

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 09:15 AM EDT

PDB ID	:	60VR
Title	:	X-ray crystal structure of a bacterial reiterative transcription complex of pyrG
		promoter variant -1G
Authors	:	Shin, Y.; Murakami, K.S.
Deposited on	:	2019-05-08
Resolution	:	2.84 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

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 2.84 Å.

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



Metric	Whole archive	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
R_{free}	130704	$1031 \ (2.86-2.82)$
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)
RNA backbone	3102	1077 (3.10-2.58)

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	Q	uality of chain		
1	А	315	-% 	24%	28%	
1	В	315	35%	36%	29%	
2	С	1119	4% 61%		35%	••
3	D	1524	3% 59%		36%	••



Mol	Chain	Length	Quali	ty of chain	
4	Е	99	59%		32% • 5%
5	F	423	45%	34%	• 18%
6	G	22	50%	32%	5% 14%
7	Н	27	44%	22% •	30%
8	Ι	8	25%	25%	38%



60VR

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28535 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	226	Total	С	Ν	Ο	S	0	0	0
1	Л	220	1782	1138	310	332	2	0	0	0
1	В	224	Total	С	Ν	Ο	S	0	0	0
	D	224	1767	1129	307	329	2	0	U	0

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
2	С	1107	Total 8726	C 5523	N 1551	O 1628	S 24	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
3	D	1484	Total 11722	С 7431	N 2065	O 2191	${ m S}\ 35$	0	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues		Atoms					AltConf	Trace
4	Е	94	Total 761	C 486	N 132	0 139	$\frac{S}{4}$	0	0	0

• Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues		Atoms					AltConf	Trace
5	F	346	Total 2790	C 1760	N 508	0 518	${f S}{4}$	0	0	0

• Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP *AP*GP*CP*CP*CP*GP*AP*AP*A)-3').



Mol	Chain	Residues		Atoms					AltConf	Trace
6	G	19	Total 387	C 183	N 75	O 110	Р 19	0	0	0

• Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP* TP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
7	Н	19	Total 394	C 188	N 76	O 112	Р 18	0	0	0

• Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Ι	8	Total 193	C 80	N 40	O 63	Р 10	0	0	0

• Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0

• Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	С	1	Total 9	0 7	Р 2	0	0

• Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
11	D	2	Total Zn 2 2	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: DNA-directed RNA polymerase subunit alpha

• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 61% 35%







T97 P98 A99	H101 1102	F104 V105	K106	K111 K111	2117	L116 D117	L118	E122	L123 E124	Q125 V126	L127	Y128	K131	1132 1133	V134	D136	P137	L142	N143 G144	V147	E148	K149	L152	D155 5156	E157	Y158 R159	E160 1161	1017	K165 Q166	E167 T168	Y169 P170 L171
P172 P173 G174	L178 V179 V180	D181 0182 6182	E183 E184	V185 V186	6188	Q189 E190	L191	76TU	V195 V196	S197	L199	D200	A203	L204 Y205	R206	F20/ P208	R209 R210	V211	K212 V213	E214 Y215		K218 E219	R220 A221	G222	R224	V231	Jenv	1230 K237	E240	1241 L242	L245 P246
E247 P248 Y249	R252 A253 F254	V258		E266	A268 F269	L270 V271	L272 P273	R274	E275 D276	E277 D770	V279	A280 T281	Y282	F283 L284	P285	0287 G287	M288	E296	129/ V298	E299 K300	G301	1302	E306	(309	L311	R312 M313	P314 P315	(316 (316	V317	A320 Q321	E326 E327
L333 T334 T334		K343	D344	v 347 Q 348	M351	N352 V353	V354 V355	P356	E357 G358	A359	V361	E362	G364	D365 K366	1367 1369	A 369	A370 T371	D372	E374	V377	I378	A3/9 E380	A381 E382	G383 V204	V 304	H386 L387	H388 5200	P390	A391 S392	1393 L394	V395 V396 K397
A398 ¥401	D405 D406 11407	V ±01 E408 V 409	5410 T411	6412 D413	V420	G425	VA31	Y432	G433 R434	V435	V437	D438	R441	V443	V444	V446 V446	V447 F.448	S449	Y450 D451	I452 D453	A454	K455 M456	G457	A460	L465	L468	D469	L4/0	E474	M481 K482	H483 P484 S485
R486 A487 R488 P100	K491 K491	K494 R495	L496	0094	T-PO3	R508 P509	E510 U611	M512	I513	V517	L520	P521		K526 P526	M527	v 528 Q529	V530 D531		K534	T537	Y544	1548	R553	L554 Vees	K556	L557 L558	TERE	1566	I 567	E570 K571	R572 M573 L574
Q575 D579	L581 L582	R587	S602 L603	R613	R622	<mark>V623</mark> D624	7625 3676	G627	R628 S629	V630 T634	1031 V632	P635	Q636	L63/ K638	L639 11640	но40 Q641	C642 G643	L644	P045	P655 F656	L657	K660	M661	K664	1666	N669	V670	T / OV	R674 R675	M676 L677	0680 R681
D682 1683 K684	E686 V687	0000 D689 A690		GROT	V699 V700	L701 L702	N703 P704	F O N	H709 R710	L711 6710	I713	Q714	0717	V/18 V719	L720	0724	0727		F / 36	D739 F740	D741	G742 D743	Q744 M745	A746 1777	4746 H748	V749 P750	E L	r / 34 A755	<mark>q 756</mark>	1761 Q762	M763 H767
A773	D784	L787	1792 T793	U7 95 V7 95	K797	E7 98 K7 99	K800	L804	T808	P809	E010 E811	A812 1.813		K818 G819	E820	N824	1827	K828	67.81	R832 F833	T834	R838	V842	MO A F	N040	E848	L860	Tooh	T865	E874 T875	S876 R879
I880 L881 Tooe	1000 V886 A887	A889 V890	V895	A896 V897	L899 L899	1900 01	L902	V904	P905 Q906	E907	8910	<u>Y916</u>	q917	L920	R921	TA22	Y936 Y937	G938	F939 T940	F941	1947	1948 1949	D952	TOFE	OCET	E975	• 87978	F982	L983 T984	D985 R986	E987 R988 Y989
1992 1992	V1003	V1007	F1011		6101A	M1023	A1028	670TV	01033 01034	1 1000	C1039	G1040 1.1041	R1042	M1045	Q1046	N104/ P1048	S1049 G1050	E1051	T1052 F1053	E1054	V1057	V1067	L1068	11072	H1075	G1076	T1084	T1088	G1092	L1098	V1099 V1107
R1108 E1109 A1110 D111	C1112 C1112 G1113	D1126	E1127 V1128	R1129 R1130	R1137	E1141	A1142	L1144	Y1145 G1146	R1147 V1140	OTTA	R1151	V1155	R1159	1 1 6 1	K1164 Y1165	L1166 S1167	M1168	V1171	A1177		V1188 R1189	R1197	Y1198	V1200	K1203	C1204	P1214	11217	A1225	11229
T1234 Q1235 L1236 T1236	ARG	PHE HIS	THR GLY	GLY VAL	GLY	ALA ALA	ASP	THR	01254	R1258	E1261	L1262	A1265	R1266 R1267	P1268	K1271	A1272 V1273	11274	512/5 E1276	11277 D1278	G1279	V1280 V1281	R1282	T1286 E1.287	E1288	K1289 L1290	<mark>81291</mark>	F1293	V1294 E1295	S1296 E1297	G1298 • F1299 • <mark>S1300</mark>
K1301 E1302 Y1303 V1304	L1305	E1308 A1309 A1309	R1310 L1311		K1314 D1315	G1316 D1317	Y1318	T1326	R1327	D1331	H1333	1.1.336		E1342 A1343	V1344	E1351	1.1363	H1364	D1365 K1366	V1371	V1372	R13/3 Q1374	M1375	V1379	D1386	S1387	L1390 E1301	терта	W1398 D1399	E1405	A1409 E1410





ARG ALA ALA ALA ARG GLY VAL LYS GLV GLU GLN CGLN CGLN CGLN ALA ALA

• Molecule 4: DNA-directed RNA polymerase subunit omega



P*AP*AP*A)-3')



• Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP *AP*GP*G)-3')







4 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	185.90Å 101.42Å 295.19Å	Depositor	
a, b, c, α , β , γ	90.00° 98.64° 90.00°	Depositor	
Bosolution(A)	41.69 - 2.84	Depositor	
Resolution (A)	41.69 - 2.84	EDS	
% Data completeness	96.5 (41.69-2.84)	Depositor	
(in resolution range)	96.5(41.69-2.84)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.72 (at 2.86 \text{\AA})$	Xtriage	
Refinement program	PHENIX (1.14_3260: ???)	Depositor	
P. P.	0.222 , 0.268	Depositor	
n, n_{free}	0.222 , 0.268	DCC	
R_{free} test set	1994 reflections (1.61%)	wwPDB-VP	
Wilson B-factor $(Å^2)$	79.0	Xtriage	
Anisotropy	0.659	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 64.0	EDS	
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	28535	wwPDB-VP	
Average B, all atoms $(Å^2)$	102.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.

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, ZN, POP, GTP

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	Bo	ond lengths	B	ond angles
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.50	1/1814~(0.1%)	0.70	1/2466~(0.0%)
1	В	0.53	0/1799	0.72	0/2447
2	С	0.52	3/8892~(0.0%)	0.72	5/12028~(0.0%)
3	D	0.57	3/11928~(0.0%)	0.75	12/16127~(0.1%)
4	Е	0.52	0/775	0.80	3/1045~(0.3%)
5	F	0.58	5/2835~(0.2%)	0.74	6/3816~(0.2%)
6	G	1.14	1/434~(0.2%)	1.06	1/666~(0.2%)
7	Н	0.87	0/442	1.00	2/680~(0.3%)
8	Ι	0.79	0/181	1.36	1/283~(0.4%)
All	All	0.57	13/29100~(0.0%)	0.75	31/39558~(0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
3	D	0	2
5	F	0	1
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	F	249	ARG	CB-CG	10.78	1.81	1.52
2	С	37	GLU	CB-CG	-10.32	1.32	1.52
2	С	37	GLU	CD-OE1	-8.63	1.16	1.25
5	F	249	ARG	CZ-NH2	-8.59	1.21	1.33
5	F	249	ARG	NE-CZ	8.53	1.44	1.33
2	C 37		GLU	CD-OE2	7.38	1.33	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	G	19	DA	P-O5'	6.97	1.66	1.59
3	D	1148	VAL	CB-CG2	-6.40	1.39	1.52
3	D	749	VAL	CB-CG2	-5.64	1.41	1.52
3	D	299	GLU	CB-CG	5.47	1.62	1.52
5	F	249	ARG	CD-NE	5.30	1.55	1.46
1	А	75	VAL	CB-CG1	-5.05	1.42	1.52
5	F	265	VAL	CB-CG1	-5.04	1.42	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	F	249	ARG	NE-CZ-NH2	13.02	126.81	120.30
6	G	19	DA	O4'-C4'-C3'	-8.25	101.05	106.00
5	F	249	ARG	NH1-CZ-NH2	-7.98	110.62	119.40
3	D	513	ILE	CG1-CB-CG2	-7.95	93.91	111.40
3	D	35	ARG	NE-CZ-NH2	-7.32	116.64	120.30
3	D	1151	ARG	CA-CB-CG	7.21	129.26	113.40
5	F	249	ARG	CD-NE-CZ	7.10	133.54	123.60
3	D	152	LEU	CA-CB-CG	6.97	131.34	115.30
3	D	1151	ARG	NE-CZ-NH1	-6.76	116.92	120.30
3	D	170	PRO	C-N-CA	-6.73	104.88	121.70
4	Е	85	LEU	CB-CG-CD1	-6.34	100.22	111.00
3	D	204	LEU	CB-CG-CD1	-6.32	100.26	111.00
5	F	127	ILE	CG1-CB-CG2	-6.13	97.91	111.40
4	Е	30	LEU	CB-CG-CD1	-5.99	100.83	111.00
2	С	203	ASP	CB-CG-OD1	5.87	123.58	118.30
3	D	191	LEU	CB-CG-CD2	-5.82	101.10	111.00
2	С	260	LEU	CA-CB-CG	5.78	128.60	115.30
4	Е	26	ARG	CG-CD-NE	5.72	123.80	111.80
7	Н	1	DT	O4'-C1'-N1	5.70	111.99	108.00
1	А	99	LEU	CB-CG-CD2	-5.46	101.72	111.00
7	Н	5	DA	O4'-C1'-N9	5.43	111.80	108.00
5	F	282	LEU	CA-CB-CG	5.43	127.79	115.30
2	С	241	LEU	CA-CB-CG	5.43	127.78	115.30
5	F	383	LEU	CA-CB-CG	5.29	127.47	115.30
2	С	1055	LEU	CA-CB-CG	5.23	127.33	115.30
8	Ι	2	G	O4'-C1'-N9	-5.22	104.03	108.20
3	D	1422	MET	CA-CB-CG	5.18	122.11	113.30
3	D	739	ASP	CB-CG-OD2	5.05	122.85	118.30
3	D	713	ILE	CG1-CB-CG2	-5.02	100.35	111.40
2	С	37	GLU	CB-CA-C	-5.02	100.36	110.40
3	D	191	LEU	CA-CB-CG	5.02	126.84	115.30



There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group		
1	А	161	ARG	Peptide		
3	D	1129	THR	Peptide		
3	D	65	ARG	Peptide		
5	F	389	PHE	Peptide		

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	1782	0	1834	86	0
1	В	1767	0	1816	118	0
2	С	8726	0	8814	428	0
3	D	11722	0	11950	601	13
4	Е	761	0	778	43	0
5	F	2790	0	2853	183	11
6	G	387	0	212	9	0
7	Н	394	0	217	9	0
8	Ι	193	0	88	3	0
9	В	1	0	0	0	0
9	D	1	0	0	0	0
10	С	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28535	0	28562	1358	13

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 24.

All (1358) 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)
5:F:249:ARG:CG	5:F:249:ARG:CB	1.81	1.58
3:D:371:ILE:CD1	3:D:372:ASP:H	1.36	1.38
2:C:605:LYS:HB3	2:C:610:ARG:NH2	1.35	1.36
3:D:411:THR:O	5:F:178:ARG:NH2	1.58	1.36



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:411:THR:C	5:F:178:ARG:NH2	1.90	1.23
2:C:605:LYS:CB	2:C:610:ARG:NH2	2.06	1.19
5:F:258:ILE:O	5:F:258:ILE:HD12	1.39	1.17
3:D:371:ILE:HD12	3:D:372:ASP:N	1.58	1.16
2:C:367:LEU:HA	2:C:371:LYS:HE3	1.29	1.13
3:D:411:THR:O	5:F:178:ARG:CZ	1.97	1.11
2:C:13:ILE:HD12	2:C:14:PRO:HD2	1.33	1.11
2:C:68:PHE:HA	2:C:98:LEU:HD12	1.28	1.10
3:D:135:LEU:O	3:D:149:LYS:HE2	1.52	1.09
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.34	1.07
3:D:411:THR:O	5:F:178:ARG:NE	1.88	1.06
2:C:366:SER:O	2:C:371:LYS:NZ	1.90	1.04
2:C:1101:THR:OG1	2:C:1111:ILE:HD11	1.55	1.04
3:D:572:ARG:HH12	5:F:83:GLN:HG2	1.22	1.03
3:D:218:LYS:NZ	3:D:338:GLU:CA	2.23	1.01
3:D:992:ILE:HD11	3:D:1054:GLU:HB3	1.42	1.01
1:A:57:TYR:CD1	1:A:161:ARG:NH1	2.28	1.01
3:D:371:ILE:CD1	3:D:372:ASP:N	2.17	1.01
3:D:890:VAL:CG1	3:D:922:LEU:HD13	1.90	1.00
3:D:1047:LYS:CE	3:D:1048:PRO:HG2	1.93	0.99
5:F:230:LYS:O	5:F:232:ARG:HD2	1.63	0.98
3:D:218:LYS:HE3	3:D:338:GLU:HG2	1.45	0.97
5:F:258:ILE:O	5:F:258:ILE:CD1	2.12	0.97
1:B:71:VAL:HG12	1:B:132:LEU:HG	1.45	0.97
3:D:218:LYS:NZ	3:D:338:GLU:HA	1.78	0.96
2:C:605:LYS:CB	2:C:610:ARG:HH22	1.70	0.96
3:D:371:ILE:HD13	3:D:372:ASP:CG	1.84	0.96
1:A:57:TYR:CE2	1:A:161:ARG:NH2	2.34	0.96
2:C:1067:TYR:OH	3:D:674:ARG:NH1	1.99	0.96
3:D:36:THR:HG23	3:D:38:LYS:H	1.29	0.96
2:C:723:THR:HG22	2:C:725:ASP:H	1.29	0.95
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.47	0.94
3:D:218:LYS:NZ	3:D:339:TRP:N	2.17	0.92
2:C:486:MET:HG3	2:C:490:GLU:HG3	1.48	0.92
3:D:168:THR:HG22	3:D:394:LEU:HD13	1.52	0.92
3:D:361:VAL:HG23	3:D:365:ASP:HB2	1.49	0.92
3:D:371:ILE:HD12	3:D:372:ASP:H	0.75	0.91
3:D:371:ILE:HD13	3:D:372:ASP:OD1	1.69	0.91
3:D:218:LYS:CE	3:D:338:GLU:CB	2.49	0.90
1:B:102:LYS:HG3	1:B:139:ASN:HB2	1.51	0.90
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.52	0.90



	h h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:F:237:THR:HG1	7:H:4:DA:H8	1.13	0.90
3:D:205:TYR:HD1	3:D:390:PRO:HB3	1.36	0.90
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.52	0.89
3:D:218:LYS:HZ2	3:D:338:GLU:HA	1.33	0.89
1:B:124:ASN:HD22	1:B:127:LEU:CD1	1.85	0.89
3:D:828:LYS:HD2	3:D:833:GLU:HB3	1.55	0.88
1:B:124:ASN:ND2	1:B:127:LEU:HD12	1.89	0.88
3:D:174:GLY:H	3:D:209:ARG:HH12	1.20	0.88
2:C:367:LEU:HA	2:C:371:LYS:CE	2.04	0.87
1:A:99:LEU:HD11	1:A:114:PHE:HB3	1.54	0.87
2:C:575:GLN:OE1	2:C:671:ASN:N	2.07	0.86
3:D:116:LEU:HD11	3:D:465:LEU:HD21	1.55	0.86
2:C:210:GLU:HB3	2:C:211:LEU:HD22	1.55	0.86
3:D:142:LEU:HD12	3:D:161:LEU:HD11	1.56	0.86
3:D:181:ASP:HB2	3:D:205:TYR:HD2	1.40	0.86
3:D:209:ARG:HA	3:D:347:VAL:HG12	1.55	0.86
5:F:372:ARG:HH12	5:F:380:GLU:HA	1.40	0.85
3:D:208:PRO:O	3:D:347:VAL:HG11	1.75	0.85
5:F:372:ARG:O	5:F:372:ARG:NH1	2.08	0.85
2:C:605:LYS:HB3	2:C:610:ARG:HH22	0.77	0.84
3:D:241:ILE:HD11	3:D:310:LEU:HD11	1.59	0.84
3:D:631:ILE:HD11	3:D:745:MET:SD	2.17	0.84
3:D:1047:LYS:HE2	3:D:1048:PRO:CG	2.08	0.84
3:D:173:PRO:HA	3:D:209:ARG:HH22	1.43	0.84
3:D:218:LYS:HZ1	3:D:338:GLU:CA	1.91	0.84
3:D:1047:LYS:NZ	3:D:1048:PRO:HG2	1.93	0.84
3:D:896:ALA:O	3:D:900:ILE:HD12	1.78	0.83
1:A:76:VAL:O	1:A:79:ILE:HG22	1.79	0.83
2:C:428:ARG:NH2	2:C:447:ALA:O	2.12	0.83
1:B:112:ARG:HG2	1:B:125:PRO:HB2	1.59	0.83
3:D:496:LEU:HD23	3:D:1390:LEU:HD21	1.60	0.82
1:A:57:TYR:CZ	1:A:161:ARG:NH2	2.44	0.82
1:A:85:LEU:HD21	1:A:87:VAL:HG13	1.61	0.82
2:C:23:VAL:HA	2:C:121:MET:HE1	1.61	0.82
2:C:607:ASP:HB3	2:C:610:ARG:HG3	1.62	0.82
5:F:116:LEU:HD22	5:F:127:ILE:HG21	1.61	0.82
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.61	0.81
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.60	0.81
2:C:367:LEU:HD12	2:C:371:LYS:NZ	1.93	0.81
3:D:890:VAL:HG11	3:D:922:LEU:CD1	2.09	0.81
3:D:218:LYS:HZ1	3:D:338:GLU:C	1.84	0.81



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.45	0.81
6:G:18:DG:H2'	6:G:19:DA:H5'	1.62	0.81
2:C:716:LYS:HE2	2:C:716:LYS:H	1.45	0.80
3:D:1047:LYS:CE	3:D:1048:PRO:CG	2.58	0.80
3:D:218:LYS:HE3	3:D:338:GLU:CG	2.11	0.80
2:C:503:LEU:HD12	2:C:508:ILE:HA	1.63	0.80
3:D:218:LYS:CE	3:D:338:GLU:HB3	2.11	0.80
3:D:413:ASP:H	5:F:178:ARG:HH22	1.28	0.80
3:D:628:ARG:HH21	3:D:746:ALA:HB2	1.43	0.80
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.47	0.80
1:A:57:TYR:CD2	1:A:161:ARG:NH2	2.50	0.79
2:C:229:MET:HG3	2:C:233:GLU:HB2	1.64	0.79
3:D:203:ALA:HB1	3:D:393:ILE:HD11	1.64	0.79
3:D:218:LYS:HZ2	3:D:339:TRP:H	1.31	0.79
3:D:800:LYS:NZ	3:D:819:GLY:O	2.16	0.79
2:C:728:HIS:ND1	5:F:422:LEU:O	2.15	0.79
2:C:890:LEU:HD23	2:C:890:LEU:O	1.82	0.79
3:D:65:ARG:HH21	5:F:377:ASP:H	1.28	0.79
2:C:367:LEU:HD12	2:C:371:LYS:HZ2	1.45	0.78
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.18	0.78
2:C:589:ARG:HE	2:C:596:TYR:HE2	1.32	0.78
3:D:218:LYS:NZ	3:D:339:TRP:H	1.80	0.78
3:D:218:LYS:HE2	3:D:338:GLU:HB3	1.66	0.78
3:D:218:LYS:CE	3:D:338:GLU:CG	2.62	0.78
3:D:259:VAL:HG12	3:D:296:GLU:O	1.85	0.77
5:F:116:LEU:HD21	5:F:163:LEU:HD21	1.65	0.77
1:A:108:GLU:HG2	1:A:131:THR:HG23	1.67	0.77
2:C:474:VAL:HG11	2:C:529:VAL:HG22	1.65	0.77
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.66	0.77
3:D:371:ILE:HD13	3:D:372:ASP:CB	2.14	0.77
3:D:209:ARG:HA	3:D:347:VAL:CG1	2.14	0.77
3:D:224:ARG:NH1	3:D:254:GLU:OE1	2.16	0.77
4:E:26:ARG:HD3	4:E:30:LEU:HD11	1.64	0.77
5:F:131:VAL:HG13	5:F:178:ARG:HG2	1.66	0.77
3:D:1047:LYS:HE2	3:D:1048:PRO:HD2	1.65	0.77
4:E:80:VAL:CG2	4:E:85:LEU:HD11	2.14	0.77
1:A:111:ALA:HA	1:A:114:PHE:HE2	1.50	0.76
3:D:218:LYS:NZ	3:D:338:GLU:C	2.39	0.76
3:D:631:ILE:HD11	3:D:745:MET:HB2	1.66	0.76
3:D:1047:LYS:HE2	3:D:1048:PRO:CD	2.15	0.76
3:D:33:ASN:HB3	3:D:36:THR:HG22	1.66	0.76



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:19:GLU:HA	1:A:201:THR:HG22	1.67	0.76
2:C:162:ILE:HD11	2:C:172:ILE:HD12	1.66	0.76
2:C:711:GLU:OE1	2:C:713:ARG:NH2	2.20	0.75
1:B:18:ARG:NH1	1:B:204:SER:O	2.20	0.75
5:F:265:VAL:O	5:F:269:ASN:ND2	2.19	0.75
4:E:50:THR:HG22	4:E:53:GLY:O	1.86	0.75
2:C:226:VAL:O	2:C:229:MET:HE2	1.87	0.75
2:C:78:PHE:HB3	2:C:82:GLU:HG2	1.68	0.75
2:C:150:PRO:HA	2:C:158:TYR:HD1	1.50	0.75
3:D:1126:ASP:O	3:D:1130:ARG:HA	1.87	0.75
3:D:675:ARG:HH22	5:F:420:ASP:HA	1.50	0.74
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.68	0.74
3:D:171:LEU:HD21	3:D:390:PRO:HG2	1.69	0.74
1:B:206:THR:HG22	1:B:209:GLU:HB2	1.69	0.74
3:D:224:ARG:HH11	3:D:254:GLU:CD	1.90	0.74
3:D:808:THR:HG23	3:D:811:GLU:HB2	1.70	0.74
1:A:111:ALA:HA	1:A:114:PHE:CE2	2.22	0.73
2:C:23:VAL:HA	2:C:121:MET:CE	2.18	0.73
3:D:691:LEU:HD22	3:D:720:LEU:HD21	1.69	0.73
5:F:120:THR:HB	5:F:122:LEU:HD13	1.67	0.73
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.71	0.73
1:A:79:ILE:HD11	1:A:167:VAL:CG2	2.19	0.73
1:B:128:HIS:HE1	1:B:131:THR:HG22	1.54	0.73
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.03	0.73
2:C:605:LYS:HB2	2:C:610:ARG:NH2	2.04	0.73
2:C:267:TYR:CZ	2:C:290:LEU:HD11	2.24	0.73
3:D:1286:THR:O	3:D:1307:LYS:NZ	2.18	0.72
4:E:39:VAL:HG11	4:E:72:ARG:HB2	1.69	0.72
2:C:280:LYS:HE3	2:C:323:ASP:OD2	1.89	0.72
3:D:686:GLU:OE1	3:D:686:GLU:N	2.22	0.72
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.21	0.72
2:C:495:THR:HG23	2:C:530:GLU:OE1	1.90	0.72
3:D:572:ARG:NH1	5:F:83:GLN:HG2	2.01	0.72
3:D:798:GLU:OE2	3:D:824:ASN:ND2	2.20	0.72
3:D:828:LYS:CD	3:D:833:GLU:HB3	2.20	0.72
3:D:100:ALA:HB3	3:D:575:GLN:HE22	1.54	0.72
3:D:625:TYR:HB3	3:D:749:VAL:HG22	1.71	0.72
3:D:767:HIS:CE1	4:E:6:ILE:HD13	2.24	0.72
3:D:975:GLU:OE2	3:D:988:ARG:NH1	2.21	0.72
3:D:1155:VAL:HG11	3:D:1177:ALA:HB2	1.71	0.72
3:D:218:LYS:HZ2	3:D:339:TRP:N	1.85	0.72



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:875:THR:HG21	3:D:902:LEU:HD21	1.72	0.72
1:A:94:LEU:O	1:A:146:ARG:NH1	2.23	0.71
5:F:122:LEU:HB3	5:F:127:ILE:HD11	1.72	0.71
1:B:124:ASN:HB2	1:B:127:LEU:HG	1.70	0.71
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.70	0.71
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.71	0.71
1:A:104:GLU:HG2	1:A:137:ARG:HD3	1.72	0.71
3:D:169:TYR:HE1	3:D:395:VAL:HG12	1.56	0.71
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.71	0.71
1:A:39:PRO:O	1:A:43:ILE:HG13	1.91	0.71
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.24	0.71
3:D:218:LYS:CE	3:D:338:GLU:HA	2.21	0.71
3:D:1305:LEU:HD21	3:D:1309:ALA:HB3	1.72	0.71
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.23	0.70
3:D:231:VAL:O	3:D:236:TYR:OH	2.08	0.70
3:D:408:GLU:HA	5:F:164:LYS:NZ	2.07	0.70
3:D:297:ILE:HD12	3:D:297:ILE:O	1.92	0.70
3:D:581:LEU:HD23	3:D:582:LEU:HD23	1.73	0.70
3:D:1267:ARG:NH1	3:D:1331:ASP:OD2	2.23	0.70
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.74	0.70
3:D:513:ILE:O	3:D:513:ILE:HD12	1.92	0.70
3:D:36:THR:HG23	3:D:38:LYS:N	2.02	0.70
3:D:116:LEU:HD21	3:D:465:LEU:CD2	2.22	0.70
3:D:809:PRO:HG3	3:D:829:VAL:HG11	1.74	0.70
1:B:101:LEU:HD21	1:B:113:ASP:O	1.92	0.69
3:D:1282:ARG:HA	3:D:1315:ASP:OD1	1.91	0.69
1:A:222:LEU:HD22	1:B:215:VAL:HG23	1.75	0.69
2:C:753:ASP:OD2	3:D:681:ARG:NH2	2.25	0.69
3:D:368:VAL:HG22	3:D:377:VAL:HG22	1.73	0.69
3:D:984:THR:HB	3:D:987:GLU:H	1.55	0.69
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.73	0.69
2:C:150:PRO:HA	2:C:158:TYR:CD1	2.26	0.69
2:C:242:LEU:N	2:C:242:LEU:HD22	2.08	0.69
1:A:101:LEU:HD12	1:A:114:PHE:CE1	2.28	0.69
3:D:64:LYS:O	3:D:65:ARG:HG3	1.93	0.69
2:C:495:THR:HG22	2:C:517:ARG:HD3	1.73	0.69
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.28	0.69
2:C:719:PRO:HB3	2:C:820:ARG:HH12	1.58	0.68
3:D:1294:VAL:O	3:D:1300:SER:HB3	1.93	0.68
2:C:13:ILE:HD12	2:C:14:PRO:CD	2.19	0.68
1:B:58:ILE:HG13	1:B:61:VAL:HG12	1.74	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:85:LEU:HD21	1:B:122:ILE:HG23	1.76	0.68
2:C:395:LYS:HD3	2:C:397:GLU:HB3	1.74	0.68
2:C:754:ILE:HG13	2:C:791:ARG:HE	1.58	0.68
2:C:890:LEU:HD21	2:C:901:TYR:CD2	2.28	0.68
3:D:218:LYS:HZ1	3:D:338:GLU:HB3	1.58	0.68
1:B:58:ILE:HD11	1:B:61:VAL:HB	1.75	0.68
3:D:413:ASP:N	5:F:178:ARG:HH22	1.92	0.68
5:F:363:GLU:O	5:F:367:MET:N	2.27	0.68
3:D:179:VAL:HG21	3:D:191:LEU:HD12	1.74	0.67
2:C:163:ILE:HG13	2:C:171:TRP:HD1	1.59	0.67
3:D:218:LYS:NZ	3:D:338:GLU:CB	2.56	0.67
3:D:411:THR:HA	3:D:435:VAL:HG13	1.76	0.67
3:D:371:ILE:HD13	3:D:372:ASP:N	2.09	0.67
3:D:245:LEU:HD12	3:D:309:GLY:O	1.94	0.67
5:F:365:GLU:HG2	5:F:403:LYS:HE3	1.76	0.67
2:C:535:SER:OG	2:C:537:LYS:HG3	1.95	0.67
3:D:992:ILE:CD1	3:D:1054:GLU:HB3	2.22	0.67
1:B:124:ASN:HD22	1:B:127:LEU:HD11	1.57	0.67
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.75	0.67
3:D:133:ILE:HD12	3:D:152:LEU:HB3	1.76	0.67
3:D:218:LYS:CE	3:D:338:GLU:HG2	2.22	0.67
3:D:1271:LYS:HD2	3:D:1331:ASP:HB2	1.77	0.67
2:C:244:PRO:O	5:F:82:ARG:NH1	2.27	0.67
3:D:218:LYS:HZ1	3:D:338:GLU:CB	2.08	0.67
3:D:485:SER:O	3:D:487:ALA:N	2.24	0.67
3:D:1019:PRO:O	3:D:1023:MET:HG3	1.95	0.67
3:D:1273:VAL:H	3:D:1326:THR:HG22	1.59	0.67
1:A:4:SER:O	1:A:189:ARG:NH1	2.27	0.66
2:C:189:ARG:NH1	2:C:242:LEU:O	2.27	0.66
2:C:390:GLN:NE2	2:C:414:GLY:HA2	2.09	0.66
2:C:835:VAL:HA	2:C:849:VAL:HG23	1.76	0.66
5:F:110:MET:HG2	5:F:128:ARG:HH22	1.60	0.66
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.11	0.66
3:D:1235:GLN:O	3:D:1236:LEU:HD12	1.96	0.66
1:A:211:LEU:O	1:A:215:VAL:HG12	1.95	0.66
2:C:241:LEU:CB	2:C:242:LEU:HD22	2.26	0.66
2:C:728:HIS:C	2:C:729:LEU:HD22	2.16	0.66
3:D:640:HIS:CD2	3:D:641:GLN:HG3	2.30	0.66
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.77	0.66
3:D:191:LEU:HD21	3:D:197:SER:CB	2.26	0.66
4:E:39:VAL:HG12	4:E:72:ARG:HH11	1.60	0.66



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:F:193:ARG:HB3	7:H:7:DG:H5'	1.78	0.66
2:C:154:ARG:NH2	2:C:175:GLU:OE2	2.29	0.66
2:C:615:TYR:HD2	2:C:619:ARG:HE	1.42	0.66
3:D:407:VAL:O	5:F:164:LYS:NZ	2.29	0.66
5:F:104:ARG:O	5:F:108:GLU:HG3	1.96	0.66
1:B:110:LYS:HZ2	1:B:112:ARG:HG3	1.59	0.66
3:D:1046:GLN:HE21	3:D:1076:GLY:HA3	1.60	0.66
2:C:168:ARG:NH2	2:C:265:ARG:O	2.29	0.65
2:C:503:LEU:CD1	2:C:508:ILE:HA	2.25	0.65
2:C:229:MET:CE	2:C:237:ARG:HE	2.08	0.65
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.65
2:C:913:GLU:O	2:C:917:LEU:HD12	1.95	0.65
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.10	0.65
1:B:153:ALA:O	1:B:155:LYS:N	2.29	0.65
2:C:233:GLU:OE1	2:C:233:GLU:N	2.20	0.65
3:D:93:ILE:HB	3:D:517:VAL:HG12	1.79	0.65
2:C:1047:HIS:CE1	3:D:1471:LEU:HD11	2.31	0.65
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.77	0.65
2:C:495:THR:HG22	2:C:517:ARG:CD	2.26	0.65
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.77	0.65
3:D:1151:ARG:HB3	3:D:1151:ARG:CZ	2.22	0.65
5:F:154:LYS:NZ	5:F:155:THR:HG22	2.12	0.65
3:D:218:LYS:CE	3:D:338:GLU:CA	2.75	0.65
3:D:762:GLN:OE1	4:E:20:THR:HG21	1.96	0.65
2:C:105:THR:HG23	2:C:106:GLY:H	1.60	0.65
2:C:884:GLN:O	2:C:888:THR:HG23	1.97	0.65
5:F:322:GLY:O	5:F:324:GLU:N	2.30	0.65
5:F:372:ARG:NH1	5:F:380:GLU:HA	2.10	0.64
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.79	0.64
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.77	0.64
3:D:1144:LEU:O	3:D:1147:ARG:HG3	1.96	0.64
5:F:363:GLU:OE1	5:F:363:GLU:HA	1.95	0.64
1:B:95:GLN:HE21	1:B:146:ARG:HD2	1.62	0.64
3:D:1033:GLN:N	3:D:1033:GLN:OE1	2.30	0.64
3:D:408:GLU:HA	5:F:164:LYS:HZ1	1.61	0.64
1:A:215:VAL:HG23	1:B:222:LEU:HD22	1.78	0.64
1:B:124:ASN:HD22	1:B:127:LEU:HD12	1.47	0.64
1:A:57:TYR:CE1	1:A:161:ARG:NH1	2.62	0.64
2:C:68:PHE:HA	2:C:98:LEU:CD1	2.16	0.64
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.79	0.64
3:D:1047:LYS:CD	3:D:1048:PRO:HG2	2.27	0.64



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:674:VAL:HG23	2:C:869:VAL:HG13	1.79	0.64
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.78	0.64
5:F:326:ASP:O	6:G:19:DA:N6	2.31	0.64
2:C:853:LEU:HB2	2:C:858:MET:CE	2.28	0.64
3:D:361:VAL:CG2	3:D:365:ASP:HB2	2.24	0.64
1:B:95:GLN:NE2	1:B:146:ARG:HD2	2.12	0.64
3:D:205:TYR:CD1	3:D:390:PRO:HB3	2.27	0.64
5:F:365:GLU:HG3	5:F:404:ALA:HB2	1.80	0.64
3:D:280:ALA:HB1	3:D:282:TYR:CE2	2.33	0.64
5:F:265:VAL:HG22	5:F:269:ASN:HD21	1.63	0.64
3:D:218:LYS:NZ	3:D:338:GLU:HB3	2.14	0.63
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.13	0.63
3:D:116:LEU:HD21	3:D:465:LEU:HD22	1.80	0.63
1:B:61:VAL:CG2	1:B:66:SER:HB2	2.29	0.63
5:F:122:LEU:CB	5:F:127:ILE:HD11	2.27	0.63
1:B:110:LYS:HZ1	1:B:112:ARG:HD2	1.63	0.63
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.81	0.63
4:E:80:VAL:HG21	4:E:85:LEU:HD11	1.80	0.63
5:F:101:GLU:O	5:F:105:LYS:HG3	1.97	0.63
1:B:124:ASN:ND2	1:B:127:LEU:CD1	2.53	0.63
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.80	0.63
3:D:218:LYS:HE2	3:D:338:GLU:CB	2.24	0.63
5:F:116:LEU:O	5:F:120:THR:OG1	2.08	0.63
5:F:132:ARG:HH21	5:F:184:ARG:CZ	2.11	0.63
2:C:238:LEU:O	2:C:242:LEU:CD2	2.47	0.63
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.81	0.63
3:D:1273:VAL:HG12	3:D:1326:THR:HG22	1.81	0.62
2:C:716:LYS:NZ	3:D:529:GLN:HE22	1.96	0.62
4:E:88:GLU:O	4:E:92:LEU:HD13	1.99	0.62
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.33	0.62
2:C:473:ARG:O	2:C:480:THR:HG22	1.99	0.62
3:D:631:ILE:CD1	3:D:745:MET:HB2	2.29	0.62
3:D:367:ILE:HB	3:D:377:VAL:HG23	1.82	0.62
5:F:269:ASN:O	5:F:273:ARG:HG3	2.00	0.62
1:B:72:LYS:HE2	1:B:133:GLU:HG3	1.82	0.61
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.30	0.61
2:C:163:ILE:HG13	2:C:171:TRP:CD1	2.34	0.61
2:C:495:THR:CG2	2:C:517:ARG:HE	2.13	0.61
2:C:946:ARG:HH12	3:D:861:GLN:HE22	1.46	0.61
3:D:808:THR:CG2	3:D:811:GLU:HB2	2.29	0.61
1:A:35:THR:OG1	1:B:42:ARG:HD3	2.01	0.61



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:937:ASP:HB3	2:C:940:GLU:HG3	1.82	0.61
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.83	0.61
8:I:3:G:N3	8:I:4:G:N2	2.48	0.61
2:C:238:LEU:O	2:C:242:LEU:HD23	2.00	0.61
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.81	0.61
3:D:116:LEU:HB3	3:D:118:LEU:HD13	1.81	0.61
3:D:412:GLY:N	5:F:178:ARG:NH2	2.47	0.61
2:C:390:GLN:HE21	2:C:414:GLY:HA2	1.65	0.61
3:D:1151:ARG:CZ	3:D:1151:ARG:CB	2.78	0.61
2:C:1101:THR:OG1	2:C:1111:ILE:CD1	2.43	0.61
3:D:530:VAL:HG22	3:D:531:ASP:H	1.64	0.61
1:A:57:TYR:CD1	1:A:161:ARG:CZ	2.84	0.61
2:C:97:ARG:NH1	2:C:112:GLU:OE2	2.34	0.61
2:C:390:GLN:O	2:C:390:GLN:HG2	2.01	0.61
2:C:545:ASN:O	2:C:581:THR:HG21	2.01	0.61
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.83	0.61
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.81	0.61
1:A:85:LEU:HD21	1:A:87:VAL:CG1	2.31	0.61
2:C:468:ARG:NH2	2:C:490:GLU:OE2	2.34	0.61
3:D:258:VAL:HG12	3:D:297:ILE:HG22	1.83	0.61
3:D:500:ARG:NH1	3:D:1390:LEU:HD11	2.15	0.61
3:D:761:ILE:HD12	4:E:20:THR:HB	1.83	0.61
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.83	0.60
2:C:241:LEU:HB2	2:C:242:LEU:HD22	1.83	0.60
2:C:640:ARG:HD3	2:C:642:ARG:HH22	1.64	0.60
3:D:286:VAL:O	3:D:311:LEU:HD12	2.01	0.60
3:D:671:LYS:HE3	5:F:421:PHE:HA	1.83	0.60
3:D:956:ILE:HD13	3:D:1039:CYS:O	2.01	0.60
2:C:598:GLU:HG3	2:C:623:TYR:OH	2.01	0.60
5:F:185:GLN:O	5:F:189:GLU:HG3	2.01	0.60
3:D:199:LEU:HD11	3:D:397:LYS:HD2	1.83	0.60
3:D:500:ARG:HH11	3:D:1390:LEU:HD11	1.66	0.60
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.34	0.60
2:C:64:LEU:N	2:C:103:LYS:HB3	2.17	0.60
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.84	0.60
1:B:110:LYS:NZ	1:B:112:ARG:HG3	2.16	0.60
1:B:206:THR:HG22	1:B:209:GLU:CB	2.31	0.60
2:C:277:ALA:O	2:C:281:LEU:HD12	2.02	0.60
3:D:199:LEU:HD21	3:D:397:LYS:HG3	1.84	0.60
8:I:2:G:N3	8:I:2:G:H2'	2.16	0.60
2:C:711:GLU:O	2:C:758:ARG:NH1	2.33	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:572:ARG:HH12	5:F:83:GLN:CG	2.07	0.60
1:B:206:THR:HG22	1:B:209:GLU:CG	2.32	0.60
3:D:631:ILE:HD11	3:D:745:MET:CB	2.31	0.60
3:D:631:ILE:HG22	3:D:740:PHE:CE2	2.37	0.60
2:C:727:PRO:O	2:C:729:LEU:HD23	2.01	0.59
2:C:607:ASP:CB	2:C:610:ARG:HG3	2.31	0.59
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.00	0.59
1:B:64:GLU:HG2	1:B:76:VAL:HG12	1.84	0.59
3:D:208:PRO:HG3	3:D:387:LEU:HD12	1.84	0.59
3:D:988:ARG:HG3	3:D:989:TYR:N	2.17	0.59
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.34	0.59
3:D:410:SER:O	3:D:435:VAL:HG11	2.03	0.59
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.01	0.59
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.85	0.59
2:C:154:ARG:CZ	2:C:175:GLU:OE2	2.51	0.59
2:C:501:THR:O	2:C:503:LEU:HD22	2.01	0.59
5:F:109:GLY:O	5:F:113:ILE:HG13	2.02	0.59
2:C:723:THR:O	2:C:741:GLY:HA3	2.03	0.59
4:E:30:LEU:HD12	4:E:30:LEU:N	2.18	0.59
5:F:164:LYS:HZ2	5:F:171:LYS:HE3	1.67	0.59
5:F:372:ARG:HH22	5:F:380:GLU:HB3	1.68	0.59
2:C:586:ARG:O	2:C:586:ARG:HG3	2.00	0.59
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.38	0.59
3:D:65:ARG:NH2	5:F:376:ILE:HA	2.17	0.59
3:D:241:ILE:HD11	3:D:310:LEU:CD1	2.31	0.59
3:D:1405:GLU:OE2	3:D:1409:ALA:N	2.35	0.59
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.84	0.59
1:A:18:ARG:O	1:A:201:THR:HG21	2.02	0.58
3:D:65:ARG:HH21	5:F:376:ILE:HA	1.68	0.58
3:D:288:MET:HB2	3:D:311:LEU:HD11	1.85	0.58
5:F:376:ILE:O	5:F:377:ASP:HB3	2.03	0.58
1:B:86:VAL:HG13	1:B:123:MET:HB2	1.84	0.58
2:C:436:GLY:HA2	2:C:538:GLN:O	2.02	0.58
2:C:238:LEU:O	2:C:241:LEU:HB2	2.03	0.58
2:C:768:THR:HG23	2:C:771:GLU:H	1.66	0.58
3:D:184:GLU:N	3:D:184:GLU:OE1	2.36	0.58
3:D:209:ARG:CA	3:D:347:VAL:HG12	2.29	0.58
4:E:26:ARG:HD3	4:E:30:LEU:CD1	2.31	0.58
3:D:82:LYS:HB2	3:D:84:ILE:HG22	1.86	0.58
2:C:711:GLU:HB2	2:C:713:ARG:HH21	1.68	0.58
2:C:890:LEU:HD21	2:C:901:TYR:CG	2.38	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:985:ASP:HA	3:D:988:ARG:HG2	1.86	0.58
5:F:361:LEU:HD13	5:F:407:LYS:HB3	1.84	0.58
1:A:85:LEU:CD2	1:A:87:VAL:HG13	2.32	0.58
1:B:85:LEU:HD22	1:B:87:VAL:HG13	1.86	0.58
2:C:162:ILE:HD13	2:C:290:LEU:HD21	1.85	0.58
2:C:290:LEU:N	2:C:290:LEU:HD12	2.18	0.58
3:D:174:GLY:N	3:D:209:ARG:HH12	1.97	0.58
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.86	0.58
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.03	0.58
2:C:745:ILE:HD12	2:C:745:ILE:H	1.68	0.58
1:A:44:LEU:O	1:A:174:VAL:HG11	2.04	0.58
3:D:465:LEU:N	3:D:465:LEU:HD23	2.18	0.58
2:C:719:PRO:CB	2:C:820:ARG:HH12	2.15	0.58
3:D:218:LYS:HZ1	3:D:339:TRP:N	1.99	0.58
3:D:1495:ILE:O	3:D:1499:ARG:HG3	2.04	0.58
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.68	0.57
1:B:110:LYS:NZ	1:B:112:ARG:HD2	2.18	0.57
2:C:15:LEU:O	2:C:586:ARG:NH2	2.31	0.57
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.68	0.57
3:D:1272:ALA:HA	3:D:1326:THR:HG23	1.85	0.57
5:F:398:ARG:O	5:F:398:ARG:NH1	2.37	0.57
6:G:5:DT:H2"	6:G:6:DG:C8	2.39	0.57
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.86	0.57
5:F:162:LYS:HE2	5:F:165:SER:HB2	1.86	0.57
5:F:230:LYS:O	5:F:232:ARG:CD	2.47	0.57
3:D:352:ASN:HB3	5:F:104:ARG:CZ	2.34	0.57
2:C:173:ASP:HB2	2:C:185:LYS:HE3	1.86	0.57
3:D:165:LYS:HD2	3:D:166:GLN:H	1.69	0.57
3:D:312:ARG:NH1	3:D:315:ARG:HH22	2.03	0.57
2:C:209:ARG:HG3	2:C:210:GLU:N	2.19	0.57
3:D:218:LYS:HZ2	3:D:338:GLU:CA	1.99	0.57
3:D:218:LYS:HE2	3:D:338:GLU:CG	2.32	0.57
2:C:475:VAL:O	2:C:477:GLY:N	2.37	0.57
5:F:111:GLU:HA	5:F:114:LYS:HG2	1.87	0.57
5:F:91:VAL:O	5:F:193:ARG:NH2	2.33	0.57
1:A:64:GLU:O	1:A:75:VAL:HG13	2.05	0.57
1:B:94:LEU:HD11	1:B:96:THR:O	2.05	0.57
2:C:272:ALA:HA	2:C:464:LEU:HD13	1.86	0.57
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.86	0.57
3:D:1048:PRO:HD3	3:D:1075:HIS:ND1	2.19	0.57
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.07	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:34:VAL:HG23	2:C:39:ARG:HG2	1.86	0.56
2:C:179:ASN:ND2	2:C:181:VAL:HG12	2.19	0.56
3:D:218:LYS:HE3	3:D:338:GLU:HA	1.87	0.56
1:A:201:THR:HG23	1:A:203:GLY:H	1.70	0.56
2:C:367:LEU:CD1	2:C:371:LYS:HZ2	2.16	0.56
2:C:650:ARG:HH11	2:C:650:ARG:HB2	1.70	0.56
3:D:956:ILE:CD1	3:D:1039:CYS:O	2.53	0.56
1:B:38:ASN:O	1:B:42:ARG:HG3	2.06	0.56
2:C:249:LYS:HB2	2:C:252:LYS:HG2	1.86	0.56
2:C:1060:ILE:HD11	2:C:1083:GLU:HG2	1.87	0.56
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.69	0.56
3:D:122:GLU:HG2	3:D:152:LEU:HD21	1.88	0.56
3:D:170:PRO:HA	3:D:392:SER:OG	2.04	0.56
3:D:347:VAL:CG2	3:D:351:MET:HG3	2.36	0.56
3:D:628:ARG:NH2	3:D:746:ALA:HB2	2.17	0.56
5:F:398:ARG:HH12	5:F:402:ASN:ND2	2.03	0.56
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.86	0.56
1:B:41:ARG:HG3	1:B:177:VAL:CG2	2.35	0.56
2:C:916:GLU:O	2:C:920:GLN:HG3	2.06	0.56
2:C:366:SER:O	2:C:367:LEU:HD12	2.06	0.56
1:B:132:LEU:HD21	1:B:136:GLY:HA3	1.88	0.56
3:D:565:ILE:HD12	3:D:565:ILE:H	1.70	0.56
1:B:110:LYS:NZ	1:B:112:ARG:CG	2.69	0.56
1:B:132:LEU:HD21	1:B:136:GLY:CA	2.35	0.56
2:C:198:ARG:HH22	2:C:230:ARG:HA	1.70	0.56
3:D:699:VAL:N	3:D:756:GLN:OE1	2.36	0.56
3:D:1047:LYS:HD3	3:D:1048:PRO:HG2	1.88	0.56
5:F:91:VAL:HG11	5:F:189:GLU:O	2.05	0.56
5:F:154:LYS:HD3	5:F:155:THR:HG22	1.87	0.56
1:B:58:ILE:HD13	1:B:68:ILE:HD11	1.88	0.55
1:B:153:ALA:C	1:B:155:LYS:H	2.09	0.55
2:C:146:VAL:HG13	2:C:162:ILE:HG22	1.88	0.55
2:C:238:LEU:HG	2:C:242:LEU:HD21	1.88	0.55
4:E:57:ASP:O	4:E:63:TRP:NE1	2.38	0.55
2:C:668:LEU:HD12	2:C:668:LEU:H	1.70	0.55
3:D:258:VAL:HG22	3:D:273:ARG:O	2.06	0.55
3:D:272:LEU:HD21	3:D:298:VAL:CG1	2.36	0.55
1:B:101:LEU:HG	1:B:114:PHE:HA	1.88	0.55
1:B:170:VAL:HG11	3:D:848:GLU:HG3	1.87	0.55
2:C:14:PRO:HB2	2:C:586:ARG:NH2	2.21	0.55
3:D:405:ASP:CG	3:D:406:ASP:H	2.10	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.89	0.55
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.88	0.55
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.87	0.55
2:C:1101:THR:HB	3:D:5:VAL:HG13	1.89	0.55
2:C:750:LYS:HE3	3:D:680:GLN:OE1	2.07	0.55
3:D:173:PRO:HA	3:D:209:ARG:NH2	2.17	0.55
3:D:508:ARG:NH1	3:D:509:PRO:HD2	2.22	0.55
2:C:376:ARG:HE	5:F:276:ARG:HG2	1.71	0.55
2:C:602:GLU:CG	2:C:648:ARG:HE	2.19	0.55
3:D:203:ALA:O	3:D:204:LEU:HD23	2.07	0.55
3:D:1372:VAL:HA	3:D:1375:MET:SD	2.47	0.55
1:A:57:TYR:CG	1:A:161:ARG:CZ	2.89	0.55
1:B:58:ILE:HG22	1:B:140:MET:HB3	1.88	0.55
1:B:208:LEU:H	1:B:208:LEU:HD23	1.72	0.55
3:D:95:LEU:HD22	3:D:574:LEU:HD21	1.89	0.55
3:D:185:VAL:HG13	3:D:189:GLN:HB3	1.89	0.55
3:D:326:GLU:N	3:D:326:GLU:OE2	2.40	0.55
3:D:348:GLN:HB2	3:D:351:MET:CE	2.37	0.55
3:D:704:ARG:HB2	3:D:745:MET:CE	2.37	0.55
5:F:232:ARG:HG2	5:F:232:ARG:HH11	1.72	0.55
1:B:85:LEU:HD22	1:B:87:VAL:CG1	2.36	0.54
3:D:481:MET:O	3:D:489:ARG:HD3	2.08	0.54
1:B:108:GLU:HA	1:B:131:THR:HA	1.90	0.54
3:D:669:ASN:HB3	5:F:417:LYS:HE2	1.88	0.54
3:D:808:THR:HG23	3:D:811:GLU:H	1.72	0.54
3:D:875:THR:HG21	3:D:902:LEU:CD2	2.36	0.54
3:D:881:LEU:O	3:D:885:ILE:HG12	2.07	0.54
3:D:886:VAL:O	3:D:890:VAL:HG23	2.08	0.54
3:D:1145:TYR:CD1	3:D:1168:MET:HE2	2.43	0.54
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.87	0.54
1:A:87:VAL:CG2	1:A:144:VAL:HG11	2.37	0.54
1:A:201:THR:HG23	1:A:203:GLY:N	2.22	0.54
3:D:317:VAL:HG12	3:D:339:TRP:CB	2.36	0.54
3:D:666:ILE:HD11	3:D:684:LYS:HZ2	1.72	0.54
5:F:401:GLU:O	5:F:405:LEU:HD13	2.07	0.54
3:D:100:ALA:HA	3:D:513:ILE:HG22	1.88	0.54
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.89	0.54
3:D:1047:LYS:CE	3:D:1048:PRO:HD2	2.35	0.54
1:A:99:LEU:CD1	1:A:114:PHE:HB3	2.34	0.54
3:D:171:LEU:HD11	3:D:390:PRO:O	2.07	0.54
3:D:181:ASP:CB	3:D:205:TYR:HD2	2.15	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:554:LEU:HB2	3:D:570:GLU:HG2	1.88	0.54
3:D:1046:GLN:NE2	3:D:1076:GLY:HA3	2.23	0.54
5:F:299:TRP:HA	5:F:303:ARG:HD3	1.89	0.54
1:B:206:THR:HG22	1:B:209:GLU:CD	2.28	0.54
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.90	0.54
2:C:480:THR:HG21	2:C:482:GLU:HG2	1.89	0.54
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.90	0.54
2:C:1111:ILE:HD12	2:C:1111:ILE:H	1.73	0.54
3:D:661:MET:CE	3:D:677:LEU:HD11	2.38	0.54
5:F:129:GLU:HG3	5:F:147:LEU:HD21	1.90	0.54
1:A:57:TYR:CE1	1:A:161:ARG:NH2	2.72	0.54
3:D:890:VAL:HG13	3:D:922:LEU:HD13	1.87	0.54
3:D:361:VAL:O	3:D:382:GLU:HA	2.08	0.54
3:D:544:TYR:O	3:D:548:ILE:HG13	2.08	0.54
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.88	0.54
1:B:72:LYS:HG3	1:B:131:THR:OG1	2.07	0.54
3:D:200:ASP:O	3:D:397:LYS:HG2	2.08	0.54
3:D:661:MET:HE2	3:D:677:LEU:HD11	1.90	0.54
3:D:1295:GLU:OE2	3:D:1300:SER:HB2	2.08	0.54
5:F:164:LYS:NZ	5:F:171:LYS:HE3	2.23	0.54
5:F:277:GLN:O	5:F:281:GLU:HG2	2.07	0.54
3:D:275:GLU:OE1	3:D:275:GLU:N	2.40	0.54
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.89	0.54
5:F:132:ARG:HH21	5:F:184:ARG:NH2	2.06	0.54
1:B:110:LYS:HZ1	1:B:112:ARG:CD	2.20	0.53
2:C:64:LEU:HA	2:C:103:LYS:H	1.72	0.53
2:C:816:LYS:O	2:C:819:VAL:HG12	2.08	0.53
3:D:135:LEU:O	3:D:149:LYS:CE	2.42	0.53
3:D:695:ILE:HD12	3:D:718:PRO:HG2	1.90	0.53
3:D:1273:VAL:H	3:D:1326:THR:CG2	2.20	0.53
2:C:179:ASN:HD21	2:C:181:VAL:HG12	1.71	0.53
2:C:227:PHE:O	2:C:229:MET:N	2.41	0.53
2:C:666:LEU:HG	2:C:668:LEU:HD11	1.91	0.53
3:D:828:LYS:CD	3:D:833:GLU:CB	2.86	0.53
2:C:3:ILE:HA	2:C:900:ARG:O	2.08	0.53
2:C:280:LYS:HE3	2:C:323:ASP:CG	2.28	0.53
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.42	0.53
3:D:669:ASN:ND2	5:F:417:LYS:HG2	2.24	0.53
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.90	0.53
2:C:262:ALA:HA	2:C:289:THR:OG1	2.07	0.53
3:D:936:TYR:O	3:D:940:THR:HG23	2.08	0.53



	1 +	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:1286:THR:HG22	3:D:1287:GLU:H	1.74	0.53
2:C:97:ARG:O	2:C:98:LEU:HD13	2.09	0.53
2:C:890:LEU:CD2	2:C:901:TYR:CD2	2.92	0.53
1:B:132:LEU:HD23	1:B:133:GLU:N	2.24	0.53
2:C:367:LEU:CA	2:C:371:LYS:HE3	2.21	0.53
2:C:495:THR:HG22	2:C:517:ARG:NE	2.23	0.53
2:C:683:ASN:CB	2:C:872:ASN:HD22	2.22	0.53
2:C:1109:VAL:O	2:C:1111:ILE:HD12	2.08	0.53
3:D:15:PRO:O	3:D:19:ARG:HG3	2.08	0.53
3:D:666:ILE:CD1	3:D:684:LYS:HZ2	2.21	0.53
3:D:675:ARG:HH22	5:F:420:ASP:CA	2.20	0.53
3:D:865:THR:HG22	3:D:874:GLU:HG2	1.91	0.53
1:B:68:ILE:HB	1:B:71:VAL:HG22	1.90	0.53
7:H:17:DT:H2'	7:H:18:DG:C8	2.44	0.53
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.91	0.53
1:A:70:GLY:N	2:C:607:ASP:OD1	2.42	0.53
1:B:110:LYS:HZ1	1:B:112:ARG:CG	2.22	0.53
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.41	0.53
3:D:142:LEU:HD12	3:D:161:LEU:CD1	2.33	0.53
3:D:657:LEU:HG	3:D:661:MET:CE	2.39	0.53
5:F:278:LEU:C	5:F:282:LEU:HD12	2.29	0.53
2:C:595:LEU:C	2:C:596:TYR:HD1	2.13	0.53
2:C:1100:GLN:OE1	2:C:1108:PRO:HB3	2.08	0.53
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.90	0.53
2:C:102:HIS:HE1	2:C:365:ASP:HA	1.73	0.53
2:C:473:ARG:NE	2:C:482:GLU:OE2	2.33	0.53
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.23	0.53
3:D:1155:VAL:HG11	3:D:1177:ALA:CB	2.38	0.53
5:F:154:LYS:HD3	5:F:155:THR:CG2	2.38	0.53
5:F:398:ARG:NH2	5:F:399:GLN:HG3	2.24	0.53
1:B:216:GLU:OE1	1:B:219:ARG:NE	2.43	0.52
2:C:97:ARG:HG2	2:C:112:GLU:HB2	1.90	0.52
2:C:229:MET:HE1	2:C:237:ARG:HE	1.73	0.52
3:D:361:VAL:HG23	3:D:365:ASP:CB	2.30	0.52
3:D:491:LYS:HD2	3:D:494:LYS:HE3	1.90	0.52
3:D:1286:THR:HG22	3:D:1287:GLU:N	2.24	0.52
3:D:1487:VAL:HG23	4:E:74:VAL:HG13	1.91	0.52
5:F:106:VAL:O	5:F:110:MET:HG3	2.10	0.52
1:A:209:GLU:O	1:A:213:GLN:HG2	2.09	0.52
2:C:492:ASP:HB3	2:C:518:LYS:HG2	1.92	0.52
3:D:581:LEU:O	3:D:603:LEU:HD12	2.09	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:473:ARG:HB3	2:C:480:THR:HG21	1.91	0.52
2:C:495:THR:HG22	2:C:517:ARG:HE	1.74	0.52
2:C:654:LEU:HD11	2:C:656:ALA:O	2.09	0.52
3:D:809:PRO:O	3:D:813:LEU:HD12	2.09	0.52
3:D:1033:GLN:CD	3:D:1033:GLN:H	2.13	0.52
1:A:110:LYS:HD3	1:A:128:HIS:HA	1.91	0.52
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.92	0.52
2:C:911:GLU:O	2:C:915:LYS:HG2	2.10	0.52
3:D:1290:LEU:HD12	3:D:1307:LYS:HD3	1.90	0.52
2:C:154:ARG:CB	2:C:157:ARG:HG2	2.40	0.52
2:C:470:PRO:HD3	2:C:485:TYR:CE1	2.44	0.52
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.91	0.52
3:D:1492:LEU:CD1	3:D:1493:LYS:HE2	2.39	0.52
4:E:26:ARG:CD	4:E:30:LEU:HD11	2.36	0.52
4:E:39:VAL:HG12	4:E:72:ARG:NH1	2.25	0.52
1:B:14:ARG:HG2	1:B:14:ARG:HH11	1.74	0.52
1:B:31:GLY:N	1:B:193:ASP:OD1	2.43	0.52
3:D:191:LEU:HD21	3:D:197:SER:HB3	1.91	0.52
3:D:1287:GLU:C	3:D:1307:LYS:HZ2	2.12	0.52
5:F:256:ARG:HH21	5:F:258:ILE:HD11	1.74	0.52
2:C:214:TYR:O	2:C:218:VAL:HG23	2.09	0.52
2:C:611:ILE:O	2:C:611:ILE:HG13	2.09	0.52
2:C:793:PRO:HG2	2:C:796:GLU:OE1	2.10	0.52
3:D:804:LEU:O	3:D:827:ILE:HG23	2.10	0.52
1:A:65:PHE:CE2	2:C:703:ILE:HD13	2.45	0.52
2:C:154:ARG:HB3	2:C:157:ARG:HG2	1.91	0.52
2:C:727:PRO:HB2	2:C:728:HIS:CD2	2.45	0.52
3:D:750:PRO:O	3:D:756:GLN:NE2	2.43	0.52
3:D:828:LYS:NZ	3:D:833:GLU:HB2	2.25	0.52
3:D:1047:LYS:HZ2	3:D:1048:PRO:HG2	1.73	0.52
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.90	0.52
5:F:96:LEU:O	5:F:100:VAL:HG12	2.10	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.91	0.52
1:A:57:TYR:CG	1:A:161:ARG:NH2	2.77	0.51
2:C:179:ASN:CG	2:C:181:VAL:H	2.12	0.51
2:C:603:VAL:HA	2:C:613:VAL:HG23	1.91	0.51
2:C:758:ARG:HH21	2:C:788:THR:HG22	1.74	0.51
3:D:65:ARG:HH21	5:F:377:ASP:N	2.01	0.51
3:D:470:LEU:HB2	3:D:503:LEU:HD21	1.91	0.51
3:D:1486:VAL:HG13	4:E:29:GLN:NE2	2.24	0.51
5:F:403:LYS:O	5:F:407:LYS:HB2	2.10	0.51



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:101:LEU:HD11	1:A:109:VAL:HG11	1.92	0.51
1:B:58:ILE:HG22	1:B:140:MET:CB	2.39	0.51
1:B:107:LYS:HE2	1:B:108:GLU:O	2.11	0.51
2:C:1055:LEU:HD13	2:C:1079:PRO:HB3	1.91	0.51
2:C:764:GLU:HA	2:C:766:GLU:OE1	2.10	0.51
2:C:770:GLU:OE2	2:C:770:GLU:N	2.37	0.51
2:C:788:THR:HG22	2:C:788:THR:O	2.10	0.51
5:F:166:LEU:HB2	5:F:171:LYS:CG	2.41	0.51
1:A:9:PRO:HD2	1:B:224:TYR:CD1	2.46	0.51
3:D:116:LEU:CD1	3:D:465:LEU:HD21	2.34	0.51
3:D:178:LEU:HD23	3:D:190:GLU:OE1	2.10	0.51
3:D:371:ILE:CD1	3:D:372:ASP:CB	2.87	0.51
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.40	0.51
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.93	0.51
2:C:263:ASP:O	2:C:265:ARG:N	2.40	0.51
3:D:93:ILE:HB	3:D:517:VAL:CG1	2.40	0.51
3:D:413:ASP:H	5:F:178:ARG:NH2	2.04	0.51
2:C:412:ALA:O	2:C:417:GLY:HA3	2.11	0.51
5:F:349:LEU:HD22	5:F:421:PHE:HZ	1.76	0.51
2:C:236:ILE:O	2:C:240:THR:HG23	2.11	0.51
3:D:208:PRO:O	3:D:347:VAL:CG1	2.54	0.51
3:D:285:PRO:HG2	3:D:311:LEU:HG	1.92	0.51
3:D:702:LEU:O	3:D:713:ILE:HA	2.11	0.51
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.46	0.51
3:D:374:GLU:OE2	3:D:374:GLU:N	2.31	0.51
3:D:522:PRO:HA	3:D:525:ARG:HG3	1.92	0.51
6:G:12:DG:H5"	6:G:12:DG:H8	1.76	0.51
3:D:527:MET:HE2	3:D:537:THR:HB	1.92	0.51
2:C:502:PRO:O	2:C:503:LEU:HD13	2.11	0.51
2:C:1031:ARG:HB2	3:D:622:ARG:NH1	2.26	0.51
3:D:258:VAL:O	3:D:272:LEU:HA	2.11	0.51
4:E:33:HIS:O	4:E:36:LYS:HG3	2.11	0.51
2:C:267:TYR:CE1	2:C:290:LEU:HD11	2.46	0.50
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.93	0.50
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.27	0.50
2:C:768:THR:OG1	2:C:770:GLU:OE2	2.30	0.50
3:D:657:LEU:HG	3:D:661:MET:HE2	1.93	0.50
3:D:1485:GLN:O	4:E:75:PHE:HA	2.11	0.50
5:F:162:LYS:HE2	5:F:162:LYS:HA	1.92	0.50
5:F:394:ARG:NH1	5:F:395:GLU:OE2	2.44	0.50
1:A:79:ILE:HD11	1:A:167:VAL:HG22	1.91	0.50



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.46	0.50
3:D:65:ARG:NH2	5:F:377:ASP:H	2.05	0.50
3:D:988:ARG:O	3:D:992:ILE:HG23	2.10	0.50
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.11	0.50
5:F:129:GLU:HA	5:F:132:ARG:HB2	1.92	0.50
1:A:9:PRO:HB3	1:A:27:PRO:O	2.12	0.50
1:A:19:GLU:HA	1:A:201:THR:CG2	2.41	0.50
2:C:589:ARG:NE	2:C:596:TYR:HE2	2.05	0.50
3:D:288:MET:HA	3:D:306:GLU:O	2.11	0.50
3:D:631:ILE:HD11	3:D:745:MET:CG	2.41	0.50
3:D:1280:VAL:HG12	3:D:1318:TYR:HA	1.93	0.50
2:C:64:LEU:HD13	2:C:102:HIS:CD2	2.47	0.50
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.93	0.50
2:C:575:GLN:HG3	2:C:670:GLN:HA	1.92	0.50
1:A:65:PHE:HE2	2:C:703:ILE:HD13	1.76	0.50
2:C:286:SER:OG	2:C:301:GLU:OE1	2.28	0.50
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.46	0.50
3:D:124:GLU:OE2	3:D:128:TYR:CD1	2.64	0.50
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.93	0.50
1:A:170:VAL:O	1:A:170:VAL:HG23	2.12	0.50
1:B:112:ARG:CG	1:B:125:PRO:HB2	2.35	0.50
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.94	0.50
2:C:1067:TYR:CZ	5:F:342:VAL:HG12	2.46	0.50
3:D:412:GLY:CA	5:F:178:ARG:NH2	2.74	0.50
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.46	0.50
2:C:650:ARG:HB2	2:C:650:ARG:NH1	2.26	0.50
3:D:1159:ARG:HG3	3:D:1159:ARG:O	2.11	0.50
2:C:283:ILE:HD13	2:C:305:PRO:HB3	1.94	0.50
6:G:12:DG:N2	7:H:17:DT:O2	2.45	0.50
2:C:31:GLN:HB3	2:C:34:VAL:HG22	1.94	0.49
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.47	0.49
3:D:695:ILE:CD1	3:D:720:LEU:HD11	2.42	0.49
1:A:19:GLU:CA	1:A:201:THR:HG22	2.39	0.49
2:C:1111:ILE:HD12	2:C:1111:ILE:N	2.27	0.49
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.94	0.49
2:C:719:PRO:HB3	2:C:820:ARG:HH22	1.77	0.49
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.94	0.49
3:D:1289:LYS:C	3:D:1307:LYS:HE2	2.33	0.49
5:F:154:LYS:O	5:F:158:GLU:HG2	2.12	0.49
1:A:74:ASP:HB3	2:C:627:ARG:NH2	2.28	0.49
3:D:1305:LEU:HD23	3:D:1306:PRO:O	2.12	0.49



	h h h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:D:1364:HIS:CE1	3:D:1366:LYS:HB2	2.47	0.49
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.95	0.49
2:C:69:LEU:HB2	2:C:97:ARG:O	2.13	0.49
2:C:835:VAL:HA	2:C:849:VAL:CG2	2.42	0.49
2:C:877:PRO:HG3	3:D:1023:MET:CE	2.42	0.49
3:D:218:LYS:HE3	3:D:338:GLU:CB	2.35	0.49
3:D:362:GLU:HG3	3:D:363:ALA:N	2.27	0.49
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.49
3:D:513:ILE:HD12	3:D:513:ILE:C	2.31	0.49
4:E:30:LEU:HD12	4:E:30:LEU:H	1.78	0.49
5:F:128:ARG:NH1	5:F:181:GLU:OE1	2.45	0.49
5:F:265:VAL:HG22	5:F:269:ASN:ND2	2.28	0.49
2:C:209:ARG:NE	2:C:210:GLU:OE1	2.45	0.49
2:C:597:ALA:HB2	2:C:655:LEU:HD11	1.94	0.49
2:C:719:PRO:HB3	2:C:820:ARG:NH1	2.26	0.49
3:D:82:LYS:O	3:D:85:VAL:HG22	2.13	0.49
3:D:102:ILE:HB	3:D:579:ASP:OD2	2.12	0.49
3:D:581:LEU:O	3:D:602:SER:HB2	2.12	0.49
3:D:810:GLU:OE2	3:D:810:GLU:N	2.30	0.49
3:D:907:GLU:OE2	3:D:910:SER:N	2.33	0.49
4:E:39:VAL:CG1	4:E:72:ARG:HH11	2.25	0.49
5:F:365:GLU:OE2	5:F:365:GLU:HA	2.13	0.49
2:C:148:PHE:HD1	2:C:280:LYS:NZ	2.11	0.49
2:C:640:ARG:HB2	2:C:642:ARG:NH2	2.28	0.49
2:C:838:LYS:HE3	3:D:741:ASP:O	2.12	0.49
2:C:97:ARG:HG2	2:C:112:GLU:CB	2.43	0.49
2:C:633:GLN:N	2:C:633:GLN:OE1	2.46	0.49
5:F:349:LEU:HD22	5:F:421:PHE:CZ	2.48	0.49
2:C:682:TYR:CE1	3:D:635:PRO:HD2	2.48	0.49
5:F:166:LEU:HB2	5:F:171:LYS:HG3	1.94	0.49
1:B:220:GLU:O	1:B:223:THR:OG1	2.24	0.48
2:C:97:ARG:HH11	2:C:97:ARG:HG3	1.78	0.48
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.93	0.48
2:C:890:LEU:HD21	2:C:901:TYR:CE2	2.47	0.48
3:D:34:TYR:CB	5:F:260:ILE:HG22	2.43	0.48
3:D:66:GLN:HB3	5:F:376:ILE:CG2	2.43	0.48
3:D:270:LEU:HB2	3:D:284:LEU:HD11	1.95	0.48
3:D:553:ARG:HG3	3:D:557:LEU:HD13	1.95	0.48
3:D:695:ILE:HD11	3:D:720:LEU:HD11	1.95	0.48
3:D:1165:TYR:CE1	3:D:1214:PRO:HB3	2.48	0.48
5:F:162:LYS:CE	5:F:165:SER:HB2	2.43	0.48



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (\AA)
5:F:229:TYR:CE1	5:F:230:LYS:HD3	2.47	0.48
2:C:157:ARG:HD2	2:C:157:ARG:N	2.27	0.48
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.94	0.48
2:C:1009:SER:O	3:D:624:ASP:HB3	2.13	0.48
3:D:207:PHE:CE2	5:F:97:GLU:HB2	2.48	0.48
5:F:365:GLU:CD	5:F:400:ILE:HB	2.33	0.48
1:A:66:SER:O	1:A:75:VAL:HG12	2.13	0.48
1:A:85:LEU:C	1:A:85:LEU:HD23	2.34	0.48
3:D:33:ASN:HB2	3:D:40:GLU:OE2	2.12	0.48
3:D:191:LEU:HD21	3:D:197:SER:HB2	1.96	0.48
3:D:556:LYS:NZ	5:F:222:ARG:HH21	2.11	0.48
5:F:398:ARG:O	5:F:401:GLU:HB3	2.13	0.48
1:A:103:ALA:O	1:A:104:GLU:HG3	2.12	0.48
1:A:111:ALA:O	1:A:114:PHE:HD2	1.95	0.48
1:B:206:THR:HG23	1:B:209:GLU:H	1.79	0.48
2:C:234:ALA:O	2:C:237:ARG:HB2	2.14	0.48
2:C:243:ARG:HD3	2:C:256:TYR:CE2	2.48	0.48
3:D:137:PRO:HA	3:D:452:ILE:CD1	2.42	0.48
3:D:437:VAL:HG21	5:F:175:HIS:CE1	2.48	0.48
5:F:386:VAL:HG13	5:F:390:PHE:CE1	2.48	0.48
3:D:179:VAL:HG12	3:D:180:LYS:N	2.29	0.48
3:D:828:LYS:HZ2	3:D:833:GLU:HB2	1.79	0.48
5:F:234:LYS:HD2	7:H:5:DA:OP2	2.12	0.48
1:A:97:VAL:HG13	1:A:98:THR:N	2.29	0.48
2:C:64:LEU:HD12	2:C:101:ILE:O	2.13	0.48
2:C:194:VAL:HG23	2:C:197:LEU:HD12	1.95	0.48
2:C:586:ARG:HA	2:C:589:ARG:HB3	1.96	0.48
2:C:728:HIS:CE1	5:F:422:LEU:O	2.67	0.48
2:C:734:LEU:HD23	2:C:737:LEU:HD12	1.96	0.48
2:C:765:SER:O	2:C:765:SER:OG	2.31	0.48
3:D:186:VAL:HG12	3:D:189:GLN:HB2	1.94	0.48
3:D:834:THR:HB	3:D:838:ARG:HD2	1.95	0.48
3:D:204:LEU:HD11	3:D:445:ARG:HH11	1.78	0.48
3:D:347:VAL:HG23	3:D:351:MET:HG3	1.96	0.48
7:H:17:DT:H2"	7:H:18:DG:H5'	1.96	0.48
1:B:132:LEU:HD21	1:B:136:GLY:C	2.34	0.48
3:D:556:LYS:NZ	5:F:222:ARG:NH2	2.61	0.48
3:D:1047:LYS:CG	3:D:1048:PRO:HD2	2.44	0.48
3:D:1084:THR:O	3:D:1088:THR:HG23	2.14	0.48
3:D:1379:VAL:HA	3:D:1420:LEU:HB2	1.95	0.48
5:F:287:THR:HG22	5:F:290:GLU:OE2	2.13	0.48



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:148:PHE:HD1	2:C:280:LYS:HZ2	1.62	0.48
2:C:242:LEU:N	2:C:242:LEU:CD2	2.77	0.48
3:D:701:LEU:HB2	3:D:748:HIS:HB2	1.96	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.48
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.13	0.48
4:E:80:VAL:HG23	4:E:85:LEU:HD11	1.95	0.48
5:F:372:ARG:HH12	5:F:380:GLU:CA	2.19	0.48
1:A:53:VAL:HG21	1:A:82:LEU:O	2.14	0.48
1:B:159:LYS:HE2	1:B:164:ALA:O	2.13	0.48
2:C:31:GLN:O	2:C:34:VAL:HG22	2.13	0.48
2:C:627:ARG:NH1	2:C:640:ARG:HA	2.29	0.48
3:D:1047:LYS:CD	3:D:1048:PRO:HD2	2.44	0.48
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.96	0.48
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.49	0.48
3:D:1499:ARG:NH1	4:E:84:ARG:HG2	2.28	0.48
1:A:99:LEU:HD12	1:A:100:LEU:H	1.79	0.47
2:C:290:LEU:O	2:C:301:GLU:HB2	2.14	0.47
3:D:348:GLN:HB2	3:D:351:MET:HE2	1.95	0.47
3:D:401:TYR:C	3:D:443:VAL:HG23	2.34	0.47
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.96	0.47
2:C:777:ILE:HD13	5:F:408:LEU:HD13	1.95	0.47
3:D:896:ALA:O	3:D:900:ILE:CD1	2.57	0.47
3:D:1266:ARG:CZ	7:H:18:DG:H4'	2.45	0.47
4:E:44:GLU:O	4:E:66:LYS:HE2	2.14	0.47
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.94	0.47
1:B:64:GLU:HG3	1:B:79:ILE:HD12	1.94	0.47
3:D:1047:LYS:NZ	3:D:1048:PRO:CG	2.71	0.47
3:D:1282:ARG:HD2	3:D:1293:PHE:HB2	1.95	0.47
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.29	0.47
1:A:222:LEU:HD11	1:B:218:LEU:HD23	1.96	0.47
1:B:112:ARG:HG2	1:B:125:PRO:CB	2.37	0.47
2:C:14:PRO:HB2	2:C:586:ARG:HH21	1.79	0.47
2:C:568:ALA:CB	2:C:668:LEU:HB3	2.45	0.47
2:C:367:LEU:HD12	2:C:371:LYS:HZ1	1.75	0.47
2:C:627:ARG:HA	2:C:638:ASP:OD1	2.14	0.47
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.50	0.47
3:D:411:THR:HG22	5:F:178:ARG:HB2	1.97	0.47
3:D:897:TRP:CH2	3:D:902:LEU:HD13	2.49	0.47
3:D:1293:PHE:CD1	3:D:1302:GLU:HB3	2.50	0.47
5:F:130:VAL:HG11	5:F:159:ILE:HG22	1.95	0.47
1:B:9:PRO:HB2	1:B:25:LEU:HD11	1.97	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:468:ARG:HG3	2:C:485:TYR:HB3	1.97	0.47
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.49	0.47
3:D:126:VAL:O	3:D:457:GLY:N	2.42	0.47
3:D:212:ARG:HG3	3:D:344:ASP:OD1	2.14	0.47
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.45	0.47
2:C:247:PRO:O	2:C:252:LYS:HD3	2.14	0.47
2:C:730:SER:O	2:C:734:LEU:HD12	2.15	0.47
2:C:1111:ILE:HG22	2:C:1111:ILE:O	2.15	0.47
3:D:266:GLU:OE2	3:D:315:ARG:NH2	2.43	0.47
3:D:420:VAL:HG23	3:D:425:GLY:HA2	1.96	0.47
3:D:885:ILE:HD12	3:D:937:TYR:CG	2.50	0.47
3:D:1275:SER:OG	3:D:1277:ILE:O	2.33	0.47
3:D:1305:LEU:HD11	3:D:1326:THR:HB	1.97	0.47
2:C:190:LYS:HE3	2:C:190:LYS:HB3	1.50	0.47
2:C:283:ILE:HG22	2:C:284:ARG:N	2.30	0.47
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.49	0.47
3:D:316:GLN:O	3:D:316:GLN:HG3	2.15	0.47
3:D:357:GLU:HB2	3:D:387:LEU:HD23	1.97	0.47
3:D:530:VAL:HG22	3:D:531:ASP:N	2.28	0.47
3:D:613:ARG:HA	3:D:613:ARG:HD3	1.76	0.47
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.97	0.47
5:F:147:LEU:HD23	5:F:151:LEU:HD11	1.95	0.47
2:C:185:LYS:HB2	2:C:190:LYS:HD2	1.96	0.47
3:D:207:PHE:HB2	3:D:391:ALA:HB2	1.96	0.47
3:D:398:ALA:HB2	3:D:447:VAL:HG12	1.96	0.47
4:E:30:LEU:HB3	4:E:35:PHE:CD1	2.49	0.47
3:D:156:GLU:H	3:D:156:GLU:CD	2.14	0.46
3:D:252:ARG:HB3	3:D:301:GLY:HA2	1.97	0.46
5:F:403:LYS:HG3	5:F:404:ALA:N	2.30	0.46
1:A:4:SER:HB3	1:A:189:ARG:HH22	1.80	0.46
1:A:11:PHE:O	1:B:228:PRO:HA	2.14	0.46
1:A:76:VAL:O	1:A:80:LEU:HD13	2.14	0.46
1:A:176:ARG:NH2	2:C:865:THR:HG22	2.30	0.46
1:B:117:VAL:HB	1:B:120:VAL:HG22	1.98	0.46
2:C:243:ARG:HD3	2:C:256:TYR:CZ	2.50	0.46
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.48	0.46
3:D:8:VAL:HG12	3:D:1434:TRP:HZ2	1.81	0.46
3:D:237:LYS:O	3:D:240:GLU:HB2	2.15	0.46
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.44	0.46
3:D:999:THR:O	3:D:1003:VAL:HG13	2.14	0.46
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	2.16	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:13:ILE:HG13	2:C:14:PRO:O	2.16	0.46
2:C:928:LYS:HG3	2:C:932:GLU:OE1	2.15	0.46
2:C:1004:LYS:HD3	3:D:744:GLN:HE22	1.80	0.46
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.97	0.46
2:C:82:GLU:HG3	2:C:86:LYS:NZ	2.31	0.46
2:C:727:PRO:O	2:C:729:LEU:CD2	2.63	0.46
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.50	0.46
2:C:1101:THR:CG2	2:C:1111:ILE:HD11	2.46	0.46
1:A:191:ASP:OD1	2:C:938:LYS:NZ	2.37	0.46
6:G:12:DG:C6	6:G:13:DA:C6	3.04	0.46
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.50	0.46
3:D:1399:ASP:OD2	3:D:1432:LYS:NZ	2.49	0.46
3:D:1492:LEU:HD11	3:D:1493:LYS:HE2	1.98	0.46
5:F:105:LYS:HE2	5:F:179:GLU:OE2	2.15	0.46
2:C:97:ARG:NH1	2:C:97:ARG:HG3	2.30	0.46
2:C:238:LEU:HG	2:C:242:LEU:CD2	2.45	0.46
3:D:347:VAL:HG22	3:D:351:MET:HG3	1.97	0.46
3:D:409:VAL:HG23	3:D:435:VAL:HG21	1.96	0.46
3:D:666:ILE:HD11	3:D:684:LYS:NZ	2.30	0.46
1:A:99:LEU:HD21	1:A:114:PHE:CG	2.50	0.46
1:B:97:VAL:HG13	1:B:144:VAL:HG22	1.96	0.46
1:B:124:ASN:HB2	1:B:127:LEU:CG	2.42	0.46
1:B:153:ALA:HB2	1:B:168:ASP:N	2.31	0.46
2:C:31:GLN:HB3	2:C:34:VAL:CG2	2.46	0.46
2:C:337:GLY:O	2:C:341:THR:HG23	2.15	0.46
2:C:497:ALA:HB3	2:C:532:MET:HG3	1.98	0.46
2:C:668:LEU:HD12	2:C:668:LEU:N	2.30	0.46
2:C:762:LYS:HE2	2:C:783:ARG:O	2.14	0.46
3:D:704:ARG:HD3	3:D:736:PHE:O	2.15	0.46
1:A:185:ARG:CZ	1:A:187:GLY:HA2	2.46	0.46
1:B:64:GLU:HB2	1:B:165:ILE:HG21	1.98	0.46
2:C:501:THR:CG2	2:C:513:VAL:HG23	2.35	0.46
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.37	0.46
2:C:602:GLU:HG3	2:C:648:ARG:HE	1.81	0.46
2:C:716:LYS:HZ2	3:D:529:GLN:HE22	1.64	0.46
3:D:556:LYS:HZ1	5:F:222:ARG:HH21	1.64	0.46
5:F:107:GLU:O	5:F:111:GLU:HG3	2.16	0.46
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.97	0.46
2:C:204:GLN:HA	2:C:207:LEU:HD23	1.98	0.46
2:C:627:ARG:HD2	2:C:639:GLN:O	2.16	0.46
2:C:929:ARG:NH2	2:C:940:GLU:OE2	2.49	0.46



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.81	0.46
2:C:946:ARG:NH1	3:D:861:GLN:HE22	2.14	0.46
3:D:155:ASP:OD1	3:D:159:ARG:NH2	2.49	0.46
3:D:683:ILE:CG2	3:D:687:VAL:HG11	2.45	0.46
5:F:382:THR:HB	5:F:383:LEU:HD12	1.96	0.46
2:C:68:PHE:HD2	2:C:98:LEU:HD11	1.81	0.45
2:C:627:ARG:NH1	2:C:639:GLN:O	2.49	0.45
2:C:810:ASP:HB2	2:C:813:VAL:CG1	2.46	0.45
3:D:97:THR:HG22	3:D:98:PRO:O	2.15	0.45
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.98	0.45
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.30	0.45
3:D:1410:GLU:HB3	3:D:1412:LYS:HE2	1.97	0.45
5:F:366:ALA:O	5:F:370:LYS:HB2	2.16	0.45
2:C:206:THR:HA	2:C:209:ARG:HD3	1.98	0.45
2:C:366:SER:O	2:C:366:SER:OG	2.29	0.45
3:D:1148:VAL:HG22	3:D:1189:ARG:HB2	1.97	0.45
4:E:26:ARG:HD2	4:E:67:GLU:OE1	2.17	0.45
1:A:104:GLU:HG2	1:A:137:ARG:CD	2.43	0.45
2:C:282:GLY:C	2:C:283:ILE:HD12	2.37	0.45
2:C:739:GLU:CD	2:C:739:GLU:H	2.20	0.45
3:D:169:TYR:O	3:D:392:SER:HB3	2.16	0.45
3:D:556:LYS:HD3	5:F:218:GLN:NE2	2.32	0.45
2:C:236:ILE:HG23	2:C:248:PRO:HB2	1.99	0.45
2:C:716:LYS:HZ1	3:D:529:GLN:HE22	1.64	0.45
3:D:437:VAL:HG11	5:F:175:HIS:ND1	2.32	0.45
3:D:773:ALA:HB1	3:D:1363:LEU:HD12	1.99	0.45
4:E:84:ARG:HG3	4:E:88:GLU:OE1	2.16	0.45
2:C:769:PRO:HD2	3:D:65:ARG:NH1	2.32	0.45
3:D:1148:VAL:HA	3:D:1164:ARG:O	2.17	0.45
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.51	0.45
2:C:5:ARG:HH11	2:C:5:ARG:HB3	1.82	0.45
2:C:1001:VAL:HG22	3:D:724:GLN:HB2	1.98	0.45
3:D:131:LYS:N	3:D:456:MET:HE2	2.32	0.45
3:D:199:LEU:HG	3:D:200:ASP:O	2.15	0.45
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.56	0.45
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.31	0.45
5:F:164:LYS:HD2	5:F:171:LYS:CD	2.45	0.45
5:F:278:LEU:O	5:F:282:LEU:HD12	2.15	0.45
2:C:175:GLU:O	2:C:183:SER:OG	2.20	0.45
2:C:687:ALA:HB1	2:C:850:ALA:HB2	1.99	0.45
4:E:85:LEU:N	4:E:85:LEU:HD12	2.32	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
5:F:162:LYS:NZ	5:F:165:SER:HB2	2.31	0.45
1:A:133:GLU:OE2	2:C:610:ARG:NH2	2.49	0.45
3:D:3:LYS:HG3	3:D:4:GLU:H	1.82	0.45
3:D:432:TYR:O	3:D:448:GLU:HA	2.17	0.45
3:D:628:ARG:HE	3:D:628:ARG:HB2	1.70	0.45
3:D:632:VAL:O	3:D:727:GLN:HA	2.16	0.45
3:D:1295:GLU:HA	3:D:1300:SER:CB	2.47	0.45
5:F:181:GLU:O	5:F:185:GLN:HG2	2.17	0.45
5:F:232:ARG:HG2	5:F:232:ARG:NH1	2.31	0.45
5:F:369:LEU:O	5:F:372:ARG:HB3	2.17	0.45
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.81	0.45
2:C:681:GLY:HA2	3:D:939:PHE:CE1	2.52	0.45
2:C:820:ARG:H	2:C:820:ARG:HG2	1.65	0.45
3:D:199:LEU:HD12	3:D:199:LEU:HA	1.72	0.45
3:D:354:VAL:HG22	3:D:354:VAL:O	2.17	0.45
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.50	0.45
3:D:1003:VAL:HG21	3:D:1041:LEU:HD22	1.98	0.45
1:B:161:ARG:HG3	1:B:162:ILE:O	2.17	0.45
2:C:278:GLU:HG2	2:C:284:ARG:HA	1.99	0.45
2:C:882:LEU:HD23	2:C:882:LEU:HA	1.70	0.45
3:D:23:TYR:CE1	3:D:89:ARG:HD3	2.51	0.45
3:D:63:TYR:CZ	3:D:71:LYS:HE2	2.51	0.45
3:D:431:VAL:HG11	3:D:448:GLU:CD	2.38	0.45
5:F:368:VAL:O	5:F:390:PHE:HE2	1.99	0.45
2:C:195:LEU:HD22	2:C:238:LEU:HB2	1.98	0.44
2:C:263:ASP:C	2:C:265:ARG:H	2.20	0.44
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.18	0.44
3:D:1054:GLU:H	3:D:1054:GLU:HG3	1.62	0.44
5:F:97:GLU:HA	5:F:100:VAL:HG12	2.00	0.44
2:C:68:PHE:CA	2:C:98:LEU:HD12	2.21	0.44
2:C:583:LEU:O	2:C:587:VAL:HG23	2.17	0.44
2:C:766:GLU:O	2:C:767:PRO:C	2.55	0.44
3:D:669:ASN:HD22	5:F:417:LYS:HG2	1.82	0.44
3:D:916:TYR:CZ	3:D:920:LEU:HD21	2.52	0.44
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.50	0.44
1:A:36:LEU:O	1:A:39:PRO:HD2	2.18	0.44
1:B:29:GLU:HG2	1:B:30:ARG:N	2.33	0.44
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.97	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.53	0.44
2:C:259:GLY:HA2	2:C:263:ASP:CB	2.48	0.44
2:C:385:PHE:O	2:C:389:SER:HB3	2.18	0.44



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:573:ARG:HB2	2:C:670:GLN:HE21	1.81	0.44
3:D:165:LYS:HD2	3:D:166:GLN:N	2.32	0.44
3:D:361:VAL:HG21	3:D:379:ALA:CB	2.47	0.44
3:D:792:ILE:HD13	3:D:941:PHE:CE2	2.53	0.44
1:A:16:GLN:OE1	1:A:17:GLY:N	2.51	0.44
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.52	0.44
2:C:650:ARG:NH1	2:C:653:ASP:OD1	2.49	0.44
3:D:171:LEU:HD21	3:D:390:PRO:CG	2.44	0.44
3:D:187:LYS:HG2	3:D:200:ASP:OD2	2.18	0.44
3:D:310:LEU:HD12	3:D:310:LEU:HA	1.68	0.44
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.98	0.44
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.69	0.44
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.38	0.44
4:E:17:TYR:O	4:E:21:VAL:HG23	2.18	0.44
5:F:252:ALA:HB1	5:F:265:VAL:HG11	2.00	0.44
1:B:40:LEU:HD21	1:B:218:LEU:HD22	1.98	0.44
3:D:56:TYR:HA	3:D:80:VAL:HG23	1.99	0.44
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.77	0.44
3:D:348:GLN:HB2	3:D:351:MET:HE3	2.00	0.44
3:D:1047:LYS:CD	3:D:1048:PRO:CD	2.96	0.44
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.52	0.44
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.53	0.44
2:C:34:VAL:CG2	2:C:39:ARG:HG2	2.47	0.44
2:C:280:LYS:HE3	2:C:323:ASP:OD1	2.17	0.44
2:C:290:LEU:HD12	2:C:290:LEU:H	1.82	0.44
2:C:470:PRO:HB2	2:C:534:VAL:HG21	2.00	0.44
2:C:1053:LEU:HD11	3:D:1466:VAL:HG13	2.00	0.44
3:D:297:ILE:HD12	3:D:297:ILE:C	2.37	0.44
3:D:799:LYS:NZ	3:D:1014:ASN:HA	2.32	0.44
3:D:1314:LYS:O	3:D:1317:ASP:HB2	2.18	0.44
5:F:101:GLU:O	5:F:104:ARG:HB3	2.17	0.44
5:F:364:ARG:HE	5:F:364:ARG:C	2.20	0.44
1:A:18:ARG:O	1:A:201:THR:CG2	2.66	0.44
2:C:404:LEU:O	2:C:408:ARG:HG3	2.18	0.44
3:D:124:GLU:OE2	3:D:128:TYR:HD1	1.99	0.44
3:D:169:TYR:HE1	3:D:395:VAL:CG1	2.26	0.44
3:D:186:VAL:HG13	3:D:187:LYS:O	2.18	0.44
3:D:1045:MET:HB3	3:D:1045:MET:HE2	1.88	0.44
3:D:1053:PHE:CE2	3:D:1072:ILE:HD12	2.53	0.44
5:F:105:LYS:HB3	5:F:105:LYS:HE3	1.53	0.44
5:F:412:GLU:OE1	5:F:418:LEU:HB2	2.18	0.44



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:58:ILE:HG13	1:B:61:VAL:CG1	2.44	0.44
2:C:207:LEU:C	2:C:207:LEU:HD12	2.38	0.44
2:C:719:PRO:CB	2:C:820:ARG:HH22	2.31	0.44
2:C:732:ALA:O	2:C:735:ARG:HG2	2.17	0.44
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.36	0.44
3:D:85:VAL:C	3:D:87:ARG:H	2.20	0.44
3:D:1048:PRO:HD3	3:D:1075:HIS:CG	2.53	0.44
3:D:1053:PHE:CD2	3:D:1072:ILE:HG23	2.52	0.44
3:D:1262:LEU:CD1	3:D:1351:GLU:HB3	2.47	0.44
3:D:1442:ASN:OD1	6:G:11:DA:H4'	2.18	0.44
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.76	0.44
2:C:304:LEU:HD22	2:C:304:LEU:HA	1.71	0.44
2:C:759:THR:HB	2:C:785:VAL:HB	1.99	0.44
2:C:905:ILE:O	2:C:907:ASP:N	2.51	0.44
3:D:808:THR:OG1	3:D:810:GLU:OE2	2.28	0.44
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.17	0.44
3:D:1267:ARG:HD2	3:D:1331:ASP:OD2	2.17	0.44
3:D:1386:ASP:OD2	3:D:1413:THR:HG22	2.17	0.44
5:F:354:LEU:O	5:F:358:LEU:HD13	2.18	0.44
1:B:128:HIS:CE1	1:B:131:THR:CG2	2.97	0.43
1:B:173:PRO:HB2	1:B:205:VAL:HG12	1.99	0.43
3:D:34:TYR:HB3	5:F:260:ILE:HG22	1.99	0.43
3:D:231:VAL:HG22	3:D:242:LEU:O	2.18	0.43
3:D:794:GLN:HG3	3:D:795:VAL:N	2.32	0.43
3:D:876:SER:OG	3:D:879:ARG:HG3	2.18	0.43
5:F:172:ARG:HG3	5:F:173:TYR:CD1	2.53	0.43
1:B:219:ARG:HG2	1:B:219:ARG:HH11	1.83	0.43
2:C:675:ALA:HA	2:C:989:VAL:HG22	2.00	0.43
2:C:1022:GLY:O	2:C:1026:GLN:NE2	2.51	0.43
3:D:204:LEU:O	3:D:393:ILE:HD12	2.17	0.43
3:D:483:HIS:O	3:D:489:ARG:HG2	2.18	0.43
3:D:660:LYS:HA	3:D:660:LYS:HD3	1.82	0.43
3:D:711:LEU:HD13	3:D:778:LEU:CD1	2.49	0.43
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.34	0.43
2:C:230:ARG:HB2	2:C:233:GLU:OE1	2.18	0.43
2:C:755:LEU:HD11	2:C:792:VAL:HG22	2.00	0.43
3:D:209:ARG:N	3:D:389:GLU:O	2.32	0.43
3:D:684:LYS:O	3:D:687:VAL:HG12	2.18	0.43
1:A:152:PRO:O	1:A:155:LYS:HB2	2.17	0.43
1:B:170:VAL:HG23	1:B:170:VAL:O	2.17	0.43
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.01	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:187:LYS:HE3	3:D:200:ASP:OD2	2.17	0.43
3:D:520:LEU:O	3:D:525:ARG:HD3	2.18	0.43
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.54	0.43
3:D:900:ILE:HD12	3:D:900:ILE:H	1.83	0.43
5:F:193:ARG:NH1	7:H:7:DG:N7	2.66	0.43
2:C:64:LEU:HD11	2:C:100:LEU:HD11	2.00	0.43
2:C:229:MET:HE2	2:C:229:MET:HB3	1.82	0.43
2:C:627:ARG:HE	2:C:627:ARG:HB3	1.61	0.43
2:C:763:GLY:O	2:C:765:SER:N	2.52	0.43
2:C:890:LEU:HD23	2:C:890:LEU:C	2.37	0.43
2:C:905:ILE:C	2:C:907:ASP:H	2.21	0.43
3:D:317:VAL:HG12	3:D:339:TRP:HB3	2.00	0.43
3:D:818:ARG:HB3	3:D:820:GLU:HG3	2.00	0.43
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.19	0.43
5:F:164:LYS:HZ2	5:F:171:LYS:CE	2.32	0.43
1:A:176:ARG:CZ	2:C:865:THR:HG22	2.48	0.43
1:B:48:ILE:C	1:B:148:VAL:HG12	2.39	0.43
1:B:85:LEU:HD23	1:B:86:VAL:N	2.34	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.66	0.43
3:D:266:GLU:CD	3:D:315:ARG:HD2	2.39	0.43
4:E:79:LEU:HD23	4:E:79:LEU:HA	1.70	0.43
5:F:184:ARG:O	5:F:188:ILE:HG13	2.18	0.43
1:B:13:VAL:HG22	1:B:23:PHE:CD1	2.54	0.43
2:C:754:ILE:CG1	2:C:791:ARG:HE	2.27	0.43
3:D:362:GLU:HG3	3:D:363:ALA:H	1.82	0.43
3:D:526:PRO:HG2	5:F:317:LEU:HD11	2.01	0.43
3:D:631:ILE:CG1	3:D:745:MET:HB2	2.48	0.43
3:D:1047:LYS:HD3	3:D:1048:PRO:CG	2.49	0.43
3:D:1293:PHE:CE1	3:D:1302:GLU:HG2	2.54	0.43
1:A:97:VAL:HG12	1:A:144:VAL:HB	1.99	0.43
2:C:713:ARG:HG2	2:C:720:GLU:OE1	2.18	0.43
2:C:748:GLU:HA	2:C:799:ILE:HD13	1.99	0.43
3:D:41:ARG:HH21	3:D:48:ARG:NH1	2.17	0.43
3:D:116:LEU:CB	3:D:118:LEU:HD13	2.48	0.43
3:D:408:GLU:HA	5:F:164:LYS:CE	2.49	0.43
3:D:1371:VAL:O	3:D:1374:GLN:N	2.52	0.43
3:D:1487:VAL:HG23	4:E:74:VAL:CG1	2.49	0.43
5:F:132:ARG:NH2	5:F:184:ARG:NH2	2.66	0.43
5:F:200:LYS:O	5:F:203:THR:HG23	2.19	0.43
2:C:605:LYS:HD3	2:C:610:ARG:HH12	1.84	0.43
2:C:763:GLY:C	2:C:765:SER:H	2.22	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:890:LEU:CD2	2:C:901:TYR:CE2	3.02	0.43
3:D:208:PRO:CG	3:D:387:LEU:HD12	2.49	0.43
1:A:185:ARG:NH2	1:A:187:GLY:O	2.52	0.43
2:C:274:ARG:HH22	2:C:284:ARG:CZ	2.32	0.43
2:C:283:ILE:CG2	2:C:284:ARG:N	2.82	0.43
2:C:508:ILE:HG21	2:C:526:PRO:HB3	2.01	0.43
3:D:335:LEU:HD23	3:D:335:LEU:HA	1.82	0.43
3:D:1262:LEU:HD11	3:D:1351:GLU:HB3	2.01	0.43
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.01	0.42
2:C:172:ILE:HG12	2:C:186:VAL:CG2	2.45	0.42
2:C:206:THR:HA	2:C:209:ARG:HG2	2.00	0.42
3:D:361:VAL:HG22	3:D:362:GLU:O	2.18	0.42
3:D:626:SER:HA	3:D:747:VAL:O	2.19	0.42
3:D:640:HIS:CD2	3:D:640:HIS:H	2.37	0.42
5:F:396:ARG:O	5:F:400:ILE:HG12	2.19	0.42
1:B:104:GLU:HA	1:B:132:LEU:HD13	2.00	0.42
2:C:229:MET:SD	2:C:237:ARG:HG3	2.58	0.42
3:D:272:LEU:CD2	3:D:298:VAL:CG1	2.97	0.42
5:F:163:LEU:HD23	5:F:163:LEU:HA	1.52	0.42
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.39	0.42
3:D:128:TYR:CE1	3:D:587:ARG:HD2	2.54	0.42
3:D:213:VAL:HG13	3:D:215:TYR:CE2	2.54	0.42
3:D:1148:VAL:CG2	3:D:1189:ARG:HG3	2.49	0.42
1:B:94:LEU:HD12	1:B:95:GLN:N	2.33	0.42
2:C:595:LEU:C	2:C:596:TYR:CD1	2.93	0.42
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.50	0.42
2:C:736:ASP:O	2:C:744:ARG:HG2	2.19	0.42
2:C:876:VAL:H	2:C:877:PRO:HD2	1.85	0.42
3:D:33:ASN:HB3	3:D:36:THR:CG2	2.45	0.42
3:D:352:ASN:OD1	3:D:352:ASN:N	2.52	0.42
3:D:486:ARG:O	3:D:489:ARG:HB2	2.20	0.42
3:D:984:THR:HG22	3:D:986:ARG:H	1.84	0.42
3:D:1092:GLY:HA3	6:G:14:DG:O4'	2.20	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.54	0.42
5:F:240:THR:O	5:F:244:ARG:HG3	2.19	0.42
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	2.00	0.42
3:D:258:VAL:HG12	3:D:297:ILE:CG2	2.48	0.42
3:D:273:ARG:HB2	3:D:277:GLU:O	2.20	0.42
3:D:314:PRO:HB2	3:D:317:VAL:HG22	2.01	0.42
3:D:413:ASP:N	5:F:178:ARG:NH2	2.65	0.42
3:D:684:LYS:HZ3	3:D:684:LYS:HG3	1.76	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:D:949:ILE:HD11	3:D:1023:MET:HE1	2.00	0.42
3:D:1286:THR:HB	3:D:1289:LYS:H	1.85	0.42
2:C:241:LEU:HB2	2:C:242:LEU:CD2	2.50	0.42
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.53	0.42
2:C:773:LEU:O	2:C:777:ILE:HG13	2.19	0.42
2:C:783:ARG:CZ	2:C:783:ARG:HB3	2.49	0.42
3:D:352:ASN:HB3	5:F:104:ARG:NH2	2.35	0.42
3:D:1286:THR:N	3:D:1289:LYS:O	2.49	0.42
3:D:1291:SER:HB2	3:D:1304:LYS:HG2	2.01	0.42
5:F:320:PRO:HA	5:F:327:SER:O	2.20	0.42
1:A:57:TYR:CD1	1:A:161:ARG:NH2	2.87	0.42
2:C:280:LYS:CE	2:C:323:ASP:OD2	2.62	0.42
2:C:1063:ARG:HG3	5:F:341:PRO:HG3	2.02	0.42
3:D:128:TYR:HD2	3:D:128:TYR:HA	1.70	0.42
3:D:210:ARG:HG2	3:D:388:HIS:HB2	2.02	0.42
3:D:317:VAL:HG12	3:D:339:TRP:HB2	2.01	0.42
3:D:394:LEU:HD11	3:D:396:VAL:HG12	2.01	0.42
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.42
5:F:166:LEU:O	5:F:171:LYS:NZ	2.30	0.42
5:F:364:ARG:CZ	5:F:368:VAL:HG23	2.50	0.42
1:B:185:ARG:NH1	1:B:187:GLY:O	2.53	0.42
1:B:212:ASN:HA	1:B:215:VAL:HG12	2.02	0.42
2:C:762:LYS:HD2	2:C:784:ASP:C	2.40	0.42
2:C:926:PHE:O	2:C:929:ARG:HB3	2.19	0.42
1:B:73:GLU:OE1	1:B:73:GLU:N	2.40	0.42
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.01	0.42
3:D:112:ILE:HG23	3:D:465:LEU:HD11	2.02	0.42
3:D:148:GLU:H	3:D:148:GLU:HG2	1.49	0.42
3:D:553:ARG:HG3	3:D:557:LEU:CD1	2.50	0.42
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.55	0.42
5:F:260:ILE:CD1	5:F:265:VAL:HB	2.49	0.42
5:F:351:SER:HA	5:F:354:LEU:HB2	2.02	0.42
2:C:64:LEU:HD12	2:C:65:VAL:H	1.85	0.42
3:D:71:LYS:O	3:D:80:VAL:HG12	2.20	0.42
3:D:371:ILE:CD1	3:D:372:ASP:CA	2.95	0.42
3:D:1047:LYS:CE	3:D:1048:PRO:CD	2.88	0.42
1:A:97:VAL:HG22	1:A:98:THR:H	1.85	0.41
2:C:121:MET:CE	2:C:125:GLY:HA2	2.50	0.41
2:C:283:ILE:CD1	2:C:305:PRO:HB3	2.50	0.41
2:C:331:ARG:NH1	2:C:427:VAL:HG23	2.34	0.41
2:C:611:ILE:HD11	2:C:655:LEU:HB3	2.02	0.41



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:1015:LEU:HD21	5:F:333:ILE:HG22	2.02	0.41
3:D:128:TYR:HE1	3:D:587:ARG:HD2	1.85	0.41
3:D:273:ARG:HH11	3:D:278:PRO:HD3	1.85	0.41
3:D:641:GLN:HE21	3:D:717:GLN:NE2	2.18	0.41
3:D:711:LEU:HB3	3:D:714:GLN:OE1	2.20	0.41
3:D:1034:GLN:O	3:D:1038:LEU:HD12	2.20	0.41
3:D:1098:LEU:HD23	3:D:1098:LEU:HA	1.82	0.41
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.20	0.41
4:E:30:LEU:HD23	4:E:35:PHE:HD1	1.85	0.41
4:E:50:THR:CG2	4:E:53:GLY:H	2.32	0.41
5:F:95:THR:OG1	5:F:98:GLU:HG3	2.20	0.41
1:A:30:ARG:HB2	1:A:191:ASP:O	2.19	0.41
2:C:207:LEU:O	2:C:211:LEU:HD23	2.21	0.41
2:C:768:THR:HG23	2:C:771:GLU:N	2.33	0.41
2:C:834:GLN:HG2	2:C:837:ASP:OD2	2.20	0.41
2:C:959:PRO:O	2:C:963:LEU:HG	2.19	0.41
2:C:1059:ASP:OD2	2:C:1080:SER:HB3	2.20	0.41
3:D:36:THR:C	3:D:38:LYS:H	2.23	0.41
4:E:40:LEU:HA	4:E:72:ARG:HH12	1.85	0.41
5:F:154:LYS:HZ3	5:F:155:THR:HG22	1.83	0.41
1:A:213:GLN:HG2	1:A:213:GLN:H	1.57	0.41
1:B:106:PRO:HD3	1:B:134:GLU:HG2	2.03	0.41
2:C:388:ARG:HG2	2:C:388:ARG:HH11	1.83	0.41
3:D:14:SER:HB2	3:D:16:GLU:OE2	2.20	0.41
3:D:437:VAL:HG11	5:F:175:HIS:CE1	2.56	0.41
3:D:450:TYR:C	3:D:452:ILE:H	2.23	0.41
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	2.01	0.41
5:F:157:GLU:O	5:F:161:GLN:HG2	2.20	0.41
6:G:5:DT:O2	7:H:24:DG:N2	2.53	0.41
2:C:719:PRO:HG2	2:C:721:ARG:NH2	2.35	0.41
1:B:128:HIS:CE1	1:B:131:THR:HG22	2.43	0.41
2:C:365:ASP:N	2:C:365:ASP:OD2	2.54	0.41
2:C:717:LEU:HD21	2:C:763:GLY:HA2	2.02	0.41
3:D:127:LEU:HD23	3:D:127:LEU:HA	1.78	0.41
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.56	0.41
3:D:222:GLY:HA2	3:D:333:LEU:O	2.21	0.41
3:D:272:LEU:HD21	3:D:298:VAL:HG11	2.01	0.41
3:D:431:VAL:HG12	3:D:432:TYR:N	2.35	0.41
3:D:860:LEU:O	3:D:876:SER:HB2	2.21	0.41
4:E:26:ARG:O	4:E:29:GLN:HB2	2.20	0.41
1:B:23:PHE:HE1	1:B:208:LEU:HB3	1.85	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:C:19:THR:O	2:C:23:VAL:HG23	2.20	0.41
2:C:495:THR:HA	2:C:517:ARG:HG2	2.01	0.41
2:C:754:ILE:CG2	2:C:789:SER:HB3	2.51	0.41
3:D:105:VAL:O	3:D:110:SER:HB2	2.21	0.41
3:D:800:LYS:HZ3	3:D:820:GLU:C	2.23	0.41
3:D:1110:ALA:O	3:D:1203:LYS:HG2	2.20	0.41
5:F:383:LEU:HB2	5:F:384:GLU:OE2	2.20	0.41
1:B:150:TYR:CE2	1:B:170:VAL:HG12	2.56	0.41
1:B:188:GLN:CD	1:B:188:GLN:H	2.23	0.41
2:C:580:MET:HE1	2:C:665:PHE:CE2	2.55	0.41
2:C:763:GLY:C	2:C:765:SER:N	2.74	0.41
2:C:808:ARG:NH1	2:C:820:ARG:HD2	2.36	0.41
3:D:116:LEU:HD11	3:D:465:LEU:CD2	2.38	0.41
3:D:137:PRO:HB3	3:D:147:VAL:CG1	2.50	0.41
3:D:313:MET:HA	3:D:314:PRO:HD3	1.94	0.41
3:D:720:LEU:H	3:D:720:LEU:HD12	1.85	0.41
1:B:32:PHE:HA	1:B:35:THR:HB	2.02	0.41
1:B:53:VAL:HG22	1:B:144:VAL:HG12	2.02	0.41
2:C:91:GLN:HG3	2:C:117:HIS:HB3	2.02	0.41
2:C:207:LEU:HD11	2:C:222:MET:CE	2.51	0.41
2:C:487:THR:OG1	2:C:490:GLU:HG2	2.21	0.41
2:C:810:ASP:HB2	2:C:813:VAL:HG11	2.02	0.41
2:C:944:LEU:HA	2:C:944:LEU:HD23	1.90	0.41
3:D:191:LEU:N	3:D:191:LEU:HD22	2.35	0.41
3:D:218:LYS:HE2	3:D:338:GLU:CD	2.41	0.41
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.41	0.41
5:F:363:GLU:OE1	5:F:366:ALA:HB3	2.21	0.41
1:B:36:LEU:O	1:B:39:PRO:HD2	2.21	0.41
2:C:151:ASP:HB3	2:C:157:ARG:O	2.21	0.41
2:C:714:ASP:OD2	2:C:820:ARG:HD3	2.20	0.41
2:C:884:GLN:HB2	2:C:992:MET:CE	2.51	0.41
3:D:181:ASP:N	3:D:205:TYR:HE2	2.19	0.41
3:D:231:VAL:O	3:D:231:VAL:HG23	2.21	0.41
3:D:245:LEU:CD2	3:D:249:TYR:HB3	2.50	0.41
3:D:1217:ILE:HG21	3:D:1480:PHE:CG	2.55	0.41
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.91	0.41
5:F:172:ARG:O	5:F:176:ILE:HG12	2.21	0.41
5:F:276:ARG:O	5:F:280:GLN:HB2	2.21	0.41
8:I:3:G:C2	8:I:4:G:N2	2.89	0.41
2:C:546:LEU:HA	2:C:581:THR:HG21	2.03	0.41
3:D:1145:TYR:CG	3:D:1168:MET:HE2	2.54	0.41



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
4:E:50:THR:HG23	4:E:53:GLY:H	1.86	0.41
5:F:166:LEU:HB2	5:F:171:LYS:HG2	2.03	0.41
1:B:18:ARG:O	1:B:207:PRO:HD3	2.22	0.40
3:D:169:TYR:CE1	3:D:395:VAL:HG12	2.46	0.40
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.65	0.40
3:D:1237:THR:O	3:D:1237:THR:HG22	2.22	0.40
3:D:1471:LEU:HD21	3:D:1477:GLY:HA2	2.03	0.40
4:E:44:GLU:O	4:E:66:LYS:CE	2.69	0.40
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.92	0.40
1:B:40:LEU:N	1:B:40:LEU:HD23	2.36	0.40
1:B:124:ASN:OD1	1:B:124:ASN:N	2.47	0.40
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.54	0.40
1:B:211:LEU:O	1:B:215:VAL:HG12	2.21	0.40
2:C:195:LEU:CD2	2:C:238:LEU:HB2	2.51	0.40
2:C:1086:ARG:HE	2:C:1111:ILE:HG22	1.86	0.40
3:D:355:VAL:CG1	3:D:367:ILE:HA	2.51	0.40
3:D:845:ASN:OD1	3:D:848:GLU:N	2.46	0.40
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.22	0.40
2:C:376:ARG:NE	5:F:276:ARG:HG2	2.36	0.40
2:C:494:TYR:CD2	2:C:531:PHE:CE2	3.09	0.40
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.36	0.40
2:C:758:ARG:HE	2:C:788:THR:HG22	1.86	0.40
2:C:799:ILE:O	2:C:801:VAL:HG13	2.21	0.40
2:C:876:VAL:HG22	2:C:884:GLN:NE2	2.37	0.40
2:C:877:PRO:HG3	3:D:1023:MET:HE3	2.01	0.40
3:D:359:ALA:H	3:D:385:VAL:HG22	1.85	0.40
1:A:190:THR:OG1	1:A:191:ASP:N	2.55	0.40
1:B:75:VAL:O	1:B:79:ILE:HG13	2.21	0.40
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.86	0.40
2:C:598:GLU:HG3	2:C:615:TYR:OH	2.21	0.40
2:C:861:LEU:HD13	2:C:865:THR:OG1	2.21	0.40
3:D:16:GLU:OE2	3:D:16:GLU:N	2.30	0.40
3:D:703:ASN:HA	3:D:712:GLY:O	2.22	0.40
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.22	0.40
3:D:1265:ALA:O	3:D:1333:HIS:HE1	2.04	0.40
5:F:140:ARG:HE	5:F:140:ARG:HB2	1.62	0.40
5:F:358:LEU:CB	5:F:366:ALA:HB1	2.51	0.40
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.77	0.40
2:C:486:MET:SD	2:C:491:GLU:HA	2.62	0.40
2:C:1093:GLN:HG2	3:D:21:TRP:CH2	2.56	0.40
3:D:204:LEU:CD1	3:D:445:ARG:HH11	2.35	0.40



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:86:HIS:O	5:F:90:GLN:NE2	2.53	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:301:GLY:N	5:F:249:ARG:NH1[4_1349]	1.44	0.76
3:D:300:LYS:O	5:F:249:ARG:NE[4_1349]	1.58	0.62
3:D:302:GLN:N	5:F:249:ARG:NH2[4_1349]	1.66	0.54
3:D:302:GLN:N	5:F:249:ARG:CZ[4_1349]	1.77	0.43
3:D:300:LYS:C	5:F:249:ARG:NE[4_1349]	1.80	0.40
3:D:302:GLN:CG	5:F:249:ARG:NH2[4_1349]	1.81	0.39
3:D:301:GLY:N	5:F:249:ARG:CZ[4_1349]	1.91	0.29
3:D:35:ARG:NH2	3:D:327:GLU:OE1[4_1359]	1.98	0.22
3:D:300:LYS:C	5:F:249:ARG:NH1[4_1349]	2.00	0.20
3:D:299:GLU:O	5:F:249:ARG:NH1[4_1349]	2.14	0.06
3:D:301:GLY:C	5:F:249:ARG:CZ[4_1349]	2.16	0.04
3:D:985:ASP:CB	3:D:1497:GLU:OE2[1_545]	2.16	0.04
3:D:300:LYS:C	5:F:249:ARG:CZ[4_1349]	2.19	0.01

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	Perce	ntiles
1	А	224/315~(71%)	211 (94%)	13~(6%)	0	100	100
1	В	222/315~(70%)	202 (91%)	18 (8%)	2(1%)	17	34
2	С	1101/1119 (98%)	1036 (94%)	53~(5%)	12 (1%)	14	30
3	D	1480/1524~(97%)	1398 (94%)	71 (5%)	11 (1%)	22	42
4	Ε	92/99~(93%)	89~(97%)	3~(3%)	0	100	100
5	F	344/423~(81%)	316 (92%)	23~(7%)	5 (2%)	10	22



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3463/3795~(91%)	3252 (94%)	181 (5%)	30 (1%)	17 34

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	154	GLU
2	С	363	SER
2	С	418	LEU
2	С	419	THR
3	D	486	ARG
3	D	664	LYS
3	D	1130	ARG
5	F	323	ASP
5	F	377	ASP
2	С	362	GLY
2	С	476	GLY
3	D	743	ASP
3	D	984	THR
2	С	228	ALA
3	D	320	ALA
3	D	442	ASN
2	С	229	MET
3	D	37	LEU
3	D	86	ARG
3	D	187	LYS
3	D	484	PRO
2	С	766	GLU
2	С	1015	LEU
2	С	1034	GLU
5	F	325	LYS
5	F	378	GLY
5	F	416	ARG
1	В	59	GLU
2	С	728	HIS
2	С	765	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	\mathbf{ntiles}
1	А	199/273~(73%)	192~(96%)	7~(4%)	36	61
1	В	197/273~(72%)	194~(98%)	3~(2%)	65	82
2	С	931/941~(99%)	892~(96%)	39~(4%)	30	54
3	D	1250/1279~(98%)	1213~(97%)	37 (3%)	41	65
4	Е	83/88~(94%)	80~(96%)	3~(4%)	35	60
5	F	296/371~(80%)	281~(95%)	15 (5%)	24	45
All	All	2956/3225~(92%)	2852~(96%)	104 (4%)	36	61

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

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	16	GLN
1	А	126	ASP
1	А	145	ASP
1	А	161	ARG
1	А	175	ARG
1	А	188	GLN
1	А	219	ARG
1	В	74	ASP
1	В	110	LYS
1	В	126	ASP
2	С	38	LYS
2	С	103	LYS
2	С	134	ARG
2	С	141	HIS
2	С	154	ARG
2	С	157	ARG
2	С	168	ARG
2	С	171	TRP
2	С	179	ASN
2	С	189	ARG
2	С	238	LEU
2	С	243	ARG
2	С	275	TYR
2	С	284	ARG
2	С	293	PHE
2	С	342	ASP
2	С	353	ARG



Mol	Chain	Res	Type
2	С	365	ASP
2	С	366	SER
2	С	371	LYS
2	С	434	HIS
2	С	454	SER
2	С	482	GLU
2	С	557	ARG
2	С	586	ARG
2	С	610	ARG
2	С	617	ASP
2	С	626	ARG
2	С	648	ARG
2	С	680	ASP
2	С	716	LYS
2	С	721	ARG
2	С	735	ARG
2	С	765	SER
2	С	791	ARG
2	С	834	GLN
2	С	879	ARG
2	С	929	ARG
2	С	1026	GLN
3	D	3	LYS
3	D	9	ARG
3	D	106	LYS
3	D	190	GLU
3	D	220	ARG
3	D	224	ARG
3	D	247	GLU
3	D	276	ASP
3	D	302	GLN
3	D	316	GLN
3	D	351	MET
3	D	434	ARG
3	D	500	ARG
3	D	508	ARG
3	D	525	ARG
3	D	638	LYS
3	D	640	HIS
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU



Mol	Chain	Res	Type
3	D	784	ASP
3	D	797	LYS
3	D	832	ARG
3	D	907	GLU
3	D	982	PHE
3	D	986	ARG
3	D	988	ARG
3	D	1011	PHE
3	D	1159	ARG
3	D	1188	VAL
3	D	1234	THR
3	D	1282	ARG
3	D	1308	GLU
3	D	1317	ASP
3	D	1363	LEU
3	D	1418	LYS
3	D	1426	LYS
4	Е	15	SER
4	Е	84	ARG
4	Е	87	LYS
5	F	93	LEU
5	F	162	LYS
5	F	172	ARG
5	F	186	HIS
5	F	205	ARG
5	F	232	ARG
5	F	302	LYS
5	F	355	GLU
5	F	377	ASP
5	F	396	ARG
5	F	398	ARG
5	F	409	LYS
5	F	411	HIS
5	F	413	SER
5	F	419	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	128	HIS
1	А	213	GLN
1	В	95	GLN



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Mol	Chain	\mathbf{Res}	Type
1	В	124	ASN
1	В	163	ASN
1	В	229	GLN
2	С	102	HIS
2	С	139	GLN
2	С	204	GLN
2	С	647	GLN
2	С	1047	HIS
3	D	33	ASN
3	D	151	GLN
3	D	529	GLN
3	D	611	GLN
3	D	640	HIS
3	D	717	GLN
3	D	744	GLN
3	D	861	GLN
3	D	1046	GLN
3	D	1445	HIS
5	F	175	HIS
5	F	248	ASN
5	F	402	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Ι	7/8~(87%)	3~(42%)	2(28%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Ι	3	G
8	Ι	4	G
8	Ι	5	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	Ι	1	GTP
8	Ι	4	G



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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mal	Tuno	Chain	Dog	Tink	B	ond leng	gths	В	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
10	POP	C	1201	-	6,8,8	0.51	0	$13,\!13,\!13$	1.31	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	POP	С	1201	-	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
10	С	1201	POP	P2-O-P1	-2.86	123.03	132.83

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	$OWAB(Å^2)$	Q<0.9
1	А	226/315~(71%)	-0.11	3 (1%) 77 74	71, 95, 118, 132	0
1	В	224/315~(71%)	-0.02	1 (0%) 92 91	68, 96, 127, 146	0
2	С	1107/1119~(98%)	0.16	48 (4%) 35 27	54, 94, 165, 203	0
3	D	1484/1524~(97%)	0.13	47 (3%) 47 41	49, 87, 149, 204	0
4	Е	94/99~(94%)	0.01	0 100 100	64, 102, 152, 157	0
5	F	346/423~(81%)	0.65	52~(15%) 2 1	62, 107, 206, 228	0
6	G	19/22~(86%)	0.63	$3\ (15\%)\ 2\ 1$	66, 123, 229, 241	0
7	Н	19/27~(70%)	0.11	$3\ (15\%)\ 2\ 1$	92, 125, 233, 239	0
8	Ι	7/8~(87%)	1.04	2(28%) 0 0	68, 83, 172, 195	0
All	All	3526/3852~(91%)	0.17	159 (4%) 33 25	49, 94, 165, 241	0

All (159) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
5	F	392	VAL	9.6
5	F	397	ILE	8.2
5	F	376	ILE	8.1
5	F	396	ARG	8.0
5	F	374	GLY	7.7
5	F	375	LEU	7.5
5	F	419	ARG	6.6
5	F	390	PHE	6.1
5	F	422	LEU	6.1
3	D	173	PRO	5.8
5	F	356	LYS	5.6
5	F	400	ILE	5.5
5	F	149	GLU	5.5
5	F	357	ALA	5.4
5	F	361	LEU	5.4



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Mol	Chain	Res	Type	RSRZ
5	F	414	ARG	5.1
5	F	147	LEU	5.0
5	F	370	LYS	4.9
5	F	148	LYS	4.9
6	G	3	DC	4.8
5	F	394	ARG	4.8
2	С	107	LEU	4.7
5	F	391	GLY	4.7
2	С	188	LYS	4.6
5	F	393	THR	4.6
3	D	1129	THR	4.5
3	D	144	GLY	4.5
5	F	367	MET	4.5
2	С	245	GLY	4.5
2	С	311	PHE	4.4
5	F	371	LEU	4.3
3	D	1128	VAL	4.3
3	D	1301	LYS	4.2
3	D	1297	GLU	4.1
5	F	349	LEU	4.1
2	С	219	GLN	4.0
2	С	194	VAL	4.0
5	F	389	PHE	3.9
7	Н	25	DG	3.9
7	Н	24	DG	3.9
2	С	216	GLU	3.8
3	D	1502	ALA	3.8
5	F	386	VAL	3.8
8	Ι	4	G	3.8
5	F	352	GLU	3.7
5	F	395	GLU	3.7
5	F	369	LEU	3.7
2	С	617	ASP	3.6
5	F	413	SER	3.6
5	F	416	ARG	3.6
7	Н	23	DA	3.6
5	F	417	LYS	3.6
3	D	1298	GLY	3.6
3	D	174	GLY	3.6
2	С	104	ASP	3.3
5	F	353	GLU	3.3
5	F	362	SER	3.3



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Mol	Chain	Res	Type	RSRZ
1	В	138	LEU	3.3
2	С	304	LEU	3.2
5	F	150	THR	3.2
5	F	381	HIS	3.2
5	F	410	TYR	3.1
5	F	173	TYR	3.1
3	D	188	GLY	3.1
3	D	409	VAL	3.1
3	D	310	LEU	3.1
2	С	416	GLY	3.1
5	F	142	ARG	3.0
2	С	102	HIS	3.0
5	F	385	GLU	2.9
3	D	268	ALA	2.9
2	С	254	VAL	2.9
5	F	143	HIS	2.9
3	D	1299	PHE	2.9
3	D	363	ALA	2.9
2	С	64	LEU	2.8
2	С	811	PRO	2.8
2	С	417	GLY	2.8
2	С	221	LEU	2.8
3	D	67	ARG	2.7
3	D	1278	ASP	2.7
3	D	1294	VAL	2.7
2	С	109	LYS	2.7
2	С	189	ARG	2.7
3	D	1289	LYS	2.7
3	D	384	VAL	2.7
3	D	1293	PHE	2.7
3	D	1313	VAL	2.7
3	D	142	LEU	2.6
5	F	379	ARG	2.6
3	D	170	PRO	2.6
2	С	208	ALA	2.6
2	C	217	LEU	2.5
2	С	251	ASP	2.5
8	Ι	3	G	2.5
3	D	978	TYR	2.5
3	D	152	LEU	2.5
2	C	181	VAL	2.5
3	D	1497	$\mathrm{GL}\overline{\mathrm{U}}$	2.5



Mol	Chain	Res	Type	RSRZ	
5	F	323	ASP	2.5	
2	С	215 GLY		2.5	
5	F	360 LYS		2.5	
2	С	367	LEU	2.5	
1	А	137	ARG	2.4	
2	С	195	LEU	2.4	
5	F	420	ASP	2.4	
2	С	778	PHE	2.4	
3	D	143	ASN	2.4	
2	С	153	ALA	2.4	
1	А	99 LEU		2.4	
2	С	12 VAL		2.4	
2	С	106	GLY	2.4	
5	F	373	LYS	2.4	
2	С	250	ARG	2.3	
3	D	183	GLU	2.3	
3	D	241	ILE	2.3	
3	D	1305 LEU		2.3	
3	D	1288	GLU	2.3	
3	D	1327	ARG	2.3	
3	D	369	ALA	2.3	
5	F	350	LEU	2.3	
3	D	195	VAL	2.3	
5	F	359	SER	2.3	
2	С	224	GLU	2.3	
3	D	1387	SER	2.3	
2	С	650	ARG	2.3	
5	F	404	ALA	2.3	
6	G	4	DC	2.2	
2	C	320	HIS	2.2	
3	D	63	TYR	2.2	
3	D	1501	GLU	2.2	
6	G	19	DA	2.2	
2	С	299	LYS	2.2	
2	С	241	LEU	2.2	
3	D	1292	VAL	2.2	
2	С	154	ARG	2.2	
5	F	423	ASP	2.2	
3	D	189	GLN	2.2	
2	С	507	ARG	2.2	
2	С	253	ALA	2.2	
2	С	508	ILE	2.2	



Mol	Chain	Res	Type	RSRZ	
3	D	1436	SER	2.2	
2	С	222	MET	2.2	
2	С	300	ASP	2.2	
3	D	321	GLN	2.2	
3	D	1311	LEU	2.1	
2	С	414	GLY	2.1	
3	D	203	ALA	2.1	
1	А	100	LEU	2.1	
2	С	298	PHE	2.1	
2	С	451	LEU	2.1	
2	С	616	GLU	2.1	
5	F	144	ILE	2.1	
2	С	511	GLU	2.1	
3	D	339	TRP	2.1	
3	D	236	TYR	2.1	
2	С	615	TYR	2.0	
5	F	159	ILE	2.0	
3	D	1499	ARG	2.0	

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

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

6.3 Carbohydrates (i)

There are no 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	$B-factors(A^2)$	Q<0.9
10	POP	С	1201	9/9	0.91	0.15	78,95,107,114	0
9	MG	D	2001	1/1	0.92	0.25	48,48,48,48	0
9	MG	В	1001	1/1	0.93	0.37	78,78,78,78	0
11	ZN	D	2002	1/1	0.97	0.12	113,113,113,113	0
11	ZN	D	2003	1/1	0.99	0.28	116,116,116,116	0



6.5 Other polymers (i)

There are no such residues in this entry.

