	TRP	ENGINEERED	UNP O93627
H	329	ILE	ASP	ENGINEERED	UNP O93627
H	330	THR	VAL	ENGINEERED	UNP O93627
H	331	LEU	ILE	ENGINEERED	UNP O93627
H	332	GLY	GLN	ENGINEERED	UNP O93627
H	333	PHE	ASN	ENGINEERED	UNP O93627
H	334	VAL	ALA	ENGINEERED	UNP O93627
H	335	ASP	ARG	ENGINEERED	UNP O93627
H	336	LEU	ILE	ENGINEERED	UNP O93627
I	326	GLU	GLY	ENGINEERED	UNP O93627
I	327	ARG	LYS	ENGINEERED	UNP O93627
I	328	ASP	TRP	ENGINEERED	UNP O93627
I	329	ILE	ASP	ENGINEERED	UNP O93627
I	330	THR	VAL	ENGINEERED	UNP O93627

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	331	LEU	ILE	ENGINEERED	UNP O93627
I	332	GLY	GLN	ENGINEERED	UNP O93627
I	333	PHE	ASN	ENGINEERED	UNP O93627
I	334	VAL	ALA	ENGINEERED	UNP O93627
I	335	ASP	ARG	ENGINEERED	UNP O93627
I	336	LEU	ILE	ENGINEERED	UNP O93627
J	326	GLU	GLY	ENGINEERED	UNP O93627
J	327	ARG	LYS	ENGINEERED	UNP O93627
J	328	ASP	TRP	ENGINEERED	UNP O93627
J	329	ILE	ASP	ENGINEERED	UNP O93627
J	330	THR	VAL	ENGINEERED	UNP O93627
J	331	LEU	ILE	ENGINEERED	UNP O93627
J	332	GLY	GLN	ENGINEERED	UNP O93627
J	333	PHE	ASN	ENGINEERED	UNP O93627
J	334	VAL	ALA	ENGINEERED	UNP O93627
J	335	ASP	ARG	ENGINEERED	UNP O93627
J	336	LEU	ILE	ENGINEERED	UNP O93627

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			21	6	13	2		
2	B	1	Total	C	O	P	0	0
			21	6	13	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			21	6	13	2		
2	D	1	Total	C	O	P	0	0
			21	6	13	2		
2	E	1	Total	C	O	P	0	0
			21	6	13	2		
2	F	1	Total	C	O	P	0	0
			21	6	13	2		
2	G	1	Total	C	O	P	0	0
			21	6	13	2		
2	H	1	Total	C	O	P	0	0
			21	6	13	2		
2	I	1	Total	C	O	P	0	0
			21	6	13	2		
2	J	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

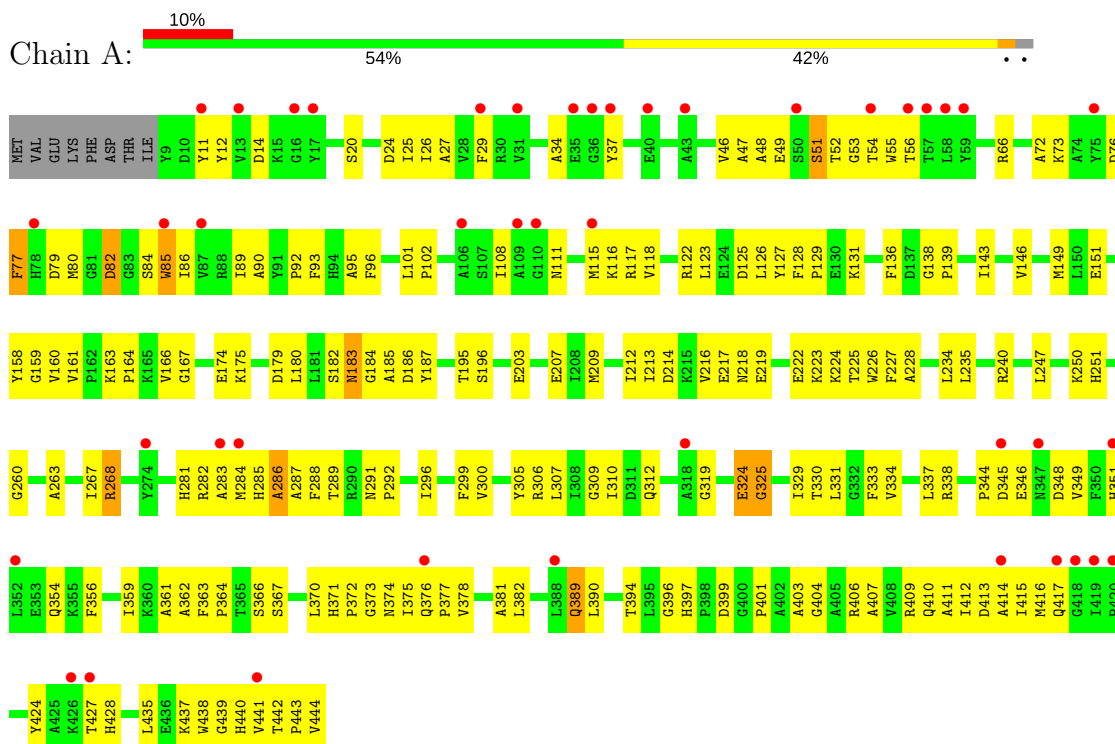
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total 97	O 97	0	0
4	B	175	Total 175	O 175	0	0
4	C	226	Total 226	O 226	0	0
4	D	239	Total 239	O 239	0	0
4	E	197	Total 197	O 197	0	0
4	F	179	Total 179	O 179	0	0
4	G	174	Total 174	O 174	0	0
4	H	123	Total 123	O 123	0	0
4	I	192	Total 192	O 192	0	0
4	J	209	Total 209	O 209	0	0

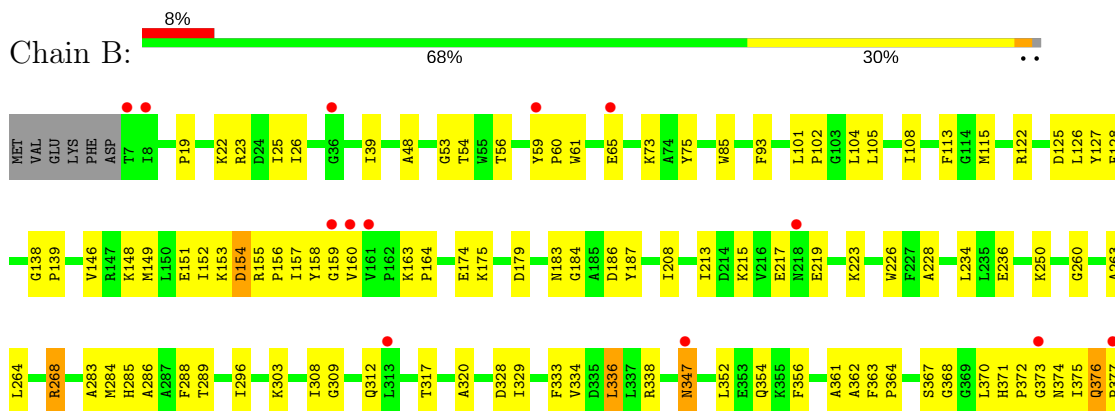
3 Residue-property plots

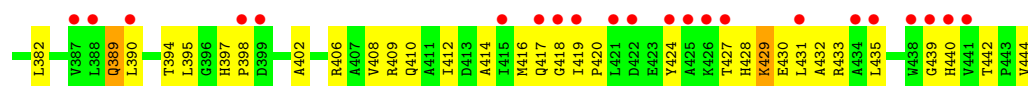
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Ribulose biphosphate carboxylase

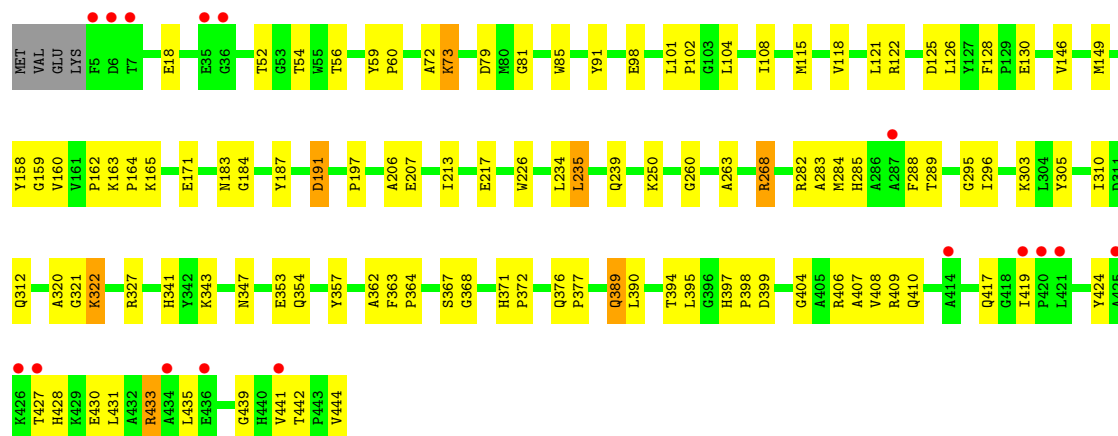
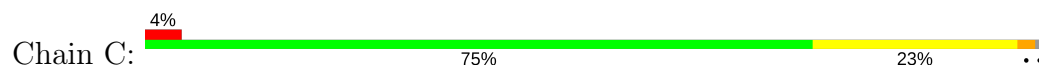


• Molecule 1: Ribulose biphosphate carboxylase

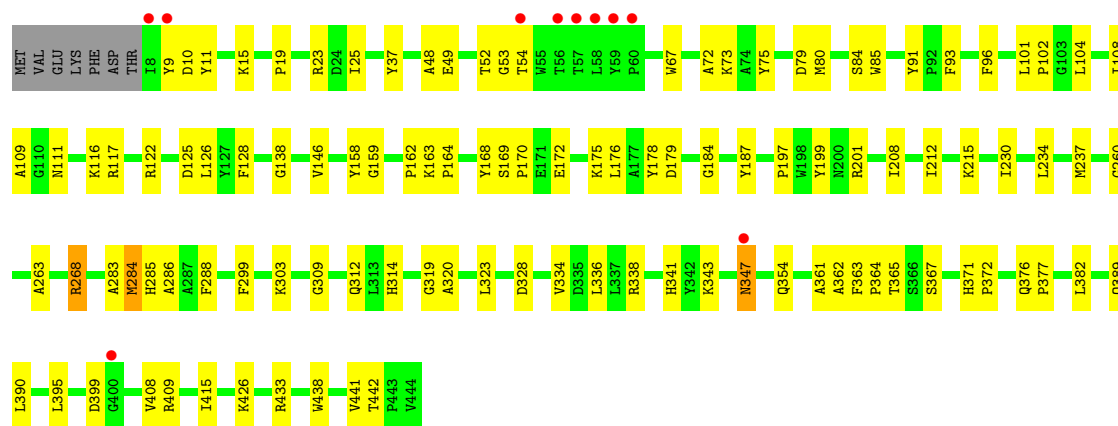
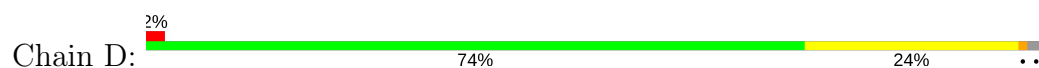




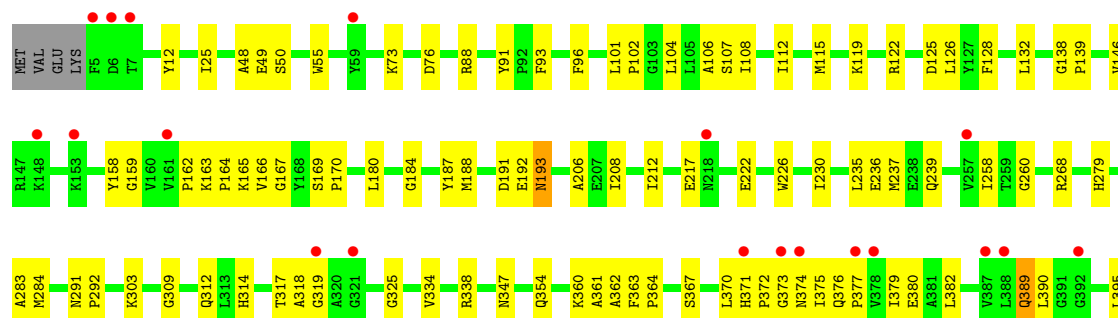
• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase

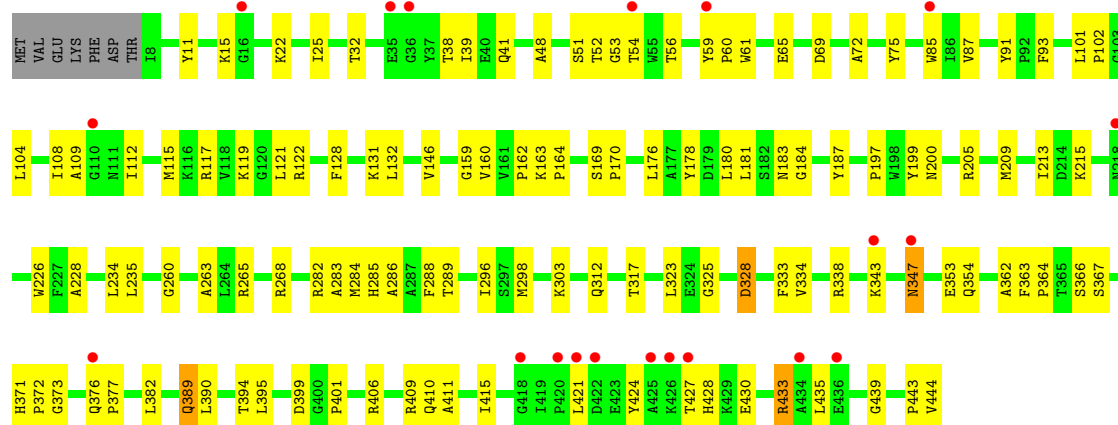


• Molecule 1: Ribulose biphosphate carboxylase

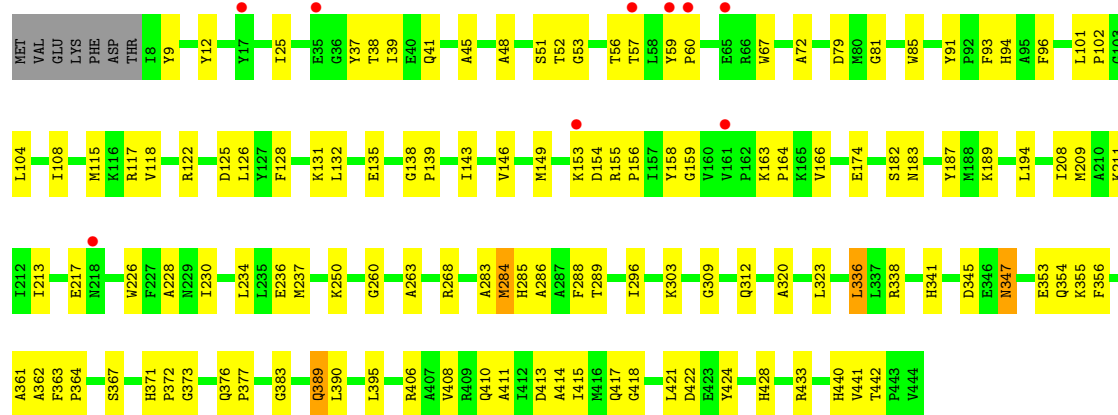




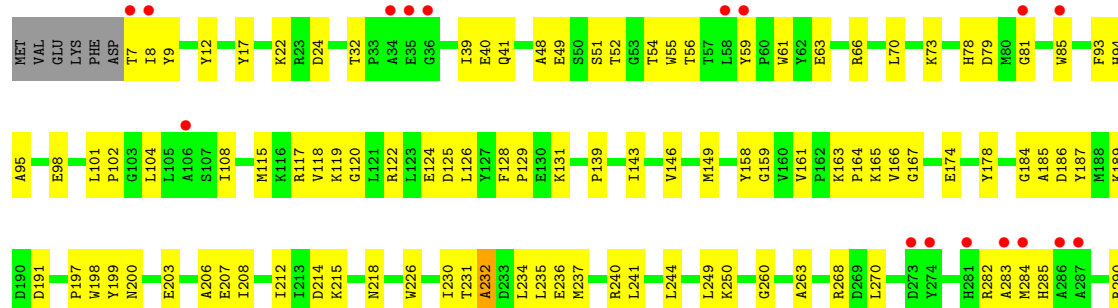
• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.48Å 246.57Å 134.83Å 90.00° 104.73° 90.00°	Depositor
Resolution (Å)	38.46 – 2.36 38.46 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (38.46-2.36) 99.4 (38.46-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.219 , 0.264 0.213 , 0.252	Depositor DCC
R_{free} test set	12530 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	36065	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CAP, KCX

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	0.21	0/3415	0.36	0/4642
1	B	0.22	0/3467	0.37	0/4712
1	C	0.22	0/3496	0.38	0/4750
1	D	0.22	0/3494	0.39	0/4739
1	E	0.22	0/3494	0.38	0/4744
1	F	0.22	0/3491	0.38	0/4738
1	G	0.21	0/3499	0.38	0/4747
1	H	0.21	0/3458	0.37	0/4700
1	I	0.22	0/3485	0.38	0/4730
1	J	0.22	0/3491	0.39	0/4738
All	All	0.22	0/34790	0.38	0/47240

There are no bond length outliers.

There are no bond angle outliers.

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	3341	0	3185	218	0
1	B	3391	0	3252	153	0
1	C	3420	0	3289	121	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3419	0	3317	102	0
1	E	3418	0	3303	121	0
1	F	3415	0	3313	126	0
1	G	3423	0	3328	129	0
1	H	3382	0	3257	207	0
1	I	3410	0	3301	112	0
1	J	3415	0	3310	143	0
2	A	21	0	8	0	0
2	B	21	0	7	1	0
2	C	21	0	9	1	0
2	D	21	0	8	0	0
2	E	21	0	8	2	0
2	F	21	0	8	0	0
2	G	21	0	8	1	0
2	H	21	0	8	0	0
2	I	21	0	8	0	0
2	J	21	0	7	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	97	0	0	12	0
4	B	175	0	0	10	0
4	C	226	0	0	7	0
4	D	239	0	0	4	0
4	E	197	0	0	9	0
4	F	179	0	0	9	0
4	G	174	0	0	8	0
4	H	123	0	0	6	0
4	I	192	0	0	7	0
4	J	209	0	0	15	0
All	All	36065	0	32934	1362	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 20.

All (1362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:397:HIS:ND1	1:H:398:PRO:HD2	1.29	1.44
1:H:397:HIS:CG	1:H:398:PRO:HD2	1.61	1.32
1:A:149:MET:HE3	1:A:250:LYS:CB	1.65	1.26
1:H:397:HIS:ND1	1:H:398:PRO:CD	2.06	1.18
1:I:72:ALA:O	1:I:73:LYS:HD2	1.43	1.17
1:H:282:ARG:HD2	1:H:285:HIS:CD2	1.81	1.15
1:H:397:HIS:CE1	1:H:398:PRO:HD2	1.81	1.15
1:A:108:ILE:CD1	1:A:126:LEU:HD11	1.80	1.11
1:F:433:ARG:HH11	1:F:433:ARG:HG2	1.01	1.10
1:E:91:TYR:CZ	1:E:108:ILE:HD11	1.88	1.08
1:B:317:THR:HG21	1:B:370:LEU:HD11	1.35	1.08
1:B:149:MET:HE3	1:B:250:LYS:HB2	1.36	1.07
1:A:108:ILE:HD11	1:A:126:LEU:HD11	1.36	1.07
1:A:149:MET:HE2	1:A:250:LYS:HD2	1.36	1.07
1:C:433:ARG:HH11	1:C:433:ARG:HG2	0.98	1.06
1:A:149:MET:HE3	1:A:250:LYS:HB3	1.04	1.04
1:J:343:LYS:HE2	1:J:353:GLU:OE2	1.57	1.03
1:E:91:TYR:CE2	1:E:108:ILE:HD11	1.94	1.03
1:C:433:ARG:CG	1:C:433:ARG:HH11	1.72	1.03
1:A:108:ILE:HD12	1:A:126:LEU:HD21	1.40	1.03
1:F:433:ARG:HH11	1:F:433:ARG:CG	1.72	1.03
1:A:444:VAL:O	1:H:117:ARG:HD2	1.60	1.02
1:A:282:ARG:HD2	1:A:285:HIS:CD2	1.96	1.01
1:I:159:GLY:HA3	1:I:187:TYR:CZ	1.96	1.00
1:H:149:MET:HE1	1:H:250:LYS:HB2	1.41	1.00
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.44	0.99
1:C:397:HIS:CG	1:C:398:PRO:HD2	1.99	0.98
1:E:319:GLY:HA2	4:E:496:HOH:O	1.61	0.97
1:A:86:ILE:CD1	1:A:349:VAL:HG23	1.95	0.97
1:F:131:LYS:HE2	4:F:1817:HOH:O	1.65	0.95
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.00	0.95
1:H:302:ALA:HB1	1:H:337:LEU:HD11	1.48	0.95
1:C:163:LYS:H	1:C:395:LEU:CD2	1.78	0.95
1:A:149:MET:CE	1:A:250:LYS:HB3	1.96	0.95
1:H:397:HIS:CG	1:H:398:PRO:CD	2.47	0.95
1:E:193:ASN:HD22	1:E:193:ASN:H	1.13	0.93
1:A:366:SER:HA	4:A:1262:HOH:O	1.68	0.92
1:C:433:ARG:NH1	1:C:433:ARG:HG2	1.79	0.91
1:I:209:MET:O	1:I:213:ILE:HG13	1.69	0.91
1:H:159:GLY:HA3	1:H:187:TYR:CZ	2.06	0.91
1:H:424:TYR:O	1:H:427:THR:HG22	1.71	0.91
1:E:91:TYR:CZ	1:E:108:ILE:CD1	2.53	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:ARG:NH1	1:F:433:ARG:HG2	1.82	0.91
1:H:334:VAL:CG1	1:H:338:ARG:NH2	2.33	0.90
1:G:347:ASN:ND2	1:G:347:ASN:H	1.70	0.90
1:G:38:THR:HG23	1:G:41:GLN:OE1	1.72	0.90
1:D:116:LYS:HE2	4:J:1843:HOH:O	1.69	0.90
1:B:371:HIS:O	1:B:375:ILE:HG23	1.72	0.89
1:H:334:VAL:HG11	1:H:338:ARG:NH2	1.87	0.89
1:A:86:ILE:CD1	1:A:349:VAL:CG2	2.50	0.89
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.08	0.89
1:A:86:ILE:HD13	1:A:349:VAL:HG23	1.53	0.88
1:B:183:ASN:ND2	1:B:402:ALA:HB1	1.89	0.88
1:C:149:MET:HE1	1:C:250:LYS:HB2	1.53	0.88
1:B:317:THR:CG2	1:B:370:LEU:HD11	2.04	0.87
1:G:347:ASN:HD22	1:G:347:ASN:H	0.88	0.87
1:B:303:LYS:HZ3	1:B:354:GLN:HE21	1.23	0.87
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.10	0.86
1:H:397:HIS:CE1	1:H:398:PRO:CD	2.56	0.86
1:A:149:MET:CE	1:A:250:LYS:CB	2.52	0.86
1:E:180:LEU:HD12	1:E:188:MET:CE	2.04	0.86
1:C:399:ASP:OD2	1:C:433:ARG:HD3	1.75	0.86
1:B:149:MET:HE2	1:B:250:LYS:HD2	1.56	0.85
1:A:108:ILE:CD1	1:A:126:LEU:CD1	2.55	0.85
1:A:108:ILE:CD1	1:A:126:LEU:HD21	2.06	0.85
1:F:32:THR:HG21	1:F:119:LYS:HE2	1.58	0.85
1:A:14:ASP:CB	4:A:2019:HOH:O	2.25	0.85
1:H:149:MET:HE1	1:H:250:LYS:CB	2.06	0.85
1:J:443:PRO:O	1:J:444:VAL:HG23	1.76	0.85
1:B:149:MET:HE3	1:B:250:LYS:CB	2.07	0.85
1:A:381:ALA:O	1:A:382:LEU:HD12	1.76	0.85
1:J:353:GLU:HB3	4:J:1285:HOH:O	1.76	0.85
1:F:347:ASN:HD22	1:F:347:ASN:H	1.25	0.85
1:J:413:ASP:HA	4:J:1924:HOH:O	1.77	0.84
1:A:438:TRP:O	1:A:441:VAL:HG12	1.76	0.84
1:A:76:ASP:OD1	1:A:77:PHE:N	2.10	0.84
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.12	0.84
1:F:159:GLY:HA3	1:F:187:TYR:CZ	2.13	0.84
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.13	0.84
1:B:373:GLY:O	1:B:440:HIS:HA	1.77	0.84
1:J:397:HIS:CG	1:J:398:PRO:HD2	2.13	0.84
1:H:32:THR:HG22	1:H:119:LYS:HB3	1.59	0.83
1:G:411:ALA:O	1:G:415:ILE:HG13	1.79	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:PHE:O	1:H:337:LEU:HD13	1.79	0.83
1:B:371:HIS:CE1	1:B:373:GLY:C	2.52	0.83
1:C:389:GLN:C	1:C:390:LEU:HD12	1.98	0.83
1:A:444:VAL:O	1:H:117:ARG:CD	2.27	0.83
1:F:32:THR:CG2	1:F:119:LYS:HE2	2.08	0.82
1:I:15:LYS:HG3	4:I:468:HOH:O	1.79	0.82
1:A:108:ILE:HD12	1:A:126:LEU:HD11	1.60	0.82
1:A:14:ASP:HB2	4:A:2019:HOH:O	1.78	0.82
1:C:347:ASN:HB3	4:C:1690:HOH:O	1.80	0.82
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.14	0.82
1:J:303:LYS:NZ	1:J:354:GLN:HE21	1.78	0.81
1:G:153:LYS:HG2	1:G:154:ASP:OD1	1.80	0.81
1:H:419:ILE:N	1:H:419:ILE:HD12	1.94	0.81
1:I:376:GLN:HB3	1:I:377:PRO:HD3	1.61	0.81
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.16	0.81
1:G:347:ASN:HD22	1:G:347:ASN:N	1.68	0.81
1:F:376:GLN:HB3	1:F:377:PRO:HD3	1.62	0.80
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.16	0.80
1:C:397:HIS:CD2	1:C:398:PRO:HD2	2.16	0.80
1:H:163:LYS:HA	1:H:164:PRO:O	1.82	0.80
1:J:153:LYS:CE	1:J:154:ASP:OD1	2.29	0.80
1:J:427:THR:HB	4:J:2029:HOH:O	1.81	0.80
1:A:149:MET:HE3	1:A:250:LYS:HB2	1.64	0.79
1:H:417:GLN:CB	1:H:419:ILE:HD13	2.13	0.79
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.18	0.79
1:C:149:MET:HE1	1:C:250:LYS:CB	2.13	0.79
1:G:128:PHE:H	1:G:354:GLN:HE22	1.27	0.79
1:H:149:MET:HE3	1:H:250:LYS:CD	2.11	0.79
1:H:406:ARG:O	1:H:410:GLN:HG3	1.83	0.79
1:J:165:LYS:HB3	1:J:191:ASP:OD1	1.82	0.79
1:F:427:THR:HG22	4:F:494:HOH:O	1.82	0.79
1:A:149:MET:HE2	1:A:250:LYS:CD	2.11	0.79
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.18	0.79
1:F:163:LYS:H	1:F:395:LEU:HD13	1.48	0.78
1:B:317:THR:HG21	1:B:370:LEU:CD1	2.13	0.78
1:H:397:HIS:CE1	1:H:398:PRO:HG2	2.19	0.78
1:D:37:TYR:OH	1:J:444:VAL:HG12	1.84	0.77
1:A:76:ASP:C	1:A:77:PHE:CD2	2.58	0.77
1:I:128:PHE:H	1:I:354:GLN:HE22	1.31	0.77
1:B:371:HIS:ND1	1:B:373:GLY:N	2.33	0.77
1:H:397:HIS:CD2	1:H:398:PRO:HD2	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ASP:HB2	1:G:85:TRP:CZ3	2.20	0.77
1:A:149:MET:CE	1:A:250:LYS:HD2	2.14	0.77
1:A:376:GLN:HA	1:A:415:ILE:HD13	1.65	0.77
1:C:419:ILE:HD12	1:C:419:ILE:H	1.50	0.77
1:J:331:LEU:HD13	1:J:381:ALA:O	1.85	0.77
1:C:149:MET:HE3	1:C:250:LYS:HD2	1.65	0.76
1:B:60:PRO:HA	4:B:2001:HOH:O	1.84	0.76
1:E:180:LEU:HD12	1:E:188:MET:HE2	1.65	0.76
1:A:108:ILE:HD12	1:A:126:LEU:CD2	2.14	0.76
1:E:159:GLY:HA3	1:E:187:TYR:CZ	2.21	0.76
1:A:334:VAL:CG1	1:A:338:ARG:NH2	2.48	0.76
1:C:419:ILE:N	1:C:419:ILE:HD12	2.01	0.76
1:A:424:TYR:CZ	1:A:428:HIS:CE1	2.74	0.75
1:J:443:PRO:O	1:J:444:VAL:CG2	2.34	0.75
1:D:176:LEU:HD11	1:D:395:LEU:HD21	1.67	0.75
1:H:371:HIS:HB2	1:H:372:PRO:CD	2.16	0.75
1:J:303:LYS:HZ3	1:J:354:GLN:HE21	1.34	0.75
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.21	0.75
1:B:149:MET:HE2	1:B:250:LYS:CD	2.16	0.75
1:A:334:VAL:HG21	1:A:382:LEU:HG	1.67	0.75
1:A:14:ASP:CG	4:A:2019:HOH:O	2.24	0.75
1:B:371:HIS:HE1	1:B:373:GLY:C	1.90	0.75
1:C:149:MET:HE3	1:C:250:LYS:CD	2.17	0.75
1:H:334:VAL:HG12	1:H:338:ARG:HH21	1.52	0.75
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.35	0.74
1:B:371:HIS:CE1	1:B:373:GLY:CA	2.70	0.74
1:J:397:HIS:ND1	1:J:398:PRO:HD2	2.03	0.74
1:A:406:ARG:O	1:A:410:GLN:HG3	1.87	0.74
1:G:163:LYS:H	1:G:395:LEU:HD22	1.52	0.74
1:A:108:ILE:HD11	1:A:126:LEU:CD1	2.14	0.74
1:H:125:ASP:OD1	1:H:126:LEU:N	2.21	0.74
1:H:334:VAL:CG1	1:H:338:ARG:HH21	1.98	0.74
1:A:268:ARG:HD3	1:A:268:ARG:C	2.08	0.74
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.23	0.73
1:H:410:GLN:HE21	1:H:431:LEU:HB2	1.52	0.73
1:F:376:GLN:CB	1:F:377:PRO:HD3	2.18	0.73
1:A:159:GLY:HA3	1:A:187:TYR:CE2	2.23	0.73
1:E:163:LYS:H	1:E:395:LEU:CD1	2.02	0.73
1:C:163:LYS:H	1:C:395:LEU:HD22	1.51	0.73
1:B:149:MET:CE	1:B:250:LYS:HD2	2.17	0.73
1:H:163:LYS:HA	1:H:164:PRO:C	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:H	1:D:395:LEU:HD13	1.54	0.73
1:C:263:ALA:HB2	1:F:263:ALA:HB2	1.71	0.73
1:F:25:ILE:HD11	1:F:132:LEU:HD21	1.69	0.73
1:H:282:ARG:NH1	1:H:285:HIS:CE1	2.56	0.73
1:H:410:GLN:HE22	1:H:431:LEU:H	1.35	0.73
1:B:429:LYS:O	1:B:432:ALA:N	2.22	0.72
1:G:104:LEU:O	1:G:104:LEU:HD23	1.89	0.72
1:A:424:TYR:CE2	1:A:428:HIS:CE1	2.77	0.72
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.17	0.72
1:D:117:ARG:NH2	1:J:444:VAL:O	2.22	0.72
1:D:108:ILE:HD12	1:D:108:ILE:C	2.10	0.72
1:F:347:ASN:N	1:F:347:ASN:HD22	1.87	0.72
1:H:208:ILE:O	1:H:212:ILE:HG13	1.90	0.72
1:F:399:ASP:OD2	1:F:433:ARG:HD3	1.89	0.72
1:A:125:ASP:OD1	1:A:126:LEU:N	2.23	0.72
1:A:334:VAL:HG11	1:A:338:ARG:NH2	2.03	0.72
1:B:373:GLY:HA3	1:B:439:GLY:O	1.89	0.72
1:G:389:GLN:C	1:G:390:LEU:HD12	2.09	0.72
1:H:128:PHE:H	1:H:354:GLN:HE22	1.37	0.72
1:H:400:GLY:O	1:H:403:ALA:HB3	1.90	0.71
1:J:153:LYS:HE2	1:J:154:ASP:OD1	1.89	0.71
1:H:425:ALA:C	1:H:427:THR:H	1.92	0.71
1:D:268:ARG:HD3	1:D:268:ARG:C	2.11	0.71
1:G:376:GLN:HB3	1:G:377:PRO:HD3	1.71	0.71
1:G:104:LEU:C	1:G:104:LEU:HD23	2.11	0.71
1:B:419:ILE:HD12	1:B:419:ILE:N	2.06	0.71
1:H:349:VAL:HG12	1:H:349:VAL:O	1.90	0.70
1:H:397:HIS:CE1	1:H:398:PRO:CG	2.73	0.70
1:H:318:ALA:HA	1:H:325:GLY:O	1.91	0.70
1:H:371:HIS:HB2	1:H:372:PRO:HD2	1.73	0.70
1:B:397:HIS:ND1	1:B:398:PRO:HD2	2.06	0.70
1:C:128:PHE:H	1:C:354:GLN:HE22	1.40	0.70
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.25	0.70
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.25	0.70
1:I:319:GLY:HA2	4:I:459:HOH:O	1.90	0.70
1:J:268:ARG:C	1:J:268:ARG:HD3	2.10	0.70
1:J:362:ALA:O	1:J:364:PRO:HD3	1.91	0.70
1:C:79:ASP:HB2	1:C:85:TRP:CZ3	2.26	0.70
1:H:318:ALA:HB1	1:H:327:ARG:HA	1.73	0.70
1:B:236:GLU:N	1:B:236:GLU:OE1	2.24	0.70
1:J:370:LEU:HA	1:J:374:ASN:HD21	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.26	0.70
1:I:285:HIS:HD2	1:I:289:THR:OG1	1.75	0.70
1:G:79:ASP:HB2	1:G:85:TRP:CH2	2.27	0.69
1:A:367:SER:N	4:A:1262:HOH:O	2.23	0.69
1:H:419:ILE:H	1:H:419:ILE:HD12	1.55	0.69
1:I:406:ARG:O	1:I:410:GLN:HG3	1.92	0.69
1:J:153:LYS:HE3	1:J:154:ASP:OD1	1.91	0.69
1:I:72:ALA:C	1:I:73:LYS:HD2	2.11	0.69
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.28	0.69
1:C:417:GLN:CB	1:C:419:ILE:HD13	2.21	0.69
1:B:303:LYS:NZ	1:B:354:GLN:HE21	1.90	0.69
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.28	0.69
1:B:389:GLN:C	1:B:390:LEU:HD12	2.13	0.69
1:J:411:ALA:O	1:J:415:ILE:HG13	1.93	0.68
1:A:376:GLN:HB3	1:A:377:PRO:HD3	1.75	0.68
1:J:98:GLU:HG3	1:J:135:GLU:OE2	1.93	0.68
1:C:162:PRO:HA	1:C:395:LEU:HD21	1.74	0.68
1:F:54:THR:HG23	1:F:56:THR:O	1.94	0.68
1:A:260:GLY:HA3	1:H:260:GLY:HA3	1.75	0.68
1:I:376:GLN:HA	1:I:415:ILE:HD13	1.74	0.68
1:I:268:ARG:C	1:I:268:ARG:HD3	2.13	0.68
1:F:362:ALA:O	1:F:364:PRO:HD3	1.93	0.68
1:H:178:TYR:CE1	1:H:215:LYS:HE3	2.29	0.68
1:F:38:THR:OG1	1:F:41:GLN:HG3	1.92	0.68
1:I:163:LYS:H	1:I:395:LEU:HD12	1.58	0.68
1:J:104:LEU:HD23	1:J:104:LEU:C	2.13	0.68
1:B:268:ARG:C	1:B:268:ARG:HD3	2.15	0.68
1:B:183:ASN:HD21	1:B:402:ALA:HB1	1.56	0.68
1:B:54:THR:HG23	1:B:56:THR:O	1.93	0.68
1:A:444:VAL:O	1:H:117:ARG:HB2	1.93	0.68
1:A:139:PRO:HD3	1:A:306:ARG:O	1.94	0.68
1:B:125:ASP:OD1	1:B:126:LEU:N	2.27	0.68
1:H:391:GLY:O	1:H:395:LEU:HD23	1.94	0.68
1:H:397:HIS:CD2	1:H:404:GLY:HA2	2.29	0.68
1:E:435:LEU:O	1:E:439:GLY:N	2.25	0.67
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.29	0.67
1:H:427:THR:HG23	1:H:428:HIS:ND1	2.09	0.67
1:A:128:PHE:H	1:A:354:GLN:HE22	1.41	0.67
1:A:175:LYS:CG	4:A:1729:HOH:O	2.43	0.67
1:C:376:GLN:HB3	1:C:377:PRO:HD3	1.75	0.67
1:E:279:HIS:NE2	1:E:314:HIS:HE1	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:407:ALA:O	1:J:410:GLN:HB2	1.94	0.67
1:H:425:ALA:O	1:H:427:THR:N	2.28	0.67
1:B:424:TYR:HE1	4:B:963:HOH:O	1.77	0.67
1:E:371:HIS:ND1	1:E:373:GLY:N	2.42	0.67
1:F:159:GLY:HA3	1:F:187:TYR:CE1	2.29	0.67
1:G:376:GLN:CB	1:G:377:PRO:HD3	2.25	0.67
1:B:328:ASP:CB	4:B:1794:HOH:O	2.43	0.67
1:E:389:GLN:C	1:E:390:LEU:HD12	2.15	0.67
1:H:282:ARG:HD2	1:H:285:HIS:NE2	2.10	0.67
1:I:25:ILE:HD11	1:I:132:LEU:HD21	1.75	0.67
1:A:413:ASP:O	1:A:417:GLN:HG3	1.95	0.66
1:B:60:PRO:CA	4:B:2001:HOH:O	2.42	0.66
1:A:334:VAL:CG1	1:A:338:ARG:CZ	2.74	0.66
1:H:376:GLN:HA	1:H:415:ILE:HD13	1.76	0.66
1:B:334:VAL:HG21	1:B:382:LEU:HD22	1.78	0.66
1:C:283:ALA:O	1:C:284:MET:HB3	1.95	0.66
1:J:334:VAL:HG21	1:J:382:LEU:HD22	1.78	0.66
1:B:424:TYR:CE1	4:B:963:HOH:O	2.49	0.66
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.30	0.66
1:A:66:ARG:HD2	1:H:167:GLY:O	1.96	0.65
1:B:444:VAL:O	1:G:117:ARG:NH2	2.22	0.65
1:I:162:PRO:HA	1:I:395:LEU:HD11	1.78	0.65
1:I:72:ALA:O	1:I:73:LYS:CD	2.32	0.65
1:I:319:GLY:CA	4:I:459:HOH:O	2.43	0.65
1:I:163:LYS:H	1:I:395:LEU:CD1	2.09	0.65
1:A:175:LYS:HE3	1:A:179:ASP:OD2	1.96	0.65
1:H:104:LEU:C	1:H:104:LEU:HD23	2.16	0.65
1:I:215:LYS:HE2	1:I:219:GLU:OE2	1.97	0.65
1:E:371:HIS:CE1	1:E:373:GLY:CA	2.79	0.65
1:F:54:THR:HA	4:F:492:HOH:O	1.96	0.65
1:A:122:ARG:HD3	1:A:292:PRO:O	1.95	0.65
1:H:283:ALA:O	1:H:284:MET:HB3	1.96	0.65
1:I:371:HIS:HB2	1:I:372:PRO:HD2	1.79	0.65
1:A:283:ALA:O	1:A:284:MET:HB3	1.96	0.65
1:C:59:TYR:CD1	1:C:60:PRO:HD2	2.32	0.65
1:J:343:LYS:HG2	1:J:353:GLU:HG3	1.78	0.65
1:C:320:ALA:O	1:C:442:THR:HG23	1.97	0.65
1:F:430:GLU:OE1	1:F:430:GLU:N	2.25	0.65
1:I:389:GLN:C	1:I:390:LEU:HD12	2.15	0.65
1:E:128:PHE:H	1:E:354:GLN:HE22	1.45	0.64
1:H:334:VAL:HG12	1:H:338:ARG:NH2	2.10	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396:GLY:O	1:I:437:LYS:NZ	2.24	0.64
1:H:418:GLY:O	1:H:420:PRO:HD3	1.97	0.64
1:H:54:THR:HG23	1:H:56:THR:H	1.61	0.64
1:B:215:LYS:HE2	1:B:219:GLU:OE2	1.97	0.64
1:H:108:ILE:HG22	1:H:108:ILE:O	1.96	0.64
1:J:317:THR:HG21	1:J:370:LEU:HD11	1.78	0.64
1:A:376:GLN:HA	1:A:415:ILE:CD1	2.27	0.64
1:B:158:TYR:O	1:B:186:ASP:HB2	1.97	0.64
1:G:338:ARG:HA	1:G:361:ALA:HB1	1.78	0.64
1:H:334:VAL:CG1	1:H:338:ARG:CZ	2.76	0.64
1:E:260:GLY:HA3	1:I:260:GLY:HA3	1.79	0.64
1:I:410:GLN:NE2	1:I:428:HIS:HB3	2.13	0.64
1:B:371:HIS:HE1	1:B:373:GLY:CA	2.10	0.64
1:F:343:LYS:HE2	1:F:353:GLU:OE2	1.97	0.64
1:A:108:ILE:CD1	1:A:126:LEU:CD2	2.74	0.64
1:B:163:LYS:HA	1:B:164:PRO:C	2.18	0.64
1:C:160:VAL:HG11	1:C:395:LEU:HD11	1.78	0.64
1:D:376:GLN:HB3	1:D:377:PRO:HD3	1.80	0.64
1:H:419:ILE:H	1:H:419:ILE:CD1	2.09	0.64
1:D:117:ARG:HH21	1:J:444:VAL:C	2.01	0.64
1:F:159:GLY:HA3	1:F:187:TYR:CE2	2.33	0.64
1:B:234:LEU:HD21	1:G:234:LEU:HD21	1.80	0.64
1:D:168:TYR:HA	1:J:66:ARG:HH21	1.63	0.64
1:E:125:ASP:OD1	1:E:126:LEU:N	2.31	0.63
1:B:283:ALA:O	1:B:284:MET:HB3	1.99	0.63
1:C:410:GLN:HE22	1:C:431:LEU:H	1.45	0.63
1:F:433:ARG:CG	1:F:433:ARG:NH1	2.43	0.63
1:B:376:GLN:HB3	1:B:377:PRO:HD3	1.80	0.63
1:D:263:ALA:HB2	1:J:263:ALA:HB2	1.78	0.63
1:H:149:MET:CE	1:H:250:LYS:HB2	2.24	0.63
1:H:419:ILE:N	1:H:419:ILE:CD1	2.61	0.63
1:E:371:HIS:CE1	1:E:373:GLY:C	2.72	0.63
1:E:429:LYS:CB	4:E:2023:HOH:O	2.46	0.63
1:H:149:MET:CE	1:H:250:LYS:CB	2.77	0.63
1:C:260:GLY:HA3	1:F:260:GLY:HA3	1.80	0.63
1:H:417:GLN:CB	1:H:419:ILE:CD1	2.77	0.63
1:C:419:ILE:CD1	1:C:419:ILE:H	2.11	0.63
1:J:128:PHE:H	1:J:354:GLN:HE22	1.45	0.63
1:A:362:ALA:O	1:A:364:PRO:HD3	1.99	0.63
1:H:303:LYS:HZ1	1:H:354:GLN:HE21	1.47	0.63
1:H:441:VAL:HG12	1:H:442:THR:N	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ALA:HB1	1:G:115:MET:CE	2.28	0.63
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.28	0.63
1:G:48:ALA:HB1	1:G:53:GLY:HA3	1.80	0.63
1:H:101:LEU:HB3	1:H:102:PRO:HD3	1.81	0.63
1:D:128:PHE:H	1:D:354:GLN:HE22	1.47	0.63
1:H:341:HIS:NE2	1:H:353:GLU:OE2	2.28	0.62
1:J:406:ARG:O	1:J:410:GLN:HG3	1.99	0.62
1:B:149:MET:CE	1:B:250:LYS:CD	2.77	0.62
1:H:282:ARG:HH11	1:H:285:HIS:CE1	2.15	0.62
1:B:128:PHE:H	1:B:354:GLN:HE22	1.48	0.62
1:F:25:ILE:HD11	1:F:132:LEU:CD2	2.29	0.62
1:H:41:GLN:HB3	1:H:117:ARG:HH11	1.61	0.62
1:A:381:ALA:C	1:A:382:LEU:HD12	2.20	0.62
1:B:184:GLY:HA3	1:B:409:ARG:HG3	1.82	0.62
1:D:389:GLN:C	1:D:390:LEU:HD12	2.20	0.62
1:H:399:ASP:HB2	1:H:403:ALA:CB	2.30	0.62
1:A:46:VAL:HG22	1:A:115:MET:CE	2.29	0.62
1:B:419:ILE:H	1:B:419:ILE:HD12	1.64	0.62
1:I:213:ILE:O	1:I:217:GLU:HG3	1.99	0.62
1:I:283:ALA:O	1:I:284:MET:HB3	2.00	0.62
1:F:389:GLN:C	1:F:390:LEU:HD12	2.19	0.62
1:B:412:ILE:O	1:B:416:MET:HG2	1.99	0.62
1:E:444:VAL:O	1:I:117:ARG:NH2	2.25	0.62
1:F:289:THR:HG22	1:F:296:ILE:O	2.00	0.62
1:H:302:ALA:HB1	1:H:337:LEU:CD1	2.27	0.62
1:H:435:LEU:O	1:H:439:GLY:N	2.33	0.62
1:A:86:ILE:HG21	1:A:349:VAL:O	2.00	0.61
1:C:371:HIS:HB2	1:C:372:PRO:HD2	1.81	0.61
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.81	0.61
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.82	0.61
1:A:376:GLN:CB	1:A:377:PRO:HD3	2.28	0.61
1:E:180:LEU:CD1	1:E:188:MET:HE1	2.28	0.61
1:F:268:ARG:HD3	1:F:268:ARG:C	2.20	0.61
1:F:347:ASN:H	1:F:347:ASN:ND2	1.97	0.61
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.35	0.61
1:E:303:LYS:NZ	1:E:354:GLN:HE21	1.97	0.61
1:G:371:HIS:HB2	1:G:372:PRO:HD2	1.83	0.61
1:F:32:THR:HG21	1:F:119:LYS:CE	2.29	0.61
1:H:319:GLY:N	1:H:325:GLY:O	2.33	0.61
1:A:214:ASP:O	1:A:218:ASN:HB2	2.00	0.61
1:H:268:ARG:C	1:H:268:ARG:HD3	2.21	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:376:GLN:N	1:H:377:PRO:CD	2.63	0.61
1:D:37:TYR:CZ	1:J:444:VAL:HG12	2.35	0.61
1:F:163:LYS:HA	1:F:164:PRO:C	2.21	0.61
1:A:143:ILE:HD11	1:A:338:ARG:HG2	1.83	0.60
1:B:159:GLY:HA3	1:B:187:TYR:CD1	2.35	0.60
1:E:163:LYS:HA	1:E:164:PRO:C	2.20	0.60
1:G:163:LYS:H	1:G:395:LEU:CD2	2.14	0.60
1:A:115:MET:O	1:A:118:VAL:HG22	2.00	0.60
1:E:268:ARG:HD3	1:E:268:ARG:C	2.21	0.60
1:H:174:GLU:HG3	1:H:212:ILE:HD11	1.82	0.60
1:B:430:GLU:OE1	1:B:430:GLU:N	2.34	0.60
1:B:260:GLY:HA3	1:G:260:GLY:HA3	1.83	0.60
1:E:180:LEU:CD1	1:E:188:MET:CE	2.79	0.60
1:E:370:LEU:HB2	4:E:1679:HOH:O	2.01	0.60
1:G:345:ASP:HB3	1:G:347:ASN:HD21	1.66	0.60
1:E:410:GLN:NE2	1:E:430:GLU:HB2	2.15	0.60
1:B:263:ALA:HB2	1:G:263:ALA:HB2	1.83	0.60
1:G:38:THR:H	1:G:41:GLN:CD	2.05	0.60
1:B:427:THR:HG23	1:B:428:HIS:ND1	2.17	0.60
1:H:410:GLN:NE2	1:H:431:LEU:H	1.99	0.60
1:B:427:THR:HG23	1:B:428:HIS:CE1	2.37	0.60
1:D:108:ILE:CD1	1:D:108:ILE:C	2.70	0.60
1:D:172:GLU:OE1	1:J:66:ARG:NH2	2.35	0.60
1:G:336:LEU:CD2	1:G:356:PHE:HZ	2.15	0.60
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.37	0.60
1:C:163:LYS:HA	1:C:164:PRO:C	2.22	0.60
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.36	0.60
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.31	0.60
1:E:396:GLY:O	1:E:437:LYS:NZ	2.35	0.60
1:F:163:LYS:H	1:F:395:LEU:CD1	2.13	0.60
1:A:203:GLU:O	1:A:207:GLU:HG2	2.01	0.59
1:A:345:ASP:O	1:A:348:ASP:N	2.32	0.59
1:A:80:MET:SD	1:A:86:ILE:CD1	2.90	0.59
1:J:317:THR:CG2	1:J:370:LEU:HD11	2.32	0.59
1:H:395:LEU:N	1:H:395:LEU:HD22	2.17	0.59
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.37	0.59
1:F:427:THR:HG23	1:F:428:HIS:ND1	2.16	0.59
1:A:86:ILE:HD11	1:A:349:VAL:HG23	1.81	0.59
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.38	0.59
1:B:183:ASN:ND2	1:B:402:ALA:CB	2.63	0.59
1:A:182:SER:C	1:A:183:ASN:HD22	2.06	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:GLY:O	1:A:437:LYS:NZ	2.27	0.59
1:B:158:TYR:CE1	1:B:408:VAL:HG11	2.37	0.59
1:C:424:TYR:CE2	1:C:428:HIS:CE1	2.90	0.59
1:F:104:LEU:C	1:F:104:LEU:HD23	2.23	0.59
1:J:162:PRO:HA	1:J:395:LEU:HD11	1.85	0.59
1:A:80:MET:SD	1:A:86:ILE:HD11	2.42	0.59
1:B:371:HIS:HB2	1:B:372:PRO:HD2	1.84	0.59
1:D:37:TYR:OH	1:J:444:VAL:CG1	2.51	0.59
1:C:108:ILE:CG2	1:C:108:ILE:O	2.51	0.59
1:D:320:ALA:O	1:D:442:THR:HG23	2.03	0.59
1:H:17:TYR:CE1	1:H:73:LYS:HE3	2.37	0.59
1:A:108:ILE:HD12	1:A:126:LEU:CD1	2.28	0.58
1:B:406:ARG:O	1:B:410:GLN:HG3	2.03	0.58
1:H:149:MET:CE	1:H:250:LYS:HD2	2.27	0.58
1:C:427:THR:HG23	1:C:428:HIS:CE1	2.39	0.58
1:I:285:HIS:CD2	1:I:289:THR:OG1	2.56	0.58
1:I:72:ALA:HB2	1:I:91:TYR:CD1	2.38	0.58
1:C:165:LYS:NZ	1:C:191:ASP:OD1	2.20	0.58
1:I:159:GLY:CA	1:I:187:TYR:CZ	2.80	0.58
1:A:375:ILE:O	1:A:378:VAL:N	2.32	0.58
1:H:231:THR:O	1:H:232:ALA:HB2	2.02	0.58
1:H:317:THR:O	1:H:318:ALA:HB3	2.02	0.58
1:I:371:HIS:HB2	1:I:372:PRO:CD	2.33	0.58
1:J:319:GLY:CA	4:J:1255:HOH:O	2.52	0.58
1:E:165:LYS:HG2	1:E:191:ASP:OD2	2.04	0.58
1:H:439:GLY:O	1:H:440:HIS:CD2	2.57	0.58
1:J:183:ASN:OD1	1:J:406:ARG:NH1	2.36	0.58
1:J:373:GLY:O	1:J:440:HIS:HA	2.04	0.58
1:B:410:GLN:OE1	1:B:431:LEU:HB2	2.04	0.58
1:D:283:ALA:O	1:D:284:MET:HB3	2.04	0.58
1:B:175:LYS:HE3	1:B:179:ASP:OD2	2.04	0.58
1:A:282:ARG:HD2	1:A:285:HIS:NE2	2.18	0.58
1:B:183:ASN:HD22	1:B:402:ALA:CA	2.17	0.58
2:E:600:CAP:O7	2:E:600:CAP:H4	2.04	0.58
1:H:191:ASP:HB2	4:H:470:HOH:O	2.04	0.57
1:I:362:ALA:O	1:I:364:PRO:HD3	2.04	0.57
1:G:149:MET:HE3	1:G:250:LYS:HD2	1.85	0.57
1:J:397:HIS:ND1	1:J:398:PRO:CD	2.67	0.57
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.86	0.57
1:B:213:ILE:O	1:B:217:GLU:HG3	2.05	0.57
1:I:163:LYS:HA	1:I:164:PRO:C	2.25	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ALA:HB1	1:B:53:GLY:HA3	1.85	0.57
1:B:59:TYR:O	1:B:61:TRP:HD1	1.87	0.57
1:F:104:LEU:O	1:F:104:LEU:HD23	2.04	0.57
1:G:289:THR:HG22	1:G:296:ILE:O	2.05	0.57
1:J:108:ILE:O	1:J:108:ILE:CG2	2.52	0.57
1:B:215:LYS:CE	1:B:219:GLU:OE2	2.52	0.57
1:B:347:ASN:C	1:B:347:ASN:HD22	2.08	0.57
1:G:149:MET:HE1	1:G:250:LYS:HB3	1.87	0.57
1:H:118:VAL:HG22	1:H:120:GLY:H	1.70	0.57
1:J:443:PRO:C	1:J:444:VAL:HG23	2.24	0.57
1:E:180:LEU:HD12	1:E:188:MET:HE1	1.85	0.57
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.86	0.57
1:G:414:ALA:HB2	1:G:424:TYR:CG	2.40	0.57
1:H:159:GLY:HA3	1:H:187:TYR:CD1	2.40	0.57
4:E:722:HOH:O	1:I:265:ARG:HB3	2.04	0.57
1:A:86:ILE:HD13	1:A:349:VAL:CG2	2.26	0.57
1:B:370:LEU:HB2	4:B:1246:HOH:O	2.05	0.57
1:C:389:GLN:O	1:C:390:LEU:HD12	2.04	0.57
1:G:373:GLY:O	1:G:440:HIS:CD2	2.58	0.57
1:F:128:PHE:H	1:F:354:GLN:HE22	1.52	0.56
1:H:178:TYR:CE1	1:H:215:LYS:CE	2.88	0.56
1:J:283:ALA:O	1:J:284:MET:HB3	2.05	0.56
1:A:282:ARG:NH1	1:A:285:HIS:CE1	2.74	0.56
1:A:283:ALA:O	1:A:284:MET:CB	2.53	0.56
1:B:362:ALA:O	1:B:364:PRO:HD3	2.04	0.56
1:H:425:ALA:C	1:H:427:THR:N	2.57	0.56
1:I:338:ARG:HA	1:I:361:ALA:HB1	1.87	0.56
1:J:108:ILE:O	1:J:108:ILE:HG22	2.03	0.56
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.87	0.56
1:B:226:TRP:CZ3	1:B:228:ALA:HB2	2.40	0.56
1:C:149:MET:CE	1:C:250:LYS:HD2	2.36	0.56
1:E:376:GLN:N	1:E:377:PRO:HD2	2.21	0.56
1:C:343:LYS:HG2	1:C:353:GLU:HG3	1.86	0.56
1:H:184:GLY:CA	1:H:409:ARG:HG3	2.36	0.56
1:C:433:ARG:CG	1:C:433:ARG:NH1	2.43	0.56
1:D:260:GLY:HA3	1:J:260:GLY:HA3	1.86	0.56
1:A:330:THR:CG2	1:A:382:LEU:HD21	2.35	0.56
1:B:419:ILE:CG2	1:B:424:TYR:HB2	2.36	0.56
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.36	0.56
1:E:283:ALA:O	1:E:284:MET:HB3	2.06	0.56
1:A:442:THR:O	1:A:444:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.88	0.56
1:D:67:TRP:CD1	1:J:164:PRO:HG3	2.41	0.56
1:J:158:TYR:CE1	1:J:408:VAL:HG11	2.41	0.56
1:J:163:LYS:H	1:J:395:LEU:CD1	2.19	0.56
1:B:431:LEU:O	1:B:435:LEU:HG	2.06	0.56
1:C:79:ASP:HB2	1:C:85:TRP:CH2	2.41	0.56
1:D:376:GLN:HA	1:D:415:ILE:HD13	1.87	0.56
1:G:38:THR:N	1:G:41:GLN:OE1	2.33	0.56
1:H:184:GLY:HA3	1:H:409:ARG:HG3	1.88	0.56
1:B:288:PHE:HB3	1:G:288:PHE:HB3	1.87	0.56
1:H:290:ARG:N	4:H:461:HOH:O	2.27	0.56
1:J:163:LYS:HA	1:J:164:PRO:C	2.26	0.56
1:J:201:ARG:HB2	1:J:204:GLU:HG3	1.88	0.56
1:A:163:LYS:HA	1:A:164:PRO:C	2.27	0.56
1:F:395:LEU:HD23	1:F:401:PRO:HG3	1.88	0.56
1:I:203:GLU:HG3	4:I:448:HOH:O	2.05	0.55
1:J:442:THR:HG23	1:J:442:THR:O	2.07	0.55
1:B:347:ASN:ND2	1:B:347:ASN:C	2.59	0.55
1:E:319:GLY:CA	4:E:496:HOH:O	2.32	0.55
1:F:334:VAL:CG1	1:F:338:ARG:CZ	2.84	0.55
1:A:305:TYR:O	1:A:310:ILE:HG12	2.06	0.55
1:G:341:HIS:ND1	1:G:355:LYS:HG2	2.21	0.55
1:H:236:GLU:OE1	1:H:236:GLU:N	2.38	0.55
1:B:22:LYS:HD3	1:F:65:GLU:HG3	1.87	0.55
1:J:375:ILE:O	1:J:379:ILE:HG13	2.06	0.55
1:E:101:LEU:HB3	1:E:102:PRO:HD3	1.88	0.55
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.87	0.55
1:F:424:TYR:CE2	1:F:428:HIS:CE1	2.94	0.55
1:A:209:MET:O	1:A:213:ILE:HG13	2.07	0.55
1:C:362:ALA:O	1:C:364:PRO:HD3	2.06	0.55
1:G:45:ALA:HB1	1:G:115:MET:HE1	1.87	0.55
1:H:397:HIS:ND1	1:H:398:PRO:N	2.54	0.55
1:B:368:GLY:O	1:B:370:LEU:CD1	2.54	0.55
1:C:441:VAL:HG12	1:C:442:THR:N	2.22	0.55
1:C:52:THR:O	1:F:164:PRO:HB3	2.07	0.55
1:J:289:THR:HG22	1:J:296:ILE:O	2.07	0.55
1:A:76:ASP:O	1:A:77:PHE:CD2	2.59	0.55
1:C:419:ILE:N	1:C:419:ILE:CD1	2.70	0.55
1:D:163:LYS:HA	1:D:164:PRO:C	2.27	0.55
1:D:48:ALA:HB1	1:D:53:GLY:HA3	1.89	0.55
1:G:174:GLU:OE2	1:G:211:LYS:NZ	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:318:ALA:CA	1:H:325:GLY:O	2.54	0.55
1:J:376:GLN:CB	1:J:377:PRO:HD3	2.36	0.55
1:A:92:PRO:HG2	1:A:95:ALA:HB2	1.87	0.55
1:C:160:VAL:HG11	1:C:395:LEU:CD1	2.37	0.55
1:D:362:ALA:O	1:D:364:PRO:HD3	2.08	0.54
1:A:51:SER:OG	1:A:52:THR:N	2.39	0.54
1:G:209:MET:O	1:G:213:ILE:HG13	2.06	0.54
1:H:397:HIS:HD2	1:H:404:GLY:HA2	1.71	0.54
1:J:165:LYS:CB	1:J:191:ASP:OD1	2.54	0.54
1:B:183:ASN:HD22	1:B:402:ALA:HA	1.73	0.54
1:B:226:TRP:CH2	1:B:228:ALA:HB2	2.42	0.54
1:C:59:TYR:CG	1:C:60:PRO:HD2	2.43	0.54
1:G:149:MET:HE1	1:G:250:LYS:CB	2.38	0.54
1:H:427:THR:HG23	1:H:428:HIS:HD1	1.72	0.54
1:A:183:ASN:HD22	1:A:183:ASN:N	2.05	0.54
1:A:55:TRP:O	1:A:55:TRP:CE3	2.60	0.54
1:G:158:TYR:CE1	1:G:408:VAL:HG11	2.43	0.54
1:G:79:ASP:OD1	1:G:81:GLY:N	2.34	0.54
1:E:193:ASN:ND2	1:E:193:ASN:H	1.95	0.54
1:H:165:LYS:NZ	1:H:191:ASP:OD2	2.35	0.54
1:H:244:LEU:HD23	1:H:249:LEU:HD12	1.89	0.54
1:I:9:TYR:C	1:I:11:TYR:N	2.60	0.54
1:E:49:GLU:HG3	1:E:115:MET:SD	2.48	0.54
1:G:104:LEU:CD2	1:G:104:LEU:C	2.76	0.54
1:H:143:ILE:HD11	1:H:338:ARG:HG2	1.87	0.54
1:H:343:LYS:HG2	1:H:353:GLU:HG3	1.89	0.54
1:H:395:LEU:H	1:H:395:LEU:HD22	1.71	0.54
1:H:410:GLN:NE2	1:H:431:LEU:HB2	2.22	0.54
1:F:93:PHE:CD2	4:F:496:HOH:O	2.61	0.54
1:I:162:PRO:HA	1:I:395:LEU:CD1	2.38	0.54
1:J:317:THR:HG21	1:J:370:LEU:CD1	2.37	0.54
1:A:184:GLY:HA3	1:A:409:ARG:HG3	1.89	0.54
1:A:285:HIS:CG	1:A:286:ALA:N	2.76	0.54
1:A:330:THR:HG21	1:A:382:LEU:HD21	1.88	0.54
1:A:435:LEU:O	1:A:439:GLY:HA2	2.08	0.54
1:B:397:HIS:CE1	1:B:398:PRO:HD2	2.43	0.54
1:C:163:LYS:N	1:C:395:LEU:HD22	2.21	0.54
1:E:314:HIS:HD2	2:E:600:CAP:O6P	1.91	0.54
1:E:371:HIS:O	1:E:375:ILE:HG23	2.08	0.54
1:G:138:GLY:C	1:G:309:GLY:HA2	2.28	0.54
1:G:38:THR:CG2	1:G:41:GLN:OE1	2.53	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:GLY:CA	1:H:187:TYR:CZ	2.86	0.54
1:A:86:ILE:HD11	1:A:349:VAL:CG2	2.35	0.54
1:C:424:TYR:CZ	1:C:428:HIS:CE1	2.96	0.54
1:D:341:HIS:NE2	1:D:343:LYS:HE2	2.23	0.54
1:G:45:ALA:CB	1:G:117:ARG:HD2	2.38	0.54
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.04	0.54
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.89	0.54
1:C:397:HIS:ND1	1:C:398:PRO:HD2	2.23	0.54
1:E:380:GLU:HA	4:E:1249:HOH:O	2.08	0.54
1:F:32:THR:HG22	1:F:119:LYS:HE2	1.87	0.54
1:G:303:LYS:NZ	1:G:354:GLN:HE21	2.06	0.54
1:I:411:ALA:O	1:I:415:ILE:HG13	2.08	0.54
1:A:424:TYR:CE2	1:A:428:HIS:ND1	2.76	0.53
1:A:76:ASP:C	1:A:77:PHE:HD2	2.08	0.53
1:C:321:GLY:HA3	1:C:368:GLY:O	2.07	0.53
1:F:160:VAL:HG21	1:F:394:THR:HG21	1.90	0.53
1:F:406:ARG:O	1:F:410:GLN:HG3	2.06	0.53
1:I:180:LEU:HD11	1:I:395:LEU:HD21	1.89	0.53
1:H:429:LYS:O	1:H:433:ARG:N	2.26	0.53
1:I:76:ASP:HB3	1:I:88:ARG:HG3	1.90	0.53
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.43	0.53
1:A:356:PHE:HB3	1:A:359:ILE:HB	1.90	0.53
1:C:79:ASP:OD1	1:C:81:GLY:N	2.38	0.53
1:A:175:LYS:HG3	4:A:1729:HOH:O	2.06	0.53
1:D:172:GLU:CD	1:J:66:ARG:HH22	2.11	0.53
1:I:108:ILE:C	1:I:108:ILE:HD12	2.29	0.53
1:A:381:ALA:C	1:A:382:LEU:CD1	2.77	0.53
1:A:86:ILE:CD1	1:A:349:VAL:HG21	2.35	0.53
1:F:101:LEU:HB3	1:F:102:PRO:HD3	1.89	0.53
1:E:165:LYS:HE2	1:I:49:GLU:O	2.09	0.53
1:D:288:PHE:HB3	1:J:288:PHE:HB3	1.90	0.53
1:H:139:PRO:HD3	1:H:306:ARG:O	2.08	0.53
1:A:115:MET:O	1:A:118:VAL:CG2	2.57	0.53
1:B:105:LEU:HD23	1:B:108:ILE:HD11	1.90	0.53
1:E:192:GLU:OE2	1:I:111:ASN:ND2	2.42	0.53
1:C:163:LYS:NZ	1:C:191:ASP:OD2	2.42	0.53
1:F:72:ALA:HB2	1:F:91:TYR:CD1	2.44	0.53
1:I:101:LEU:HB3	1:I:102:PRO:HD3	1.90	0.53
1:J:174:GLU:OE1	1:J:211:LYS:CE	2.57	0.53
1:C:441:VAL:CG1	1:C:442:THR:N	2.72	0.53
1:D:9:TYR:CD2	1:D:117:ARG:NH1	2.76	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PRO:HB2	1:D:199:TYR:CE2	2.44	0.53
1:E:430:GLU:OE1	1:E:430:GLU:N	2.27	0.53
1:F:176:LEU:HD11	1:F:395:LEU:HD21	1.91	0.53
1:J:435:LEU:O	1:J:439:GLY:N	2.41	0.53
1:A:116:LYS:O	1:A:118:VAL:N	2.43	0.52
1:A:225:THR:HG1	1:A:251:HIS:HD1	1.57	0.52
1:H:284:MET:O	1:H:284:MET:HG2	2.09	0.52
1:B:334:VAL:CG1	1:B:338:ARG:CZ	2.88	0.52
1:D:299:PHE:CZ	1:D:336:LEU:HD22	2.44	0.52
1:F:421:LEU:HD13	4:F:1429:HOH:O	2.08	0.52
1:B:429:LYS:O	1:B:430:GLU:C	2.48	0.52
1:G:345:ASP:HB3	1:G:347:ASN:ND2	2.24	0.52
1:H:59:TYR:O	1:H:61:TRP:HD1	1.93	0.52
1:A:11:TYR:CZ	1:A:73:LYS:HE2	2.45	0.52
1:A:337:LEU:HD22	1:A:362:ALA:HB3	1.89	0.52
1:D:367:SER:HB2	1:D:389:GLN:HB3	1.92	0.52
1:E:397:HIS:ND1	1:E:398:PRO:HD2	2.23	0.52
1:F:112:ILE:HD12	1:F:121:LEU:HD21	1.89	0.52
1:G:163:LYS:HA	1:G:164:PRO:C	2.29	0.52
1:H:22:LYS:HE3	4:H:1185:HOH:O	2.10	0.52
1:D:117:ARG:NE	1:J:444:VAL:O	2.43	0.52
1:D:347:ASN:C	1:D:347:ASN:HD22	2.11	0.52
1:G:428:HIS:HA	4:G:852:HOH:O	2.09	0.52
1:H:283:ALA:O	1:H:284:MET:CB	2.57	0.52
1:J:371:HIS:CE1	1:J:373:GLY:C	2.83	0.52
1:A:324:GLU:OE1	1:A:325:GLY:N	2.42	0.52
1:C:417:GLN:CB	1:C:419:ILE:CD1	2.88	0.52
1:D:15:LYS:HD2	4:D:948:HOH:O	2.09	0.52
1:D:371:HIS:HB2	1:D:372:PRO:HD2	1.92	0.52
1:F:178:TYR:HE1	1:F:215:LYS:CD	2.23	0.52
1:F:283:ALA:O	1:F:284:MET:HB3	2.09	0.52
1:G:226:TRP:CZ3	1:G:228:ALA:HB2	2.44	0.52
1:G:283:ALA:O	1:G:284:MET:HB3	2.08	0.52
1:H:104:LEU:HD23	1:H:104:LEU:O	2.08	0.52
1:B:336:LEU:O	1:B:336:LEU:HD23	2.10	0.52
1:G:336:LEU:CD2	1:G:356:PHE:CZ	2.92	0.52
1:A:180:LEU:O	1:A:183:ASN:N	2.30	0.52
1:F:399:ASP:OD2	1:F:433:ARG:CD	2.57	0.52
1:F:427:THR:HG23	1:F:428:HIS:CE1	2.44	0.52
1:H:8:ILE:O	1:H:8:ILE:HG12	2.08	0.52
1:A:37:TYR:OH	1:H:444:VAL:CB	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:HD3	1:C:268:ARG:C	2.30	0.52
1:F:59:TYR:O	1:F:61:TRP:HD1	1.93	0.52
1:D:328:ASP:HB2	4:D:457:HOH:O	2.10	0.52
1:D:49:GLU:O	1:J:165:LYS:HE3	2.08	0.52
1:E:370:LEU:HA	1:E:374:ASN:HD21	1.74	0.52
1:J:209:MET:O	1:J:213:ILE:HG13	2.10	0.52
1:D:283:ALA:O	1:D:284:MET:CB	2.58	0.51
1:G:341:HIS:NE2	1:G:353:GLU:OE2	2.36	0.51
1:B:264:LEU:HD23	1:B:308:ILE:CD1	2.39	0.51
1:H:203:GLU:O	1:H:207:GLU:HG3	2.09	0.51
1:I:26:ILE:HD13	1:I:75:TYR:OH	2.11	0.51
1:A:26:ILE:HB	1:A:127:TYR:HB3	1.92	0.51
1:A:366:SER:CA	4:A:1262:HOH:O	2.40	0.51
1:E:338:ARG:HA	1:E:361:ALA:HB1	1.92	0.51
1:C:104:LEU:C	1:C:104:LEU:HD23	2.31	0.51
1:G:413:ASP:O	1:G:417:GLN:HG3	2.10	0.51
1:H:338:ARG:HA	1:H:361:ALA:HB1	1.93	0.51
1:H:9:TYR:CE1	1:H:54:THR:O	2.64	0.51
1:J:226:TRP:CZ3	1:J:228:ALA:HB2	2.45	0.51
1:A:268:ARG:HD3	1:A:268:ARG:O	2.11	0.51
1:B:104:LEU:HD23	1:B:108:ILE:HG13	1.92	0.51
1:E:410:GLN:NE2	1:E:431:LEU:H	2.09	0.51
1:A:207:GLU:OE1	1:A:247:LEU:HD21	2.11	0.51
1:F:285:HIS:CG	1:F:286:ALA:N	2.78	0.51
1:H:400:GLY:O	1:H:403:ALA:N	2.44	0.51
1:J:371:HIS:ND1	1:J:373:GLY:N	2.56	0.51
1:A:217:GLU:HG2	1:A:222:GLU:O	2.11	0.51
1:E:404:GLY:O	1:E:407:ALA:HB3	2.11	0.51
1:H:349:VAL:CG1	1:H:349:VAL:O	2.56	0.51
1:I:11:TYR:O	1:I:73:LYS:HE2	2.11	0.51
1:H:159:GLY:HA3	1:H:187:TYR:CD2	2.46	0.51
1:I:397:HIS:CE1	1:I:399:ASP:HB2	2.46	0.51
1:I:399:ASP:OD2	1:I:433:ARG:HG3	2.10	0.51
1:D:116:LYS:HE3	1:J:323:LEU:O	2.11	0.51
1:A:289:THR:HG22	1:A:296:ILE:O	2.11	0.51
1:B:390:LEU:N	1:B:390:LEU:HD12	2.26	0.51
1:C:234:LEU:HD21	1:F:234:LEU:HD21	1.93	0.51
1:E:334:VAL:CG1	1:E:338:ARG:CZ	2.89	0.51
1:G:174:GLU:HG3	1:G:208:ILE:HG23	1.93	0.51
1:H:158:TYR:O	1:H:186:ASP:HB2	2.11	0.51
1:J:319:GLY:HA2	4:J:1255:HOH:O	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:C	1:B:108:ILE:HD12	2.32	0.51
1:D:23:ARG:NE	1:I:69:ASP:OD1	2.44	0.51
1:H:439:GLY:C	1:H:440:HIS:CD2	2.84	0.51
1:C:158:TYR:CE1	1:C:408:VAL:HG11	2.46	0.50
1:C:149:MET:HE3	1:C:250:LYS:HD3	1.92	0.50
1:C:435:LEU:O	1:C:439:GLY:HA2	2.11	0.50
1:D:303:LYS:HZ3	1:D:354:GLN:HE21	1.58	0.50
1:E:166:VAL:HG23	1:I:52:THR:HG22	1.93	0.50
1:A:389:GLN:C	1:A:390:LEU:HD12	2.31	0.50
1:A:427:THR:HG22	1:A:427:THR:O	2.11	0.50
1:A:443:PRO:O	1:A:444:VAL:CG2	2.60	0.50
1:D:9:TYR:HD2	1:D:117:ARG:NH1	2.09	0.50
1:E:106:ALA:HA	1:I:258:ILE:CD1	2.41	0.50
1:F:169:SER:HB2	1:F:170:PRO:HD2	1.91	0.50
1:B:320:ALA:O	1:B:442:THR:HG23	2.11	0.50
1:E:180:LEU:HD21	1:E:401:PRO:HB3	1.92	0.50
1:G:236:GLU:N	1:G:236:GLU:OE1	2.45	0.50
1:G:418:GLY:HA2	4:G:1310:HOH:O	2.10	0.50
1:D:178:TYR:CE1	1:D:215:LYS:HD3	2.47	0.50
1:G:362:ALA:O	1:G:364:PRO:HD3	2.11	0.50
1:H:334:VAL:HG21	1:H:382:LEU:HD22	1.93	0.50
1:E:138:GLY:C	1:E:309:GLY:HA2	2.32	0.50
1:E:371:HIS:HB2	1:E:372:PRO:HD2	1.93	0.50
4:B:1128:HOH:O	1:F:65:GLU:HG2	2.11	0.50
1:G:115:MET:O	1:G:118:VAL:HG22	2.11	0.50
1:B:283:ALA:O	1:B:284:MET:CB	2.60	0.50
1:E:334:VAL:HG21	1:E:382:LEU:HD22	1.93	0.50
1:H:93:PHE:CD1	1:H:93:PHE:C	2.84	0.50
1:I:335:ASP:HA	4:I:1735:HOH:O	2.11	0.50
1:J:338:ARG:HA	1:J:361:ALA:HB1	1.93	0.50
1:B:104:LEU:O	1:B:104:LEU:HD23	2.12	0.50
1:C:108:ILE:HG22	1:C:108:ILE:O	2.12	0.50
1:C:18:GLU:HG3	4:C:1961:HOH:O	2.12	0.50
1:E:376:GLN:H	1:E:377:PRO:HD2	1.76	0.50
1:I:390:LEU:HD12	1:I:390:LEU:N	2.27	0.50
1:I:412:ILE:O	1:I:416:MET:HG2	2.11	0.50
1:B:153:LYS:CB	1:B:154:ASP:OD1	2.60	0.50
1:A:319:GLY:N	1:A:325:GLY:O	2.45	0.49
1:D:230:ILE:O	1:D:237:MET:HG2	2.12	0.49
1:B:152:ILE:HD12	1:B:157:ILE:HD12	1.93	0.49
1:B:371:HIS:HA	1:B:390:LEU:HD23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:TYR:C	1:I:11:TYR:H	2.15	0.49
1:I:371:HIS:O	1:I:375:ILE:HG23	2.12	0.49
1:D:303:LYS:NZ	1:D:354:GLN:HE21	2.09	0.49
1:H:230:ILE:O	1:H:237:MET:HG2	2.13	0.49
1:H:402:ALA:O	1:H:406:ARG:NH1	2.45	0.49
1:H:441:VAL:CG1	1:H:442:THR:N	2.74	0.49
1:H:51:SER:OG	1:H:52:THR:N	2.46	0.49
1:J:159:GLY:HA3	1:J:187:TYR:CD1	2.48	0.49
1:A:116:LYS:C	1:A:118:VAL:H	2.14	0.49
1:B:104:LEU:C	1:B:104:LEU:HD23	2.32	0.49
1:B:183:ASN:HD22	1:B:402:ALA:CB	2.24	0.49
1:C:419:ILE:HG22	1:C:424:TYR:HB2	1.95	0.49
1:D:176:LEU:HD11	1:D:395:LEU:CD2	2.39	0.49
1:D:72:ALA:O	1:D:73:LYS:HD3	2.12	0.49
1:E:362:ALA:O	1:E:364:PRO:HD3	2.11	0.49
1:E:371:HIS:HE1	1:E:373:GLY:C	2.14	0.49
1:E:390:LEU:N	1:E:390:LEU:HD12	2.27	0.49
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.95	0.49
1:A:226:TRP:CZ3	1:A:228:ALA:HB2	2.47	0.49
1:A:77:PHE:N	1:A:77:PHE:CD2	2.80	0.49
1:H:411:ALA:O	1:H:414:ALA:HB3	2.13	0.49
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.77	0.49
1:I:47:ALA:O	1:I:51:SER:HB2	2.13	0.49
1:A:299:PHE:CE2	1:A:351:HIS:CD2	3.00	0.49
1:A:80:MET:HB2	1:A:84:SER:O	2.11	0.49
1:E:193:ASN:HD22	1:E:193:ASN:N	1.87	0.49
1:F:347:ASN:ND2	4:F:1415:HOH:O	2.45	0.49
1:H:108:ILE:O	1:H:108:ILE:CG2	2.61	0.49
1:I:235:LEU:O	1:I:239:GLN:HG3	2.13	0.49
1:I:318:ALA:HB1	1:I:327:ARG:HA	1.95	0.49
1:B:26:ILE:HB	1:B:127:TYR:HB3	1.94	0.49
1:D:347:ASN:C	1:D:347:ASN:ND2	2.66	0.49
1:E:406:ARG:O	1:E:410:GLN:HG2	2.13	0.49
1:F:303:LYS:NZ	1:F:354:GLN:HE21	2.10	0.49
1:B:444:VAL:HG12	1:G:117:ARG:HB3	1.94	0.49
1:A:411:ALA:O	1:A:414:ALA:HB3	2.12	0.49
1:C:397:HIS:CG	1:C:398:PRO:CD	2.84	0.49
1:E:217:GLU:HG2	1:E:222:GLU:O	2.11	0.49
1:J:371:HIS:HB2	1:J:372:PRO:HD2	1.95	0.49
1:C:404:GLY:O	1:C:408:VAL:HG23	2.13	0.49
1:C:427:THR:HG23	1:C:428:HIS:ND1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:ILE:O	1:J:212:ILE:HG12	2.13	0.49
1:J:353:GLU:CG	4:J:1285:HOH:O	2.61	0.49
1:F:54:THR:CG2	1:F:56:THR:O	2.60	0.49
1:B:25:ILE:HD12	1:B:25:ILE:N	2.28	0.48
1:E:158:TYR:CE1	1:E:408:VAL:HG11	2.48	0.48
1:E:165:LYS:HB3	1:E:191:ASP:OD2	2.13	0.48
1:E:367:SER:HB2	1:E:389:GLN:HB3	1.93	0.48
1:G:213:ILE:O	1:G:217:GLU:HG3	2.13	0.48
1:G:373:GLY:O	1:G:440:HIS:HD2	1.96	0.48
1:J:26:ILE:HB	1:J:127:TYR:HB3	1.95	0.48
1:A:345:ASP:O	1:A:346:GLU:C	2.51	0.48
1:A:86:ILE:HD13	1:A:349:VAL:O	2.13	0.48
1:C:303:LYS:NZ	1:C:354:GLN:HE21	2.11	0.48
1:H:391:GLY:O	1:H:395:LEU:CD2	2.59	0.48
1:H:79:ASP:HB2	1:H:85:TRP:CZ3	2.48	0.48
1:I:15:LYS:CB	4:I:468:HOH:O	2.61	0.48
1:E:371:HIS:HE1	1:E:373:GLY:CA	2.22	0.48
1:A:93:PHE:CE1	1:A:131:LYS:HD3	2.49	0.48
1:A:54:THR:HG23	1:A:56:THR:H	1.78	0.48
1:B:419:ILE:CD1	1:B:419:ILE:N	2.76	0.48
1:C:149:MET:CE	1:C:250:LYS:CD	2.89	0.48
1:C:410:GLN:HE21	1:C:431:LEU:HB2	1.78	0.48
1:F:178:TYR:CE1	1:F:215:LYS:HD2	2.47	0.48
1:H:371:HIS:CB	1:H:372:PRO:CD	2.88	0.48
1:A:158:TYR:O	1:A:186:ASP:HB2	2.14	0.48
1:B:368:GLY:O	1:B:370:LEU:HD12	2.13	0.48
1:C:410:GLN:NE2	1:C:431:LEU:H	2.11	0.48
1:D:111:ASN:ND2	1:J:192:GLU:OE2	2.46	0.48
1:E:412:ILE:O	1:E:416:MET:HG2	2.14	0.48
1:G:45:ALA:HB1	1:G:115:MET:HE2	1.94	0.48
1:I:223:LYS:O	1:I:224:LYS:HD3	2.13	0.48
1:J:146:VAL:HG21	1:J:312:GLN:HE21	1.77	0.48
1:J:371:HIS:O	1:J:374:ASN:OD1	2.31	0.48
1:J:397:HIS:CE1	1:J:398:PRO:HD2	2.48	0.48
1:A:330:THR:O	1:A:334:VAL:HG23	2.13	0.48
1:A:441:VAL:HG22	1:A:442:THR:N	2.28	0.48
1:B:174:GLU:HG3	1:B:208:ILE:HG23	1.95	0.48
1:C:122:ARG:HD2	4:C:448:HOH:O	2.11	0.48
1:G:283:ALA:O	1:G:284:MET:CB	2.62	0.48
1:J:153:LYS:HB3	1:J:154:ASP:OD1	2.13	0.48
1:J:41:GLN:HA	4:J:1290:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:MET:HG2	1:A:284:MET:O	2.13	0.48
1:A:435:LEU:O	1:A:439:GLY:N	2.46	0.48
1:B:54:THR:CG2	1:B:56:THR:O	2.59	0.48
1:C:283:ALA:O	1:C:284:MET:CB	2.61	0.48
1:C:399:ASP:OD2	1:C:433:ARG:CD	2.56	0.48
1:F:209:MET:O	1:F:213:ILE:HG13	2.14	0.48
1:F:39:ILE:HG12	1:F:85:TRP:CG	2.48	0.48
1:I:334:VAL:HG21	1:I:382:LEU:HD22	1.96	0.48
1:A:282:ARG:CD	1:A:285:HIS:CD2	2.85	0.48
1:D:72:ALA:HB2	1:D:91:TYR:CD1	2.48	0.48
1:A:116:LYS:C	1:A:118:VAL:N	2.66	0.48
1:A:20:SER:N	1:A:24:ASP:OD2	2.38	0.48
1:A:334:VAL:HG12	1:A:338:ARG:NH2	2.26	0.48
1:D:371:HIS:HB2	1:D:372:PRO:CD	2.44	0.48
1:H:159:GLY:CA	1:H:187:TYR:CE2	2.95	0.48
1:H:98:GLU:OE2	1:H:131:LYS:NZ	2.47	0.48
1:A:324:GLU:OE1	1:A:324:GLU:C	2.52	0.48
1:A:46:VAL:HG22	1:A:115:MET:HE1	1.95	0.48
1:D:197:PRO:O	1:D:201:ARG:HD3	2.14	0.48
1:D:178:TYR:CE1	1:D:215:LYS:CE	2.97	0.48
1:E:159:GLY:HA3	1:E:187:TYR:CD1	2.49	0.48
1:H:197:PRO:HB2	1:H:199:TYR:CE2	2.48	0.48
1:B:419:ILE:H	1:B:419:ILE:CD1	2.27	0.47
1:D:159:GLY:CA	1:D:187:TYR:CZ	2.89	0.47
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.43	0.47
1:G:108:ILE:HD12	1:G:108:ILE:C	2.34	0.47
1:J:323:LEU:HB2	4:J:455:HOH:O	2.14	0.47
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.14	0.47
1:F:443:PRO:O	1:F:444:VAL:CG2	2.62	0.47
1:I:226:TRP:CZ3	1:I:228:ALA:HB2	2.49	0.47
1:J:370:LEU:HA	1:J:374:ASN:ND2	2.28	0.47
1:B:338:ARG:HA	1:B:361:ALA:HB1	1.96	0.47
1:C:130:GLU:OE1	1:J:66:ARG:HD3	2.14	0.47
1:E:371:HIS:CE1	1:E:373:GLY:HA3	2.47	0.47
1:B:234:LEU:CD2	1:G:234:LEU:HD21	2.44	0.47
1:G:367:SER:HB2	1:G:389:GLN:HB3	1.96	0.47
1:H:9:TYR:CZ	1:H:55:TRP:HA	2.50	0.47
1:J:139:PRO:O	1:J:360:LYS:HD2	2.13	0.47
1:J:343:LYS:O	4:J:2115:HOH:O	2.20	0.47
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.79	0.47
1:A:397:HIS:CE1	1:A:399:ASP:HB2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:O	1:A:416:MET:HG2	2.14	0.47
1:B:164:PRO:HG3	1:G:67:TRP:CD1	2.50	0.47
1:I:399:ASP:HB2	1:I:403:ALA:CB	2.45	0.47
1:E:25:ILE:HD11	1:E:132:LEU:HD21	1.97	0.47
1:H:362:ALA:O	1:H:364:PRO:HD3	2.14	0.47
1:A:79:ASP:HA	1:A:85:TRP:NE1	2.30	0.47
1:D:175:LYS:HE3	1:D:179:ASP:OD2	2.14	0.47
1:H:163:LYS:CA	1:H:164:PRO:O	2.58	0.47
1:H:206:ALA:HA	1:H:226:TRP:CH2	2.50	0.47
1:H:250:LYS:HE2	4:H:624:HOH:O	2.15	0.47
1:I:441:VAL:O	1:I:443:PRO:HD3	2.14	0.47
1:J:283:ALA:O	1:J:284:MET:CB	2.61	0.47
1:J:410:GLN:HG2	4:J:456:HOH:O	2.13	0.47
1:A:399:ASP:HB2	1:A:403:ALA:CB	2.44	0.47
1:H:400:GLY:O	1:H:403:ALA:CB	2.61	0.47
1:H:410:GLN:NE2	1:H:428:HIS:HB3	2.29	0.47
1:A:187:TYR:CE1	1:A:227:PHE:CE2	3.03	0.47
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.95	0.47
1:H:118:VAL:HG22	1:H:120:GLY:N	2.29	0.47
1:H:197:PRO:HD2	1:H:200:ASN:O	2.15	0.47
1:H:226:TRP:CZ3	1:H:249:LEU:HD13	2.50	0.47
4:E:722:HOH:O	1:I:265:ARG:CB	2.62	0.47
2:B:600:CAP:O6P	4:B:482:HOH:O	2.21	0.47
1:D:108:ILE:HD12	1:D:109:ALA:N	2.30	0.47
1:D:9:TYR:HD2	1:D:117:ARG:HH12	1.62	0.47
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.80	0.47
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.49	0.47
1:F:178:TYR:CE1	1:F:215:LYS:CD	2.97	0.47
1:F:180:LEU:HD21	1:F:401:PRO:HB3	1.97	0.47
1:I:46:VAL:HG22	1:I:115:MET:HE1	1.97	0.47
1:J:334:VAL:CG1	1:J:338:ARG:CZ	2.93	0.47
1:C:444:VAL:O	1:F:117:ARG:NH2	2.32	0.47
1:F:328:ASP:N	1:F:328:ASP:OD2	2.48	0.47
1:H:161:VAL:CG2	1:H:189:KCX:HD2	2.44	0.47
1:H:395:LEU:H	1:H:395:LEU:CD2	2.28	0.47
1:J:226:TRP:CH2	1:J:228:ALA:HB2	2.50	0.47
1:A:216:VAL:C	1:A:218:ASN:N	2.69	0.47
1:A:441:VAL:CG2	1:A:442:THR:N	2.77	0.47
1:B:138:GLY:C	1:B:309:GLY:HA2	2.35	0.47
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.80	0.47
1:B:159:GLY:CA	1:B:187:TYR:CZ	2.90	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:MET:HG2	1:E:284:MET:O	2.14	0.47
1:E:411:ALA:O	1:E:415:ILE:HG12	2.15	0.47
1:G:59:TYR:CD1	1:G:60:PRO:HD2	2.50	0.47
1:C:213:ILE:O	1:C:217:GLU:HG3	2.15	0.46
1:F:376:GLN:CB	1:F:377:PRO:CD	2.89	0.46
1:I:17:TYR:CE2	1:I:19:PRO:HA	2.50	0.46
1:J:353:GLU:CB	4:J:1285:HOH:O	2.49	0.46
1:A:108:ILE:HD12	1:A:126:LEU:CG	2.45	0.46
1:A:376:GLN:HG3	1:A:377:PRO:N	2.31	0.46
1:C:98:GLU:CD	4:C:1818:HOH:O	2.53	0.46
1:F:226:TRP:CZ3	1:F:228:ALA:HB2	2.50	0.46
1:G:126:LEU:O	1:G:303:LYS:NZ	2.48	0.46
1:A:282:ARG:HH11	1:A:285:HIS:CE1	2.33	0.46
1:D:111:ASN:HD21	1:J:192:GLU:CD	2.18	0.46
1:G:125:ASP:OD1	1:G:126:LEU:N	2.48	0.46
1:H:93:PHE:CD1	1:H:94:HIS:N	2.83	0.46
1:B:376:GLN:N	1:B:377:PRO:CD	2.79	0.46
1:C:184:GLY:HA3	1:C:409:ARG:HG3	1.98	0.46
1:E:236:GLU:HA	1:E:239:GLN:HE21	1.81	0.46
1:G:159:GLY:CA	1:G:187:TYR:CZ	2.87	0.46
1:H:438:TRP:O	1:H:441:VAL:HG23	2.15	0.46
1:A:407:ALA:O	1:A:410:GLN:HB2	2.15	0.46
1:B:22:LYS:HD3	1:F:65:GLU:CG	2.45	0.46
1:E:375:ILE:O	1:E:379:ILE:HG13	2.16	0.46
1:G:226:TRP:CH2	1:G:228:ALA:HB2	2.51	0.46
1:G:395:LEU:N	1:G:395:LEU:HD12	2.30	0.46
1:H:9:TYR:OH	1:H:55:TRP:HA	2.16	0.46
1:J:303:LYS:HZ2	1:J:354:GLN:HE21	1.58	0.46
1:A:54:THR:HG21	1:A:56:THR:O	2.15	0.46
1:E:139:PRO:O	1:E:360:LYS:HD2	2.15	0.46
1:G:285:HIS:CG	1:G:286:ALA:N	2.82	0.46
1:H:427:THR:HG23	1:H:428:HIS:CE1	2.50	0.46
1:J:152:ILE:HD12	1:J:157:ILE:HD12	1.96	0.46
1:A:334:VAL:HG12	1:A:338:ARG:HH21	1.81	0.46
1:B:22:LYS:CG	1:F:65:GLU:HG3	2.46	0.46
1:A:159:GLY:CA	1:A:187:TYR:CE2	2.96	0.46
1:A:180:LEU:HD21	1:A:401:PRO:HB3	1.97	0.46
1:B:148:LYS:HB3	4:B:1301:HOH:O	2.16	0.46
1:B:371:HIS:HB2	1:B:372:PRO:HD3	1.97	0.46
1:D:441:VAL:HG22	1:D:442:THR:N	2.31	0.46
1:E:396:GLY:O	1:E:397:HIS:C	2.53	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:GLY:HA3	1:F:409:ARG:HG3	1.98	0.46
1:E:91:TYR:CE1	1:E:108:ILE:CD1	2.98	0.46
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.80	0.46
1:E:379:ILE:HD12	1:E:415:ILE:HG21	1.97	0.46
1:G:336:LEU:CD2	1:G:336:LEU:O	2.64	0.46
1:G:389:GLN:O	1:G:390:LEU:HD12	2.16	0.46
1:I:25:ILE:HD11	1:I:132:LEU:CD2	2.42	0.46
1:A:443:PRO:C	1:A:444:VAL:HG23	2.36	0.46
1:B:433:ARG:CB	4:B:1637:HOH:O	2.63	0.46
1:C:322:LYS:O	1:C:322:LYS:HG2	2.16	0.46
1:E:279:HIS:NE2	1:E:314:HIS:CE1	2.80	0.46
1:I:159:GLY:HA3	1:I:187:TYR:CD1	2.49	0.46
1:I:283:ALA:O	1:I:284:MET:CB	2.62	0.46
1:J:59:TYR:O	1:J:61:TRP:HD1	1.99	0.46
1:A:234:LEU:HD21	1:H:234:LEU:HD21	1.96	0.45
1:A:329:ILE:HG22	1:A:333:PHE:CE2	2.51	0.45
1:C:122:ARG:NH1	4:C:1829:HOH:O	2.24	0.45
1:C:160:VAL:CG1	1:C:395:LEU:HD11	2.46	0.45
1:D:163:LYS:H	1:D:395:LEU:CD1	2.25	0.45
1:D:399:ASP:OD2	1:D:433:ARG:HG3	2.17	0.45
1:F:159:GLY:CA	1:F:187:TYR:CZ	2.95	0.45
1:F:265:ARG:NH1	4:F:501:HOH:O	2.49	0.45
1:G:155:ARG:HB2	1:G:156:PRO:HD2	1.98	0.45
1:G:376:GLN:HG3	1:G:377:PRO:N	2.30	0.45
1:H:399:ASP:HB2	1:H:403:ALA:HB1	1.98	0.45
1:H:17:TYR:CD1	1:H:73:LYS:CD	2.99	0.45
1:I:215:LYS:CE	1:I:219:GLU:OE2	2.64	0.45
1:C:115:MET:HA	1:F:323:LEU:HD23	1.98	0.45
1:C:322:LYS:NZ	2:C:600:CAP:O3P	2.47	0.45
1:E:371:HIS:HE1	1:E:373:GLY:HA3	1.80	0.45
1:A:27:ALA:HB1	1:A:29:PHE:CE2	2.52	0.45
1:B:395:LEU:N	1:B:395:LEU:HD12	2.32	0.45
1:D:376:GLN:N	1:D:377:PRO:CD	2.80	0.45
1:E:158:TYR:CD1	1:E:408:VAL:HG11	2.51	0.45
1:G:104:LEU:HD23	1:G:108:ILE:HG13	1.98	0.45
1:H:39:ILE:HG23	1:H:40:GLU:N	2.31	0.45
1:D:117:ARG:CZ	1:J:444:VAL:O	2.64	0.45
1:A:149:MET:CE	1:A:250:LYS:CD	2.83	0.45
1:A:370:LEU:HA	1:A:374:ASN:HD21	1.81	0.45
1:B:263:ALA:CB	1:G:263:ALA:HB2	2.46	0.45
1:C:305:TYR:O	1:C:310:ILE:HG12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:GLY:O	1:D:409:ARG:HD3	2.17	0.45
1:H:369:GLY:HA3	1:H:443:PRO:HG2	1.97	0.45
1:H:389:GLN:C	1:H:390:LEU:HD12	2.37	0.45
1:H:390:LEU:HD12	1:H:390:LEU:N	2.32	0.45
1:J:101:LEU:HB3	1:J:102:PRO:HD3	1.98	0.45
1:J:101:LEU:N	1:J:102:PRO:CD	2.79	0.45
1:J:299:PHE:CZ	1:J:336:LEU:HD22	2.52	0.45
1:J:424:TYR:CZ	1:J:428:HIS:CE1	3.04	0.45
1:D:234:LEU:HD21	1:J:234:LEU:HD21	1.99	0.45
1:B:65:GLU:HG3	1:F:22:LYS:CG	2.47	0.45
1:G:93:PHE:CD1	1:G:94:HIS:N	2.84	0.45
1:H:424:TYR:O	1:H:427:THR:CG2	2.53	0.45
1:J:123:LEU:HG	1:J:300:VAL:HG21	1.99	0.45
1:A:25:ILE:HD12	1:A:96:PHE:CE2	2.52	0.45
1:A:285:HIS:ND1	1:A:286:ALA:N	2.65	0.45
1:A:435:LEU:O	1:A:439:GLY:CA	2.65	0.45
1:B:419:ILE:HG22	1:B:424:TYR:HB2	1.99	0.45
1:C:130:GLU:HG3	1:C:357:TYR:CE2	2.51	0.45
1:D:138:GLY:C	1:D:309:GLY:HA2	2.37	0.45
1:H:240:ARG:NH1	4:H:697:HOH:O	2.48	0.45
1:J:108:ILE:N	1:J:108:ILE:HD12	2.32	0.45
1:A:111:ASN:HA	4:A:464:HOH:O	2.17	0.45
1:A:268:ARG:CD	1:A:268:ARG:C	2.78	0.45
1:B:149:MET:HE2	1:B:250:LYS:HD3	1.97	0.45
1:D:52:THR:HG22	1:J:166:VAL:HG23	1.99	0.45
1:F:334:VAL:HG21	1:F:382:LEU:HG	1.97	0.45
1:G:320:ALA:O	1:G:442:THR:HG23	2.16	0.45
1:H:343:LYS:HE2	1:H:353:GLU:OE2	2.17	0.45
1:I:105:LEU:HD23	1:I:108:ILE:HD11	1.97	0.45
1:J:263:ALA:O	1:J:267:ILE:HG12	2.17	0.45
1:A:138:GLY:C	1:A:309:GLY:HA2	2.37	0.45
1:C:122:ARG:HA	1:C:295:GLY:O	2.17	0.45
1:F:433:ARG:HH11	1:F:433:ARG:CB	2.26	0.45
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.82	0.45
1:G:39:ILE:HG12	1:G:85:TRP:CG	2.52	0.45
1:I:424:TYR:CZ	1:I:428:HIS:CE1	3.05	0.45
1:B:139:PRO:N	1:B:309:GLY:HA2	2.32	0.45
1:B:160:VAL:HG21	1:B:394:THR:HG21	1.98	0.45
1:E:435:LEU:O	1:E:437:LYS:N	2.50	0.45
1:H:424:TYR:CE2	1:H:428:HIS:CE1	3.05	0.45
1:J:141:PHE:O	1:J:145:GLY:HA3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:19:PRO:HG3	1:J:75:TYR:CZ	2.51	0.45
1:A:299:PHE:CD2	1:A:351:HIS:CD2	3.05	0.45
1:C:407:ALA:HB2	1:C:430:GLU:HB3	1.98	0.45
1:F:183:ASN:OD1	1:F:406:ARG:NH1	2.50	0.45
1:F:435:LEU:O	1:F:439:GLY:N	2.48	0.45
1:G:183:ASN:HD22	1:G:183:ASN:N	2.15	0.45
1:H:12:TYR:CD2	1:H:48:ALA:HB2	2.51	0.45
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.52	0.45
1:J:371:HIS:CE1	1:J:373:GLY:CA	3.00	0.45
1:J:371:HIS:N	1:J:374:ASN:OD1	2.27	0.45
1:A:82:ASP:OD1	1:A:82:ASP:C	2.56	0.44
1:E:283:ALA:O	1:E:284:MET:CB	2.65	0.44
1:F:108:ILE:HD12	1:F:109:ALA:N	2.32	0.44
1:H:206:ALA:HA	1:H:226:TRP:CZ3	2.52	0.44
1:H:282:ARG:NH1	1:H:285:HIS:NE2	2.64	0.44
1:H:442:THR:O	1:H:443:PRO:O	2.35	0.44
1:A:166:VAL:HG23	1:H:52:THR:HG22	1.99	0.44
1:I:284:MET:HG2	1:I:284:MET:O	2.17	0.44
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.82	0.44
1:B:39:ILE:CD1	1:B:85:TRP:HB2	2.47	0.44
1:D:159:GLY:HA3	1:D:187:TYR:CD2	2.52	0.44
1:D:285:HIS:CG	1:D:286:ALA:N	2.85	0.44
1:E:347:ASN:N	1:E:347:ASN:OD1	2.37	0.44
1:G:38:THR:OG1	1:G:41:GLN:HG2	2.18	0.44
1:I:285:HIS:CG	1:I:286:ALA:N	2.86	0.44
1:A:288:PHE:CD1	1:A:289:THR:HG23	2.53	0.44
1:C:206:ALA:HA	1:C:226:TRP:CH2	2.52	0.44
1:D:9:TYR:HE1	1:D:54:THR:O	2.00	0.44
1:E:106:ALA:HA	1:I:258:ILE:HD11	1.99	0.44
1:E:112:ILE:HG23	4:E:1890:HOH:O	2.16	0.44
1:C:288:PHE:HB3	1:F:288:PHE:HB3	2.00	0.44
1:F:15:LYS:HA	1:F:75:TYR:O	2.17	0.44
1:G:376:GLN:CB	1:G:377:PRO:CD	2.94	0.44
1:H:8:ILE:O	1:H:8:ILE:CG1	2.65	0.44
1:B:289:THR:HG22	1:B:296:ILE:O	2.18	0.44
1:C:73:LYS:HE2	4:J:641:HOH:O	2.18	0.44
1:E:163:LYS:H	1:E:395:LEU:HD11	1.81	0.44
1:G:421:LEU:HD13	4:G:1150:HOH:O	2.18	0.44
1:A:136:PHE:HB3	1:A:307:LEU:O	2.17	0.44
1:A:185:ALA:O	1:A:224:LYS:NZ	2.25	0.44
1:A:47:ALA:HB2	1:A:89:ILE:HD13	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ASP:HB3	1:E:88:ARG:HG3	2.00	0.44
1:G:406:ARG:O	1:G:410:GLN:HG3	2.16	0.44
1:E:192:GLU:CD	1:I:111:ASN:HD21	2.20	0.44
1:A:375:ILE:O	1:A:376:GLN:C	2.55	0.44
1:C:54:THR:HG23	1:C:56:THR:H	1.82	0.44
1:F:433:ARG:CB	1:F:433:ARG:NH1	2.80	0.44
1:I:174:GLU:HB2	1:I:208:ILE:HD13	2.00	0.44
1:A:46:VAL:CG2	1:A:115:MET:HE3	2.48	0.44
1:B:93:PHE:C	1:B:93:PHE:CD1	2.91	0.44
1:D:299:PHE:CE2	1:D:336:LEU:HD22	2.53	0.44
1:D:11:TYR:CE2	1:D:73:LYS:NZ	2.85	0.44
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.83	0.44
1:F:283:ALA:O	1:F:284:MET:CB	2.66	0.44
1:I:206:ALA:HA	1:I:226:TRP:CZ3	2.53	0.44
1:J:268:ARG:C	1:J:268:ARG:CD	2.84	0.44
1:A:411:ALA:O	1:A:414:ALA:N	2.50	0.44
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.83	0.44
1:C:341:HIS:NE2	1:C:353:GLU:OE2	2.40	0.44
1:D:438:TRP:O	1:D:441:VAL:HG12	2.17	0.44
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.48	0.44
1:F:39:ILE:CD1	1:F:85:TRP:HB2	2.48	0.44
1:F:93:PHE:CE2	4:F:496:HOH:O	2.56	0.44
1:I:20:SER:O	1:I:24:ASP:HB2	2.17	0.44
1:A:281:HIS:CE1	1:A:283:ALA:HB2	2.53	0.44
1:A:285:HIS:O	1:A:287:ALA:N	2.51	0.44
1:A:79:ASP:HA	1:A:85:TRP:CD1	2.52	0.44
1:C:289:THR:HG22	1:C:296:ILE:O	2.18	0.44
1:F:197:PRO:HB2	1:F:199:TYR:CE2	2.53	0.44
1:F:373:GLY:HA3	1:F:439:GLY:O	2.17	0.44
1:B:285:HIS:CG	1:B:286:ALA:N	2.86	0.43
1:D:184:GLY:HA3	1:D:409:ARG:HG3	2.00	0.43
1:B:23:ARG:NE	1:F:69:ASP:OD1	2.49	0.43
1:A:216:VAL:O	1:A:218:ASN:N	2.51	0.43
1:B:374:ASN:C	1:B:374:ASN:OD1	2.57	0.43
1:C:235:LEU:O	1:C:239:GLN:HG3	2.18	0.43
1:C:397:HIS:CE1	1:C:398:PRO:HD2	2.52	0.43
1:E:208:ILE:O	1:E:212:ILE:HG12	2.18	0.43
1:F:162:PRO:HA	1:F:395:LEU:HD11	2.00	0.43
1:G:139:PRO:N	1:G:309:GLY:HA2	2.32	0.43
1:J:389:GLN:C	1:J:390:LEU:HD12	2.38	0.43
1:J:430:GLU:N	1:J:430:GLU:OE1	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:OH	1:A:53:GLY:HA2	2.18	0.43
1:A:159:GLY:HA3	1:A:187:TYR:CD2	2.52	0.43
1:A:49:GLU:O	1:H:165:LYS:HE2	2.19	0.43
1:B:371:HIS:CB	1:B:372:PRO:CD	2.87	0.43
1:A:216:VAL:O	1:A:219:GLU:N	2.44	0.43
1:C:118:VAL:HG11	1:C:121:LEU:HB2	2.00	0.43
1:C:163:LYS:N	1:C:395:LEU:CD2	2.62	0.43
1:D:208:ILE:O	1:D:212:ILE:HG12	2.18	0.43
1:D:338:ARG:HA	1:D:361:ALA:HB1	2.01	0.43
1:D:80:MET:HB2	1:D:84:SER:O	2.18	0.43
1:D:93:PHE:C	1:D:93:PHE:CD1	2.91	0.43
1:F:51:SER:OG	1:F:52:THR:N	2.52	0.43
1:F:59:TYR:CD2	1:F:60:PRO:HD2	2.54	0.43
1:G:131:LYS:O	1:G:135:GLU:HG3	2.19	0.43
1:G:441:VAL:CG1	1:G:442:THR:N	2.82	0.43
1:I:251:HIS:NE2	1:I:312:GLN:NE2	2.64	0.43
1:I:79:ASP:HB2	1:I:85:TRP:CZ3	2.54	0.43
1:J:159:GLY:CA	1:J:187:TYR:CZ	2.96	0.43
1:A:123:LEU:HG	1:A:300:VAL:HG21	2.00	0.43
1:A:373:GLY:O	1:A:440:HIS:HA	2.18	0.43
1:B:371:HIS:CE1	1:B:373:GLY:N	2.84	0.43
1:C:72:ALA:HB2	1:C:91:TYR:CD1	2.53	0.43
1:G:166:VAL:HG12	1:G:194:LEU:HD13	2.00	0.43
1:G:51:SER:OG	1:G:52:THR:N	2.52	0.43
1:J:175:LYS:HE3	1:J:179:ASP:OD2	2.19	0.43
1:J:93:PHE:C	1:J:93:PHE:CD1	2.91	0.43
1:A:122:ARG:HD3	1:A:292:PRO:C	2.39	0.43
1:B:155:ARG:HB2	1:B:156:PRO:HD2	2.00	0.43
1:D:159:GLY:HA3	1:D:187:TYR:CD1	2.53	0.43
1:E:165:LYS:CB	1:E:191:ASP:OD2	2.65	0.43
1:E:230:ILE:O	1:E:237:MET:HG2	2.19	0.43
1:E:407:ALA:O	1:E:410:GLN:HG2	2.18	0.43
1:F:11:TYR:CD2	1:F:11:TYR:C	2.92	0.43
1:F:317:THR:HA	1:F:366:SER:HG	1.82	0.43
1:H:427:THR:CG2	1:H:428:HIS:HD1	2.32	0.43
1:A:401:PRO:O	1:A:404:GLY:N	2.51	0.43
1:B:417:GLN:CB	1:B:419:ILE:HD13	2.49	0.43
1:C:159:GLY:HA3	1:C:187:TYR:CD2	2.52	0.43
1:D:19:PRO:HG3	1:D:75:TYR:CZ	2.53	0.43
1:G:336:LEU:HD21	1:G:356:PHE:HZ	1.82	0.43
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:LYS:HG3	1:J:212:ILE:N	2.33	0.43
1:A:174:GLU:CG	1:A:212:ILE:HD11	2.49	0.43
1:A:263:ALA:HA	4:A:1589:HOH:O	2.19	0.43
1:C:125:ASP:OD1	1:C:126:LEU:N	2.49	0.43
1:C:376:GLN:N	1:C:377:PRO:CD	2.80	0.43
1:E:398:PRO:CG	1:E:433:ARG:HB3	2.49	0.43
1:F:200:ASN:OD1	1:F:205:ARG:CG	2.66	0.43
1:F:38:THR:HA	4:F:476:HOH:O	2.18	0.43
1:G:118:VAL:HG23	1:G:118:VAL:O	2.17	0.43
1:I:209:MET:HG3	1:I:226:TRP:CG	2.54	0.43
1:I:56:THR:OG1	1:I:57:THR:N	2.52	0.43
1:J:374:ASN:N	4:J:1683:HOH:O	2.51	0.43
1:A:338:ARG:HA	1:A:361:ALA:HB1	2.00	0.43
1:D:169:SER:HB2	1:D:170:PRO:HD2	2.00	0.43
1:F:376:GLN:HA	1:F:415:ILE:HD13	2.01	0.43
1:F:443:PRO:C	1:F:444:VAL:HG23	2.39	0.43
1:I:125:ASP:OD1	1:I:126:LEU:N	2.52	0.43
1:B:104:LEU:HD23	1:B:108:ILE:CG1	2.49	0.43
1:C:390:LEU:N	1:C:390:LEU:HD12	2.31	0.43
1:D:54:THR:CB	4:D:1771:HOH:O	2.67	0.43
1:F:178:TYR:HE1	1:F:215:LYS:HD2	1.84	0.43
1:H:32:THR:CG2	1:H:119:LYS:HB3	2.40	0.43
1:I:101:LEU:N	1:I:102:PRO:CD	2.82	0.43
1:D:25:ILE:CD1	1:D:93:PHE:HA	2.49	0.42
1:F:443:PRO:O	1:F:444:VAL:HG23	2.19	0.42
1:G:104:LEU:HD21	1:G:108:ILE:HG12	2.01	0.42
1:G:96:PHE:HB3	4:G:1180:HOH:O	2.19	0.42
1:H:101:LEU:N	1:H:102:PRO:CD	2.81	0.42
1:I:15:LYS:CG	4:I:468:HOH:O	2.50	0.42
1:D:389:GLN:O	1:D:390:LEU:HD12	2.19	0.42
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.83	0.42
1:I:159:GLY:CA	1:I:187:TYR:CE2	3.00	0.42
1:C:183:ASN:OD1	1:C:406:ARG:NH1	2.43	0.42
1:D:125:ASP:OD1	1:D:126:LEU:N	2.47	0.42
1:E:184:GLY:HA3	1:E:409:ARG:HG3	2.01	0.42
1:E:55:TRP:CD1	1:I:369:GLY:HA2	2.54	0.42
1:D:9:TYR:CE1	1:D:54:THR:O	2.72	0.42
1:E:25:ILE:HD12	1:E:96:PHE:CE2	2.54	0.42
1:G:48:ALA:O	1:G:53:GLY:N	2.50	0.42
1:G:56:THR:OG1	1:G:57:THR:N	2.47	0.42
1:G:25:ILE:HD13	1:G:93:PHE:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:ARG:HG2	1:H:124:GLU:OE2	2.19	0.42
1:A:184:GLY:CA	1:A:409:ARG:HG3	2.50	0.42
1:B:336:LEU:CD2	1:B:356:PHE:HZ	2.32	0.42
1:D:319:GLY:HA2	4:D:468:HOH:O	2.20	0.42
1:E:101:LEU:N	1:E:102:PRO:CD	2.82	0.42
1:E:119:LYS:HE2	4:E:2010:HOH:O	2.18	0.42
1:E:159:GLY:CA	1:E:187:TYR:CZ	2.97	0.42
1:B:444:VAL:HB	1:G:37:TYR:OH	2.19	0.42
1:H:379:ILE:HD12	1:H:415:ILE:HD12	2.02	0.42
1:A:376:GLN:CB	1:A:377:PRO:CD	2.97	0.42
1:A:161:VAL:HG23	1:A:389:GLN:CG	2.50	0.42
1:B:367:SER:HB2	1:B:389:GLN:HB3	2.00	0.42
1:E:317:THR:O	1:E:318:ALA:C	2.58	0.42
1:E:93:PHE:C	1:E:93:PHE:CD1	2.93	0.42
1:F:298:MET:HB3	1:F:333:PHE:CZ	2.54	0.42
1:H:214:ASP:O	1:H:218:ASN:HB2	2.19	0.42
1:H:70:LEU:HD22	1:H:95:ALA:HA	2.00	0.42
1:J:269:ASP:OD2	4:J:1488:HOH:O	2.21	0.42
1:G:182:SER:C	1:G:183:ASN:HD22	2.23	0.42
1:G:9:TYR:CD1	1:G:45:ALA:HA	2.55	0.42
1:H:158:TYR:CD2	1:H:185:ALA:HA	2.55	0.42
1:H:341:HIS:HB2	4:H:1700:HOH:O	2.20	0.42
1:J:158:TYR:CD1	1:J:408:VAL:HG11	2.55	0.42
1:J:414:ALA:HB1	1:J:419:ILE:O	2.19	0.42
1:A:195:THR:OG1	1:A:196:SER:N	2.52	0.42
1:B:395:LEU:N	1:B:395:LEU:CD1	2.83	0.42
1:E:162:PRO:HA	1:E:395:LEU:HD11	2.02	0.42
1:G:45:ALA:HB2	1:G:117:ARG:HD2	2.00	0.42
1:H:241:LEU:HD12	1:H:270:LEU:HD23	2.02	0.42
1:H:395:LEU:CD2	1:H:395:LEU:N	2.83	0.42
1:H:79:ASP:OD1	1:H:81:GLY:N	2.52	0.42
1:I:209:MET:HG3	1:I:226:TRP:CD2	2.55	0.42
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.49	0.42
1:D:164:PRO:HB3	1:J:52:THR:O	2.19	0.42
1:A:27:ALA:CB	1:A:29:PHE:CE2	3.03	0.42
1:A:46:VAL:HG22	1:A:115:MET:HE3	2.02	0.42
1:C:367:SER:HB2	1:C:389:GLN:HB3	2.02	0.42
1:C:433:ARG:HH11	1:C:433:ARG:CB	2.29	0.42
1:G:159:GLY:HA3	1:G:187:TYR:CD1	2.55	0.42
1:I:303:LYS:NZ	1:I:354:GLN:HE21	2.17	0.42
1:A:72:ALA:HB1	1:A:90:ALA:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:O	1:C:285:HIS:HB3	2.19	0.42
1:D:158:TYR:CE1	1:D:408:VAL:HG11	2.55	0.42
1:E:291:ASN:HA	1:E:292:PRO:HD3	1.81	0.42
1:E:319:GLY:N	1:E:325:GLY:O	2.53	0.42
1:G:143:ILE:HD11	1:G:338:ARG:HG2	2.02	0.42
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.55	0.42
1:G:149:MET:CE	1:G:250:LYS:HB3	2.48	0.41
1:B:329:ILE:HG22	1:B:333:PHE:CZ	2.55	0.41
1:C:197:PRO:HG3	4:C:565:HOH:O	2.19	0.41
1:D:314:HIS:HA	1:D:365:THR:O	2.20	0.41
1:F:108:ILE:HD12	1:F:108:ILE:C	2.40	0.41
1:F:390:LEU:N	1:F:390:LEU:HD12	2.35	0.41
1:G:12:TYR:CD2	1:G:48:ALA:HB2	2.55	0.41
1:H:104:LEU:C	1:H:104:LEU:CD2	2.87	0.41
1:A:52:THR:HG22	1:H:166:VAL:O	2.20	0.41
1:H:334:VAL:CG1	1:H:338:ARG:NE	2.84	0.41
1:J:65:GLU:H	1:J:65:GLU:CD	2.21	0.41
1:B:397:HIS:ND1	1:B:398:PRO:CD	2.78	0.41
1:B:113:PHE:HB2	1:G:286:ALA:HB3	2.01	0.41
1:J:11:TYR:CD2	1:J:11:TYR:C	2.93	0.41
1:J:169:SER:HB2	1:J:170:PRO:CD	2.49	0.41
1:A:128:PHE:H	1:A:354:GLN:NE2	2.14	0.41
1:A:282:ARG:O	1:A:283:ALA:C	2.58	0.41
1:B:115:MET:HA	1:G:323:LEU:HD23	2.03	0.41
1:B:371:HIS:HE1	1:B:373:GLY:HA3	1.83	0.41
1:E:397:HIS:ND1	1:E:398:PRO:CD	2.83	0.41
1:G:230:ILE:O	1:G:237:MET:HG2	2.19	0.41
1:G:433:ARG:NH1	4:G:1446:HOH:O	2.25	0.41
1:A:167:GLY:O	1:H:66:ARG:HD2	2.19	0.41
1:I:9:TYR:O	1:I:11:TYR:N	2.52	0.41
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.56	0.41
1:J:91:TYR:CD2	1:J:91:TYR:N	2.88	0.41
1:A:128:PHE:HA	1:A:129:PRO:HD2	1.97	0.41
1:A:240:ARG:NH1	4:A:467:HOH:O	2.47	0.41
1:B:226:TRP:CH2	1:B:228:ALA:CB	3.04	0.41
1:B:264:LEU:HD23	1:B:308:ILE:HD12	2.02	0.41
1:D:323:LEU:O	1:J:116:LYS:HE3	2.19	0.41
1:E:169:SER:HB2	1:E:170:PRO:HD2	2.03	0.41
1:F:424:TYR:CZ	1:F:428:HIS:CE1	3.08	0.41
1:G:159:GLY:CA	1:G:187:TYR:CE2	3.02	0.41
1:G:12:TYR:OH	1:G:53:GLY:HA2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:LYS:HB2	1:I:119:LYS:HE3	1.78	0.41
1:I:26:ILE:HB	1:I:127:TYR:HB3	2.02	0.41
1:I:93:PHE:C	1:I:93:PHE:CD1	2.93	0.41
1:J:367:SER:HB2	1:J:389:GLN:HB3	2.02	0.41
1:J:414:ALA:HB2	1:J:424:TYR:CG	2.54	0.41
1:A:151:GLU:OE1	1:A:223:LYS:HE2	2.21	0.41
1:D:96:PHE:CE1	1:D:104:LEU:HD12	2.56	0.41
1:G:383:GLY:HA2	4:G:1439:HOH:O	2.20	0.41
1:J:285:HIS:CG	1:J:286:ALA:N	2.88	0.41
1:J:12:TYR:CD2	1:J:48:ALA:HB2	2.56	0.41
1:A:390:LEU:HD12	1:A:390:LEU:N	2.35	0.41
1:C:433:ARG:NH1	1:C:433:ARG:CB	2.83	0.41
1:D:334:VAL:HG21	1:D:382:LEU:HD22	2.03	0.41
1:F:104:LEU:HD23	1:F:108:ILE:HG13	2.02	0.41
1:H:435:LEU:O	1:H:439:GLY:CA	2.69	0.41
1:E:12:TYR:CD2	1:E:48:ALA:HB2	2.56	0.41
1:F:112:ILE:O	1:F:115:MET:HE2	2.21	0.41
1:F:421:LEU:N	1:F:421:LEU:HD12	2.36	0.41
1:G:433:ARG:NH2	4:G:1446:HOH:O	2.50	0.41
1:H:401:PRO:C	1:H:403:ALA:N	2.74	0.41
1:J:163:LYS:H	1:J:395:LEU:HD12	1.85	0.41
1:A:263:ALA:O	1:A:267:ILE:HG12	2.21	0.41
1:B:151:GLU:OE2	1:B:223:LYS:HE2	2.21	0.41
1:E:167:GLY:O	1:I:66:ARG:HD2	2.21	0.41
1:F:101:LEU:N	1:F:102:PRO:CD	2.83	0.41
1:F:433:ARG:HB3	1:F:433:ARG:NH1	2.36	0.41
1:G:101:LEU:N	1:G:102:PRO:CD	2.83	0.41
1:G:108:ILE:HD13	1:G:126:LEU:HD11	2.01	0.41
1:H:159:GLY:HA3	1:H:187:TYR:CG	2.56	0.41
1:H:161:VAL:HG22	1:H:189:KCX:HB2	2.02	0.41
1:H:231:THR:O	1:H:232:ALA:CB	2.68	0.41
1:H:49:GLU:HG3	1:H:115:MET:SD	2.61	0.41
1:I:17:TYR:HE2	1:I:19:PRO:HA	1.85	0.41
1:B:73:LYS:HA	1:B:73:LYS:HD3	1.93	0.41
1:D:101:LEU:HB3	1:D:102:PRO:HD3	2.01	0.41
1:D:79:ASP:HB2	1:D:85:TRP:CZ3	2.56	0.41
1:H:198:TRP:CZ3	1:H:199:TYR:HB3	2.56	0.41
1:H:399:ASP:HB2	1:H:403:ALA:HB2	2.02	0.41
1:H:429:LYS:O	1:H:433:ARG:CB	2.69	0.41
1:A:443:PRO:O	1:A:444:VAL:HG23	2.21	0.41
1:I:424:TYR:CE2	1:I:428:HIS:CE1	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:ALA:O	1:I:442:THR:HG23	2.21	0.41
1:J:169:SER:HB2	1:J:170:PRO:HD2	2.03	0.41
1:J:230:ILE:O	1:J:237:MET:HG2	2.20	0.41
1:J:407:ALA:O	1:J:410:GLN:N	2.54	0.41
1:C:171:GLU:CD	1:C:171:GLU:H	2.24	0.40
1:C:159:GLY:CA	1:C:187:TYR:CE2	3.02	0.40
1:E:317:THR:HG23	1:E:367:SER:O	2.22	0.40
1:F:178:TYR:CE1	1:F:215:LYS:HD3	2.56	0.40
1:H:24:ASP:O	1:H:129:PRO:HG3	2.20	0.40
1:H:54:THR:HG23	1:H:55:TRP:N	2.36	0.40
1:I:376:GLN:N	1:I:377:PRO:CD	2.84	0.40
1:J:390:LEU:N	1:J:390:LEU:HD12	2.36	0.40
1:A:160:VAL:HG21	1:A:394:THR:HG21	2.03	0.40
1:A:428:HIS:HA	4:A:1965:HOH:O	2.22	0.40
1:B:264:LEU:HD23	1:B:308:ILE:HD13	2.03	0.40
1:C:395:LEU:N	1:C:395:LEU:HD12	2.36	0.40
1:D:268:ARG:O	1:D:268:ARG:HD3	2.21	0.40
1:D:162:PRO:HA	1:D:395:LEU:HD11	2.03	0.40
1:G:72:ALA:HB2	1:G:91:TYR:CD1	2.56	0.40
1:A:263:ALA:HB2	1:H:263:ALA:HB2	2.03	0.40
1:C:160:VAL:HG21	1:C:394:THR:HG21	2.03	0.40
1:E:191:ASP:HB3	1:E:193:ASN:ND2	2.35	0.40
1:F:411:ALA:O	1:F:415:ILE:HG13	2.20	0.40
1:B:22:LYS:CD	1:F:65:GLU:HG3	2.51	0.40
1:G:183:ASN:OD1	1:G:406:ARG:NH1	2.51	0.40
1:H:63:GLU:HG2	1:H:66:ARG:H	1.86	0.40
1:I:197:PRO:HB2	1:I:199:TYR:CE2	2.56	0.40
1:I:92:PRO:HB2	1:I:94:HIS:CE1	2.56	0.40
1:J:268:ARG:HD3	1:J:268:ARG:O	2.21	0.40
1:B:414:ALA:O	1:B:418:GLY:N	2.44	0.40
1:C:149:MET:CE	1:C:250:LYS:CB	2.91	0.40
1:E:435:LEU:O	1:E:436:GLU:C	2.59	0.40
1:E:50:SER:O	1:E:107:SER:OG	2.38	0.40
1:F:282:ARG:O	1:F:285:HIS:HB3	2.22	0.40
1:H:321:GLY:HA3	1:H:368:GLY:O	2.22	0.40
1:H:78:HIS:CD2	1:H:349:VAL:HG11	2.56	0.40
1:H:79:ASP:C	1:H:79:ASP:OD1	2.60	0.40
1:I:115:MET:HB2	1:I:115:MET:HE2	1.91	0.40
1:J:174:GLU:OE1	1:J:211:LYS:HE2	2.20	0.40
1:A:331:LEU:HD13	1:A:381:ALA:O	2.22	0.40
1:B:336:LEU:O	1:B:336:LEU:CD2	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PRO:HG3	1:B:75:TYR:CZ	2.56	0.40
1:C:18:GLU:HB2	4:C:612:HOH:O	2.22	0.40
1:E:104:LEU:HD21	1:E:128:PHE:CE1	2.56	0.40
1:F:38:THR:HG1	1:F:41:GLN:HG3	1.86	0.40
1:G:132:LEU:HG	4:G:1820:HOH:O	2.22	0.40
1:G:189:KCX:OQ1	2:G:600:CAP:O3	2.38	0.40
1:E:258:ILE:HD11	1:I:106:ALA:HA	2.04	0.40
1:J:217:GLU:HG2	1:J:222:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/444 (98%)	386 (89%)	40 (9%)	7 (2%)	11	9
1	B	435/444 (98%)	408 (94%)	25 (6%)	2 (0%)	32	37
1	C	437/444 (98%)	420 (96%)	16 (4%)	1 (0%)	51	61
1	D	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	51	61
1	E	437/444 (98%)	410 (94%)	25 (6%)	2 (0%)	32	37
1	F	434/444 (98%)	414 (95%)	19 (4%)	1 (0%)	51	61
1	G	434/444 (98%)	415 (96%)	18 (4%)	1 (0%)	51	61
1	H	435/444 (98%)	389 (89%)	39 (9%)	7 (2%)	11	9
1	I	435/444 (98%)	415 (95%)	18 (4%)	2 (0%)	32	37
1	J	435/444 (98%)	414 (95%)	20 (5%)	1 (0%)	51	61
All	All	4349/4440 (98%)	4086 (94%)	238 (6%)	25 (1%)	28	32

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	426	LYS
1	B	429	LYS
1	A	34	ALA
1	A	82	ASP
1	A	117	ARG
1	D	284	MET
1	E	420	PRO
1	H	232	ALA
1	H	443	PRO
1	A	286	ALA
1	E	436	GLU
1	H	318	ALA
1	H	420	PRO
1	I	10	ASP
1	C	327	ARG
1	G	284	MET
1	J	284	MET
1	A	51	SER
1	B	420	PRO
1	H	325	GLY
1	A	325	GLY
1	F	325	GLY
1	H	401	PRO
1	I	8	ILE
1	A	344	PRO

5.3.2 Protein sidechains [i](#)

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	321/356 (90%)	313 (98%)	8 (2%)	53	66
1	B	331/356 (93%)	322 (97%)	9 (3%)	50	63
1	C	336/356 (94%)	327 (97%)	9 (3%)	50	63
1	D	339/356 (95%)	333 (98%)	6 (2%)	64	76
1	E	335/356 (94%)	329 (98%)	6 (2%)	64	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	338/356 (95%)	329 (97%)	9 (3%)	50	63
1	G	340/356 (96%)	333 (98%)	7 (2%)	59	72
1	H	329/356 (92%)	322 (98%)	7 (2%)	59	72
1	I	336/356 (94%)	331 (98%)	5 (2%)	70	81
1	J	337/356 (95%)	333 (99%)	4 (1%)	75	86
All	All	3342/3560 (94%)	3272 (98%)	70 (2%)	59	72

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	PHE
1	A	85	TRP
1	A	183	ASN
1	A	235	LEU
1	A	268	ARG
1	A	324	GLU
1	A	363	PHE
1	A	389	GLN
1	B	122	ARG
1	B	154	ASP
1	B	268	ARG
1	B	336	LEU
1	B	347	ASN
1	B	352	LEU
1	B	363	PHE
1	B	376	GLN
1	B	389	GLN
1	C	73	LYS
1	C	191	ASP
1	C	207	GLU
1	C	235	LEU
1	C	268	ARG
1	C	322	LYS
1	C	363	PHE
1	C	389	GLN
1	C	433	ARG
1	D	10	ASP
1	D	122	ARG
1	D	268	ARG
1	D	347	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	363	PHE
1	D	426	LYS
1	E	73	LYS
1	E	122	ARG
1	E	193	ASN
1	E	235	LEU
1	E	363	PHE
1	E	389	GLN
1	F	87	VAL
1	F	122	ARG
1	F	181	LEU
1	F	235	LEU
1	F	328	ASP
1	F	347	ASN
1	F	363	PHE
1	F	389	GLN
1	F	433	ARG
1	G	122	ARG
1	G	268	ARG
1	G	336	LEU
1	G	347	ASN
1	G	363	PHE
1	G	389	GLN
1	G	422	ASP
1	H	7	THR
1	H	235	LEU
1	H	336	LEU
1	H	363	PHE
1	H	389	GLN
1	H	406	ARG
1	H	419	ILE
1	I	73	LYS
1	I	122	ARG
1	I	149	MET
1	I	268	ARG
1	I	363	PHE
1	J	122	ARG
1	J	268	ARG
1	J	363	PHE
1	J	389	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	183	ASN
1	A	312	GLN
1	A	354	GLN
1	A	417	GLN
1	B	183	ASN
1	B	312	GLN
1	B	347	ASN
1	B	354	GLN
1	B	376	GLN
1	C	312	GLN
1	C	354	GLN
1	C	376	GLN
1	C	410	GLN
1	C	440	HIS
1	D	312	GLN
1	D	347	ASN
1	D	354	GLN
1	D	417	GLN
1	D	440	HIS
1	E	193	ASN
1	E	239	GLN
1	E	312	GLN
1	E	314	HIS
1	E	354	GLN
1	E	410	GLN
1	F	64	GLN
1	F	239	GLN
1	F	312	GLN
1	F	347	ASN
1	F	354	GLN
1	G	239	GLN
1	G	312	GLN
1	G	347	ASN
1	G	354	GLN
1	G	417	GLN
1	G	440	HIS
1	H	78	HIS
1	H	312	GLN
1	H	354	GLN
1	H	410	GLN
1	H	440	HIS
1	I	218	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	239	GLN
1	I	285	HIS
1	I	312	GLN
1	I	354	GLN
1	I	376	GLN
1	I	410	GLN
1	J	64	GLN
1	J	239	GLN
1	J	312	GLN
1	J	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	189	1,3	8,11,12	0.92	0	6,12,14	1.47	1 (16%)
1	KCX	B	189	1,3	8,11,12	0.95	0	6,12,14	1.40	1 (16%)
1	KCX	C	189	1,3	8,11,12	1.06	1 (12%)	6,12,14	1.18	1 (16%)
1	KCX	D	189	1,3	8,11,12	0.99	1 (12%)	6,12,14	1.23	1 (16%)
1	KCX	E	189	1,3	8,11,12	1.06	1 (12%)	6,12,14	1.38	1 (16%)
1	KCX	F	189	1,3	8,11,12	0.94	1 (12%)	6,12,14	1.42	1 (16%)
1	KCX	G	189	1,3	8,11,12	1.02	1 (12%)	6,12,14	1.08	0
1	KCX	H	189	1,3	8,11,12	0.96	0	6,12,14	1.38	1 (16%)
1	KCX	I	189	1,3	8,11,12	1.03	1 (12%)	6,12,14	1.22	1 (16%)
1	KCX	J	189	1,3	8,11,12	0.97	1 (12%)	6,12,14	1.43	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	C	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	D	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	F	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	G	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	H	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	I	189	1,3	-	0/6/10/12	0/0/0/0
1	KCX	J	189	1,3	-	0/6/10/12	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	189	KCX	CA-C	2.02	1.52	1.50
1	F	189	KCX	CA-C	2.03	1.52	1.50
1	I	189	KCX	CA-C	2.06	1.53	1.50
1	G	189	KCX	CA-C	2.08	1.53	1.50
1	D	189	KCX	CA-C	2.13	1.53	1.50
1	C	189	KCX	CA-C	2.25	1.53	1.50
1	E	189	KCX	CA-C	2.28	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	KCX	CE-NZ-CX	-2.93	119.76	123.35
1	F	189	KCX	CE-NZ-CX	-2.86	119.85	123.35
1	B	189	KCX	CE-NZ-CX	-2.82	119.89	123.35
1	E	189	KCX	CE-NZ-CX	-2.71	120.03	123.35
1	J	189	KCX	CE-NZ-CX	-2.71	120.04	123.35
1	H	189	KCX	CE-NZ-CX	-2.62	120.14	123.35
1	D	189	KCX	CE-NZ-CX	-2.24	120.61	123.35
1	I	189	KCX	CE-NZ-CX	-2.13	120.74	123.35
1	C	189	KCX	CE-NZ-CX	-2.05	120.83	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	189	KCX	1	0
1	H	189	KCX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CAP	A	600	3	14,20,20	0.76	0	17,31,31	0.80	0
2	CAP	B	600	3	14,20,20	0.73	0	17,31,31	0.74	0
2	CAP	C	600	3	14,20,20	0.73	0	17,31,31	0.71	0
2	CAP	D	600	3	14,20,20	0.76	0	17,31,31	0.73	0
2	CAP	E	600	3	14,20,20	0.74	0	17,31,31	0.72	0
2	CAP	F	600	3	14,20,20	0.73	0	17,31,31	0.77	0
2	CAP	G	600	3	14,20,20	0.72	0	17,31,31	0.78	0
2	CAP	H	600	3	14,20,20	0.74	0	17,31,31	0.70	0
2	CAP	I	600	3	14,20,20	0.74	0	17,31,31	0.80	0
2	CAP	J	600	3	14,20,20	0.73	0	17,31,31	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	A	600	3	-	0/23/29/29	0/0/0/0
2	CAP	B	600	3	-	0/23/29/29	0/0/0/0
2	CAP	C	600	3	-	0/23/29/29	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAP	D	600	3	-	0/23/29/29	0/0/0/0
2	CAP	E	600	3	-	0/23/29/29	0/0/0/0
2	CAP	F	600	3	-	0/23/29/29	0/0/0/0
2	CAP	G	600	3	-	0/23/29/29	0/0/0/0
2	CAP	H	600	3	-	0/23/29/29	0/0/0/0
2	CAP	I	600	3	-	0/23/29/29	0/0/0/0
2	CAP	J	600	3	-	0/23/29/29	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	CAP	1	0
2	C	600	CAP	1	0
2	E	600	CAP	2	0
2	G	600	CAP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	435/444 (97%)	0.83	43 (9%) 8 12	28, 41, 56, 60	0
1	B	437/444 (98%)	0.50	35 (8%) 13 19	19, 32, 62, 65	0
1	C	439/444 (98%)	0.27	16 (3%) 43 55	17, 27, 49, 52	0
1	D	436/444 (98%)	0.10	10 (2%) 61 71	16, 24, 35, 42	0
1	E	439/444 (98%)	0.46	42 (9%) 9 13	18, 28, 58, 60	0
1	F	436/444 (98%)	0.32	20 (4%) 33 45	18, 29, 45, 51	0
1	G	436/444 (98%)	0.26	9 (2%) 64 74	18, 31, 44, 48	0
1	H	437/444 (98%)	0.79	50 (11%) 6 9	27, 37, 66, 66	0
1	I	437/444 (98%)	0.22	22 (5%) 30 41	17, 28, 47, 53	0
1	J	437/444 (98%)	0.38	35 (8%) 13 19	16, 25, 59, 60	0
All	All	4369/4440 (98%)	0.41	282 (6%) 20 27	16, 30, 52, 66	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	444	VAL	7.3
1	J	434	ALA	6.5
1	E	441	VAL	6.3
1	E	425	ALA	6.2
1	E	415	ILE	6.2
1	J	421	LEU	5.7
1	J	425	ALA	5.7
1	E	418	GLY	5.7
1	B	421	LEU	5.6
1	E	434	ALA	5.5
1	E	421	LEU	5.5
1	A	59	TYR	5.1
1	E	398	PRO	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	441	VAL	4.9
1	A	54	THR	4.8
1	H	421	LEU	4.8
1	H	426	LYS	4.7
1	J	424	TYR	4.6
1	H	441	VAL	4.6
1	D	59	TYR	4.6
1	B	424	TYR	4.4
1	I	57	THR	4.3
1	E	377	PRO	4.3
1	I	434	ALA	4.3
1	C	5	PHE	4.2
1	F	59	TYR	4.2
1	A	85	TRP	4.1
1	E	414	ALA	4.1
1	G	59	TYR	4.1
1	J	7	THR	4.1
1	B	59	TYR	4.0
1	H	425	ALA	4.0
1	A	36	GLY	4.0
1	A	13	VAL	4.0
1	H	434	ALA	4.0
1	I	59	TYR	3.9
1	E	433	ARG	3.9
1	H	36	GLY	3.9
1	J	381	ALA	3.9
1	J	427	THR	3.8
1	H	398	PRO	3.8
1	I	425	ALA	3.8
1	J	414	ALA	3.8
1	H	8	ILE	3.8
1	G	57	THR	3.8
1	I	421	LEU	3.8
1	E	426	LYS	3.8
1	E	424	TYR	3.8
1	B	419	ILE	3.7
1	C	7	THR	3.7
1	E	427	THR	3.7
1	F	427	THR	3.6
1	A	58	LEU	3.6
1	H	85	TRP	3.6
1	H	422	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	422	ASP	3.6
1	E	5	PHE	3.5
1	J	422	ASP	3.4
1	E	7	THR	3.4
1	H	396	GLY	3.4
1	I	10	ASP	3.4
1	D	54	THR	3.4
1	A	414	ALA	3.4
1	C	421	LEU	3.4
1	J	420	PRO	3.4
1	H	414	ALA	3.4
1	H	431	LEU	3.4
1	J	426	LYS	3.3
1	C	441	VAL	3.3
1	J	398	PRO	3.3
1	F	426	LYS	3.3
1	E	387	VAL	3.3
1	F	421	LEU	3.2
1	I	58	LEU	3.2
1	E	396	GLY	3.2
1	E	218	ASN	3.2
1	E	420	PRO	3.2
1	D	58	LEU	3.2
1	D	9	TYR	3.2
1	I	9	TYR	3.2
1	A	57	THR	3.2
1	C	6	ASP	3.2
1	B	398	PRO	3.1
1	A	78	HIS	3.1
1	A	11	TYR	3.1
1	C	425	ALA	3.1
1	J	415	ILE	3.1
1	J	377	PRO	3.1
1	J	387	VAL	3.1
1	H	435	LEU	3.1
1	F	418	GLY	3.1
1	E	432	ALA	3.1
1	B	435	LEU	3.0
1	E	59	TYR	3.0
1	B	417	GLN	3.0
1	C	420	PRO	3.0
1	J	418	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	418	GLY	3.0
1	A	37	TYR	2.9
1	J	396	GLY	2.9
1	A	56	THR	2.9
1	B	427	THR	2.9
1	H	373	GLY	2.9
1	B	8	ILE	2.9
1	H	7	THR	2.9
1	J	433	ARG	2.9
1	J	161	VAL	2.9
1	F	425	ALA	2.9
1	I	8	ILE	2.8
1	I	427	THR	2.8
1	H	283	ALA	2.8
1	B	373	GLY	2.8
1	J	439	GLY	2.8
1	B	422	ASP	2.8
1	B	160	VAL	2.8
1	G	65	GLU	2.8
1	H	418	GLY	2.8
1	E	6	ASP	2.8
1	H	274	TYR	2.8
1	H	293	TYR	2.8
1	H	438	TRP	2.8
1	E	444	VAL	2.8
1	F	420	PRO	2.8
1	H	432	ALA	2.7
1	C	434	ALA	2.7
1	H	35	GLU	2.7
1	J	444	VAL	2.7
1	A	35	GLU	2.7
1	A	43	ALA	2.7
1	B	418	GLY	2.7
1	B	439	GLY	2.7
1	H	379	ILE	2.7
1	A	29	PHE	2.7
1	B	218	ASN	2.7
1	A	40	GLU	2.7
1	C	35	GLU	2.7
1	B	438	TRP	2.7
1	H	424	TYR	2.7
1	H	420	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	419	ILE	2.6
1	A	16	GLY	2.6
1	A	426	LYS	2.6
1	C	426	LYS	2.6
1	E	392	GLY	2.6
1	J	373	GLY	2.6
1	B	161	VAL	2.6
1	I	426	LYS	2.6
1	D	400	GLY	2.6
1	A	115	MET	2.6
1	F	36	GLY	2.6
1	F	218	ASN	2.6
1	I	436	GLU	2.6
1	B	415	ILE	2.6
1	A	427	THR	2.5
1	J	438	TRP	2.5
1	A	87	VAL	2.5
1	J	441	VAL	2.5
1	J	59	TYR	2.5
1	A	50	SER	2.5
1	E	412	ILE	2.5
1	H	419	ILE	2.5
1	I	422	ASP	2.5
1	G	218	ASN	2.5
1	A	318	ALA	2.5
1	B	65	GLU	2.5
1	E	438	TRP	2.5
1	A	109	ALA	2.5
1	G	60	PRO	2.5
1	B	431	LEU	2.5
1	F	347	ASN	2.5
1	I	53	GLY	2.5
1	C	414	ALA	2.5
1	H	296	ILE	2.5
1	I	419	ILE	2.5
1	A	376	GLN	2.5
1	A	417	GLN	2.5
1	D	347	ASN	2.4
1	E	374	ASN	2.4
1	E	442	THR	2.4
1	H	319	GLY	2.4
1	A	106	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	351	HIS	2.4
1	H	443	PRO	2.4
1	H	284	MET	2.4
1	J	442	THR	2.4
1	E	416	MET	2.4
1	H	287	ALA	2.4
1	I	54	THR	2.4
1	A	347	ASN	2.4
1	E	388	LEU	2.4
1	B	377	PRO	2.4
1	B	425	ALA	2.4
1	B	434	ALA	2.4
1	H	345	ASP	2.4
1	H	439	GLY	2.4
1	C	427	THR	2.4
1	I	218	ASN	2.4
1	B	426	LYS	2.4
1	G	17	TYR	2.4
1	B	313	LEU	2.4
1	F	434	ALA	2.4
1	D	8	ILE	2.3
1	F	35	GLU	2.3
1	A	31	VAL	2.3
1	I	439	GLY	2.3
1	A	388	LEU	2.3
1	J	435	LEU	2.3
1	A	345	ASP	2.3
1	H	58	LEU	2.3
1	E	436	GLU	2.3
1	B	440	HIS	2.3
1	J	227	PHE	2.3
1	F	436	GLU	2.3
1	H	59	TYR	2.3
1	A	110	GLY	2.3
1	B	7	THR	2.2
1	H	323	LEU	2.2
1	E	321	GLY	2.2
1	B	387	VAL	2.2
1	A	283	ALA	2.2
1	H	286	ALA	2.2
1	A	352	LEU	2.2
1	F	343	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	36	GLY	2.2
1	C	287	ALA	2.2
1	D	57	THR	2.2
1	B	388	LEU	2.2
1	F	422	ASP	2.2
1	H	397	HIS	2.2
1	I	387	VAL	2.2
1	A	284	MET	2.2
1	A	441	VAL	2.2
1	G	161	VAL	2.2
1	C	419	ILE	2.2
1	H	437	LYS	2.2
1	H	273	ASP	2.2
1	H	318	ALA	2.2
1	J	428	HIS	2.2
1	J	8	ILE	2.2
1	H	106	ALA	2.1
1	F	376	GLN	2.1
1	E	161	VAL	2.1
1	E	257	VAL	2.1
1	B	399	ASP	2.1
1	E	153	LYS	2.1
1	I	328	ASP	2.1
1	A	274	TYR	2.1
1	B	36	GLY	2.1
1	C	436	GLU	2.1
1	E	319	GLY	2.1
1	E	148	LYS	2.1
1	A	420	PRO	2.1
1	I	60	PRO	2.1
1	I	221	GLY	2.1
1	H	375	ILE	2.1
1	D	56	THR	2.1
1	F	85	TRP	2.1
1	H	34	ALA	2.1
1	J	218	ASN	2.1
1	H	378	VAL	2.1
1	B	159	GLY	2.1
1	H	81	GLY	2.1
1	B	347	ASN	2.1
1	A	17	TYR	2.1
1	D	60	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	281	HIS	2.0
1	G	153	LYS	2.0
1	F	54	THR	2.0
1	E	378	VAL	2.0
1	J	257	VAL	2.0
1	E	371	HIS	2.0
1	B	390	LEU	2.0
1	J	388	LEU	2.0
1	E	373	GLY	2.0
1	F	110	GLY	2.0
1	J	36	GLY	2.0
1	A	75	TYR	2.0
1	G	35	GLU	2.0
1	J	419	ILE	2.0
1	F	16	GLY	2.0
1	H	410	GLN	2.0
1	E	437	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	KCX	E	189	12/13	0.97	0.21	-	22,23,24,24	0
1	KCX	A	189	12/13	0.97	0.22	-	33,33,33,34	0
1	KCX	G	189	12/13	0.98	0.21	-	21,21,22,23	0
1	KCX	C	189	12/13	0.96	0.20	-	24,24,24,24	0
1	KCX	J	189	12/13	0.97	0.23	-	22,23,23,24	0
1	KCX	H	189	12/13	0.96	0.19	-	35,36,37,37	0
1	KCX	F	189	12/13	0.98	0.20	-	22,22,22,22	0
1	KCX	D	189	12/13	0.98	0.20	-	16,18,19,19	0
1	KCX	B	189	12/13	0.97	0.23	-	30,31,32,33	0
1	KCX	I	189	12/13	0.97	0.19	-	24,25,26,26	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	CAP	E	600	21/21	0.92	0.24	0.98	31,37,40,41	0
3	MG	E	500	1/1	0.98	0.23	0.53	26,26,26,26	0
2	CAP	J	600	21/21	0.95	0.21	0.18	31,35,38,38	0
2	CAP	H	600	21/21	0.89	0.22	-0.12	41,42,42,43	0
2	CAP	C	600	21/21	0.97	0.18	-0.18	30,31,32,32	0
2	CAP	G	600	21/21	0.98	0.17	-0.52	22,25,26,26	0
2	CAP	D	600	21/21	0.98	0.13	-0.60	16,20,21,21	0
2	CAP	A	600	21/21	0.94	0.17	-1.01	36,38,38,39	0
2	CAP	B	600	21/21	0.97	0.16	-1.19	31,35,36,37	0
2	CAP	F	600	21/21	0.98	0.12	-1.49	22,24,24,25	0
2	CAP	I	600	21/21	0.98	0.10	-1.82	18,21,21,22	0
3	MG	C	500	1/1	0.94	0.16	-2.32	28,28,28,28	0
3	MG	J	500	1/1	0.99	0.13	-2.44	19,19,19,19	0
3	MG	H	500	1/1	0.94	0.16	-3.22	37,37,37,37	0
3	MG	I	500	1/1	0.94	0.10	-3.50	20,20,20,20	0
3	MG	B	500	1/1	0.93	0.10	-4.36	31,31,31,31	0
3	MG	G	500	1/1	0.97	0.09	-5.58	20,20,20,20	0
3	MG	A	500	1/1	0.98	0.13	-5.77	28,28,28,28	0
3	MG	D	500	1/1	0.99	0.08	-7.37	15,15,15,15	0
3	MG	F	500	1/1	0.99	0.10	-8.00	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.