



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:28 PM GMT

PDB ID : 4XYK
Title : Crystal structure of human phosphofructokinase-1 in complex with ADP, Northeast Structural Genomics Consortium Target HR9275
Authors : Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2015-02-02
Resolution : 3.40 Å(reported)

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

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

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

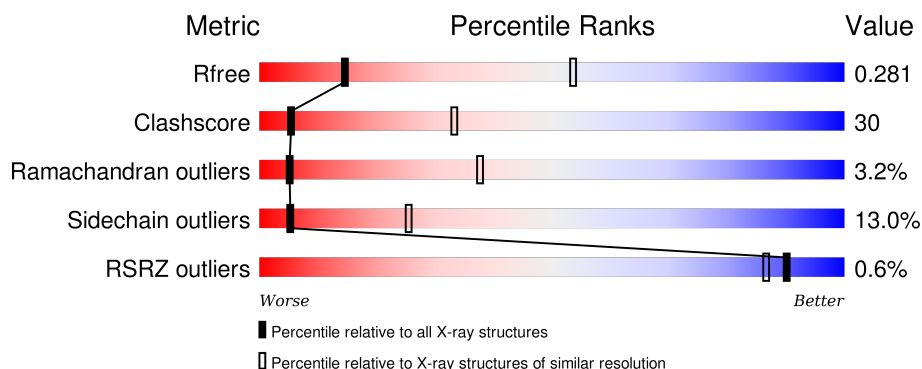
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	812	 40% 43% 7% • 9%
1	B	812	 41% 43% 7% • 8%
1	C	812	 40% 43% 8% 8%
1	D	812	 43% 41% 8% 8%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	803	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22897 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5640	3542	1000	1059	39			
1	B	749	Total	C	N	O	S	0	0	0
			5727	3595	1019	1074	39			
1	C	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			
1	D	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

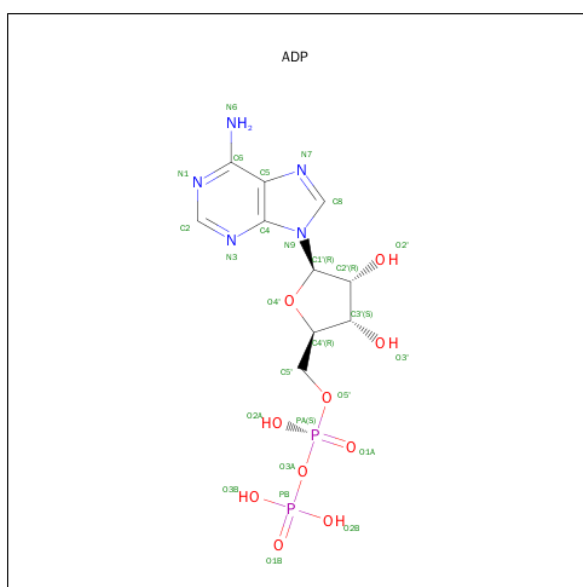
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

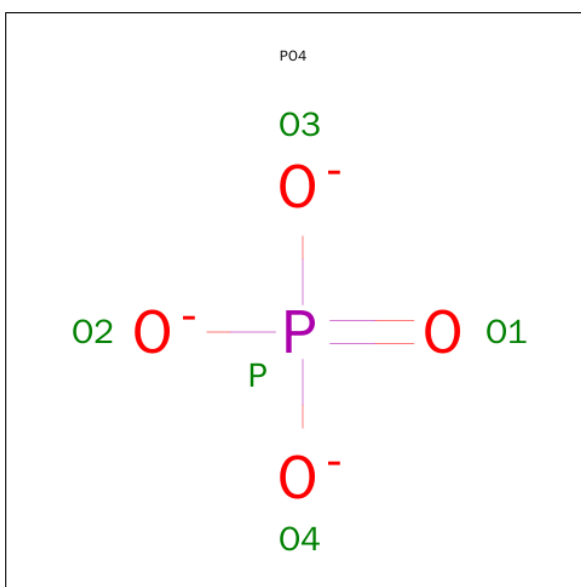
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

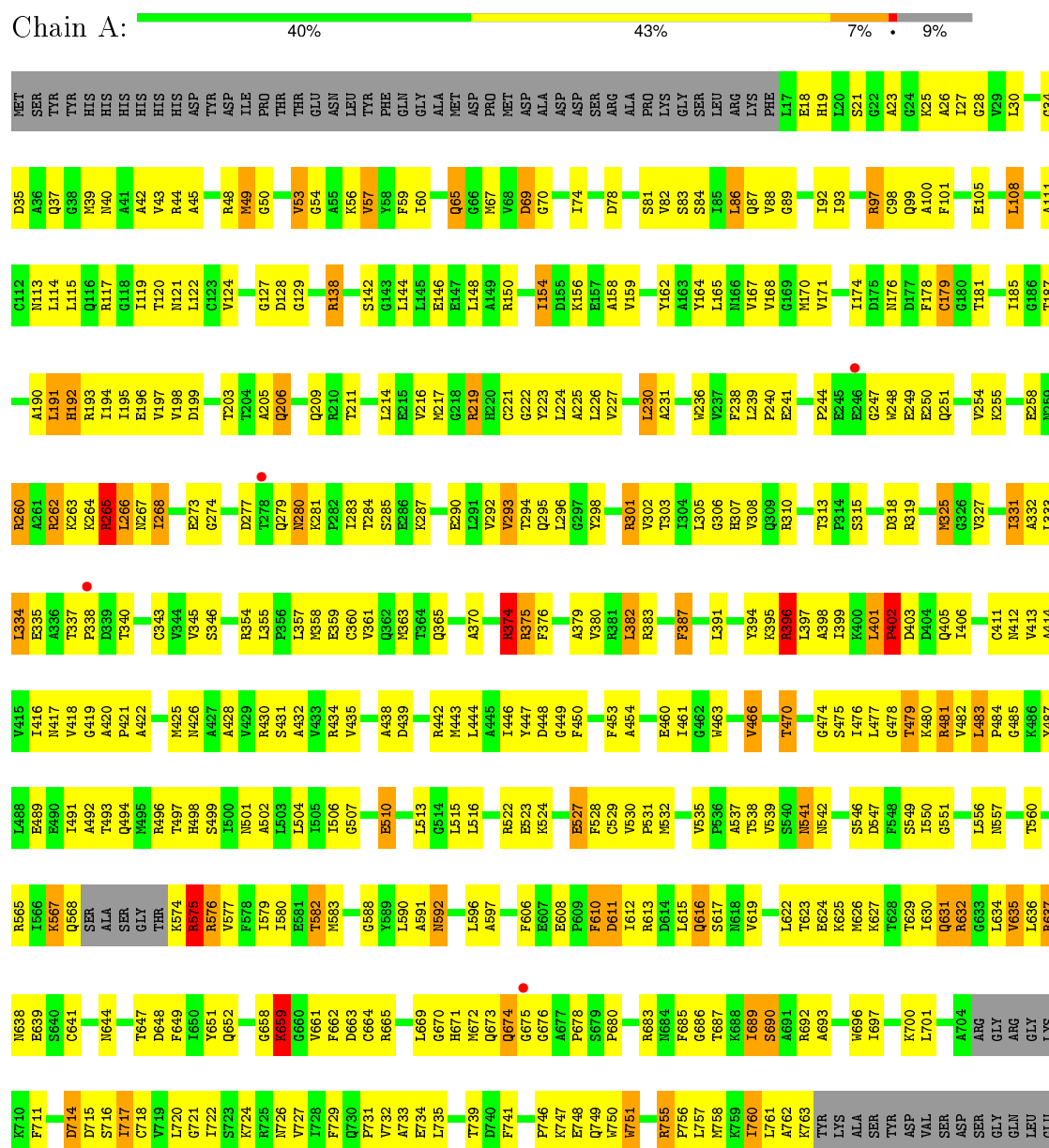


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

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

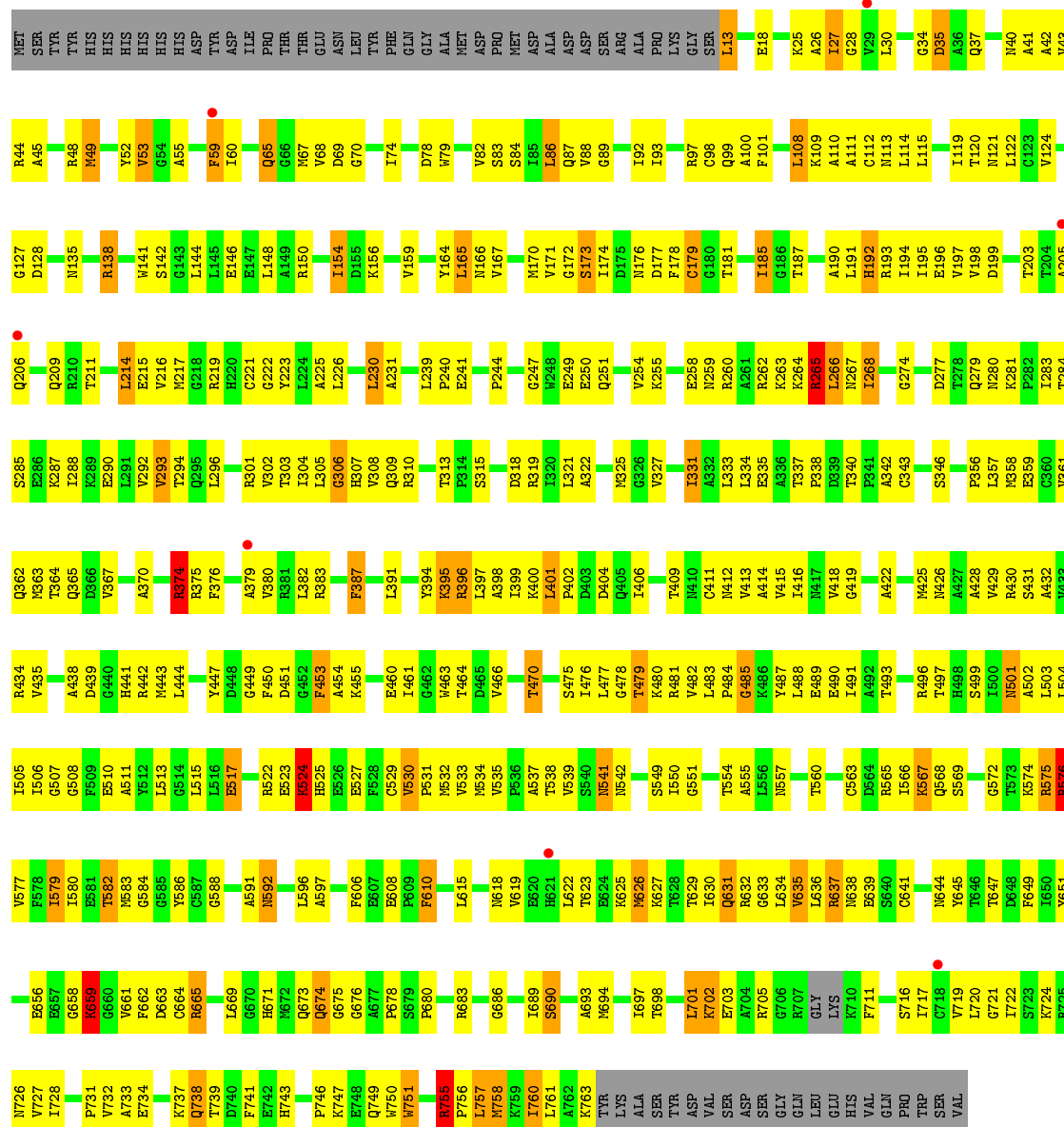
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



HIS
VAL
GLN
PRO
TRP
SER
VAL

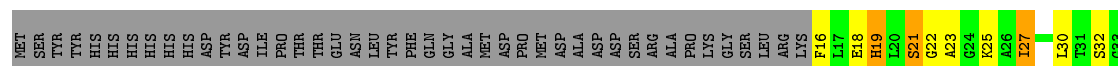
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain B: 41% 43% 7% 8%



• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain C: 40% 43% 8% 8%



V732	A733	E734	L735	K736	K737	Q738	I739	D740		H743		P746	K747	E748	Q749	W750	W751	L752		R755	P756	L757	W758	K759	I760	L761	A762	K763	TYR	LVS	ALA	SFR	TYR	ASP	VAL	GLY	SER	ASP	SER	GLY	GLN	LEU	GLU	HIS	VAL	GLN	PRO	TRP	SER	SER	VAL																
R665	L669	G670	H671	M672	Q673	Q674	G675	G676	G677	P678	S679	P680		R683	M684	P685	G686	T687	H688	L689	S690		M694	E695	H696	I697	K625	K626	K700	L701	K702		R705	GLY	ARG	GLY	GLY	LVS	LVS	F711	T712	T713	D714	D715	S716	I717	C718	V719	L720	G721	I722	S655	W723	K724	R725	N726	V727	I728	F729	Q730	P731						
I580	E581	T582	M583		Y586	C587	G588		A591	N592	L515	L516	E517	L518	S519	A520	A521		H525	E526	E527	F528	C529	V530	P531	H532	V533	M534	V535	P536	A537	T538	I539	Q540	N541		P544	G545	S546	D547	F548	S549	L550		N557		T560		R565		S566	K567	Q568		G572		R575	A576	V577	F578	C564						
L503	L504	I505	I506	G507		E510	A511	Y512		L515	L516	E517	L518	S519	A520	A521		H525	E526	E527	F528	C529	V530	P531	H532	V533	M534	V535	P536	A537	T538	I539	Q540	N541		P544	G545	S546	D547	F548	S549	L550		N557		T560		R565		S566	K567	Q568		G572		R575	A576	V577	F578	C564							
R430	S431		R434	V435		D439		R442	M443	L444		Y447	D448	G449	F450		F453	A454		I458	K459	G460	R461	S462	M463	T464	D465	V466		T470		G474	S475	I476	K400	L401	G477	P402	D403		K480	R481	V482	L483	P484	G485	K486	Y487	L488	E489	E490	I491	V418	A492		M495	R496	T497	H498	S499	I500	M501	A502				
T278	Q279	N280	K281		P282	L283	T284	S285	E286	K287		E290	L291	V292	V293	T294		Q295	L296	G297	Y298		R301	V302	T303	I304	L305	G306	H307	V308	Q309	R310		S315		D318	R319	I320		M325	G326	V327		I331	A332	L333	L334		T337	P338	D339	T340		C343	V344	V345	S346		H351		R354						
L355		M358		C360		K363	T364	Q365		A370			R374	R375	F376		A379	V380	R381	L382	R383			G384	R385	S386	F387		N390		Y394	K395	R396	L397	A398	I399	K400	L401	P402	D403		P404	Q405	L406		C411	N412	V413	A414		V415	I416	N417	D418	V418	A419	A420		P421	R422	A423	G424	M425	N426		V429	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.34Å 168.37Å 133.27Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	45.37 – 3.40 45.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	74.2 (45.37-3.40) 84.5 (45.37-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.256 , 0.290 0.269 , 0.281	Depositor DCC
R_{free} test set	3943 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 14.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 39429 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22897	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.57	1/5730 (0.0%)	0.75	15/7735 (0.2%)
1	B	0.55	0/5819	0.85	18/7854 (0.2%)
1	C	0.54	1/5773 (0.0%)	0.81	16/7795 (0.2%)
1	D	0.53	0/5773	0.89	16/7795 (0.2%)
All	All	0.55	2/23095 (0.0%)	0.83	65/31179 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	664	CYS	CB-SG	-6.17	1.71	1.82
1	A	360	CYS	CB-SG	-5.68	1.72	1.81

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-22.12	109.24	120.30
1	D	374	ARG	NE-CZ-NH1	-21.17	109.71	120.30
1	D	374	ARG	NE-CZ-NH2	21.17	130.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	ARG	NE-CZ-NH1	-20.40	110.10	120.30
1	C	97	ARG	NE-CZ-NH1	19.91	130.25	120.30
1	D	375	ARG	NE-CZ-NH2	-17.76	111.42	120.30
1	B	575	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	B	665	ARG	NE-CZ-NH2	17.37	128.98	120.30
1	D	575	ARG	NE-CZ-NH1	16.50	128.55	120.30
1	D	375	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	B	576	ARG	NE-CZ-NH1	-16.29	112.16	120.30
1	D	150	ARG	NE-CZ-NH2	16.24	128.42	120.30
1	B	575	ARG	NE-CZ-NH2	-15.79	112.40	120.30
1	B	576	ARG	NE-CZ-NH2	15.54	128.07	120.30
1	D	575	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	C	575	ARG	NE-CZ-NH2	13.23	126.91	120.30
1	D	150	ARG	NE-CZ-NH1	-12.67	113.97	120.30
1	C	575	ARG	NE-CZ-NH1	-11.81	114.40	120.30
1	D	374	ARG	CD-NE-CZ	10.69	138.56	123.60
1	C	665	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	B	374	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	C	97	ARG	CD-NE-CZ	9.45	136.83	123.60
1	A	575	ARG	NE-CZ-NH2	8.97	124.78	120.30
1	B	665	ARG	CD-NE-CZ	8.62	135.67	123.60
1	A	665	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	D	665	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	C	375	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	D	665	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	575	ARG	CD-NE-CZ	8.00	134.79	123.60
1	C	374	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	374	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	150	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	D	150	ARG	CD-NE-CZ	7.87	134.62	123.60
1	D	375	ARG	CD-NE-CZ	7.82	134.55	123.60
1	A	576	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	D	575	ARG	CD-NE-CZ	7.67	134.34	123.60
1	C	375	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	C	665	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	375	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	C	575	ARG	CD-NE-CZ	7.25	133.75	123.60
1	A	575	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	575	ARG	CD-NE-CZ	7.18	133.66	123.60
1	C	374	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	375	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	B	375	ARG	NE-CZ-NH2	7.03	123.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	ARG	CD-NE-CZ	6.93	133.31	123.60
1	C	150	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	97	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	665	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	374	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	150	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	576	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	576	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	374	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	97	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	97	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	B	97	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	150	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	150	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	150	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	744	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	D	97	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	375	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	C	576	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	579	ILE	CG1-CB-CG2	-5.02	100.35	111.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	692	ARG	Sidechain
1	B	219	ARG	Sidechain
1	B	396	ARG	Sidechain
1	B	565	ARG	Sidechain
1	B	755	ARG	Sidechain
1	C	260	ARG	Sidechain
1	C	265	ARG	Sidechain
1	C	44	ARG	Sidechain
1	C	632	ARG	Sidechain
1	D	138	ARG	Sidechain
1	D	265	ARG	Sidechain

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	5640	0	5674	340	0
1	B	5727	0	5764	340	0
1	C	5681	0	5709	358	0
1	D	5681	0	5709	376	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	20	0	0	1	0
3	D	15	0	0	1	0
All	All	22897	0	22904	1376	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 30.

All (1376) 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:D:480:LYS:HB3	1:D:482:VAL:HG23	1.29	1.05
1:B:522:ARG:HH12	1:B:529:CYS:HA	1.25	1.00
1:D:532:MET:HB2	1:D:717:ILE:HG22	1.41	1.00
1:A:539:VAL:HG11	1:A:674:GLN:HB3	1.43	0.99
1:A:121:ASN:HB3	1:A:333:LEU:HD22	1.46	0.97
1:C:121:ASN:HB3	1:C:333:LEU:HD22	1.45	0.95
1:C:44:ARG:NH1	1:C:761:LEU:HD22	1.81	0.95
1:D:327:VAL:HG21	1:D:757:LEU:HD21	1.47	0.93
1:D:30:LEU:HD21	1:D:124:VAL:HG22	1.51	0.92
1:B:30:LEU:HD21	1:B:124:VAL:HG22	1.50	0.91
1:A:181:THR:HB	1:A:346:SER:HB2	1.53	0.91
1:B:588:GLY:HA2	1:B:638:ASN:HD22	1.36	0.90
1:A:284:THR:HG23	1:A:287:LYS:H	1.32	0.90
1:C:588:GLY:HA2	1:C:638:ASN:HD22	1.37	0.90
1:D:630:ILE:HD12	1:D:630:ILE:H	1.36	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:HB3	1:B:333:LEU:HD22	1.53	0.89
1:B:630:ILE:H	1:B:630:ILE:HD12	1.37	0.89
1:D:516:LEU:HD21	1:D:736:LYS:HE2	1.54	0.89
1:A:219:ARG:HG3	1:A:273:GLU:OE1	1.72	0.88
1:C:539:VAL:HG11	1:C:674:GLN:HB3	1.56	0.88
1:A:496:ARG:HB3	1:A:527:GLU:HG3	1.53	0.88
1:D:44:ARG:HH11	1:D:44:ARG:HG3	1.38	0.87
1:A:678:PRO:HG2	1:A:683:ARG:HD3	1.57	0.87
1:C:630:ILE:HD12	1:C:630:ILE:H	1.39	0.86
1:B:284:THR:HG23	1:B:287:LYS:H	1.37	0.86
1:D:181:THR:HB	1:D:346:SER:HB2	1.54	0.86
1:D:678:PRO:HG2	1:D:683:ARG:HD3	1.55	0.86
1:D:488:LEU:H	1:D:488:LEU:HD23	1.40	0.85
1:C:534:MET:HG2	1:C:719:VAL:HG22	1.56	0.85
1:B:522:ARG:NH1	1:B:529:CYS:HA	1.91	0.84
1:C:30:LEU:HD21	1:C:124:VAL:HG22	1.59	0.84
1:C:284:THR:HG23	1:C:287:LYS:H	1.40	0.84
1:A:30:LEU:HD21	1:A:124:VAL:HG22	1.59	0.84
1:B:262:ARG:HH22	1:B:400:LYS:HD3	1.42	0.84
1:C:181:THR:HB	1:C:346:SER:HB2	1.58	0.84
1:A:480:LYS:HB3	1:A:482:VAL:HG23	1.57	0.83
1:B:539:VAL:HG11	1:B:674:GLN:HB3	1.60	0.82
1:B:669:LEU:HB3	1:B:673:GLN:HE21	1.44	0.82
1:D:121:ASN:HB3	1:D:333:LEU:HD22	1.58	0.82
1:A:630:ILE:HD12	1:A:630:ILE:H	1.44	0.82
1:D:575:ARG:HD3	1:D:661:VAL:O	1.79	0.82
1:A:515:LEU:CD2	1:A:732:VAL:HG11	2.10	0.82
1:B:678:PRO:HG2	1:B:683:ARG:HD3	1.60	0.82
1:C:658:GLY:O	1:C:661:VAL:HG12	1.80	0.81
1:D:539:VAL:HG11	1:D:674:GLN:HB3	1.61	0.81
1:C:262:ARG:HH22	1:C:400:LYS:HD3	1.43	0.81
1:A:448:ASP:OD1	1:B:574:LYS:HG3	1.81	0.81
1:D:401:LEU:H	1:D:401:LEU:HD23	1.46	0.80
1:A:45:ALA:O	1:A:49:MET:HB2	1.82	0.80
1:B:401:LEU:HD23	1:B:401:LEU:H	1.45	0.80
1:B:26:ALA:HB3	1:B:119:ILE:HA	1.60	0.80
1:B:413:VAL:HG22	1:B:502:ALA:HB3	1.63	0.80
1:B:279:GLN:HG2	1:B:374:ARG:CZ	2.11	0.80
1:C:327:VAL:HG21	1:C:757:LEU:HD21	1.64	0.79
1:C:306:GLY:CA	1:D:303:THR:HG21	2.12	0.79
1:A:658:GLY:O	1:A:661:VAL:HG12	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ARG:NH1	1:C:529:CYS:HA	1.97	0.79
1:A:48:ARG:HH12	3:A:803:PO4:P	2.06	0.79
1:D:505:ILE:HG13	1:D:515:LEU:HD21	1.64	0.78
1:C:686:GLY:O	1:C:690:SER:HB2	1.84	0.78
1:D:284:THR:HG23	1:D:287:LYS:H	1.49	0.78
1:B:401:LEU:HD21	1:B:406:ILE:HD11	1.65	0.78
1:C:401:LEU:H	1:C:401:LEU:HD23	1.49	0.78
1:D:515:LEU:HA	1:D:518:LEU:HD12	1.65	0.77
1:D:503:LEU:HB3	1:D:532:MET:HG2	1.65	0.77
1:A:527:GLU:CD	1:A:527:GLU:H	1.87	0.77
1:B:259:ASN:HD22	1:B:267:ASN:HD21	1.33	0.77
1:A:40:ASN:OD1	1:A:92:ILE:HG23	1.85	0.76
1:B:327:VAL:HG21	1:B:757:LEU:HD21	1.68	0.76
1:B:181:THR:HB	1:B:346:SER:HB2	1.66	0.76
1:B:250:GLU:O	1:B:254:VAL:HG23	1.85	0.76
1:B:480:LYS:HB3	1:B:482:VAL:HG23	1.68	0.76
1:D:630:ILE:HG22	1:D:632:ARG:HG2	1.68	0.76
1:C:522:ARG:HE	1:C:717:ILE:HD11	1.51	0.76
1:B:70:GLY:HA3	1:B:113:ASN:ND2	2.00	0.75
1:D:266:LEU:HD22	1:D:267:ASN:N	2.02	0.75
1:D:658:GLY:O	1:D:661:VAL:HG12	1.85	0.75
1:C:412:ASN:OD1	1:C:442:ARG:HD3	1.86	0.75
1:D:262:ARG:HH22	1:D:400:LYS:HD3	1.52	0.75
1:A:515:LEU:HD22	1:A:732:VAL:HG11	1.69	0.75
1:C:413:VAL:HG22	1:C:502:ALA:HB3	1.67	0.74
1:B:606:PHE:HB2	1:B:641:CYS:HA	1.69	0.74
1:B:401:LEU:HD23	1:B:401:LEU:N	2.03	0.74
1:D:43:VAL:HG11	1:D:93:ILE:HD12	1.68	0.74
1:B:588:GLY:HA2	1:B:638:ASN:ND2	2.02	0.74
1:C:401:LEU:HD21	1:C:406:ILE:HD11	1.69	0.74
1:C:495:MET:SD	1:C:500:ILE:HD12	2.28	0.74
1:C:40:ASN:OD1	1:C:92:ILE:HG23	1.86	0.74
1:A:530:VAL:HB	1:A:531:PRO:HD2	1.70	0.73
1:C:501:ASN:O	1:C:530:VAL:HB	1.88	0.73
1:D:577:VAL:HG21	1:D:622:LEU:HD21	1.70	0.73
1:C:44:ARG:NH1	1:C:761:LEU:CD2	2.52	0.73
1:D:401:LEU:H	1:D:401:LEU:CD2	2.01	0.73
1:C:431:SER:HB2	1:C:687:THR:HG23	1.70	0.73
1:D:731:PRO:HG2	1:D:734:GLU:HG2	1.68	0.73
1:B:534:MET:HB3	1:B:719:VAL:HG12	1.71	0.73
1:B:142:SER:O	1:B:146:GLU:HG2	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:ASN:HA	1:D:549:SER:OG	1.89	0.73
1:B:401:LEU:CD2	1:B:401:LEU:H	2.02	0.73
1:C:731:PRO:HG2	1:C:734:GLU:HG2	1.68	0.73
1:D:720:LEU:HD23	1:D:721:GLY:N	2.03	0.73
1:A:83:SER:HA	3:A:803:PO4:O3	1.89	0.72
1:C:588:GLY:HA2	1:C:638:ASN:ND2	2.05	0.72
1:A:108:LEU:HG	1:A:144:LEU:HD22	1.69	0.72
1:C:171:VAL:HG11	1:C:181:THR:HG21	1.70	0.72
1:A:577:VAL:HG21	1:A:622:LEU:HD21	1.70	0.72
1:C:79:TRP:CZ2	1:C:763:LYS:HB2	2.25	0.72
1:A:717:ILE:O	1:A:717:ILE:HG12	1.90	0.72
1:C:515:LEU:HD11	1:C:534:MET:HB3	1.72	0.72
1:D:250:GLU:O	1:D:254:VAL:HG23	1.90	0.72
1:B:418:VAL:O	1:B:507:GLY:HA3	1.90	0.71
1:A:522:ARG:HH21	1:A:717:ILE:HG23	1.55	0.71
1:B:108:LEU:HG	1:B:144:LEU:HD22	1.71	0.71
1:C:250:GLU:O	1:C:254:VAL:HG23	1.90	0.71
1:D:320:ILE:HD11	1:D:597:ALA:HB2	1.70	0.71
1:D:412:ASN:OD1	1:D:442:ARG:HD3	1.90	0.71
1:D:84:SER:CB	1:D:632:ARG:HH22	2.03	0.71
1:C:301:ARG:CG	1:C:301:ARG:HH21	2.03	0.71
1:C:306:GLY:HA3	1:D:303:THR:HG21	1.72	0.70
1:A:401:LEU:N	1:A:401:LEU:HD23	2.06	0.70
1:D:84:SER:HB2	1:D:632:ARG:HH22	1.55	0.70
1:B:503:LEU:HB3	1:B:532:MET:HG2	1.71	0.70
1:C:401:LEU:HD23	1:C:401:LEU:N	2.05	0.70
1:B:43:VAL:HG11	1:B:93:ILE:HD12	1.71	0.70
1:A:191:LEU:HD22	1:A:680:PRO:HB3	1.73	0.70
1:C:401:LEU:CD2	1:C:401:LEU:H	2.04	0.70
1:B:583:MET:HG2	1:B:673:GLN:OE1	1.91	0.70
1:A:522:ARG:NH2	1:A:716:SER:HB2	2.06	0.70
1:D:40:ASN:OD1	1:D:92:ILE:HG23	1.91	0.70
1:B:731:PRO:HG2	1:B:734:GLU:HG2	1.72	0.70
1:C:505:ILE:HD12	1:C:515:LEU:HD21	1.74	0.70
1:A:700:LYS:O	1:A:711:PHE:HZ	1.75	0.70
1:B:86:LEU:HD21	1:B:597:ALA:O	1.92	0.70
1:B:84:SER:HB2	1:B:632:ARG:HH22	1.56	0.69
1:D:27:ILE:HG21	1:D:333:LEU:HD13	1.74	0.69
1:A:401:LEU:H	1:A:401:LEU:CD2	2.06	0.69
1:D:44:ARG:NH1	1:D:44:ARG:HG3	2.04	0.69
1:A:420:ALA:HB2	1:A:481:ARG:HD3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:VAL:HG21	1:B:622:LEU:HD21	1.72	0.69
1:D:45:ALA:O	1:D:49:MET:HB2	1.93	0.69
1:A:142:SER:O	1:A:146:GLU:HG2	1.93	0.69
1:C:669:LEU:HB3	1:C:673:GLN:HE21	1.57	0.69
1:B:686:GLY:O	1:B:690:SER:HB2	1.91	0.69
1:D:718:CYS:HB3	1:D:731:PRO:HA	1.75	0.69
1:D:70:GLY:HA3	1:D:113:ASN:ND2	2.07	0.69
1:C:108:LEU:HG	1:C:144:LEU:HD22	1.74	0.69
1:C:306:GLY:HA2	1:D:303:THR:HG21	1.74	0.68
1:C:678:PRO:HG2	1:C:683:ARG:HD3	1.73	0.68
1:D:327:VAL:HG21	1:D:757:LEU:CD2	2.21	0.68
1:A:401:LEU:H	1:A:401:LEU:HD23	1.58	0.68
1:B:582:THR:HG21	1:B:591:ALA:HA	1.75	0.68
1:C:508:GLY:HA3	1:C:538:THR:HB	1.76	0.68
1:B:515:LEU:HD12	1:B:732:VAL:HG11	1.75	0.68
1:B:532:MET:HB2	1:B:717:ILE:HG23	1.75	0.68
1:A:583:MET:HG2	1:A:673:GLN:OE1	1.93	0.68
1:C:430:ARG:HD3	1:C:470:THR:HG23	1.73	0.68
1:B:719:VAL:HG13	1:B:732:VAL:HG12	1.76	0.68
1:C:219:ARG:HH12	3:C:805:PO4:P	2.15	0.68
1:C:623:THR:HG23	1:C:661:VAL:HG21	1.75	0.68
1:D:401:LEU:N	1:D:401:LEU:HD23	2.08	0.68
1:C:301:ARG:NH2	1:C:301:ARG:HG2	2.07	0.68
1:B:370:ALA:HB3	1:B:379:ALA:HB2	1.75	0.68
1:C:43:VAL:HG11	1:C:93:ILE:HD12	1.76	0.68
1:D:430:ARG:HD3	1:D:470:THR:HG23	1.76	0.67
1:B:428:ALA:HB1	1:B:506:ILE:HD13	1.77	0.67
1:A:756:PRO:O	1:A:760:ILE:HG23	1.94	0.67
1:B:756:PRO:O	1:B:760:ILE:HG23	1.94	0.67
1:C:483:LEU:CD1	1:C:484:PRO:HD2	2.24	0.67
1:B:532:MET:HB2	1:B:717:ILE:HG12	1.76	0.67
1:A:731:PRO:HG2	1:A:734:GLU:HG2	1.75	0.67
1:A:49:MET:O	1:A:53:VAL:HG22	1.95	0.67
1:D:370:ALA:HB3	1:D:379:ALA:HB2	1.77	0.66
1:A:430:ARG:HD3	1:A:470:THR:HG23	1.77	0.66
1:B:266:LEU:HD22	1:B:267:ASN:N	2.10	0.66
1:A:250:GLU:O	1:A:254:VAL:HG23	1.96	0.66
1:C:483:LEU:HD13	1:C:484:PRO:HD2	1.76	0.66
1:C:45:ALA:O	1:C:49:MET:HB2	1.95	0.66
1:A:669:LEU:HB3	1:A:673:GLN:HE21	1.60	0.66
1:A:294:THR:O	1:A:294:THR:HG23	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:PHE:O	1:D:380:VAL:HG23	1.96	0.66
1:D:398:ALA:O	1:D:399:ILE:HD13	1.95	0.66
1:A:717:ILE:H	1:A:717:ILE:HD13	1.61	0.65
1:C:575:ARG:H	1:C:631:GLN:HB2	1.60	0.65
1:C:478:GLY:HA2	1:D:572:GLY:O	1.96	0.65
1:C:226:LEU:HB2	1:C:239:LEU:HD11	1.77	0.65
1:D:483:LEU:HD13	1:D:484:PRO:HD2	1.78	0.65
1:B:588:GLY:CA	1:B:638:ASN:HD22	2.09	0.65
1:D:702:LYS:HA	1:D:705:ARG:HB2	1.77	0.65
1:A:418:VAL:O	1:A:507:GLY:HA3	1.96	0.65
1:D:515:LEU:HD11	1:D:534:MET:HB2	1.77	0.65
1:C:280:ASN:H	1:C:374:ARG:HH21	1.43	0.65
1:A:515:LEU:HD21	1:A:732:VAL:HG11	1.78	0.65
1:B:401:LEU:HG	1:B:406:ILE:HG12	1.78	0.65
1:D:583:MET:HG2	1:D:673:GLN:OE1	1.96	0.65
1:A:678:PRO:HG2	1:A:683:ARG:CD	2.27	0.65
1:B:483:LEU:HD22	1:B:513:LEU:HD22	1.80	0.64
1:A:358:MET:HG3	1:A:359:GLU:H	1.63	0.64
1:B:416:ILE:HD11	1:B:449:GLY:C	2.18	0.64
1:A:70:GLY:HA3	1:A:113:ASN:ND2	2.12	0.64
1:C:693:ALA:HB2	1:C:720:LEU:HD23	1.79	0.64
1:D:16:PHE:N	1:D:16:PHE:CD2	2.64	0.64
1:D:534:MET:HB3	1:D:719:VAL:HG12	1.80	0.64
1:D:108:LEU:HG	1:D:144:LEU:HD22	1.78	0.64
1:D:512:TYR:HA	1:D:534:MET:CE	2.28	0.64
1:A:419:GLY:HA2	1:A:510:GLU:HG3	1.79	0.64
1:D:669:LEU:HB3	1:D:673:GLN:HE21	1.63	0.64
1:C:70:GLY:HA3	1:C:113:ASN:ND2	2.13	0.64
1:D:412:ASN:ND2	1:D:499:SER:HB2	2.12	0.64
1:C:457:GLN:HA	1:C:457:GLN:NE2	2.12	0.64
1:D:532:MET:O	1:D:717:ILE:HA	1.98	0.64
1:A:43:VAL:HG11	1:A:93:ILE:HD12	1.79	0.63
1:A:588:GLY:HA2	1:A:638:ASN:OD1	1.98	0.63
1:B:630:ILE:HG22	1:B:632:ARG:HG2	1.80	0.63
1:D:306:GLY:C	1:D:308:VAL:H	2.01	0.63
1:B:230:LEU:HG	1:B:394:TYR:HB2	1.79	0.63
1:B:527:GLU:H	1:B:527:GLU:CD	2.01	0.63
1:B:49:MET:HG3	1:B:327:VAL:HG13	1.80	0.63
1:D:719:VAL:HG13	1:D:732:VAL:HG12	1.79	0.63
1:B:192:HIS:CE1	1:B:680:PRO:HD2	2.34	0.63
1:B:623:THR:HG23	1:B:661:VAL:HG21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:GLY:HA2	1:D:510:GLU:HG3	1.81	0.63
1:C:746:PRO:HG2	1:C:749:GLN:HG2	1.81	0.63
1:D:262:ARG:O	1:D:263:LYS:HB2	1.98	0.63
1:D:697:ILE:O	1:D:701:LEU:HB2	1.99	0.63
1:C:266:LEU:HD22	1:C:267:ASN:N	2.13	0.63
1:D:280:ASN:H	1:D:374:ARG:NH2	1.97	0.63
1:A:171:VAL:HG11	1:A:181:THR:HG21	1.80	0.63
1:D:320:ILE:CD1	1:D:597:ALA:HB2	2.28	0.63
1:B:575:ARG:H	1:B:631:GLN:HB2	1.64	0.63
1:D:507:GLY:O	1:D:537:ALA:N	2.31	0.63
1:C:416:ILE:HD11	1:C:449:GLY:C	2.19	0.62
1:A:306:GLY:C	1:A:308:VAL:H	2.02	0.62
1:A:398:ALA:O	1:A:399:ILE:HD13	1.98	0.62
1:A:280:ASN:H	1:A:374:ARG:HH21	1.45	0.62
1:C:303:THR:HG21	1:D:306:GLY:CA	2.29	0.62
1:D:226:LEU:HB2	1:D:239:LEU:HD11	1.81	0.62
1:D:280:ASN:H	1:D:374:ARG:HH21	1.47	0.62
1:C:49:MET:HG3	1:C:327:VAL:HG13	1.79	0.62
1:B:40:ASN:OD1	1:B:92:ILE:HG23	1.99	0.62
1:A:612:ILE:HG21	1:C:616:GLN:NE2	2.15	0.62
1:D:203:THR:HA	1:D:206:GLN:HG2	1.82	0.62
1:D:722:ILE:HD13	1:D:727:VAL:HG12	1.80	0.62
1:D:678:PRO:HG2	1:D:683:ARG:CD	2.28	0.62
1:D:512:TYR:HE1	1:D:516:LEU:HD12	1.64	0.62
1:D:27:ILE:HD13	1:D:57:VAL:HG12	1.82	0.62
1:B:541:ASN:HA	1:B:549:SER:OG	2.00	0.62
1:D:454:ALA:HB1	1:D:490:GLU:HB2	1.81	0.62
1:B:358:MET:HG3	1:B:359:GLU:H	1.62	0.62
1:B:480:LYS:HB3	1:B:482:VAL:CG2	2.30	0.62
1:B:505:ILE:HD12	1:B:515:LEU:HD21	1.81	0.62
1:B:18:GLU:HB2	1:B:52:TYR:OH	1.98	0.62
1:D:171:VAL:HG11	1:D:181:THR:HG21	1.80	0.62
1:A:567:LYS:HG2	1:A:632:ARG:HD3	1.82	0.61
1:B:84:SER:CB	1:B:632:ARG:HH22	2.12	0.61
1:D:702:LYS:HD2	1:D:705:ARG:CB	2.31	0.61
1:A:648:ASP:O	1:A:652:GLN:HG3	2.00	0.61
1:C:546:SER:HA	1:C:722:ILE:O	2.00	0.61
1:D:148:LEU:HB3	1:D:154:ILE:HG23	1.81	0.61
1:D:49:MET:SD	1:D:760:ILE:HD11	2.41	0.61
1:C:749:GLN:OE1	1:C:751:TRP:CZ2	2.54	0.61
1:A:422:ALA:O	1:A:425:MET:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:THR:OG1	1:D:340:THR:HB	2.00	0.61
1:D:120:THR:HG23	1:D:121:ASN:ND2	2.15	0.61
1:B:79:TRP:NE1	1:B:763:LYS:HB2	2.16	0.61
1:D:49:MET:HG3	1:D:327:VAL:HG13	1.80	0.61
1:B:658:GLY:O	1:B:661:VAL:HG12	2.00	0.61
1:B:409:THR:HB	1:B:705:ARG:HH22	1.65	0.61
1:D:538:THR:HG23	1:D:541:ASN:H	1.66	0.61
1:A:416:ILE:HD11	1:A:449:GLY:C	2.21	0.61
1:A:292:VAL:O	1:A:296:LEU:HB2	2.01	0.61
1:D:458:ILE:HD12	1:D:498:HIS:CD2	2.36	0.61
1:B:259:ASN:HD22	1:B:267:ASN:ND2	1.99	0.60
1:B:171:VAL:HG11	1:B:181:THR:HG21	1.82	0.60
1:C:292:VAL:O	1:C:296:LEU:HB2	2.01	0.60
1:A:454:ALA:HB2	1:A:491:ILE:HD12	1.82	0.60
1:C:301:ARG:NH2	1:C:301:ARG:CG	2.62	0.60
1:B:428:ALA:CB	1:B:506:ILE:HD13	2.32	0.60
1:C:65:GLN:HG2	1:C:98:CYS:HB2	1.84	0.60
1:C:514:GLY:O	1:C:518:LEU:HD23	2.01	0.60
1:B:13:LEU:N	1:B:13:LEU:HD23	2.17	0.60
1:C:148:LEU:HB3	1:C:154:ILE:HG23	1.83	0.60
1:C:32:SER:HB3	1:C:130:SER:OG	2.02	0.60
1:A:575:ARG:H	1:A:631:GLN:HB2	1.67	0.60
1:D:567:LYS:HG2	1:D:632:ARG:HD3	1.84	0.60
1:A:714:ASP:OD2	1:A:733:ALA:HB2	2.02	0.60
1:C:762:ALA:O	1:C:763:LYS:HB3	2.02	0.60
1:B:70:GLY:HA3	1:B:113:ASN:HD22	1.67	0.60
1:C:418:VAL:O	1:C:507:GLY:HA3	2.01	0.60
1:D:746:PRO:HG2	1:D:749:GLN:HG2	1.84	0.59
1:C:230:LEU:HG	1:C:394:TYR:HB2	1.84	0.59
1:B:179:CYS:SG	1:B:363:MET:HB2	2.42	0.59
1:C:171:VAL:HG11	1:C:181:THR:CG2	2.31	0.59
1:D:720:LEU:HD12	1:D:729:PHE:CE2	2.37	0.59
1:B:415:VAL:HG12	1:B:504:LEU:HD23	1.83	0.59
1:A:596:LEU:HB2	1:A:758:MET:HG3	1.83	0.59
1:D:503:LEU:HD21	1:D:505:ILE:HD11	1.83	0.59
1:C:541:ASN:HA	1:C:549:SER:OG	2.02	0.59
1:D:221:CYS:HA	1:D:383:ARG:NH2	2.17	0.59
1:B:493:THR:O	1:B:497:THR:HG23	2.02	0.59
1:B:79:TRP:CZ2	1:B:763:LYS:HA	2.36	0.59
1:A:535:VAL:HG13	1:A:689:ILE:HD11	1.83	0.59
1:C:361:VAL:HG12	1:C:365:GLN:NE2	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ALA:O	1:D:194:ILE:HG13	2.01	0.59
1:C:25:LYS:CE	1:C:120:THR:HG21	2.33	0.59
1:D:418:VAL:O	1:D:507:GLY:HA3	2.02	0.59
1:C:398:ALA:O	1:C:399:ILE:HD13	2.02	0.59
1:B:244:PRO:HD2	1:B:277:ASP:HA	1.84	0.59
1:B:398:ALA:O	1:B:399:ILE:HD13	2.02	0.59
1:D:512:TYR:CE1	1:D:516:LEU:HD12	2.37	0.59
1:C:606:PHE:HB2	1:C:641:CYS:HA	1.85	0.59
1:B:45:ALA:O	1:B:49:MET:HB2	2.02	0.59
1:B:430:ARG:HD3	1:B:470:THR:HG23	1.84	0.59
1:A:582:THR:HG21	1:A:591:ALA:HA	1.84	0.59
1:A:226:LEU:HB2	1:A:239:LEU:HD11	1.85	0.59
1:A:205:ALA:CB	1:A:266:LEU:HD23	2.33	0.59
1:B:266:LEU:HD11	1:B:268:ILE:HD11	1.84	0.59
1:D:290:GLU:O	1:D:294:THR:HG22	2.02	0.59
1:D:422:ALA:O	1:D:425:MET:HB2	2.01	0.59
1:C:473:GLY:CA	1:C:678:PRO:HD3	2.32	0.59
1:A:205:ALA:HB3	1:A:266:LEU:HD23	1.85	0.59
1:A:644:ASN:HD22	1:C:656:GLU:HB2	1.68	0.59
1:B:251:GLN:O	1:B:254:VAL:HB	2.03	0.58
1:D:702:LYS:HD2	1:D:705:ARG:HB3	1.85	0.58
1:C:579:ILE:N	1:C:579:ILE:HD12	2.18	0.58
1:D:634:LEU:HD11	1:D:636:LEU:HD21	1.85	0.58
1:D:358:MET:HG3	1:D:359:GLU:H	1.67	0.58
1:C:756:PRO:O	1:C:760:ILE:HG23	2.03	0.58
1:D:487:TYR:N	1:D:487:TYR:HD2	2.01	0.58
1:D:216:VAL:HG21	1:D:225:ALA:HA	1.85	0.58
1:D:579:ILE:HD12	1:D:579:ILE:N	2.18	0.58
1:C:676:GLY:HA2	1:D:565:ARG:HG2	1.85	0.58
1:C:221:CYS:HA	1:C:383:ARG:NH2	2.17	0.58
1:A:203:THR:HA	1:A:206:GLN:HG2	1.84	0.58
1:B:426:ASN:OD1	1:B:476:ILE:HG13	2.04	0.58
1:C:370:ALA:HB3	1:C:379:ALA:HB2	1.86	0.58
1:C:195:ILE:HD11	1:C:231:ALA:HB3	1.86	0.58
1:A:592:ASN:C	1:A:592:ASN:HD22	2.07	0.58
1:B:83:SER:O	1:B:84:SER:HB3	2.04	0.58
1:B:434:ARG:HG2	1:B:463:TRP:CD2	2.38	0.58
1:C:290:GLU:O	1:C:294:THR:HG22	2.04	0.58
1:D:623:THR:HG23	1:D:661:VAL:HG21	1.85	0.58
1:D:658:GLY:O	1:D:659:LYS:C	2.41	0.58
1:B:148:LEU:HB3	1:B:154:ILE:HG23	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:MET:HG3	1:D:309:GLN:NE2	2.19	0.58
1:A:426:ASN:OD1	1:A:476:ILE:HG13	2.04	0.58
1:C:542:ASN:O	1:C:746:PRO:HD3	2.04	0.58
1:A:477:LEU:H	1:A:477:LEU:HD12	1.67	0.57
1:B:634:LEU:HD11	1:B:636:LEU:HD21	1.86	0.57
1:A:401:LEU:CD2	1:A:401:LEU:N	2.66	0.57
1:B:190:ALA:O	1:B:194:ILE:HG13	2.04	0.57
1:B:195:ILE:HD11	1:B:231:ALA:HB3	1.86	0.57
1:C:176:ASN:C	1:C:178:PHE:H	2.08	0.57
1:A:649:PHE:CD1	1:C:649:PHE:CE1	2.93	0.57
1:D:762:ALA:O	1:D:763:LYS:HB2	2.04	0.57
1:B:630:ILE:H	1:B:630:ILE:CD1	2.14	0.57
1:A:630:ILE:HG22	1:A:632:ARG:HG2	1.87	0.57
1:D:401:LEU:HD21	1:D:406:ILE:HD11	1.86	0.57
1:B:30:LEU:H	1:B:30:LEU:HD23	1.70	0.57
1:D:431:SER:HB2	1:D:687:THR:HG23	1.86	0.57
1:B:337:THR:OG1	1:B:340:THR:HB	2.05	0.57
1:A:425:MET:HE1	1:A:475:SER:HB2	1.85	0.57
1:D:487:TYR:N	1:D:487:TYR:CD2	2.72	0.57
1:D:735:LEU:O	1:D:739:THR:HG22	2.05	0.57
1:D:719:VAL:HG23	1:D:719:VAL:O	2.04	0.57
1:C:25:LYS:HE2	1:C:120:THR:HG21	1.87	0.57
1:B:327:VAL:HG21	1:B:757:LEU:CD2	2.35	0.57
1:C:637:ARG:HE	1:C:647:THR:N	2.03	0.57
1:C:583:MET:HG2	1:C:673:GLN:OE1	2.05	0.57
1:C:676:GLY:HA3	1:D:565:ARG:CD	2.34	0.57
1:C:315:SER:O	1:C:319:ARG:HG3	2.05	0.57
1:C:483:LEU:HD12	1:C:517:GLU:OE1	2.05	0.56
1:D:756:PRO:O	1:D:760:ILE:HG23	2.04	0.56
1:B:669:LEU:CB	1:B:673:GLN:HE21	2.15	0.56
1:B:358:MET:HG3	1:B:359:GLU:N	2.19	0.56
1:D:592:ASN:HD22	1:D:592:ASN:C	2.08	0.56
1:A:539:VAL:HG11	1:A:674:GLN:CB	2.29	0.56
1:C:608:GLU:OE1	1:C:755:ARG:HG2	2.05	0.56
1:A:612:ILE:HG21	1:C:616:GLN:HE22	1.69	0.56
1:B:508:GLY:CA	1:B:538:THR:HB	2.35	0.56
1:A:479:THR:HG23	1:A:479:THR:O	2.05	0.56
1:B:292:VAL:O	1:B:296:LEU:HB2	2.05	0.56
1:A:402:PRO:HG2	1:A:405:GLN:HG3	1.88	0.56
1:B:678:PRO:HG2	1:B:683:ARG:CD	2.33	0.56
1:D:92:ILE:HG13	1:D:93:ILE:N	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:HIS:HB3	1:B:527:GLU:OE1	2.06	0.56
1:C:285:SER:HB3	1:C:302:VAL:HG21	1.87	0.56
1:B:484:PRO:HG2	1:B:517:GLU:HB3	1.87	0.56
1:A:181:THR:CB	1:A:346:SER:HB2	2.33	0.56
1:A:49:MET:HG3	1:A:327:VAL:HG13	1.86	0.56
1:C:419:GLY:HA2	1:C:510:GLU:HG3	1.86	0.56
1:D:84:SER:HB2	1:D:632:ARG:NH2	2.21	0.56
1:C:262:ARG:NH2	1:C:400:LYS:HD3	2.19	0.56
1:A:606:PHE:HB2	1:A:641:CYS:HA	1.87	0.56
1:A:575:ARG:HG2	1:A:661:VAL:O	2.05	0.56
1:D:577:VAL:HG21	1:D:622:LEU:CD2	2.36	0.56
1:C:156:LYS:O	1:C:159:VAL:HG12	2.06	0.56
1:B:531:PRO:HA	1:B:716:SER:O	2.06	0.56
1:A:401:LEU:HD21	1:A:406:ILE:HD11	1.88	0.56
1:B:701:LEU:O	1:B:705:ARG:HG3	2.06	0.56
1:A:686:GLY:O	1:A:690:SER:HB2	2.06	0.56
1:A:454:ALA:HB2	1:A:491:ILE:CD1	2.36	0.56
1:D:390:ASN:OD1	1:D:688:LYS:HE2	2.05	0.56
1:C:35:ASP:OD2	1:D:204:THR:HA	2.06	0.56
1:B:477:LEU:HD12	1:B:477:LEU:H	1.70	0.56
1:C:720:LEU:HD22	1:C:729:PHE:CE2	2.41	0.55
1:A:236:TRP:HZ3	1:A:399:ILE:HD11	1.71	0.55
1:C:487:TYR:O	1:C:491:ILE:HG13	2.06	0.55
1:C:337:THR:OG1	1:C:340:THR:HB	2.05	0.55
1:C:534:MET:CG	1:C:719:VAL:HG22	2.33	0.55
1:C:303:THR:HG21	1:D:306:GLY:HA3	1.87	0.55
1:C:579:ILE:HG13	1:C:635:VAL:CG1	2.37	0.55
1:B:577:VAL:HG21	1:B:622:LEU:CD2	2.36	0.55
1:A:416:ILE:HG13	1:A:446:ILE:HB	1.87	0.55
1:A:397:LEU:HD21	1:A:430:ARG:NH2	2.22	0.55
1:C:397:LEU:HD11	1:C:431:SER:HA	1.88	0.55
1:A:370:ALA:HB3	1:A:379:ALA:HB2	1.88	0.55
1:D:83:SER:O	1:D:84:SER:HB3	2.07	0.55
1:A:450:PHE:CE1	1:A:484:PRO:HD3	2.42	0.55
1:D:567:LYS:HD3	1:D:632:ARG:NH1	2.21	0.55
1:D:292:VAL:O	1:D:296:LEU:HB2	2.06	0.55
1:B:78:ASP:N	1:B:78:ASP:OD2	2.34	0.55
1:D:606:PHE:HB2	1:D:641:CYS:HA	1.89	0.55
1:A:195:ILE:HD11	1:A:231:ALA:HB3	1.89	0.55
1:C:634:LEU:HD11	1:C:636:LEU:HD21	1.87	0.55
1:C:680:PRO:HA	1:C:683:ARG:HG3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:722:ILE:HD13	1:D:727:VAL:CG1	2.36	0.55
1:C:579:ILE:HG13	1:C:635:VAL:HG13	1.88	0.55
1:A:478:GLY:HA2	1:B:572:GLY:O	2.05	0.55
1:A:176:ASN:C	1:A:178:PHE:H	2.10	0.55
1:D:305:LEU:H	1:D:305:LEU:HD12	1.72	0.55
1:B:192:HIS:O	1:B:196:GLU:HG3	2.06	0.55
1:B:221:CYS:HA	1:B:383:ARG:NH2	2.22	0.55
1:C:25:LYS:CD	1:C:120:THR:HG21	2.37	0.55
1:C:505:ILE:HG21	1:C:511:ALA:HB1	1.88	0.55
1:C:675:GLY:O	1:D:568:GLN:HG2	2.07	0.55
1:A:148:LEU:HB3	1:A:154:ILE:HD12	1.89	0.55
1:C:320:ILE:HD11	1:C:597:ALA:HB2	1.88	0.55
1:D:637:ARG:HE	1:D:647:THR:N	2.05	0.55
1:A:461:ILE:HD12	1:A:461:ILE:O	2.07	0.55
1:A:658:GLY:O	1:A:659:LYS:C	2.45	0.54
1:C:301:ARG:HG2	1:C:301:ARG:HH21	1.67	0.54
1:B:401:LEU:N	1:B:401:LEU:CD2	2.68	0.54
1:A:358:MET:HG3	1:A:359:GLU:N	2.22	0.54
1:A:506:ILE:HD13	1:A:535:VAL:HB	1.88	0.54
1:B:397:LEU:HD11	1:B:431:SER:HA	1.89	0.54
1:A:649:PHE:CE1	1:C:649:PHE:CE1	2.95	0.54
1:A:634:LEU:HD11	1:A:636:LEU:HD21	1.90	0.54
1:B:205:ALA:CB	1:B:266:LEU:HD23	2.37	0.54
1:A:669:LEU:HB3	1:A:673:GLN:NE2	2.22	0.54
1:B:37:GLN:NE2	1:B:310:ARG:C	2.61	0.54
1:C:240:PRO:HG3	1:C:274:GLY:O	2.08	0.54
1:B:461:ILE:HD12	1:B:461:ILE:O	2.08	0.54
1:C:630:ILE:HG22	1:C:632:ARG:HG2	1.90	0.54
1:C:327:VAL:HG21	1:C:757:LEU:CD2	2.37	0.54
1:D:582:THR:HG21	1:D:591:ALA:HA	1.90	0.54
1:B:177:ASP:O	1:B:364:THR:HG23	2.06	0.54
1:D:156:LYS:O	1:D:159:VAL:HG12	2.08	0.54
1:B:262:ARG:O	1:B:263:LYS:HB2	2.07	0.54
1:D:588:GLY:HA2	1:D:638:ASN:HD22	1.71	0.54
1:D:661:VAL:HG13	1:D:662:PHE:CD2	2.43	0.54
1:C:303:THR:HG21	1:D:306:GLY:HA2	1.89	0.54
1:A:541:ASN:HA	1:A:549:SER:OG	2.08	0.54
1:D:434:ARG:HG2	1:D:463:TRP:CD2	2.43	0.54
1:A:680:PRO:HA	1:A:683:ARG:HG3	1.88	0.54
1:D:236:TRP:CZ3	1:D:399:ILE:HD11	2.43	0.54
1:C:114:LEU:HD22	1:C:119:ILE:HB	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:SER:O	1:A:319:ARG:HG3	2.08	0.54
1:C:376:PHE:O	1:C:380:VAL:HG23	2.07	0.54
1:C:120:THR:HG23	1:C:121:ASN:ND2	2.23	0.54
1:B:669:LEU:HB3	1:B:673:GLN:NE2	2.18	0.54
1:C:658:GLY:O	1:C:659:LYS:C	2.45	0.54
1:D:370:ALA:CB	1:D:379:ALA:HB2	2.37	0.54
1:D:480:LYS:C	1:D:482:VAL:H	2.11	0.53
1:B:266:LEU:CD1	1:B:268:ILE:HD11	2.38	0.53
1:B:479:THR:HG23	1:B:479:THR:O	2.08	0.53
1:C:560:THR:HG22	1:C:597:ALA:HB3	1.90	0.53
1:A:746:PRO:HG2	1:A:749:GLN:HG2	1.90	0.53
1:A:576:ARG:HA	1:A:663:ASP:O	2.08	0.53
1:C:567:LYS:HG2	1:C:632:ARG:HD3	1.89	0.53
1:A:221:CYS:HA	1:A:383:ARG:NH2	2.24	0.53
1:C:737:LYS:HG3	1:C:738:GLN:N	2.22	0.53
1:D:503:LEU:CB	1:D:532:MET:HG2	2.36	0.53
1:A:522:ARG:HG2	1:A:528:PHE:O	2.08	0.53
1:A:434:ARG:HG2	1:A:463:TRP:CD2	2.43	0.53
1:B:240:PRO:HG3	1:B:274:GLY:O	2.08	0.53
1:D:535:VAL:HG13	1:D:689:ILE:HD11	1.91	0.53
1:D:142:SER:O	1:D:146:GLU:HG2	2.08	0.53
1:D:503:LEU:CD2	1:D:505:ILE:HD11	2.39	0.53
1:A:262:ARG:O	1:A:263:LYS:HB2	2.08	0.53
1:A:483:LEU:HD12	1:A:483:LEU:H	1.74	0.53
1:C:138:ARG:HA	1:C:165:LEU:HD12	1.91	0.53
1:A:65:GLN:HG2	1:A:98:CYS:HB2	1.90	0.53
1:D:397:LEU:HD21	1:D:430:ARG:NH2	2.24	0.53
1:D:488:LEU:H	1:D:488:LEU:CD2	2.16	0.53
1:A:577:VAL:HG21	1:A:622:LEU:CD2	2.37	0.53
1:D:236:TRP:HZ3	1:D:399:ILE:HD11	1.73	0.53
1:B:409:THR:HB	1:B:705:ARG:NH2	2.23	0.53
1:C:434:ARG:HG2	1:C:463:TRP:CD2	2.43	0.53
1:C:638:ASN:HB3	1:C:641:CYS:HB3	1.90	0.53
1:A:529:CYS:O	1:A:711:PHE:HB2	2.08	0.53
1:C:757:LEU:O	1:C:757:LEU:HD22	2.09	0.53
1:B:625:LYS:C	1:B:627:LYS:H	2.11	0.53
1:D:193:ARG:O	1:D:197:VAL:HG23	2.09	0.53
1:D:512:TYR:HA	1:D:534:MET:HE1	1.91	0.53
1:C:25:LYS:CG	1:C:120:THR:HG21	2.39	0.53
1:B:120:THR:HG23	1:B:121:ASN:ND2	2.24	0.53
1:C:538:THR:HG23	1:C:541:ASN:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ALA:HB1	1:B:170:MET:CE	2.39	0.53
1:C:669:LEU:HB3	1:C:673:GLN:NE2	2.23	0.53
1:C:37:GLN:NE2	1:C:310:ARG:C	2.62	0.53
1:A:431:SER:HB2	1:A:687:THR:HG23	1.89	0.53
1:D:171:VAL:HG11	1:D:181:THR:CG2	2.38	0.53
1:B:658:GLY:O	1:B:659:LYS:C	2.47	0.53
1:D:240:PRO:HG3	1:D:274:GLY:O	2.08	0.53
1:B:739:THR:HG23	1:B:741:PHE:CE1	2.44	0.53
1:B:306:GLY:C	1:B:308:VAL:H	2.13	0.53
1:D:480:LYS:HB3	1:D:482:VAL:CG2	2.20	0.53
1:B:84:SER:HB2	1:B:632:ARG:NH2	2.24	0.53
1:D:27:ILE:HG23	1:D:121:ASN:HB2	1.90	0.53
1:A:83:SER:O	1:A:84:SER:HB3	2.09	0.53
1:B:717:ILE:O	1:B:732:VAL:HG13	2.09	0.53
1:A:138:ARG:HA	1:A:165:LEU:HD12	1.90	0.53
1:A:412:ASN:HB2	1:A:499:SER:O	2.08	0.53
1:B:530:VAL:HB	1:B:531:PRO:HD2	1.90	0.52
1:A:515:LEU:C	1:A:515:LEU:HD23	2.29	0.52
1:C:49:MET:O	1:C:53:VAL:HG22	2.09	0.52
1:A:421:PRO:HG2	1:A:674:GLN:HE22	1.74	0.52
1:B:680:PRO:HA	1:B:683:ARG:HG3	1.91	0.52
1:D:560:THR:HG22	1:D:597:ALA:HB3	1.91	0.52
1:C:280:ASN:H	1:C:374:ARG:NH2	2.06	0.52
1:C:746:PRO:HD2	1:C:749:GLN:NE2	2.24	0.52
1:C:174:ILE:HG21	1:C:190:ALA:HB2	1.90	0.52
1:C:488:LEU:HD22	1:C:528:PHE:CZ	2.44	0.52
1:B:579:ILE:HD12	1:B:579:ILE:N	2.24	0.52
1:C:556:LEU:O	1:C:560:THR:HG23	2.09	0.52
1:B:315:SER:O	1:B:319:ARG:HG3	2.09	0.52
1:C:700:LYS:HA	1:C:703:GLU:HG2	1.90	0.52
1:C:582:THR:HG21	1:C:591:ALA:HA	1.91	0.52
1:C:356:PRO:HG2	1:C:359:GLU:HB3	1.92	0.52
1:A:487:TYR:O	1:A:491:ILE:HD13	2.10	0.52
1:D:397:LEU:HD11	1:D:431:SER:HA	1.91	0.52
1:D:27:ILE:HD12	1:D:27:ILE:N	2.24	0.52
1:A:240:PRO:HG3	1:A:274:GLY:O	2.09	0.52
1:C:435:VAL:HG21	1:C:691:ALA:CB	2.40	0.52
1:A:395:LYS:C	1:A:397:LEU:H	2.12	0.52
1:A:483:LEU:N	1:A:483:LEU:HD12	2.23	0.52
1:A:138:ARG:HD3	1:A:165:LEU:O	2.09	0.52
1:A:616:GLN:HE21	1:A:616:GLN:HA	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:MET:CB	1:B:717:ILE:HG23	2.40	0.52
1:C:508:GLY:CA	1:C:538:THR:HB	2.39	0.52
1:A:236:TRP:CZ3	1:A:399:ILE:HD11	2.45	0.52
1:D:176:ASN:C	1:D:178:PHE:H	2.13	0.52
1:B:419:GLY:HA2	1:B:481:ARG:HG2	1.90	0.52
1:C:516:LEU:HD22	1:C:732:VAL:HB	1.92	0.52
1:C:757:LEU:C	1:C:757:LEU:HD22	2.30	0.52
1:C:592:ASN:C	1:C:592:ASN:HD22	2.13	0.52
1:D:416:ILE:HD11	1:D:449:GLY:C	2.30	0.52
1:C:424:GLY:N	1:C:678:PRO:HB3	2.24	0.52
1:A:268:ILE:N	1:A:268:ILE:HD12	2.25	0.52
1:D:477:LEU:HD12	1:D:477:LEU:H	1.74	0.52
1:D:625:LYS:C	1:D:627:LYS:H	2.14	0.52
1:A:435:VAL:HG12	1:A:435:VAL:O	2.09	0.52
1:C:477:LEU:HD12	1:C:477:LEU:H	1.74	0.52
1:D:680:PRO:HA	1:D:683:ARG:HG3	1.91	0.51
1:D:420:ALA:HB2	1:D:481:ARG:HH11	1.76	0.51
1:A:720:LEU:HD22	1:A:729:PHE:CE2	2.46	0.51
1:B:176:ASN:C	1:B:178:PHE:H	2.13	0.51
1:A:50:GLY:O	1:A:53:VAL:HG23	2.11	0.51
1:B:114:LEU:HD22	1:B:119:ILE:HB	1.93	0.51
1:B:483:LEU:HD21	1:B:513:LEU:HD13	1.92	0.51
1:A:206:GLN:O	1:A:265:ARG:NH2	2.44	0.51
1:C:187:THR:HG21	1:C:223:TYR:HE2	1.75	0.51
1:C:615:LEU:O	1:C:619:VAL:HG23	2.10	0.51
1:B:376:PHE:O	1:B:380:VAL:HG23	2.10	0.51
1:A:396:ARG:HB3	1:A:396:ARG:HH21	1.76	0.51
1:D:715:ASP:C	1:D:717:ILE:H	2.13	0.51
1:D:717:ILE:O	1:D:732:VAL:HG13	2.10	0.51
1:C:181:THR:CB	1:C:346:SER:HB2	2.35	0.51
1:D:48:ARG:HG2	1:D:79:TRP:CE2	2.45	0.51
1:D:621:HIS:CE1	1:D:763:LYS:HB2	2.46	0.51
1:B:226:LEU:HB2	1:B:239:LEU:HD11	1.91	0.51
1:A:42:ALA:HB1	1:A:170:MET:CE	2.40	0.51
1:B:542:ASN:O	1:B:746:PRO:HD3	2.10	0.51
1:C:479:THR:HG23	1:C:479:THR:O	2.10	0.51
1:A:527:GLU:CD	1:A:527:GLU:N	2.62	0.51
1:B:560:THR:HG22	1:B:597:ALA:HB3	1.92	0.51
1:D:65:GLN:HG2	1:D:98:CYS:HB2	1.92	0.51
1:A:337:THR:OG1	1:A:340:THR:HB	2.10	0.51
1:A:115:LEU:HD12	1:A:162:TYR:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:THR:HG23	1:A:661:VAL:HG21	1.93	0.51
1:D:412:ASN:ND2	1:D:499:SER:CB	2.74	0.51
1:B:438:ALA:HB2	1:B:463:TRP:HZ3	1.74	0.51
1:A:216:VAL:HG21	1:A:225:ALA:HA	1.93	0.51
1:B:262:ARG:NH2	1:B:400:LYS:HD3	2.18	0.51
1:B:42:ALA:HB1	1:B:170:MET:HE1	1.93	0.51
1:B:216:VAL:HG21	1:B:225:ALA:HA	1.91	0.51
1:D:32:SER:HB3	1:D:130:SER:OG	2.09	0.51
1:C:357:LEU:O	1:C:361:VAL:HG23	2.10	0.51
1:D:66:GLY:HA2	1:D:73:ASN:HD22	1.75	0.51
1:A:28:GLY:HA3	1:A:122:LEU:HD12	1.93	0.51
1:A:579:ILE:HG13	1:A:635:VAL:HG13	1.93	0.51
1:B:592:ASN:C	1:B:592:ASN:HD22	2.14	0.51
1:B:630:ILE:N	1:B:630:ILE:HD12	2.17	0.51
1:C:572:GLY:O	1:D:478:GLY:HA2	2.10	0.51
1:B:615:LEU:O	1:B:619:VAL:HG23	2.11	0.51
1:B:443:MET:O	1:B:460:GLU:HG3	2.11	0.51
1:A:99:GLN:C	1:A:101:PHE:H	2.14	0.51
1:B:760:ILE:HG12	1:B:761:LEU:HD23	1.92	0.51
1:D:450:PHE:CD1	1:D:484:PRO:HD3	2.46	0.51
1:D:16:PHE:N	1:D:16:PHE:HD2	2.09	0.51
1:B:496:ARG:HB3	1:B:527:GLU:HG2	1.92	0.51
1:B:579:ILE:HG13	1:B:635:VAL:HG13	1.93	0.51
1:B:203:THR:HA	1:B:206:GLN:HG2	1.93	0.51
1:C:305:LEU:HD12	1:C:305:LEU:H	1.75	0.51
1:D:331:ILE:HG13	1:D:354:ARG:HH22	1.76	0.51
1:C:262:ARG:HD3	1:C:464:THR:HG22	1.93	0.51
1:A:608:GLU:OE1	1:A:755:ARG:HG2	2.11	0.51
1:B:277:ASP:HB3	1:B:283:ILE:HD11	1.93	0.51
1:B:739:THR:N	1:B:747:LYS:HG3	2.26	0.51
1:C:190:ALA:O	1:C:194:ILE:HG13	2.11	0.51
1:C:522:ARG:HH12	1:C:529:CYS:HA	1.72	0.50
1:C:516:LEU:CD2	1:C:732:VAL:HB	2.41	0.50
1:A:538:THR:HG23	1:A:541:ASN:H	1.75	0.50
1:D:358:MET:HG3	1:D:359:GLU:N	2.26	0.50
1:B:750:TRP:CG	1:B:751:TRP:N	2.78	0.50
1:B:737:LYS:HG3	1:B:738:GLN:HG3	1.92	0.50
1:C:306:GLY:C	1:C:308:VAL:H	2.14	0.50
1:B:92:ILE:HG13	1:B:93:ILE:N	2.26	0.50
1:C:583:MET:HA	1:C:639:GLU:HB2	1.93	0.50
1:A:171:VAL:HG11	1:A:181:THR:CG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:GLN:O	1:B:265:ARG:NH2	2.44	0.50
1:A:127:GLY:C	2:A:801:ADP:O3B	2.49	0.50
1:D:630:ILE:CD1	1:D:630:ILE:H	2.11	0.50
1:D:424:GLY:N	1:D:678:PRO:HB3	2.26	0.50
1:B:192:HIS:HA	1:B:680:PRO:HG2	1.94	0.50
1:B:26:ALA:CB	1:B:119:ILE:HA	2.35	0.50
1:D:577:VAL:CG2	1:D:622:LEU:HD21	2.39	0.50
1:A:483:LEU:HD23	1:A:513:LEU:HD12	1.94	0.50
1:A:625:LYS:C	1:A:627:LYS:H	2.15	0.50
1:A:174:ILE:HG21	1:A:190:ALA:HB2	1.93	0.50
1:D:615:LEU:O	1:D:619:VAL:HG23	2.12	0.50
1:C:237:VAL:HG12	1:C:238:PHE:N	2.26	0.50
1:C:515:LEU:CD1	1:C:534:MET:HB3	2.42	0.50
1:B:539:VAL:HG12	1:B:551:GLY:O	2.12	0.50
1:A:717:ILE:O	1:A:717:ILE:CG1	2.58	0.50
1:D:211:THR:OG1	1:D:267:ASN:HB2	2.12	0.50
1:B:501:ASN:HA	1:B:530:VAL:HG11	1.92	0.50
1:A:195:ILE:HG13	1:A:680:PRO:HG3	1.93	0.50
1:A:254:VAL:O	1:A:258:GLU:HG3	2.11	0.50
1:B:432:ALA:HB1	1:B:504:LEU:CD2	2.42	0.50
1:C:255:LYS:HE3	1:C:399:ILE:HD13	1.93	0.50
1:B:746:PRO:HG2	1:B:749:GLN:HG2	1.94	0.50
1:A:192:HIS:O	1:A:196:GLU:HG3	2.11	0.50
1:C:396:ARG:HH21	1:C:396:ARG:HB3	1.75	0.50
1:C:565:ARG:HG2	1:D:676:GLY:HA2	1.92	0.50
1:C:522:ARG:NE	1:C:717:ILE:HD11	2.24	0.50
1:D:315:SER:O	1:D:319:ARG:HG3	2.11	0.50
1:A:305:LEU:HD12	1:A:305:LEU:H	1.77	0.50
1:C:84:SER:CB	1:C:632:ARG:HH22	2.25	0.50
1:D:580:ILE:N	1:D:580:ILE:HD12	2.26	0.50
1:A:611:ASP:OD1	1:A:613:ARG:HB2	2.11	0.50
1:D:70:GLY:HA3	1:D:113:ASN:HD22	1.77	0.50
1:B:538:THR:HG23	1:B:541:ASN:H	1.75	0.50
1:B:290:GLU:O	1:B:294:THR:HG23	2.12	0.50
1:B:453:PHE:CG	1:B:491:ILE:HD12	2.46	0.50
1:C:44:ARG:HH11	1:C:761:LEU:CD2	2.21	0.49
1:A:630:ILE:HD12	1:A:630:ILE:N	2.21	0.49
1:A:238:PHE:CD2	1:A:283:ILE:HG21	2.47	0.49
1:A:539:VAL:O	1:A:590:LEU:HD11	2.12	0.49
1:B:49:MET:O	1:B:53:VAL:HG22	2.12	0.49
1:C:201:ILE:HD11	1:D:308:VAL:HG12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:GLY:C	1:D:308:VAL:N	2.65	0.49
1:C:429:VAL:HG11	1:C:477:LEU:HD11	1.93	0.49
1:A:114:LEU:HD22	1:A:119:ILE:HB	1.94	0.49
1:C:262:ARG:O	1:C:263:LYS:HB2	2.11	0.49
1:B:211:THR:OG1	1:B:267:ASN:HB2	2.12	0.49
1:A:290:GLU:O	1:A:294:THR:HG22	2.12	0.49
1:B:255:LYS:HE3	1:B:399:ILE:HD13	1.93	0.49
1:A:266:LEU:HD22	1:A:267:ASN:N	2.26	0.49
1:A:560:THR:HG22	1:A:597:ALA:HB3	1.94	0.49
1:D:279:GLN:O	1:D:281:LYS:N	2.46	0.49
1:D:395:LYS:C	1:D:397:LEU:H	2.15	0.49
1:D:447:TYR:HD2	1:D:477:LEU:HA	1.77	0.49
1:A:230:LEU:HG	1:A:394:TYR:HB2	1.94	0.49
1:B:193:ARG:O	1:B:197:VAL:HG23	2.11	0.49
1:D:461:ILE:HD12	1:D:461:ILE:O	2.11	0.49
1:A:331:ILE:HG13	1:A:354:ARG:HH22	1.78	0.49
1:A:280:ASN:H	1:A:374:ARG:NH2	2.09	0.49
1:D:429:VAL:HG11	1:D:477:LEU:HD11	1.93	0.49
1:C:447:TYR:HD2	1:C:477:LEU:HA	1.77	0.49
1:B:422:ALA:O	1:B:425:MET:HB2	2.12	0.49
1:A:474:GLY:HA3	1:B:568:GLN:HE21	1.77	0.49
1:B:111:ALA:O	1:B:115:LEU:HD22	2.12	0.49
1:B:181:THR:CB	1:B:346:SER:HB2	2.41	0.49
1:D:669:LEU:HB3	1:D:673:GLN:NE2	2.28	0.49
1:B:48:ARG:HG2	1:B:79:TRP:CE2	2.48	0.49
1:A:417:ASN:ND2	1:A:506:ILE:HB	2.28	0.49
1:A:266:LEU:HD11	1:A:268:ILE:HD11	1.94	0.49
1:A:542:ASN:O	1:A:746:PRO:HD3	2.13	0.49
1:B:579:ILE:HG13	1:B:635:VAL:CG1	2.42	0.49
1:A:693:ALA:HB2	1:A:720:LEU:HD23	1.93	0.49
1:C:42:ALA:HB1	1:C:170:MET:CE	2.43	0.49
1:D:238:PHE:CD2	1:D:283:ILE:HG21	2.48	0.49
1:D:49:MET:O	1:D:53:VAL:HG22	2.12	0.49
1:B:539:VAL:HG11	1:B:674:GLN:CB	2.38	0.49
1:C:179:CYS:SG	1:C:363:MET:HB2	2.53	0.49
1:A:493:THR:O	1:A:497:THR:HB	2.13	0.49
1:B:395:LYS:C	1:B:397:LEU:H	2.15	0.49
1:A:44:ARG:HD3	1:A:86:LEU:HB2	1.95	0.49
1:D:696:TRP:CZ2	1:D:700:LYS:HD2	2.47	0.49
1:D:195:ILE:HD11	1:D:231:ALA:HB3	1.95	0.49
1:C:539:VAL:HG12	1:C:551:GLY:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:O	1:A:683:ARG:HD2	2.13	0.49
1:B:669:LEU:CB	1:B:673:GLN:NE2	2.75	0.49
1:D:412:ASN:HB2	1:D:499:SER:O	2.12	0.49
1:D:411:CYS:O	1:D:442:ARG:HG2	2.12	0.49
1:C:264:LYS:HG2	1:C:266:LEU:O	2.12	0.49
1:C:65:GLN:HG2	1:C:98:CYS:CB	2.42	0.49
1:A:244:PRO:HD2	1:A:277:ASP:HA	1.94	0.49
1:C:537:ALA:HA	1:C:550:ILE:HB	1.94	0.49
1:D:27:ILE:HG21	1:D:333:LEU:CD1	2.43	0.49
1:C:605:ILE:HG12	1:C:755:ARG:HH21	1.76	0.49
1:C:397:LEU:HD21	1:C:430:ARG:NH2	2.28	0.49
1:B:737:LYS:HG3	1:B:738:GLN:N	2.27	0.49
1:D:99:GLN:C	1:D:101:PHE:H	2.16	0.49
1:C:610:PHE:N	1:C:610:PHE:CD1	2.80	0.49
1:A:268:ILE:HD12	1:A:268:ILE:H	1.77	0.48
1:D:739:THR:N	1:D:747:LYS:HG3	2.28	0.48
1:D:501:ASN:HA	1:D:530:VAL:HG11	1.94	0.48
1:D:192:HIS:O	1:D:196:GLU:HG3	2.13	0.48
1:A:532:MET:HB2	1:A:717:ILE:HG22	1.95	0.48
1:D:205:ALA:CB	1:D:266:LEU:HD23	2.43	0.48
1:A:266:LEU:CD1	1:A:268:ILE:HD11	2.42	0.48
1:C:325:MET:HE2	1:C:345:VAL:HB	1.96	0.48
1:C:501:ASN:O	1:C:531:PRO:HD2	2.13	0.48
1:D:746:PRO:HG2	1:D:749:GLN:CG	2.43	0.48
1:B:174:ILE:HG21	1:B:190:ALA:HB2	1.94	0.48
1:B:645:TYR:CE1	1:D:656:GLU:HG2	2.48	0.48
1:D:715:ASP:C	1:D:717:ILE:N	2.66	0.48
1:A:644:ASN:ND2	1:C:656:GLU:HB2	2.27	0.48
1:A:156:LYS:O	1:A:159:VAL:HG12	2.13	0.48
1:C:99:GLN:C	1:C:101:PHE:H	2.15	0.48
1:B:722:ILE:HD13	1:B:727:VAL:HG12	1.95	0.48
1:A:37:GLN:NE2	1:A:310:ARG:C	2.67	0.48
1:A:92:ILE:HG13	1:A:93:ILE:N	2.29	0.48
1:A:583:MET:HA	1:A:639:GLU:HB2	1.96	0.48
1:A:292:VAL:HG23	1:A:293:VAL:N	2.28	0.48
1:B:504:LEU:HD22	1:B:694:MET:HE1	1.95	0.48
1:B:583:MET:HA	1:B:639:GLU:HB2	1.94	0.48
1:A:522:ARG:NH1	1:A:529:CYS:HA	2.29	0.48
1:C:266:LEU:CD1	1:C:268:ILE:HD11	2.44	0.48
1:B:508:GLY:HA2	1:B:538:THR:HB	1.94	0.48
1:B:535:VAL:HG13	1:B:689:ILE:HD11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLU:HB2	1:D:644:ASN:ND2	2.28	0.48
1:D:181:THR:CB	1:D:346:SER:HB2	2.37	0.48
1:A:577:VAL:CG2	1:A:622:LEU:HD21	2.41	0.48
1:C:750:TRP:CG	1:C:751:TRP:N	2.81	0.48
1:C:461:ILE:HD12	1:C:461:ILE:O	2.13	0.48
1:D:515:LEU:HG	1:D:534:MET:HE1	1.95	0.48
1:A:539:VAL:CG1	1:A:674:GLN:HB3	2.30	0.48
1:A:284:THR:HG22	1:A:287:LYS:HB2	1.96	0.48
1:D:174:ILE:HG21	1:D:190:ALA:HB2	1.95	0.48
1:C:244:PRO:HD2	1:C:277:ASP:HA	1.93	0.48
1:C:533:VAL:HG22	1:C:696:TRP:CZ3	2.49	0.48
1:A:443:MET:O	1:A:460:GLU:HG3	2.12	0.48
1:A:241:GLU:OE2	1:A:387:PHE:HE1	1.97	0.48
1:D:49:MET:SD	1:D:760:ILE:CD1	3.01	0.48
1:D:52:TYR:CE2	1:D:760:ILE:HB	2.49	0.48
1:B:638:ASN:HB3	1:B:641:CYS:HB3	1.96	0.48
1:D:255:LYS:HE3	1:D:399:ILE:HD13	1.95	0.48
1:C:238:PHE:CD2	1:C:283:ILE:HG21	2.48	0.48
1:A:539:VAL:HG12	1:A:551:GLY:O	2.14	0.47
1:C:27:ILE:CG2	1:C:121:ASN:HB2	2.44	0.47
1:D:87:GLN:HE22	1:D:567:LYS:HE3	1.79	0.47
1:D:560:THR:CG2	1:D:597:ALA:HB3	2.44	0.47
1:C:211:THR:OG1	1:C:267:ASN:HB2	2.14	0.47
1:A:337:THR:O	1:A:340:THR:HG22	2.13	0.47
1:B:156:LYS:O	1:B:159:VAL:HG12	2.13	0.47
1:D:596:LEU:HB2	1:D:758:MET:HG3	1.96	0.47
1:B:530:VAL:CB	1:B:531:PRO:HD2	2.45	0.47
1:C:48:ARG:HG2	1:C:79:TRP:CE2	2.49	0.47
1:C:539:VAL:O	1:C:590:LEU:HD11	2.14	0.47
1:A:191:LEU:HD22	1:A:680:PRO:CB	2.44	0.47
1:C:411:CYS:O	1:C:442:ARG:HG2	2.13	0.47
1:C:720:LEU:HD13	1:C:729:PHE:CD2	2.49	0.47
1:C:205:ALA:CB	1:C:266:LEU:HD23	2.44	0.47
1:B:750:TRP:CD2	1:B:751:TRP:N	2.82	0.47
1:B:65:GLN:HG2	1:B:98:CYS:HB2	1.96	0.47
1:D:27:ILE:CG2	1:D:333:LEU:HD13	2.41	0.47
1:B:719:VAL:HG23	1:B:719:VAL:O	2.15	0.47
1:A:750:TRP:CG	1:A:751:TRP:N	2.82	0.47
1:C:27:ILE:HG13	1:C:57:VAL:HG12	1.96	0.47
1:B:262:ARG:HD3	1:B:464:THR:HG22	1.96	0.47
1:B:205:ALA:HB3	1:B:266:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:HIS:CE1	1:C:680:PRO:HD2	2.48	0.47
1:D:450:PHE:CE1	1:D:484:PRO:HG3	2.49	0.47
1:D:262:ARG:HD3	1:D:464:THR:HG22	1.97	0.47
1:C:197:VAL:HG13	1:D:308:VAL:HG11	1.95	0.47
1:D:138:ARG:HA	1:D:165:LEU:HD12	1.95	0.47
1:D:164:TYR:CD2	1:D:338:PRO:HB3	2.50	0.47
1:C:451:ASP:O	1:C:455:LYS:HG3	2.14	0.47
1:B:435:VAL:O	1:B:435:VAL:HG12	2.14	0.47
1:D:27:ILE:HD12	1:D:56:LYS:O	2.14	0.47
1:A:651:TYR:HE2	1:A:664:CYS:O	1.98	0.47
1:B:44:ARG:HD3	1:B:86:LEU:HB2	1.96	0.47
1:C:148:LEU:HB3	1:C:154:ILE:CG2	2.45	0.47
1:B:478:GLY:O	1:B:479:THR:HB	2.15	0.47
1:A:494:GLN:O	1:A:497:THR:HG22	2.14	0.47
1:A:547:ASP:HB3	1:A:750:TRP:NE1	2.30	0.47
1:C:414:ALA:HA	1:C:444:LEU:O	2.13	0.47
1:D:191:LEU:HD22	1:D:680:PRO:HB3	1.95	0.47
1:C:661:VAL:HG13	1:C:662:PHE:CD2	2.50	0.47
1:A:661:VAL:HG13	1:A:662:PHE:CD2	2.49	0.47
1:C:193:ARG:O	1:C:197:VAL:HG23	2.14	0.47
1:A:306:GLY:C	1:A:308:VAL:N	2.68	0.47
1:C:241:GLU:OE2	1:C:387:PHE:HE1	1.97	0.47
1:A:579:ILE:HG13	1:A:635:VAL:CG1	2.44	0.47
1:A:23:ALA:HB1	1:A:54:GLY:O	2.14	0.47
1:B:567:LYS:HG2	1:B:632:ARG:HD3	1.97	0.47
1:A:487:TYR:CD2	1:A:487:TYR:N	2.81	0.47
1:B:171:VAL:HG11	1:B:181:THR:CG2	2.44	0.47
1:B:254:VAL:O	1:B:258:GLU:HG3	2.15	0.47
1:D:337:THR:O	1:D:340:THR:HG22	2.14	0.47
1:A:221:CYS:SG	1:A:223:TYR:HB2	2.55	0.47
1:B:99:GLN:C	1:B:101:PHE:H	2.18	0.47
1:A:565:ARG:O	1:A:568:GLN:HB3	2.15	0.47
1:C:443:MET:O	1:C:460:GLU:HG3	2.15	0.47
1:D:610:PHE:CD1	1:D:610:PHE:N	2.82	0.47
1:B:630:ILE:CG2	1:B:632:ARG:HG2	2.45	0.47
1:B:580:ILE:HG23	1:B:669:LEU:HG	1.96	0.47
1:C:502:ALA:HB2	1:C:701:LEU:HD11	1.95	0.47
1:B:508:GLY:HA3	1:B:538:THR:HB	1.96	0.47
1:C:361:VAL:HG12	1:C:365:GLN:HE22	1.80	0.47
1:A:260:ARG:NH2	1:A:267:ASN:HD22	2.13	0.47
1:B:241:GLU:O	1:B:376:PHE:HB3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:THR:N	1:A:747:LYS:HG3	2.30	0.47
1:C:209:GLN:HA	1:C:265:ARG:O	2.15	0.47
1:C:651:TYR:HE2	1:C:664:CYS:O	1.97	0.47
1:D:332:ALA:HA	1:D:354:ARG:NH1	2.30	0.47
1:D:546:SER:HA	1:D:722:ILE:O	2.15	0.47
1:C:213:VAL:O	1:C:302:VAL:HG23	2.15	0.47
1:C:596:LEU:HB2	1:C:758:MET:HG3	1.96	0.47
1:A:726:ASN:OD1	1:A:726:ASN:N	2.48	0.47
1:B:726:ASN:OD1	1:B:726:ASN:N	2.47	0.47
1:D:713:THR:O	1:D:715:ASP:N	2.49	0.46
1:C:121:ASN:OD1	1:C:166:ASN:HB2	2.15	0.46
1:C:199:ASP:CG	1:C:683:ARG:HH22	2.19	0.46
1:C:676:GLY:HA3	1:D:565:ARG:HD2	1.96	0.46
1:A:319:ARG:HD2	1:A:597:ALA:O	2.14	0.46
1:D:101:PHE:C	1:D:103:THR:H	2.17	0.46
1:B:722:ILE:HD13	1:B:727:VAL:CG1	2.45	0.46
1:A:750:TRP:CD2	1:A:751:TRP:N	2.83	0.46
1:B:720:LEU:HD23	1:B:721:GLY:N	2.29	0.46
1:A:413:VAL:HG22	1:A:502:ALA:HB3	1.97	0.46
1:B:414:ALA:HA	1:B:444:LEU:O	2.15	0.46
1:D:414:ALA:HA	1:D:444:LEU:O	2.14	0.46
1:A:198:VAL:HG12	1:A:199:ASP:N	2.29	0.46
1:B:198:VAL:HG22	1:B:214:LEU:HD21	1.96	0.46
1:D:430:ARG:HA	1:D:466:VAL:HB	1.97	0.46
1:B:661:VAL:HG13	1:B:662:PHE:CD2	2.50	0.46
1:D:481:ARG:HH12	3:D:801:PO4:P	2.39	0.46
1:C:750:TRP:CD2	1:C:751:TRP:N	2.83	0.46
1:A:428:ALA:HB1	1:A:506:ILE:HD12	1.98	0.46
1:D:579:ILE:HG13	1:D:635:VAL:CG1	2.45	0.46
1:A:42:ALA:HB1	1:A:170:MET:HE1	1.97	0.46
1:C:420:ALA:HB2	1:C:481:ARG:NH1	2.31	0.46
1:D:752:LEU:O	1:D:755:ARG:HB2	2.14	0.46
1:A:711:PHE:HD2	1:A:716:SER:HB3	1.81	0.46
1:D:262:ARG:NH2	1:D:400:LYS:HD3	2.27	0.46
1:D:65:GLN:HG2	1:D:98:CYS:CB	2.46	0.46
1:D:426:ASN:OD1	1:D:476:ILE:HG13	2.15	0.46
1:C:509:PHE:HE2	1:C:513:LEU:HD21	1.80	0.46
1:D:115:LEU:HD12	1:D:162:TYR:CD2	2.50	0.46
1:D:42:ALA:HB1	1:D:170:MET:HE1	1.98	0.46
1:C:755:ARG:N	1:C:756:PRO:HD2	2.31	0.46
1:A:638:ASN:HB3	1:A:641:CYS:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:PHE:CE2	1:D:689:ILE:HG21	2.51	0.46
1:A:396:ARG:O	1:A:396:ARG:HD2	2.15	0.46
1:C:535:VAL:HG13	1:C:689:ILE:HD11	1.98	0.46
1:D:496:ARG:HB2	1:D:527:GLU:HG2	1.98	0.46
1:D:718:CYS:HA	1:D:732:VAL:HG13	1.97	0.46
1:B:406:ILE:HG22	1:B:406:ILE:O	2.16	0.46
1:B:493:THR:HG22	1:B:496:ARG:NH2	2.30	0.46
1:B:185:ILE:HD11	1:B:322:ALA:HA	1.98	0.46
1:C:92:ILE:HG13	1:C:93:ILE:N	2.30	0.46
1:B:702:LYS:HA	1:B:705:ARG:HD2	1.97	0.46
1:A:492:ALA:HB1	1:A:527:GLU:OE1	2.15	0.46
1:C:525:HIS:HB2	1:C:528:PHE:CE1	2.51	0.46
1:C:700:LYS:HA	1:C:703:GLU:CG	2.45	0.46
1:C:577:VAL:HG21	1:C:622:LEU:HD21	1.98	0.46
1:B:529:CYS:HB3	1:B:711:PHE:O	2.16	0.46
1:C:762:ALA:O	1:C:763:LYS:CB	2.64	0.46
1:A:69:ASP:O	1:A:113:ASN:ND2	2.48	0.46
1:A:325:MET:HE2	1:A:345:VAL:HB	1.98	0.46
1:B:610:PHE:N	1:B:610:PHE:CD1	2.84	0.46
1:C:630:ILE:HD12	1:C:630:ILE:N	2.19	0.46
1:A:717:ILE:N	1:A:717:ILE:HD13	2.30	0.46
1:A:622:LEU:O	1:A:626:MET:HG2	2.16	0.46
1:B:576:ARG:HD3	1:B:663:ASP:HB3	1.96	0.46
1:B:663:ASP:O	1:B:664:CYS:HB3	2.16	0.46
1:D:214:LEU:HB3	1:D:305:LEU:HD11	1.98	0.46
1:A:735:LEU:O	1:A:739:THR:HG22	2.16	0.46
1:C:417:ASN:HB3	1:C:425:MET:HE3	1.98	0.46
1:A:546:SER:HB2	1:A:721:GLY:HA3	1.98	0.46
1:A:522:ARG:C	1:A:524:LYS:H	2.18	0.45
1:A:532:MET:O	1:A:717:ILE:HA	2.16	0.45
1:D:262:ARG:O	1:D:263:LYS:CB	2.64	0.45
1:C:236:TRP:CZ3	1:C:399:ILE:HD11	2.51	0.45
1:A:148:LEU:HB3	1:A:154:ILE:HG23	1.97	0.45
1:A:174:ILE:HD11	1:A:217:MET:SD	2.56	0.45
1:B:523:GLU:O	1:B:524:LYS:C	2.54	0.45
1:D:401:LEU:HG	1:D:406:ILE:HG12	1.98	0.45
1:A:260:ARG:NH2	1:A:267:ASN:ND2	2.64	0.45
1:A:138:ARG:CD	1:A:165:LEU:O	2.64	0.45
1:A:412:ASN:OD1	1:A:442:ARG:HD3	2.17	0.45
1:B:241:GLU:OE2	1:B:387:PHE:HE1	1.98	0.45
1:B:596:LEU:HB2	1:B:758:MET:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:VAL:HG12	1:B:89:GLY:N	2.31	0.45
1:B:135:ASN:HB2	1:B:357:LEU:HD22	1.99	0.45
1:A:27:ILE:HD13	1:A:57:VAL:CG1	2.46	0.45
1:D:504:LEU:HD23	1:D:504:LEU:O	2.16	0.45
1:C:522:ARG:HE	1:C:717:ILE:CD1	2.23	0.45
1:C:395:LYS:C	1:C:397:LEU:H	2.19	0.45
1:D:507:GLY:N	1:D:537:ALA:HB3	2.32	0.45
1:C:223:TYR:O	1:C:225:ALA:N	2.48	0.45
1:D:42:ALA:HB1	1:D:170:MET:CE	2.47	0.45
1:C:426:ASN:OD1	1:C:476:ILE:HG13	2.16	0.45
1:D:306:GLY:O	1:D:308:VAL:N	2.50	0.45
1:D:487:TYR:O	1:D:491:ILE:HD12	2.17	0.45
1:C:489:GLU:OE2	1:C:525:HIS:CD2	2.69	0.45
1:C:115:LEU:HD12	1:C:162:TYR:CD2	2.52	0.45
1:D:750:TRP:CG	1:D:751:TRP:N	2.83	0.45
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.99	0.45
1:C:746:PRO:HG2	1:C:749:GLN:CG	2.45	0.45
1:B:447:TYR:HD2	1:B:477:LEU:HA	1.82	0.45
1:C:277:ASP:HB3	1:C:283:ILE:HD11	1.99	0.45
1:C:577:VAL:HG22	1:C:633:GLY:HA3	1.99	0.45
1:D:536:PRO:HD3	1:D:720:LEU:O	2.16	0.45
1:D:580:ILE:HG23	1:D:669:LEU:HG	1.99	0.45
1:B:483:LEU:CD2	1:B:513:LEU:HD22	2.45	0.45
1:B:363:MET:O	1:B:367:VAL:HG23	2.17	0.45
1:D:755:ARG:N	1:D:756:PRO:HD2	2.31	0.45
1:D:470:THR:O	1:D:683:ARG:HD2	2.17	0.45
1:A:332:ALA:HA	1:A:354:ARG:NH1	2.31	0.45
1:C:327:VAL:O	1:C:331:ILE:HG23	2.16	0.45
1:D:729:PHE:N	1:D:729:PHE:CD1	2.85	0.45
1:C:450:PHE:CE1	1:C:484:PRO:HD3	2.52	0.45
1:D:701:LEU:HD23	1:D:701:LEU:HA	1.83	0.45
1:C:67:MET:HE2	1:C:110:ALA:HB1	1.99	0.45
1:B:537:ALA:HA	1:B:550:ILE:HB	1.98	0.45
1:A:120:THR:HG23	1:A:121:ASN:ND2	2.31	0.45
1:D:485:GLY:O	1:D:488:LEU:HD22	2.17	0.45
1:C:473:GLY:HA2	1:C:678:PRO:HD3	1.98	0.45
1:D:481:ARG:HG3	1:D:510:GLU:CG	2.47	0.45
1:D:419:GLY:CA	1:D:510:GLU:HG3	2.47	0.45
1:B:356:PRO:HG2	1:B:359:GLU:HB3	1.99	0.45
1:D:685:PHE:HE2	1:D:689:ILE:HG21	1.81	0.45
1:C:409:THR:HB	1:C:705:ARG:NH2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG13	1:A:168:VAL:O	2.16	0.45
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.98	0.45
1:A:354:ARG:O	1:A:355:LEU:HD23	2.16	0.45
1:A:293:VAL:HG23	1:A:298:TYR:O	2.16	0.45
1:A:556:LEU:O	1:A:560:THR:HG23	2.16	0.45
1:C:670:GLY:C	1:C:672:MET:H	2.20	0.45
1:D:435:VAL:O	1:D:435:VAL:HG12	2.16	0.45
1:B:285:SER:HB3	1:B:302:VAL:HG21	1.98	0.45
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.99	0.45
1:C:519:SER:O	1:C:522:ARG:HD2	2.16	0.45
1:B:450:PHE:HD1	1:B:482:VAL:O	2.00	0.45
1:B:515:LEU:HD11	1:B:534:MET:HB2	1.98	0.45
1:A:258:GLU:O	1:A:262:ARG:HG3	2.17	0.45
1:A:70:GLY:HA3	1:A:113:ASN:HD22	1.79	0.45
1:A:417:ASN:HD22	1:A:506:ILE:HB	1.82	0.45
1:A:187:THR:HG21	1:A:223:TYR:HE2	1.82	0.45
1:A:39:MET:O	1:A:42:ALA:HB3	2.16	0.45
1:D:59:PHE:O	1:D:74:ILE:HA	2.17	0.45
1:D:285:SER:HB3	1:D:302:VAL:HG21	1.99	0.45
1:B:586:TYR:CG	1:B:743:HIS:HB3	2.51	0.45
1:D:726:ASN:OD1	1:D:726:ASN:N	2.48	0.45
1:A:397:LEU:HD11	1:A:431:SER:HA	1.99	0.44
1:B:577:VAL:CG2	1:B:622:LEU:HD21	2.44	0.44
1:A:247:GLY:O	1:A:251:GLN:HG2	2.17	0.44
1:B:662:PHE:C	1:B:662:PHE:CD1	2.90	0.44
1:B:79:TRP:CZ2	1:B:763:LYS:CA	3.00	0.44
1:A:685:PHE:CE2	1:A:689:ILE:HG21	2.53	0.44
1:C:488:LEU:HD22	1:C:528:PHE:CE1	2.52	0.44
1:C:735:LEU:O	1:C:739:THR:HG22	2.17	0.44
1:B:25:LYS:O	1:B:55:ALA:HB1	2.17	0.44
1:A:284:THR:CG2	1:A:287:LYS:HB2	2.46	0.44
1:C:83:SER:O	1:C:84:SER:HB3	2.18	0.44
1:C:50:GLY:O	1:C:53:VAL:HG23	2.18	0.44
1:D:583:MET:HA	1:D:639:GLU:HB2	1.98	0.44
1:B:533:VAL:HG21	1:B:693:ALA:HB1	1.99	0.44
1:A:174:ILE:CG2	1:A:190:ALA:HB2	2.48	0.44
1:A:26:ALA:HA	1:A:56:LYS:O	2.16	0.44
1:D:512:TYR:C	1:D:512:TYR:CD1	2.91	0.44
1:D:52:TYR:CD2	1:D:760:ILE:HB	2.52	0.44
1:A:696:TRP:CZ2	1:A:700:LYS:HD2	2.52	0.44
1:B:79:TRP:CE2	1:B:763:LYS:HB2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:CYS:HA	1:D:383:ARG:HH21	1.80	0.44
1:D:579:ILE:HA	1:D:635:VAL:HG13	1.98	0.44
1:C:320:ILE:CD1	1:C:597:ALA:HB2	2.47	0.44
1:D:530:VAL:HG12	1:D:531:PRO:HD2	1.99	0.44
1:D:521:ALA:O	1:D:525:HIS:HB2	2.17	0.44
1:C:165:LEU:HD13	1:C:167:VAL:HG13	2.00	0.44
1:D:387:PHE:HD2	1:D:387:PHE:O	2.01	0.44
1:B:215:GLU:OE1	1:B:304:ILE:HG12	2.18	0.44
1:D:416:ILE:HG22	1:D:505:ILE:HD13	1.99	0.44
1:A:496:ARG:HH21	1:A:496:ARG:HG3	1.83	0.44
1:D:266:LEU:HD11	1:D:268:ILE:HD11	1.99	0.44
1:B:483:LEU:CD2	1:B:513:LEU:HB3	2.48	0.44
1:B:221:CYS:HA	1:B:383:ARG:HH21	1.82	0.44
1:C:223:TYR:C	1:C:225:ALA:N	2.69	0.44
1:D:293:VAL:HG23	1:D:298:TYR:O	2.18	0.44
1:B:138:ARG:HA	1:B:165:LEU:HD12	1.98	0.44
1:D:27:ILE:HD12	1:D:27:ILE:H	1.83	0.44
1:B:205:ALA:HB1	1:B:266:LEU:HD23	1.99	0.44
1:B:608:GLU:OE1	1:B:755:ARG:HG2	2.18	0.44
1:D:537:ALA:HA	1:D:550:ILE:HB	1.99	0.44
1:C:578:PHE:C	1:C:579:ILE:HD12	2.38	0.44
1:D:479:THR:HG23	1:D:479:THR:O	2.16	0.44
1:C:208:HIS:O	1:C:209:GLN:C	2.56	0.44
1:B:524:LYS:HD3	1:B:524:LYS:H	1.82	0.44
1:B:644:ASN:HD21	1:D:655:SER:HB3	1.83	0.44
1:D:495:MET:C	1:D:497:THR:H	2.21	0.44
1:C:326:GLY:O	1:C:330:VAL:HG23	2.18	0.44
1:D:413:VAL:HA	1:D:502:ALA:HB3	1.98	0.44
1:A:285:SER:HB3	1:A:302:VAL:HG21	2.00	0.44
1:B:451:ASP:O	1:B:455:LYS:HG3	2.17	0.44
1:C:23:ALA:HA	1:C:54:GLY:O	2.17	0.44
1:D:512:TYR:CE2	1:D:544:PRO:HG2	2.53	0.44
1:B:30:LEU:N	1:B:30:LEU:HD23	2.32	0.44
1:B:84:SER:C	1:B:87:GLN:HE22	2.21	0.44
1:B:327:VAL:O	1:B:331:ILE:HG23	2.18	0.44
1:A:306:GLY:O	1:A:308:VAL:N	2.51	0.44
1:C:221:CYS:HA	1:C:383:ARG:HH21	1.80	0.44
1:A:720:LEU:HD13	1:A:729:PHE:CD2	2.53	0.44
1:B:209:GLN:HA	1:B:265:ARG:O	2.18	0.44
1:D:74:ILE:HG21	1:D:117:ARG:HG3	1.99	0.44
1:A:78:ASP:OD2	1:A:78:ASP:N	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HG12	1:B:333:LEU:HD13	1.99	0.44
1:D:26:ALA:HA	1:D:56:LYS:O	2.17	0.44
1:C:266:LEU:HD11	1:C:268:ILE:HD11	1.99	0.44
1:A:260:ARG:HH22	1:A:267:ASN:HD22	1.66	0.44
1:B:223:TYR:C	1:B:225:ALA:N	2.70	0.44
1:D:244:PRO:HB2	1:D:248:TRP:CG	2.53	0.44
1:B:554:THR:HG22	1:B:555:ALA:N	2.33	0.44
1:A:327:VAL:O	1:A:331:ILE:HG23	2.18	0.44
1:C:701:LEU:HD23	1:C:701:LEU:HA	1.89	0.44
1:A:718:CYS:SG	1:A:731:PRO:HA	2.58	0.44
1:A:411:CYS:O	1:A:442:ARG:HG2	2.17	0.44
1:B:566:ILE:C	1:B:568:GLN:H	2.21	0.44
1:A:279:GLN:O	1:A:281:LYS:N	2.51	0.44
1:D:717:ILE:HG13	1:D:717:ILE:O	2.18	0.43
1:C:580:ILE:N	1:C:580:ILE:HD12	2.33	0.43
1:B:541:ASN:O	1:B:541:ASN:ND2	2.48	0.43
1:B:504:LEU:HD12	1:B:533:VAL:HG13	1.99	0.43
1:A:370:ALA:HB2	1:A:375:ARG:NH1	2.33	0.43
1:B:454:ALA:N	1:B:491:ILE:HD11	2.33	0.43
1:D:740:ASP:CG	1:D:743:HIS:HD1	2.21	0.43
1:B:411:CYS:O	1:B:442:ARG:HG2	2.17	0.43
1:A:414:ALA:HA	1:A:444:LEU:O	2.18	0.43
1:D:37:GLN:NE2	1:D:310:ARG:C	2.71	0.43
1:D:327:VAL:O	1:D:331:ILE:HG23	2.17	0.43
1:A:480:LYS:C	1:A:482:VAL:H	2.20	0.43
1:A:327:VAL:HG21	1:A:757:LEU:HD21	2.01	0.43
1:B:577:VAL:O	1:B:664:CYS:HA	2.18	0.43
1:B:370:ALA:CB	1:B:379:ALA:HB2	2.45	0.43
1:C:70:GLY:HA3	1:C:113:ASN:HD22	1.83	0.43
1:A:211:THR:OG1	1:A:267:ASN:HB2	2.17	0.43
1:B:429:VAL:HG11	1:B:477:LEU:HD11	1.99	0.43
1:D:244:PRO:HD2	1:D:277:ASP:HA	1.99	0.43
1:C:414:ALA:O	1:C:503:LEU:HA	2.18	0.43
1:D:496:ARG:HD3	1:D:527:GLU:OE1	2.17	0.43
1:B:412:ASN:OD1	1:B:442:ARG:HD3	2.19	0.43
1:D:230:LEU:HG	1:D:394:TYR:HB2	2.00	0.43
1:A:193:ARG:O	1:A:197:VAL:HG23	2.18	0.43
1:A:670:GLY:C	1:A:672:MET:H	2.21	0.43
1:D:187:THR:HG21	1:D:223:TYR:HE2	1.83	0.43
1:B:419:GLY:HA2	1:B:510:GLU:HG3	2.00	0.43
1:C:311:GLY:HA3	1:D:200:ALA:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:VAL:HG21	1:C:466:VAL:HG11	1.99	0.43
1:D:27:ILE:HD13	1:D:57:VAL:CG1	2.47	0.43
1:A:535:VAL:HG13	1:A:689:ILE:CD1	2.48	0.43
1:A:209:GLN:HA	1:A:265:ARG:O	2.19	0.43
1:A:649:PHE:CD1	1:C:649:PHE:CD1	3.06	0.43
1:A:739:THR:HG23	1:A:741:PHE:CE1	2.53	0.43
1:D:738:GLN:HG2	1:D:738:GLN:O	2.18	0.43
1:C:262:ARG:HD3	1:C:464:THR:CG2	2.48	0.43
1:B:755:ARG:HA	1:B:755:ARG:HD2	1.70	0.43
1:A:255:LYS:HE3	1:A:399:ILE:HD13	2.01	0.43
1:B:187:THR:HG21	1:B:223:TYR:HE2	1.82	0.43
1:A:244:PRO:HB2	1:A:248:TRP:CG	2.54	0.43
1:B:425:MET:HE2	1:B:475:SER:HB2	2.00	0.43
1:D:25:LYS:H	1:D:25:LYS:HG3	1.50	0.43
1:B:637:ARG:HE	1:B:647:THR:N	2.17	0.43
1:B:217:MET:HG3	1:B:309:GLN:NE2	2.33	0.43
1:D:87:GLN:NE2	1:D:567:LYS:HE3	2.33	0.43
1:B:717:ILE:O	1:B:717:ILE:HG22	2.18	0.43
1:C:579:ILE:HA	1:C:635:VAL:HG13	2.00	0.43
1:C:370:ALA:HB2	1:C:375:ARG:NH1	2.34	0.43
1:A:170:MET:HG3	1:A:345:VAL:HG23	2.01	0.43
1:C:565:ARG:HG2	1:D:676:GLY:CA	2.49	0.43
1:B:649:PHE:HD1	1:D:652:GLN:OE1	2.01	0.43
1:B:67:MET:HE2	1:B:110:ALA:HB1	2.00	0.43
1:C:608:GLU:OE1	1:C:755:ARG:CG	2.66	0.43
1:B:35:ASP:O	1:B:310:ARG:HD2	2.19	0.43
1:C:402:PRO:HB2	1:C:405:GLN:HG3	2.01	0.43
1:C:568:GLN:HG3	1:D:474:GLY:HA3	2.01	0.43
1:B:284:THR:O	1:B:288:ILE:HG13	2.18	0.43
1:B:493:THR:O	1:B:496:ARG:N	2.49	0.43
1:A:477:LEU:N	1:A:477:LEU:HD12	2.33	0.43
1:D:277:ASP:HB3	1:D:283:ILE:HD11	2.01	0.43
1:A:722:ILE:HD13	1:A:727:VAL:HG12	2.01	0.43
1:C:402:PRO:HG2	1:C:405:GLN:HG3	2.01	0.43
1:C:88:VAL:HG12	1:C:89:GLY:N	2.34	0.43
1:D:526:GLU:HA	1:D:529:CYS:SG	2.59	0.43
1:A:59:PHE:O	1:A:74:ILE:HA	2.18	0.43
1:A:30:LEU:HD23	1:A:30:LEU:N	2.34	0.43
1:B:41:ALA:CB	1:B:86:LEU:HD12	2.48	0.43
1:C:601:ASP:O	1:C:602:ALA:HB2	2.19	0.43
1:D:519:SER:OG	1:D:717:ILE:HD11	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD23	1:C:30:LEU:N	2.33	0.43
1:C:49:MET:HG2	1:C:760:ILE:HD11	2.01	0.43
1:C:308:VAL:HG12	1:D:201:ILE:HD11	2.00	0.43
1:B:331:ILE:O	1:B:335:GLU:HB2	2.19	0.43
1:D:481:ARG:HG3	1:D:510:GLU:HB3	2.00	0.43
1:D:148:LEU:HB3	1:D:154:ILE:CG2	2.47	0.43
1:B:292:VAL:HG23	1:B:293:VAL:N	2.34	0.43
1:A:438:ALA:HB2	1:A:463:TRP:HZ3	1.84	0.43
1:C:324:ARG:NE	1:C:754:LEU:HD21	2.34	0.43
1:C:25:LYS:HG2	1:C:120:THR:HG21	1.99	0.42
1:B:121:ASN:OD1	1:B:166:ASN:HB2	2.18	0.42
1:B:567:LYS:HD3	1:B:632:ARG:NH1	2.33	0.42
1:B:247:GLY:O	1:B:251:GLN:HG2	2.19	0.42
1:C:483:LEU:HD13	1:C:484:PRO:CD	2.47	0.42
1:B:702:LYS:HD2	1:B:705:ARG:HD2	2.01	0.42
1:A:685:PHE:HE2	1:A:689:ILE:HG21	1.84	0.42
1:D:638:ASN:HB3	1:D:641:CYS:HB3	1.99	0.42
1:C:739:THR:HG23	1:C:741:PHE:CE1	2.54	0.42
1:B:68:VAL:O	1:B:109:LYS:HG3	2.19	0.42
1:B:321:LEU:O	1:B:321:LEU:HD23	2.19	0.42
1:A:610:PHE:CD1	1:A:610:PHE:N	2.87	0.42
1:B:199:ASP:CG	1:B:683:ARG:HH22	2.23	0.42
1:B:279:GLN:O	1:B:281:LYS:N	2.52	0.42
1:B:629:THR:O	1:B:631:GLN:HG3	2.18	0.42
1:C:42:ALA:HB1	1:C:170:MET:HE1	2.01	0.42
1:D:179:CYS:SG	1:D:363:MET:CB	3.07	0.42
1:D:443:MET:O	1:D:460:GLU:HG3	2.18	0.42
1:C:177:ASP:O	1:C:364:THR:HG23	2.19	0.42
1:D:87:GLN:CD	1:D:87:GLN:H	2.23	0.42
1:A:629:THR:O	1:A:631:GLN:HG3	2.19	0.42
1:C:541:ASN:O	1:C:541:ASN:ND2	2.53	0.42
1:D:223:TYR:O	1:D:225:ALA:N	2.52	0.42
1:B:337:THR:O	1:B:340:THR:HG22	2.19	0.42
1:C:86:LEU:HD21	1:C:597:ALA:O	2.19	0.42
1:D:637:ARG:CG	1:D:637:ARG:HH11	2.32	0.42
1:B:222:GLY:HA3	1:B:240:PRO:HD2	2.01	0.42
1:A:222:GLY:HA3	1:A:240:PRO:HD2	2.01	0.42
1:D:402:PRO:HB2	1:D:405:GLN:HG3	2.00	0.42
1:C:755:ARG:HA	1:C:755:ARG:HD2	1.83	0.42
1:D:540:SER:O	1:D:541:ASN:HB3	2.19	0.42
1:D:694:MET:O	1:D:697:ILE:HB	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:TYR:C	1:C:225:ALA:H	2.23	0.42
1:B:164:TYR:CD2	1:B:338:PRO:HB3	2.54	0.42
1:C:217:MET:HG3	1:C:309:GLN:NE2	2.35	0.42
1:A:357:LEU:O	1:A:361:VAL:HG23	2.19	0.42
1:C:625:LYS:C	1:C:627:LYS:H	2.22	0.42
1:C:27:ILE:HG23	1:C:121:ASN:HB2	2.01	0.42
1:C:662:PHE:CD1	1:C:662:PHE:C	2.93	0.42
1:A:84:SER:C	1:A:87:GLN:HE22	2.23	0.42
1:A:731:PRO:C	1:A:733:ALA:N	2.72	0.42
1:A:731:PRO:O	1:A:733:ALA:N	2.52	0.42
1:A:476:ILE:C	1:A:478:GLY:H	2.23	0.42
1:C:438:ALA:HB2	1:C:463:TRP:HZ3	1.84	0.42
1:A:190:ALA:O	1:A:194:ILE:HG13	2.18	0.42
1:B:441:HIS:NE2	1:B:698:THR:HG23	2.34	0.42
1:B:28:GLY:HA3	1:B:122:LEU:HD12	2.01	0.42
1:A:376:PHE:O	1:A:380:VAL:HG23	2.19	0.42
1:D:492:ALA:HB2	1:D:528:PHE:CZ	2.55	0.42
1:C:408:LYS:HG2	1:C:408:LYS:H	1.68	0.42
1:D:78:ASP:OD2	1:D:78:ASP:N	2.42	0.42
1:A:171:VAL:HG23	1:A:171:VAL:O	2.19	0.42
1:C:505:ILE:HD12	1:C:515:LEU:CD2	2.48	0.42
1:D:577:VAL:O	1:D:664:CYS:HA	2.20	0.42
1:A:422:ALA:HB2	1:A:538:THR:HA	2.01	0.42
1:B:477:LEU:HD12	1:B:477:LEU:N	2.33	0.42
1:A:411:CYS:SG	1:A:701:LEU:HD21	2.60	0.42
1:A:74:ILE:HG21	1:A:117:ARG:HG3	2.01	0.42
1:A:380:VAL:C	1:A:382:LEU:H	2.22	0.42
1:C:492:ALA:O	1:C:495:MET:HB2	2.19	0.42
1:D:380:VAL:C	1:D:382:LEU:H	2.23	0.42
1:C:236:TRP:HZ3	1:C:399:ILE:HD11	1.85	0.42
1:B:112:CYS:HB2	1:B:148:LEU:CD2	2.49	0.42
1:A:277:ASP:HB3	1:A:283:ILE:HD11	2.00	0.42
1:D:179:CYS:SG	1:D:363:MET:HB2	2.59	0.42
1:C:21:SER:HB2	1:C:22:GLY:H	1.60	0.42
1:A:580:ILE:HD12	1:A:580:ILE:N	2.34	0.42
1:C:84:SER:HB2	1:C:632:ARG:HH22	1.83	0.42
1:A:630:ILE:H	1:A:630:ILE:CD1	2.18	0.42
1:C:241:GLU:O	1:C:376:PHE:HB3	2.20	0.42
1:C:355:LEU:HB3	1:C:356:PRO:HD2	2.01	0.42
1:C:435:VAL:O	1:C:435:VAL:HG12	2.20	0.42
1:D:478:GLY:O	1:D:479:THR:HB	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:ASP:HB3	1:D:750:TRP:NE1	2.35	0.42
1:C:307:HIS:NE2	1:D:301:ARG:HG2	2.34	0.42
1:B:127:GLY:HA3	2:B:801:ADP:O2B	2.19	0.42
1:C:667:ASN:HD22	1:C:667:ASN:HA	1.64	0.42
1:A:537:ALA:HA	1:A:550:ILE:HB	2.01	0.42
1:D:416:ILE:CG2	1:D:505:ILE:HD13	2.50	0.42
1:D:534:MET:HB2	1:D:534:MET:HE2	1.87	0.42
1:A:447:TYR:HD2	1:A:477:LEU:HA	1.83	0.42
1:C:521:ALA:O	1:C:528:PHE:HD1	2.02	0.42
1:A:156:LYS:HD2	1:A:156:LYS:HA	1.84	0.42
1:D:413:VAL:HG22	1:D:502:ALA:HB3	2.01	0.42
1:C:402:PRO:HG2	1:C:405:GLN:CD	2.40	0.42
1:D:670:GLY:C	1:D:672:MET:H	2.23	0.42
1:C:293:VAL:HG23	1:C:298:TYR:O	2.20	0.42
1:C:48:ARG:HD3	1:C:761:LEU:O	2.20	0.42
1:D:567:LYS:HD3	1:D:632:ARG:CD	2.50	0.42
1:C:717:ILE:O	1:C:732:VAL:HG22	2.20	0.42
1:D:61:TYR:HA	1:D:93:ILE:O	2.20	0.42
1:C:729:PHE:N	1:C:729:PHE:CD1	2.88	0.42
1:B:148:LEU:HB3	1:B:154:ILE:CG2	2.49	0.42
1:A:729:PHE:CD1	1:A:729:PHE:N	2.87	0.42
1:C:244:PRO:HB2	1:C:248:TRP:CG	2.55	0.42
1:C:179:CYS:SG	1:C:363:MET:CB	3.08	0.42
1:C:422:ALA:O	1:C:425:MET:HB2	2.20	0.42
1:D:717:ILE:O	1:D:732:VAL:HG22	2.21	0.41
1:D:205:ALA:HB3	1:D:266:LEU:HD23	2.02	0.41
1:C:412:ASN:OD1	1:C:442:ARG:CD	2.63	0.41
1:C:412:ASN:ND2	1:C:498:HIS:O	2.53	0.41
1:B:504:LEU:HD22	1:B:694:MET:CE	2.50	0.41
1:B:504:LEU:CD1	1:B:533:VAL:HG13	2.50	0.41
1:B:156:LYS:HD2	1:B:156:LYS:HA	1.85	0.41
1:A:637:ARG:HE	1:A:647:THR:N	2.18	0.41
1:D:174:ILE:CG2	1:D:190:ALA:HB2	2.50	0.41
1:B:223:TYR:C	1:B:225:ALA:H	2.24	0.41
1:B:656:GLU:HB2	1:D:644:ASN:HD22	1.84	0.41
1:D:387:PHE:C	1:D:387:PHE:CD2	2.93	0.41
1:C:648:ASP:O	1:C:652:GLN:HG3	2.20	0.41
1:B:59:PHE:O	1:B:74:ILE:HA	2.19	0.41
1:B:530:VAL:HA	1:B:711:PHE:CD2	2.55	0.41
1:B:264:LYS:C	1:B:266:LEU:H	2.24	0.41
1:A:501:ASN:O	1:A:531:PRO:HD2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HG22	1:A:406:ILE:O	2.20	0.41
1:D:294:THR:O	1:D:294:THR:HG23	2.19	0.41
1:C:370:ALA:CB	1:C:379:ALA:HB2	2.49	0.41
1:D:48:ARG:NE	1:D:79:TRP:NE1	2.68	0.41
1:B:214:LEU:HB3	1:B:305:LEU:HD11	2.02	0.41
1:A:546:SER:HA	1:A:722:ILE:O	2.20	0.41
1:C:74:ILE:HG21	1:C:117:ARG:HG3	2.02	0.41
1:D:208:HIS:C	1:D:209:GLN:HG2	2.40	0.41
1:D:354:ARG:O	1:D:355:LEU:HD23	2.20	0.41
1:A:219:ARG:HG3	1:A:273:GLU:CD	2.38	0.41
1:A:717:ILE:O	1:A:732:VAL:HG13	2.20	0.41
1:B:430:ARG:HH21	1:B:470:THR:CG2	2.33	0.41
1:C:176:ASN:C	1:C:178:PHE:N	2.72	0.41
1:D:735:LEU:O	1:D:739:THR:CG2	2.67	0.41
1:B:357:LEU:O	1:B:361:VAL:HG23	2.20	0.41
1:A:432:ALA:HB1	1:A:504:LEU:HD23	2.02	0.41
1:D:512:TYR:HD1	1:D:512:TYR:C	2.24	0.41
1:B:731:PRO:C	1:B:733:ALA:N	2.74	0.41
1:B:622:LEU:O	1:B:626:MET:HG2	2.20	0.41
1:A:264:LYS:C	1:A:266:LEU:H	2.24	0.41
1:A:478:GLY:O	1:A:479:THR:HB	2.20	0.41
1:D:176:ASN:C	1:D:178:PHE:N	2.73	0.41
1:B:65:GLN:HG2	1:B:98:CYS:CB	2.50	0.41
1:A:88:VAL:HG12	1:A:89:GLY:N	2.35	0.41
1:D:731:PRO:C	1:D:733:ALA:N	2.74	0.41
1:D:424:GLY:CA	1:D:678:PRO:HB3	2.50	0.41
1:D:481:ARG:HD3	1:D:510:GLU:OE1	2.20	0.41
1:D:223:TYR:C	1:D:225:ALA:N	2.74	0.41
1:A:86:LEU:HD21	1:A:597:ALA:O	2.20	0.41
1:A:129:GLY:N	2:A:801:ADP:O3B	2.53	0.41
1:A:494:GLN:C	1:A:497:THR:HG22	2.41	0.41
1:B:412:ASN:ND2	1:B:442:ARG:HH11	2.17	0.41
1:B:284:THR:CG2	1:B:287:LYS:HB2	2.51	0.41
1:C:52:TYR:CE2	1:C:760:ILE:HB	2.56	0.41
1:B:268:ILE:HD12	1:B:268:ILE:H	1.85	0.41
1:B:397:LEU:HD21	1:B:430:ARG:NH2	2.36	0.41
1:B:138:ARG:HH11	1:B:342:ALA:HA	1.86	0.41
1:D:586:TYR:HB2	1:D:743:HIS:O	2.21	0.41
1:C:512:TYR:O	1:C:516:LEU:HD23	2.21	0.41
1:A:30:LEU:HB3	1:A:60:ILE:HB	2.02	0.41
1:C:731:PRO:C	1:C:733:ALA:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HD11	1:D:308:VAL:CG1	2.50	0.41
1:C:130:SER:HB2	2:C:801:ADP:O2A	2.20	0.41
1:B:476:ILE:C	1:B:478:GLY:H	2.22	0.41
1:D:79:TRP:CZ2	1:D:763:LYS:HA	2.55	0.41
1:C:354:ARG:O	1:C:355:LEU:HD23	2.21	0.41
1:A:122:LEU:O	1:A:167:VAL:HA	2.21	0.41
1:B:524:LYS:CD	1:B:524:LYS:H	2.34	0.41
1:B:122:LEU:O	1:B:167:VAL:HA	2.20	0.41
1:B:172:GLY:O	1:B:173:SER:HB2	2.19	0.41
1:D:712:THR:O	1:D:713:THR:C	2.58	0.41
1:A:331:ILE:O	1:A:335:GLU:HB2	2.21	0.41
1:D:284:THR:CG2	1:D:287:LYS:HB2	2.51	0.41
1:B:755:ARG:N	1:B:756:PRO:HD2	2.36	0.41
1:D:254:VAL:O	1:D:258:GLU:HG3	2.20	0.41
1:A:755:ARG:N	1:A:756:PRO:HD2	2.35	0.41
1:C:264:LYS:C	1:C:266:LEU:H	2.23	0.41
1:D:486:LYS:C	1:D:487:TYR:HD2	2.24	0.41
1:A:447:TYR:CD2	1:A:477:LEU:HA	2.56	0.41
1:A:697:ILE:O	1:A:701:LEU:N	2.51	0.41
1:C:216:VAL:HG21	1:C:225:ALA:HA	2.01	0.41
1:D:387:PHE:C	1:D:387:PHE:HD2	2.24	0.41
1:B:412:ASN:HB2	1:B:499:SER:O	2.21	0.41
1:D:209:GLN:HA	1:D:265:ARG:O	2.20	0.41
1:A:164:TYR:CD2	1:A:338:PRO:HB3	2.56	0.41
1:A:334:LEU:HG	1:A:334:LEU:H	1.68	0.41
1:C:214:LEU:N	1:C:214:LEU:CD1	2.84	0.41
1:B:485:GLY:O	1:B:488:LEU:HB2	2.21	0.41
1:C:539:VAL:HG11	1:C:674:GLN:CB	2.36	0.41
1:C:515:LEU:HB3	1:C:717:ILE:CG2	2.51	0.41
1:D:266:LEU:CD1	1:D:268:ILE:HD11	2.51	0.41
1:C:580:ILE:HG23	1:C:669:LEU:HG	2.03	0.41
1:D:222:GLY:HA3	1:D:240:PRO:HD2	2.01	0.41
1:D:579:ILE:HG13	1:D:635:VAL:HG13	2.02	0.41
1:B:223:TYR:O	1:B:225:ALA:N	2.54	0.41
1:D:67:MET:HB3	1:D:67:MET:HE2	1.89	0.41
1:D:67:MET:HE3	1:D:114:LEU:HG	2.02	0.41
1:A:67:MET:HB3	1:A:67:MET:HE2	1.92	0.41
1:D:416:ILE:HG12	1:D:417:ASN:N	2.36	0.40
1:A:81:SER:C	1:A:83:SER:H	2.24	0.40
1:C:530:VAL:HB	1:C:531:PRO:HD2	2.02	0.40
1:B:511:ALA:HB1	1:B:534:MET:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLN:O	1:A:254:VAL:HB	2.21	0.40
1:D:239:LEU:HA	1:D:240:PRO:HD3	1.86	0.40
1:C:111:ALA:O	1:C:115:LEU:HD22	2.21	0.40
1:D:750:TRP:CD2	1:D:751:TRP:N	2.89	0.40
1:C:215:GLU:OE1	1:C:304:ILE:HG12	2.21	0.40
1:C:78:ASP:OD2	1:C:81:SER:HB2	2.21	0.40
1:B:577:VAL:HG22	1:B:633:GLY:HA3	2.03	0.40
1:C:473:GLY:HA3	1:C:678:PRO:HD3	2.03	0.40
1:C:205:ALA:HB1	1:C:266:LEU:HD23	2.03	0.40
1:C:268:ILE:HD12	1:C:268:ILE:H	1.86	0.40
1:A:255:LYS:HE2	1:A:255:LYS:HB2	1.91	0.40
1:A:425:MET:CE	1:A:475:SER:HB2	2.49	0.40
1:C:174:ILE:CG2	1:C:190:ALA:HB2	2.50	0.40
1:A:722:ILE:HD13	1:A:727:VAL:CG1	2.51	0.40
1:B:141:TRP:CG	1:B:165:LEU:HB2	2.56	0.40
1:A:615:LEU:O	1:A:619:VAL:HG23	2.22	0.40
1:C:139:LYS:HD3	1:C:139:LYS:HA	1.80	0.40
1:D:534:MET:HB3	1:D:534:MET:HE2	1.86	0.40
1:D:83:SER:O	1:D:84:SER:CB	2.69	0.40
1:A:430:ARG:HA	1:A:466:VAL:HB	2.02	0.40
1:B:502:ALA:HB1	1:B:697:ILE:CG2	2.51	0.40
1:C:506:ILE:HG22	1:C:537:ALA:CB	2.52	0.40
1:C:307:HIS:C	1:C:309:GLN:H	2.24	0.40
1:D:251:GLN:OE1	1:D:251:GLN:HA	2.21	0.40
1:C:25:LYS:HB3	1:C:120:THR:CG2	2.50	0.40
1:D:81:SER:C	1:D:83:SER:H	2.25	0.40
1:B:756:PRO:HG2	1:B:757:LEU:H	1.86	0.40
1:C:476:ILE:C	1:C:478:GLY:H	2.23	0.40
1:C:544:PRO:HB3	1:C:746:PRO:HB3	2.04	0.40
1:A:111:ALA:O	1:A:115:LEU:HD22	2.21	0.40
1:A:579:ILE:HD12	1:A:579:ILE:N	2.36	0.40
1:D:531:PRO:HD3	1:D:711:PHE:CD1	2.57	0.40
1:C:425:MET:HE1	1:C:475:SER:HB2	2.03	0.40
1:B:728:ILE:HA	1:B:728:ILE:HD12	1.97	0.40
1:A:224:LEU:HA	1:A:227:VAL:CG2	2.51	0.40
1:D:512:TYR:HA	1:D:534:MET:HE3	2.03	0.40
1:A:491:ILE:HG22	1:A:492:ALA:N	2.36	0.40
1:A:496:ARG:C	1:A:498:HIS:H	2.25	0.40
1:A:530:VAL:HB	1:A:531:PRO:CD	2.47	0.40
1:A:577:VAL:O	1:A:664:CYS:HA	2.21	0.40
1:B:651:TYR:HE2	1:B:664:CYS:O	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:ILE:HG23	1:D:537:ALA:HB2	2.03	0.40
1:D:156:LYS:HD2	1:D:156:LYS:HA	1.82	0.40
1:B:239:LEU:HA	1:B:240:PRO:HD3	1.83	0.40
1:B:586:TYR:CE1	1:B:743:HIS:HD2	2.40	0.40
1:D:23:ALA:O	1:D:25:LYS:HG3	2.21	0.40
1:C:667:ASN:OD1	1:D:670:GLY:HA3	2.22	0.40
1:C:390:ASN:OD1	1:C:688:LYS:HE2	2.21	0.40
1:A:179:CYS:SG	1:A:363:MET:HB2	2.62	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	731/812 (90%)	610 (83%)	95 (13%)	26 (4%)	4	34
1	B	745/812 (92%)	631 (85%)	87 (12%)	27 (4%)	4	34
1	C	739/812 (91%)	620 (84%)	97 (13%)	22 (3%)	5	39
1	D	739/812 (91%)	618 (84%)	101 (14%)	20 (3%)	6	41
All	All	2954/3248 (91%)	2479 (84%)	380 (13%)	95 (3%)	5	38

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	724	LYS
1	B	724	LYS
1	C	19	HIS
1	C	724	LYS
1	D	714	ASP
1	A	402	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	523	GLU
1	A	659	LYS
1	A	675	GLY
1	B	69	ASP
1	B	374	ARG
1	B	402	PRO
1	B	485	GLY
1	B	659	LYS
1	B	675	GLY
1	B	676	GLY
1	C	69	ASP
1	C	486	LYS
1	C	659	LYS
1	C	675	GLY
1	D	69	ASP
1	D	280	ASN
1	D	307	HIS
1	D	402	PRO
1	D	659	LYS
1	D	675	GLY
1	D	724	LYS
1	D	751	TRP
1	A	19	HIS
1	A	34	GLY
1	A	158	ALA
1	A	280	ASN
1	A	307	HIS
1	A	751	TRP
1	A	762	ALA
1	B	82	VAL
1	B	280	ASN
1	B	490	GLU
1	B	524	LYS
1	B	703	GLU
1	B	751	TRP
1	C	35	ASP
1	C	82	VAL
1	C	173	SER
1	C	185	ILE
1	C	307	HIS
1	C	402	PRO
1	C	524	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	82	VAL
1	D	100	ALA
1	D	466	VAL
1	D	676	GLY
1	D	713	THR
1	D	715	ASP
1	A	18	GLU
1	A	35	ASP
1	A	265	ARG
1	A	396	ARG
1	A	466	VAL
1	A	676	GLY
1	B	35	ASP
1	B	100	ALA
1	B	173	SER
1	B	185	ILE
1	B	265	ARG
1	B	307	HIS
1	B	466	VAL
1	B	479	THR
1	C	34	GLY
1	C	100	ALA
1	C	280	ASN
1	D	34	GLY
1	D	35	ASP
1	D	498	HIS
1	A	82	VAL
1	A	295	GLN
1	A	479	THR
1	A	485	GLY
1	A	527	GLU
1	B	626	MET
1	C	265	ARG
1	C	466	VAL
1	C	607	GLU
1	D	265	ARG
1	A	100	ALA
1	B	489	GLU
1	C	751	TRP
1	C	306	GLY
1	C	485	GLY
1	D	306	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	34	GLY
1	B	306	GLY
1	A	185	ILE
1	B	584	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	594/658 (90%)	516 (87%)	78 (13%)	5	25
1	B	602/658 (92%)	529 (88%)	73 (12%)	6	28
1	C	598/658 (91%)	518 (87%)	80 (13%)	5	24
1	D	598/658 (91%)	517 (86%)	81 (14%)	5	24
All	All	2392/2632 (91%)	2080 (87%)	312 (13%)	5	25

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	25	LYS
1	A	49	MET
1	A	53	VAL
1	A	57	VAL
1	A	65	GLN
1	A	86	LEU
1	A	97	ARG
1	A	105	GLU
1	A	108	LEU
1	A	128	ASP
1	A	138	ARG
1	A	154	ILE
1	A	179	CYS
1	A	191	LEU
1	A	192	HIS
1	A	206	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	LEU
1	A	230	LEU
1	A	249	GLU
1	A	260	ARG
1	A	265	ARG
1	A	266	LEU
1	A	268	ILE
1	A	293	VAL
1	A	301	ARG
1	A	303	THR
1	A	313	THR
1	A	318	ASP
1	A	325	MET
1	A	331	ILE
1	A	334	LEU
1	A	343	CYS
1	A	365	GLN
1	A	374	ARG
1	A	382	LEU
1	A	387	PHE
1	A	391	LEU
1	A	396	ARG
1	A	401	LEU
1	A	402	PRO
1	A	403	ASP
1	A	439	ASP
1	A	453	PHE
1	A	470	THR
1	A	481	ARG
1	A	483	LEU
1	A	489	GLU
1	A	510	GLU
1	A	516	LEU
1	A	541	ASN
1	A	557	ASN
1	A	567	LYS
1	A	574	LYS
1	A	575	ARG
1	A	582	THR
1	A	592	ASN
1	A	610	PHE
1	A	611	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	616	GLN
1	A	617	SER
1	A	624	GLU
1	A	631	GLN
1	A	635	VAL
1	A	637	ARG
1	A	659	LYS
1	A	671	HIS
1	A	674	GLN
1	A	689	ILE
1	A	690	SER
1	A	714	ASP
1	A	715	ASP
1	A	717	ILE
1	A	748	GLU
1	A	755	ARG
1	A	760	ILE
1	A	761	LEU
1	A	763	LYS
1	B	13	LEU
1	B	27	ILE
1	B	49	MET
1	B	53	VAL
1	B	59	PHE
1	B	65	GLN
1	B	86	LEU
1	B	108	LEU
1	B	128	ASP
1	B	138	ARG
1	B	154	ILE
1	B	165	LEU
1	B	179	CYS
1	B	191	LEU
1	B	192	HIS
1	B	214	LEU
1	B	230	LEU
1	B	249	GLU
1	B	260	ARG
1	B	265	ARG
1	B	266	LEU
1	B	268	ILE
1	B	293	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	ARG
1	B	303	THR
1	B	313	THR
1	B	318	ASP
1	B	325	MET
1	B	331	ILE
1	B	334	LEU
1	B	343	CYS
1	B	362	GLN
1	B	365	GLN
1	B	382	LEU
1	B	387	PHE
1	B	391	LEU
1	B	395	LYS
1	B	396	ARG
1	B	401	LEU
1	B	404	ASP
1	B	439	ASP
1	B	453	PHE
1	B	470	THR
1	B	487	TYR
1	B	501	ASN
1	B	517	GLU
1	B	524	LYS
1	B	530	VAL
1	B	541	ASN
1	B	557	ASN
1	B	563	CYS
1	B	567	LYS
1	B	569	SER
1	B	576	ARG
1	B	582	THR
1	B	592	ASN
1	B	610	PHE
1	B	618	ASN
1	B	631	GLN
1	B	635	VAL
1	B	637	ARG
1	B	659	LYS
1	B	665	ARG
1	B	671	HIS
1	B	674	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	690	SER
1	B	701	LEU
1	B	702	LYS
1	B	738	GLN
1	B	755	ARG
1	B	757	LEU
1	B	758	MET
1	B	760	ILE
1	C	16	PHE
1	C	18	GLU
1	C	19	HIS
1	C	21	SER
1	C	27	ILE
1	C	49	MET
1	C	57	VAL
1	C	59	PHE
1	C	65	GLN
1	C	86	LEU
1	C	87	GLN
1	C	108	LEU
1	C	128	ASP
1	C	130	SER
1	C	138	ARG
1	C	139	LYS
1	C	146	GLU
1	C	154	ILE
1	C	179	CYS
1	C	191	LEU
1	C	192	HIS
1	C	214	LEU
1	C	219	ARG
1	C	230	LEU
1	C	249	GLU
1	C	258	GLU
1	C	260	ARG
1	C	265	ARG
1	C	266	LEU
1	C	268	ILE
1	C	293	VAL
1	C	301	ARG
1	C	303	THR
1	C	308	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	318	ASP
1	C	325	MET
1	C	331	ILE
1	C	334	LEU
1	C	343	CYS
1	C	351	HIS
1	C	358	MET
1	C	365	GLN
1	C	374	ARG
1	C	382	LEU
1	C	385	ARG
1	C	387	PHE
1	C	391	LEU
1	C	396	ARG
1	C	401	LEU
1	C	403	ASP
1	C	439	ASP
1	C	453	PHE
1	C	457	GLN
1	C	470	THR
1	C	503	LEU
1	C	524	LYS
1	C	526	GLU
1	C	530	VAL
1	C	541	ASN
1	C	557	ASN
1	C	568	GLN
1	C	575	ARG
1	C	582	THR
1	C	583	MET
1	C	592	ASN
1	C	610	PHE
1	C	624	GLU
1	C	631	GLN
1	C	635	VAL
1	C	637	ARG
1	C	659	LYS
1	C	674	GLN
1	C	689	ILE
1	C	690	SER
1	C	711	PHE
1	C	715	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	755	ARG
1	C	757	LEU
1	C	760	ILE
1	C	761	LEU
1	D	16	PHE
1	D	20	LEU
1	D	27	ILE
1	D	29	VAL
1	D	44	ARG
1	D	49	MET
1	D	53	VAL
1	D	59	PHE
1	D	65	GLN
1	D	86	LEU
1	D	87	GLN
1	D	97	ARG
1	D	99	GLN
1	D	108	LEU
1	D	128	ASP
1	D	130	SER
1	D	138	ARG
1	D	142	SER
1	D	154	ILE
1	D	179	CYS
1	D	191	LEU
1	D	192	HIS
1	D	206	GLN
1	D	214	LEU
1	D	219	ARG
1	D	230	LEU
1	D	249	GLU
1	D	260	ARG
1	D	265	ARG
1	D	266	LEU
1	D	268	ILE
1	D	293	VAL
1	D	301	ARG
1	D	303	THR
1	D	318	ASP
1	D	325	MET
1	D	331	ILE
1	D	334	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	351	HIS
1	D	365	GLN
1	D	374	ARG
1	D	382	LEU
1	D	385	ARG
1	D	387	PHE
1	D	396	ARG
1	D	401	LEU
1	D	403	ASP
1	D	439	ASP
1	D	453	PHE
1	D	470	THR
1	D	475	SER
1	D	487	TYR
1	D	488	LEU
1	D	489	GLU
1	D	510	GLU
1	D	512	TYR
1	D	516	LEU
1	D	519	SER
1	D	530	VAL
1	D	534	MET
1	D	540	SER
1	D	541	ASN
1	D	557	ASN
1	D	567	LYS
1	D	582	THR
1	D	592	ASN
1	D	610	PHE
1	D	624	GLU
1	D	630	ILE
1	D	637	ARG
1	D	671	HIS
1	D	674	GLN
1	D	690	SER
1	D	701	LEU
1	D	714	ASP
1	D	715	ASP
1	D	718	CYS
1	D	755	ARG
1	D	757	LEU
1	D	760	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	763	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	73	ASN
1	A	87	GLN
1	A	116	GLN
1	A	135	ASN
1	A	206	GLN
1	A	417	ASN
1	A	616	GLN
1	A	618	ASN
1	A	667	ASN
1	A	674	GLN
1	B	65	GLN
1	B	113	ASN
1	B	116	GLN
1	B	135	ASN
1	B	153	GLN
1	B	192	HIS
1	B	208	HIS
1	B	267	ASN
1	B	417	ASN
1	B	568	GLN
1	B	644	ASN
1	B	652	GLN
1	B	673	GLN
1	C	65	GLN
1	C	73	ASN
1	C	113	ASN
1	C	116	GLN
1	C	153	GLN
1	C	192	HIS
1	C	295	GLN
1	C	365	GLN
1	C	457	GLN
1	C	498	HIS
1	C	592	ASN
1	C	616	GLN
1	C	652	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	65	GLN
1	D	73	ASN
1	D	113	ASN
1	D	116	GLN
1	D	135	ASN
1	D	153	GLN
1	D	192	HIS
1	D	206	GLN
1	D	208	HIS
1	D	417	ASN
1	D	457	GLN
1	D	494	GLN
1	D	498	HIS
1	D	541	ASN
1	D	592	ASN
1	D	667	ASN
1	D	674	GLN
1	D	730	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	801	-	22,29,29	1.41	2 (9%)	27,45,45	1.21	4 (14%)
3	PO4	A	802	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	A	803	-	4,4,4	0.89	0	6,6,6	0.27	0
3	PO4	A	804	-	4,4,4	1.11	0	6,6,6	0.27	0
2	ADP	B	801	-	22,29,29	1.67	3 (13%)	27,45,45	1.20	2 (7%)
3	PO4	B	802	-	4,4,4	1.01	0	6,6,6	0.27	0
3	PO4	B	803	-	4,4,4	1.01	0	6,6,6	0.27	0
2	ADP	C	801	-	22,29,29	1.58	3 (13%)	27,45,45	1.09	3 (11%)
3	PO4	C	802	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	C	803	-	4,4,4	1.06	0	6,6,6	0.28	0
3	PO4	C	804	-	4,4,4	0.97	0	6,6,6	0.27	0
3	PO4	C	805	-	4,4,4	1.04	0	6,6,6	0.27	0
3	PO4	D	801	-	4,4,4	1.03	0	6,6,6	0.27	0
2	ADP	D	802	-	22,29,29	1.85	4 (18%)	27,45,45	1.38	4 (14%)
3	PO4	D	803	-	4,4,4	1.08	0	6,6,6	0.27	0
3	PO4	D	804	-	4,4,4	1.05	0	6,6,6	0.27	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	ADP	A	801	-	-	0/12/32/32	0/3/3/3
3	PO4	A	802	-	-	0/0/0/0	0/0/0/0
3	PO4	A	803	-	-	0/0/0/0	0/0/0/0
3	PO4	A	804	-	-	0/0/0/0	0/0/0/0
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
3	PO4	B	802	-	-	0/0/0/0	0/0/0/0
3	PO4	B	803	-	-	0/0/0/0	0/0/0/0
2	ADP	C	801	-	-	0/12/32/32	0/3/3/3
3	PO4	C	802	-	-	0/0/0/0	0/0/0/0
3	PO4	C	803	-	-	0/0/0/0	0/0/0/0
3	PO4	C	804	-	-	0/0/0/0	0/0/0/0
3	PO4	C	805	-	-	0/0/0/0	0/0/0/0
3	PO4	D	801	-	-	0/0/0/0	0/0/0/0
2	ADP	D	802	-	-	0/12/32/32	0/3/3/3
3	PO4	D	803	-	-	0/0/0/0	0/0/0/0
3	PO4	D	804	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ADP	PB-O2B	-2.13	1.47	1.54
2	D	802	ADP	C4-N3	2.15	1.38	1.35
2	B	801	ADP	O4'-C1'	2.52	1.44	1.41
2	B	801	ADP	C4-N3	2.53	1.39	1.35
2	C	801	ADP	O4'-C1'	2.77	1.44	1.41
2	C	801	ADP	C4-N3	2.82	1.39	1.35
2	A	801	ADP	O4'-C1'	3.61	1.45	1.41
2	D	802	ADP	O4'-C1'	3.73	1.45	1.41
2	A	801	ADP	PB-O3B	3.84	1.68	1.54
2	C	801	ADP	PB-O3B	4.16	1.69	1.54
2	B	801	ADP	PB-O1B	5.64	1.69	1.51
2	D	802	ADP	PB-O1B	6.09	1.71	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	ADP	O2B-PB-O1B	-2.51	102.49	110.58
2	D	802	ADP	C1'-N9-C4	-2.36	123.38	126.94
2	C	801	ADP	C1'-N9-C4	-2.11	123.75	126.94
2	B	801	ADP	O3A-PA-O5'	2.02	108.30	102.94
2	C	801	ADP	O3A-PA-O5'	2.05	108.38	102.94
2	A	801	ADP	O3A-PA-O5'	2.08	108.46	102.94
2	B	801	ADP	O5'-C5'-C4'	2.18	117.17	109.12
2	C	801	ADP	O5'-C5'-C4'	2.27	117.50	109.12
2	A	801	ADP	O2B-PB-O3A	2.40	115.98	105.09
2	A	801	ADP	O5'-C5'-C4'	2.52	118.42	109.12
2	A	801	ADP	O4'-C1'-N9	2.69	113.72	108.10
2	D	802	ADP	O5'-C5'-C4'	2.93	119.92	109.12
2	D	802	ADP	O4'-C1'-N9	3.17	114.73	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	2	0
3	A	803	PO4	2	0
2	B	801	ADP	1	0
2	C	801	ADP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	805	PO4	1	0
3	D	801	PO4	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	737/812 (90%)	-0.14	4 (0%) 91 89	27, 73, 113, 162	0
1	B	749/812 (92%)	-0.09	7 (0%) 85 81	25, 75, 114, 162	0
1	C	743/812 (91%)	-0.14	3 (0%) 93 91	26, 73, 112, 161	0
1	D	743/812 (91%)	-0.12	4 (0%) 91 89	29, 74, 113, 162	0
All	All	2972/3248 (91%)	-0.12	18 (0%) 90 86	25, 74, 113, 162	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.3
1	D	343	CYS	3.0
1	B	205	ALA	2.9
1	B	59	PHE	2.9
1	C	347	LEU	2.6
1	B	206	GLN	2.5
1	B	621	HIS	2.5
1	A	246	GLU	2.4
1	D	360	CYS	2.3
1	A	675	GLY	2.3
1	B	379	ALA	2.2
1	B	29	VAL	2.2
1	D	344	VAL	2.2
1	D	122	LEU	2.2
1	A	278	THR	2.2
1	C	59	PHE	2.1
1	B	718	CYS	2.1
1	C	164	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	C	801	27/27	0.93	0.18	-0.20	35,98,135,151	0
3	PO4	C	804	5/5	0.90	0.19	-0.24	6,89,105,127	0
2	ADP	A	801	27/27	0.94	0.19	-0.30	1,73,118,137	0
2	ADP	B	801	27/27	0.91	0.17	-0.40	21,98,154,163	0
2	ADP	D	802	27/27	0.94	0.21	-0.63	1,91,129,134	0
3	PO4	B	803	5/5	0.95	0.16	-1.02	7,34,89,107	0
3	PO4	A	803	5/5	0.91	0.17	-1.13	17,29,126,144	0
3	PO4	D	801	5/5	0.96	0.14	-1.15	14,27,57,97	0
3	PO4	A	804	5/5	0.99	0.13	-1.35	4,10,57,70	0
3	PO4	C	802	5/5	0.97	0.12	-1.38	1,66,70,97	0
3	PO4	A	802	5/5	0.97	0.13	-1.41	1,67,103,108	0
3	PO4	B	802	5/5	0.95	0.12	-1.62	16,71,134,135	0
3	PO4	D	804	5/5	0.98	0.13	-1.64	18,41,68,78	0
3	PO4	C	803	5/5	0.94	0.15	-1.73	1,20,85,87	0
3	PO4	D	803	5/5	0.97	0.10	-2.43	31,32,74,82	0
3	PO4	C	805	5/5	0.91	0.12	-2.51	65,81,155,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.