

Full wwPDB X-ray Structure Validation Report (i)

Jan 29, 2024 - 06:45 PM EST

PDB ID	:	1F4A
Title	:	E. COLI (LACZ) BETA-GALACTOSIDASE (NCS CONSTRAINED MONO
		MER-ORTHORHOMBIC)
Authors	:	Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud,
		D.E.; Matthews, B.W.
Deposited on	:	2000-06-07
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	А	1021	% 4 9%	38%	11%	•
1	В	1021	49%	38%	11%	•
1	С	1021	49%	38%	11%	•
1	D	1021	49%	38%	11%	•



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34424 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace	
1	Δ	1021	Total	С	Ν	Ο	S	84	7	0	
1	Л	1021	8238	5209	1466	1525	38	04	I	U	
1	В	1021	Total	С	Ν	Ο	S	84	7	0	
1	D	1021	8238	5209	1466	1525	38	04	1	0	
1	С	1021	Total	С	Ν	Ο	S	84	7	0	
1		1021	8238	5209	1466	1525	38	04	1	0	
1	П	1021	Total	С	Ν	Ο	S	84	7	0	
		1021	8238	5209	1466	1525	38	04	1	U	

• Molecule 1 is a protein called BETA-GALACTOSIDASE.

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mg 2 2	0	0
2	В	2	Total Mg 2 2	0	0
2	С	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	365	Total O 365 365	0	0
3	В	366	Total O 366 366	0	0
3	С	367	Total O 367 367	0	0
3	D	366	Total O 366 366	0	0



3 Residue-property plots (i)

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: BETA-GALACTOSIDASE

• Molecule 1: BETA-GALACTOSIDASE

Chain B: 49% 38% 11% . N18 P19 Q23 L24 13 14 N110 P111 P112 F113 V114 V114 R140 872 W73 1141 1141 N355 3356 1357 1357 H360 1361 1362 1362 R388 354 0507 3508 W568 D569 596 597 1570 3647 0648 1583 K661 P662 L663 A664 S665 G666 E667 V668 P669 P669 D671 V672 P674 P674 R677 K677 N649 E650 q678 L679 E681 E681 L682 P683 P685 P686 P686 P688 P688 P688 P688 L651 L652 H653 W654 W656 V656 V656 A657 L658 L658 D659 Q7 19 <u>3660</u> 1778 1779 780 767 1878 834 919 920 921 948





 \bullet Molecule 1: BETA-GALACTOSIDASE

Cha	in	I C): '								49	%													3	8%)						1	1%		•		
I3 T4 D5	SG	L7 A8	6A		Q12 B13	R14	D15	E17	N18	P19	<mark>023</mark>	L24 MDF	R26		A29 H30	P31	P32	F33 A34	335	W36 B37	N38	S39 F40	E41	A42 B43	T44	D45 R46		049	E57	W58 R59		W62 F63	P64	A65 P66	E67	E71	S72 W73	L74 E75
C76 D77 L78	P79	E80 A81	D82	183 V84	V85 V96	000 P87	S88	06M	Q91	M92	Y95	D96	V100	T101	N102	T104	Y105	P106	N110	F113	V114	P115 T116	E117	N118 D110		C122 V123	S124	L125 T126	F127	N128 V129	D130	E131 S132	W133	L134 0135	E136	0138	T139 R140	1141 1142
F143 D144 G145	V146	N147 S148	A149	H.150	W153	R157		D164 S165	R166	L167 P168	S169	E170	P1/1 D172	L173	<mark>г176</mark>		G180	E181 N182	R183	L184	M187	R 100		D193	E198	D199	D201	M202 W203		R210 D211		L214 L215	H216	K217 P218	T219	<mark>\$223</mark>	D224 F225	H226 V227
A228 T229 R230		D233 D234	F235	8236 R237	A238	v233 L240	E241	A242 E243	V244	Q245 M246	C247	G248 F240	E249 L250	R251	D252 V753	L254	R255	V256 T257	V258	5259 1.260	W261	0262 2763	E264	6760	G270	T271 4979	P273	F274	E277	1278 1279	D280	E281 R282	-	A286 D287	R288 V789	T290	L291 R292	L293
E296 E304	I 305	P306	R310	E314	L315 U216	T317	A318	G320	T321	L322	E326		D329	R333	E334 V335	R336	1337 1337	E338	K347	R.35.2	G353	V354 N355	R356	H357 5358	H359	H360 P361	L362	H363	M367	D368 E369		M372 V373	Q374	D375 1376	L377	M379	K380	N385 A386
<mark>V387</mark> R388	Y392	P393 N394	H395	P396	Y399 TADO	00	D403	G406	L407	E412		E416	M423	N424	R425	T427	D428	D429	R431	W432 1,433	P434	A435 M436	S437	E438 D/130	V440	T441 R442		Q445 R446	D447	R448	P451	S457		N460 E461	MAG7	H468	D469	Y472 R473
<u>W474 1475</u> K476	S477	V478 D479	P480	S481 R482		4400 Y486	E487	4 400	D492	1499		M502	R505	V506	D507 FEOR	D509	0510	F512	P513	A514 V515	P516	K517 W518	S519	1520 VE24		L524 S525	L526	F.579	T530	R531 P532	L533	E537		M542	5545 1 546		W553 Q554	Y559
P560 R561 L562		W568 D569	W570	V5/1 D572	0573	I576	K577	D579	E580	N581 G582	N583	P584	D591		<u>D594</u> теас	P596	N597	D598 R599	0000 000	F601 C602	MGO3	N604	D610	R611 T612	7101	T618 F619	A620	K621 H622	Q623	0624 0625	r	R630	0634	T635 1636	E637 V638	T639	S640 E641	R645
H646 S647 D648	N649	E650 L651	L652	H653 W654	M655	A657	L658	0990 0960	K661	P662 L663	A664	8665 8665	E667	V668	P669 1 670	D671	V672	A6/3 P674	Q675	G676 K677	Q678	L679 T680	E681	L682 D683	E684	L685 P686	Q687	P688 E689	8690	0693	L694	<mark>4695</mark> L696	T697	V698 R699	V701	Q702	P703	W708 S709
E710 A711 G712		Q719 W720	R721	E724	00211	T729	L730	A732	A733	S734	1737	P738	T742	S743	E744 M745	D746	F747	C/48 I749	E750	R755	W756	Q757 Е758	N759	R760 0761	8762	G763 F764	L765	S766 D767	M768	W769 1770	G771	D772 K773	K774	Q775	T778 D770	L780	R781 D782	R786
A787 P788	D792	E797	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	1801 1801	E000	R809	W810	TIQU	Q817	A818 E819		L822	L823 0824	C825	1828	T829	L830	A831 D832	A833	V834 1.835	1836	T837	H840		H844	Q845	L8 <mark>49</mark>	VB56	R857	I 858 D 859	G860	0863	M864	T867	V868 D860	V870	E871 V872	A873 S874
D875 T876 P877	H878	P879 A880	R881	1882	<mark>C886</mark>	0890	V891	A692 E893	R894	0903		Y906	D908	R909	L910 T011	1911 A912		P15 D916	R917	N918	L920	P921	S923	D924	P928	F931		E934	R938	R942	E943	L944 N945	Y946	H949	0360	G953	D954	N958 1959
0965 0965		E969 T970	S971	H972 R973	H974 1 075		E979	00673	1986	D987 G988	F989	066H	ТААМ	D996	c 1004	A1005	E1006	F1007 Q1008	L1009	01017	L1018	V1019 W1020	C1021	Q1022 x1023														

• Molecule 1: BETA-GALACTOSIDASE



Chain D:	49%	38%	11% •
13 14 15 15 15 15 15 16 11 113 113 115 115 115 115 115 115 115	923 124 125 125 125 125 125 133 133 1335 1335 1	N37 N38 N38 S39 E41 E41 T44 P45 R43 R43 C49 C49 C49 C49 C49 C49 C49 C49 C49 C49	R59 W62 F63 F64 A65 E67 V69 V69 F70 F70 S72 S72 W73
L74 E75 E75 E76 E76 E80 E80 V84 V84 V84 V84 V88 V88 V86 V86 V86 V86 V86 V86 V86 V86	M92 995 996 7100 1101 1104 1104 7106 7104	M10 P112 F113 F113 F113 F115 F115 F115 F125 F125 F126 F126 F127 F126	M128 M129 D130 E131 S132 M138 G138 G137 G138 G137 C138 R140 R141
1142 1144 1145 1145 1145 1147 1147 1147 1147	F168 8169 8169 8170 717 717 717 717 717 8180 8181 8181	M187 R190 D193 D193 D198 D198 Q200 Q200 M202 W203 W203 W203 W203	L214 L215 H216 H217 7219 T219 T219 S223 F226 H226 H226 H226 H227
1229 1229 1236 1234 1235 1236 1236 1236 1236 1236 1236 1236 1240 1240 1240 1240 1244 1240 1244	2445 2445 2246 2252 2253 2254 7255 7255 7255 7255 7255 7255 7255	0262 0263 5264 5264 5264 6270 6270 7271 7271 7271 7277 7277 7277 7277 7	E281 R282 A286 A286 D287 T229 T229 T2295 T2295 E295 E295
E304 1306 1306 1316 1314 1316 1314 1316 1316 1316 131	62 20 132 20 133 20 133 33 133	G353 V354 N355 H357 H357 H355 F351 F355 F361 F362 F362 F365 F365 F365 F365 F365 F365 F365 F365	M372 V373 V373 C374 C374 C374 C377 C376 C377 C376 C377 C376 C378 C376 C378 C378 C378 C378 C378 C378 C378 C378
R388 Y332 Y332 N334 N334 P335 P335 P335 P335 P335 P335 P335 P	T417 T417 H418 H418 G419 G419 H423 M423 L426 L426 L426 L426 L427 D429 P430 P431	W432 L433 P434 P434 A435 R435 R435 R440 T441 R442 R445 R446 R445 R446	R448 P451 S451 8457 B461 B461 B468 D469 D469 D469
R473 W474 W474 K476 K476 847 V477 V477 V478 V480 S481 9485 S481 9485 S481 1499 1499 1499 1499 V506	b500 b500 b500 b500 b500 b510 b514 b514 b514 b514 b514 b514 b514 b514	1520 1524 1524 1525 1530 1530 1530 1533 1533 1533 1533	M642 S545 L546 L546 Q554 Q554 Q554 P560 P560 R561 L552 L552 L552 N566
0569 W570 W571 W571 W572 Q572 Q572 Q572 Q572 Q572 Q572 Q572 Q572 Q573 Q541 Q541 Q541 Q541	D564 1595 P596 N599 N599 N599 R599 R599 R599 R500 F601 F601 F601 D610	R611 1612 1612 1618 6619 1618 1620 1622 1622 1623 1623 1633	1685 1685 1685 1685 1685 1685 1684 1684 1644 1644 1644 1644 1645 1644 1645 1644 1645 1644 1645 1644 1645 1644 1645 1644 1645 1644 1645 1644
L661 L662 L662 H662 H663 M664 V665 C666 C666 C666 C666 C666 C666 C666	P669 1670 1671 1672 1673 1673 1673 1677 1677 1677 1680 1680	1682 1682 1685 1685 1685 1685 1685 1685 1689 1693 1693 1693 1693	R 698 R 698 R 700 V 701 V 701 R 703 S 703 S 703 S 703 S 710 C 712 C 712 C 712
4720 8724 8724 8728 7728 7728 7733 7733 8734 7733 8734 7733 8734 7733 8734 7738 7738	E7445 E7445 M745 D7466 E746 E748 E748 E750 B756 M756 M756 N758	8760 4761 4761 5763 5763 6763 6764 4767 4767 1770 6771 6771 6771 7772	4775 1778 1779 1779 1778 1778 1781 1782 1788 1787 1787 1792
E 297 R800 1801 1801 1801 808 811 811 811 811 8	0,000 1829 1829 1833 1833 1834 1834 1835 1836 1836 1836 1836 1836	444 1844 1844 1844 1849 1858 1858 1858 1858 1855 1855 1855 185	4863 4864 1867 1867 1867 1868 1887 8874 8874 8873 8874 1876 1876
H878 H879 P879 P879 R881 R881 R881 R882 R882 R889 R893 R893 R894 R893 R894 R993 R894 R993 R894 R996 R996 R996	D900 D908 R909 1911 1912 A912 F915 B916 B916 D919 C922 P921	1922 1923 1924 1928 1928 1934 1934 1934 1942 1944	Y 945 Y 946 H 950 Q 953 Q 954 N 958 1 959 Q 964 Q 965
1970 1970 1970 1971 1973 1973 1975 1975 1975 1975 1986 1986 1988 1990 1990	D996 D996 S1005 F1005 F1005 F1005 F1006 L1009 L1009 L1010 L1011 L1018	N1 020 C1 021 01 022 K1 023	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	153.40Å 173.40Å 204.40Å	Dopositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	25.00 - 2.80	Depositor
Resolution (A)	24.97 - 2.82	EDS
% Data completeness	88.0 (25.00-2.80)	Depositor
(in resolution range)	80.5(24.97-2.82)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 2.80 \text{\AA})$	Xtriage
Refinement program	TNT 5E	Depositor
P. P.	0.167 , 0.198	Depositor
II, II free	0.149 , 0.178	DCC
R_{free} test set	1590 reflections (1.50%)	wwPDB-VP
Wilson B-factor $(Å^2)$	40.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.26 , 100.6	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34424	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: MG

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).

Mal	Chain	B	ond lengths	Bond angles						
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5					
1	А	1.08	52/8515~(0.6%)	1.61	173/11615~(1.5%)					
1	В	1.08	52/8515~(0.6%)	1.61	175/11615~(1.5%)					
1	С	1.08	52/8515~(0.6%)	1.61	174/11615~(1.5%)					
1	D	1.08	52/8515~(0.6%)	1.61	176/11615~(1.5%)					
All	All	1.08	208/34060~(0.6%)	1.61	698/46460~(1.5%)					

All (208) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	75	GLU	CD-OE2	9.53	1.36	1.25
1	С	75	GLU	CD-OE2	9.53	1.36	1.25
1	D	75	GLU	CD-OE2	9.49	1.36	1.25
1	В	75	GLU	CD-OE2	9.46	1.36	1.25
1	D	710	GLU	CD-OE2	7.62	1.34	1.25
1	В	710	GLU	CD-OE2	7.61	1.34	1.25
1	А	710	GLU	CD-OE2	7.61	1.34	1.25
1	С	710	GLU	CD-OE2	7.61	1.34	1.25
1	В	136	GLU	CD-OE2	7.46	1.33	1.25
1	D	136	GLU	CD-OE2	7.44	1.33	1.25
1	А	181	GLU	CD-OE2	7.44	1.33	1.25
1	С	181	GLU	CD-OE2	7.43	1.33	1.25
1	D	181	GLU	CD-OE2	7.43	1.33	1.25
1	D	264	GLU	CD-OE2	7.43	1.33	1.25
1	А	136	GLU	CD-OE2	7.42	1.33	1.25
1	В	181	GLU	CD-OE2	7.41	1.33	1.25
1	В	40	GLU	CD-OE2	7.41	1.33	1.25
1	А	508	GLU	CD-OE2	7.40	1.33	1.25
1	А	264	GLU	CD-OE2	7.39	1.33	1.25
1	А	681	GLU	CD-OE2	7.38	1.33	1.25
1	В	264	GLU	CD-OE2	7.38	1.33	1.25
1	С	264	GLU	CD-OE2	7.38	1.33	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	508	GLU	CD-OE2	7.38	1.33	1.25
1	В	508	GLU	CD-OE2	7.37	1.33	1.25
1	С	681	GLU	CD-OE2	7.37	1.33	1.25
1	В	681	GLU	CD-OE2	7.36	1.33	1.25
1	С	40	GLU	CD-OE2	7.36	1.33	1.25
1	С	136	GLU	CD-OE2	7.36	1.33	1.25
1	D	40	GLU	CD-OE2	7.36	1.33	1.25
1	А	40	GLU	CD-OE2	7.35	1.33	1.25
1	С	508	GLU	CD-OE2	7.35	1.33	1.25
1	D	681	GLU	CD-OE2	7.34	1.33	1.25
1	В	314	GLU	CD-OE2	7.32	1.33	1.25
1	С	943	GLU	CD-OE2	7.26	1.33	1.25
1	А	314	GLU	CD-OE2	7.25	1.33	1.25
1	А	943	GLU	CD-OE2	7.24	1.33	1.25
1	С	314	GLU	CD-OE2	7.24	1.33	1.25
1	В	943	GLU	CD-OE2	7.22	1.33	1.25
1	D	314	GLU	CD-OE2	7.21	1.33	1.25
1	D	943	GLU	CD-OE2	7.18	1.33	1.25
1	С	369	GLU	CD-OE2	7.11	1.33	1.25
1	В	369	GLU	CD-OE2	7.07	1.33	1.25
1	А	797	GLU	CD-OE2	7.05	1.33	1.25
1	С	797	GLU	CD-OE2	7.04	1.33	1.25
1	D	369	GLU	CD-OE2	7.04	1.33	1.25
1	В	797	GLU	CD-OE2	7.04	1.33	1.25
1	А	369	GLU	CD-OE2	7.03	1.33	1.25
1	D	797	GLU	CD-OE2	7.02	1.33	1.25
1	С	979	GLU	CD-OE2	6.94	1.33	1.25
1	D	979	GLU	CD-OE2	6.92	1.33	1.25
1	A	650	GLU	CD-OE2	6.88	1.33	1.25
1	A	979	GLU	CD-OE2	6.87	1.33	1.25
1	D	650	GLU	CD-OE2	6.85	1.33	1.25
1	B	650	GLU	CD-OE2	6.85	1.33	1.25
1	C	650	GLU	CD-OE2	6.82	1.33	1.25
1	D	969	GLU	CD-OE2	6.81	1.33	1.25
1	C	750	GLU	CD-OE2	6.79	1.33	1.25
	A	326	GLU	CD-OE2	6.77	1.33	1.25
	B	979	GLU	CD-OE2	6.77	1.33	1.25
	В	326	GLU	CD-OE2	6.76	1.33	1.25
	A	969	GLU	CD-OE2	0.76	1.33	1.25
	D	326	GLU	CD-OE2	6.76	1.33	1.25
	D	724	GLU	CD-OE2	6.76	1.33	1.25
1	C	969	GLU	CD-OE2	6.75	1.33	1.25



Conti	inuea fron	i previc	rus page.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	750	GLU	CD-OE2	6.75	1.33	1.25
1	С	326	GLU	CD-OE2	6.75	1.33	1.25
1	В	969	GLU	CD-OE2	6.74	1.33	1.25
1	В	724	GLU	CD-OE2	6.73	1.33	1.25
1	С	724	GLU	CD-OE2	6.73	1.33	1.25
1	В	198	GLU	CD-OE2	6.72	1.33	1.25
1	А	724	GLU	CD-OE2	6.72	1.33	1.25
1	В	750	GLU	CD-OE2	6.69	1.33	1.25
1	D	241	GLU	CD-OE2	6.68	1.32	1.25
1	А	198	GLU	CD-OE2	6.67	1.32	1.25
1	С	198	GLU	CD-OE2	6.66	1.32	1.25
1	С	241	GLU	CD-OE2	6.66	1.32	1.25
1	А	241	GLU	CD-OE2	6.66	1.32	1.25
1	D	198	GLU	CD-OE2	6.65	1.32	1.25
1	D	750	GLU	CD-OE2	6.64	1.32	1.25
1	В	241	GLU	CD-OE2	6.61	1.32	1.25
1	С	338	GLU	CD-OE2	6.55	1.32	1.25
1	А	338	GLU	CD-OE2	6.50	1.32	1.25
1	В	338	GLU	CD-OE2	6.50	1.32	1.25
1	D	338	GLU	CD-OE2	6.45	1.32	1.25
1	А	461	GLU	CD-OE2	6.38	1.32	1.25
1	С	438	GLU	CD-OE2	6.37	1.32	1.25
1	В	461	GLU	CD-OE2	6.35	1.32	1.25
1	D	461	GLU	CD-OE2	6.35	1.32	1.25
1	В	438	GLU	CD-OE2	6.34	1.32	1.25
1	А	438	GLU	CD-OE2	6.34	1.32	1.25
1	С	461	GLU	CD-OE2	6.32	1.32	1.25
1	В	296	GLU	CD-OE2	6.32	1.32	1.25
1	D	438	GLU	CD-OE2	6.32	1.32	1.25
1	А	296	GLU	CD-OE2	6.31	1.32	1.25
1	D	296	GLU	CD-OE2	6.30	1.32	1.25
1	С	296	GLU	CD-OE2	6.26	1.32	1.25
1	С	249	GLU	CD-OE2	6.22	1.32	1.25
1	А	249	GLU	CD-OE2	6.21	1.32	1.25
1	D	249	GLU	CD-OE2	6.21	1.32	1.25
1	В	537	GLU	CD-OE2	6.20	1.32	1.25
1	A	744	GLU	CD-OE2	6.20	1.32	1.25
1	D	744	GLU	CD-OE2	6.19	1.32	1.25
1	В	744	GLU	CD-OE2	6.19	1.32	1.25
1	С	637	GLU	CD-OE2	6.17	1.32	1.25

Continued from previous page.

С

С

GLU

GLU

 CD-OE2

CD-OE2

Continued on next page...

1.25

1.25

1.32

1.32



6.17

6.17

Mol

 $\frac{1}{1}$

1

1

1

1

1

1

1

 $\frac{1}{1}$

1

1

1

1

1

1

1

1

1

 $\frac{1}{1}$

1

1

 $\frac{1}{1}$

1

1

1

1

1

1

1

1

1

1

1

1

1

1

Observed(Å)

Ideal(Å)

Ζ

Atoms

808	GLU	CD-OE2	6.16	1.32	1.25
637	GLU	CD-OE2	6.15	1.32	1.25
537	GLU	CD-OE2	6.15	1.32	1.25
808	GLU	CD-OE2	6.14	1.32	1.25
57	GLU	CD-OE2	6.14	1.32	1.25
637	GLU	CD-OE2	6.14	1.32	1.25
537	GLU	CD-OE2	6.14	1.32	1.25
808	GLU	CD-OE2	6.14	1.32	1.25
537	GLU	CD-OE2	6.14	1.32	1.25
249	GLU	CD-OE2	6.12	1.32	1.25
57	GLU	CD-OE2	6.12	1.32	1.25
57	GLU	CD-OE2	6.10	1.32	1.25
57	GLU	CD-OE2	6.10	1.32	1.25
637	GLU	CD-OE2	6.10	1.32	1.25
667	GLU	CD-OE2	6.08	1.32	1.25
641	GLU	CD-OE2	6.05	1.32	1.25
281	GLU	CD-OE2	6.04	1.32	1.25
667	GLU	CD-OE2	6.03	1.32	1.25
667	GLU	CD-OE2	6.03	1.32	1.25
641	GLU	CD-OE2	6.03	1.32	1.25
641	GLU	CD-OE2	6.00	1.32	1.25
80	GLU	CD-OE2	6.00	1.32	1.25
80	GLU	CD-OE2	5.99	1.32	1.25
667	GLU	CD-OE2	5.99	1.32	1.25
80	GLU	CD-OE2	5.99	1.32	1.25
80	GLU	CD-OE2	5.97	1.32	1.25
281	GLU	CD-OE2	5.97	1.32	1.25
641	GLU	CD-OE2	5.96	1.32	1.25
281	GLU	CD-OE2	5.96	1.32	1.25
281	GLU	CD-OE2	5.94	1.32	1.25
871	GLU	CD-OE2	5.90	1.32	1.25

Continued from previous page...

 \mathbf{Res}

Type

Chain

В

B C

А

 $\overline{\mathbf{C}}$

А

D

D

A B

D

А

В

D

D

D

D

Α

С

A B

 $\frac{B}{C}$

В

D

A A

С

 $\overline{\mathbf{C}}$

B C

С

А

D

D

А

В

В

В

А

D

 $\overline{\mathrm{C}}$

41

871

871

41

41

871

41

334

334

334

334

GLU

CD-OE2

5.89

5.88

5.88

5.87

5.84

5.84

5.83

5.77

5.74

5.73

5.68

1.32

1.32

1.32

1.32

1.32

1.32

1.32

1.31

1.31

1.31

1.31

Continued on next page...

1.25

1.25

1.25

1.25

1.25

1.25

 $1.25 \\ 1.25$

1.25

1.25

1.25



	$1\mathrm{F4}$	A

Conti	nued from	n previo	ous page.				
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	71	GLU	CD-OE2	5.55	1.31	1.25
1	С	71	GLU	CD-OE2	5.52	1.31	1.25
1	А	71	GLU	CD-OE2	5.50	1.31	1.25
1	D	71	GLU	CD-OE2	5.48	1.31	1.25
1	В	619	GLU	CD-OE2	5.45	1.31	1.25
1	В	1006	GLU	CD-OE2	5.42	1.31	1.25
1	А	619	GLU	CD-OE2	5.41	1.31	1.25
1	С	1006	GLU	CD-OE2	5.39	1.31	1.25
1	С	619	GLU	CD-OE2	5.39	1.31	1.25
1	С	412	GLU	CD-OE2	5.39	1.31	1.25
1	D	1006	GLU	CD-OE2	5.38	1.31	1.25
1	D	131	GLU	CD-OE2	5.37	1.31	1.25
1	В	412	GLU	CD-OE2	5.36	1.31	1.25
1	А	1006	GLU	CD-OE2	5.36	1.31	1.25
1	В	131	GLU	CD-OE2	5.36	1.31	1.25
1	D	980	GLU	CD-OE2	5.36	1.31	1.25
1	D	580	GLU	CD-OE2	5.35	1.31	1.25
1	D	619	GLU	CD-OE2	5.35	1.31	1.25
1	А	412	GLU	CD-OE2	5.33	1.31	1.25
1	С	131	GLU	CD-OE2	5.33	1.31	1.25
1	А	17	GLU	CD-OE2	5.32	1.31	1.25
1	D	412	GLU	CD-OE2	5.31	1.31	1.25
1	А	131	GLU	CD-OE2	5.31	1.31	1.25
1	А	277	GLU	CD-OE2	5.31	1.31	1.25
1	В	277	GLU	CD-OE2	5.31	1.31	1.25
1	А	980	GLU	CD-OE2	5.30	1.31	1.25
1	А	580	GLU	CD-OE2	5.30	1.31	1.25
1	D	117	GLU	CD-OE2	5.30	1.31	1.25
1	С	17	GLU	CD-OE2	5.30	1.31	1.25
1	D	17	GLU	CD-OE2	5.29	1.31	1.25
1	В	17	GLU	CD-OE2	5.29	1.31	1.25
1	А	934	GLU	CD-OE2	5.29	1.31	1.25
1	С	580	GLU	CD-OE2	5.28	1.31	1.25
1	С	277	GLU	CD-OE2	5.28	1.31	1.25
1	А	117	GLU	CD-OE2	5.28	1.31	1.25
1	D	277	GLU	CD-OE2	5.28	1.31	1.25
1	В	934	GLU	CD-OE2	5.27	1.31	1.25
1	C	980	GLU	CD-OE2	5.27	1.31	1.25
1	В	893	GLU	CD-OE2	5.27	1.31	1.25
_ 1	В	580	GLU	CD-OE2	5.27	1.31	1.25
1	A	684	GLU	CD-OE2	5.27	1.31	1.25
1	В	980	GLU	CD-OE2	5.27	1.31	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	689	GLU	CD-OE2	5.26	1.31	1.25
1	D	934	GLU	CD-OE2	5.26	1.31	1.25
1	А	893	GLU	CD-OE2	5.26	1.31	1.25
1	С	117	GLU	CD-OE2	5.26	1.31	1.25
1	С	934	GLU	CD-OE2	5.26	1.31	1.25
1	В	689	GLU	CD-OE2	5.25	1.31	1.25
1	С	893	GLU	CD-OE2	5.24	1.31	1.25
1	D	684	GLU	CD-OE2	5.23	1.31	1.25
1	D	689	GLU	CD-OE2	5.22	1.31	1.25
1	А	689	GLU	CD-OE2	5.22	1.31	1.25
1	С	819	GLU	CD-OE2	5.21	1.31	1.25
1	В	819	GLU	CD-OE2	5.21	1.31	1.25
1	С	684	GLU	CD-OE2	5.21	1.31	1.25
1	В	684	GLU	CD-OE2	5.20	1.31	1.25
1	D	893	GLU	CD-OE2	5.20	1.31	1.25
1	В	117	GLU	CD-OE2	5.20	1.31	1.25
1	А	819	GLU	CD-OE2	5.19	1.31	1.25
1	D	819	GLU	CD-OE2	5.16	1.31	1.25

All (698) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	809[A]	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	В	809[B]	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	А	809[A]	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	А	809[B]	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	D	809[A]	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	D	809[B]	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	С	809[A]	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	С	809[B]	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	С	881	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	D	881	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	С	881	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	А	881	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	D	881	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	А	881	ARG	NE-CZ-NH2	-10.95	114.82	120.30
1	В	881	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	В	881	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	А	531	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	В	531	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	D	531	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	С	531	ARG	NE-CZ-NH1	10.71	125.65	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	385	ASN	CB-CA-C	-10.44	89.51	110.40
1	А	385	ASN	CB-CA-C	-10.44	89.52	110.40
1	В	385	ASN	CB-CA-C	-10.44	89.53	110.40
1	С	385	ASN	CB-CA-C	-10.43	89.54	110.40
1	D	507	ASP	CB-CG-OD2	-10.36	108.97	118.30
1	С	507	ASP	CB-CG-OD2	-10.34	109.00	118.30
1	А	507	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	В	507	ASP	CB-CG-OD2	-10.26	109.07	118.30
1	С	356	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	А	13	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	С	13	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	D	13	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	А	356	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	В	356	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	В	13	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	D	356	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	D	237	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	D	591	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	С	591	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	А	237	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	В	237	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	С	237	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	А	591	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	D	439	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	А	439	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	В	439	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	В	591	ASP	CB-CG-OD2	-9.48	109.77	118.30
1	С	439	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	С	249	GLU	N-CA-CB	9.26	127.27	110.60
1	А	249	GLU	N-CA-CB	9.24	127.24	110.60
1	В	249	GLU	N-CA-CB	9.24	127.23	110.60
1	D	249	GLU	N-CA-CB	9.22	127.20	110.60
1	D	509	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	А	509	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	В	509	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	С	509	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	С	424	ASN	CB-CA-C	-9.11	92.18	110.40
1	В	424	ASN	CB-CA-C	-9.11	92.19	110.40
1	А	424	ASN	CB-CA-C	-9.10	92.20	110.40
1	D	424	ASN	CB-CA-C	-9.10	92.20	110.40
1	С	938	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	А	938	ARG	NE-CZ-NH2	-8.81	115.90	120.30



Mol	Chain	Res	Type	Atoms	Ζ	Observed(°)	$Ideal(^{o})$
1	В	938	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	В	429	ASP	CB-CG-OD1	8.80	126.22	118.30
1	D	938	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	А	429	ASP	CB-CG-OD1	8.74	126.17	118.30
1	С	429	ASP	CB-CG-OD1	8.74	126.16	118.30
1	D	429	ASP	CB-CG-OD1	8.71	126.14	118.30
1	В	210	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	А	210	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	С	210	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	D	210	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	С	509	ASP	CB-CG-OD1	8.49	125.94	118.30
1	D	509	ASP	CB-CG-OD1	8.46	125.92	118.30
1	А	509	ASP	CB-CG-OD1	8.43	125.89	118.30
1	В	509	ASP	CB-CG-OD1	8.41	125.87	118.30
1	В	233	ASP	CB-CG-OD1	8.23	125.70	118.30
1	А	233	ASP	CB-CG-OD1	8.22	125.70	118.30
1	D	233	ASP	CB-CG-OD1	8.20	125.68	118.30
1	С	233	ASP	CB-CG-OD1	8.19	125.67	118.30
1	В	130	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	D	226	HIS	CB-CA-C	-8.16	94.08	110.40
1	С	226	HIS	CB-CA-C	-8.16	94.08	110.40
1	А	130	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	В	226	HIS	CB-CA-C	-8.15	94.10	110.40
1	А	226	HIS	CB-CA-C	-8.14	94.11	110.40
1	D	287	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	А	287	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	В	287	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	С	130	ASP	CB-CG-OD2	-8.12	111.00	118.30
1	С	287	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	130	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	479	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	А	479	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	В	479	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	С	479	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	В	211	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	211	ASP	CB-CG-OD1	7.97	125.48	118.30
1	A	211	ASP	CB-CG-OD1	7.96	$1\overline{25.47}$	118.30
1	В	828	ASP	$CB-\overline{CG}-\overline{OD2}$	-7.95	$1\overline{11.15}$	118.30
1	C	211	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	828	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	D	792	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	D	828	ASP	CB-CG-OD2	-7.92	111.17	118.30



tion Report		1
$served(^{o})$	$Ideal(^{o})$	
111.18	118.30	
111.19	118.30	
111.22	118.30	
111.22	118.30	
124.20	120.30	
124.20	120.30	
124.19	120.30	
96.62	110.60	
96.62	110.60	
116.42	120.30	
96.63	110.60	
06 62	110 60	

Continued from previous page...

 Mol
 Chain
 Res
 Type

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	828	ASP	CB-CG-OD2	-7.92	111.18	118.30
1	В	792	ASP	CB-CG-OD2	-7.91	111.19	118.30
1	А	792	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	С	792	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	D	13	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	А	13	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	С	13	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	А	385	ASN	N-CA-CB	-7.77	96.62	110.60
1	В	385	ASN	N-CA-CB	-7.77	96.62	110.60
1	D	288	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	D	385	ASN	N-CA-CB	-7.76	96.63	110.60
1	С	385	ASN	N-CA-CB	-7.76	96.63	110.60
1	С	310	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	310	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	С	648	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	В	13	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	А	659	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	А	648	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	С	659	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	В	310	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	В	648	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	D	648	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	А	310	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	С	832	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	В	659	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	А	288	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	В	288	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	С	288	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	D	659	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	D	832	ASP	CB-CG-OD1	7.64	125.17	118.30
1	В	832	ASP	CB-CG-OD1	7.63	125.17	118.30
1	А	832	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	В	832	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	А	832	ASP	CB-CG-OD1	7.61	125.15	118.30
1	D	479	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	479	ASP	CB-CG-OD1	7.61	125.15	118.30
1	С	479	ASP	CB-CG-OD1	7.60	125.14	118.30
1	С	832	ASP	CB-CG-OD1	7.60	125.14	118.30
1	D	832	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	В	479	ASP	CB-CG-OD1	7.59	125.14	118.30
1	В	639	THR	CA-CB-CG2	-7.47	101.94	112.40
1	C	639	THR	CA-CB-CG2	-7.46	101.95	112.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	431[A]	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	431[B]	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	С	252	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	А	639	THR	CA-CB-CG2	-7.45	101.97	112.40
1	D	639	THR	CA-CB-CG2	-7.44	101.98	112.40
1	В	199	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	D	252	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	А	252	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	В	448	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	С	199	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	А	199	ASP	CB-CG-OD2	-7.39	111.64	118.30
1	В	252	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	D	211	ASP	CB-CG-OD2	-7.38	111.65	118.30
1	В	431[A]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	В	431[B]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	А	431[A]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	А	431[B]	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	А	1004	SER	N-CA-CB	7.36	121.55	110.50
1	С	1004	SER	N-CA-CB	7.36	121.54	110.50
1	С	211	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	D	1004	SER	N-CA-CB	7.36	121.53	110.50
1	В	211	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	А	211	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	D	199	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	В	1004	SER	N-CA-CB	7.33	121.50	110.50
1	А	448	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	403	ASP	CB-CG-OD1	7.32	124.89	118.30
1	В	403	ASP	CB-CG-OD1	7.29	124.86	118.30
1	С	448	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	D	448	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	С	403	ASP	CB-CG-OD1	7.27	124.84	118.30
1	С	431[A]	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	С	431[B]	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	А	403	ASP	CB-CG-OD1	7.25	124.83	118.30
1	D	96	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	В	648	ASP	CB-CG-OD1	7.20	124.78	118.30
1	С	96	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	924	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	В	924	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	В	96	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	А	96	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	В	336	ARG	NE-CZ-NH1	7.19	123.89	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	924	ASP	CB-CG-OD1	7.18	124.77	118.30
1	D	924	ASP	CB-CG-OD1	7.18	124.77	118.30
1	В	126	THR	CA-CB-CG2	-7.17	102.36	112.40
1	С	924	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	А	924	ASP	CB-CG-OD1	7.16	124.75	118.30
1	С	648	ASP	CB-CG-OD1	7.16	124.74	118.30
1	D	924	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	А	126	THR	CA-CB-CG2	-7.15	102.39	112.40
1	С	126	THR	CA-CB-CG2	-7.15	102.39	112.40
1	D	126	THR	CA-CB-CG2	-7.14	102.40	112.40
1	В	924	ASP	CB-CG-OD1	7.14	124.73	118.30
1	А	648	ASP	CB-CG-OD1	7.14	124.72	118.30
1	С	336	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	D	336	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	А	336	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	648	ASP	CB-CG-OD1	7.11	124.70	118.30
1	А	553	TRP	CA-CB-CG	-7.08	100.25	113.70
1	В	553	TRP	CA-CB-CG	-7.08	100.25	113.70
1	С	553	TRP	CA-CB-CG	-7.08	100.25	113.70
1	С	252	ASP	CB-CG-OD1	7.08	124.67	118.30
1	В	746	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	С	356	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	553	TRP	CA-CB-CG	-7.06	100.28	113.70
1	А	252	ASP	CB-CG-OD1	7.05	124.64	118.30
1	А	746	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	С	746	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	252	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	746	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	D	400	THR	CA-CB-CG2	-7.01	102.59	112.40
1	В	252	ASP	CB-CG-OD1	7.00	124.60	118.30
1	В	859	ASP	CB-CG-OD1	6.99	124.59	118.30
1	А	400	THR	CA-CB-CG2	-6.97	102.64	112.40
1	С	400	THR	CA-CB-CG2	-6.97	102.64	112.40
1	D	356	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	В	356	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	859	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	233	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	В	233	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	В	287	ASP	CB-CG-OD1	6.95	124.55	118.30
1	C	591	ASP	CB-CG-OD1	6.95	$1\overline{24.55}$	118.30
1	А	859	ASP	CB-CG-OD1	6.94	124.55	118.30
1	В	400	THR	CA-CB-CG2	-6.94	102.68	112.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	233	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	С	233	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	А	287	ASP	CB-CG-OD1	6.93	124.53	118.30
1	А	591	ASP	CB-CG-OD1	6.92	124.53	118.30
1	В	429	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	В	859	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	А	569	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	С	96	ASP	CB-CG-OD1	6.91	124.52	118.30
1	D	287	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	591	ASP	CB-CG-OD1	6.90	124.51	118.30
1	В	403	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	С	859	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	859	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	С	287	ASP	CB-CG-OD1	6.88	124.49	118.30
1	А	859	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	С	569	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	А	429	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	D	96	ASP	CB-CG-OD1	6.87	124.49	118.30
1	А	356	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	С	859	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	569	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	429	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	В	591	ASP	CB-CG-OD1	6.86	124.47	118.30
1	А	96	ASP	CB-CG-OD1	6.86	124.47	118.30
1	С	429	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	В	569	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	D	403	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	В	881	ARG	CD-NE-CZ	6.82	133.14	123.60
1	А	403	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	С	881	ARG	CD-NE-CZ	6.81	133.13	123.60
1	D	881	ARG	CD-NE-CZ	6.81	133.13	123.60
1	А	881	ARG	CD-NE-CZ	6.80	133.12	123.60
1	В	96	ASP	CB-CG-OD1	6.79	124.42	118.30
1	С	403	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	С	659	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	375	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	659	ASP	CB-CG-OD1	6.65	124.28	118.30
1	С	571	VAL	CB-CA-C	-6.65	98.77	111.40
1	В	375	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	С	375	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	571	VAL	CB-CA-C	-6.63	98.80	111.40
1	D	571	VAL	CB-CA-C	-6.63	98.81	111.40

Continued from previous page...



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	659	ASP	CB-CG-OD1	6.63	124.27	118.30
1	В	571	VAL	CB-CA-C	-6.62	98.83	111.40
1	А	375	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	D	672	VAL	CB-CA-C	-6.60	98.86	111.40
1	С	672	VAL	CB-CA-C	-6.60	98.86	111.40
1	В	424	ASN	N-CA-CB	-6.59	98.74	110.60
1	D	659	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	424	ASN	N-CA-CB	-6.58	98.75	110.60
1	А	424	ASN	N-CA-CB	-6.58	98.75	110.60
1	А	672	VAL	CB-CA-C	-6.58	98.89	111.40
1	С	424	ASN	N-CA-CB	-6.57	98.77	110.60
1	В	672	VAL	CB-CA-C	-6.57	98.92	111.40
1	С	507	ASP	CB-CG-OD1	6.57	124.21	118.30
1	В	166	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	А	507	ASP	CB-CG-OD1	6.53	124.18	118.30
1	D	507	ASP	CB-CG-OD1	6.52	124.17	118.30
1	А	166	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	В	507	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	166	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	919	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	В	15	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	А	15	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	С	919	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	D	15	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	15	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	А	919	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	С	15	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	С	166	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	С	875	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	С	15	ASP	CB-CG-OD1	6.43	124.08	118.30
1	С	5	ASP	CB-CG-OD1	6.42	124.08	118.30
1	В	875	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	А	15	ASP	CB-CG-OD1	6.41	124.07	118.30
1	А	875	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	В	5	ASP	CB-CG-OD1	6.40	124.06	118.30
1	С	600	GLN	N-CA-CB	6.39	122.10	110.60
1	В	600	GLN	N-CA-CB	6.39	122.10	110.60
1	В	919	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	5	ASP	CB-CG-OD1	6.39	124.05	118.30
1	В	938	ARG	N-CA-CB	6.38	122.09	110.60
1	D	5	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	875	ASP	CB-CG-OD2	-6.38	112.56	118.30

Continued from previous page...



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	938	ARG	N-CA-CB	6.38	122.08	110.60
1	В	15	ASP	CB-CG-OD1	6.38	124.04	118.30
1	А	600	GLN	N-CA-CB	6.37	122.07	110.60
1	D	938	ARG	N-CA-CB	6.37	122.07	110.60
1	D	750	GLU	N-CA-CB	6.37	122.06	110.60
1	С	938	ARG	N-CA-CB	6.37	122.06	110.60
1	С	750	GLU	N-CA-CB	6.36	122.05	110.60
1	В	750	GLU	N-CA-CB	6.35	122.03	110.60
1	D	319	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	D	600	GLN	N-CA-CB	6.35	122.02	110.60
1	А	750	GLU	N-CA-CB	6.34	122.01	110.60
1	В	319	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	А	319	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	В	782	ASP	CB-CG-OD1	6.31	123.98	118.30
1	А	782	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	782	ASP	CB-CG-OD1	6.30	123.97	118.30
1	С	319	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	С	782	ASP	CB-CG-OD1	6.27	123.94	118.30
1	С	908	ASP	CB-CG-OD1	6.27	123.94	118.30
1	В	439	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	А	439	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	А	651	LEU	CB-CA-C	-6.25	98.31	110.20
1	В	651	LEU	CB-CA-C	-6.25	98.32	110.20
1	D	651	LEU	CB-CA-C	-6.25	98.32	110.20
1	D	428	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	D	439	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	С	651	LEU	CB-CA-C	-6.23	98.36	110.20
1	С	439	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	С	938	ARG	CG-CD-NE	-6.22	98.73	111.80
1	А	428	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	В	938	ARG	CG-CD-NE	-6.21	98.76	111.80
1	В	428	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	А	938	ARG	CG-CD-NE	-6.20	98.78	111.80
1	D	938	ARG	CG-CD-NE	-6.19	98.80	111.80
1	А	908	ASP	CB-CG-OD1	6.18	123.86	118.30
1	В	954	ASP	CB-CG-OD1	6.18	123.86	118.30
1	С	428	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	С	572	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	D	572	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	В	908	ASP	CB-CG-OD1	6.16	123.84	118.30
1	В	172	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	В	431[A]	ARG	NE-CZ-NH2	-6.14	117.23	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	431[B]	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	В	572	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	D	954	ASP	CB-CG-OD1	6.13	123.82	118.30
1	А	572	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	А	954	ASP	CB-CG-OD1	6.12	123.81	118.30
1	В	772	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	D	908	ASP	CB-CG-OD1	6.12	123.81	118.30
1	А	172	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	D	431[A]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	431[B]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	С	954	ASP	CB-CG-OD1	6.11	123.80	118.30
1	А	431[A]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	А	431[B]	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	172	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	С	172	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	А	772	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	772	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	А	569	ASP	CB-CG-OD1	6.07	123.76	118.30
1	С	336	ARG	CB-CA-C	-6.07	98.27	110.40
1	С	772	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	D	336	ARG	CB-CA-C	-6.05	98.30	110.40
1	А	336	ARG	CB-CA-C	-6.05	98.30	110.40
1	В	336	ARG	CB-CA-C	-6.05	98.31	110.40
1	С	431[A]	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	С	431[B]	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	С	679	LEU	CA-CB-CG	-6.03	101.44	115.30
1	А	679	LEU	CA-CB-CG	-6.01	101.48	115.30
1	D	679	LEU	CA-CB-CG	-6.00	101.50	115.30
1	В	679	LEU	CA-CB-CG	-6.00	101.51	115.30
1	А	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	С	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	С	569	ASP	CB-CG-OD1	5.97	123.68	118.30
1	В	136	GLU	CB-CA-C	-5.97	98.45	110.40
1	А	142	ILE	CB-CA-C	-5.97	99.66	111.60
1	В	142	ILE	CB-CA-C	-5.97	99.67	111.60
1	С	45	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	D	136	GLU	CB-CA-C	-5.97	98.47	110.40
1	С	142	ILE	CB-CA-C	-5.96	99.67	111.60
1	D	569	ASP	CB-CG-OD1	5.96	123.67	118.30
1	В	569	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	45	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	В	45	ASP	CB-CG-OD2	-5.95	112.94	118.30

Continued from previous page...



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	5	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	45	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	142	ILE	CB-CA-C	-5.95	99.70	111.60
1	С	908	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	D	5	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	908	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	А	908	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	В	5	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	С	199	ASP	CB-CG-OD1	5.91	123.62	118.30
1	В	1018	LEU	CB-CA-C	-5.89	99.01	110.20
1	А	1018	LEU	CB-CA-C	-5.88	99.02	110.20
1	В	43	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	В	199	ASP	CB-CG-OD1	5.88	123.59	118.30
1	А	769	TRP	CB-CA-C	-5.88	98.65	110.40
1	В	908	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	D	769	TRP	CB-CA-C	-5.87	98.65	110.40
1	А	5	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	С	769	TRP	CB-CA-C	-5.87	98.66	110.40
1	А	199	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	199	ASP	CB-CG-OD1	5.86	123.58	118.30
1	D	1018	LEU	CB-CA-C	-5.86	99.06	110.20
1	С	82	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	С	1018	LEU	CB-CA-C	-5.85	99.08	110.20
1	В	769	TRP	CB-CA-C	-5.85	98.70	110.40
1	D	77	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	С	423	MET	C-N-CA	5.84	136.29	121.70
1	А	82	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	С	77	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	А	77	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	А	423	MET	C-N-CA	5.82	136.24	121.70
1	D	82	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	77	ASP	CB-CG-OD1	5.82	123.53	118.30
1	А	77	ASP	CB-CG-OD1	5.81	123.53	118.30
1	В	144	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	В	423	MET	C-N-CA	5.80	136.21	121.70
1	D	423	MET	C-N-CA	5.80	136.21	121.70
1	В	954	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	В	610	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	D	130	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	368	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	В	77	ASP	CB-CG-OD1	5.79	123.51	118.30
1	С	130	ASP	CB-CG-OD1	5.79	123.51	118.30

Continued from previous page...



1 1

1

1 1

1

1

1

1

1

1 1

1

1

1

1 1

1

1

1

1 1

1

1

1

1

1

1 1

1

1

1

1

1

1

1

1

1

1

1

1

1

in	Res	Type	Atoms	Ζ	Observed(°)	$Ideal(^{o})$
	82	ASP	CB-CG-OD2	-5.79	113.09	118.30
	610	ASP	CB-CG-OD2	-5.79	113.09	118.30
	134	LEU	N-CA-CB	5.78	121.97	110.40
	134	LEU	N-CA-CB	5.78	121.97	110.40
	134	LEU	N-CA-CB	5.78	121.97	110.40
	954	ASP	CB-CG-OD2	-5.78	113.09	118.30
	144	ASP	CB-CG-OD2	-5.78	113.10	118.30
	43	ARG	NE-CZ-NH1	5.78	123.19	120.30
	130	ASP	CB-CG-OD1	5.78	123.50	118.30
	134	LEU	N-CA-CB	5.78	121.96	110.40
	987	ASP	CB-CG-OD1	5.78	123.50	118.30
	130	ASP	CB-CG-OD1	5.78	123.50	118.30
	77	ASP	CB-CG-OD2	-5.77	113.11	118.30
	77	ASP	CB-CG-OD1	5.77	123.49	118.30
	610	ASP	CB-CG-OD2	-5.77	113.11	118.30
	239	VAL	CA-CB-CG2	-5.77	102.25	110.90
	239	VAL	CA-CB-CG2	-5.76	102.26	110.90
	144	ASP	CB-CG-OD2	-5.75	113.12	118.30
	792	ASP	CB-CG-OD1	5.75	123.48	118.30
	610	ASP	CB-CG-OD2	-5.75	113.13	118.30
	43	ARG	NE-CZ-NH1	5.75	123.17	120.30
	954	ASP	CB-CG-OD2	-5.75	113.13	118.30
	954	ASP	CB-CG-OD2	-5.74	113.13	118.30
	239	VAL	CA-CB-CG2	-5.74	102.29	110.90
	144	ASP	CB-CG-OD2	-5.73	113.14	118.30
	368	ASP	CB-CG-OD2	-5.73	113.14	118.30
	987	ASP	CB-CG-OD1	5.72	123.45	118.30
	368	ASP	CB-CG-OD2	-5.72	113.15	118.30
	368	ASP	CB-CG-OD2	-5.72	113.15	118.30
	43	ARG	NE-CZ-NH1	5.72	123.16	120.30
	792	ASP	CB-CG-OD1	5.72	123.45	118.30
	292	ARG	NE-CZ-NH2	-5.72	117.44	120.30
	792	ASP	CB-CG-OD1	5.72	123.44	118.30
	469	ASP	CB-CG-OD1	5.71	123.44	118.30
	239	VAL	CA-CB-CG2	-5.71	102.34	110.90
	987	ASP	CB-CG-OD1	5.71	123.44	118.30

Continued fr Mol Chai

В

D А

С

D D

А

С

А

В

С

В В

С

С

D

С D

В

А

А

А С

А

С

А

А

С

В D

D

С

С

А

В

D

В

С

А

В

В

С

ASP

ASP

ASP

ARG

ASP

ARG

987

469

792

230

469

230

CB-CG-OD1

CB-CG-OD1

CB-CG-OD1

NE-CZ-NH1

CB-CG-OD1

NE-CZ-NH1

Continued on next page...

118.30

118.30

118.30

120.30

118.30

120.30

123.42

123.42

123.42

123.14

123.41

123.14



5.69

5.69

5.69

5.68

5.68

5.68

1F4A

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
1	D	144	ASP	CB-CG-OD1	5.67	123.41	118.30
1	А	164	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	В	144	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	469	ASP	CB-CG-OD1	5.67	123.40	118.30
1	В	164	ASP	CB-CG-OD1	5.67	123.40	118.30
1	В	635	THR	CA-CB-CG2	-5.66	104.47	112.40
1	D	635	THR	CA-CB-CG2	-5.66	104.48	112.40
1	А	144	ASP	CB-CG-OD1	5.66	123.39	118.30
1	А	635	THR	CA-CB-CG2	-5.66	104.48	112.40
1	С	45	ASP	CB-CG-OD1	5.66	123.39	118.30
1	В	164	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	С	635	THR	CA-CB-CG2	-5.64	104.50	112.40
1	D	230	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	164	ASP	CB-CG-OD1	5.64	123.38	118.30
1	D	164	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	С	164	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	С	144	ASP	CB-CG-OD1	5.63	123.37	118.30
1	С	288	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	А	164	ASP	CB-CG-OD1	5.63	123.36	118.30
1	А	288	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	В	288	ARG	CD-NE-CZ	-5.62	115.72	123.60
1	D	45	ASP	CB-CG-OD1	5.62	123.36	118.30
1	В	772	ASP	CB-CG-OD1	5.62	123.36	118.30
1	В	45	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	594	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	А	45	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	288	ARG	CD-NE-CZ	-5.61	115.74	123.60
1	В	210	ARG	N-CA-CB	5.61	120.69	110.60
1	А	210	ARG	N-CA-CB	5.61	120.69	110.60
1	D	210	ARG	N-CA-CB	5.60	120.68	110.60
1	А	594	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	С	210	ARG	N-CA-CB	5.59	120.67	110.60
1	С	292	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	А	230	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	772	ASP	CB-CG-OD1	5.59	123.33	118.30
1	С	164	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	772	ASP	CB-CG-OD1	5.58	123.32	118.30
1	В	594	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	916	ASP	CB-CG-OD1	5.57	123.31	118.30
1	С	594	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	С	916	ASP	CB-CG-OD1	5.56	123.31	118.30
1	D	292	ARG	NE-CZ-NH2	-5.56	117.52	120.30



1F4A

α \cdot \cdot \cdot	C		
Continued	trom	previous	page
• • • • • • • • • • • •	J	<i>r</i> · · · · · · · · · · · · · · · · · · ·	r ~g ····

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	292	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	В	492	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	С	772	ASP	CB-CG-OD1	5.56	123.30	118.30
1	А	492	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	В	292	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	А	292	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	А	828	ASP	CB-CG-OD1	5.53	123.28	118.30
1	В	916	ASP	CB-CG-OD1	5.53	123.27	118.30
1	С	492	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	D	492	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	А	916	ASP	CB-CG-OD1	5.51	123.26	118.30
1	С	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	В	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	С	987	ASP	CB-CG-OD2	-5.50	113.34	118.30
1	В	292	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	292	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	В	561	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	561	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	987	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	А	987	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	В	987	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	С	829	THR	CA-CB-CG2	-5.47	104.74	112.40
1	В	829	THR	CA-CB-CG2	-5.47	104.74	112.40
1	А	829	THR	CA-CB-CG2	-5.45	104.77	112.40
1	D	829	THR	CA-CB-CG2	-5.45	104.77	112.40
1	D	671	ASP	CB-CG-OD1	5.44	123.20	118.30
1	А	561	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	В	917	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	С	561	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	А	447	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	С	447	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	В	863	GLN	CB-CA-C	-5.42	99.56	110.40
1	D	863	GLN	CB-CA-C	-5.42	99.56	110.40
1	А	863	GLN	CB-CA-C	-5.41	99.57	110.40
1	А	917	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	С	863	GLN	CB-CA-C	-5.41	99.58	110.40
1	D	447	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	В	447	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	319	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	506	VAL	CA-CB-CG1	-5.38	102.82	110.90
1	А	671	ASP	CB-CG-OD1	5.38	123.14	118.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	219	THR	CA-CB-CG2	-5.38	104.88	112.40
1	А	219	THR	CA-CB-CG2	-5.37	104.88	112.40
1	А	506	VAL	CA-CB-CG1	-5.37	102.85	110.90
1	С	219	THR	CA-CB-CG2	-5.37	104.89	112.40
1	В	748	CYS	N-CA-CB	5.36	120.25	110.60
1	С	506	VAL	CA-CB-CG1	-5.36	102.86	110.90
1	С	671	ASP	CB-CG-OD1	5.36	123.12	118.30
1	В	506	VAL	CA-CB-CG1	-5.35	102.87	110.90
1	С	917	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	В	782	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	А	319	ASP	CB-CG-OD1	5.34	123.11	118.30
1	В	219	THR	CA-CB-CG2	-5.34	104.92	112.40
1	D	748	CYS	N-CA-CB	5.34	120.20	110.60
1	А	748	CYS	N-CA-CB	5.33	120.20	110.60
1	В	671	ASP	CB-CG-OD1	5.33	123.10	118.30
1	С	748	CYS	N-CA-CB	5.33	120.19	110.60
1	В	319	ASP	CB-CG-OD1	5.32	123.09	118.30
1	С	579	ASP	CB-CG-OD1	5.32	123.09	118.30
1	С	319	ASP	CB-CG-OD1	5.32	123.09	118.30
1	В	980	GLU	N-CA-CB	5.31	120.16	110.60
1	D	579	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	917	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	А	782	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	С	782	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	С	980	GLU	N-CA-CB	5.29	120.12	110.60
1	А	980	GLU	N-CA-CB	5.29	120.12	110.60
1	D	261	TRP	CB-CA-C	-5.29	99.82	110.40
1	В	579	ASP	CB-CG-OD1	5.29	123.06	118.30
1	В	386	ALA	N-CA-CB	-5.29	102.70	110.10
1	D	980	GLU	N-CA-CB	5.28	120.11	110.60
1	D	782	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	386	ALA	N-CA-CB	-5.28	102.71	110.10
1	В	261	TRP	CB-CA-C	-5.28	99.84	110.40
1	С	386	ALA	N-CA-CB	-5.28	102.71	110.10
1	А	261	TRP	CB-CA-C	-5.27	99.87	110.40
1	А	579	ASP	CB-CG-OD1	5.26	123.04	118.30
1	С	261	TRP	CB-CA-C	-5.26	99.87	110.40
1	А	386	ALA	N-CA-CB	-5.26	102.73	110.10
1	A	269	SER	N-CA-CB	5.24	118.36	110.50
1	С	916	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	С	329	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	201	ASP	CB-CG-OD2	-5.22	113.61	118.30



1F4A

Continued from previous page							
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	329	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	572	ASP	CB-CG-OD1	5.21	122.99	118.30
1	В	269	SER	N-CA-CB	5.21	118.31	110.50
1	А	329	ASP	CB-CG-OD2	-5.21	113.62	118.30
1	С	599	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	916	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	В	710	GLU	CB-CA-C	-5.20	100.00	110.40
1	D	269	SER	N-CA-CB	5.20	118.30	110.50
1	А	710	GLU	CB-CA-C	-5.19	100.01	110.40
1	D	710	GLU	CB-CA-C	-5.19	100.02	110.40
1	С	710	GLU	CB-CA-C	-5.19	100.03	110.40
1	В	104	THR	CA-CB-CG2	-5.18	105.14	112.40
1	С	269	SER	N-CA-CB	5.18	118.27	110.50
1	С	572	ASP	CB-CG-OD1	5.18	122.96	118.30
1	А	104	THR	CA-CB-CG2	-5.17	105.16	112.40
1	С	671	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	248	GLY	C-N-CA	-5.17	108.77	121.70
1	D	329	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	А	201	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	46	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	А	518	TRP	CB-CA-C	-5.17	100.07	110.40
1	А	248	GLY	C-N-CA	-5.16	108.79	121.70
1	D	671	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	С	46	ARG	C-N-CD	-5.16	109.25	120.60
1	С	201	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	В	248	GLY	C-N-CA	-5.16	108.80	121.70
1	D	104	THR	CA-CB-CG2	-5.16	105.18	112.40
1	А	864	MET	N-CA-CB	5.16	119.88	110.60
1	А	599	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	В	916	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	А	671	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	С	518	TRP	CB-CA-C	-5.15	100.10	110.40
1	D	46	ARG	C-N-CD	-5.15	109.27	120.60
1	D	518	TRP	CB-CA-C	-5.15	100.09	110.40
1	С	248	GLY	C-N-CA	-5.15	108.82	121.70
1	С	864	MET	N-CA-CB	5.15	119.87	110.60
1	А	46	ARG	C-N-CD	-5.15	109.28	120.60
1	А	572	ASP	CB-CG-OD1	5.14	122.93	118.30
1	В	201	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	599	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	В	572	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	610	ASP	CB-CG-OD1	5.14	122.93	118.30



1F4A

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
1	D	864	MET	N-CA-CB	5.14	119.85	110.60
1	D	903[A]	GLN	N-CA-CB	5.14	119.85	110.60
1	D	903[B]	GLN	N-CA-CB	5.14	119.85	110.60
1	В	864	MET	N-CA-CB	5.14	119.85	110.60
1	С	104	THR	CA-CB-CG2	-5.14	105.21	112.40
1	В	193	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	В	518	TRP	CB-CA-C	-5.13	100.13	110.40
1	В	903[A]	GLN	N-CA-CB	5.13	119.84	110.60
1	В	903[B]	GLN	N-CA-CB	5.13	119.84	110.60
1	А	903[A]	GLN	N-CA-CB	5.13	119.83	110.60
1	А	903[B]	GLN	N-CA-CB	5.13	119.83	110.60
1	С	903[A]	GLN	N-CA-CB	5.13	119.83	110.60
1	С	903[B]	GLN	N-CA-CB	5.13	119.83	110.60
1	D	651	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	В	651	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	В	46	ARG	C-N-CD	-5.12	109.34	120.60
1	В	671	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	А	916	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	237	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	С	193	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	А	651	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	А	193	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	С	651	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	В	599	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	А	610	ASP	CB-CG-OD1	5.08	122.88	118.30
1	D	310	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	В	610	ASP	CB-CG-OD1	5.07	122.86	118.30
1	С	610	ASP	CB-CG-OD1	5.07	122.86	118.30
1	В	46	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	193	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	С	310	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	С	721	ARG	N-CA-CB	5.05	119.69	110.60
1	D	363	HIS	CA-CB-CG	-5.05	105.02	113.60
1	D	721	ARG	N-CA-CB	5.04	119.68	110.60
1	А	721	ARG	N-CA-CB	5.04	119.67	110.60
1	С	919	ASP	CB-CG-OD1	5.04	122.83	118.30
1	С	363	HIS	CA-CB-CG	-5.03	105.05	113.60
1	В	721	ARG	N-CA-CB	5.03	119.66	110.60
1	А	919	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	363	HIS	CA-CB-CG	-5.02	105.06	113.60
1	С	869	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	В	869	ASP	CB-CG-OD2	-5.02	113.78	118.30



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	D	919	ASP	CB-CG-OD1	5.01	122.81	118.30
1	В	363	HIS	CA-CB-CG	-5.01	105.08	113.60
1	А	237	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	D	114	VAL	CA-CB-CG1	5.01	118.41	110.90
1	В	919	ASP	CB-CG-OD1	5.00	122.80	118.30
1	В	420	MET	CG-SD-CE	-5.00	92.19	100.20

Continued from previous page...

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	А	8238	0	7824	394	0
1	В	8238	0	7824	374	0
1	С	8238	0	7824	379	0
1	D	8238	0	7824	374	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
3	А	365	0	0	10	0
3	В	366	0	0	10	0
3	С	367	0	0	10	0
3	D	366	0	0	10	0
All	All	34424	0	31296	1496	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:THR:HA	1:B:436:MET:HE1	1.21	1.11
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.34	1.10



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.34	1.09
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.34	1.09
1:C:427:THR:HA	1:C:436:MET:HE1	1.28	1.08
1:A:427:THR:HA	1:A:436:MET:HE1	1.32	1.07
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.34	1.06
1:D:427:THR:HA	1:D:436:MET:HE1	1.35	1.05
1:B:693:GLN:HG2	1:B:721:ARG:HD3	1.39	1.05
1:D:693:GLN:HG2	1:D:721:ARG:HD3	1.39	1.04
1:A:693:GLN:HG2	1:A:721:ARG:HD3	1.39	1.03
1:C:693:GLN:HG2	1:C:721:ARG:HD3	1.39	1.01
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.44	0.99
1:C:597:ASN:HD22	1:C:599:ARG:H	1.11	0.98
1:D:597:ASN:HD22	1:D:599:ARG:H	1.11	0.98
1:C:597:ASN:ND2	1:C:599:ARG:H	1.65	0.95
1:B:38:ASN:ND2	1:B:41:GLU:H	1.66	0.94
1:A:38:ASN:ND2	1:A:41:GLU:H	1.66	0.94
1:A:597:ASN:ND2	1:A:599:ARG:H	1.65	0.94
1:D:597:ASN:ND2	1:D:599:ARG:H	1.65	0.94
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.34	0.93
1:B:427:THR:HA	1:B:436:MET:CE	1.99	0.93
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.34	0.93
1:C:38:ASN:ND2	1:C:41:GLU:H	1.66	0.93
1:B:597:ASN:ND2	1:B:599:ARG:H	1.65	0.92
1:C:255:ARG:HG2	1:C:255:ARG:HH11	1.34	0.92
1:D:38:ASN:ND2	1:D:41:GLU:H	1.66	0.92
1:C:427:THR:HA	1:C:436:MET:CE	1.99	0.92
1:A:427:THR:HA	1:A:436:MET:CE	1.99	0.92
1:B:597:ASN:HD22	1:B:599:ARG:H	1.11	0.92
1:D:427:THR:HA	1:D:436:MET:CE	1.99	0.91
1:A:597:ASN:HD22	1:A:599:ARG:H	1.11	0.91
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.34	0.89
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.58	0.86
1:A:734:SER:HB3	1:A:860:GLY:HA3	1.57	0.86
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.57	0.86
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.58	0.85
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.58	0.85
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.58	0.85
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.57	0.85
1:D:856:TYR:HB3	1:D:864:MET:CE	2.07	0.85
1:A:856:TYR:HB3	1:A:864:MET:CE	2.07	0.84
1:C:856:TYR:HB3	1:C:864:MET:CE	2.07	0.84



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.57	0.84
1:B:856:TYR:HB3	1:B:864:MET:CE	2.07	0.83
1:D:734:SER:CB	1:D:860:GLY:HA3	2.08	0.83
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.94	0.83
1:B:734:SER:CB	1:B:860:GLY:HA3	2.08	0.82
1:A:734:SER:CB	1:A:860:GLY:HA3	2.09	0.82
1:C:654:TRP:NE1	1:C:666:GLY:HA3	1.94	0.82
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	1.98	0.82
1:B:654:TRP:NE1	1:B:666:GLY:HA3	1.94	0.82
1:C:734:SER:CB	1:C:860:GLY:HA3	2.09	0.82
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	1.98	0.82
1:A:654:TRP:NE1	1:A:666:GLY:HA3	1.94	0.81
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.11	0.81
1:A:830:LEU:CD2	1:A:835:LEU:HB2	2.11	0.81
1:C:830:LEU:CD2	1:C:835:LEU:HB2	2.11	0.81
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	1.98	0.81
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	1.98	0.80
1:D:830:LEU:CD2	1:D:835:LEU:HB2	2.11	0.80
1:C:134:LEU:HD12	1:C:134:LEU:N	1.97	0.80
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.97	0.80
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.97	0.80
1:A:134:LEU:N	1:A:134:LEU:HD12	1.97	0.79
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.97	0.79
1:B:77:ASP:O	1:B:78:LEU:HD23	1.83	0.79
1:D:436:MET:HE1	1:D:467:ASN:HD22	1.46	0.79
1:C:77:ASP:O	1:C:78:LEU:HD23	1.83	0.79
1:B:134:LEU:N	1:B:134:LEU:HD12	1.97	0.78
1:D:77:ASP:O	1:D:78:LEU:HD23	1.83	0.78
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.65	0.78
1:A:77:ASP:O	1:A:78:LEU:HD23	1.83	0.78
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.97	0.77
1:A:928:PRO:HB2	1:A:973:ARG:NH1	1.99	0.77
1:B:9:VAL:O	1:B:12:GLN:HB3	1.85	0.77
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.65	0.77
1:C:928:PRO:HB2	1:C:973:ARG:NH1	1.99	0.77
1:D:134:LEU:N	1:D:134:LEU:HD12	1.97	0.77
1:A:11:LEU:HD21	1:A:187:MET:CE	2.15	0.77
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.66	0.77
1:B:928:PRO:HB2	1:B:973:ARG:NH1	1.99	0.77
1:C:1004:SER:HB2	1:C:1006:GLU:OE2	1.85	0.77
1:A:1004:SER:HB2	1:A:1006:GLU:OE2	1.85	0.77



Atom-1	Atom 2	Interatomic	Clash
	Atom-2	distance (\AA)	overlap (Å)
1:D:928:PRO:HB2	1:D:973:ARG:NH1	1.99	0.77
1:D:9:VAL:O	1:D:12:GLN:HB3	1.85	0.76
1:B:11:LEU:HD21	1:B:187:MET:CE	2.15	0.76
1:D:11:LEU:HD21	1:D:187:MET:CE	2.15	0.76
1:A:9:VAL:O	1:A:12:GLN:HB3	1.85	0.76
1:C:9:VAL:O	1:C:12:GLN:HB3	1.85	0.76
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.14	0.76
1:C:11:LEU:HD21	1:C:187:MET:CE	2.15	0.76
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.14	0.76
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.49	0.76
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.65	0.76
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.68	0.76
1:D:1004:SER:HB2	1:D:1006:GLU:OE2	1.85	0.76
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.69	0.75
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.68	0.75
1:B:746:ASP:CA	1:B:760:ARG:HG3	2.14	0.75
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.68	0.75
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.35	0.75
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.85	0.75
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.68	0.75
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.68	0.74
1:C:38:ASN:HD22	1:C:41:GLU:H	1.35	0.74
1:A:38:ASN:HD22	1:A:41:GLU:H	1.35	0.74
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.69	0.74
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.68	0.74
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.14	0.74
1:D:655:MET:HG3	1:D:656:VAL:N	2.03	0.74
1:C:436:MET:HE1	1:C:467:ASN:HD22	1.53	0.73
1:D:579:ASP:OD1	1:D:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.53	0.73
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.70	0.73
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.70	0.73
1:B:237:ARG:HH11	1:B:237:ARG:HB3	1.54	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.71	0.73
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.02	0.73
1:A:579:ASP:OD1	1:A:583:ASN:HB2	1.89	0.72
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.70	0.72
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.54	0.72
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.54	0.72



Atom-1	Atom-2	Interatomic	Clash
1100111-1	1100111-2	distance (Å)	overlap (Å)
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.70	0.72
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.71	0.72
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.35	0.72
1:B:3:ILE:HG13	1:B:4:THR:N	2.04	0.72
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.71	0.72
1:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.35	0.72
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.71	0.72
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.71	0.72
1:D:3:ILE:HG13	1:D:4:THR:N	2.04	0.72
1:D:380:LYS:HE2	3:D:4077:HOH:O	1.90	0.72
1:A:652:LEU:HD11	1:A:698:VAL:HB	1.71	0.72
1:D:436:MET:CE	1:D:467:ASN:HD22	2.03	0.72
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.55	0.72
1:B:237:ARG:HH11	1:B:237:ARG:CB	2.02	0.72
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.35	0.72
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.72	0.71
1:A:436:MET:CE	1:A:467:ASN:HD22	2.03	0.71
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.55	0.71
1:C:655:MET:HG3	1:C:656:VAL:N	2.03	0.71
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.55	0.71
1:A:3:ILE:HG13	1:A:4:THR:N	2.04	0.71
1:B:38:ASN:HD22	1:B:41:GLU:H	1.35	0.71
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.55	0.71
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.02	0.71
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.02	0.71
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.71	0.71
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.71	0.71
1:C:3:ILE:HG13	1:C:4:THR:N	2.04	0.71
1:C:436:MET:CE	1:C:467:ASN:HD22	2.03	0.71
1:B:380:LYS:HE2	3:B:4134:HOH:O	1.90	0.71
1:B:436:MET:CE	1:B:467:ASN:HD22	2.03	0.71
1:C:380:LYS:HE2	3:C:4174:HOH:O	1.90	0.71
1:C:650:GLU:HB3	1:C:670:LEU:HD12	1.73	0.71
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.73	0.70
1:B:11:LEU:HD21	1:B:187:MET:HE3	1.72	0.70
1:C:836:ILE:HD13	1:C:836:ILE:N	2.07	0.69
1:D:38:ASN:HD22	1:D:41:GLU:H	1.35	0.69
1:A:655:MET:HG3	1:A:656:VAL:N	2.03	0.69
1:C:11:LEU:HD21	1:C:187:MET:HE3	1.74	0.69
1:A:380:LYS:HE2	3:A:4077:HOH:O	1.90	0.69
1:A:836:ILE:HD13	1:A:836:ILE:N	2.07	0.69



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.73	0.69
1:B:655:MET:HG3	1:B:656:VAL:N	2.03	0.69
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.75	0.69
1:D:836:ILE:HD13	1:D:836:ILE:N	2.07	0.69
1:B:836:ILE:HD13	1:B:836:ILE:N	2.07	0.69
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.73	0.68
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.75	0.68
1:A:11:LEU:HD21	1:A:187:MET:HE3	1.73	0.68
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.92	0.68
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.07	0.68
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.91	0.68
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.91	0.68
1:B:35:SER:OG	1:B:37:ARG:NH1	2.27	0.68
1:C:923:SER:HB3	3:C:4345:HOH:O	1.94	0.68
1:D:35:SER:OG	1:D:37:ARG:NH1	2.27	0.68
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.68
1:A:923:SER:HB3	3:A:4380:HOH:O	1.94	0.67
1:D:923:SER:HB3	3:D:4380:HOH:O	1.94	0.67
1:D:211:ASP:OD1	1:D:211:ASP:N	2.27	0.67
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.76	0.67
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.07	0.67
1:D:856:TYR:CD2	1:D:864:MET:HE1	2.29	0.67
1:D:965:GLN:O	1:D:969:GLU:HG3	1.94	0.67
1:B:965:GLN:O	1:B:969:GLU:HG3	1.94	0.67
1:C:59:ARG:NH2	1:C:81:ALA:O	2.28	0.67
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.77	0.67
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.91	0.67
1:C:965:GLN:O	1:C:969:GLU:HG3	1.94	0.67
1:A:211:ASP:N	1:A:211:ASP:OD1	2.27	0.67
1:A:35:SER:OG	1:A:37:ARG:NH1	2.27	0.67
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.75	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.28	0.66
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.07	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.77	0.66
1:C:375:ASP:O	1:C:379:MET:HG3	1.95	0.66
1:D:11:LEU:HD21	1:D:187:MET:HE3	1.76	0.66
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.77	0.66
1:A:965:GLN:O	1:A:969:GLU:HG3	1.94	0.66
1:A:7:LEU:N	1:A:71:GLU:OE2	2.28	0.66
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.75	0.66
1:B:824:GLN:HG3	1:B:825:CYS:N	2.11	0.66


Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:923:SER:HB3	3:B:4305:HOH:O	1.94	0.66
1:B:856:TYR:CD2	1:B:864:MET:HE1	2.31	0.66
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.77	0.66
1:D:824:GLN:HG3	1:D:825:CYS:N	2.11	0.66
1:A:856:TYR:HB3	1:A:864:MET:HE1	1.77	0.66
1:B:7:LEU:N	1:B:71:GLU:OE2	2.28	0.66
1:D:59:ARG:NH2	1:D:81:ALA:O	2.28	0.66
1:B:59:ARG:NH2	1:B:81:ALA:O	2.28	0.66
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.77	0.66
1:A:375:ASP:O	1:A:379:MET:HG3	1.95	0.66
1:B:211:ASP:OD1	1:B:211:ASP:N	2.27	0.65
1:C:30:HIS:HB2	1:C:31:PRO:HD2	1.77	0.65
1:C:824:GLN:HG3	1:C:825:CYS:N	2.11	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.28	0.65
1:D:7:LEU:N	1:D:71:GLU:OE2	2.28	0.65
1:D:775:GLN:OE1	1:D:890:GLN:NE2	2.30	0.65
1:D:856:TYR:HD2	1:D:864:MET:HE1	1.61	0.65
1:B:375:ASP:O	1:B:379:MET:HG3	1.95	0.65
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.77	0.65
1:C:210:ARG:HD3	3:C:4138:HOH:O	1.97	0.65
1:D:375:ASP:O	1:D:379:MET:HG3	1.95	0.65
1:A:824:GLN:HG3	1:A:825:CYS:N	2.10	0.65
1:B:742:THR:HG22	1:B:743:SER:N	2.12	0.65
1:B:775:GLN:OE1	1:B:890:GLN:NE2	2.30	0.65
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.30	0.65
1:D:742:THR:HG22	1:D:743:SER:N	2.12	0.65
1:A:742:THR:HG22	1:A:743:SER:N	2.12	0.64
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.77	0.64
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.80	0.64
1:C:742:THR:HG22	1:C:743:SER:N	2.12	0.64
1:A:499:ILE:HB	1:A:533:LEU:HB2	1.79	0.64
1:A:210:ARG:HD3	3:A:4036:HOH:O	1.97	0.64
1:A:775:GLN:OE1	1:A:890:GLN:NE2	2.30	0.64
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.62	0.64
1:D:856:TYR:HB3	1:D:864:MET:HE1	1.78	0.64
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.64
1:D:499:ILE:HB	1:D:533:LEU:HB2	1.79	0.64
1:B:210:ARG:HD3	3:B:4098:HOH:O	1.97	0.64
1:B:797:GLU:O	1:B:801:ILE:HD12	1.98	0.64
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.77	0.64
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.79	0.64



A + a 1	A + a == 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:210:ARG:HD3	3:D:4036:HOH:O	1.97	0.64
1:A:287:ASP:CG	1:D:425:ARG:HH22	2.00	0.63
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.81	0.63
1:A:835:LEU:C	1:A:836:ILE:HD13	2.19	0.63
1:B:835:LEU:C	1:B:836:ILE:HD13	2.19	0.63
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.81	0.63
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.81	0.63
1:B:746:ASP:HA	1:B:760:ARG:CG	2.22	0.63
1:C:746:ASP:HA	1:C:760:ARG:CG	2.22	0.63
1:C:797:GLU:O	1:C:801:ILE:HD12	1.98	0.63
1:B:649:ASN:OD1	1:B:703:PRO:HD2	1.99	0.63
1:B:66:PRO:HD2	1:B:67:GLU:HG2	1.81	0.63
1:A:66:PRO:HD2	1:A:67:GLU:HG2	1.81	0.63
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.34	0.63
1:C:211:ASP:N	1:C:211:ASP:OD1	2.27	0.63
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.81	0.63
1:D:649:ASN:OD1	1:D:703:PRO:HD2	1.99	0.63
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.81	0.62
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.34	0.62
1:A:797:GLU:O	1:A:801:ILE:HD12	1.98	0.62
1:D:746:ASP:HA	1:D:760:ARG:CG	2.22	0.62
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.07	0.62
1:A:649:ASN:OD1	1:A:703:PRO:HD2	1.99	0.62
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.34	0.62
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.34	0.62
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.81	0.62
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.34	0.62
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.99	0.62
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.81	0.62
1:C:835:LEU:C	1:C:836:ILE:HD13	2.19	0.62
1:A:906:TYR:HB3	1:A:907:PRO:HD2	1.81	0.62
1:C:767:GLN:HG3	1:C:768:MET:N	2.15	0.62
1:A:767:GLN:HG3	1:A:768:MET:N	2.15	0.62
1:D:835:LEU:C	1:D:836:ILE:HD13	2.19	0.62
1:C:66:PRO:HD2	1:C:67:GLU:HG2	1.81	0.62
1:C:778:THR:CG2	1:C:779:PRO:HD2	2.30	0.62
1:D:797:GLU:O	1:D:801:ILE:HD12	1.98	0.62
1:B:767:GLN:HG3	1:B:768:MET:N	2.15	0.61
1:D:66:PRO:HD2	1:D:67:GLU:HG2	1.81	0.61
1:A:778:THR:CG2	1:A:779:PRO:HD2	2.30	0.61
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.81	0.61



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:822:LEU:HD12	1:B:824:GLN:N	2.16	0.61
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.81	0.61
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.81	0.61
1:C:928:PRO:O	1:C:973:ARG:NH1	2.33	0.61
1:A:651:LEU:HD12	1:A:669:PRO:HA	1.83	0.61
1:B:856:TYR:HD2	1:B:864:MET:HE1	1.63	0.61
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.01	0.61
1:A:928:PRO:O	1:A:973:ARG:NH1	2.34	0.61
1:C:227:VAL:HG13	1:C:240:LEU:HD11	1.83	0.61
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.30	0.61
1:C:651:LEU:HD12	1:C:669:PRO:HA	1.83	0.61
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.81	0.61
1:B:928:PRO:O	1:B:973:ARG:NH1	2.34	0.61
1:D:928:PRO:O	1:D:973:ARG:NH1	2.34	0.61
1:B:227:VAL:HG13	1:B:240:LEU:HD11	1.83	0.60
1:D:102:ASN:ND2	1:D:201:ASP:HB2	2.16	0.60
1:D:778:THR:CG2	1:D:779:PRO:HD2	2.30	0.60
1:D:822:LEU:HD12	1:D:824:GLN:N	2.16	0.60
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.16	0.60
1:A:822:LEU:HD12	1:A:824:GLN:N	2.16	0.60
1:B:822:LEU:HD11	1:B:824:GLN:O	2.01	0.60
1:C:595:THR:HG23	1:C:596:PRO:HA	1.82	0.60
1:D:822:LEU:HD11	1:D:824:GLN:O	2.01	0.60
1:A:610:ASP:OD2	1:A:612:THR:HG23	2.01	0.60
1:C:102:ASN:ND2	1:C:201:ASP:HB2	2.16	0.60
1:C:822:LEU:HD11	1:C:824:GLN:O	2.01	0.60
1:C:870:VAL:HG12	1:C:871:GLU:N	2.16	0.60
1:D:595:THR:HG23	1:D:596:PRO:HA	1.82	0.60
1:A:595:THR:HG23	1:A:596:PRO:HA	1.82	0.60
1:B:102:ASN:ND2	1:B:201:ASP:HB2	2.16	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.84	0.60
1:B:80:GLU:H	1:B:80:GLU:CD	2.01	0.60
1:B:140:ARG:NH1	1:B:170:GLU:OE1	2.31	0.60
1:B:595:THR:HG23	1:B:596:PRO:HA	1.82	0.60
1:B:734:SER:HB3	1:B:860:GLY:CA	2.30	0.60
1:C:822:LEU:HD12	1:C:824:GLN:N	2.16	0.60
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.36	0.60
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.02	0.60
1:C:511:PRO:HA	1:C:516:PRO:HB3	1.84	0.60
1:C:734:SER:HB3	1:C:860:GLY:CA	2.30	0.60
1:A:282:ARG:HD3	1:D:418:HIS:O	2.01	0.60



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:651:LEU:HD12	1:D:669:PRO:HA	1.83	0.60
1:A:128:ASN:HA	1:A:180:GLY:O	2.02	0.60
1:B:610:ASP:OD2	1:B:612:THR:HG23	2.01	0.60
1:B:651:LEU:HD12	1:B:669:PRO:HA	1.83	0.60
1:C:128:ASN:HA	1:C:180:GLY:O	2.02	0.60
1:A:734:SER:HB3	1:A:860:GLY:CA	2.30	0.59
1:A:830:LEU:HD21	1:A:835:LEU:HB2	1.84	0.59
1:B:870:VAL:HG12	1:B:871:GLU:N	2.16	0.59
1:D:227:VAL:HG13	1:D:240:LEU:HD11	1.83	0.59
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.84	0.59
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.02	0.59
1:C:759:ASN:OD1	1:C:761:GLN:N	2.35	0.59
1:D:734:SER:HB3	1:D:860:GLY:CA	2.30	0.59
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.83	0.59
1:A:759:ASN:OD1	1:A:761:GLN:N	2.35	0.59
1:A:822:LEU:HD11	1:A:824:GLN:O	2.01	0.59
1:C:610:ASP:OD2	1:C:612:THR:HG23	2.01	0.59
1:D:701:VAL:HG12	1:D:702:GLN:N	2.17	0.59
1:D:767:GLN:HG3	1:D:768:MET:N	2.15	0.59
1:A:696:LEU:HD12	1:A:697:THR:N	2.18	0.59
1:A:870:VAL:HG12	1:A:871:GLU:N	2.16	0.59
1:B:696:LEU:HD12	1:B:697:THR:N	2.18	0.59
1:D:128:ASN:HA	1:D:180:GLY:O	2.02	0.59
1:A:505:ARG:HG2	1:A:996:ASP:OD2	2.02	0.59
1:D:696:LEU:HD12	1:D:697:THR:N	2.18	0.59
1:A:282:ARG:HH12	1:D:419:GLY:C	2.06	0.59
1:B:128:ASN:HA	1:B:180:GLY:O	2.02	0.59
1:D:505:ARG:HG2	1:D:996:ASP:OD2	2.02	0.59
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.84	0.59
1:D:870:VAL:HG12	1:D:871:GLU:N	2.16	0.59
1:A:701:VAL:HG12	1:A:702:GLN:N	2.17	0.58
1:B:336:ARG:NH2	1:B:338:GLU:OE1	2.36	0.58
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.31	0.58
1:C:696:LEU:HD12	1:C:697:THR:N	2.17	0.58
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.84	0.58
1:B:6:SER:HB2	1:B:71:GLU:OE2	2.04	0.58
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.19	0.58
1:C:473:ARG:O	1:C:473:ARG:HD3	2.04	0.58
1:C:533:LEU:C	1:C:533:LEU:HD12	2.24	0.58
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.36	0.58
1:B:511:PRO:HA	1:B:516:PRO:HB3	1.84	0.58



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.39	0.58
1:B:473:ARG:O	1:B:473:ARG:HD3	2.04	0.58
1:C:336:ARG:NH2	1:C:338:GLU:OE1	2.36	0.58
1:A:62:TRP:CD1	1:A:95:TYR:HB3	2.39	0.58
1:A:473:ARG:O	1:A:473:ARG:HD3	2.04	0.58
1:B:701:VAL:HG12	1:B:702:GLN:N	2.17	0.58
1:B:737:ILE:HG13	1:B:738:PRO:N	2.17	0.58
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.68	0.58
1:D:336:ARG:NH2	1:D:338:GLU:OE1	2.36	0.58
1:D:473:ARG:HD3	1:D:473:ARG:O	2.04	0.58
1:D:737:ILE:HG13	1:D:738:PRO:N	2.17	0.58
1:A:769:TRP:NE1	1:A:774:LYS:HG3	2.19	0.58
1:B:759:ASN:OD1	1:B:761:GLN:N	2.35	0.57
1:C:701:VAL:HG12	1:C:702:GLN:N	2.17	0.57
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.19	0.57
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.04	0.57
1:B:316:HIS:HD2	1:B:317:THR:O	1.87	0.57
1:A:533:LEU:HD12	1:A:533:LEU:C	2.24	0.57
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.86	0.57
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	0.57
1:B:533:LEU:HD12	1:B:533:LEU:C	2.24	0.57
1:C:618:THR:HG22	1:C:912:ALA:HB1	1.86	0.57
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.04	0.57
1:D:618:THR:HG22	1:D:912:ALA:HB1	1.86	0.57
1:A:6:SER:HB2	1:A:71:GLU:OE2	2.03	0.57
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.39	0.57
1:C:737:ILE:HG13	1:C:738:PRO:N	2.17	0.57
1:C:769:TRP:NE1	1:C:774:LYS:HG3	2.19	0.57
1:D:80:GLU:H	1:D:80:GLU:CD	2.01	0.57
1:C:830:LEU:HD21	1:C:835:LEU:HB2	1.84	0.57
1:A:737:ILE:HG13	1:A:738:PRO:N	2.17	0.57
1:B:460:ASN:ND2	1:B:461:GLU:HG2	2.20	0.57
1:B:618:THR:HG22	1:B:912:ALA:HB1	1.86	0.57
1:C:62:TRP:CD1	1:C:95:TYR:HB3	2.39	0.57
1:C:134:LEU:HD12	1:C:134:LEU:H	1.69	0.57
1:D:533:LEU:HD12	1:D:533:LEU:C	2.24	0.57
1:C:26:ARG:HD2	1:C:169:SER:HA	1.87	0.57
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.04	0.57
1:D:140:ARG:NH1	1:D:170:GLU:OE1	2.31	0.57
1:D:316:HIS:HD2	1:D:317:THR:O	1.87	0.57
1:A:597:ASN:HD22	1:A:599:ARG:N	1.94	0.57



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:166:ARG:HD3	3:C:4137:HOH:O	2.05	0.57
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.40	0.57
1:A:316:HIS:HD2	1:A:317:THR:O	1.87	0.57
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.40	0.57
1:A:419:GLY:C	1:D:282:ARG:HH12	2.08	0.57
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.87	0.57
1:B:26:ARG:HD2	1:B:169:SER:HA	1.87	0.57
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.40	0.57
1:B:763:GLY:HA3	1:B:822:LEU:HD21	1.87	0.57
1:C:6:SER:HB2	1:C:71:GLU:OE2	2.03	0.57
1:C:460:ASN:ND2	1:C:461:GLU:HG2	2.20	0.57
1:A:460:ASN:ND2	1:A:461:GLU:HG2	2.20	0.57
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.40	0.56
1:A:166:ARG:HD3	3:A:4035:HOH:O	2.05	0.56
1:A:457:SER:HA	1:A:485:GLN:O	2.06	0.56
1:B:166:ARG:HD3	3:B:4097:HOH:O	2.05	0.56
1:B:834:VAL:HG12	1:B:835:LEU:N	2.19	0.56
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.20	0.56
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.41	0.56
1:B:18:ASN:OD1	1:B:19:PRO:HD2	2.06	0.56
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.05	0.56
1:C:763:GLY:HA3	1:C:822:LEU:HD21	1.87	0.56
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.87	0.56
1:D:18:ASN:OD1	1:D:19:PRO:HD2	2.06	0.56
1:A:26:ARG:HD2	1:A:169:SER:HA	1.87	0.56
1:C:834:VAL:HG12	1:C:835:LEU:N	2.19	0.56
1:D:38:ASN:HD21	1:D:41:GLU:H	1.53	0.56
1:D:166:ARG:HD3	3:D:4035:HOH:O	2.05	0.56
1:D:457:SER:HA	1:D:485:GLN:O	2.06	0.56
1:A:304:GLU:C	1:A:305:ILE:HG13	2.26	0.56
1:A:531:ARG:O	1:A:561:ARG:NH1	2.39	0.56
1:A:834:VAL:HG12	1:A:835:LEU:N	2.19	0.56
1:B:531:ARG:O	1:B:561:ARG:NH1	2.39	0.56
1:C:457:SER:HA	1:C:485:GLN:O	2.06	0.56
1:D:834:VAL:HG12	1:D:835:LEU:N	2.19	0.56
1:A:577:LYS:O	1:A:584:PRO:HA	2.06	0.56
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.05	0.56
1:B:763:GLY:HA3	1:B:822:LEU:CD2	2.36	0.56
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.40	0.56
1:D:134:LEU:HD12	1:D:134:LEU:H	1.69	0.56
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.05	0.56



A + am 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.06	0.56
1:A:80:GLU:H	1:A:80:GLU:CD	2.01	0.56
1:B:457:SER:HA	1:B:485:GLN:O	2.05	0.56
1:C:316:HIS:HD2	1:C:317:THR:O	1.88	0.56
1:C:833:ALA:HB1	1:C:858:ILE:O	2.06	0.56
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.05	0.56
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.36	0.56
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.71	0.56
1:D:429:ASP:OD1	1:D:430:PRO:HD2	2.04	0.55
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.74	0.55
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.39	0.55
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.41	0.55
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.22	0.55
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.42	0.55
1:A:833:ALA:HB1	1:A:858:ILE:O	2.06	0.55
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.42	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.36	0.55
1:B:38:ASN:HD21	1:B:41:GLU:H	1.53	0.55
1:B:134:LEU:HD12	1:B:134:LEU:H	1.69	0.55
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.22	0.55
1:B:833:ALA:HB1	1:B:858:ILE:O	2.06	0.55
1:C:304:GLU:C	1:C:305:ILE:HG13	2.26	0.55
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.22	0.55
1:C:531:ARG:O	1:C:561:ARG:NH1	2.39	0.55
1:A:140:ARG:NH1	1:A:170:GLU:OE1	2.31	0.55
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.42	0.55
1:C:18:ASN:OD1	1:C:19:PRO:HD2	2.06	0.55
1:D:304:GLU:C	1:D:305:ILE:HG13	2.26	0.55
1:B:304:GLU:C	1:B:305:ILE:HG13	2.26	0.55
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.55
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.41	0.55
1:A:942:ARG:HA	1:A:953:GLY:O	2.07	0.55
1:C:942:ARG:HA	1:C:953:GLY:O	2.07	0.55
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.36	0.55
1:C:786:ARG:HA	1:C:964:GLN:OE1	2.07	0.55
1:D:577:LYS:O	1:D:584:PRO:HA	2.06	0.55
1:D:668:VAL:HG13	1:D:669:PRO:HD2	1.89	0.55
1:D:833:ALA:HB1	1:D:858:ILE:O	2.06	0.55
1:C:577:LYS:O	1:C:584:PRO:HA	2.06	0.54
1:D:531:ARG:O	1:D:561:ARG:NH1	2.39	0.54
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.11	0.54



Atom 1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:786:ARG:HA	1:A:964:GLN:OE1	2.07	0.54
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.89	0.54
1:C:749:ILE:O	1:C:755:ARG:HG3	2.07	0.54
1:A:749:ILE:O	1:A:755:ARG:HG3	2.08	0.54
1:B:942:ARG:HA	1:B:953:GLY:O	2.07	0.54
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.42	0.54
1:B:786:ARG:HA	1:B:964:GLN:OE1	2.07	0.54
1:B:894:ARG:NH1	1:B:919:ASP:OD1	2.34	0.54
1:D:26:ARG:HD2	1:D:169:SER:HA	1.87	0.54
1:A:746:ASP:HA	1:A:760:ARG:CG	2.22	0.54
1:B:79:PRO:N	1:B:80:GLU:OE2	2.41	0.54
1:D:79:PRO:N	1:D:80:GLU:OE2	2.41	0.54
1:D:942:ARG:HA	1:D:953:GLY:O	2.07	0.54
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.74	0.54
1:A:134:LEU:HD12	1:A:134:LEU:H	1.69	0.54
1:C:79:PRO:N	1:C:80:GLU:OE2	2.41	0.54
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.11	0.54
1:D:759:ASN:OD1	1:D:761:GLN:N	2.35	0.54
1:A:79:PRO:N	1:A:80:GLU:OE2	2.41	0.54
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.22	0.54
1:A:418:HIS:O	1:D:282:ARG:HD3	2.08	0.54
1:B:29:ALA:HA	3:B:4295:HOH:O	2.07	0.54
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.38	0.54
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.89	0.54
1:D:38:ASN:ND2	1:D:41:GLU:N	2.48	0.54
1:D:749:ILE:O	1:D:755:ARG:HG3	2.08	0.54
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.38	0.54
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.11	0.54
1:C:38:ASN:HD21	1:C:41:GLU:H	1.53	0.54
1:C:80:GLU:H	1:C:80:GLU:CD	2.01	0.54
1:D:29:ALA:HA	3:D:4347:HOH:O	2.07	0.54
1:C:30:HIS:HB2	1:C:31:PRO:CD	2.38	0.54
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.91	0.54
1:C:903[A]:GLN:HB2	3:C:4239:HOH:O	2.08	0.54
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.54
1:D:786:ARG:HA	1:D:964:GLN:OE1	2.07	0.54
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.89	0.53
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.38	0.53
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.11	0.53
1:B:749:ILE:O	1:B:755:ARG:HG3	2.07	0.53
1:A:29:ALA:HA	3:A:4347:HOH:O	2.07	0.53



Atom_1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:A:357:HIS:HD2	1:A:392:TYR:OH	1.91	0.53
1:A:903[A]:GLN:HB2	3:A:4157:HOH:O	2.09	0.53
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.09	0.53
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.38	0.53
1:B:1017:GLN:O	1:B:1018:LEU:HD23	2.09	0.53
1:B:742:THR:HG22	1:B:743:SER:H	1.74	0.53
1:C:6:SER:OG	1:C:9:VAL:HB	2.09	0.53
1:C:110:ASN:O	1:C:113:PHE:N	2.39	0.53
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.53
1:C:894:ARG:NH1	1:C:919:ASP:OD1	2.34	0.53
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.92	0.53
1:D:597:ASN:HD22	1:D:599:ARG:N	1.94	0.53
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.11	0.53
1:D:696:LEU:HD12	1:D:697:THR:H	1.74	0.53
1:A:959:ILE:HG23	1:A:959:ILE:O	2.09	0.53
1:B:597:ASN:HD22	1:B:599:ARG:N	1.94	0.53
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.44	0.53
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.38	0.53
1:A:6:SER:OG	1:A:9:VAL:HB	2.09	0.52
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.09	0.52
1:C:29:ALA:HA	3:C:4335:HOH:O	2.07	0.52
1:C:416:GLU:OE1	1:C:461:GLU:HG3	2.09	0.52
1:D:416:GLU:OE1	1:D:461:GLU:HG3	2.09	0.52
1:C:696:LEU:HD12	1:C:697:THR:H	1.74	0.52
1:C:959:ILE:HG23	1:C:959:ILE:O	2.09	0.52
1:C:1017:GLN:O	1:C:1018:LEU:HD23	2.09	0.52
1:D:742:THR:HG22	1:D:743:SER:H	1.74	0.52
1:A:416:GLU:OE1	1:A:461:GLU:HG3	2.09	0.52
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.39	0.52
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.09	0.52
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.25	0.52
1:A:696:LEU:HD12	1:A:697:THR:H	1.74	0.52
1:B:959:ILE:HG23	1:B:959:ILE:O	2.09	0.52
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.09	0.52
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.09	0.52
1:D:808:GLU:HA	1:D:808:GLU:OE1	2.10	0.52
1:B:696:LEU:HD12	1:B:697:THR:H	1.74	0.52
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.74	0.52
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.44	0.52
1:A:749:ILE:HD12	1:A:749:ILE:N	2.25	0.52
1:B:251:ARG:NH1	1:B:251:ARG:HG2	2.25	0.52



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:749:ILE:N	1:C:749:ILE:HD12	2.25	0.52
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.10	0.52
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.91	0.52
1:B:436:MET:HE3	1:B:467:ASN:HD22	1.72	0.52
1:A:742:THR:HG22	1:A:743:SER:H	1.74	0.52
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.10	0.52
1:D:749:ILE:HD12	1:D:749:ILE:N	2.25	0.52
1:D:1017:GLN:O	1:D:1018:LEU:HD23	2.09	0.52
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.38	0.52
1:B:903[A]:GLN:HB2	3:B:4199:HOH:O	2.08	0.52
1:D:110:ASN:O	1:D:113:PHE:N	2.39	0.52
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.43	0.52
1:B:130:ASP:OD2	1:B:132:SER:OG	2.28	0.52
1:B:770:ILE:O	1:B:770:ILE:HG22	2.10	0.52
1:D:6:SER:OG	1:D:9:VAL:HB	2.09	0.52
1:D:130:ASP:OD2	1:D:132:SER:OG	2.28	0.52
1:D:148:SER:HB3	1:D:190:ARG:O	2.10	0.52
1:A:654:TRP:CE2	1:A:666:GLY:HA3	2.44	0.51
1:B:6:SER:OG	1:B:9:VAL:HB	2.09	0.51
1:C:742:THR:HG22	1:C:743:SER:H	1.74	0.51
1:D:542:MET:HA	1:D:604:ASN:HA	1.92	0.51
1:B:148:SER:HB3	1:B:190:ARG:O	2.10	0.51
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.92	0.51
1:B:749:ILE:N	1:B:749:ILE:HD12	2.25	0.51
1:C:878:HIS:HB3	1:C:1009:LEU:O	2.10	0.51
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.44	0.51
1:B:808:GLU:HA	1:B:808:GLU:OE1	2.10	0.51
1:C:542:MET:HA	1:C:604:ASN:HA	1.92	0.51
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.11	0.51
1:B:416:GLU:OE1	1:B:461:GLU:HG3	2.09	0.51
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.10	0.51
1:D:959:ILE:HG23	1:D:959:ILE:O	2.09	0.51
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.25	0.51
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.10	0.51
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.41	0.51
1:C:531:ARG:HB3	1:C:532:PRO:HD2	1.92	0.51
1:A:130:ASP:OD2	1:A:132:SER:OG	2.28	0.51
1:A:531:ARG:HB3	1:A:532:PRO:HD2	1.92	0.51
1:A:808:GLU:OE1	1:A:808:GLU:HA	2.10	0.51
1:C:38:ASN:ND2	1:C:41:GLU:N	2.48	0.51
1:D:230:ARG:HH11	1:D:230:ARG:CG	2.24	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:903[A]:GLN:HB2	3:D:4157:HOH:O	2.08	0.51
1:A:26:ARG:CD	1:A:169:SER:HB3	2.41	0.51
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.14	0.51
1:B:822:LEU:HD12	1:B:824:GLN:H	1.76	0.51
1:C:148:SER:HB3	1:C:190:ARG:O	2.10	0.51
1:A:254:LEU:O	1:A:255:ARG:NH1	2.44	0.51
1:A:894:ARG:HD3	1:A:919:ASP:OD1	2.11	0.51
1:A:906:TYR:HB3	1:A:907:PRO:CD	2.41	0.51
1:C:597:ASN:HD22	1:C:599:ARG:N	1.94	0.51
1:B:26:ARG:CD	1:B:169:SER:HB3	2.41	0.51
1:B:254:LEU:O	1:B:255:ARG:NH1	2.44	0.51
1:A:38:ASN:ND2	1:A:41:GLU:N	2.48	0.51
1:A:770:ILE:O	1:A:770:ILE:HG22	2.10	0.50
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.41	0.50
1:C:26:ARG:CD	1:C:169:SER:HB3	2.41	0.50
1:C:95:TYR:CD1	1:C:95:TYR:N	2.79	0.50
1:D:254:LEU:O	1:D:255:ARG:NH1	2.44	0.50
1:D:894:ARG:NH1	1:D:919:ASP:OD1	2.34	0.50
1:A:134:LEU:N	1:A:134:LEU:CD1	2.73	0.50
1:A:282:ARG:CG	1:D:423:MET:HB2	2.42	0.50
1:B:542:MET:HA	1:B:604:ASN:HA	1.92	0.50
1:D:65:ALA:HB1	1:D:66:PRO:CD	2.41	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.50
1:D:531:ARG:HB3	1:D:532:PRO:HD2	1.92	0.50
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.47	0.50
1:A:836:ILE:HG22	1:A:837:THR:N	2.26	0.50
1:D:822:LEU:HD12	1:D:824:GLN:H	1.76	0.50
1:D:906:TYR:HB3	1:D:907:PRO:CD	2.41	0.50
1:A:38:ASN:HD21	1:A:41:GLU:H	1.53	0.50
1:A:767:GLN:CG	1:A:768:MET:N	2.75	0.50
1:B:134:LEU:N	1:B:134:LEU:CD1	2.73	0.50
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.24	0.50
1:D:770:ILE:HG22	1:D:770:ILE:O	2.10	0.50
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.47	0.50
1:D:26:ARG:CD	1:D:169:SER:HB3	2.41	0.50
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.24	0.50
1:A:542:MET:HA	1:A:604:ASN:HA	1.92	0.50
1:A:662:PRO:C	1:A:663:LEU:HD23	2.32	0.50
1:B:662:PRO:C	1:B:663:LEU:HD23	2.32	0.50
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.47	0.50
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.47	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.47	0.50
1:B:65:ALA:HB1	1:B:66:PRO:CD	2.41	0.50
1:B:882:ILE:O	1:B:882:ILE:HG22	2.12	0.50
1:A:652:LEU:HD12	1:A:699:ARG:O	2.12	0.50
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.47	0.50
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.16	0.50
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.24	0.50
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.47	0.50
1:B:433:LEU:O	1:B:437:SER:HB3	2.12	0.50
1:B:836:ILE:HG22	1:B:837:THR:N	2.26	0.50
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.47	0.50
1:C:360:HIS:CG	1:C:361:PRO:HD2	2.47	0.50
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.50
1:B:894:ARG:HD3	1:B:919:ASP:OD1	2.11	0.50
1:C:662:PRO:C	1:C:663:LEU:HD23	2.32	0.50
1:D:95:TYR:CD1	1:D:95:TYR:N	2.79	0.50
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.47	0.50
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.11	0.50
1:C:433:LEU:O	1:C:437:SER:HB3	2.12	0.49
1:A:148:SER:HB3	1:A:190:ARG:O	2.10	0.49
1:C:30:HIS:ND1	1:C:31:PRO:O	2.40	0.49
1:C:254:LEU:O	1:C:255:ARG:NH1	2.44	0.49
1:C:822:LEU:HD12	1:C:824:GLN:H	1.76	0.49
1:A:12:GLN:HG3	1:A:13:ARG:N	2.27	0.49
1:A:638:VAL:O	1:A:677:LYS:HA	2.12	0.49
1:A:822:LEU:HD12	1:A:824:GLN:H	1.76	0.49
1:B:767:GLN:CG	1:B:768:MET:N	2.75	0.49
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.16	0.49
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.25	0.49
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.48	0.49
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.42	0.49
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.47	0.49
1:D:882:ILE:O	1:D:882:ILE:HG22	2.12	0.49
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.41	0.49
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.43	0.49
1:B:638:VAL:O	1:B:677:LYS:HA	2.12	0.49
1:B:763:GLY:CA	1:B:822:LEU:HD21	2.42	0.49
1:C:153:TRP:HA	1:C:157:ARG:O	2.13	0.49
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.43	0.49
1:C:595:THR:HG23	1:C:596:PRO:CA	2.43	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:638:VAL:O	1:C:677:LYS:HA	2.12	0.49
1:C:770:ILE:O	1:C:770:ILE:HG22	2.10	0.49
1:D:12:GLN:HG3	1:D:13:ARG:N	2.27	0.49
1:D:595:THR:HG23	1:D:596:PRO:CA	2.43	0.49
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.16	0.49
1:A:95:TYR:CD1	1:A:95:TYR:N	2.79	0.49
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.48	0.49
1:A:153:TRP:HA	1:A:157:ARG:O	2.13	0.49
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.48	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:B:652:LEU:HD12	1:B:699:ARG:O	2.12	0.49
1:A:110:ASN:O	1:A:113:PHE:N	2.39	0.49
1:A:200:GLN:OE1	1:A:200:GLN:N	2.44	0.49
1:C:660:GLY:O	1:C:662:PRO:HD3	2.13	0.49
1:C:763:GLY:CA	1:C:822:LEU:HD21	2.42	0.49
1:D:660:GLY:O	1:D:662:PRO:HD3	2.13	0.49
1:A:660:GLY:O	1:A:662:PRO:HD3	2.13	0.49
1:B:12:GLN:HG3	1:B:13:ARG:N	2.27	0.49
1:C:143:PHE:CD1	1:C:143:PHE:N	2.81	0.49
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.47	0.49
1:D:767:GLN:CG	1:D:768:MET:N	2.75	0.49
1:C:130:ASP:OD2	1:C:132:SER:OG	2.28	0.49
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.48	0.49
1:C:830:LEU:HD22	1:C:835:LEU:HB2	1.95	0.49
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.41	0.49
1:C:938:ARG:NH2	3:C:4307:HOH:O	2.45	0.49
1:D:652:LEU:HD12	1:D:699:ARG:O	2.12	0.49
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.39	0.49
1:B:595:THR:HG23	1:B:596:PRO:CA	2.43	0.49
1:B:938:ARG:NH2	3:B:4267:HOH:O	2.45	0.49
1:C:134:LEU:N	1:C:134:LEU:CD1	2.73	0.49
1:D:662:PRO:C	1:D:663:LEU:HD23	2.32	0.49
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.42	0.49
1:D:836:ILE:HG22	1:D:837:THR:N	2.26	0.49
1:A:143:PHE:N	1:A:143:PHE:CD1	2.81	0.48
1:A:433:LEU:O	1:A:437:SER:HB3	2.12	0.48
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.46	0.48
1:B:646:HIS:O	1:B:648:ASP:N	2.47	0.48
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.48	0.48
1:C:835:LEU:CD1	1:C:857:ARG:HB2	2.43	0.48
1:C:836:ILE:HG22	1:C:837:THR:N	2.26	0.48



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.16	0.48
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.48
1:C:882:ILE:HG22	1:C:882:ILE:O	2.12	0.48
1:A:787:ALA:HA	1:A:788:PRO:HD3	1.66	0.48
1:C:12:GLN:HG3	1:C:13:ARG:N	2.27	0.48
1:C:652:LEU:HD12	1:C:699:ARG:O	2.12	0.48
1:D:143:PHE:N	1:D:143:PHE:CD1	2.81	0.48
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.48
1:A:835:LEU:CD1	1:A:857:ARG:HB2	2.43	0.48
1:B:597:ASN:ND2	1:B:599:ARG:N	2.48	0.48
1:B:651:LEU:HD12	1:B:651:LEU:HA	1.46	0.48
1:B:660:GLY:O	1:B:662:PRO:HD3	2.13	0.48
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.44	0.48
1:B:835:LEU:CD1	1:B:857:ARG:HB2	2.43	0.48
1:D:433:LEU:O	1:D:437:SER:HB3	2.12	0.48
1:D:646:HIS:O	1:D:648:ASP:N	2.47	0.48
1:C:26:ARG:HD3	1:C:169:SER:HB3	1.96	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.65	0.48
1:C:257:THR:OG1	1:C:316:HIS:HE1	1.97	0.48
1:D:651:LEU:HD12	1:D:651:LEU:HA	1.46	0.48
1:A:595:THR:HG23	1:A:596:PRO:CA	2.43	0.48
1:A:651:LEU:HD23	1:A:653[A]:HIS:HE1	1.79	0.48
1:B:257:THR:OG1	1:B:316:HIS:HE1	1.97	0.48
1:C:646:HIS:O	1:C:648:ASP:N	2.46	0.48
1:C:651:LEU:HD23	1:C:653[A]:HIS:HE1	1.79	0.48
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.96	0.48
1:D:30:HIS:ND1	1:D:31:PRO:O	2.40	0.48
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.79	0.48
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.49	0.48
1:A:513:PRO:O	1:A:514:ALA:HB3	2.14	0.48
1:A:597:ASN:ND2	1:A:599:ARG:N	2.48	0.48
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.14	0.48
1:A:646:HIS:O	1:A:648:ASP:N	2.46	0.48
1:A:894:ARG:NH1	1:A:919:ASP:OD1	2.34	0.48
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.62	0.48
1:C:599:ARG:HD2	1:C:600:GLN:OE1	2.14	0.48
1:C:856:TYR:HD2	1:C:864:MET:CE	2.27	0.48
1:A:257:THR:OG1	1:A:316:HIS:HE1	1.97	0.48
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.43	0.48
1:B:26:ARG:HD3	1:B:169:SER:HB3	1.96	0.48
1:B:143:PHE:CD1	1:B:143:PHE:N	2.81	0.48



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:147:ASN:HA	1:B:148:SER:HA	1.65	0.48
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.44	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:A:30:HIS:ND1	1:A:31:PRO:O	2.40	0.47
1:B:67:GLU:HG2	1:B:67:GLU:H	1.15	0.47
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.49	0.47
1:B:970:THR:CG2	1:B:975:LEU:HB2	2.44	0.47
1:C:573:GLN:HB2	1:C:602:CYS:O	2.14	0.47
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.49	0.47
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.47	0.47
1:A:668:VAL:HA	1:A:669:PRO:HD3	1.66	0.47
1:A:701:VAL:CG1	1:A:702:GLN:N	2.77	0.47
1:C:742:THR:CG2	1:C:743:SER:N	2.77	0.47
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.43	0.47
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.96	0.47
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.49	0.47
1:C:210:ARG:NH1	1:C:358:GLU:OE1	2.47	0.47
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.62	0.47
1:D:668:VAL:CG1	1:D:669:PRO:HD2	2.44	0.47
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.95	0.47
1:A:292:ARG:C	1:A:293:LEU:HD23	2.35	0.47
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.62	0.47
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.47
1:A:830:LEU:HD22	1:A:835:LEU:HB2	1.95	0.47
1:A:882:ILE:HG22	1:A:882:ILE:O	2.12	0.47
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.48	0.47
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.97	0.47
1:D:210:ARG:NH1	1:D:358:GLU:OE1	2.47	0.47
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.14	0.47
1:A:18:ASN:HA	1:A:19:PRO:HD3	1.56	0.47
1:A:423:MET:HB2	1:D:282:ARG:CG	2.43	0.47
1:A:856:TYR:HD2	1:A:864:MET:CE	2.27	0.47
1:A:970:THR:CG2	1:A:975:LEU:HB2	2.44	0.47
1:B:251:ARG:HG2	1:B:251:ARG:HH11	1.79	0.47
1:C:701:VAL:CG1	1:C:702:GLN:N	2.77	0.47
1:D:635:THR:OG1	1:D:681:GLU:HG3	2.15	0.47
1:D:651:LEU:HD23	1:D:653[A]:HIS:HE1	1.79	0.47
1:A:26:ARG:HD3	1:A:169:SER:HB3	1.96	0.47
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.97	0.47
1:B:110:ASN:O	1:B:113:PHE:N	2.39	0.47
1:B:651:LEU:HD23	1:B:653[A]:HIS:HE1	1.79	0.47



Atom-1	Atom-2	Interatomic	Clash
1100111-1	1100111-2	distance (Å)	overlap (Å)
1:B:780:LEU:HA	1:B:886:CYS:HB3	1.97	0.47
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.96	0.47
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.97	0.47
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:B:599:ARG:HD2	1:B:600:GLN:OE1	2.14	0.47
1:B:701:VAL:CG1	1:B:702:GLN:N	2.78	0.47
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.61	0.47
1:C:513:PRO:O	1:C:514:ALA:HB3	2.14	0.47
1:C:661:LYS:HA	1:C:662:PRO:HD2	1.71	0.47
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.44	0.47
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.97	0.47
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.43	0.47
1:D:830:LEU:HD22	1:D:835:LEU:HB2	1.95	0.47
1:D:938:ARG:NH2	3:D:4279:HOH:O	2.45	0.47
1:D:970:THR:CG2	1:D:975:LEU:HB2	2.44	0.47
1:A:80:GLU:OE2	1:A:80:GLU:N	2.29	0.47
1:A:261:TRP:CD1	1:A:261:TRP:N	2.83	0.47
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.62	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.77	0.47
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.80	0.47
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.47
1:C:292:ARG:C	1:C:293:LEU:HD23	2.35	0.47
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.79	0.47
1:A:849:LEU:N	1:A:849:LEU:HD23	2.30	0.47
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.96	0.47
1:B:830:LEU:HD22	1:B:835:LEU:HB2	1.95	0.47
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.50	0.47
1:A:282:ARG:NH1	1:D:419:GLY:C	2.68	0.46
1:A:419:GLY:C	1:D:282:ARG:NH1	2.68	0.46
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.50	0.46
1:B:200:GLN:OE1	1:B:200:GLN:N	2.44	0.46
1:B:272:ALA:HB1	1:B:273:PRO:CD	2.43	0.46
1:D:441:THR:HG22	1:D:474:TRP:CH2	2.50	0.46
1:D:573:GLN:HB2	1:D:602:CYS:O	2.14	0.46
1:D:701:VAL:CG1	1:D:702:GLN:N	2.77	0.46
1:B:95:TYR:N	1:B:95:TYR:CD1	2.79	0.46
1:B:292:ARG:C	1:B:293:LEU:HD23	2.35	0.46
1:B:513:PRO:O	1:B:514:ALA:HB3	2.14	0.46
1:B:573:GLN:HB2	1:B:602:CYS:O	2.14	0.46
1:C:234:ASP:O	1:C:235:PHE:HB2	2.15	0.46
1:C:635:THR:OG1	1:C:681:GLU:HG3	2.15	0.46



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:230:ARG:HH11	1:D:230:ARG:HG2	1.81	0.46
1:D:234:ASP:O	1:D:235:PHE:HB2	2.15	0.46
1:D:292:ARG:C	1:D:293:LEU:HD23	2.35	0.46
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.81	0.46
1:A:282:ARG:HG2	1:D:423:MET:HB2	1.97	0.46
1:A:429:ASP:OD1	1:A:431[A]:ARG:HG3	2.16	0.46
1:B:202:MET:HE3	1:B:357:HIS:CD2	2.50	0.46
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.16	0.46
1:D:834:VAL:CG1	1:D:835:LEU:N	2.79	0.46
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.63	0.46
1:B:226:HIS:CD2	1:B:226:HIS:N	2.83	0.46
1:B:429:ASP:OD1	1:B:431[A]:ARG:HG3	2.16	0.46
1:B:429:ASP:HA	1:B:430:PRO:HD3	1.82	0.46
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.46
1:C:226:HIS:N	1:C:226:HIS:CD2	2.83	0.46
1:C:227:VAL:HG12	1:C:228:ALA:N	2.31	0.46
1:C:1018:LEU:HD23	1:C:1018:LEU:HA	1.53	0.46
1:D:261:TRP:CD1	1:D:261:TRP:N	2.83	0.46
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.51	0.46
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.36	0.46
1:B:234:ASP:O	1:B:235:PHE:HB2	2.15	0.46
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.50	0.46
1:C:11:LEU:CD2	1:C:187:MET:HE3	2.45	0.46
1:C:84:VAL:HG13	1:C:85:VAL:N	2.31	0.46
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.80	0.46
1:D:200:GLN:OE1	1:D:200:GLN:N	2.44	0.46
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.69	0.46
1:A:423:MET:HB2	1:D:282:ARG:HG2	1.97	0.46
1:A:742:THR:CG2	1:A:743:SER:N	2.77	0.46
1:B:166:ARG:HG3	1:B:392:TYR:CG	2.51	0.46
1:B:254:LEU:C	1:B:255:ARG:HG2	2.36	0.46
1:B:261:TRP:CD1	1:B:261:TRP:N	2.83	0.46
1:C:261:TRP:CD1	1:C:261:TRP:N	2.83	0.46
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.96	0.46
1:C:620:ALA:O	1:C:624:GLN:HG3	2.16	0.46
1:D:597:ASN:ND2	1:D:599:ARG:N	2.48	0.46
1:D:630:ARG:HE	1:D:630:ARG:HB3	1.31	0.46
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.78	0.46
1:B:620:ALA:O	1:B:624:GLN:HG3	2.16	0.46
1:B:635:THR:OG1	1:B:681:GLU:HG3	2.15	0.46
1:B:849:LEU:N	1:B:849:LEU:HD23	2.30	0.46



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.16	0.46
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.51	0.46
1:D:227:VAL:HG12	1:D:228:ALA:N	2.31	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.46
1:A:679:LEU:HA	1:A:679:LEU:HD23	1.13	0.46
1:B:111:PRO:HA	1:B:112:PRO:HA	1.57	0.46
1:B:369:GLU:O	1:B:373:VAL:HG23	2.16	0.46
1:B:742:THR:CG2	1:B:743:SER:N	2.77	0.46
1:B:834:VAL:CG1	1:B:835:LEU:N	2.79	0.46
1:B:856:TYR:HD2	1:B:864:MET:CE	2.27	0.46
1:C:141:ILE:CG1	1:C:142:ILE:N	2.79	0.46
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.36	0.46
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.80	0.46
1:D:316:HIS:HB2	1:D:321:THR:O	2.16	0.46
1:D:701:VAL:O	1:D:703:PRO:HD3	2.16	0.46
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.31	0.46
1:A:881:ARG:HD3	1:A:987:ASP:CG	2.36	0.46
1:B:701:VAL:O	1:B:703:PRO:HD3	2.16	0.46
1:C:441:THR:HG22	1:C:474:TRP:CH2	2.50	0.46
1:D:254:LEU:C	1:D:255:ARG:HG2	2.36	0.46
1:D:658:LEU:O	1:D:659:ASP:C	2.54	0.46
1:D:870:VAL:CG1	1:D:871:GLU:N	2.79	0.46
1:A:141:ILE:CG1	1:A:142:ILE:N	2.79	0.46
1:A:369:GLU:O	1:A:373:VAL:HG23	2.16	0.46
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.31	0.46
1:B:168:PRO:O	1:B:442:ARG:NH2	2.48	0.46
1:B:870:VAL:CG1	1:B:871:GLU:N	2.79	0.46
1:B:881:ARG:HD3	1:B:987:ASP:CG	2.36	0.46
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.51	0.46
1:D:84:VAL:HG13	1:D:85:VAL:N	2.31	0.46
1:A:234:ASP:O	1:A:235:PHE:HB2	2.15	0.45
1:A:254:LEU:C	1:A:255:ARG:HG2	2.36	0.45
1:B:3:ILE:O	1:B:3:ILE:HD12	2.16	0.45
1:B:316:HIS:HB2	1:B:321:THR:O	2.16	0.45
1:C:230:ARG:HH11	1:C:230:ARG:HG2	1.81	0.45
1:C:403:ASP:CG	1:C:451:PRO:HD2	2.36	0.45
1:C:834:VAL:CG1	1:C:835:LEU:N	2.79	0.45
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.52	0.45
1:D:856:TYR:HD2	1:D:864:MET:CE	2.27	0.45
1:A:3:ILE:HD12	1:A:3:ILE:O	2.16	0.45
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.32	0.45



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:226:HIS:CD2	1:A:226:HIS:N	2.83	0.45
1:A:441:THR:HG22	1:A:474:TRP:CH2	2.50	0.45
1:A:658:LEU:O	1:A:659:ASP:C	2.54	0.45
1:A:938:ARG:NH2	3:A:4279:HOH:O	2.45	0.45
1:B:38:ASN:ND2	1:B:41:GLU:HG3	2.31	0.45
1:B:80:GLU:OE2	1:B:80:GLU:N	2.29	0.45
1:B:403:ASP:CG	1:B:451:PRO:HD2	2.36	0.45
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	1.53	0.45
1:C:242:ALA:O	1:C:290:THR:HA	2.16	0.45
1:C:701:VAL:O	1:C:703:PRO:HD3	2.16	0.45
1:D:226:HIS:N	1:D:226:HIS:CD2	2.83	0.45
1:D:369:GLU:O	1:D:373:VAL:HG23	2.16	0.45
1:D:881:ARG:HD3	1:D:987:ASP:CG	2.36	0.45
1:D:908:ASP:HB3	1:D:1007:PHE:CD1	2.52	0.45
1:D:945:ASN:OD1	1:D:950:GLN:HB2	2.16	0.45
1:A:227:VAL:HG12	1:A:228:ALA:N	2.31	0.45
1:A:701:VAL:O	1:A:703:PRO:HD3	2.16	0.45
1:A:834:VAL:CG1	1:A:835:LEU:N	2.79	0.45
1:A:1018:LEU:HD23	1:A:1018:LEU:HA	1.53	0.45
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.45
1:B:757:GLN:HG2	1:B:758:PHE:N	2.31	0.45
1:B:832:ASP:OD1	1:B:832:ASP:N	2.50	0.45
1:C:230:ARG:CG	1:C:230:ARG:NH1	2.79	0.45
1:C:369:GLU:O	1:C:373:VAL:HG23	2.16	0.45
1:D:531:ARG:CB	1:D:532:PRO:HD2	2.46	0.45
1:A:84:VAL:HG13	1:A:85:VAL:N	2.31	0.45
1:A:202:MET:HE3	1:A:357:HIS:CD2	2.52	0.45
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.61	0.45
1:A:242:ALA:O	1:A:290:THR:HA	2.16	0.45
1:A:524:LEU:HB2	3:A:4198:HOH:O	2.16	0.45
1:A:620:ALA:O	1:A:624:GLN:HG3	2.16	0.45
1:B:141:ILE:CG1	1:B:142:ILE:N	2.79	0.45
1:B:242:ALA:O	1:B:290:THR:HA	2.16	0.45
1:B:352:ARG:O	1:B:385:ASN:HB2	2.17	0.45
1:B:531:ARG:CB	1:B:532:PRO:HD2	2.46	0.45
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.39	0.45
1:C:67:GLU:HG2	1:C:67:GLU:H	1.15	0.45
1:C:80:GLU:OE2	1:C:80:GLU:N	2.29	0.45
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.79	0.45
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.45
1:D:3:ILE:HD12	1:D:3:ILE:O	2.16	0.45



Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.45	0.45
1:D:620:ALA:O	1:D:624:GLN:HG3	2.16	0.45
1:A:352:ARG:O	1:A:385:ASN:HB2	2.17	0.45
1:A:559:TYR:HA	1:A:560:PRO:HD2	1.85	0.45
1:A:915:PHE:O	1:A:916:ASP:HB2	2.17	0.45
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.45
1:B:679:LEU:HA	1:B:679:LEU:HD23	1.13	0.45
1:C:38:ASN:ND2	1:C:41:GLU:HG3	2.32	0.45
1:C:63:PHE:HB3	1:C:64:PRO:CD	2.45	0.45
1:C:531:ARG:CB	1:C:532:PRO:HD2	2.46	0.45
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.36	0.45
1:B:227:VAL:HG12	1:B:228:ALA:N	2.31	0.45
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.50	0.45
1:B:650:GLU:HA	1:B:701:VAL:O	2.17	0.45
1:D:111:PRO:HA	1:D:112:PRO:HA	1.56	0.45
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.51	0.45
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.45
1:A:945:ASN:OD1	1:A:950:GLN:HB2	2.16	0.45
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.95	0.45
1:B:878:HIS:HA	1:B:879:PRO:HD3	1.69	0.45
1:C:524:LEU:HB2	3:C:4262:HOH:O	2.16	0.45
1:C:650:GLU:HA	1:C:701:VAL:O	2.17	0.45
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.45
1:D:38:ASN:ND2	1:D:41:GLU:HG3	2.32	0.45
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.80	0.45
1:D:757:GLN:HG2	1:D:758:PHE:N	2.31	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.45
1:B:84:VAL:HG13	1:B:85:VAL:N	2.31	0.45
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.99	0.45
1:B:894:ARG:NH2	1:B:921:PRO:HD3	2.31	0.45
1:C:3:ILE:HD12	1:C:3:ILE:O	2.16	0.45
1:C:730:LEU:H	1:C:730:LEU:HG	1.41	0.45
1:C:832:ASP:OD1	1:C:832:ASP:N	2.49	0.45
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.45
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.80	0.45
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.69	0.45
1:B:255:ARG:NH1	1:B:255:ARG:CG	2.79	0.45
1:B:915:PHE:O	1:B:916:ASP:HB2	2.17	0.45
1:C:849:LEU:N	1:C:849:LEU:HD23	2.30	0.45
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	2.16	0.45
1:D:524:LEU:HB2	3:D:4198:HOH:O	2.16	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:77:ASP:C	1:A:78:LEU:HD23	2.37	0.45
1:A:399:TYR:CD1	1:A:399:TYR:N	2.85	0.45
1:B:230:ARG:HH11	1:B:230:ARG:HG2	1.81	0.45
1:B:599:ARG:HB2	1:B:600:GLN:H	1.54	0.45
1:C:77:ASP:C	1:C:78:LEU:HD23	2.37	0.45
1:C:945:ASN:OD1	1:C:950:GLN:HB2	2.16	0.45
1:D:441:THR:HG22	1:D:474:TRP:CZ3	2.52	0.45
1:D:832:ASP:OD1	1:D:832:ASP:N	2.50	0.45
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.99	0.44
1:B:38:ASN:ND2	1:B:41:GLU:N	2.48	0.44
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.99	0.44
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.61	0.44
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.44
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	0.44
1:C:352:ARG:O	1:C:385:ASN:HB2	2.17	0.44
1:C:399:TYR:CD1	1:C:399:TYR:N	2.85	0.44
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.52	0.44
1:D:230:ARG:CG	1:D:230:ARG:NH1	2.79	0.44
1:D:352:ARG:O	1:D:385:ASN:HB2	2.17	0.44
1:D:1018:LEU:HD23	1:D:1018:LEU:HA	1.53	0.44
1:A:78:LEU:HB3	1:A:80:GLU:OE2	2.18	0.44
1:A:531:ARG:CB	1:A:532:PRO:HD2	2.46	0.44
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.52	0.44
1:B:136:GLU:O	1:B:216:HIS:HE1	2.01	0.44
1:C:18:ASN:HA	1:C:19:PRO:HD3	1.56	0.44
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.51	0.44
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.44
1:C:668:VAL:HA	1:C:669:PRO:HD3	1.66	0.44
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.31	0.44
1:D:141:ILE:CG1	1:D:142:ILE:N	2.79	0.44
1:D:650:GLU:HA	1:D:701:VAL:O	2.17	0.44
1:A:230:ARG:CG	1:A:230:ARG:NH1	2.79	0.44
1:A:708:TRP:CD1	1:A:708:TRP:N	2.85	0.44
1:A:870:VAL:CG1	1:A:871:GLU:N	2.79	0.44
1:A:989:PHE:CD1	1:A:989:PHE:N	2.86	0.44
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.52	0.44
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.36	0.44
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.52	0.44
1:C:316:HIS:HB2	1:C:321:THR:O	2.16	0.44
1:C:870:VAL:CG1	1:C:871:GLU:N	2.79	0.44
1:C:881:ARG:HD3	1:C:987:ASP:OD2	2.17	0.44



A 4 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:849:LEU:N	1:D:849:LEU:HD23	2.30	0.44
1:A:136:GLU:O	1:A:216:HIS:HE1	2.01	0.44
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.36	0.44
1:B:77:ASP:C	1:B:78:LEU:HD23	2.37	0.44
1:B:143:PHE:O	1:B:168:PRO:HA	2.17	0.44
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.53	0.44
1:C:708:TRP:CD1	1:C:708:TRP:N	2.85	0.44
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.99	0.44
1:D:708:TRP:CD1	1:D:708:TRP:N	2.85	0.44
1:A:63:PHE:CD1	1:A:63:PHE:N	2.86	0.44
1:A:650:GLU:HA	1:A:701:VAL:O	2.17	0.44
1:B:441:THR:HG22	1:B:474:TRP:CZ3	2.52	0.44
1:B:947:GLY:HA3	1:B:948:PRO:HD2	1.89	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.51	0.44
1:C:737:ILE:HA	1:C:738:PRO:HD3	1.78	0.44
1:C:989:PHE:CD1	1:C:989:PHE:N	2.86	0.44
1:D:77:ASP:C	1:D:78:LEU:HD23	2.38	0.44
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.18	0.44
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.00	0.44
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.61	0.44
1:A:168:PRO:O	1:A:442:ARG:NH2	2.48	0.44
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.83	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.18	0.44
1:C:79:PRO:HB2	1:C:80:GLU:HG3	2.00	0.44
1:D:18:ASN:HA	1:D:19:PRO:HD3	1.56	0.44
1:D:242:ALA:O	1:D:290:THR:HA	2.16	0.44
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.51	0.44
1:B:399:TYR:CD1	1:B:399:TYR:N	2.85	0.44
1:B:524:LEU:HB2	3:B:4222:HOH:O	2.16	0.44
1:C:63:PHE:CD1	1:C:63:PHE:N	2.86	0.44
1:C:202:MET:HE3	1:C:357:HIS:CD2	2.53	0.44
1:D:136:GLU:O	1:D:216:HIS:HE1	2.01	0.44
1:B:30:HIS:CE1	1:B:33:PHE:CD1	3.06	0.44
1:B:78:LEU:HB3	1:B:80:GLU:OE2	2.18	0.44
1:C:441:THR:HG22	1:C:474:TRP:CZ3	2.52	0.44
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.44
1:A:441:THR:HG22	1:A:474:TRP:CZ3	2.52	0.44
1:B:11:LEU:CD2	1:B:187:MET:HE3	2.44	0.44
1:C:136:GLU:O	1:C:216:HIS:HE1	2.01	0.44
1:D:134:LEU:N	1:D:134:LEU:CD1	2.73	0.44
1:D:989:PHE:CD1	1:D:989:PHE:N	2.86	0.44



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:316:HIS:HB2	1:A:321:THR:O	2.16	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:A:832:ASP:OD1	1:A:832:ASP:N	2.50	0.43
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.18	0.43
1:C:145:GLY:HA3	1:C:210:ARG:HG3	2.00	0.43
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.36	0.43
1:C:915:PHE:O	1:C:916:ASP:HB2	2.17	0.43
1:A:3:ILE:C	1:A:5:ASP:H	2.22	0.43
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.06	0.43
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.48	0.43
1:B:630:ARG:HE	1:B:630:ARG:HB3	1.31	0.43
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.51	0.43
1:B:748:CYS:C	1:B:749:ILE:HD12	2.39	0.43
1:B:989:PHE:CD1	1:B:989:PHE:N	2.86	0.43
1:C:255:ARG:NH1	1:C:255:ARG:CG	2.79	0.43
1:C:597:ASN:ND2	1:C:599:ARG:N	2.48	0.43
1:D:30:HIS:CE1	1:D:33:PHE:CD1	3.06	0.43
1:D:79:PRO:HB2	1:D:80:GLU:HG3	2.00	0.43
1:D:915:PHE:O	1:D:916:ASP:HB2	2.17	0.43
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.52	0.43
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.59	0.43
1:A:742:THR:CG2	1:A:743:SER:H	2.31	0.43
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.53	0.43
1:C:3:ILE:C	1:C:5:ASP:H	2.22	0.43
1:C:634:GLN:NE2	1:C:682:LEU:O	2.51	0.43
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.43
1:D:145:GLY:HA3	1:D:210:ARG:HG3	2.00	0.43
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.36	0.43
1:A:285:TYR:OH	1:D:424:ASN:HB3	2.19	0.43
1:A:881:ARG:HD3	1:A:987:ASP:OD2	2.17	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:B:433:LEU:HB3	1:B:434:PRO:HD3	2.00	0.43
1:B:682:LEU:HA	1:B:683:PRO:HD3	1.91	0.43
1:C:168:PRO:O	1:C:442:ARG:NH2	2.48	0.43
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.43
1:C:657:ALA:O	1:C:694:LEU:HD12	2.18	0.43
1:D:399:TYR:CD1	1:D:399:TYR:N	2.85	0.43
1:D:881:ARG:HD3	1:D:987:ASP:OD2	2.18	0.43
1:A:67:GLU:HG2	1:A:67:GLU:H	1.15	0.43
1:A:79:PRO:HB2	1:A:80:GLU:HG3	2.00	0.43
1:A:143:PHE:O	1:A:168:PRO:HA	2.17	0.43



A + 1	Atom-2	Interatomic	Clash
Atom-1		distance (\AA)	overlap (Å)
1:B:79:PRO:HB2	1:B:80:GLU:HG3	2.00	0.43
1:B:145:GLY:HA3	1:B:210:ARG:HG3	2.00	0.43
1:B:742:THR:CG2	1:B:743:SER:H	2.31	0.43
1:D:11:LEU:CD2	1:D:187:MET:HE3	2.48	0.43
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.82	0.43
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.51	0.43
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.84	0.43
1:B:118:ASN:HA	1:B:119:PRO:HD2	1.61	0.43
1:B:657:ALA:O	1:B:694:LEU:HD12	2.18	0.43
1:C:176:PHE:CD1	1:C:176:PHE:N	2.87	0.43
1:C:217:LYS:HB3	1:C:218:PRO:HD2	2.00	0.43
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.57	0.43
1:C:878:HIS:HA	1:C:879:PRO:HD3	1.69	0.43
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.39	0.43
1:D:657:ALA:O	1:D:694:LEU:HD12	2.18	0.43
1:D:748:CYS:C	1:D:749:ILE:HD12	2.39	0.43
1:A:77:ASP:HA	3:A:4132:HOH:O	2.19	0.43
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.95	0.43
1:A:822:LEU:HD12	1:A:823:LEU:N	2.34	0.43
1:C:30:HIS:CE1	1:C:33:PHE:CD1	3.06	0.43
1:C:114:VAL:HA	1:C:115:PRO:HD3	1.77	0.43
1:C:200:GLN:OE1	1:C:200:GLN:N	2.44	0.43
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.82	0.43
1:C:630:ARG:HE	1:C:630:ARG:HB3	1.31	0.43
1:C:645:ARG:NH2	1:C:650:GLU:OE2	2.45	0.43
1:C:679:LEU:HA	1:C:679:LEU:HD23	1.13	0.43
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.53	0.43
1:D:787:ALA:HA	1:D:788:PRO:HD3	1.66	0.43
1:A:217:LYS:HB3	1:A:218:PRO:HD2	2.00	0.43
1:A:630:ARG:HE	1:A:630:ARG:HB3	1.31	0.43
1:A:634:GLN:NE2	1:A:682:LEU:O	2.51	0.43
1:A:730:LEU:H	1:A:730:LEU:HG	1.41	0.43
1:A:748:CYS:C	1:A:749:ILE:HD12	2.39	0.43
1:B:708:TRP:CD1	1:B:708:TRP:N	2.85	0.43
1:C:173:LEU:HD23	1:C:173:LEU:HA	1.80	0.43
1:D:354:VAL:HG22	1:D:355:ASN:N	2.34	0.43
1:D:910:LEU:HD12	1:D:910:LEU:C	2.39	0.43
1:A:105:TYR:HB3	1:A:106:PRO:HD2	2.01	0.43
1:A:251:ARG:HH11	1:A:251:ARG:CG	2.32	0.43
1:A:257:THR:HA	1:A:270:GLY:O	2.19	0.43
1:A:687:GLN:HA	1:A:688:PRO:HD3	1.82	0.43



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:227:VAL:CG1	1:B:240:LEU:HD11	2.48	0.43	
1:B:251:ARG:HH11	1:B:251:ARG:CG	2.32	0.43	
1:B:634:GLN:NE2	1:B:682:LEU:O	2.51	0.43	
1:C:734:SER:HB2	1:C:860:GLY:HA3	1.95	0.43	
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	0.43	
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.43	
1:D:685:LEU:CB	1:D:686:PRO:HD2	2.38	0.43	
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.89	0.43	
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.54	0.43	
1:B:30:HIS:ND1	1:B:31:PRO:O	2.40	0.43	
1:B:63:PHE:CD1	1:B:63:PHE:N	2.86	0.43	
1:B:187:MET:O	1:B:187:MET:HG3	2.19	0.43	
1:B:622:HIS:HD2	1:B:625:GLN:OE1	2.02	0.43	
1:C:234:ASP:OD1	1:C:236:SER:OG	2.31	0.43	
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.81	0.43	
1:C:840:HIS:ND1	1:C:840:HIS:N	2.67	0.43	
1:D:105:TYR:HB3	1:D:106:PRO:HD2	2.01	0.43	
1:D:257:THR:HA	1:D:270:GLY:O	2.19	0.43	
1:D:622:HIS:HD2	1:D:625:GLN:OE1	2.02	0.43	
1:A:11:LEU:CD2	1:A:187:MET:HE3	2.45	0.42	
1:A:145:GLY:HA3	1:A:210:ARG:HG3	2.01	0.42	
1:A:354:VAL:HG22	1:A:355:ASN:N	2.34	0.42	
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.53	0.42	
1:A:635:THR:HA	1:A:680:ILE:O	2.19	0.42	
1:A:822:LEU:HD13	1:A:822:LEU:HA	1.79	0.42	
1:B:77:ASP:HA	3:B:4178:HOH:O	2.19	0.42	
1:B:114:VAL:HA	1:B:115:PRO:HD3	1.77	0.42	
1:B:257:THR:HA	1:B:270:GLY:O	2.19	0.42	
1:B:910:LEU:C	1:B:910:LEU:HD12	2.39	0.42	
1:C:187:MET:O	1:C:187:MET:HG3	2.19	0.42	
1:D:634:GLN:NE2	1:D:682:LEU:O	2.51	0.42	
1:A:429:ASP:HA	1:A:430:PRO:HD3	1.82	0.42	
1:B:570:TRP:CD1	1:B:571:VAL:HG22	2.54	0.42	
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.66	0.42	
1:D:217:LYS:HB3	1:D:218:PRO:HD2	2.00	0.42	
1:D:225:PHE:HA	1:D:243:GLU:O	2.19	0.42	
1:A:225:PHE:HA	1:A:243:GLU:O	2.19	0.42	
1:A:657:ALA:O	1:A:694:LEU:HD12	2.18	0.42	
1:B:635:THR:HA	1:B:680:ILE:O	2.19	0.42	
1:C:183:ARG:HH11	1:C:183:ARG:HD3	1.55	0.42	
1:C:257:THR:HA	1:C:270:GLY:O	2.19	0.42	



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:367:MET:HB3	1:C:372:MET:CE	2.50	0.42
1:D:187:MET:O	1:D:187:MET:HG3	2.19	0.42
1:A:622:HIS:HD2	1:A:625:GLN:OE1	2.02	0.42
1:B:278:ILE:HD12	1:B:278:ILE:HA	1.88	0.42
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.42
1:C:227:VAL:CG1	1:C:240:LEU:HD11	2.48	0.42
1:C:576:ILE:HD13	1:C:584:PRO:HB2	2.02	0.42
1:C:822:LEU:HD12	1:C:823:LEU:N	2.34	0.42
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.73	0.42
1:D:782:ASP:OD1	1:D:854:LYS:NZ	2.52	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.20	0.42
1:A:282:ARG:NH1	1:D:418:HIS:O	2.52	0.42
1:B:52[A]:ARG:HH11	1:B:52[A]:ARG:HD3	1.65	0.42
1:B:227:VAL:CG1	1:B:228:ALA:N	2.83	0.42
1:B:737:ILE:HA	1:B:738:PRO:HD3	1.78	0.42
1:C:635:THR:HA	1:C:680:ILE:O	2.19	0.42
1:D:576:ILE:HD13	1:D:584:PRO:HB2	2.02	0.42
1:A:187:MET:O	1:A:187:MET:HG3	2.19	0.42
1:A:255:ARG:NH1	1:A:255:ARG:CG	2.79	0.42
1:A:367:MET:HB3	1:A:372:MET:CE	2.50	0.42
1:A:858:ILE:HG12	1:A:864:MET:HB3	2.02	0.42
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.42
1:C:274:PHE:HB3	1:C:286:ALA:O	2.20	0.42
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.54	0.42
1:C:742:THR:CG2	1:C:743:SER:H	2.31	0.42
1:D:367:MET:HB3	1:D:372:MET:CE	2.50	0.42
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.91	0.42
1:A:274:PHE:HB3	1:A:286:ALA:O	2.20	0.42
1:B:105:TYR:HB3	1:B:106:PRO:HD2	2.01	0.42
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.84	0.42
1:C:77:ASP:HA	3:C:4218:HOH:O	2.19	0.42
1:C:479:ASP:HA	1:C:480:PRO:HD2	1.73	0.42
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.61	0.42
1:D:570:TRP:CD1	1:D:571:VAL:HG22	2.54	0.42
1:A:910:LEU:HD12	1:A:910:LEU:C	2.39	0.42
1:B:685:LEU:CB	1:B:686:PRO:HD2	2.38	0.42
1:B:822:LEU:HD12	1:B:823:LEU:N	2.34	0.42
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.78	0.42
1:C:354:VAL:HG22	1:C:355:ASN:N	2.34	0.42
1:C:622:HIS:HD2	1:C:625:GLN:OE1	2.02	0.42



Atom_1	Atom_2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:757:GLN:HG2	1:C:758:PHE:N	2.31	0.42	
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.66	0.42	
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.32	0.42	
1:D:274:PHE:HB3	1:D:286:ALA:O	2.20	0.42	
1:D:822:LEU:HD12	1:D:823:LEU:N	2.34	0.42	
1:D:835:LEU:HA	1:D:835:LEU:HD12	1.90	0.42	
1:A:424:ASN:HD22	1:A:424:ASN:HA	1.40	0.42	
1:B:11:LEU:N	1:B:11:LEU:HD23	2.35	0.42	
1:B:217:LYS:HB3	1:B:218:PRO:HD2	2.01	0.42	
1:B:274:PHE:HB3	1:B:286:ALA:O	2.20	0.42	
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.80	0.42	
1:C:63:PHE:CB	1:C:64:PRO:CD	2.98	0.42	
1:C:251:ARG:HH11	1:C:251:ARG:CG	2.32	0.42	
1:D:202:MET:HE3	1:D:357:HIS:CD2	2.54	0.42	
1:D:635:THR:HA	1:D:680:ILE:O	2.19	0.42	
1:D:840:HIS:ND1	1:D:840:HIS:N	2.67	0.42	
1:D:858:ILE:HG12	1:D:864:MET:HB3	2.02	0.42	
1:A:11:LEU:N	1:A:11:LEU:HD23	2.35	0.42	
1:A:441:THR:O	1:A:445:GLN:HG3	2.20	0.42	
1:A:474:TRP:CZ2	1:A:478:VAL:HG21	2.55	0.42	
1:B:3:ILE:C	1:B:5:ASP:H	2.22	0.42	
1:B:124:SER:HA	1:B:184:LEU:O	2.20	0.42	
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.42	
1:C:472:TYR:O	1:C:476:LYS:HG2	2.20	0.42	
1:C:474:TRP:CZ2	1:C:478:VAL:HG21	2.55	0.42	
1:C:651:LEU:HD12	1:C:651:LEU:HA	1.46	0.42	
1:C:856:TYR:CD1	1:C:856:TYR:N	2.88	0.42	
1:C:910:LEU:C	1:C:910:LEU:HD12	2.39	0.42	
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.84	0.42	
1:D:378:LEU:HA	1:D:378:LEU:HD23	1.75	0.42	
1:D:856:TYR:N	1:D:856:TYR:CD1	2.88	0.42	
1:A:111:PRO:HA	1:A:112:PRO:HA	1.56	0.41	
1:A:645:ARG:NH2	1:A:650:GLU:OE2	2.46	0.41	
1:A:856:TYR:CD1	1:A:856:TYR:N	2.88	0.41	
1:B:262:GLN:O	1:B:262:GLN:HG2	2.19	0.41	
1:B:576:ILE:HD13	1:B:584:PRO:HB2	2.02	0.41	
1:D:441:THR:O	1:D:445:GLN:HG3	2.20	0.41	
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.85	0.41	
1:A:176:PHE:CD1	1:A:176:PHE:N	2.87	0.41	
1:A:721:ARG:HE	1:B:874:SER:CB	2.32	0.41	
1:A:757:GLN:HG2	1:A:758:PHE:N	2.31	0.41	



Atom-1 Atom-2		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:176:PHE:CD1	1:B:176:PHE:N	2.87	0.41
1:B:288:ARG:HH11	1:B:288:ARG:HD3	1.48	0.41
1:C:105:TYR:HB3	1:C:106:PRO:HD2	2.01	0.41
1:C:227:VAL:CG1	1:C:228:ALA:N	2.83	0.41
1:C:395:HIS:HA	1:C:396:PRO:HD3	1.83	0.41
1:C:599:ARG:HB2	1:C:600:GLN:H	1.54	0.41
1:D:141:ILE:HG12	1:D:142:ILE:N	2.35	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.55	0.41
1:D:559:TYR:HB2	1:D:562:LEU:CD1	2.47	0.41
1:A:141:ILE:HG12	1:A:142:ILE:N	2.35	0.41
1:A:524:LEU:O	1:A:561:ARG:NH2	2.50	0.41
1:B:23:GLN:HG2	3:B:4413:HOH:O	2.20	0.41
1:C:141:ILE:HG12	1:C:142:ILE:N	2.35	0.41
1:C:262:GLN:O	1:C:262:GLN:HG2	2.19	0.41
1:C:578:TYR:HA	1:C:583:ASN:O	2.20	0.41
1:C:858:ILE:HG12	1:C:864:MET:HB3	2.02	0.41
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.86	0.41
1:D:835:LEU:HD12	1:D:857:ARG:HB2	2.03	0.41
1:A:23:GLN:HG2	3:A:7533:HOH:O	2.20	0.41
1:A:63:PHE:CB	1:A:64:PRO:CD	2.98	0.41
1:A:682:LEU:HA	1:A:683:PRO:HD3	1.91	0.41
1:A:835:LEU:HD12	1:A:857:ARG:HB2	2.03	0.41
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.56	0.41
1:B:41:GLU:HG2	1:B:46:ARG:NH1	2.35	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.58	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.90	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.86	0.41
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.85	0.41
1:D:41:GLU:HG2	1:D:46:ARG:NH1	2.35	0.41
1:D:524:LEU:O	1:D:561:ARG:NH2	2.50	0.41
1:D:742:THR:CG2	1:D:743:SER:H	2.32	0.41
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.55	0.41
1:A:599:ARG:HB2	1:A:600:GLN:H	1.54	0.41
1:B:63:PHE:CB	1:B:64:PRO:CD	2.98	0.41
1:B:822:LEU:HD13	1:B:822:LEU:HA	1.79	0.41
1:D:77:ASP:HA	3:D:4132:HOH:O	2.19	0.41
1:D:124:SER:HA	1:D:184:LEU:O	2.20	0.41
1:D:352:ARG:NH2	1:D:641:GLU:OE1	2.54	0.41
1:D:559:TYR:HA	1:D:560:PRO:HD2	1.86	0.41
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.41



Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.88	0.41
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.41
1:B:367:MET:HB3	1:B:372:MET:CE	2.50	0.41
1:B:649:ASN:O	1:B:702:GLN:HG3	2.21	0.41
1:B:856:TYR:CD1	1:B:856:TYR:N	2.88	0.41
1:C:11:LEU:N	1:C:11:LEU:HD23	2.35	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	0.41
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.88	0.41
1:A:380:LYS:HE3	1:A:406:GLY:O	2.21	0.41
1:A:578:TYR:HA	1:A:583:ASN:O	2.20	0.41
1:B:63:PHE:HB3	1:B:64:PRO:CD	2.45	0.41
1:B:69:VAL:HG13	1:B:70:PRO:HD2	2.03	0.41
1:B:352:ARG:NH2	1:B:641:GLU:OE1	2.54	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.03	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41
1:B:655:MET:O	1:B:696:LEU:HD12	2.21	0.41
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.56	0.41
1:C:26:ARG:HD2	1:C:169:SER:HB3	2.02	0.41
1:C:41:GLU:HG2	1:C:46:ARG:NH1	2.35	0.41
1:C:559:TYR:HB2	1:C:562:LEU:CD1	2.47	0.41
1:C:649:ASN:O	1:C:702:GLN:HG3	2.21	0.41
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.91	0.41
1:C:970:THR:HG22	1:C:972:HIS:O	2.21	0.41
1:D:63:PHE:CB	1:D:64:PRO:CD	2.98	0.41
1:A:227:VAL:CG1	1:A:228:ALA:N	2.83	0.41
1:A:282:ARG:HG3	1:D:423:MET:HB2	2.03	0.41
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.38	0.41
1:A:840:HIS:N	1:A:840:HIS:ND1	2.67	0.41
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.36	0.41
1:A:949:HIS:CD2	1:A:1020:TRP:NE1	2.79	0.41
1:C:441:THR:O	1:C:445:GLN:HG3	2.20	0.41
1:C:511:PRO:HA	1:C:516:PRO:CB	2.51	0.41
1:D:26:ARG:HD2	1:D:169:SER:HB3	2.02	0.41
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.56	0.41
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.36	0.41
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.35	0.41
1:A:63:PHE:HB3	1:A:64:PRO:CD	2.45	0.41
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.56	0.41
1:A:262:GLN:O	1:A:262:GLN:HG2	2.19	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.41
1:A:649:ASN:O	1:A:702:GLN:HG3	2.21	0.41



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:655:MET:O	1:A:696:LEU:HD12	2.21	0.41	
1:A:778:THR:HG22	1:A:779:PRO:N	2.35	0.41	
1:A:970:THR:HG22	1:A:972:HIS:O	2.21	0.41	
1:B:105:TYR:HA	1:B:106:PRO:HD3	1.91	0.41	
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.55	0.41	
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.81	0.41	
1:B:778:THR:HG22	1:B:779:PRO:N	2.35	0.41	
1:B:858:ILE:HG12	1:B:864:MET:HB3	2.02	0.41	
1:C:305:ILE:HA	1:C:306:PRO:HD2	1.88	0.41	
1:C:380:LYS:HE3	1:C:406:GLY:O	2.21	0.41	
1:C:524:LEU:O	1:C:561:ARG:NH2	2.50	0.41	
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.03	0.41	
1:C:652:LEU:O	1:C:667:GLU:HA	2.20	0.41	
1:C:835:LEU:HD12	1:C:857:ARG:HB2	2.03	0.41	
1:D:11:LEU:N	1:D:11:LEU:HD23	2.35	0.41	
1:D:114:VAL:HA	1:D:115:PRO:HD3	1.77	0.41	
1:D:168:PRO:O	1:D:442:ARG:NH2	2.48	0.41	
1:D:649:ASN:O	1:D:702:GLN:HG3	2.21	0.41	
1:D:655:MET:O	1:D:696:LEU:HD12	2.21	0.41	
1:D:778:THR:CG2	1:D:779:PRO:CD	2.99	0.41	
1:D:778:THR:HG22	1:D:779:PRO:N	2.35	0.41	
1:D:917:ARG:NH2	1:D:943:GLU:OE1	2.54	0.41	
1:A:26:ARG:HD2	1:A:169:SER:HB3	2.02	0.41	
1:A:161:TYR:OH	1:A:163:GLN:NE2	2.50	0.41	
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.75	0.41	
1:A:868:VAL:HG12	1:A:869:ASP:N	2.36	0.41	
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.23	0.41	
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.19	0.41	
1:B:588:TYR:O	1:B:589:GLY:C	2.59	0.41	
1:B:868:VAL:HG12	1:B:869:ASP:N	2.36	0.41	
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.84	0.41	
1:C:778:THR:HG22	1:C:779:PRO:N	2.35	0.41	
1:D:176:PHE:CD1	1:D:176:PHE:N	2.87	0.41	
1:D:578:TYR:HA	1:D:583:ASN:O	2.21	0.41	
1:D:970:THR:HG22	1:D:972:HIS:O	2.21	0.41	
1:A:149:ALA:O	1:A:150:PHE:HB3	2.21	0.40	
1:A:576:ILE:HD13	1:A:584:PRO:HB2	2.02	0.40	
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.56	0.40	
1:B:26:ARG:HD2	1:B:169:SER:HB3	2.02	0.40	
1:B:141:ILE:HG12	1:B:142:ILE:N	2.35	0.40	
1:B:840:HIS:ND1	1:B:840:HIS:N	2.67	0.40	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:352:ARG:NH2	1:C:641:GLU:OE1	2.54	0.40	
1:D:69:VAL:HG13	1:D:70:PRO:HD2	2.03	0.40	
1:A:272:ALA:CB	1:A:273:PRO:CD	2.99	0.40	
1:A:278:ILE:N	1:A:278:ILE:HD13	2.37	0.40	
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.54	0.40	
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.61	0.40	
1:B:380:LYS:HE3	1:B:406:GLY:O	2.21	0.40	
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.42	0.40	
1:B:658:LEU:HG	1:B:661:LYS:HZ2	1.86	0.40	
1:C:23:GLN:HG2	3:C:4454:HOH:O	2.20	0.40	
1:C:149:ALA:O	1:C:150:PHE:HB3	2.21	0.40	
1:C:762:SER:C	1:C:822:LEU:HD23	2.42	0.40	
1:D:23:GLN:HG2	3:D:7533:HOH:O	2.20	0.40	
1:A:502:MET:HA	1:A:537:GLU:O	2.22	0.40	
1:A:588:TYR:O	1:A:589:GLY:C	2.59	0.40	
1:B:272:ALA:CB	1:B:273:PRO:CD	2.99	0.40	
1:B:780:LEU:HA	1:B:780:LEU:HD12	1.89	0.40	
1:C:89:ASN:O	1:C:92:MET:HB2	2.21	0.40	
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.86	0.40	
1:C:502:MET:HA	1:C:537:GLU:O	2.22	0.40	
1:D:3:ILE:C	1:D:5:ASP:H	2.22	0.40	
1:D:149:ALA:O	1:D:150:PHE:HB3	2.21	0.40	
1:A:90:TRP:NE1	1:A:96:ASP:OD1	2.55	0.40	
1:A:147:ASN:HA	1:A:148:SER:HA	1.65	0.40	
1:A:244:VAL:O	1:A:288:ARG:HA	2.22	0.40	
1:A:762:SER:C	1:A:822:LEU:HD23	2.42	0.40	
1:B:578:TYR:HA	1:B:583:ASN:O	2.21	0.40	
1:B:970:THR:HG22	1:B:972:HIS:O	2.21	0.40	
1:C:38:ASN:HD21	1:C:41:GLU:N	2.17	0.40	
1:C:65:ALA:CB	1:C:66:PRO:CD	3.00	0.40	
1:C:128:ASN:HD22	1:C:180:GLY:C	2.25	0.40	
1:D:89:ASN:O	1:D:92:MET:HB2	2.22	0.40	
1:D:227:VAL:CG1	1:D:240:LEU:HD11	2.48	0.40	
1:D:702:GLN:O	1:D:712:GLY:N	2.50	0.40	
1:D:868:VAL:HG12	1:D:869:ASP:N	2.36	0.40	
1:A:100:TYR:O	1:A:597:ASN:HB2	2.22	0.40	
1:A:128:ASN:HD22	1:A:180:GLY:C	2.25	0.40	
1:B:90:TRP:CD1	1:B:90:TRP:C	2.95	0.40	
1:B:844:HIS:ND1	1:B:845:GLN:HG2	2.36	0.40	
1:C:244:VAL:O	1:C:288:ARG:HA	2.22	0.40	
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.56	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:TYR:HA	1:C:560:PRO:HD2	1.86	0.40
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.42	0.40
1:C:702:GLN:O	1:C:712:GLY:N	2.50	0.40
1:C:868:VAL:HG12	1:C:869:ASP:N	2.36	0.40
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.54	0.40
1:D:237:ARG:CB	1:D:237:ARG:NH1	2.79	0.40
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entiles
1	А	1026/1021~(100%)	953~(93%)	67~(6%)	6 (1%)	25	56
1	В	1026/1021~(100%)	953~(93%)	67~(6%)	6 (1%)	25	56
1	С	1026/1021~(100%)	953~(93%)	67~(6%)	6 (1%)	25	56
1	D	1026/1021~(100%)	953~(93%)	67~(6%)	6 (1%)	25	56
All	All	4104/4084 (100%)	3812 (93%)	268 (6%)	24 (1%)	25	56

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	647	SER
1	В	647	SER
1	С	647	SER
1	D	647	SER
1	А	77	ASP
1	А	601	PHE
1	В	77	ASP
1	В	601	PHE



Mol	Chain	Res	Type
1	С	77	ASP
1	С	601	PHE
1	D	77	ASP
1	D	601	PHE
1	А	164	ASP
1	В	164	ASP
1	С	164	ASP
1	D	164	ASP
1	А	690	SER
1	В	690	SER
1	С	690	SER
1	D	690	SER
1	А	10	VAL
1	В	10	VAL
1	С	10	VAL
1	D	10	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	880/873~(101%)	755~(86%)	125~(14%)	3	10
1	В	880/873~(101%)	755~(86%)	125~(14%)	3	10
1	С	880/873~(101%)	755~(86%)	125~(14%)	3	10
1	D	880/873~(101%)	755~(86%)	125 (14%)	3	10
All	All	3520/3492~(101%)	3020 (86%)	500 (14%)	3	10

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	ILE
1	А	12	GLN
1	А	24	LEU
1	А	37	ARG
1	А	38	ASN



Mol	Chain	Res	Type
1	А	39	SER
1	А	49	GLN
1	А	67	GLU
1	А	71	GLU
1	А	72	SER
1	А	80	GLU
1	А	85	VAL
1	А	90	TRP
1	А	102	ASN
1	А	114	VAL
1	А	116	THR
1	А	134	LEU
1	А	135	GLN
1	А	136	GLU
1	А	138	GLN
1	А	148	SER
1	А	169	SER
1	А	187	MET
1	А	190	ARG
1	А	202	MET
1	А	210	ARG
1	А	211	ASP
1	А	214	LEU
1	А	219	THR
1	А	223	SER
1	А	230	ARG
1	А	237	ARG
1	А	246	MET
1	А	249	GLU
1	А	251	ARG
1	A	255	ARG
1	A	259	SER
1	A	269	SER
1	A	277	GLU
1	A	278	ILE
1	A	279	ILE
1	A	282	ARG
1	A	288	ARG
1	A	310	ARG
1	A	322	LEU
1	A	333	ARG
1	A	347	LYS



Mol	Chain	Res	Type
1	А	385	ASN
1	А	394	ASN
1	А	424	ASN
1	А	425	ARG
1	А	437	SER
1	А	448	ARG
1	А	473	ARG
1	А	481	SER
1	А	519	SER
1	А	521	LYS
1	А	525	SER
1	А	526	LEU
1	А	529	GLU
1	А	533	LEU
1	А	545	SER
1	А	546	LEU
1	А	554	GLN
1	А	571	VAL
1	А	576	ILE
1	А	580	GLU
1	А	581	ASN
1	А	600	GLN
1	А	645	ARG
1	А	647	SER
1	А	655	MET
1	А	661	LYS
1	А	665	SER
1	А	672	VAL
1	A	675	GLN
1	A	687	GLN
1	A	690	SER
1	A	719	GLN
1	A	721	ARG
1	A	728	VAL
1	A	730	LEU
1	A	734	SER
1	A	737	ILE
1	A	743	SER
1	A	746	ASP
1	A	750	GLU
1	A	755	ARG
1	A	761	GLN



Mol	Chain	Res	Type
1	А	765	LEU
1	А	766	SER
1	А	768	MET
1	А	770	ILE
1	А	772	ASP
1	А	773	LYS
1	А	774	LYS
1	А	797	GLU
1	А	800	ARG
1	А	801	ILE
1	А	811	LYS
1	А	817	GLN
1	А	822	LEU
1	А	824	GLN
1	А	830	LEU
1	А	843	GLN
1	А	845	GLN
1	А	856	TYR
1	А	857	ARG
1	А	867	THR
1	А	874	SER
1	А	881	ARG
1	А	894	ARG
1	А	917	ARG
1	А	923	SER
1	А	931	PHE
1	А	938	ARG
1	А	950	GLN
1	А	958	ASN
1	А	969	GLU
1	А	986	ILE
1	А	991	MET
1	А	1004	SER
1	А	1006	GLU
1	A	1017	GLN
1	A	1023	LYS
1	В	3	ILE
1	В	12	GLN
1	В	24	LEU
1	В	37	ARG
1	В	38	ASN
1	В	39	SER


1 B 49 GLN 1 B 67 GLU	
1 B 67 GLU	
1 B 71 GLU	
1 B 72 SER	
1 B 80 GLU	
1 B 85 VAL	
1 B 90 TRP	
1 B 102 ASN	
1 B 114 VAL	
1 B 116 THR	
1 B 134 LEU	
1 B 135 GLN	
1 B 136 GLU	
1 B 138 GLN	
1 B 148 SER	
1 B 169 SER	
1 B 187 MET	
1 B 190 ARG	
1 B 202 MET	
1 B 210 ARG	
1 B 211 ASP	
1 B 214 LEU	
1 B 219 THR	
1 B 223 SER	
1 B 230 ARG	
1 B 237 ARG	
1 B 246 MET	
1 B 249 GLU	
1 B 251 ARG	
1 B 255 ARG	
1 B 259 SER	
1 B 269 SER	
1 B 277 GLU	
1 B 278 ILE	
1 B 279 ILE	
1 B 282 ARG	
1 B 288 ARG	
1 B 310 ARG	
1 B 322 LEU	
1 B 333 ARG	
1 B 347 LYS	
1 B 385 ASN	



Mol	Chain	Res	Type
1	В	394	ASN
1	В	424	ASN
1	В	425	ARG
1	В	437	SER
1	В	448	ARG
1	В	473	ARG
1	В	481	SER
1	В	519	SER
1	В	521	LYS
1	В	525	SER
1	В	526	LEU
1	В	529	GLU
1	В	533	LEU
1	В	545	SER
1	В	546	LEU
1	В	554	GLN
1	В	571	VAL
1	В	576	ILE
1	В	580	GLU
1	В	581	ASN
1	В	600	GLN
1	В	645	ARG
1	В	647	SER
1	В	655	MET
1	В	661	LYS
1	В	665	SER
1	В	672	VAL
1	В	675	GLN
1	В	687	GLN
1	В	690	SER
1	В	719	GLN
1	В	721	ARG
1	В	728	VAL
1	В	730	LEU
1	В	734	SER
1	В	737	ILE
1	В	743	SER
1	В	746	ASP
1	В	750	GLU
1	В	755	ARG
1	В	761	GLN
1	В	765	LEU



\mathbf{Mol}	Chain	Res	Type
1	В	766	SER
1	В	768	MET
1	В	770	ILE
1	В	772	ASP
1	В	773	LYS
1	В	774	LYS
1	В	797	GLU
1	В	800	ARG
1	В	801	ILE
1	В	811	LYS
1	В	817	GLN
1	В	822	LEU
1	В	824	GLN
1	В	830	LEU
1	В	843	GLN
1	В	845	GLN
1	В	856	TYR
1	В	857	ARG
1	В	867	THR
1	В	874	SER
1	В	881	ARG
1	В	894	ARG
1	В	917	ARG
1	В	923	SER
1	В	931	PHE
1	В	938	ARG
1	В	950	GLN
1	В	958	ASN
1	В	969	GLU
1	В	986	ILE
1	В	991	MET
1	В	1004	SER
1	В	1006	GLU
1	В	1017	GLN
1	В	1023	LYS
1	С	3	ILE
1	С	12	GLN
1	С	24	LEU
1	С	37	ARG
1	С	38	ASN
1	С	39	SER
1	С	49	GLN



\mathbf{Mol}	Chain	Res	Type
1	С	67	GLU
1	С	71	GLU
1	С	72	SER
1	С	80	GLU
1	С	85	VAL
1	С	90	TRP
1	С	102	ASN
1	С	114	VAL
1	С	116	THR
1	С	134	LEU
1	С	135	GLN
1	С	136	GLU
1	С	138	GLN
1	С	148	SER
1	С	169	SER
1	С	187	MET
1	С	190	ARG
1	С	202	MET
1	С	210	ARG
1	С	211	ASP
1	С	214	LEU
1	С	219	THR
1	С	223	SER
1	С	230	ARG
1	С	237	ARG
1	С	246	MET
1	С	249	GLU
1	С	251	ARG
1	С	255	ARG
1	С	259	SER
1	C	269	SER
1	С	277	GLU
1	С	278	ILE
1	С	279	ILE
1	С	282	ARG
1	С	288	ARG
1	С	310	ARG
1	С	322	LEU
1	С	333	ARG
1	C	347	LYS
1	С	385	ASN
1	С	394	ASN



Mol	Chain	Res	Type
1	С	424	ASN
1	С	425	ARG
1	С	437	SER
1	С	448	ARG
1	С	473	ARG
1	С	481	SER
1	С	519	SER
1	С	521	LYS
1	С	525	SER
1	С	526	LEU
1	С	529	GLU
1	С	533	LEU
1	С	545	SER
1	С	546	LEU
1	С	554	GLN
1	С	571	VAL
1	С	576	ILE
1	С	580	GLU
1	С	581	ASN
1	С	600	GLN
1	С	645	ARG
1	С	647	SER
1	С	655	MET
1	С	661	LYS
1	С	665	SER
1	С	672	VAL
1	С	675	GLN
1	С	687	GLN
1	С	690	SER
1	С	719	GLN
1	С	721	ARG
1	C	728	VAL
1	С	730	LEU
1	С	734	SER
1	С	737	ILE
1	C	743	SER
1	С	746	ASP
1	C	750	GLU
1	C	755	ARG
1	С	761	GLN
1	С	765	LEU
1	С	766	SER



Mol	Chain	Res	Type
1	С	768	MET
1	С	770	ILE
1	С	772	ASP
1	С	773	LYS
1	С	774	LYS
1	С	797	GLU
1	С	800	ARG
1	С	801	ILE
1	С	811	LYS
1	С	817	GLN
1	С	822	LEU
1	С	824	GLN
1	С	830	LEU
1	С	843	GLN
1	С	845	GLN
1	С	856	TYR
1	С	857	ARG
1	С	867	THR
1	С	874	SER
1	С	881	ARG
1	С	894	ARG
1	С	917	ARG
1	С	923	SER
1	С	931	PHE
1	С	938	ARG
1	С	950	GLN
1	С	958	ASN
1	С	969	GLU
1	С	986	ILE
1	С	991	MET
1	С	1004	SER
1	C	1006	GLU
1	С	1017	GLN
1	C	1023	LYS
1	D	3	ILE
1	D	12	GLN
1	D	24	LEU
1	D	37	ARG
1	D	38	ASN
1	D	39	SER
1	D	49	GLN
1	D	67	GLU



Mol	Chain	Res	Type
1	D	71	GLU
1	D	72	SER
1	D	80	GLU
1	D	85	VAL
1	D	90	TRP
1	D	102	ASN
1	D	114	VAL
1	D	116	THR
1	D	134	LEU
1	D	135	GLN
1	D	136	GLU
1	D	138	GLN
1	D	148	SER
1	D	169	SER
1	D	187	MET
1	D	190	ARG
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	214	LEU
1	D	219	THR
1	D	223	SER
1	D	230	ARG
1	D	237	ARG
1	D	246	MET
1	D	249	GLU
1	D	251	ARG
1	D	255	ARG
1	D	259	SER
1	D	269	SER
1	D	277	GLU
1	D	278	ILE
1	D	279	ILE
1	D	282	ARG
1	D	288	ARG
1	D	310	ARG
1	D	322	LEU
1	D	333	ARG
1	D	347	LYS
1	D	385	ASN
1	D	394	ASN
1	D	424	ASN



Mol	Chain	Res	Type
1	D	425	ARG
1	D	437	SER
1	D	448	ARG
1	D	473	ARG
1	D	481	SER
1	D	519	SER
1	D	521	LYS
1	D	525	SER
1	D	526	LEU
1	D	529	GLU
1	D	533	LEU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	576	ILE
1	D	580	GLU
1	D	581	ASN
1	D	600	GLN
1	D	645	ARG
1	D	647	SER
1	D	655	MET
1	D	661	LYS
1	D	665	SER
1	D	672	VAL
1	D	675	GLN
1	D	687	GLN
1	D	690	SER
1	D	719	GLN
1	D	721	ARG
1	D	728	VAL
1	D	730	LEU
1	D	734	SER
1	D	737	ILE
1	D	743	SER
1	D	746	ASP
1	D	750	GLU
1	D	755	ARG
1	D	761	GLN
1	D	765	LEU
1	D	766	SER
1	D	768	MET



Mol	Chain	Res	Type
1	D	770	ILE
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	797	GLU
1	D	800	ARG
1	D	801	ILE
1	D	811	LYS
1	D	817	GLN
1	D	822	LEU
1	D	824	GLN
1	D	830	LEU
1	D	843	GLN
1	D	845	GLN
1	D	856	TYR
1	D	857	ARG
1	D	867	THR
1	D	874	SER
1	D	881	ARG
1	D	894	ARG
1	D	917	ARG
1	D	923	SER
1	D	931	PHE
1	D	938	ARG
1	D	950	GLN
1	D	958	ASN
1	D	969	GLU
1	D	986	ILE
1	D	991	MET
1	D	1004	SER
1	D	1006	GLU
1	D	1017	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	38	ASN
1	А	50	GLN
1	А	102	ASN
1	А	128	ASN
1	А	163	GLN



Mol	Chain	Res	Type
1	А	216	HIS
1	А	226	HIS
1	А	316	HIS
1	А	357	HIS
1	А	385	ASN
1	А	424	ASN
1	А	467	ASN
1	А	554	GLN
1	А	581	ASN
1	А	597	ASN
1	А	604	ASN
1	А	622	HIS
1	А	624	GLN
1	А	634	GLN
1	А	817	GLN
1	A	890	GLN
1	А	949	HIS
1	А	990	HIS
1	А	1017	GLN
1	В	38	ASN
1	В	50	GLN
1	В	102	ASN
1	В	128	ASN
1	В	163	GLN
1	В	216	HIS
1	В	226	HIS
1	В	316	HIS
1	В	357	HIS
1	В	385	ASN
1	В	424	ASN
1	В	467	ASN
1	B	554	GLN
1	B	581	ASN
1	B	597	ASN
1	B	604	ASN
1	В	622	HIS
1	B	624	GLN
1	B	634	GLN
1	В	817	GLN
1	В	890	GLN
1	В	949	HIS
1	В	990	HIS



Mol	Chain	Res	Type
1	В	1017	GLN
1	С	38	ASN
1	С	50	GLN
1	С	102	ASN
1	С	128	ASN
1	С	216	HIS
1	С	226	HIS
1	С	316	HIS
1	С	357	HIS
1	С	385	ASN
1	С	424	ASN
1	С	467	ASN
1	С	554	GLN
1	С	581	ASN
1	С	597	ASN
1	С	604	ASN
1	С	622	HIS
1	С	624	GLN
1	С	634	GLN
1	С	817	GLN
1	С	890	GLN
1	С	949	HIS
1	С	990	HIS
1	С	1017	GLN
1	D	38	ASN
1	D	50	GLN
1	D	102	ASN
1	D	128	ASN
1	D	216	HIS
1	D	226	HIS
1	D	316	HIS
1	D	357	HIS
1	D	385	ASN
1	D	424	ASN
1	D	467	ASN
1	D	554	GLN
1	D	581	ASN
1	D	597	ASN
1	D	604	ASN
1	D	622	HIS
1	D	624	GLN
1	D	634	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	D	817	GLN
1	D	890	GLN
1	D	949	HIS
1	D	990	HIS
1	D	1017	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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 (i)

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, 95^{th} 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		$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	1021/1021~(100%)	-0.82	7 (0%) 87	84	8, 29, 70, 100	19 (1%)
1	В	1021/1021~(100%)	-0.82	4 (0%) 92	91	8, 29, 70, 100	19 (1%)
1	С	1021/1021~(100%)	-0.85	4 (0%) 92	91	8, 29, 70, 100	19 (1%)
1	D	1021/1021~(100%)	-0.82	5 (0%) 91	88	8, 29, 70, 100	19 (1%)
All	All	4084/4084~(100%)	-0.83	20 (0%) 91	88	8, 29, 71, 100	76 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ	
1	D	732	ALA	4.5	
1	А	732	ALA	4.1	
1	С	581	ASN	3.7	
1	А	581	ASN	3.3	
1	В	732	ALA	3.2	
1	А	801	ILE	3.1	
1	С	732	ALA	2.9	
1	А	733	ALA	2.9	
1	А	734	SER	2.7	
1	А	730	LEU	2.7	
1	D	733	ALA	2.6	
1	В	583	ASN	2.4	
1	С	596	PRO	2.4	
1	В	798	ALA	2.3	
1	D	730	LEU	2.2	
1	С	734	SER	2.2	
1	D	734	SER	2.2	
1	А	729	THR	2.2	
1	D	731	PRO	2.1	
1	В	799	THR	2.1	



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 monosaccharides 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, 95^{th} 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)	$\mathbf{Q} < 0.9$
2	MG	В	3002	1/1	0.93	0.09	31,31,31,31	0
2	MG	A	3001	1/1	0.96	0.08	28,28,28,28	0
2	MG	С	3002	1/1	0.96	0.09	31,31,31,31	0
2	MG	D	3002	1/1	0.96	0.12	31,31,31,31	0
2	MG	А	3002	1/1	0.98	0.11	31,31,31,31	0
2	MG	В	3001	1/1	0.99	0.08	28,28,28,28	0
2	MG	D	3001	1/1	0.99	0.08	28,28,28,28	0
2	MG	С	3001	1/1	0.99	0.05	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.

