



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:56 PM UTC

PDB ID : 3BG9 / pdb_00003bg9
Title : Crystal Structure of Human Pyruvate Carboxylase (missing the biotin carboxylase domain at the N-terminus) F1077A Mutant
Authors : Xiang, S.; Tong, L.
Deposited on : 2007-11-26
Resolution : 3.00 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

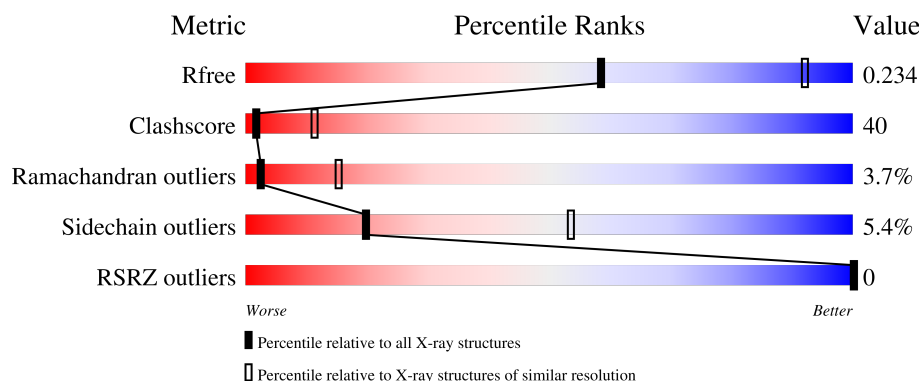
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

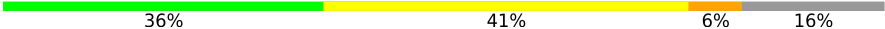
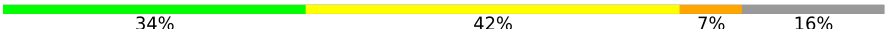
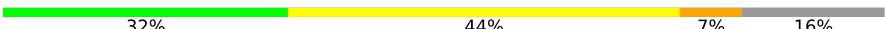
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	718	
1	B	718	
1	C	718	
1	D	718	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18516 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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	B	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	C	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	D	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	MET	-	expression tag	UNP P11498
A	462	GLY	-	expression tag	UNP P11498
A	463	SER	-	expression tag	UNP P11498
A	464	SER	-	expression tag	UNP P11498
A	465	HIS	-	expression tag	UNP P11498
A	466	HIS	-	expression tag	UNP P11498
A	467	HIS	-	expression tag	UNP P11498
A	468	HIS	-	expression tag	UNP P11498
A	469	HIS	-	expression tag	UNP P11498
A	470	HIS	-	expression tag	UNP P11498
A	471	SER	-	expression tag	UNP P11498
A	472	SER	-	expression tag	UNP P11498
A	473	GLY	-	expression tag	UNP P11498
A	474	LEU	-	expression tag	UNP P11498
A	475	VAL	-	expression tag	UNP P11498
A	476	PRO	-	expression tag	UNP P11498
A	477	ARG	-	expression tag	UNP P11498
A	478	GLY	-	expression tag	UNP P11498
A	479	SER	-	expression tag	UNP P11498
A	480	HIS	-	expression tag	UNP P11498
A	481	MET	-	expression tag	UNP P11498

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP P11498
B	461	MET	-	expression tag	UNP P11498
B	462	GLY	-	expression tag	UNP P11498
B	463	SER	-	expression tag	UNP P11498
B	464	SER	-	expression tag	UNP P11498
B	465	HIS	-	expression tag	UNP P11498
B	466	HIS	-	expression tag	UNP P11498
B	467	HIS	-	expression tag	UNP P11498
B	468	HIS	-	expression tag	UNP P11498
B	469	HIS	-	expression tag	UNP P11498
B	470	HIS	-	expression tag	UNP P11498
B	471	SER	-	expression tag	UNP P11498
B	472	SER	-	expression tag	UNP P11498
B	473	GLY	-	expression tag	UNP P11498
B	474	LEU	-	expression tag	UNP P11498
B	475	VAL	-	expression tag	UNP P11498
B	476	PRO	-	expression tag	UNP P11498
B	477	ARG	-	expression tag	UNP P11498
B	478	GLY	-	expression tag	UNP P11498
B	479	SER	-	expression tag	UNP P11498
B	480	HIS	-	expression tag	UNP P11498
B	481	MET	-	expression tag	UNP P11498
B	1077	ALA	PHE	engineered mutation	UNP P11498
C	461	MET	-	expression tag	UNP P11498
C	462	GLY	-	expression tag	UNP P11498
C	463	SER	-	expression tag	UNP P11498
C	464	SER	-	expression tag	UNP P11498
C	465	HIS	-	expression tag	UNP P11498
C	466	HIS	-	expression tag	UNP P11498
C	467	HIS	-	expression tag	UNP P11498
C	468	HIS	-	expression tag	UNP P11498
C	469	HIS	-	expression tag	UNP P11498
C	470	HIS	-	expression tag	UNP P11498
C	471	SER	-	expression tag	UNP P11498
C	472	SER	-	expression tag	UNP P11498
C	473	GLY	-	expression tag	UNP P11498
C	474	LEU	-	expression tag	UNP P11498
C	475	VAL	-	expression tag	UNP P11498
C	476	PRO	-	expression tag	UNP P11498
C	477	ARG	-	expression tag	UNP P11498
C	478	GLY	-	expression tag	UNP P11498
C	479	SER	-	expression tag	UNP P11498

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	480	HIS	-	expression tag	UNP P11498
C	481	MET	-	expression tag	UNP P11498
C	1077	ALA	PHE	engineered mutation	UNP P11498
D	461	MET	-	expression tag	UNP P11498
D	462	GLY	-	expression tag	UNP P11498
D	463	SER	-	expression tag	UNP P11498
D	464	SER	-	expression tag	UNP P11498
D	465	HIS	-	expression tag	UNP P11498
D	466	HIS	-	expression tag	UNP P11498
D	467	HIS	-	expression tag	UNP P11498
D	468	HIS	-	expression tag	UNP P11498
D	469	HIS	-	expression tag	UNP P11498
D	470	HIS	-	expression tag	UNP P11498
D	471	SER	-	expression tag	UNP P11498
D	472	SER	-	expression tag	UNP P11498
D	473	GLY	-	expression tag	UNP P11498
D	474	LEU	-	expression tag	UNP P11498
D	475	VAL	-	expression tag	UNP P11498
D	476	PRO	-	expression tag	UNP P11498
D	477	ARG	-	expression tag	UNP P11498
D	478	GLY	-	expression tag	UNP P11498
D	479	SER	-	expression tag	UNP P11498
D	480	HIS	-	expression tag	UNP P11498
D	481	MET	-	expression tag	UNP P11498
D	1077	ALA	PHE	engineered mutation	UNP P11498

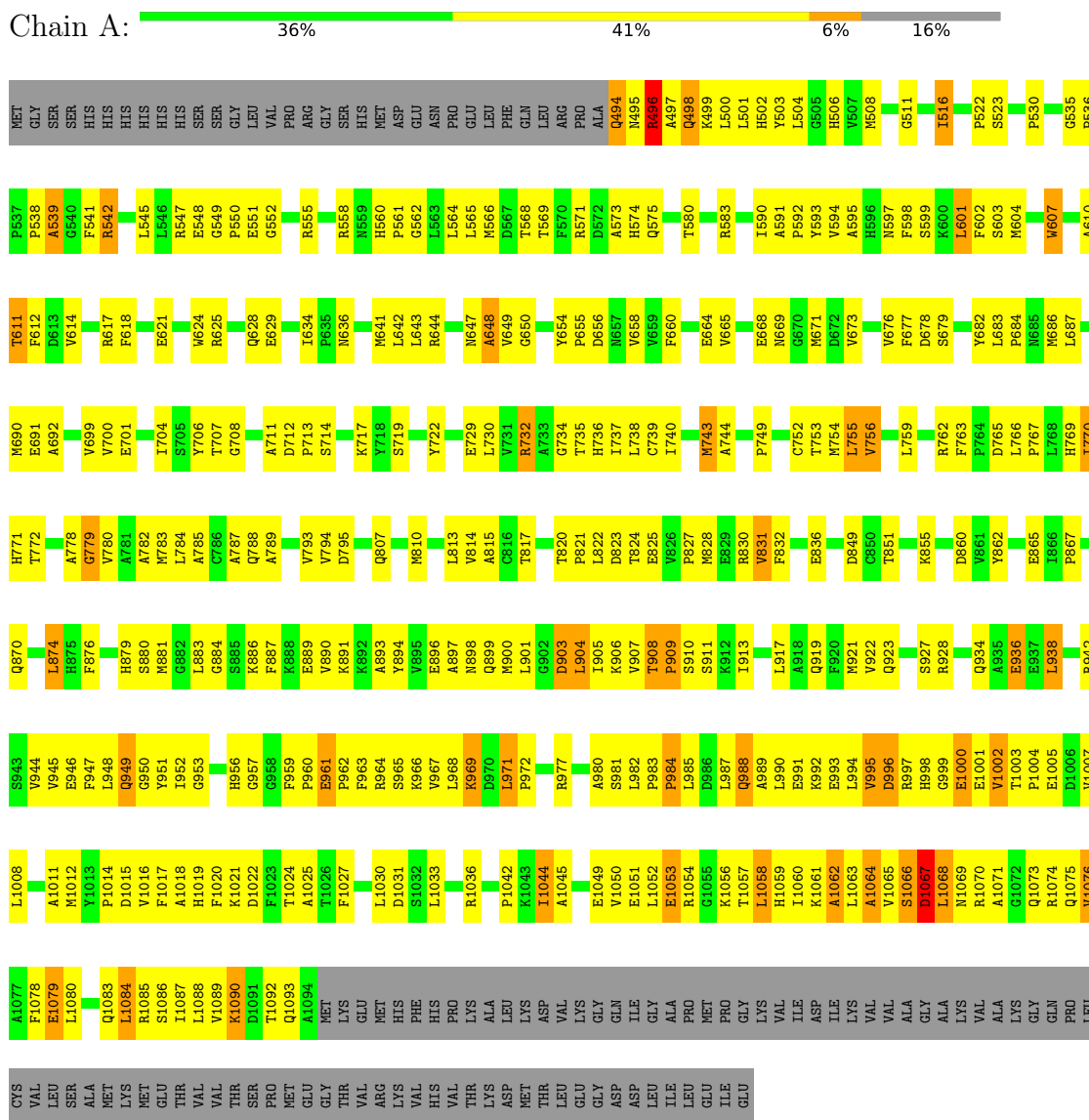
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

3 Residue-property plots

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

• Molecule 1: Pyruvate carboxylase, mitochondrial

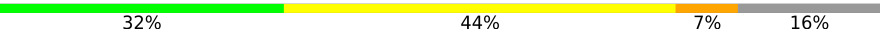


• Molecule 1: Pyruvate carboxylase, mitochondrial



VAL	V1065	V995	R928	K855	F763	M686	F612	G535
ALA	S1066	D996		S856	P764	L687		P536
GLY	D1067	R997			G765	L688	R617	P537
ALA	L1068	H998	A935	S859	L766	G689		P538
LYS	N1069	G999	E936	S859	P767	M690		A539
VAL	R1070	E1000	E937	D860	L768	E691	W624	G540
ALA	A1071	E1001	L938	V861	H769		R625	F541
LYS	G1072	V1002	S939	N864	T772	S695	Q628	R542
GLY	Q1073	T1003	F940	E865			E629	D543
GLN	R1074	P1004	P941		A778	G698	L630	I544
PRO	Q1075		R942	Q870	G779	V699	R631	L545
LEU	V1076	V1007			V790	G699		L546
CYS	A1077	L1008	V945	N873		V700	E632	R547
VAL	F1078	S1009	E946	L874	M783	E701	L633	G548
LEU	E1079	A1010	F947		A702	G549	I634	E549
SER	L1080	A1011	L948		A703	P635		P550
ALA		M1012	Q949	Q877	L785	I704	N636	E551
MET	Q1083	Y1013		A878	G786	S705	I637	G552
LYS	L1084	D1014	G952	H879	A787			
MET	R1085	P1015	Y953	Q788	T707	F639		R555
GLU	S1086	V1016	V954	L883	G708		Q640	
THR	L1087	M1017	P955	G884	D709	M641		R558
VAL	L1088	A1018	H956	S885	V710	L642		
VAL	V1089	H1019	G957	K886	A711	L643		P561
THR	K1090	F1020	G958	E889	S802	R644		
SER	D1091	K1021	F959	V890	P713	L564		L564
PRO	T1092	D1022	P960	K891	G845	A546		L565
MET	Q1093		E961	S892	Q807	N647		M566
GLY	A1094	T1024	P962		A648			
MET		A1025	F963	A893	S719			
GLY		T1026	R964	R894		V649		T569
THR	LYS	F1027	S965	V895	Y722	G650		F570
VAL	GLU	G1028	K966	E896		R571		ARG
ARG	MET	P1029	V967	R897	L726	N652		D572
LYS	THR	L1030	L968	N898	R732	Y654		A573
VAL	PHE	D1031	K969	Q899	A733	P655		H574
HIS					G734	P655		Q575
VAL	PRO		P970	M900	T817	D656		
VAL	THR	T1035	L971	G902	R818	N657		T580
LYS	ALA		P972	L901	G819	V658		
ASP	LYS	P1042	R973	D903	T820			L500
MET	LYS	K1043	V974	L904	R821	L738		L501
MET	ASP	I1044		I905	L822	C739		L502
LEU	VAL	A1045		K906	D823			
LEU	GLY		R977	V907	T824	D742		E590
GLY	GLY	E1049	G979	P908		M743		A591
ASP	GLN	V1050	A980	P909	P827			P592
ASP	ILE	E1051	S981	S910	M828	L747		Y593
LEU	GLY	L1052	L982	S911	E829	K748		V594
ILE	ALA	E1053	P983		R830	P749		A595
PRO	ALA	R1054	P984	I913	W831	T750		M508
LEU	PRO	G1055	L985	V914	F832	A751		N597
GLU	MET	K1056	D986	G915	D833	C752		F598
ILE	PRO	T1057	L987	D916		V676		N510
GLY	GLY			L917		D678		S599
LYS	LYS	L1058	Q988	L918	E836	T753		K600
VAL	VAL	H1059	A989	A918		S679		L601
ILE	ILE	L1060	L990	Q919	L755	L680		F602
ASP	ASP	K1061	E991	N881	V756	N681		S603
ILE	ILE	A1062	K992	F848	L759	Y682		M604
VAL	VAL	L1063	F993	D850		L683		E532
VAL	VAL	A1064	L994	T851		P684		N606
VAL	VAL							F533
VAL	VAL							I534

• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain C:  32% 44% 7% 16%

V756	V676	K600	T534	MET
L759	F677	L601	G535	GLY
R762	F678	F602	P536	SER
F763	S679	S603	P537	SER
P764	L680	M604	P538	HIS
D765	K681	E605	A539	HIS
L766	Y682	N606		HIS
P767	L683	W607	R542	HIS
L768	P684		D543	HIS
H769	N685	F612	I544	HIS
T770	M686	D613	L545	SER
H771	L687	V614	L546	SER
T772	M690	R617	E548	GLY
A778	E691		G549	LEU
G779	A696	W624	P550	PRO
V780	V699		E551	ARG
M783	V700	Q628	G552	GLY
L784	E701	P553	P553	SER
A787	T704	E632	A554	HIS
Q788	S705	L633	R555	MET
A789	Y706	I634	A556	ASP
	T707	K635	V557	GLU
V793	G708	N636	R558	ASN
V794	T709	I637	N559	PRO
D795	G710	P638	H560	GLU
	A711		P561	LEU
Q807	P712	M641	G562	PHE
S809	D713	L642	L563	GLN
M810	S714	L643	L564	LEU
	K717	R644	L565	ARG
L813	T718	G645	M566	PRO
V814	S719	A646		ALA
A815	Y722	E648	T569	Q494
C816		V649	F570	N495
T817	R732	G650	R571	R496
R818	A733	T651	D572	A497
G819	G734	R552	A573	Q498
T820	T735	N653	H574	K499
P821	H736	N654	Q575	L500
L822	L737	P658		L501
D823	L738	V659	A579	H502
T824	C739	F660	T580	Y503
	I740	K661	L584	L504
E825			G586	G505
V826	M743	E664	L587	H506
P827	A744	V665		V507
R829		A666	T590	M508
R830	P749	K667	A591	V509
V831	T750	E668	P592	N510
F832	A751	N669	L593	G511
	L752	G670	V594	I516
Y837	T753	M671	A595	P517
	M754	D672	H596	P527
	L755	F673	N597	V528
			F598	P530
			S599	A531
				V532
				N533
				I534

GLY	T1057	E991	A918	F848
LYS	L1068	K992	Q919	D849
VAL	H1059	E993	F920	C850
ILE	I1060	L994	M921	T851
ASP	K1061	V995	V922	K855
ILE	A1062	D996	Q923	
LYS	L1063	E997	N924	
VAL	A1064	H998		S859
VAL	V1065	G999	R928	D860
ALA	S1066	E1000		V861
GLY	D1067	E1001	E932	
ALA	L1068	V1002	A933	N864
LYS	R1069	T1003	Q934	E865
VAL	A1070	P1004	A935	I866
ALA	G1072	E1005	E936	P867
GLY	Q1073	V1007	E937	
GLN	R1074	L1008	L938	Q870
PRO	Q1075	S1009	R942	L874
LEU	V1076	A1010		F876
MET	A1077	V945		
LYS	L1083	E946		H879
MET	R1084	F947		S880
GLY	L1085	L948		M881
GLN	S1086	Q949		G882
THR	I1087	I952		L883
VAL	L1088	G953		G884
VAL	V1089	V954		S885
THR	K1090	P955		K886
THR	A1091	H956		F887
GLY	T1092	G957		G888
MET	Q1093	G958		E889
GLY	A1094	F959		K892
THR	MET	P960		N898
GLY	GLY	E961		Q899
THR	THR	P962		L901
VAL	GLU	F963		G902
VAL	L500	S965		D903
ARG	L501	K966		L904
LYS	H502	V967		I905
VAL	Y503	L968		K906
HIS	L504	K969		V907
VAL	G505	D970		T908
THR	V507	L971		P909
ASP	M508			S910
THR	G511			G912
LEU	T516			I913
GLY	P517			V914
ASP	P530			G915
ILE	G535			D916
GLU	P536			A988
P537	R617			E989
P538				L990

• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain D:  36% 41% 7% 16%

MET	E691	I770	Q870	R942	D1006	A1077	GLY
GLY	V699	A778	N873	S943	V1007	F1078	LYS
SER	E701	G779	L874	V944	L1008	E1079	VAL
HIS	I704	V780	H879	E946	A1010	N1081	ILE
HIS	S705	M783	S860	F947	M1012	G1082	ASP
HIS	T706	L784	M881	N948	P1014	Q1083	ILE
HIS	G708	A785	G882	G950	P1016	L1084	VAL
GLY	G708	C786	L883	Y951	D1015	S1086	VAL
GLY	A711	G884	G884	Y952	V1016	I1087	LYS
LEU	D712	A787	S885	Q963	A1017	L1088	VAL
VAL	P713	Q807	K866	V954	F1018	V1089	VAL
PRO	S714	M810	F887	H956	H1019	K1090	ALA
ARG	R715	D795	E889	G957	F1020	D1091	GLY
SER	T716	V794	V890	G958	K1021	T1092	GLY
PRO	K717	D795	K891	P960	D1022	Q1093	GLY
HIS	Y718	Q807	K892	E961	A1025	A1094	VAL
MET	S719	M810	A945	F962	T1026		LYS
ASP	L720	V895	Y894	P963	F1027		GLY
GLU	Q721	V895	R964	F964	G1028		ALA
ASN	Y722	L813	E896	S965	P1029		HIS
PRO	Y723	V814	A937	K966	L1030		PHE
GLU	H724	T817	N898	V967	D1031		HIS
LEU	A727	T820	Q999	L968	P1042		PRO
GLN	L730	P821	M900	K969	K1043		LYS
ARG	H574	P821	L901	S910	I1044		ALA
ARG	Q575	R731	G902	S911	A1045		LYS
PRO	N657	R732	D823	R912	E1046		ASP
ALA	T580	A733	T824	S981	E1049		VAL
ALA	R581	G734	E825	G976	V1050		LYS
ASP	T584	L735	V826	R977	E1051		GLY
GLY	K588	I737	P827	S981	L1052		ILE
GLY	A591	L737	M828	P909	E1053		GLY
THR	P592	L738	E829	S910	R1054		ALA
THR	P592	C739	R830	S911	G1055		PRO
GLY	E668	I740	V831	L985	T1057		PRO
GLY	E668	M743	F832	D986	L1058		GLY
GLY	E668	A744	E836	Q988	H1059		LYS
GLY	E668	A744	E836	A989	I1060		VAL
GLY	E668	A744	E836	L990	K1061		ILE
GLY	E668	A744	E836	E991	A1062		ASP
GLY	E668	A744	E836	K992	L1063		ILE
GLY	E668	A744	E836	E993	A1064		LYS
GLY	E668	A744	E836	L994	V1065		VAL
GLY	E668	A744	E836	V995	S1066		VAL
GLY	E668	A744	E836	D996	D1067		ALA
GLY	E668	A744	E836	R997	N1068		GLY
GLY	E668	A744	E836	H998	N1069		ALA
GLY	E668	A744	E836	G999	R1070		LYS
GLY	E668	A744	E836	E1001	A1071		VAL
GLY	E668	A744	E836	V1002	G1073		ALA
GLY	E668	A744	E836	E937	R1074		LYS
GLY	E668	A744	E836	P1004	Q1075		GLY
GLY	E668	A744	E836	E1005	V1076		PRO

LEU	CYS	VAL	LEU	SER	ALA	MET	LYS	MET	GLU	THR	VAL	VAL	THR	SER	PRO	MET	GLU	GLY	THR	VAL	ARG	LYS	VAL	HIS	VAL	THR	LYS	ASP	MET	THR	LEU	GLU	GLY	ASP	ASP	LEU	ILE	LEU	GLU	ILE	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.54Å 107.54Å 524.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	80.8 (30.00-3.00) 88.9 (30.00-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.236 0.193 , 0.234	Depositor DCC
R_{free} test set	2799 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.370 for -h,-k,l	Xtriage
Reported twinning fraction	0.366 for -h,-k,l	Depositor
Outliers	0 of 63285 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18516	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.58	0/4736	1.08	22/6428 (0.3%)
1	B	0.59	1/4736 (0.0%)	1.10	28/6428 (0.4%)
1	C	0.58	0/4736	1.09	32/6428 (0.5%)
1	D	0.60	0/4736	1.10	33/6428 (0.5%)
All	All	0.58	1/18944 (0.0%)	1.09	115/25712 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	536	PRO	CA-C	5.27	1.54	1.51

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	GLY	CA-C-N	13.55	129.56	119.66
1	B	535	GLY	C-N-CA	13.55	129.56	119.66
1	A	535	GLY	CA-C-N	8.91	129.56	120.38
1	A	535	GLY	C-N-CA	8.91	129.56	120.38
1	D	535	GLY	CA-C-N	8.74	129.38	120.38
1	D	535	GLY	C-N-CA	8.74	129.38	120.38
1	B	536	PRO	N-CA-C	8.69	118.82	110.47
1	D	904	LEU	N-CA-C	8.03	121.52	109.95
1	C	535	GLY	CA-C-N	8.02	128.64	120.38
1	C	535	GLY	C-N-CA	8.02	128.64	120.38
1	D	536	PRO	N-CA-C	7.72	120.12	110.70
1	A	995	VAL	N-CA-C	-7.67	103.06	110.42
1	B	904	LEU	N-CA-C	7.66	120.73	109.69
1	C	971	LEU	CA-C-N	7.60	128.79	119.98
1	C	971	LEU	C-N-CA	7.60	128.79	119.98
1	D	712	ASP	CA-C-N	7.38	127.09	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	712	ASP	C-N-CA	7.38	127.09	119.56
1	B	511	GLY	CA-C-N	7.35	129.02	119.84
1	B	511	GLY	C-N-CA	7.35	129.02	119.84
1	C	1065	VAL	N-CA-C	-7.31	97.80	107.88
1	A	511	GLY	CA-C-N	7.29	128.95	119.84
1	A	511	GLY	C-N-CA	7.29	128.95	119.84
1	A	1000	GLU	N-CA-C	-7.22	104.56	113.15
1	A	516	ILE	CA-C-N	7.04	127.02	119.28
1	A	516	ILE	C-N-CA	7.04	127.02	119.28
1	C	908	THR	CA-C-N	-6.94	111.16	119.84
1	C	908	THR	C-N-CA	-6.94	111.16	119.84
1	A	904	LEU	N-CA-C	6.92	119.65	109.69
1	A	536	PRO	N-CA-C	6.79	118.99	110.70
1	D	957	GLY	N-CA-C	-6.76	105.17	114.64
1	C	536	PRO	N-CA-C	6.59	118.74	110.70
1	A	949	GLN	N-CA-C	-6.58	104.83	112.92
1	D	1000	GLU	N-CA-C	-6.57	105.58	112.93
1	A	770	ILE	N-CA-C	6.55	117.30	107.80
1	B	971	LEU	CA-C-N	6.55	127.58	119.98
1	B	971	LEU	C-N-CA	6.55	127.58	119.98
1	C	1069	ASN	N-CA-C	6.46	121.95	113.30
1	C	516	ILE	CA-C-N	6.41	126.91	119.47
1	C	516	ILE	C-N-CA	6.41	126.91	119.47
1	C	957	GLY	N-CA-C	-6.39	105.80	115.00
1	C	961	GLU	N-CA-C	6.34	121.50	113.25
1	B	969	LYS	CB-CA-C	-6.33	109.28	116.63
1	D	961	GLU	N-CA-C	6.33	122.25	113.45
1	A	541	PHE	N-CA-C	6.29	119.11	111.82
1	A	961	GLU	N-CA-C	6.21	121.32	113.25
1	D	511	GLY	CA-C-N	6.18	127.56	119.84
1	D	511	GLY	C-N-CA	6.18	127.56	119.84
1	A	969	LYS	CB-CA-C	-6.16	109.48	116.63
1	C	1028	GLY	CA-C-N	5.91	127.23	119.84
1	C	1028	GLY	C-N-CA	5.91	127.23	119.84
1	A	927	SER	N-CA-C	-5.90	102.74	110.53
1	C	826	VAL	CA-C-N	5.90	127.22	119.84
1	C	826	VAL	C-N-CA	5.90	127.22	119.84
1	C	1000	GLU	N-CA-C	-5.90	106.32	112.93
1	C	763	PHE	CA-C-N	5.88	127.19	119.84
1	C	763	PHE	C-N-CA	5.88	127.19	119.84
1	B	961	GLU	N-CA-C	5.84	120.84	113.25
1	D	631	ARG	N-CA-C	-5.81	105.03	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	496	ARG	N-CA-C	-5.80	103.94	111.02
1	B	509	VAL	N-CA-C	5.80	115.99	110.42
1	D	541	PHE	N-CA-C	5.77	117.65	111.36
1	A	496	ARG	N-CA-C	-5.74	104.02	111.02
1	B	637	ILE	N-CA-C	5.70	114.11	107.89
1	C	614	VAL	N-CA-C	5.64	117.05	110.62
1	B	541	PHE	N-CA-C	5.63	118.36	111.82
1	B	631	ARG	N-CA-C	-5.63	105.14	111.28
1	C	949	GLN	N-CA-C	-5.63	106.18	113.16
1	C	905	ILE	N-CA-C	-5.63	99.04	107.37
1	B	938	LEU	N-CA-C	-5.60	100.23	108.79
1	B	1069	ASN	N-CA-C	5.57	120.96	113.72
1	B	957	GLY	N-CA-C	-5.57	106.98	115.00
1	D	1069	ASN	N-CA-C	5.55	120.94	113.72
1	D	516	ILE	CA-C-N	5.55	125.64	119.32
1	D	516	ILE	C-N-CA	5.55	125.64	119.32
1	B	763	PHE	CA-C-N	5.54	126.76	119.84
1	B	763	PHE	C-N-CA	5.54	126.76	119.84
1	B	908	THR	CA-C-N	-5.45	113.03	119.84
1	B	908	THR	C-N-CA	-5.45	113.03	119.84
1	B	1057	THR	N-CA-C	-5.43	107.20	113.88
1	C	706	TYR	N-CA-C	5.42	118.08	109.24
1	C	712	ASP	CA-C-N	5.42	125.24	119.28
1	C	712	ASP	C-N-CA	5.42	125.24	119.28
1	A	1053	GLU	CB-CA-C	-5.42	109.86	117.23
1	B	516	ILE	CA-C-N	5.39	125.47	119.32
1	B	516	ILE	C-N-CA	5.39	125.47	119.32
1	D	722	TYR	N-CA-C	-5.36	105.08	111.03
1	B	496	ARG	N-CA-C	-5.35	104.69	111.11
1	B	905	ILE	N-CA-C	-5.34	99.56	107.51
1	B	1065	VAL	N-CA-C	-5.33	98.26	109.34
1	D	927	SER	N-CA-C	-5.32	103.50	110.53
1	C	511	GLY	CA-C-N	5.31	126.48	119.84
1	C	511	GLY	C-N-CA	5.31	126.48	119.84
1	D	954	VAL	N-CA-C	5.29	113.26	107.60
1	D	581	ARG	N-CA-C	5.28	119.71	113.16
1	D	969	LYS	CB-CA-C	-5.25	110.09	117.23
1	B	596	HIS	N-CA-C	5.24	118.14	111.69
1	D	507	VAL	N-CA-C	-5.24	105.27	110.62
1	A	938	LEU	N-CA-C	-5.24	100.78	108.79
1	D	989	ALA	N-CA-C	-5.23	104.83	111.11
1	A	957	GLY	N-CA-C	-5.23	107.32	114.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	637	ILE	N-CA-C	5.22	113.58	107.89
1	C	536	PRO	CA-C-N	5.21	125.75	120.38
1	C	536	PRO	C-N-CA	5.21	125.75	120.38
1	D	549	GLY	CA-C-N	5.20	124.92	119.82
1	D	549	GLY	C-N-CA	5.20	124.92	119.82
1	A	971	LEU	CA-C-N	5.20	126.01	119.98
1	A	971	LEU	C-N-CA	5.20	126.01	119.98
1	D	995	VAL	N-CA-C	-5.20	104.82	110.23
1	D	1065	VAL	N-CA-C	-5.19	98.55	109.34
1	D	888	LYS	N-CA-C	-5.17	104.72	111.02
1	C	904	LEU	N-CA-C	5.12	117.06	109.69
1	D	826	VAL	N-CA-C	5.10	112.20	107.56
1	D	496	ARG	N-CA-C	-5.10	105.00	111.11
1	D	906	LYS	N-CA-C	5.07	116.86	108.20
1	D	770	ILE	N-CA-C	5.01	115.19	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4628	0	4579	375	1
1	B	4628	0	4579	379	0
1	C	4628	0	4579	395	1
1	D	4628	0	4579	353	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	18516	0	18316	1488	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (1488) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HB3	1:C:1052:LEU:HD11	1.27	1.12
1:D:1044:ILE:H	1:D:1044:ILE:HD12	1.18	1.07
1:D:496:ARG:HB3	1:D:1052:LEU:HD11	1.37	1.06
1:A:496:ARG:HB3	1:A:1052:LEU:HD11	1.38	1.02
1:A:700:VAL:H	1:A:736:HIS:HD2	1.11	0.98
1:C:641:MET:HB3	1:C:671:MET:HE3	1.47	0.97
1:B:665:VAL:HG21	1:B:1008:LEU:HD11	1.45	0.96
1:B:1044:ILE:HD12	1:B:1044:ILE:H	1.28	0.95
1:B:700:VAL:H	1:B:736:HIS:HD2	1.14	0.94
1:B:496:ARG:HB3	1:B:1052:LEU:HD11	1.49	0.94
1:B:641:MET:HB3	1:B:671:MET:HE3	1.50	0.93
1:D:641:MET:HB3	1:D:671:MET:HE3	1.48	0.93
1:A:732:ARG:HH11	1:A:732:ARG:HB2	1.33	0.93
1:A:1044:ILE:HD12	1:A:1044:ILE:H	1.32	0.92
1:A:752:CYS:O	1:A:756:VAL:HG12	1.71	0.91
1:A:1068:LEU:HD13	1:A:1074:ARG:NH2	1.85	0.91
1:D:700:VAL:H	1:D:736:HIS:HD2	1.15	0.91
1:C:711:ALA:HA	1:C:754:MET:HE1	1.53	0.91
1:B:1068:LEU:HD13	1:B:1074:ARG:NH2	1.85	0.90
1:C:913:ILE:HD13	1:C:947:PHE:HB2	1.54	0.89
1:A:571:ARG:HH11	1:A:575:GLN:NE2	1.70	0.88
1:A:913:ILE:HD13	1:A:947:PHE:HB2	1.56	0.88
1:D:1068:LEU:HD13	1:D:1074:ARG:NH2	1.89	0.88
1:C:1065:VAL:HG13	1:C:1076:VAL:HG12	1.56	0.88
1:D:991:GLU:O	1:D:995:VAL:HG23	1.74	0.88
1:B:913:ILE:HD13	1:B:947:PHE:HB2	1.56	0.87
1:D:732:ARG:HH11	1:D:732:ARG:HB2	1.40	0.87
1:C:679:SER:HB3	1:C:909:PRO:HD2	1.59	0.85
1:B:870:GLN:O	1:B:874:LEU:HD13	1.77	0.85
1:A:571:ARG:HH11	1:A:575:GLN:HE22	1.24	0.84
1:C:665:VAL:HG21	1:C:1008:LEU:HD11	1.57	0.84
1:B:624:TRP:O	1:B:628:GLN:HG3	1.77	0.84
1:B:732:ARG:HB2	1:B:732:ARG:HH11	1.42	0.84
1:C:564:LEU:HB2	1:C:793:VAL:HG22	1.60	0.84
1:C:1068:LEU:HD13	1:C:1074:ARG:NH2	1.92	0.84
1:D:679:SER:HB3	1:D:909:PRO:HD2	1.60	0.83
1:C:1044:ILE:HD12	1:C:1044:ILE:H	1.44	0.83
1:D:665:VAL:HG21	1:D:1008:LEU:HD11	1.60	0.83
1:D:496:ARG:CB	1:D:1052:LEU:HD11	2.09	0.82
1:D:870:GLN:O	1:D:874:LEU:HD13	1.79	0.82
1:A:991:GLU:O	1:A:995:VAL:HG23	1.80	0.82
1:C:989:ALA:O	1:C:993:GLU:HB2	1.80	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ARG:HH11	1:B:575:GLN:HE22	1.27	0.82
1:C:870:GLN:O	1:C:874:LEU:HD13	1.80	0.82
1:C:1066:SER:O	1:C:1068:LEU:HD23	1.80	0.82
1:A:649:VAL:H	1:A:1012:MET:HE1	1.44	0.81
1:D:752:CYS:O	1:D:756:VAL:HG12	1.80	0.81
1:A:989:ALA:O	1:A:993:GLU:HB2	1.79	0.81
1:C:601:LEU:HD22	1:C:603:SER:O	1.81	0.81
1:B:571:ARG:HH11	1:B:575:GLN:NE2	1.78	0.81
1:B:539:ALA:HA	1:B:636:ASN:HB2	1.63	0.80
1:C:700:VAL:H	1:C:736:HIS:HD2	1.28	0.80
1:C:995:VAL:HG22	1:C:1002:VAL:CG2	2.11	0.80
1:C:612:PHE:CB	1:C:649:VAL:HG11	2.12	0.80
1:B:706:TYR:O	1:B:743:MET:HE1	1.82	0.80
1:C:571:ARG:HH11	1:C:575:GLN:HE22	1.29	0.79
1:D:913:ILE:HD13	1:D:947:PHE:HB2	1.62	0.79
1:C:942:ARG:O	1:C:945:VAL:HG22	1.82	0.79
1:A:732:ARG:HB2	1:A:732:ARG:NH1	1.97	0.79
1:C:571:ARG:HH11	1:C:575:GLN:NE2	1.80	0.79
1:A:641:MET:HB3	1:A:671:MET:HE3	1.62	0.78
1:A:496:ARG:CB	1:A:1052:LEU:HD11	2.11	0.78
1:C:624:TRP:O	1:C:628:GLN:HG3	1.83	0.78
1:C:504:LEU:HD22	1:C:1042:PRO:HD3	1.63	0.78
1:B:900:MET:HE1	1:B:921:MET:SD	2.24	0.78
1:B:1066:SER:O	1:B:1068:LEU:HD23	1.84	0.78
1:C:566:MET:HE3	1:C:605:GLU:HB2	1.65	0.78
1:C:991:GLU:O	1:C:995:VAL:HG23	1.84	0.78
1:B:595:ALA:HB2	1:B:634:ILE:HG23	1.64	0.77
1:B:989:ALA:O	1:B:993:GLU:HB2	1.84	0.77
1:B:711:ALA:HA	1:B:754:MET:HE1	1.64	0.77
1:B:849:ASP:HB3	1:B:851:THR:HG22	1.65	0.77
1:D:992:LYS:O	1:D:996:ASP:HB3	1.84	0.77
1:D:706:TYR:O	1:D:743:MET:HE1	1.83	0.77
1:D:989:ALA:O	1:D:993:GLU:HB2	1.84	0.77
1:B:991:GLU:O	1:B:995:VAL:HG23	1.85	0.77
1:C:591:ALA:HB3	1:C:592:PRO:HD3	1.65	0.77
1:A:1051:GLU:OE1	1:A:1057:THR:HG23	1.85	0.77
1:D:571:ARG:HH11	1:D:575:GLN:NE2	1.83	0.77
1:A:679:SER:HB3	1:A:909:PRO:HD2	1.67	0.76
1:B:564:LEU:HB2	1:B:793:VAL:HG22	1.67	0.76
1:C:977:ARG:HH11	1:C:977:ARG:HB3	1.50	0.76
1:D:612:PHE:CB	1:D:649:VAL:HG11	2.15	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:PRO:O	1:A:658:VAL:HG22	1.84	0.76
1:D:1022:ASP:O	1:D:1025:ALA:HB3	1.85	0.76
1:A:995:VAL:HG22	1:A:1002:VAL:CG2	2.16	0.76
1:B:988:GLN:N	1:B:988:GLN:CD	2.43	0.76
1:B:898:ASN:HD21	1:B:904:LEU:H	1.34	0.76
1:D:649:VAL:H	1:D:1012:MET:HE1	1.50	0.76
1:A:992:LYS:O	1:A:996:ASP:HB3	1.86	0.76
1:C:995:VAL:HG22	1:C:1002:VAL:HG21	1.66	0.76
1:A:665:VAL:HG21	1:A:1008:LEU:HD11	1.67	0.75
1:C:498:GLN:HA	1:C:501:LEU:HD12	1.67	0.75
1:D:732:ARG:HB2	1:D:732:ARG:NH1	2.01	0.75
1:A:849:ASP:HB3	1:A:851:THR:HG22	1.66	0.75
1:C:687:LEU:O	1:C:691:GLU:HG2	1.87	0.75
1:C:906:LYS:C	1:C:911:SER:HB3	2.11	0.75
1:D:784:LEU:O	1:D:788:GLN:HG2	1.86	0.75
1:B:752:CYS:O	1:B:756:VAL:HG12	1.87	0.75
1:D:655:PRO:O	1:D:658:VAL:HG22	1.85	0.74
1:A:908:THR:HB	1:A:909:PRO:HD3	1.68	0.74
1:A:988:GLN:CD	1:A:988:GLN:N	2.46	0.74
1:C:641:MET:HB3	1:C:671:MET:CE	2.17	0.74
1:A:995:VAL:HG22	1:A:1002:VAL:HG21	1.68	0.74
1:B:649:VAL:H	1:B:1012:MET:HE1	1.52	0.74
1:B:1054:ARG:O	1:B:1054:ARG:HD3	1.87	0.74
1:C:977:ARG:HB3	1:C:977:ARG:NH1	2.02	0.74
1:B:886:LYS:HA	1:B:889:GLU:OE1	1.87	0.74
1:C:496:ARG:CB	1:C:1052:LEU:HD11	2.11	0.74
1:D:719:SER:O	1:D:722:TYR:HB3	1.88	0.73
1:B:732:ARG:HB2	1:B:732:ARG:NH1	2.03	0.73
1:B:898:ASN:ND2	1:B:904:LEU:H	1.85	0.73
1:D:648:ALA:HB3	1:D:1012:MET:HE1	1.69	0.73
1:D:886:LYS:HA	1:D:889:GLU:OE1	1.87	0.73
1:B:612:PHE:CB	1:B:649:VAL:HG11	2.17	0.73
1:B:711:ALA:O	1:B:713:PRO:HD3	1.88	0.73
1:C:883:LEU:O	1:C:886:LYS:HB2	1.88	0.73
1:A:687:LEU:O	1:A:691:GLU:HG2	1.88	0.73
1:D:624:TRP:O	1:D:628:GLN:HG3	1.88	0.73
1:C:1083:GLN:CD	1:C:1085:ARG:HH21	1.97	0.73
1:D:498:GLN:HA	1:D:501:LEU:HD12	1.69	0.73
1:B:906:LYS:C	1:B:911:SER:HB3	2.14	0.73
1:A:883:LEU:O	1:A:886:LYS:HB2	1.89	0.72
1:A:899:GLN:HA	1:A:899:GLN:NE2	2.04	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ALA:HA	1:C:636:ASN:HB2	1.71	0.72
1:C:1045:ALA:CA	1:C:1063:LEU:HG	2.19	0.72
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.35	0.72
1:D:711:ALA:HA	1:D:754:MET:HE1	1.70	0.72
1:D:1065:VAL:HG13	1:D:1076:VAL:HG12	1.70	0.72
1:B:1045:ALA:CA	1:B:1063:LEU:HG	2.19	0.72
1:D:504:LEU:O	1:D:508:MET:HG3	1.90	0.72
1:D:1044:ILE:H	1:D:1044:ILE:CD1	1.91	0.72
1:A:906:LYS:C	1:A:911:SER:HB3	2.14	0.72
1:B:995:VAL:HG22	1:B:1002:VAL:CG2	2.20	0.72
1:B:601:LEU:HD22	1:B:603:SER:O	1.89	0.72
1:D:936:GLU:HB3	1:D:966:LYS:NZ	2.04	0.72
1:A:898:ASN:ND2	1:A:904:LEU:H	1.87	0.72
1:B:784:LEU:O	1:B:788:GLN:HG2	1.90	0.71
1:A:612:PHE:CB	1:A:649:VAL:HG11	2.20	0.71
1:B:923:GLN:O	1:B:923:GLN:HG2	1.89	0.71
1:C:1051:GLU:OE1	1:C:1057:THR:HG23	1.90	0.71
1:B:604:MET:HE1	1:B:634:ILE:HD13	1.71	0.71
1:A:601:LEU:HD22	1:A:603:SER:O	1.90	0.71
1:C:1003:THR:O	1:C:1007:VAL:HG23	1.91	0.71
1:D:883:LEU:O	1:D:886:LYS:HB2	1.90	0.71
1:A:539:ALA:HA	1:A:636:ASN:HB2	1.72	0.71
1:B:687:LEU:O	1:B:691:GLU:HG2	1.89	0.71
1:D:988:GLN:N	1:D:988:GLN:CD	2.48	0.71
1:A:575:GLN:HG3	1:A:580:THR:OG1	1.90	0.71
1:A:612:PHE:HB2	1:A:649:VAL:HG11	1.72	0.71
1:C:817:THR:HG21	1:C:824:THR:HG23	1.73	0.71
1:A:1065:VAL:HG13	1:A:1076:VAL:HG12	1.72	0.71
1:A:1066:SER:C	1:A:1068:LEU:H	1.99	0.70
1:D:538:PRO:HG2	1:D:599:SER:HB3	1.73	0.70
1:A:644:ARG:HD2	1:A:647:ASN:OD1	1.91	0.70
1:C:992:LYS:O	1:C:996:ASP:HB3	1.92	0.70
1:D:942:ARG:O	1:D:945:VAL:HG22	1.91	0.70
1:D:505:GLY:O	1:D:508:MET:HB2	1.91	0.70
1:C:643:LEU:CD1	1:C:648:ALA:HA	2.21	0.70
1:A:711:ALA:HA	1:A:754:MET:HE1	1.74	0.70
1:D:1067:ASP:OD2	1:D:1067:ASP:N	2.22	0.70
1:A:569:THR:HA	1:A:573:ALA:HB3	1.74	0.70
1:B:1065:VAL:HG22	1:B:1076:VAL:HG12	1.74	0.70
1:A:886:LYS:HA	1:A:889:GLU:OE1	1.92	0.69
1:A:498:GLN:HA	1:A:501:LEU:HD12	1.72	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ALA:HB3	1:B:592:PRO:HD3	1.73	0.69
1:C:810:MET:O	1:C:814:VAL:HG23	1.91	0.69
1:A:494:GLN:HG2	1:A:1056:LYS:NZ	2.08	0.69
1:A:591:ALA:HB3	1:A:592:PRO:HD3	1.74	0.69
1:B:904:LEU:N	1:B:904:LEU:HD12	2.07	0.69
1:C:1089:VAL:HG12	1:C:1090:LYS:H	1.58	0.69
1:C:936:GLU:HB3	1:C:966:LYS:NZ	2.05	0.69
1:C:1066:SER:C	1:C:1068:LEU:H	2.00	0.69
1:A:564:LEU:HB2	1:A:793:VAL:HG22	1.73	0.69
1:B:496:ARG:CB	1:B:1052:LEU:HD11	2.22	0.69
1:C:550:PRO:HB3	1:C:699:VAL:HG22	1.74	0.69
1:C:617:ARG:HH21	1:C:1016:VAL:HG21	1.57	0.69
1:C:706:TYR:O	1:C:743:MET:HE1	1.92	0.69
1:C:1089:VAL:HG12	1:C:1090:LYS:N	2.07	0.69
1:A:898:ASN:HD21	1:A:904:LEU:H	1.40	0.69
1:C:1027:PHE:HB3	1:C:1030:LEU:HD21	1.75	0.69
1:D:641:MET:HB3	1:D:671:MET:CE	2.22	0.69
1:C:598:PHE:O	1:C:601:LEU:HB2	1.93	0.68
1:D:664:GLU:O	1:D:668:GLU:HG3	1.92	0.68
1:A:682:TYR:CE1	1:A:684:PRO:HB2	2.27	0.68
1:B:679:SER:HB3	1:B:909:PRO:HD2	1.74	0.68
1:C:649:VAL:HG12	1:C:649:VAL:O	1.93	0.68
1:A:1076:VAL:O	1:A:1086:SER:HB2	1.94	0.68
1:B:612:PHE:HB3	1:B:649:VAL:HG11	1.73	0.68
1:A:649:VAL:HG12	1:A:649:VAL:O	1.94	0.68
1:A:995:VAL:HA	1:A:999:GLY:O	1.94	0.68
1:C:597:ASN:HB3	1:C:830:ARG:HD3	1.76	0.68
1:A:1067:ASP:OD2	1:A:1067:ASP:N	2.27	0.68
1:B:1003:THR:O	1:B:1007:VAL:HG23	1.93	0.68
1:B:899:GLN:HA	1:B:899:GLN:NE2	2.06	0.68
1:C:604:MET:HE1	1:C:634:ILE:HD13	1.76	0.68
1:C:977:ARG:NH1	1:C:980:ALA:HB2	2.07	0.68
1:B:1073:GLN:HB3	1:B:1089:VAL:O	1.94	0.67
1:D:1066:SER:C	1:D:1068:LEU:H	2.01	0.67
1:C:737:ILE:HG23	1:C:767:PRO:HB2	1.75	0.67
1:C:977:ARG:HH12	1:C:980:ALA:HB2	1.58	0.67
1:D:810:MET:O	1:D:814:VAL:HG23	1.94	0.67
1:A:504:LEU:HD22	1:A:1042:PRO:HD3	1.76	0.67
1:A:538:PRO:HG2	1:A:599:SER:HB3	1.76	0.67
1:D:1065:VAL:O	1:D:1066:SER:HB3	1.94	0.67
1:C:988:GLN:CD	1:C:988:GLN:N	2.52	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:LEU:HD22	1:D:603:SER:O	1.93	0.67
1:B:499:LYS:NZ	1:B:1025:ALA:O	2.22	0.67
1:C:612:PHE:HB2	1:C:649:VAL:HG11	1.76	0.67
1:B:1089:VAL:HG12	1:B:1090:LYS:N	2.09	0.67
1:D:612:PHE:HB2	1:D:649:VAL:HG11	1.76	0.67
1:B:1083:GLN:CD	1:B:1085:ARG:HH21	2.03	0.66
1:D:737:ILE:HG23	1:D:767:PRO:HB2	1.75	0.66
1:D:1003:THR:O	1:D:1007:VAL:HG23	1.96	0.66
1:C:595:ALA:HB2	1:C:634:ILE:HG23	1.77	0.66
1:C:752:CYS:O	1:C:756:VAL:HG12	1.95	0.66
1:C:1045:ALA:HA	1:C:1063:LEU:HG	1.77	0.66
1:A:569:THR:HA	1:A:573:ALA:CB	2.25	0.66
1:A:706:TYR:O	1:A:743:MET:HE1	1.95	0.66
1:B:504:LEU:HD22	1:B:1042:PRO:HD3	1.76	0.66
1:D:591:ALA:HB3	1:D:592:PRO:HD3	1.76	0.66
1:A:648:ALA:HB3	1:A:1012:MET:HE1	1.77	0.66
1:C:784:LEU:O	1:C:788:GLN:HG2	1.96	0.66
1:B:936:GLU:HB3	1:B:966:LYS:NZ	2.11	0.66
1:A:1089:VAL:HG12	1:A:1090:LYS:N	2.10	0.66
1:B:737:ILE:HG23	1:B:767:PRO:HB2	1.77	0.66
1:B:922:VAL:HG23	1:B:923:GLN:N	2.11	0.66
1:B:1065:VAL:HG22	1:B:1076:VAL:CG1	2.26	0.66
1:C:612:PHE:HB3	1:C:649:VAL:HG11	1.76	0.66
1:D:1090:LYS:H	1:D:1090:LYS:HD2	1.59	0.66
1:B:550:PRO:HB3	1:B:699:VAL:HG22	1.78	0.66
1:B:644:ARG:HD2	1:B:647:ASN:OD1	1.95	0.66
1:B:992:LYS:O	1:B:996:ASP:HB3	1.95	0.66
1:D:612:PHE:HB3	1:D:649:VAL:HG11	1.77	0.66
1:D:897:ALA:HB2	1:D:921:MET:HE2	1.78	0.66
1:D:901:LEU:HB2	1:D:904:LEU:HD11	1.78	0.66
1:A:683:LEU:O	1:A:687:LEU:HG	1.96	0.66
1:C:649:VAL:H	1:C:1012:MET:HE1	1.59	0.66
1:C:908:THR:HB	1:C:909:PRO:HD3	1.76	0.65
1:B:995:VAL:HG22	1:B:1002:VAL:HG21	1.77	0.65
1:C:901:LEU:HB2	1:C:904:LEU:HD11	1.78	0.65
1:A:700:VAL:H	1:A:736:HIS:CD2	2.03	0.65
1:A:1044:ILE:HA	1:A:1062:ALA:HB3	1.78	0.65
1:B:649:VAL:HG12	1:B:649:VAL:O	1.97	0.65
1:B:1089:VAL:HG12	1:B:1090:LYS:H	1.60	0.65
1:C:849:ASP:HB3	1:C:851:THR:HG22	1.78	0.65
1:A:624:TRP:O	1:A:628:GLN:HG3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:PHE:O	1:A:967:VAL:HG23	1.96	0.65
1:B:1022:ASP:O	1:B:1025:ALA:HB3	1.97	0.65
1:D:687:LEU:O	1:D:691:GLU:HG2	1.96	0.65
1:C:612:PHE:HB3	1:C:649:VAL:CG1	2.27	0.65
1:C:1044:ILE:HG22	1:C:1063:LEU:HD23	1.77	0.65
1:B:1051:GLU:OE1	1:B:1057:THR:HG23	1.97	0.65
1:D:1060:ILE:N	1:D:1060:ILE:HD12	2.11	0.65
1:B:1045:ALA:HA	1:B:1063:LEU:HG	1.76	0.65
1:D:1083:GLN:CD	1:D:1085:ARG:HH21	2.05	0.65
1:D:995:VAL:HA	1:D:999:GLY:O	1.97	0.65
1:D:1051:GLU:OE1	1:D:1057:THR:HG23	1.97	0.64
1:D:1065:VAL:HG22	1:D:1076:VAL:HG12	1.78	0.64
1:A:784:LEU:O	1:A:788:GLN:HG2	1.96	0.64
1:B:538:PRO:HG2	1:B:599:SER:HB3	1.78	0.64
1:A:1003:THR:O	1:A:1007:VAL:HG23	1.97	0.64
1:B:908:THR:HB	1:B:909:PRO:HD3	1.80	0.64
1:A:719:SER:O	1:A:722:TYR:HB3	1.97	0.64
1:A:1054:ARG:O	1:A:1054:ARG:HD3	1.98	0.64
1:A:1083:GLN:CD	1:A:1085:ARG:HH21	2.05	0.64
1:B:643:LEU:O	1:B:676:VAL:HA	1.97	0.64
1:D:923:GLN:O	1:D:923:GLN:HG2	1.96	0.64
1:B:1044:ILE:H	1:B:1044:ILE:CD1	1.98	0.64
1:C:1065:VAL:O	1:C:1066:SER:HB3	1.97	0.64
1:B:617:ARG:HH21	1:B:1016:VAL:HG21	1.63	0.64
1:B:1060:ILE:N	1:B:1060:ILE:HD12	2.13	0.64
1:C:886:LYS:HA	1:C:889:GLU:OE1	1.97	0.64
1:D:1065:VAL:O	1:D:1066:SER:CB	2.45	0.64
1:D:682:TYR:CE1	1:D:684:PRO:HB2	2.33	0.64
1:A:1066:SER:O	1:A:1068:LEU:HD23	1.97	0.64
1:A:922:VAL:HG23	1:A:923:GLN:N	2.12	0.63
1:A:947:PHE:HD1	1:A:952:ILE:HD11	1.61	0.63
1:A:1065:VAL:O	1:A:1066:SER:CB	2.45	0.63
1:B:942:ARG:O	1:B:945:VAL:HG22	1.97	0.63
1:C:899:GLN:HA	1:C:899:GLN:NE2	2.12	0.63
1:B:743:MET:N	1:B:743:MET:HE2	2.13	0.63
1:C:923:GLN:HG2	1:C:923:GLN:O	1.98	0.63
1:A:947:PHE:CD1	1:A:952:ILE:HD11	2.34	0.63
1:A:1067:ASP:OD1	1:A:1075:GLN:HB3	1.98	0.63
1:A:1065:VAL:O	1:A:1066:SER:HB3	1.99	0.63
1:B:707:THR:HG22	1:B:708:GLY:N	2.14	0.63
1:B:1058:LEU:HB3	1:B:1060:ILE:HD11	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:GLN:HG2	1:C:1056:LYS:NZ	2.14	0.63
1:D:995:VAL:HG22	1:D:1002:VAL:CG2	2.28	0.63
1:A:595:ALA:HB2	1:A:634:ILE:HG23	1.80	0.63
1:C:569:THR:HA	1:C:573:ALA:HB3	1.80	0.63
1:A:900:MET:HE1	1:A:921:MET:SD	2.39	0.63
1:D:550:PRO:HB3	1:D:699:VAL:HG22	1.79	0.63
1:A:900:MET:CE	1:A:928:ARG:HG3	2.29	0.63
1:B:883:LEU:O	1:B:886:LYS:HB2	1.98	0.63
1:D:1044:ILE:O	1:D:1045:ALA:HB3	1.97	0.63
1:A:1027:PHE:HB3	1:A:1030:LEU:HD21	1.80	0.62
1:B:1073:GLN:O	1:B:1074:ARG:HB2	1.98	0.62
1:C:643:LEU:HD12	1:C:648:ALA:HA	1.81	0.62
1:D:678:ASP:HB2	1:D:686:MET:HG3	1.80	0.62
1:B:506:HIS:HD2	1:B:1090:LYS:HE2	1.62	0.62
1:B:990:LEU:O	1:B:994:LEU:HG	2.00	0.62
1:A:558:ARG:O	1:A:558:ARG:NH1	2.31	0.62
1:D:498:GLN:NE2	1:D:498:GLN:C	2.57	0.62
1:B:963:PHE:O	1:B:967:VAL:HG23	1.98	0.62
1:D:498:GLN:C	1:D:498:GLN:HE21	2.07	0.62
1:B:865:GLU:HB2	1:B:906:LYS:NZ	2.14	0.62
1:C:778:ALA:O	1:C:780:VAL:N	2.32	0.62
1:D:566:MET:HE3	1:D:605:GLU:HB2	1.81	0.62
1:A:711:ALA:O	1:A:713:PRO:HD3	2.00	0.62
1:D:496:ARG:NH1	1:D:1056:LYS:NZ	2.47	0.62
1:D:539:ALA:HA	1:D:636:ASN:HB2	1.82	0.62
1:D:1073:GLN:HB3	1:D:1089:VAL:O	1.99	0.62
1:B:1044:ILE:HG22	1:B:1063:LEU:HD23	1.80	0.62
1:C:780:VAL:HG13	1:C:813:LEU:HD22	1.82	0.62
1:B:641:MET:HB3	1:B:671:MET:CE	2.27	0.61
1:B:900:MET:HE2	1:B:928:ARG:HG3	1.81	0.61
1:C:1067:ASP:OD2	1:C:1067:ASP:N	2.32	0.61
1:D:569:THR:HA	1:D:573:ALA:HB3	1.82	0.61
1:D:778:ALA:O	1:D:780:VAL:N	2.33	0.61
1:C:1062:ALA:O	1:C:1063:LEU:HB2	1.99	0.61
1:D:711:ALA:O	1:D:713:PRO:HD3	2.01	0.61
1:A:778:ALA:O	1:A:780:VAL:N	2.33	0.61
1:B:1067:ASP:N	1:B:1067:ASP:OD2	2.33	0.61
1:C:1060:ILE:HD12	1:C:1060:ILE:N	2.15	0.61
1:B:766:LEU:HD12	1:B:767:PRO:HD2	1.82	0.61
1:C:907:VAL:N	1:C:911:SER:HB3	2.16	0.61
1:C:1065:VAL:O	1:C:1066:SER:CB	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:820:THR:HB	1:D:821:PRO:HD2	1.83	0.61
1:B:1065:VAL:O	1:B:1066:SER:CB	2.49	0.61
1:C:1022:ASP:O	1:C:1025:ALA:HB3	2.01	0.61
1:A:1065:VAL:HG22	1:A:1076:VAL:HG12	1.82	0.61
1:B:644:ARG:HH11	1:B:644:ARG:HB3	1.65	0.61
1:D:574:HIS:CD2	1:D:580:THR:HA	2.36	0.61
1:D:1092:THR:HG22	1:D:1092:THR:O	2.00	0.61
1:A:900:MET:HE2	1:A:928:ARG:HG3	1.81	0.61
1:C:1044:ILE:O	1:C:1045:ALA:HB3	2.01	0.61
1:A:1060:ILE:N	1:A:1060:ILE:HD12	2.16	0.61
1:B:575:GLN:HG3	1:B:580:THR:OG1	2.00	0.61
1:A:717:LYS:NZ	1:A:956:HIS:O	2.27	0.60
1:C:644:ARG:HH11	1:C:644:ARG:HB3	1.65	0.60
1:D:644:ARG:HB3	1:D:644:ARG:HH11	1.64	0.60
1:D:900:MET:HE2	1:D:928:ARG:HG3	1.83	0.60
1:D:1045:ALA:CA	1:D:1063:LEU:HG	2.30	0.60
1:B:897:ALA:HB2	1:B:921:MET:HE2	1.83	0.60
1:C:732:ARG:HH11	1:C:732:ARG:HB2	1.66	0.60
1:C:738:LEU:HD12	1:C:739:CYS:N	2.16	0.60
1:B:604:MET:HE1	1:B:634:ILE:CD1	2.32	0.60
1:C:1044:ILE:HA	1:C:1062:ALA:HB3	1.81	0.60
1:D:564:LEU:HB2	1:D:793:VAL:HG22	1.83	0.60
1:A:1044:ILE:O	1:A:1045:ALA:HB3	2.01	0.60
1:A:1045:ALA:CA	1:A:1063:LEU:HG	2.32	0.60
1:D:612:PHE:HB3	1:D:649:VAL:CG1	2.32	0.60
1:D:922:VAL:HG23	1:D:923:GLN:N	2.16	0.60
1:A:494:GLN:HA	1:A:496:ARG:NH2	2.17	0.60
1:A:560:HIS:CD2	1:A:564:LEU:HD21	2.37	0.60
1:B:1044:ILE:HA	1:B:1062:ALA:HB3	1.82	0.60
1:B:1066:SER:C	1:B:1068:LEU:H	2.09	0.60
1:C:538:PRO:HG2	1:C:599:SER:HB3	1.84	0.60
1:D:977:ARG:NH1	1:D:977:ARG:HB3	2.17	0.60
1:A:860:ASP:HA	1:B:832:PHE:CZ	2.36	0.60
1:B:566:MET:HE3	1:B:605:GLU:HB2	1.84	0.60
1:D:849:ASP:HB3	1:D:851:THR:HG22	1.82	0.60
1:B:508:MET:SD	1:B:1042:PRO:HG2	2.42	0.60
1:B:1065:VAL:HG13	1:B:1076:VAL:HG12	1.84	0.60
1:C:1076:VAL:O	1:C:1086:SER:HB2	2.01	0.60
1:D:547:ARG:C	1:D:548:GLU:HG3	2.26	0.60
1:D:717:LYS:NZ	1:D:956:HIS:O	2.28	0.60
1:C:502:HIS:HE1	1:C:1090:LYS:NZ	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:ASP:OD1	1:C:751:ALA:HB2	2.01	0.60
1:D:1008:LEU:O	1:D:1011:ALA:HB3	2.02	0.60
1:A:828:MET:O	1:A:831:VAL:HG22	2.01	0.59
1:D:683:LEU:O	1:D:687:LEU:HG	2.02	0.59
1:B:772:THR:HG21	1:B:783:MET:HE3	1.84	0.59
1:C:655:PRO:O	1:C:658:VAL:HG22	2.02	0.59
1:C:711:ALA:O	1:C:713:PRO:HD3	2.01	0.59
1:D:1089:VAL:HG12	1:D:1090:LYS:N	2.17	0.59
1:B:595:ALA:CB	1:B:634:ILE:HG23	2.33	0.59
1:B:612:PHE:HB2	1:B:649:VAL:HG11	1.83	0.59
1:B:743:MET:SD	1:B:907:VAL:HG22	2.43	0.59
1:B:665:VAL:HG12	1:B:669:ASN:ND2	2.17	0.59
1:D:947:PHE:CD1	1:D:952:ILE:HD11	2.37	0.59
1:B:787:ALA:HB1	1:B:822:LEU:HD13	1.83	0.59
1:C:766:LEU:HD12	1:C:767:PRO:HD2	1.84	0.59
1:D:947:PHE:HD1	1:D:952:ILE:HD11	1.65	0.59
1:D:1069:ASN:O	1:D:1071:ALA:N	2.35	0.59
1:D:990:LEU:O	1:D:994:LEU:HG	2.01	0.59
1:C:642:LEU:HD11	1:C:677:PHE:CD2	2.38	0.59
1:C:977:ARG:HH11	1:C:977:ARG:CB	2.16	0.59
1:A:1089:VAL:HG12	1:A:1090:LYS:H	1.67	0.59
1:B:1067:ASP:OD1	1:B:1075:GLN:HB3	2.03	0.59
1:C:539:ALA:HB1	1:C:543:ASP:OD2	2.01	0.59
1:C:560:HIS:CD2	1:C:564:LEU:HD21	2.38	0.59
1:D:495:ASN:OD1	1:D:499:LYS:HE3	2.02	0.59
1:D:707:THR:HG22	1:D:708:GLY:N	2.17	0.59
1:A:1065:VAL:HG22	1:A:1076:VAL:CG1	2.32	0.59
1:A:1069:ASN:O	1:A:1071:ALA:N	2.35	0.59
1:B:612:PHE:HB3	1:B:649:VAL:CG1	2.32	0.59
1:C:719:SER:O	1:C:722:TYR:HB3	2.02	0.59
1:A:550:PRO:HB3	1:A:699:VAL:HG22	1.84	0.59
1:A:1015:ASP:HB3	1:A:1019:HIS:NE2	2.18	0.59
1:D:780:VAL:HG13	1:D:813:LEU:HD22	1.85	0.59
1:D:952:ILE:HG13	1:D:953:GLY:N	2.18	0.59
1:A:1058:LEU:HB3	1:A:1060:ILE:HD11	1.85	0.58
1:C:678:ASP:HB2	1:C:686:MET:HG3	1.85	0.58
1:C:865:GLU:HB2	1:C:906:LYS:HZ2	1.66	0.58
1:C:565:LEU:O	1:C:602:PHE:HB3	2.02	0.58
1:A:952:ILE:HG13	1:A:953:GLY:N	2.19	0.58
1:B:574:HIS:CD2	1:B:580:THR:HA	2.38	0.58
1:C:502:HIS:HE1	1:C:1090:LYS:HZ3	1.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:GLU:OE2	1:C:937:GLU:N	2.36	0.58
1:A:664:GLU:O	1:A:668:GLU:HG3	2.03	0.58
1:A:936:GLU:HB3	1:A:966:LYS:NZ	2.17	0.58
1:B:498:GLN:HA	1:B:501:LEU:HD12	1.84	0.58
1:B:807:GLN:H	1:B:807:GLN:NE2	2.01	0.58
1:C:1069:ASN:O	1:C:1071:ALA:N	2.37	0.58
1:D:756:VAL:HG11	1:D:789:ALA:HB3	1.85	0.58
1:D:907:VAL:N	1:D:911:SER:HB3	2.17	0.58
1:A:499:LYS:NZ	1:A:1025:ALA:O	2.27	0.58
1:A:917:LEU:O	1:A:921:MET:HG3	2.03	0.58
1:B:590:ILE:O	1:B:594:VAL:HG23	2.03	0.58
1:D:814:VAL:O	1:D:817:THR:HG22	2.03	0.58
1:A:949:GLN:HG3	1:A:968:LEU:CD2	2.34	0.58
1:A:1045:ALA:HA	1:A:1063:LEU:HG	1.85	0.58
1:B:749:PRO:O	1:B:752:CYS:HB2	2.04	0.58
1:D:644:ARG:HB3	1:D:644:ARG:NH1	2.19	0.58
1:D:1045:ALA:HA	1:D:1063:LEU:HG	1.86	0.58
1:A:1065:VAL:HG22	1:A:1076:VAL:HB	1.85	0.58
1:B:955:PRO:HD2	1:B:959:PHE:CE1	2.39	0.58
1:D:917:LEU:O	1:D:921:MET:HG3	2.03	0.58
1:A:650:GLY:HA3	1:A:654:TYR:OH	2.04	0.58
1:C:900:MET:HE2	1:C:928:ARG:HG3	1.84	0.58
1:A:832:PHE:CZ	1:B:860:ASP:HA	2.39	0.58
1:A:977:ARG:HB3	1:A:977:ARG:NH1	2.18	0.58
1:A:516:ILE:O	1:A:516:ILE:HG13	2.03	0.57
1:B:597:ASN:HB3	1:B:830:ARG:HD3	1.86	0.57
1:B:570:PHE:CD2	1:B:587:LEU:HD22	2.38	0.57
1:D:597:ASN:HB3	1:D:830:ARG:HD3	1.85	0.57
1:A:1022:ASP:O	1:A:1025:ALA:HB3	2.03	0.57
1:B:661:LYS:O	1:B:665:VAL:HG23	2.04	0.57
1:B:996:ASP:OD1	1:B:997:ARG:N	2.38	0.57
1:B:1068:LEU:HA	1:B:1074:ARG:HE	1.68	0.57
1:A:665:VAL:HG12	1:A:669:ASN:ND2	2.18	0.57
1:C:570:PHE:CD2	1:C:587:LEU:HD22	2.40	0.57
1:C:655:PRO:HB2	1:C:984:PRO:HA	1.87	0.57
1:C:1005:GLU:H	1:C:1005:GLU:CD	2.12	0.57
1:D:494:GLN:HA	1:D:496:ARG:NH2	2.18	0.57
1:D:649:VAL:O	1:D:649:VAL:HG12	2.04	0.57
1:A:907:VAL:O	1:A:908:THR:C	2.47	0.57
1:A:495:ASN:OD1	1:A:499:LYS:HE3	2.04	0.57
1:B:678:ASP:OD1	1:B:682:TYR:HB3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1044:ILE:CG2	1:B:1063:LEU:HA	2.34	0.57
1:C:807:GLN:H	1:C:807:GLN:NE2	2.02	0.57
1:D:1027:PHE:HB3	1:D:1030:LEU:HD21	1.86	0.57
1:B:762:ARG:HG3	1:B:763:PHE:CE1	2.40	0.57
1:B:1044:ILE:HD12	1:B:1044:ILE:N	2.09	0.57
1:B:1044:ILE:O	1:B:1045:ALA:HB3	2.04	0.57
1:A:899:GLN:HA	1:A:899:GLN:HE21	1.68	0.57
1:B:949:GLN:HG3	1:B:968:LEU:CD2	2.35	0.57
1:C:575:GLN:HG3	1:C:580:THR:OG1	2.05	0.57
1:C:963:PHE:O	1:C:967:VAL:HG23	2.05	0.57
1:D:504:LEU:HD22	1:D:1042:PRO:HD3	1.86	0.57
1:D:904:LEU:HD12	1:D:904:LEU:N	2.20	0.57
1:C:820:THR:HB	1:C:821:PRO:HD2	1.87	0.57
1:C:898:ASN:HD22	1:C:906:LYS:HD3	1.70	0.57
1:C:1080:LEU:HD23	1:C:1085:ARG:CZ	2.35	0.57
1:D:906:LYS:C	1:D:911:SER:HB3	2.29	0.57
1:D:908:THR:HB	1:D:909:PRO:HD3	1.86	0.57
1:C:961:GLU:OE1	1:C:964:ARG:HD3	2.05	0.56
1:D:1065:VAL:HG22	1:D:1076:VAL:CG1	2.35	0.56
1:B:700:VAL:H	1:B:736:HIS:CD2	2.06	0.56
1:B:1065:VAL:O	1:B:1066:SER:HB3	2.05	0.56
1:D:617:ARG:HH21	1:D:1016:VAL:HG21	1.70	0.56
1:A:1044:ILE:H	1:A:1044:ILE:CD1	2.01	0.56
1:B:952:ILE:HG13	1:B:953:GLY:N	2.21	0.56
1:C:504:LEU:O	1:C:508:MET:HG3	2.05	0.56
1:C:900:MET:HE1	1:C:921:MET:SD	2.46	0.56
1:D:644:ARG:NH1	1:D:644:ARG:CB	2.68	0.56
1:D:995:VAL:HG22	1:D:1002:VAL:HG21	1.86	0.56
1:D:1044:ILE:HD12	1:D:1044:ILE:N	2.03	0.56
1:C:707:THR:HG22	1:C:708:GLY:N	2.21	0.56
1:D:1067:ASP:O	1:D:1069:ASN:N	2.39	0.56
1:B:648:ALA:HB3	1:B:1012:MET:HE1	1.87	0.56
1:B:817:THR:HG21	1:B:824:THR:HG23	1.87	0.56
1:C:653:ASN:HB3	1:C:982:LEU:HD11	1.87	0.56
1:C:701:GLU:HG3	1:C:737:ILE:HB	1.85	0.56
1:A:1065:VAL:HG22	1:A:1076:VAL:CB	2.36	0.56
1:B:919:GLN:HA	1:B:922:VAL:HG22	1.86	0.56
1:B:1044:ILE:HG22	1:B:1063:LEU:HA	1.86	0.56
1:D:743:MET:SD	1:D:907:VAL:HG22	2.46	0.56
1:C:1058:LEU:HB3	1:C:1060:ILE:HD11	1.88	0.56
1:C:1060:ILE:HG22	1:C:1061:LYS:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:VAL:CG1	1:C:1076:VAL:HG12	2.33	0.56
1:D:600:LYS:HE3	1:D:825:GLU:HB3	1.88	0.56
1:A:907:VAL:HG12	1:A:908:THR:H	1.70	0.56
1:A:1090:LYS:H	1:A:1090:LYS:HD2	1.70	0.56
1:B:778:ALA:O	1:B:780:VAL:N	2.39	0.56
1:C:644:ARG:HD2	1:C:647:ASN:OD1	2.05	0.56
1:C:1044:ILE:CG2	1:C:1063:LEU:HA	2.36	0.56
1:D:542:ARG:H	1:D:638:PRO:HD3	1.71	0.56
1:D:558:ARG:O	1:D:558:ARG:NH1	2.38	0.56
1:C:500:LEU:O	1:C:503:TYR:HB3	2.06	0.56
1:C:647:ASN:ND2	1:C:650:GLY:O	2.39	0.56
1:D:727:ALA:O	1:D:731:VAL:HG23	2.05	0.56
1:D:766:LEU:HD12	1:D:767:PRO:HD2	1.88	0.56
1:D:1063:LEU:O	1:D:1064:ALA:CB	2.53	0.56
1:A:881:MET:O	1:A:883:LEU:HG	2.05	0.56
1:A:897:ALA:HB2	1:A:921:MET:HE2	1.88	0.56
1:C:1068:LEU:HA	1:C:1074:ARG:HE	1.70	0.56
1:D:604:MET:HE1	1:D:634:ILE:HD13	1.87	0.56
1:D:1068:LEU:HA	1:D:1074:ARG:HE	1.71	0.56
1:A:1001:GLU:O	1:A:1002:VAL:C	2.49	0.55
1:C:922:VAL:HG23	1:C:923:GLN:N	2.22	0.55
1:C:952:ILE:HG13	1:C:953:GLY:N	2.20	0.55
1:D:565:LEU:O	1:D:602:PHE:HB3	2.06	0.55
1:A:961:GLU:OE1	1:A:964:ARG:HD3	2.06	0.55
1:B:569:THR:HA	1:B:573:ALA:HB3	1.87	0.55
1:B:655:PRO:O	1:B:658:VAL:HG22	2.06	0.55
1:D:936:GLU:HB3	1:D:966:LYS:HZ1	1.69	0.55
1:A:990:LEU:O	1:A:994:LEU:HG	2.07	0.55
1:B:539:ALA:HA	1:B:636:ASN:CB	2.34	0.55
1:B:995:VAL:HA	1:B:999:GLY:O	2.07	0.55
1:A:707:THR:HG22	1:A:708:GLY:N	2.21	0.55
1:A:949:GLN:HG3	1:A:968:LEU:HD22	1.89	0.55
1:C:502:HIS:CE1	1:C:1090:LYS:HZ3	2.24	0.55
1:D:700:VAL:H	1:D:736:HIS:CD2	2.08	0.55
1:D:968:LEU:O	1:D:971:LEU:HD12	2.06	0.55
1:A:502:HIS:HE1	1:A:1090:LYS:NZ	2.04	0.55
1:A:961:GLU:O	1:A:962:PRO:C	2.47	0.55
1:A:1092:THR:O	1:A:1093:GLN:C	2.50	0.55
1:C:1065:VAL:HG22	1:C:1076:VAL:HB	1.87	0.55
1:A:502:HIS:CE1	1:A:1090:LYS:NZ	2.75	0.55
1:B:665:VAL:HG21	1:B:1008:LEU:CD1	2.27	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:THR:HG22	1:B:909:PRO:N	2.21	0.55
1:B:1065:VAL:HG22	1:B:1076:VAL:CB	2.37	0.55
1:C:558:ARG:O	1:C:558:ARG:NH1	2.36	0.55
1:D:949:GLN:HG3	1:D:968:LEU:CD2	2.36	0.55
1:A:995:VAL:HG13	1:A:1000:GLU:HA	1.87	0.55
1:A:999:GLY:C	1:A:1001:GLU:H	2.14	0.55
1:A:1068:LEU:HA	1:A:1074:ARG:HE	1.71	0.55
1:C:961:GLU:OE2	1:C:965:SER:HB3	2.07	0.55
1:D:917:LEU:HB2	1:D:944:VAL:HG21	1.88	0.55
1:A:665:VAL:HG12	1:A:669:ASN:HD22	1.72	0.55
1:A:907:VAL:N	1:A:911:SER:HB3	2.21	0.55
1:B:494:GLN:HG2	1:B:1056:LYS:NZ	2.22	0.55
1:B:644:ARG:HB3	1:B:644:ARG:NH1	2.22	0.55
1:B:917:LEU:O	1:B:921:MET:HG3	2.07	0.55
1:B:1065:VAL:HG22	1:B:1076:VAL:HB	1.89	0.55
1:C:494:GLN:HA	1:C:496:ARG:NH2	2.21	0.55
1:C:983:PRO:O	1:C:984:PRO:O	2.25	0.55
1:D:898:ASN:ND2	1:D:904:LEU:H	2.04	0.55
1:A:780:VAL:HG13	1:A:813:LEU:HD22	1.88	0.55
1:A:810:MET:O	1:A:814:VAL:HG23	2.07	0.55
1:B:907:VAL:N	1:B:911:SER:HB3	2.22	0.55
1:C:643:LEU:HD11	1:C:648:ALA:HA	1.89	0.55
1:B:682:TYR:CE1	1:B:684:PRO:HB2	2.42	0.54
1:B:945:VAL:HG23	1:B:946:GLU:N	2.22	0.54
1:C:569:THR:HA	1:C:573:ALA:CB	2.37	0.54
1:C:1052:LEU:HD23	1:C:1053:GLU:HB2	1.89	0.54
1:A:644:ARG:HH11	1:A:644:ARG:HB3	1.72	0.54
1:A:1092:THR:O	1:A:1092:THR:HG22	2.07	0.54
1:B:569:THR:HA	1:B:573:ALA:CB	2.37	0.54
1:C:1008:LEU:O	1:C:1011:ALA:HB3	2.08	0.54
1:C:1044:ILE:HG22	1:C:1063:LEU:HA	1.89	0.54
1:D:678:ASP:HB2	1:D:686:MET:CG	2.38	0.54
1:A:787:ALA:HB1	1:A:822:LEU:HD13	1.90	0.54
1:C:894:TYR:CE2	1:C:906:LYS:HD2	2.42	0.54
1:C:945:VAL:HG23	1:C:946:GLU:N	2.22	0.54
1:A:571:ARG:NH1	1:A:575:GLN:NE2	2.50	0.54
1:A:817:THR:HG21	1:A:824:THR:HG23	1.90	0.54
1:A:899:GLN:HE22	1:A:903:ASP:HB2	1.72	0.54
1:A:952:ILE:HG13	1:A:953:GLY:H	1.73	0.54
1:B:558:ARG:O	1:B:558:ARG:NH1	2.37	0.54
1:C:502:HIS:CE1	1:C:1090:LYS:NZ	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:919:GLN:HA	1:C:922:VAL:HG22	1.89	0.54
1:C:1090:LYS:H	1:C:1090:LYS:HD2	1.72	0.54
1:D:1078:PHE:C	1:D:1079:GLU:OE1	2.50	0.54
1:A:612:PHE:HB3	1:A:649:VAL:HG11	1.89	0.54
1:A:1049:GLU:HA	1:A:1058:LEU:O	2.08	0.54
1:B:860:ASP:OD2	1:B:860:ASP:C	2.50	0.54
1:B:965:SER:C	1:B:967:VAL:H	2.15	0.54
1:B:974:VAL:HG11	1:B:978:PRO:HG3	1.88	0.54
1:B:1020:PHE:O	1:B:1024:THR:HG23	2.08	0.54
1:C:656:ASP:CG	1:C:977:ARG:HH21	2.15	0.54
1:C:955:PRO:HD2	1:C:959:PHE:CE1	2.42	0.54
1:D:595:ALA:HB2	1:D:634:ILE:HG23	1.89	0.54
1:B:719:SER:O	1:B:722:TYR:HB3	2.08	0.54
1:C:887:PHE:CE2	1:C:891:LYS:HE3	2.43	0.54
1:A:1063:LEU:O	1:A:1064:ALA:CB	2.55	0.54
1:B:498:GLN:C	1:B:498:GLN:HE21	2.16	0.54
1:D:494:GLN:HG2	1:D:1056:LYS:NZ	2.23	0.54
1:D:516:ILE:O	1:D:516:ILE:HG13	2.08	0.54
1:A:598:PHE:O	1:A:601:LEU:HB2	2.08	0.54
1:A:678:ASP:HB2	1:A:686:MET:HG3	1.90	0.54
1:A:743:MET:N	1:A:743:MET:HE2	2.23	0.54
1:B:502:HIS:HE1	1:B:1090:LYS:NZ	2.05	0.54
1:B:686:MET:O	1:B:690:MET:HG3	2.08	0.54
1:D:901:LEU:HA	1:D:960:PRO:HG3	1.90	0.54
1:A:643:LEU:CD1	1:A:648:ALA:HA	2.38	0.53
1:A:860:ASP:OD2	1:A:860:ASP:C	2.51	0.53
1:B:849:ASP:CB	1:B:851:THR:HG22	2.36	0.53
1:C:595:ALA:CB	1:C:634:ILE:HG23	2.37	0.53
1:C:902:GLY:O	1:C:903:ASP:O	2.24	0.53
1:D:749:PRO:O	1:D:752:CYS:HB2	2.08	0.53
1:A:621:GLU:HG2	1:A:1031:ASP:HB3	1.90	0.53
1:A:942:ARG:O	1:A:945:VAL:HG22	2.09	0.53
1:B:903:ASP:C	1:B:904:LEU:HD12	2.32	0.53
1:C:1073:GLN:HB3	1:C:1089:VAL:O	2.08	0.53
1:A:917:LEU:HB2	1:A:944:VAL:HG21	1.90	0.53
1:C:865:GLU:HB2	1:C:906:LYS:NZ	2.23	0.53
1:B:498:GLN:C	1:B:498:GLN:NE2	2.66	0.53
1:B:711:ALA:HA	1:B:754:MET:CE	2.35	0.53
1:A:766:LEU:HD12	1:A:767:PRO:HD2	1.90	0.53
1:A:907:VAL:HG12	1:A:908:THR:N	2.24	0.53
1:A:1066:SER:O	1:A:1068:LEU:N	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1062:ALA:O	1:B:1063:LEU:HB2	2.08	0.53
1:C:678:ASP:OD1	1:C:682:TYR:HB3	2.08	0.53
1:C:717:LYS:NZ	1:C:956:HIS:O	2.36	0.53
1:C:832:PHE:CZ	1:D:860:ASP:HA	2.43	0.53
1:D:496:ARG:NH1	1:D:1056:LYS:HZ2	2.07	0.53
1:A:494:GLN:CG	1:A:1056:LYS:HZ1	2.22	0.53
1:A:771:HIS:HB2	1:A:795:ASP:OD2	2.09	0.53
1:B:701:GLU:OE2	1:B:769:HIS:ND1	2.35	0.53
1:B:1027:PHE:HB3	1:B:1030:LEU:HD21	1.91	0.53
1:B:1063:LEU:O	1:B:1064:ALA:CB	2.56	0.53
1:C:965:SER:C	1:C:967:VAL:N	2.67	0.53
1:D:569:THR:HA	1:D:573:ALA:CB	2.38	0.53
1:B:807:GLN:NE2	1:B:807:GLN:N	2.57	0.53
1:B:1015:ASP:HB3	1:B:1019:HIS:NE2	2.24	0.53
1:B:1092:THR:O	1:B:1092:THR:HG22	2.08	0.53
1:C:644:ARG:O	1:C:645:GLY:C	2.52	0.53
1:C:743:MET:HE2	1:C:744:ALA:H	1.73	0.53
1:C:1049:GLU:HA	1:C:1058:LEU:O	2.09	0.53
1:D:919:GLN:HA	1:D:922:VAL:HG22	1.90	0.53
1:B:678:ASP:HB2	1:B:686:MET:CG	2.39	0.53
1:B:678:ASP:HB2	1:B:686:MET:HG3	1.91	0.53
1:C:732:ARG:HB2	1:C:732:ARG:NH1	2.24	0.53
1:A:737:ILE:HG23	1:A:767:PRO:HB2	1.89	0.53
1:B:565:LEU:O	1:B:602:PHE:HB3	2.08	0.53
1:C:915:GLY:O	1:C:919:GLN:HG3	2.08	0.53
1:D:817:THR:HG21	1:D:824:THR:HG23	1.91	0.53
1:A:612:PHE:HB3	1:A:649:VAL:CG1	2.40	0.53
1:C:860:ASP:OD2	1:C:860:ASP:C	2.52	0.53
1:C:1044:ILE:H	1:C:1044:ILE:CD1	2.11	0.53
1:A:649:VAL:N	1:A:1012:MET:HE1	2.19	0.52
1:B:642:LEU:HD11	1:B:677:PHE:CD2	2.44	0.52
1:B:1088:LEU:HD23	1:B:1089:VAL:N	2.23	0.52
1:A:701:GLU:HG3	1:A:737:ILE:HB	1.92	0.52
1:A:1044:ILE:HD12	1:A:1044:ILE:N	2.15	0.52
1:C:829:GLU:O	1:C:832:PHE:HB2	2.08	0.52
1:C:738:LEU:HD12	1:C:739:CYS:H	1.74	0.52
1:D:899:GLN:HA	1:D:899:GLN:NE2	2.24	0.52
1:D:655:PRO:HB2	1:D:657:ASN:OD1	2.09	0.52
1:D:922:VAL:HG23	1:D:923:GLN:H	1.75	0.52
1:C:506:HIS:HD2	1:C:1090:LYS:HE2	1.73	0.52
1:C:887:PHE:O	1:C:890:VAL:HG22	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:THR:HB	1:A:821:PRO:HD2	1.92	0.52
1:B:879:HIS:CE1	1:B:884:GLY:HA3	2.45	0.52
1:B:977:ARG:NH1	1:B:977:ARG:HB3	2.25	0.52
1:C:766:LEU:HD12	1:C:767:PRO:CD	2.39	0.52
1:C:898:ASN:ND2	1:C:904:LEU:H	2.08	0.52
1:A:504:LEU:O	1:A:508:MET:HG3	2.10	0.52
1:B:736:HIS:O	1:B:737:ILE:HD13	2.09	0.52
1:C:601:LEU:CD2	1:C:603:SER:O	2.56	0.52
1:C:936:GLU:HB3	1:C:966:LYS:HZ1	1.75	0.52
1:D:793:VAL:HG12	1:D:794:VAL:N	2.24	0.52
1:A:988:GLN:CD	1:A:988:GLN:H	2.17	0.52
1:C:644:ARG:NH1	1:C:644:ARG:CB	2.73	0.52
1:A:1073:GLN:HB3	1:A:1089:VAL:O	2.10	0.52
1:C:683:LEU:O	1:C:687:LEU:HG	2.10	0.52
1:C:1045:ALA:N	1:C:1063:LEU:HG	2.25	0.52
1:D:928:ARG:O	1:D:932:GLU:HG3	2.09	0.52
1:A:500:LEU:O	1:A:503:TYR:HB3	2.09	0.51
1:C:1066:SER:O	1:C:1068:LEU:N	2.34	0.51
1:D:648:ALA:HB3	1:D:1012:MET:CE	2.39	0.51
1:B:644:ARG:NH1	1:B:644:ARG:CB	2.73	0.51
1:B:704:ILE:HG23	1:B:726:LEU:HD23	1.91	0.51
1:D:898:ASN:HD21	1:D:904:LEU:H	1.56	0.51
1:D:1066:SER:O	1:D:1068:LEU:N	2.37	0.51
1:B:810:MET:O	1:B:814:VAL:HG23	2.10	0.51
1:A:965:SER:C	1:A:967:VAL:H	2.19	0.51
1:A:1008:LEU:O	1:A:1011:ALA:HB3	2.09	0.51
1:C:643:LEU:O	1:C:676:VAL:HA	2.10	0.51
1:A:923:GLN:O	1:A:923:GLN:HG2	2.10	0.51
1:A:1078:PHE:C	1:A:1079:GLU:OE1	2.53	0.51
1:B:756:VAL:O	1:B:759:LEU:HB2	2.11	0.51
1:C:644:ARG:HB3	1:C:644:ARG:NH1	2.26	0.51
1:C:547:ARG:C	1:C:548:GLU:HG3	2.35	0.51
1:C:1089:VAL:CG1	1:C:1090:LYS:H	2.22	0.51
1:D:907:VAL:HG12	1:D:908:THR:H	1.76	0.51
1:A:1052:LEU:HD22	1:A:1056:LYS:HD2	1.92	0.51
1:A:1068:LEU:HD13	1:A:1074:ARG:HH22	1.72	0.51
1:C:553:PHE:O	1:C:557:VAL:HG23	2.10	0.51
1:C:1065:VAL:HG22	1:C:1076:VAL:CB	2.41	0.51
1:D:502:HIS:HA	1:D:1087:ILE:HG21	1.91	0.51
1:D:1017:PHE:CZ	1:D:1021:LYS:HD3	2.45	0.51
1:A:887:PHE:HA	1:A:890:VAL:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:GLU:OE1	1:A:1001:GLU:HA	2.11	0.51
1:B:899:GLN:HA	1:B:899:GLN:HE21	1.75	0.51
1:B:988:GLN:CD	1:B:988:GLN:H	2.16	0.51
1:B:1076:VAL:O	1:B:1086:SER:HB2	2.11	0.51
1:C:574:HIS:CD2	1:C:580:THR:HA	2.46	0.51
1:C:900:MET:CE	1:C:928:ARG:HG3	2.41	0.51
1:D:720:LEU:HD22	1:D:754:MET:SD	2.50	0.51
1:D:867:PRO:HG2	1:D:870:GLN:HB3	1.93	0.51
1:A:1062:ALA:O	1:A:1063:LEU:HB2	2.11	0.51
1:C:1054:ARG:O	1:C:1054:ARG:HD3	2.10	0.51
1:D:656:ASP:CG	1:D:977:ARG:HH21	2.19	0.51
1:D:787:ALA:HB1	1:D:822:LEU:HD13	1.92	0.51
1:A:936:GLU:HB3	1:A:966:LYS:HZ1	1.75	0.51
1:C:561:PRO:HG2	1:C:562:GLY:H	1.76	0.51
1:D:649:VAL:N	1:D:1012:MET:HE1	2.24	0.51
1:D:1073:GLN:O	1:D:1074:ARG:HB2	2.09	0.51
1:A:625:ARG:HH21	1:A:629:GLU:CD	2.19	0.50
1:A:1080:LEU:HD23	1:A:1085:ARG:CZ	2.41	0.50
1:B:653:ASN:HB3	1:B:982:LEU:HD11	1.92	0.50
1:B:1069:ASN:O	1:B:1071:ALA:N	2.44	0.50
1:C:665:VAL:HG12	1:C:669:ASN:ND2	2.26	0.50
1:A:749:PRO:HD3	1:B:816:CYS:SG	2.51	0.50
1:A:1068:LEU:HA	1:A:1074:ARG:NE	2.26	0.50
1:B:506:HIS:CD2	1:B:1090:LYS:HE2	2.45	0.50
1:C:928:ARG:O	1:C:932:GLU:HG3	2.11	0.50
1:D:496:ARG:HH11	1:D:1056:LYS:HZ2	1.59	0.50
1:D:547:ARG:NH1	1:D:548:GLU:OE1	2.43	0.50
1:D:651:TYR:CD1	1:D:652:THR:HG23	2.46	0.50
1:D:686:MET:O	1:D:690:MET:HG3	2.11	0.50
1:D:881:MET:O	1:D:883:LEU:HG	2.11	0.50
1:D:900:MET:CE	1:D:928:ARG:HG3	2.41	0.50
1:A:648:ALA:HB3	1:A:1012:MET:CE	2.42	0.50
1:B:665:VAL:CG2	1:B:1008:LEU:HD11	2.30	0.50
1:B:1029:PRO:C	1:B:1031:ASP:H	2.18	0.50
1:C:678:ASP:HB2	1:C:686:MET:CG	2.41	0.50
1:C:887:PHE:CD2	1:C:891:LYS:HE3	2.46	0.50
1:C:949:GLN:HG3	1:C:968:LEU:CD2	2.41	0.50
1:C:965:SER:C	1:C:967:VAL:H	2.19	0.50
1:A:1073:GLN:O	1:A:1074:ARG:HB2	2.10	0.50
1:B:502:HIS:CE1	1:B:1090:LYS:NZ	2.79	0.50
1:B:965:SER:C	1:B:967:VAL:N	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:PRO:HB2	1:C:837:TYR:CE1	2.47	0.50
1:C:743:MET:HE2	1:C:743:MET:N	2.27	0.50
1:C:1015:ASP:HB3	1:C:1019:HIS:NE2	2.27	0.50
1:A:655:PRO:HB2	1:A:984:PRO:HA	1.92	0.50
1:B:833:ASP:O	1:B:836:GLU:HB3	2.11	0.50
1:B:898:ASN:HD21	1:B:904:LEU:N	2.06	0.50
1:D:506:HIS:HD2	1:D:1090:LYS:HE2	1.77	0.50
1:A:498:GLN:C	1:A:498:GLN:NE2	2.70	0.50
1:A:1067:ASP:O	1:A:1069:ASN:N	2.45	0.50
1:B:644:ARG:O	1:B:645:GLY:C	2.53	0.50
1:B:683:LEU:O	1:B:687:LEU:HG	2.11	0.50
1:C:879:HIS:CE1	1:C:884:GLY:HA3	2.46	0.50
1:D:779:GLY:O	1:D:783:MET:HG2	2.11	0.50
1:D:894:TYR:CE2	1:D:906:LYS:HD2	2.46	0.50
1:B:807:GLN:H	1:B:807:GLN:HE21	1.59	0.50
1:C:505:GLY:O	1:C:508:MET:HB2	2.11	0.50
1:C:552:GLY:HA2	1:C:555:ARG:HD2	1.93	0.50
1:C:590:ILE:O	1:C:594:VAL:HG23	2.11	0.50
1:C:749:PRO:O	1:C:752:CYS:HB2	2.12	0.50
1:C:995:VAL:HA	1:C:999:GLY:O	2.12	0.50
1:C:1066:SER:C	1:C:1068:LEU:N	2.68	0.50
1:D:604:MET:HE1	1:D:634:ILE:HG21	1.94	0.50
1:D:936:GLU:HB3	1:D:966:LYS:HZ2	1.77	0.50
1:D:977:ARG:HB3	1:D:977:ARG:HH11	1.77	0.50
1:D:995:VAL:HG13	1:D:1000:GLU:HA	1.93	0.50
1:B:738:LEU:HD12	1:B:739:CYS:N	2.27	0.50
1:B:922:VAL:HG23	1:B:923:GLN:H	1.77	0.50
1:B:1001:GLU:O	1:B:1002:VAL:C	2.53	0.50
1:B:1090:LYS:H	1:B:1090:LYS:HD2	1.76	0.50
1:C:495:ASN:OD1	1:C:499:LYS:HE3	2.12	0.50
1:C:665:VAL:CG2	1:C:1008:LEU:HD11	2.36	0.50
1:C:1089:VAL:CG1	1:C:1090:LYS:N	2.74	0.50
1:D:1060:ILE:HG22	1:D:1061:LYS:N	2.26	0.50
1:A:655:PRO:HG3	1:A:985:LEU:HB2	1.93	0.49
1:A:1054:ARG:HD3	1:A:1054:ARG:C	2.36	0.49
1:A:1060:ILE:HG22	1:A:1061:LYS:N	2.28	0.49
1:A:1063:LEU:O	1:A:1064:ALA:HB3	2.11	0.49
1:C:1001:GLU:O	1:C:1002:VAL:C	2.54	0.49
1:D:865:GLU:HB2	1:D:906:LYS:NZ	2.27	0.49
1:B:598:PHE:O	1:B:601:LEU:HB2	2.11	0.49
1:B:664:GLU:O	1:B:668:GLU:HG3	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:SER:HB2	1:B:807:GLN:O	2.12	0.49
1:C:828:MET:O	1:C:831:VAL:HG22	2.11	0.49
1:D:874:LEU:N	1:D:874:LEU:CD1	2.75	0.49
1:D:907:VAL:O	1:D:908:THR:C	2.54	0.49
1:D:1001:GLU:O	1:D:1002:VAL:C	2.54	0.49
1:D:1044:ILE:HA	1:D:1062:ALA:HB3	1.94	0.49
1:A:922:VAL:HG23	1:A:923:GLN:H	1.78	0.49
1:A:965:SER:C	1:A:967:VAL:N	2.70	0.49
1:B:650:GLY:HA3	1:B:654:TYR:CE1	2.48	0.49
1:C:762:ARG:HG3	1:C:763:PHE:CE1	2.47	0.49
1:C:934:GLN:O	1:C:938:LEU:HG	2.12	0.49
1:C:949:GLN:HG3	1:C:968:LEU:HD22	1.94	0.49
1:C:996:ASP:OD1	1:C:997:ARG:N	2.45	0.49
1:D:893:ALA:CB	1:D:922:VAL:HG13	2.42	0.49
1:A:590:ILE:O	1:A:594:VAL:HG23	2.12	0.49
1:A:919:GLN:HA	1:A:922:VAL:HG22	1.93	0.49
1:B:1010:ALA:HB2	1:B:1017:PHE:CD2	2.47	0.49
1:C:516:ILE:O	1:C:516:ILE:HG13	2.12	0.49
1:D:538:PRO:O	1:D:539:ALA:HB3	2.11	0.49
1:D:661:LYS:O	1:D:665:VAL:HG23	2.12	0.49
1:D:1066:SER:O	1:D:1068:LEU:HD23	2.12	0.49
1:A:650:GLY:HA3	1:A:654:TYR:CE1	2.47	0.49
1:A:1066:SER:C	1:A:1068:LEU:N	2.67	0.49
1:C:549:GLY:C	1:C:551:GLU:H	2.20	0.49
1:D:887:PHE:HA	1:D:890:VAL:HG22	1.95	0.49
1:A:599:SER:C	1:A:601:LEU:H	2.19	0.49
1:B:772:THR:CG2	1:B:783:MET:HE3	2.41	0.49
1:C:779:GLY:O	1:C:783:MET:HG2	2.13	0.49
1:C:867:PRO:HD2	1:C:870:GLN:OE1	2.12	0.49
1:C:887:PHE:HA	1:C:890:VAL:HG22	1.95	0.49
1:C:893:ALA:HB2	1:C:922:VAL:CG1	2.41	0.49
1:D:496:ARG:NH1	1:D:1056:LYS:HZ1	2.11	0.49
1:A:617:ARG:HH21	1:A:1016:VAL:HG21	1.77	0.49
1:A:643:LEU:O	1:A:676:VAL:HA	2.12	0.49
1:C:591:ALA:HB3	1:C:633:LEU:HD13	1.94	0.49
1:D:807:GLN:H	1:D:807:GLN:NE2	2.11	0.49
1:D:945:VAL:HG23	1:D:946:GLU:N	2.28	0.49
1:D:997:ARG:HD2	1:D:998:HIS:CD2	2.47	0.49
1:D:1002:VAL:O	1:D:1002:VAL:HG23	2.12	0.49
1:A:1057:THR:HB	1:A:1059:HIS:CE1	2.48	0.49
1:B:539:ALA:HB1	1:B:543:ASP:OD2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:GLY:HA3	1:C:654:TYR:CE1	2.48	0.49
1:C:942:ARG:O	1:C:945:VAL:CG2	2.55	0.49
1:C:995:VAL:CG2	1:C:1002:VAL:HG21	2.38	0.49
1:D:996:ASP:OD1	1:D:997:ARG:N	2.46	0.49
1:A:824:THR:O	1:A:825:GLU:HB2	2.12	0.49
1:A:1044:ILE:O	1:A:1045:ALA:CB	2.61	0.49
1:B:766:LEU:HD12	1:B:767:PRO:CD	2.43	0.49
1:C:1015:ASP:O	1:C:1016:VAL:C	2.54	0.49
1:C:1079:GLU:HA	1:C:1084:LEU:HB3	1.94	0.49
1:D:606:ASN:OD1	1:D:606:ASN:C	2.56	0.49
1:D:701:GLU:HG3	1:D:737:ILE:HB	1.94	0.49
1:D:736:HIS:O	1:D:737:ILE:HD13	2.13	0.49
1:D:828:MET:O	1:D:831:VAL:HG22	2.12	0.49
1:A:887:PHE:CE2	1:A:891:LYS:HE3	2.48	0.49
1:A:904:LEU:HD12	1:A:904:LEU:N	2.27	0.49
1:A:1044:ILE:HG22	1:A:1063:LEU:HA	1.95	0.49
1:A:1058:LEU:HD22	1:A:1080:LEU:HD11	1.95	0.49
1:A:1076:VAL:HG23	1:A:1078:PHE:CE1	2.48	0.49
1:B:780:VAL:HG13	1:B:813:LEU:HD22	1.94	0.49
1:B:1063:LEU:O	1:B:1064:ALA:HB3	2.13	0.49
1:C:961:GLU:HA	1:C:964:ARG:HB3	1.95	0.49
1:D:1044:ILE:O	1:D:1045:ALA:CB	2.61	0.49
1:A:673:VAL:HA	1:A:699:VAL:HB	1.94	0.48
1:A:701:GLU:HA	1:A:737:ILE:O	2.12	0.48
1:B:873:ASN:O	1:B:877:GLN:HG2	2.13	0.48
1:D:879:HIS:CE1	1:D:884:GLY:HA3	2.48	0.48
1:D:886:LYS:HD3	1:D:889:GLU:OE1	2.12	0.48
1:A:552:GLY:HA2	1:A:555:ARG:HD2	1.96	0.48
1:B:865:GLU:HB2	1:B:906:LYS:HZ2	1.78	0.48
1:D:1029:PRO:C	1:D:1031:ASP:H	2.21	0.48
1:D:1063:LEU:O	1:D:1064:ALA:HB3	2.12	0.48
1:D:771:HIS:HE1	1:D:807:GLN:OE1	1.97	0.48
1:D:952:ILE:HG13	1:D:953:GLY:H	1.77	0.48
1:D:1066:SER:C	1:D:1068:LEU:N	2.69	0.48
1:C:1065:VAL:HG22	1:C:1076:VAL:HG12	1.95	0.48
1:D:517:PRO:HG2	1:D:847:ALA:O	2.12	0.48
1:D:756:VAL:O	1:D:759:LEU:HB2	2.13	0.48
1:D:965:SER:C	1:D:967:VAL:N	2.69	0.48
1:A:494:GLN:HG2	1:A:1056:LYS:HZ1	1.76	0.48
1:B:896:GLU:O	1:B:900:MET:HB2	2.13	0.48
1:B:1001:GLU:HA	1:B:1001:GLU:OE1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:VAL:CG1	1:B:1090:LYS:H	2.26	0.48
1:C:1088:LEU:HD23	1:C:1089:VAL:N	2.29	0.48
1:D:942:ARG:O	1:D:945:VAL:CG2	2.60	0.48
1:D:1074:ARG:O	1:D:1088:LEU:HD23	2.14	0.48
1:A:899:GLN:HE21	1:A:899:GLN:CA	2.24	0.48
1:B:829:GLU:O	1:B:832:PHE:HB2	2.13	0.48
1:C:1065:VAL:HG22	1:C:1076:VAL:CG1	2.44	0.48
1:D:743:MET:N	1:D:743:MET:HE2	2.29	0.48
1:A:677:PHE:CE1	1:A:907:VAL:HG11	2.48	0.48
1:A:711:ALA:HA	1:A:754:MET:CE	2.43	0.48
1:A:743:MET:SD	1:A:907:VAL:HG22	2.54	0.48
1:A:793:VAL:HG12	1:A:794:VAL:N	2.28	0.48
1:A:870:GLN:O	1:A:874:LEU:HD13	2.14	0.48
1:C:883:LEU:HD22	1:C:886:LYS:HG3	1.95	0.48
1:C:1092:THR:HG22	1:C:1092:THR:O	2.13	0.48
1:A:959:PHE:HB2	1:A:964:ARG:HD2	1.96	0.48
1:B:859:SER:C	1:B:861:VAL:H	2.20	0.48
1:B:1049:GLU:HA	1:B:1058:LEU:O	2.13	0.48
1:C:700:VAL:H	1:C:736:HIS:CD2	2.19	0.48
1:C:901:LEU:HA	1:C:960:PRO:HG3	1.94	0.48
1:D:581:ARG:HG3	1:D:848:PHE:CD2	2.49	0.48
1:D:756:VAL:CG1	1:D:789:ALA:HB3	2.43	0.48
1:D:887:PHE:O	1:D:890:VAL:HG22	2.13	0.48
1:D:1068:LEU:HA	1:D:1074:ARG:NE	2.29	0.48
1:D:1080:LEU:HD23	1:D:1085:ARG:CZ	2.44	0.48
1:A:547:ARG:C	1:A:548:GLU:HG3	2.39	0.48
1:A:865:GLU:HB2	1:A:906:LYS:NZ	2.29	0.48
1:A:1005:GLU:CD	1:A:1005:GLU:H	2.22	0.48
1:B:665:VAL:HG12	1:B:669:ASN:HD22	1.79	0.48
1:B:893:ALA:HB2	1:B:922:VAL:CG1	2.43	0.48
1:C:517:PRO:HG2	1:C:847:ALA:O	2.13	0.48
1:B:643:LEU:CD1	1:B:648:ALA:HA	2.43	0.47
1:B:961:GLU:OE1	1:B:964:ARG:HD3	2.13	0.47
1:B:1079:GLU:HA	1:B:1084:LEU:HB3	1.95	0.47
1:C:936:GLU:HB3	1:C:966:LYS:HZ2	1.77	0.47
1:C:1001:GLU:OE1	1:C:1001:GLU:HA	2.14	0.47
1:D:679:SER:HB2	1:D:910:SER:OG	2.14	0.47
1:B:530:PRO:HB2	1:B:593:TYR:CD1	2.49	0.47
1:B:538:PRO:O	1:B:539:ALA:HB3	2.14	0.47
1:B:709:ASP:OD1	1:B:751:ALA:HB2	2.14	0.47
1:B:820:THR:HB	1:B:821:PRO:HD2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:771:HIS:HB2	1:C:795:ASP:OD2	2.13	0.47
1:D:870:GLN:HA	1:D:873:ASN:HD22	1.79	0.47
1:D:1058:LEU:HB3	1:D:1060:ILE:HD11	1.96	0.47
1:B:649:VAL:N	1:B:1012:MET:HE1	2.25	0.47
1:B:922:VAL:CG2	1:B:923:GLN:N	2.76	0.47
1:D:544:ILE:O	1:D:545:LEU:C	2.57	0.47
1:D:860:ASP:OD2	1:D:860:ASP:C	2.56	0.47
1:A:738:LEU:HD12	1:A:739:CYS:H	1.78	0.47
1:B:712:ASP:OD1	1:B:714:SER:HB2	2.15	0.47
1:C:494:GLN:HG2	1:C:1056:LYS:HZ3	1.79	0.47
1:A:1079:GLU:OE1	1:A:1079:GLU:N	2.47	0.47
1:B:935:ALA:C	1:B:937:GLU:N	2.73	0.47
1:C:864:ASN:HA	1:C:895:VAL:HG22	1.96	0.47
1:D:947:PHE:O	1:D:959:PHE:HE2	1.98	0.47
1:A:571:ARG:HD2	1:A:571:ARG:C	2.39	0.47
1:A:571:ARG:HG3	1:A:607:TRP:O	2.15	0.47
1:A:641:MET:HB3	1:A:671:MET:CE	2.41	0.47
1:C:876:PHE:O	1:C:880:SER:HB3	2.14	0.47
1:C:907:VAL:O	1:C:908:THR:C	2.57	0.47
1:D:1054:ARG:O	1:D:1054:ARG:HD3	2.15	0.47
1:A:498:GLN:C	1:A:498:GLN:HE21	2.23	0.47
1:A:502:HIS:HA	1:A:1087:ILE:HG21	1.96	0.47
1:A:565:LEU:O	1:A:602:PHE:HB3	2.14	0.47
1:A:679:SER:HB2	1:A:910:SER:OG	2.14	0.47
1:A:779:GLY:O	1:A:783:MET:HG2	2.15	0.47
1:B:680:LEU:HD11	1:B:952:ILE:HD12	1.96	0.47
1:B:904:LEU:N	1:B:904:LEU:CD1	2.77	0.47
1:C:682:TYR:CE1	1:C:684:PRO:HB2	2.50	0.47
1:C:965:SER:HA	1:C:973:ARG:NH2	2.29	0.47
1:D:503:TYR:O	1:D:507:VAL:HG23	2.14	0.47
1:D:770:ILE:HG21	1:D:783:MET:HE1	1.96	0.47
1:D:890:VAL:HG23	1:D:891:LYS:N	2.30	0.47
1:D:923:GLN:HE21	1:D:924:ASN:ND2	2.13	0.47
1:A:624:TRP:CG	1:A:1005:GLU:HB3	2.49	0.47
1:B:502:HIS:CE1	1:B:1090:LYS:HZ1	2.32	0.47
1:B:679:SER:OG	1:B:680:LEU:HD12	2.13	0.47
1:B:1074:ARG:O	1:B:1088:LEU:HD23	2.14	0.47
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.96	0.47
1:C:1063:LEU:O	1:C:1064:ALA:HB3	2.14	0.47
1:D:560:HIS:CD2	1:D:564:LEU:HD21	2.50	0.47
1:A:686:MET:O	1:A:690:MET:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:THR:O	1:C:614:VAL:HG11	2.14	0.47
1:C:1043:LYS:O	1:C:1046:GLU:HB2	2.15	0.47
1:C:1044:ILE:O	1:C:1045:ALA:CB	2.63	0.47
1:D:865:GLU:HB2	1:D:906:LYS:HZ2	1.79	0.47
1:D:1089:VAL:HG12	1:D:1090:LYS:H	1.79	0.47
1:A:656:ASP:CG	1:A:977:ARG:HH21	2.22	0.47
1:B:739:CYS:HA	1:B:769:HIS:O	2.15	0.47
1:D:1003:THR:HB	1:D:1004:PRO:HD2	1.96	0.47
1:A:738:LEU:HD12	1:A:739:CYS:N	2.31	0.46
1:A:755:LEU:HD22	1:A:759:LEU:CD1	2.45	0.46
1:B:517:PRO:HG2	1:B:847:ALA:O	2.16	0.46
1:C:904:LEU:N	1:C:904:LEU:HD12	2.30	0.46
1:D:770:ILE:CG2	1:D:783:MET:HE1	2.45	0.46
1:D:824:THR:O	1:D:825:GLU:HB2	2.14	0.46
1:D:1079:GLU:OE1	1:D:1079:GLU:N	2.47	0.46
1:A:502:HIS:CE1	1:A:1090:LYS:HZ1	2.32	0.46
1:A:583:ARG:NH1	1:A:1033:LEU:O	2.48	0.46
1:A:704:ILE:HB	1:A:740:ILE:HD13	1.97	0.46
1:A:732:ARG:C	1:A:734:GLY:N	2.72	0.46
1:A:783:MET:HA	1:A:783:MET:HE2	1.98	0.46
1:B:997:ARG:HD2	1:B:998:HIS:CD2	2.50	0.46
1:D:644:ARG:HD2	1:D:647:ASN:OD1	2.15	0.46
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.49	0.46
1:A:785:ALA:O	1:A:788:GLN:HB2	2.15	0.46
1:A:922:VAL:CG2	1:A:923:GLN:N	2.78	0.46
1:B:900:MET:CE	1:B:928:ARG:HG3	2.45	0.46
1:C:664:GLU:O	1:C:668:GLU:HG3	2.14	0.46
1:A:977:ARG:HB3	1:A:977:ARG:HH11	1.78	0.46
1:C:997:ARG:HG2	1:C:998:HIS:N	2.31	0.46
1:D:961:GLU:OE1	1:D:964:ARG:HD3	2.15	0.46
1:D:1044:ILE:CD1	1:D:1044:ILE:N	2.71	0.46
1:D:1076:VAL:HG23	1:D:1078:PHE:CE1	2.50	0.46
1:A:980:ALA:C	1:A:982:LEU:H	2.23	0.46
1:D:965:SER:C	1:D:967:VAL:H	2.22	0.46
1:D:1005:GLU:CD	1:D:1005:GLU:H	2.23	0.46
1:A:779:GLY:O	1:A:782:ALA:HB3	2.15	0.46
1:A:822:LEU:O	1:A:823:ASP:C	2.59	0.46
1:B:507:VAL:O	1:B:511:GLY:N	2.48	0.46
1:B:599:SER:C	1:B:601:LEU:H	2.22	0.46
1:B:625:ARG:HH21	1:B:629:GLU:CD	2.24	0.46
1:B:891:LYS:O	1:B:895:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:VAL:HG13	1:B:1000:GLU:HA	1.98	0.46
1:A:644:ARG:NH1	1:A:644:ARG:CB	2.78	0.46
1:A:701:GLU:OE2	1:A:769:HIS:ND1	2.36	0.46
1:A:704:ILE:HD11	1:A:730:LEU:HD12	1.97	0.46
1:B:586:ASP:OD2	1:B:1035:THR:OG1	2.32	0.46
1:C:656:ASP:OD2	1:C:977:ARG:NH2	2.48	0.46
1:C:1020:PHE:O	1:C:1024:THR:HG23	2.15	0.46
1:D:640:GLN:HG3	1:D:673:VAL:HG12	1.96	0.46
1:D:887:PHE:HD1	1:D:890:VAL:CG2	2.29	0.46
1:D:1049:GLU:HA	1:D:1058:LEU:O	2.16	0.46
1:A:862:TYR:CE1	1:B:815:ALA:HB1	2.51	0.46
1:A:1089:VAL:CG1	1:A:1090:LYS:N	2.77	0.46
1:B:631:ARG:NH2	1:B:639:PHE:CE1	2.84	0.46
1:B:899:GLN:HE21	1:B:899:GLN:CA	2.27	0.46
1:C:536:PRO:HA	1:C:537:PRO:HD3	1.75	0.46
1:C:894:TYR:HA	1:C:918:ALA:HB2	1.97	0.46
1:C:898:ASN:HD21	1:C:904:LEU:H	1.62	0.46
1:D:644:ARG:HB2	1:D:644:ARG:CZ	2.46	0.46
1:D:739:CYS:SG	1:D:740:ILE:N	2.88	0.46
1:C:498:GLN:NE2	1:C:498:GLN:C	2.74	0.46
1:C:566:MET:CE	1:C:605:GLU:HB2	2.42	0.46
1:C:965:SER:HA	1:C:973:ARG:HH22	1.81	0.46
1:D:502:HIS:HE1	1:D:1090:LYS:NZ	2.14	0.46
1:D:650:GLY:HA3	1:D:654:TYR:CE1	2.51	0.46
1:B:1017:PHE:CZ	1:B:1021:LYS:HD3	2.50	0.46
1:B:1044:ILE:O	1:B:1045:ALA:CB	2.64	0.46
1:C:499:LYS:NZ	1:C:1025:ALA:O	2.32	0.46
1:C:667:LYS:HG2	1:C:696:ALA:O	2.16	0.46
1:C:780:VAL:HG22	1:C:808:PRO:HB2	1.98	0.46
1:C:807:GLN:HB3	1:C:808:PRO:HD2	1.98	0.46
1:D:961:GLU:O	1:D:962:PRO:C	2.58	0.46
1:D:1065:VAL:CG1	1:D:1076:VAL:HG12	2.44	0.46
1:A:538:PRO:O	1:A:539:ALA:HB3	2.16	0.45
1:B:894:TYR:HA	1:B:918:ALA:HB2	1.97	0.45
1:C:539:ALA:HA	1:C:636:ASN:CB	2.44	0.45
1:C:651:TYR:CD1	1:C:652:THR:HG23	2.51	0.45
1:B:502:HIS:HD2	1:B:1087:ILE:HD11	1.81	0.45
1:B:743:MET:HE2	1:B:743:MET:H	1.81	0.45
1:B:961:GLU:N	1:B:962:PRO:HD2	2.31	0.45
1:D:707:THR:OG1	1:D:905:ILE:HG12	2.15	0.45
1:D:963:PHE:O	1:D:964:ARG:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:ASP:CG	1:A:1075:GLN:HB3	2.42	0.45
1:B:695:SER:C	1:B:697:GLY:N	2.74	0.45
1:C:814:VAL:O	1:C:817:THR:HG22	2.15	0.45
1:A:571:ARG:NH2	1:A:642:LEU:HD22	2.32	0.45
1:A:707:THR:OG1	1:A:905:ILE:HG12	2.15	0.45
1:B:547:ARG:C	1:B:548:GLU:HG3	2.42	0.45
1:B:864:ASN:HA	1:B:895:VAL:HG22	1.99	0.45
1:B:1088:LEU:HD23	1:B:1088:LEU:C	2.41	0.45
1:C:899:GLN:HA	1:C:899:GLN:HE21	1.79	0.45
1:C:899:GLN:CA	1:C:899:GLN:HE21	2.30	0.45
1:D:977:ARG:HH11	1:D:977:ARG:CB	2.30	0.45
1:B:814:VAL:O	1:B:817:THR:HG22	2.16	0.45
1:C:583:ARG:NH2	1:C:1033:LEU:O	2.49	0.45
1:D:500:LEU:O	1:D:503:TYR:HB3	2.16	0.45
1:D:506:HIS:ND1	1:D:506:HIS:C	2.75	0.45
1:D:937:GLU:O	1:D:938:LEU:HG	2.17	0.45
1:A:644:ARG:HB3	1:A:644:ARG:NH1	2.31	0.45
1:A:849:ASP:C	1:A:851:THR:N	2.74	0.45
1:B:787:ALA:O	1:B:788:GLN:C	2.60	0.45
1:B:865:GLU:HB2	1:B:906:LYS:HZ1	1.79	0.45
1:B:936:GLU:OE2	1:B:937:GLU:N	2.50	0.45
1:B:1008:LEU:O	1:B:1011:ALA:HB3	2.17	0.45
1:B:1045:ALA:HB2	1:B:1063:LEU:HG	1.99	0.45
1:C:617:ARG:HH21	1:C:1016:VAL:CG2	2.28	0.45
1:C:648:ALA:HB3	1:C:1012:MET:HE1	1.99	0.45
1:D:654:TYR:CB	1:D:658:VAL:HG21	2.46	0.45
1:D:704:ILE:HD11	1:D:730:LEU:HD12	1.98	0.45
1:D:965:SER:HA	1:D:973:ARG:HH22	1.82	0.45
1:A:762:ARG:HG3	1:A:763:PHE:CE1	2.52	0.45
1:A:901:LEU:O	1:A:904:LEU:HD11	2.16	0.45
1:A:950:GLY:O	1:A:952:ILE:N	2.50	0.45
1:B:516:ILE:O	1:B:516:ILE:HG13	2.16	0.45
1:B:855:LYS:O	1:B:856:SER:HB3	2.15	0.45
1:C:534:ILE:CG2	1:C:535:GLY:N	2.80	0.45
1:C:1067:ASP:O	1:C:1069:ASN:N	2.50	0.45
1:D:545:LEU:O	1:D:549:GLY:N	2.49	0.45
1:D:604:MET:HE1	1:D:634:ILE:CD1	2.47	0.45
1:D:907:VAL:HG12	1:D:908:THR:N	2.31	0.45
1:A:604:MET:HE1	1:A:634:ILE:HD13	1.99	0.45
1:B:701:GLU:HG3	1:B:737:ILE:HB	1.99	0.45
1:B:907:VAL:O	1:B:908:THR:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:ALA:HB1	1:D:862:TYR:CE1	2.52	0.45
1:C:967:VAL:O	1:C:969:LYS:HG3	2.16	0.45
1:D:536:PRO:HA	1:D:537:PRO:HD3	1.76	0.45
1:D:547:ARG:O	1:D:548:GLU:HG3	2.17	0.45
1:D:893:ALA:HB2	1:D:922:VAL:CG1	2.47	0.45
1:D:1010:ALA:HB2	1:D:1017:PHE:CD2	2.51	0.45
1:A:678:ASP:HB2	1:A:686:MET:CG	2.47	0.45
1:A:894:TYR:CE2	1:A:906:LYS:HD2	2.52	0.45
1:A:1003:THR:HB	1:A:1004:PRO:HD2	1.99	0.45
1:B:894:TYR:CE2	1:B:906:LYS:HD2	2.52	0.45
1:B:1002:VAL:HG23	1:B:1002:VAL:O	2.17	0.45
1:B:1060:ILE:HG22	1:B:1061:LYS:N	2.31	0.45
1:B:1089:VAL:CG1	1:B:1090:LYS:N	2.77	0.45
1:B:1092:THR:O	1:B:1093:GLN:HG2	2.17	0.45
1:C:711:ALA:HA	1:C:754:MET:CE	2.35	0.45
1:C:772:THR:HG21	1:C:783:MET:HE3	1.99	0.45
1:C:1010:ALA:HB2	1:C:1017:PHE:CD2	2.52	0.45
1:D:506:HIS:HA	1:D:1089:VAL:HG11	1.98	0.45
1:D:657:ASN:ND2	1:D:985:LEU:H	2.15	0.45
1:A:597:ASN:HB3	1:A:830:ARG:HD3	1.99	0.45
1:A:756:VAL:CG1	1:A:789:ALA:HB3	2.47	0.45
1:A:815:ALA:HB2	1:A:828:MET:CE	2.47	0.45
1:B:828:MET:O	1:B:831:VAL:HG22	2.17	0.45
1:B:859:SER:C	1:B:861:VAL:N	2.75	0.45
1:C:544:ILE:O	1:C:545:LEU:C	2.60	0.45
1:C:769:HIS:NE2	1:C:795:ASP:OD1	2.50	0.45
1:C:1063:LEU:O	1:C:1064:ALA:CB	2.63	0.45
1:C:1068:LEU:HA	1:C:1074:ARG:NE	2.31	0.45
1:D:551:GLU:OE2	1:D:551:GLU:HA	2.17	0.45
1:D:650:GLY:HA3	1:D:654:TYR:OH	2.17	0.45
1:D:679:SER:OG	1:D:909:PRO:HB2	2.17	0.45
1:A:655:PRO:HB3	1:A:983:PRO:O	2.17	0.44
1:A:860:ASP:OD1	1:A:891:LYS:NZ	2.50	0.44
1:C:496:ARG:NH1	1:C:1056:LYS:NZ	2.64	0.44
1:C:599:SER:C	1:C:601:LEU:H	2.25	0.44
1:C:807:GLN:H	1:C:807:GLN:HE21	1.64	0.44
1:C:1091:ASP:O	1:C:1092:THR:C	2.60	0.44
1:D:711:ALA:HB2	1:D:751:ALA:HA	1.99	0.44
1:D:788:GLN:OE1	1:D:788:GLN:HA	2.17	0.44
1:D:893:ALA:HB2	1:D:922:VAL:HG13	1.99	0.44
1:D:1052:LEU:HD22	1:D:1056:LYS:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLN:CG	1:A:1056:LYS:NZ	2.76	0.44
1:A:987:LEU:O	1:A:991:GLU:N	2.45	0.44
1:B:552:GLY:HA2	1:B:555:ARG:HD2	1.99	0.44
1:C:947:PHE:HD1	1:C:952:ILE:HD11	1.83	0.44
1:C:1073:GLN:NE2	1:C:1088:LEU:HD22	2.32	0.44
1:D:948:LEU:HD22	1:D:964:ARG:HG3	2.00	0.44
1:D:1065:VAL:HG22	1:D:1076:VAL:CB	2.47	0.44
1:D:1079:GLU:HA	1:D:1084:LEU:HB3	1.99	0.44
1:A:501:LEU:O	1:A:502:HIS:C	2.61	0.44
1:A:643:LEU:HD12	1:A:648:ALA:HA	1.98	0.44
1:A:766:LEU:HD12	1:A:767:PRO:CD	2.46	0.44
1:B:534:ILE:CG2	1:B:535:GLY:N	2.79	0.44
1:B:752:CYS:O	1:B:753:THR:C	2.60	0.44
1:B:908:THR:O	1:B:909:PRO:C	2.59	0.44
1:B:964:ARG:HG2	1:B:968:LEU:HD12	1.99	0.44
1:D:908:THR:HG22	1:D:909:PRO:N	2.32	0.44
1:A:660:PHE:HA	1:A:692:ALA:HB1	1.98	0.44
1:B:591:ALA:HB3	1:B:633:LEU:HD13	2.00	0.44
1:B:656:ASP:CG	1:B:977:ARG:HH21	2.26	0.44
1:B:1052:LEU:HD23	1:B:1053:GLU:HB2	1.98	0.44
1:C:959:PHE:CB	1:C:964:ARG:HD2	2.47	0.44
1:C:961:GLU:N	1:C:962:PRO:HD2	2.33	0.44
1:C:999:GLY:C	1:C:1001:GLU:H	2.25	0.44
1:C:1073:GLN:O	1:C:1074:ARG:HB2	2.17	0.44
1:A:997:ARG:HD2	1:A:998:HIS:CD2	2.52	0.44
1:A:1089:VAL:CG1	1:A:1090:LYS:H	2.30	0.44
1:B:883:LEU:HD22	1:B:886:LYS:HG3	2.00	0.44
1:D:643:LEU:O	1:D:676:VAL:HA	2.18	0.44
1:D:891:LYS:O	1:D:895:VAL:HG23	2.17	0.44
1:D:1068:LEU:HD13	1:D:1074:ARG:CZ	2.47	0.44
1:A:539:ALA:HA	1:A:636:ASN:CB	2.42	0.44
1:B:645:GLY:HA2	1:B:689:GLY:HA3	2.00	0.44
1:B:657:ASN:ND2	1:B:985:LEU:H	2.16	0.44
1:B:1045:ALA:CB	1:B:1063:LEU:HG	2.47	0.44
1:B:1054:ARG:HD3	1:B:1054:ARG:C	2.42	0.44
1:C:571:ARG:NH1	1:C:575:GLN:NE2	2.58	0.44
1:C:661:LYS:O	1:C:665:VAL:HG23	2.17	0.44
1:D:665:VAL:HG12	1:D:669:ASN:ND2	2.32	0.44
1:A:590:ILE:O	1:A:590:ILE:HG13	2.17	0.44
1:A:752:CYS:O	1:A:753:THR:C	2.60	0.44
1:A:756:VAL:HG11	1:A:789:ALA:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:VAL:O	1:A:817:THR:HG22	2.18	0.44
1:B:908:THR:CB	1:B:909:PRO:HD3	2.46	0.44
1:B:971:LEU:HA	1:B:972:PRO:HD3	1.71	0.44
1:D:708:GLY:HA2	1:D:715:ARG:NH1	2.32	0.44
1:D:743:MET:HE2	1:D:744:ALA:H	1.82	0.44
1:D:936:GLU:CD	1:D:937:GLU:N	2.76	0.44
1:A:656:ASP:OD2	1:A:977:ARG:NH2	2.51	0.44
1:A:961:GLU:N	1:A:962:PRO:HD2	2.33	0.44
1:A:995:VAL:CG1	1:A:1000:GLU:HA	2.48	0.44
1:B:949:GLN:HG3	1:B:968:LEU:HD22	1.99	0.44
1:C:1057:THR:HB	1:C:1059:HIS:CE1	2.53	0.44
1:D:644:ARG:O	1:D:645:GLY:C	2.60	0.44
1:A:1020:PHE:CE1	1:A:1024:THR:HG21	2.53	0.44
1:A:1052:LEU:HD23	1:A:1053:GLU:HB2	2.00	0.44
1:A:1074:ARG:O	1:A:1088:LEU:HD23	2.17	0.44
1:B:738:LEU:HD12	1:B:739:CYS:H	1.83	0.44
1:C:682:TYR:C	1:C:684:PRO:HD2	2.43	0.44
1:C:807:GLN:NE2	1:C:807:GLN:N	2.65	0.44
1:D:849:ASP:CB	1:D:851:THR:HG22	2.48	0.44
1:D:971:LEU:HA	1:D:972:PRO:HD3	1.85	0.44
1:A:876:PHE:O	1:A:880:SER:HB3	2.18	0.43
1:A:961:GLU:HA	1:A:964:ARG:HB3	2.00	0.43
1:B:818:ARG:HA	1:B:823:ASP:CG	2.43	0.43
1:B:987:LEU:O	1:B:991:GLU:N	2.49	0.43
1:C:884:GLY:O	1:C:885:SER:C	2.61	0.43
1:D:599:SER:C	1:D:601:LEU:H	2.26	0.43
1:D:785:ALA:O	1:D:788:GLN:HB2	2.18	0.43
1:A:770:ILE:CG2	1:A:783:MET:HE1	2.47	0.43
1:B:575:GLN:HG3	1:B:580:THR:HG1	1.81	0.43
1:C:690:MET:HE3	1:C:735:THR:HB	2.00	0.43
1:C:849:ASP:CB	1:C:851:THR:HG22	2.46	0.43
1:C:964:ARG:HE	1:C:968:LEU:HD11	1.83	0.43
1:C:1092:THR:O	1:C:1093:GLN:C	2.60	0.43
1:B:532:VAL:HG23	1:B:532:VAL:O	2.18	0.43
1:B:827:PRO:HD2	1:B:830:ARG:HD2	2.00	0.43
1:C:658:VAL:HG23	1:C:659:VAL:N	2.32	0.43
1:C:743:MET:SD	1:C:907:VAL:HG22	2.58	0.43
1:C:824:THR:O	1:C:825:GLU:HB2	2.17	0.43
1:C:1078:PHE:C	1:C:1079:GLU:OE1	2.61	0.43
1:D:829:GLU:O	1:D:832:PHE:HB2	2.19	0.43
1:D:883:LEU:HD22	1:D:886:LYS:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:TYR:CE1	1:A:597:ASN:ND2	2.86	0.43
1:A:624:TRP:CD1	1:A:1005:GLU:HB3	2.54	0.43
1:A:898:ASN:HD21	1:A:904:LEU:N	2.11	0.43
1:A:903:ASP:C	1:A:904:LEU:HD12	2.43	0.43
1:B:495:ASN:O	1:B:496:ARG:C	2.61	0.43
1:B:571:ARG:NH1	1:B:575:GLN:NE2	2.56	0.43
1:B:936:GLU:O	1:B:969:LYS:HE3	2.17	0.43
1:B:938:LEU:HB2	1:B:940:PHE:CE1	2.53	0.43
1:C:641:MET:O	1:C:641:MET:HG3	2.15	0.43
1:C:815:ALA:HB2	1:C:828:MET:HE1	1.99	0.43
1:C:860:ASP:HA	1:D:832:PHE:CZ	2.54	0.43
1:C:907:VAL:HG12	1:C:908:THR:N	2.33	0.43
1:D:1067:ASP:OD1	1:D:1075:GLN:HB3	2.18	0.43
1:A:827:PRO:HD2	1:A:830:ARG:HD2	2.00	0.43
1:B:500:LEU:O	1:B:503:TYR:HB3	2.19	0.43
1:B:549:GLY:C	1:B:551:GLU:H	2.27	0.43
1:B:707:THR:CG2	1:B:708:GLY:N	2.81	0.43
1:B:732:ARG:C	1:B:734:GLY:N	2.74	0.43
1:B:1029:PRO:C	1:B:1031:ASP:N	2.73	0.43
1:C:756:VAL:O	1:C:759:LEU:HB2	2.18	0.43
1:A:599:SER:C	1:A:601:LEU:N	2.76	0.43
1:A:948:LEU:HA	1:A:959:PHE:CE2	2.54	0.43
1:C:564:LEU:O	1:C:793:VAL:HA	2.19	0.43
1:C:679:SER:HB2	1:C:910:SER:OG	2.17	0.43
1:C:917:LEU:O	1:C:921:MET:HG3	2.18	0.43
1:A:770:ILE:HG22	1:A:783:MET:HE1	2.00	0.43
1:A:899:GLN:NE2	1:A:899:GLN:CA	2.75	0.43
1:A:977:ARG:HH11	1:A:977:ARG:CB	2.31	0.43
1:B:655:PRO:HB2	1:B:984:PRO:HA	2.01	0.43
1:C:936:GLU:CD	1:C:937:GLU:N	2.77	0.43
1:D:959:PHE:HB2	1:D:964:ARG:HD2	2.01	0.43
1:D:1015:ASP:HB3	1:D:1019:HIS:NE2	2.33	0.43
1:A:574:HIS:CD2	1:A:580:THR:HA	2.54	0.43
1:A:660:PHE:CD2	1:A:692:ALA:HA	2.54	0.43
1:A:849:ASP:CB	1:A:851:THR:HG22	2.43	0.43
1:A:865:GLU:HB2	1:A:906:LYS:HZ2	1.84	0.43
1:A:893:ALA:HB2	1:A:922:VAL:CG1	2.48	0.43
1:B:677:PHE:CE1	1:B:907:VAL:HG11	2.53	0.43
1:B:901:LEU:HB2	1:B:904:LEU:HD11	2.00	0.43
1:B:952:ILE:HG13	1:B:953:GLY:H	1.84	0.43
1:C:528:VAL:O	1:C:530:PRO:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:GLY:HA3	1:C:823:ASP:O	2.19	0.43
1:C:793:VAL:HG12	1:C:794:VAL:N	2.33	0.43
1:D:494:GLN:HE21	1:D:494:GLN:HB2	1.69	0.43
1:D:1065:VAL:HG22	1:D:1076:VAL:HB	2.00	0.43
1:A:860:ASP:HA	1:B:832:PHE:CE2	2.54	0.43
1:B:599:SER:C	1:B:601:LEU:N	2.76	0.43
1:B:680:LEU:HD12	1:B:680:LEU:N	2.34	0.43
1:B:977:ARG:NH1	1:B:980:ALA:HB2	2.33	0.43
1:C:827:PRO:O	1:C:828:MET:C	2.62	0.43
1:C:948:LEU:HA	1:C:959:PHE:CE2	2.54	0.43
1:C:1063:LEU:HD23	1:C:1063:LEU:HA	1.89	0.43
1:D:624:TRP:CZ3	1:D:665:VAL:HG12	2.53	0.43
1:A:908:THR:HG22	1:A:909:PRO:N	2.33	0.43
1:A:995:VAL:CG2	1:A:1002:VAL:HG21	2.45	0.43
1:A:1015:ASP:O	1:A:1018:ALA:N	2.51	0.43
1:C:997:ARG:HD2	1:C:998:HIS:CD2	2.54	0.43
1:D:961:GLU:OE2	1:D:965:SER:HB3	2.19	0.43
1:C:752:CYS:O	1:C:753:THR:C	2.60	0.42
1:C:1003:THR:O	1:C:1004:PRO:C	2.60	0.42
1:D:859:SER:C	1:D:861:VAL:H	2.26	0.42
1:A:919:GLN:O	1:A:922:VAL:HG22	2.19	0.42
1:A:988:GLN:N	1:A:988:GLN:OE1	2.51	0.42
1:B:564:LEU:O	1:B:793:VAL:HA	2.19	0.42
1:B:590:ILE:O	1:B:590:ILE:HG13	2.19	0.42
1:B:1068:LEU:HA	1:B:1074:ARG:NE	2.32	0.42
1:C:1074:ARG:O	1:C:1088:LEU:HD23	2.19	0.42
1:D:787:ALA:O	1:D:788:GLN:C	2.61	0.42
1:D:887:PHE:O	1:D:888:LYS:C	2.62	0.42
1:A:849:ASP:C	1:A:851:THR:H	2.26	0.42
1:B:947:PHE:HD1	1:B:952:ILE:HD11	1.84	0.42
1:C:908:THR:O	1:C:909:PRO:C	2.58	0.42
1:C:964:ARG:O	1:C:967:VAL:HB	2.19	0.42
1:A:523:SER:O	1:A:1036:ARG:NH2	2.48	0.42
1:A:967:VAL:O	1:A:969:LYS:HG3	2.19	0.42
1:B:762:ARG:CG	1:B:763:PHE:CE1	3.02	0.42
1:C:650:GLY:HA3	1:C:654:TYR:HE1	1.84	0.42
1:C:1029:PRO:C	1:C:1031:ASP:H	2.26	0.42
1:D:1003:THR:HB	1:D:1004:PRO:CD	2.48	0.42
1:A:522:PRO:O	1:A:523:SER:C	2.63	0.42
1:A:787:ALA:O	1:A:788:GLN:C	2.63	0.42
1:A:901:LEU:HA	1:A:960:PRO:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:PHE:CZ	1:A:1021:LYS:HD3	2.55	0.42
1:B:762:ARG:HG3	1:B:763:PHE:CZ	2.54	0.42
1:B:961:GLU:O	1:B:962:PRO:C	2.63	0.42
1:B:961:GLU:C	1:B:963:PHE:N	2.75	0.42
1:B:983:PRO:O	1:B:984:PRO:O	2.38	0.42
1:C:712:ASP:OD1	1:C:714:SER:HB2	2.19	0.42
1:C:881:MET:O	1:C:883:LEU:HG	2.20	0.42
1:C:947:PHE:CD1	1:C:952:ILE:HD11	2.55	0.42
1:D:502:HIS:CE1	1:D:1090:LYS:NZ	2.87	0.42
1:D:581:ARG:NH1	1:D:848:PHE:CE2	2.87	0.42
1:D:625:ARG:O	1:D:626:ARG:C	2.61	0.42
1:A:595:ALA:CB	1:A:634:ILE:HG23	2.48	0.42
1:B:601:LEU:CD2	1:B:603:SER:O	2.64	0.42
1:B:1045:ALA:N	1:B:1063:LEU:HG	2.35	0.42
1:C:990:LEU:O	1:C:994:LEU:HG	2.20	0.42
1:D:541:PHE:O	1:D:542:ARG:C	2.62	0.42
1:D:900:MET:HE1	1:D:921:MET:SD	2.60	0.42
1:D:1001:GLU:HA	1:D:1001:GLU:OE1	2.20	0.42
1:D:1092:THR:O	1:D:1093:GLN:C	2.62	0.42
1:B:501:LEU:O	1:B:502:HIS:C	2.63	0.42
1:B:1057:THR:HB	1:B:1059:HIS:CE1	2.55	0.42
1:C:907:VAL:HG12	1:C:908:THR:H	1.85	0.42
1:A:494:GLN:HG2	1:A:1056:LYS:CE	2.49	0.42
1:A:1065:VAL:CG1	1:A:1076:VAL:HG12	2.44	0.42
1:B:954:VAL:HA	1:B:955:PRO:HD2	1.90	0.42
1:C:682:TYR:HD1	1:C:685:ASN:ND2	2.18	0.42
1:C:893:ALA:CB	1:C:922:VAL:HG13	2.50	0.42
1:C:968:LEU:HB2	1:C:973:ARG:HH21	1.85	0.42
1:D:752:CYS:O	1:D:753:THR:C	2.62	0.42
1:A:551:GLU:OE2	1:A:551:GLU:HA	2.20	0.42
1:A:562:GLY:HA3	1:A:823:ASP:O	2.19	0.42
1:A:566:MET:HE3	1:A:568:THR:HG22	2.02	0.42
1:A:934:GLN:O	1:A:938:LEU:HG	2.20	0.42
1:A:945:VAL:HG23	1:A:946:GLU:N	2.35	0.42
1:A:1067:ASP:HB2	1:A:1074:ARG:HA	2.02	0.42
1:B:494:GLN:HB2	1:B:497:ALA:HB3	2.01	0.42
1:B:654:TYR:CB	1:B:658:VAL:HG21	2.49	0.42
1:B:785:ALA:O	1:B:788:GLN:HB2	2.19	0.42
1:C:603:SER:HA	1:C:638:PRO:HB2	2.00	0.42
1:C:901:LEU:HB2	1:C:904:LEU:CD1	2.48	0.42
1:C:918:ALA:O	1:C:922:VAL:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:PHE:HB2	1:C:964:ARG:HD2	2.02	0.42
1:D:597:ASN:O	1:D:830:ARG:NH1	2.53	0.42
1:D:658:VAL:HG23	1:D:659:VAL:N	2.34	0.42
1:D:987:LEU:O	1:D:991:GLU:N	2.45	0.42
1:A:614:VAL:HG13	1:A:618:PHE:HD1	1.84	0.42
1:A:893:ALA:CB	1:A:922:VAL:HG13	2.49	0.42
1:A:1003:THR:O	1:A:1004:PRO:C	2.62	0.42
1:A:1065:VAL:HA	1:A:1075:GLN:O	2.19	0.42
1:C:570:PHE:HB3	1:C:606:ASN:CB	2.50	0.42
1:C:859:SER:C	1:C:861:VAL:H	2.27	0.42
1:C:964:ARG:HG2	1:C:968:LEU:HD12	2.02	0.42
1:D:657:ASN:HD21	1:D:985:LEU:H	1.67	0.42
1:A:545:LEU:O	1:A:549:GLY:N	2.47	0.41
1:A:1092:THR:O	1:A:1093:GLN:HG2	2.20	0.41
1:B:502:HIS:HA	1:B:1087:ILE:HG12	2.01	0.41
1:B:1003:THR:O	1:B:1004:PRO:C	2.60	0.41
1:C:763:PHE:HA	1:C:764:PRO:HD2	1.81	0.41
1:C:1073:GLN:CD	1:C:1088:LEU:HD21	2.45	0.41
1:A:621:GLU:HG2	1:A:1031:ASP:CB	2.49	0.41
1:A:643:LEU:HD11	1:A:648:ALA:HA	2.01	0.41
1:A:1067:ASP:HA	1:D:1082:GLY:O	2.20	0.41
1:B:502:HIS:HA	1:B:1087:ILE:HG21	2.02	0.41
1:B:686:MET:HE3	1:B:703:ALA:O	2.20	0.41
1:C:737:ILE:HD12	1:C:767:PRO:CB	2.51	0.41
1:D:732:ARG:C	1:D:734:GLY:N	2.74	0.41
1:D:827:PRO:O	1:D:828:MET:C	2.63	0.41
1:A:772:THR:HG21	1:A:783:MET:HE3	2.02	0.41
1:A:1002:VAL:O	1:A:1002:VAL:HG23	2.20	0.41
1:B:508:MET:HE3	1:B:1042:PRO:O	2.21	0.41
1:B:536:PRO:HA	1:B:537:PRO:HD3	1.84	0.41
1:B:742:ASP:HB2	1:B:747:LEU:CD1	2.50	0.41
1:B:1066:SER:C	1:B:1068:LEU:N	2.74	0.41
1:C:560:HIS:CG	1:C:564:LEU:HD21	2.55	0.41
1:C:654:TYR:CE1	1:C:1012:MET:HE2	2.55	0.41
1:C:704:ILE:HB	1:C:740:ILE:HD13	2.02	0.41
1:C:737:ILE:HD12	1:C:767:PRO:HB2	2.02	0.41
1:C:739:CYS:SG	1:C:740:ILE:N	2.93	0.41
1:C:961:GLU:C	1:C:963:PHE:N	2.75	0.41
1:A:496:ARG:NH1	1:A:1056:LYS:NZ	2.69	0.41
1:A:749:PRO:O	1:A:752:CYS:HB2	2.20	0.41
1:A:788:GLN:HA	1:A:788:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:THR:CB	1:A:909:PRO:HD3	2.43	0.41
1:B:809:SER:O	1:B:813:LEU:HD23	2.20	0.41
1:B:897:ALA:O	1:B:901:LEU:HG	2.20	0.41
1:B:977:ARG:HB3	1:B:977:ARG:HH11	1.86	0.41
1:B:1058:LEU:HD22	1:B:1080:LEU:HD11	2.01	0.41
1:B:1065:VAL:CG2	1:B:1076:VAL:HG12	2.48	0.41
1:C:506:HIS:CE1	1:C:510:ASN:HB2	2.56	0.41
1:C:590:ILE:O	1:C:590:ILE:HG13	2.21	0.41
1:C:612:PHE:HB3	1:C:649:VAL:HG12	2.02	0.41
1:C:732:ARG:C	1:C:734:GLY:N	2.78	0.41
1:D:571:ARG:NH1	1:D:575:GLN:NE2	2.62	0.41
1:D:1089:VAL:CG1	1:D:1090:LYS:N	2.83	0.41
1:A:749:PRO:CD	1:B:816:CYS:SG	3.08	0.41
1:B:755:LEU:HD22	1:B:759:LEU:HD12	2.02	0.41
1:B:1067:ASP:O	1:B:1074:ARG:HA	2.21	0.41
1:D:624:TRP:CG	1:D:1005:GLU:HB3	2.55	0.41
1:D:950:GLY:O	1:D:952:ILE:N	2.53	0.41
1:A:690:MET:HE3	1:A:735:THR:HB	2.03	0.41
1:A:879:HIS:CE1	1:A:884:GLY:HA3	2.56	0.41
1:A:900:MET:HE3	1:A:928:ARG:HG3	2.00	0.41
1:A:1001:GLU:O	1:A:1002:VAL:O	2.39	0.41
1:A:1079:GLU:HA	1:A:1084:LEU:HB3	2.03	0.41
1:B:982:LEU:HA	1:B:983:PRO:HD3	1.91	0.41
1:C:498:GLN:C	1:C:498:GLN:HE21	2.28	0.41
1:C:545:LEU:O	1:C:549:GLY:N	2.52	0.41
1:C:579:ALA:O	1:C:581:ARG:HG2	2.20	0.41
1:C:586:ASP:OD2	1:C:1035:THR:OG1	2.27	0.41
1:C:680:LEU:HD11	1:C:952:ILE:HD12	2.02	0.41
1:C:707:THR:CG2	1:C:708:GLY:N	2.84	0.41
1:D:720:LEU:O	1:D:724:MET:HG2	2.21	0.41
1:D:923:GLN:HE21	1:D:924:ASN:HD21	1.67	0.41
1:A:565:LEU:O	1:A:601:LEU:HD23	2.20	0.41
1:A:580:THR:HG21	1:A:610:ALA:HB3	2.02	0.41
1:A:769:HIS:C	1:A:770:ILE:HD13	2.46	0.41
1:A:827:PRO:O	1:A:828:MET:C	2.62	0.41
1:B:769:HIS:CD2	1:B:793:VAL:HB	2.56	0.41
1:B:827:PRO:O	1:B:828:MET:C	2.64	0.41
1:B:874:LEU:N	1:B:874:LEU:CD1	2.83	0.41
1:B:965:SER:O	1:B:967:VAL:N	2.54	0.41
1:C:787:ALA:HB1	1:C:822:LEU:HD13	2.02	0.41
1:C:883:LEU:HB3	1:C:886:LYS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:VAL:CG2	1:C:946:GLU:N	2.84	0.41
1:D:949:GLN:HG3	1:D:968:LEU:HD22	2.02	0.41
1:D:976:GLY:O	1:D:977:ARG:C	2.64	0.41
1:A:610:ALA:O	1:A:611:THR:C	2.63	0.41
1:B:651:TYR:CD2	1:B:651:TYR:N	2.89	0.41
1:B:893:ALA:CB	1:B:922:VAL:HG13	2.50	0.41
1:B:1078:PHE:C	1:B:1079:GLU:OE1	2.64	0.41
1:C:828:MET:O	1:C:829:GLU:C	2.64	0.41
1:C:1073:GLN:CD	1:C:1088:LEU:CD2	2.94	0.41
1:C:1089:VAL:HA	1:C:1090:LYS:HZ2	1.86	0.41
1:D:603:SER:HA	1:D:638:PRO:HB2	2.01	0.41
1:D:1091:ASP:C	1:D:1093:GLN:N	2.78	0.41
1:A:502:HIS:HA	1:A:1087:ILE:HG12	2.03	0.41
1:A:506:HIS:HA	1:A:1089:VAL:HG11	2.02	0.41
1:A:743:MET:HE2	1:A:744:ALA:H	1.86	0.41
1:A:906:LYS:HB3	1:A:911:SER:CB	2.51	0.41
1:A:961:GLU:C	1:A:963:PHE:N	2.79	0.41
1:B:494:GLN:HG2	1:B:1056:LYS:HZ3	1.86	0.41
1:B:654:TYR:HB3	1:B:658:VAL:HG21	2.02	0.41
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	2.03	0.41
1:B:1013:TYR:O	1:B:1017:PHE:CB	2.69	0.41
1:C:599:SER:C	1:C:601:LEU:N	2.78	0.41
1:C:650:GLY:HA3	1:C:654:TYR:OH	2.21	0.41
1:C:673:VAL:HA	1:C:699:VAL:HB	2.03	0.41
1:C:936:GLU:O	1:C:969:LYS:HE3	2.20	0.41
1:C:961:GLU:O	1:C:962:PRO:C	2.62	0.41
1:C:1043:LYS:HB2	1:C:1046:GLU:OE1	2.21	0.41
1:D:584:THR:HG22	1:D:588:LYS:HG3	2.02	0.41
1:D:711:ALA:HA	1:D:754:MET:CE	2.44	0.41
1:D:738:LEU:HD12	1:D:739:CYS:N	2.36	0.41
1:A:542:ARG:HD3	1:A:542:ARG:O	2.21	0.41
1:A:654:TYR:CB	1:A:658:VAL:HG21	2.51	0.41
1:A:867:PRO:HD2	1:A:870:GLN:OE1	2.21	0.41
1:B:793:VAL:HG12	1:B:794:VAL:N	2.35	0.41
1:B:1050:VAL:O	1:B:1050:VAL:CG2	2.66	0.41
1:C:832:PHE:CE2	1:D:860:ASP:HA	2.55	0.41
1:C:874:LEU:N	1:C:874:LEU:CD1	2.84	0.41
1:C:876:PHE:O	1:C:880:SER:CB	2.69	0.41
1:D:769:HIS:NE2	1:D:795:ASP:OD1	2.54	0.41
1:D:885:SER:OG	1:D:886:LYS:N	2.53	0.41
1:D:999:GLY:C	1:D:1001:GLU:H	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1029:PRO:C	1:D:1031:ASP:N	2.77	0.41
1:A:959:PHE:CB	1:A:964:ARG:HD2	2.51	0.40
1:A:1003:THR:HB	1:A:1004:PRO:CD	2.51	0.40
1:B:900:MET:HB2	1:B:900:MET:HE3	1.97	0.40
1:B:963:PHE:O	1:B:964:ARG:C	2.64	0.40
1:C:494:GLN:HE21	1:C:494:GLN:HB2	1.71	0.40
1:C:818:ARG:HA	1:C:823:ASP:CG	2.46	0.40
1:C:1060:ILE:CG2	1:C:1061:LYS:N	2.84	0.40
1:D:557:VAL:HG13	1:D:564:LEU:HD12	2.03	0.40
1:D:965:SER:HA	1:D:973:ARG:NH2	2.36	0.40
1:A:814:VAL:HG13	1:A:824:THR:OG1	2.21	0.40
1:A:862:TYR:CE1	1:B:815:ALA:CB	3.04	0.40
1:A:896:GLU:O	1:A:900:MET:HB2	2.21	0.40
1:A:1075:GLN:OE1	1:D:1084:LEU:HD11	2.21	0.40
1:B:496:ARG:NH1	1:B:1056:LYS:NZ	2.69	0.40
1:B:643:LEU:HD12	1:B:648:ALA:HA	2.03	0.40
1:B:655:PRO:HB2	1:B:657:ASN:OD1	2.21	0.40
1:B:657:ASN:HD21	1:B:985:LEU:H	1.69	0.40
1:B:945:VAL:CG2	1:B:946:GLU:N	2.85	0.40
1:C:654:TYR:HB3	1:C:658:VAL:HG21	2.03	0.40
1:C:756:VAL:CG1	1:C:789:ALA:HB3	2.51	0.40
1:C:815:ALA:CB	1:D:862:TYR:CE1	3.04	0.40
1:D:898:ASN:HD22	1:D:906:LYS:HD3	1.85	0.40
1:D:997:ARG:HG3	1:D:997:ARG:NH1	2.37	0.40
1:A:1045:ALA:HB2	1:A:1063:LEU:HG	2.02	0.40
1:B:707:THR:HG22	1:B:708:GLY:H	1.86	0.40
1:B:736:HIS:C	1:B:737:ILE:HD13	2.46	0.40
1:B:767:PRO:HA	1:B:792:ASP:OD2	2.20	0.40
1:B:964:ARG:HG2	1:B:968:LEU:CD1	2.52	0.40
1:C:507:VAL:O	1:C:511:GLY:N	2.52	0.40
1:C:549:GLY:C	1:C:551:GLU:N	2.78	0.40
1:C:1003:THR:HB	1:C:1004:PRO:HD2	2.02	0.40
1:D:867:PRO:HD2	1:D:870:GLN:OE1	2.21	0.40
1:D:1065:VAL:CG2	1:D:1076:VAL:HG12	2.50	0.40
1:A:961:GLU:OE2	1:A:965:SER:HB3	2.20	0.40
1:B:544:ILE:O	1:B:545:LEU:C	2.65	0.40
1:B:915:GLY:O	1:B:919:GLN:HG3	2.22	0.40
1:B:942:ARG:O	1:B:945:VAL:CG2	2.69	0.40
1:B:1043:LYS:HD3	1:B:1043:LYS:HA	1.93	0.40
1:B:1092:THR:O	1:B:1093:GLN:C	2.64	0.40
1:C:495:ASN:H	1:C:496:ARG:HH21	1.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:922:VAL:CG2	1:C:923:GLN:N	2.85	0.40
1:D:494:GLN:HB2	1:D:497:ALA:CB	2.51	0.40
1:D:771:HIS:CE1	1:D:807:GLN:OE1	2.74	0.40
1:D:1045:ALA:HB2	1:D:1063:LEU:HG	2.03	0.40
1:A:712:ASP:OD1	1:A:714:SER:HB2	2.21	0.40
1:A:971:LEU:HA	1:A:972:PRO:HD3	1.79	0.40
1:B:807:GLN:HB3	1:B:808:PRO:HD2	2.03	0.40
1:C:923:GLN:HE21	1:C:924:ASN:ND2	2.19	0.40
1:C:942:ARG:C	1:C:945:VAL:HG22	2.45	0.40
1:C:1067:ASP:OD1	1:C:1075:GLN:HB3	2.21	0.40
1:D:1091:ASP:O	1:D:1092:THR:C	2.63	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:LYS:NZ	1:C:970:ASP:OD1[1_565]	2.18	0.02

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	599/718 (83%)	505 (84%)	72 (12%)	22 (4%)	2	15
1	B	599/718 (83%)	495 (83%)	83 (14%)	21 (4%)	3	16
1	C	599/718 (83%)	497 (83%)	80 (13%)	22 (4%)	2	15
1	D	599/718 (83%)	499 (83%)	76 (13%)	24 (4%)	2	14
All	All	2396/2872 (83%)	1996 (83%)	311 (13%)	89 (4%)	2	15

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ALA
1	A	779	GLY
1	A	984	PRO
1	A	1002	VAL
1	A	1062	ALA
1	A	1064	ALA
1	A	1066	SER
1	A	1068	LEU
1	A	1070	ARG
1	B	779	GLY
1	B	984	PRO
1	B	1062	ALA
1	B	1064	ALA
1	B	1066	SER
1	B	1070	ARG
1	C	779	GLY
1	C	903	ASP
1	C	984	PRO
1	C	1062	ALA
1	C	1066	SER
1	C	1068	LEU
1	C	1070	ARG
1	D	779	GLY
1	D	984	PRO
1	D	1062	ALA
1	D	1064	ALA
1	D	1066	SER
1	D	1068	LEU
1	D	1070	ARG
1	A	648	ALA
1	A	903	ASP
1	A	951	TYR
1	A	981	SER
1	A	1058	LEU
1	B	497	ALA
1	B	648	ALA
1	B	909	PRO
1	B	1002	VAL
1	B	1058	LEU
1	B	1068	LEU
1	C	539	ALA
1	C	648	ALA
1	C	1002	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1058	LEU
1	C	1064	ALA
1	C	1067	ASP
1	D	497	ALA
1	D	903	ASP
1	D	909	PRO
1	D	1002	VAL
1	D	1058	LEU
1	A	908	THR
1	A	909	PRO
1	A	1067	ASP
1	B	903	ASP
1	B	908	THR
1	B	936	GLU
1	B	1074	ARG
1	C	497	ALA
1	C	908	THR
1	C	909	PRO
1	C	1014	PRO
1	D	648	ALA
1	D	714	SER
1	D	951	TYR
1	D	1067	ASP
1	A	530	PRO
1	A	539	ALA
1	A	561	PRO
1	B	539	ALA
1	B	981	SER
1	D	908	THR
1	D	1074	ARG
1	B	1014	PRO
1	C	561	PRO
1	C	1074	ARG
1	D	981	SER
1	D	998	HIS
1	A	611	THR
1	B	530	PRO
1	B	561	PRO
1	C	964	ARG
1	C	998	HIS
1	D	539	ALA
1	D	561	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1014	PRO
1	A	1014	PRO
1	D	530	PRO
1	C	530	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/593 (83%)	466 (94%)	27 (6%)	19	53
1	B	493/593 (83%)	466 (94%)	27 (6%)	19	53
1	C	493/593 (83%)	467 (95%)	26 (5%)	20	54
1	D	493/593 (83%)	467 (95%)	26 (5%)	20	54
All	All	1972/2372 (83%)	1866 (95%)	106 (5%)	20	53

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	496	ARG
1	A	498	GLN
1	A	542	ARG
1	A	601	LEU
1	A	607	TRP
1	A	729	GLU
1	A	732	ARG
1	A	743	MET
1	A	755	LEU
1	A	756	VAL
1	A	765	ASP
1	A	807	GLN
1	A	831	VAL
1	A	836	GLU
1	A	855	LYS
1	A	874	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	936	GLU
1	A	988	GLN
1	A	996	ASP
1	A	1044	ILE
1	A	1050	VAL
1	A	1067	ASP
1	A	1076	VAL
1	A	1079	GLU
1	A	1084	LEU
1	A	1090	LYS
1	B	494	GLN
1	B	496	ARG
1	B	498	GLN
1	B	542	ARG
1	B	601	LEU
1	B	607	TRP
1	B	634	ILE
1	B	680	LEU
1	B	712	ASP
1	B	732	ARG
1	B	743	MET
1	B	755	LEU
1	B	756	VAL
1	B	765	ASP
1	B	807	GLN
1	B	831	VAL
1	B	855	LYS
1	B	936	GLU
1	B	988	GLN
1	B	996	ASP
1	B	1000	GLU
1	B	1044	ILE
1	B	1050	VAL
1	B	1067	ASP
1	B	1076	VAL
1	B	1084	LEU
1	B	1090	LYS
1	C	494	GLN
1	C	498	GLN
1	C	534	ILE
1	C	542	ARG
1	C	580	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	601	LEU
1	C	607	TRP
1	C	632	GLU
1	C	743	MET
1	C	755	LEU
1	C	756	VAL
1	C	765	ASP
1	C	807	GLN
1	C	831	VAL
1	C	855	LYS
1	C	936	GLU
1	C	988	GLN
1	C	996	ASP
1	C	1044	ILE
1	C	1050	VAL
1	C	1067	ASP
1	C	1068	LEU
1	C	1076	VAL
1	C	1079	GLU
1	C	1084	LEU
1	C	1090	LYS
1	D	494	GLN
1	D	496	ARG
1	D	498	GLN
1	D	542	ARG
1	D	601	LEU
1	D	607	TRP
1	D	712	ASP
1	D	732	ARG
1	D	743	MET
1	D	755	LEU
1	D	756	VAL
1	D	765	ASP
1	D	807	GLN
1	D	831	VAL
1	D	836	GLU
1	D	855	LYS
1	D	874	LEU
1	D	988	GLN
1	D	996	ASP
1	D	1044	ILE
1	D	1046	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1050	VAL
1	D	1067	ASP
1	D	1079	GLU
1	D	1084	LEU
1	D	1090	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	498	GLN
1	A	502	HIS
1	A	506	HIS
1	A	560	HIS
1	A	574	HIS
1	A	575	GLN
1	A	685	ASN
1	A	721	GLN
1	A	736	HIS
1	A	807	GLN
1	A	858	ASN
1	A	873	ASN
1	A	879	HIS
1	A	898	ASN
1	A	899	GLN
1	A	924	ASN
1	A	998	HIS
1	A	1059	HIS
1	A	1073	GLN
1	B	494	GLN
1	B	498	GLN
1	B	502	HIS
1	B	506	HIS
1	B	560	HIS
1	B	574	HIS
1	B	575	GLN
1	B	628	GLN
1	B	685	ASN
1	B	721	GLN
1	B	736	HIS
1	B	771	HIS
1	B	807	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	858	ASN
1	B	873	ASN
1	B	879	HIS
1	B	898	ASN
1	B	899	GLN
1	B	924	ASN
1	B	934	GLN
1	B	998	HIS
1	B	1073	GLN
1	C	494	GLN
1	C	498	GLN
1	C	502	HIS
1	C	506	HIS
1	C	560	HIS
1	C	574	HIS
1	C	575	GLN
1	C	628	GLN
1	C	669	ASN
1	C	685	ASN
1	C	721	GLN
1	C	736	HIS
1	C	807	GLN
1	C	858	ASN
1	C	873	ASN
1	C	879	HIS
1	C	898	ASN
1	C	899	GLN
1	C	923	GLN
1	C	924	ASN
1	C	998	HIS
1	C	1075	GLN
1	D	494	GLN
1	D	498	GLN
1	D	502	HIS
1	D	506	HIS
1	D	560	HIS
1	D	574	HIS
1	D	575	GLN
1	D	628	GLN
1	D	669	ASN
1	D	685	ASN
1	D	721	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	736	HIS
1	D	771	HIS
1	D	807	GLN
1	D	858	ASN
1	D	873	ASN
1	D	879	HIS
1	D	898	ASN
1	D	899	GLN
1	D	923	GLN
1	D	924	ASN
1	D	998	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	601/718 (83%)	-1.61	0 100 100	47, 47, 47, 78	0
1	B	601/718 (83%)	-1.60	0 100 100	47, 47, 47, 78	0
1	C	601/718 (83%)	-1.61	0 100 100	1, 47, 47, 78	0
1	D	601/718 (83%)	-1.59	0 100 100	47, 47, 47, 78	0
All	All	2404/2872 (83%)	-1.60	0 100 100	1, 47, 47, 78	0

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	MN	D	2001	1/1	0.99	0.03	87,87,87,87	0
2	MN	B	2001	1/1	1.00	0.02	87,87,87,87	0
2	MN	C	2001	1/1	1.00	0.01	87,87,87,87	0
2	MN	A	2001	1/1	1.00	0.04	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.