

Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 - 09:34 am GMT

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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 3.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	В	1054	.%	50%	11% ••
1	С	1054	35%	50%	9% • 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ANP	В	2055	Х	-	-	-
3	MG	С	2056	-	-	-	Х



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16398 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 REVERSE GYRASE.

Mol	Chain	Residues		Α	toms		ZeroOcc	AltConf	Trace	
1	В	1020	Total 8226	C 5246	N 1450	O 1505	S 25	0	0	0
1	С	1005	Total 8108	C 5169	N 1430	0 1483	S 26	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	719	LEU	PRO	engineered mutation	UNP O29238
В	1046	MET	LEU	engineered mutation	UNP O29238
С	719	LEU	PRO	engineered mutation	UNP O29238
С	1046	MET	LEU	engineered mutation	UNP O29238

• Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).





Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf			
2	В	1	Total	С	Ν	Ο	Р	0	0		
	D	1	31	10	6	12	3	0	0		
0	С	1	Total	С	Ν	0	Р	0	0		
Z	U	1	31	10	6	12	3	0	0		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	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: REVERSE GYRASE









10VE

20010

1469	E464	R465	A400 K467	L468	Y469 D470	I471	E472	F473	K474 S475	1476	D477	E478	V479	D480 E481	E482	K483	L484	T ADD	D489	E490	S491	R492 D493	R494	Y495	R496 P407	R498	Q499	E500	D502	L503	K505	P506		F509	1510	V511 EE10	S513	P514	1 1 1	A517 R518	Q519		R522 F523	F524	-
	V529	K530	V531 L532	D533	G534	V537	Y538	E539	I540 P541	M542	Q543	K544	Y545	07940	V549		1553	VEEG	V557	D558	L559 T560	1560 T561		G564	F565	V568	L569	V570 N571	G572	R573	r5/4 V575	-	S580 TE81	K582	R583	C584 DE OF	ASP	CYS	GLY	U I I	PHE	THR	GL U ASP	ARG	GLU
	PRO	LYS	GLY	SER	GLU ASN	V606	D607	N608	8609 8610	S611	R612	I613	E614	A615 1616	R617	K618	L619	A620 u621	D622	A623	E624	T627	V628	G629	T630	T634	E635	G636 F637	K638	I639	A640 W641	D642	L643	L646	L647	5648	C650	-	K654	T GER		V661	T662 R663	R664	A665
1000T	E668	A669	L673		V681 K682	A683	<mark>0684</mark>	V685	V686 R687	R688	I 689	E690	D691	TROA	1034 G695	F696	V697		K701	L702	W703	E/04 R705	F706	N707	N708 B700	N710	L711	S712	G714	R715	A/10 0717	T718	L719 V720	L721	G722	W723	1725 1725	D726	R727	<u>873</u> 1	R732	E733	R735 R735	K736	1737
1720	V740	R741	D/ 42 F743	D744	L745 V746	L747	GLU	HIS	D750	E752	E753	F754	D755	L/ 56	1758 1758	K759	L760	V761	E763	R764	E765	E/ 66	R768	T7 69	P770	4	Y774	T775 T776	E777	0 0 2 2	D/ 82 A7 83	N784	1 707	K788	F789	8790 V761	V1 31 K7 92	Q793		4797 1797		L801	1.806	1807	T808
	R811	T812	S814	T815	R816 V817	S818	D819	V820	G821	R823	I824	-	L829	G830	D832	F833	V834	G835 D026	E837	W838	C 839	G842		E845	C846 1947	R848	P849	T850 R851	P852	L853	1 854 R855	D856	D857 Veee	0859	R860	L861 T067	1 0 0 2 0 8 6 3		V869	E8/0	L872	R873	W874 E875	H876	F877
1 070	Y880	D881	L002 I883	F884	R885 R886	F887	M888	A889	5890 1891	C892	R893	P894	F895	K896	V 898	V 899	K900	K901 V002	2903	1904	E905	F906	GLY	LYS	THR	E912	E913	E914		E920	6921 R922	A923	Y924	L926	Y927	R928	V930	W931	V932	N934	E935	L936	P937 T938	6939	T940
	V943	K944	E946	V947	K948 S949	V950	P951	K952	V953	T957	<mark>0958</mark>	S959	E960	1961 TOR7	1902 []963	M964	M965	K966 F967	R968	6969	1970 1971	G971 R972		T975	Y976	T978	1979	V980 D981	R982	L983	r 984 M985	R986		066A	E991	K992	R995	-	P998	1999 K1000	L1001	G1002	11003 D1004	V1005	F1006
	L1009	V1010	R1012	Y1013		V1017	S1018	E1019	D1020 B1021	T1022	_	L1025	E1026	B1020	M1029	D1030	A1031	I1032	L1037	D1038	Y1039	T1050	K1051	S1052	11053	HOOH A																			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	132.41Å 68.69Å 134.00Å	Deperitor
a, b, c, α , β , γ	90.00° 99.70° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	34.00 - 3.20	Depositor
Resolution (A)	$34.40 \ - \ 3.20$	EDS
% Data completeness	96.6 (34.00-3.20)	Depositor
(in resolution range)	96.7 (34.40-3.20)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$2.90 (at 3.18 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.256 , 0.332	Depositor
n, n_{free}	0.247 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	69.1	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 87.2	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16398	wwPDB-VP
Average B, all atoms $(Å^2)$	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.78% 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, ANP

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	Bond	lengths	Bo	ond angles
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.47	0/8371	0.72	5/11265~(0.0%)
1	С	0.35	0/8246	0.61	3/11090~(0.0%)
All	All	0.41	0/16617	0.67	8/22355~(0.0%)

There are no bond length outliers.

All ((8)) bond	angle	outliers	are	listed	below:
1111	(0)	, bond	angre	outificity	arc	moucu	00101.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	391	ARG	N-CA-C	-7.20	91.57	111.00
1	С	305	THR	N-CA-C	6.94	129.73	111.00
1	В	388	ALA	N-CA-C	-6.79	92.68	111.00
1	В	3	PRO	N-CA-CB	5.77	110.23	103.30
1	С	11	PRO	N-CA-CB	5.54	109.95	103.30
1	С	3	PRO	N-CA-CB	5.43	109.81	103.30
1	В	11	PRO	N-CA-CB	5.42	109.80	103.30
1	В	305	THR	N-CA-C	5.24	125.13	111.00

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	В	8226	0	8310	830	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	8108	0	8178	754	0
2	В	31	0	13	5	0
2	С	31	0	13	5	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
All	All	16398	0	16514	1581	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 48.

All (1581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:379:VAL:HG12	1:B:380:ASP:H	1.12	1.12
1:B:386:LEU:H	1:B:386:LEU:HD23	1.19	1.06
1:B:638:LYS:HB2	1:B:684:GLN:HG3	1.38	1.06
1:C:192:LYS:HB3	1:C:196:LYS:HE3	1.43	1.00
1:B:540:ILE:HG13	1:B:541:PRO:HD2	1.46	0.97
1:C:334:VAL:HG12	1:C:335:ARG:HG3	1.47	0.96
1:C:379:VAL:HG12	1:C:380:ASP:H	1.30	0.95
1:C:426:LEU:HD11	1:C:466:ALA:HA	1.49	0.94
1:C:301:ILE:O	1:C:320:ILE:HG13	1.67	0.94
1:C:305:THR:OG1	1:C:329:TYR:HB3	1.66	0.94
1:B:852:PRO:O	1:B:853:LEU:HD23	1.68	0.94
1:B:760:LEU:HD23	1:B:760:LEU:H	1.34	0.93
1:C:244:ILE:HG22	1:C:245:GLY:N	1.84	0.93
1:B:771:LEU:HD12	1:B:927:TYR:HE2	1.34	0.92
1:B:358:ILE:H	1:B:358:ILE:HD12	1.31	0.92
1:C:556:VAL:HB	1:C:613:ILE:HD11	1.49	0.92
1:B:387:PRO:C	1:B:389:VAL:H	1.72	0.92
1:C:153:LEU:O	1:C:154:ARG:HB2	1.69	0.90
1:B:369:VAL:HG11	1:B:393:ILE:HG23	1.55	0.89
1:B:556:VAL:HB	1:B:613:ILE:HD11	1.52	0.88
1:C:386:LEU:HD23	1:C:386:LEU:H	1.37	0.88
1:B:904:ILE:HD11	1:B:911:ALA:HB3	1.56	0.87
1:B:784:ASN:HD22	1:B:959:SER:H	1.22	0.87
1:C:527:PRO:HB3	1:C:540:ILE:HB	1.56	0.87
1:B:869:VAL:HG21	1:B:872:LEU:HD12	1.56	0.87
1:B:556:VAL:HG23	1:B:557:VAL:HG13	1.54	0.86
1:B:784:ASN:ND2	1:B:959:SER:H	1.73	0.86
1:B:61:GLN:HE22	2:B:2055:ANP:HN61	0.91	0.86



	1 1 1 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:322:HIS:O	1:B:323:LEU:HD12	1.75	0.86
1:C:892:CYS:SG	1:C:922:ARG:HB3	2.16	0.86
1:C:198:LEU:H	1:C:198:LEU:HD12	1.39	0.86
1:B:201:LEU:O	1:B:217:ARG:HB3	1.75	0.86
1:B:301:ILE:HD12	1:B:301:ILE:H	1.40	0.86
1:C:638:LYS:HB2	1:C:684:GLN:HG3	1.57	0.86
1:B:369:VAL:HG21	1:B:393:ILE:HG21	1.56	0.86
1:B:1001:LEU:O	1:B:1005:VAL:HG23	1.76	0.86
1:B:1028:ARG:O	1:B:1032:ILE:HG22	1.76	0.85
1:B:61:GLN:NE2	2:B:2055:ANP:HN61	1.74	0.85
1:B:384:ARG:HB3	1:B:384:ARG:HH11	1.40	0.85
1:B:395:GLU:O	1:B:399:ILE:HG12	1.77	0.85
1:B:556:VAL:HB	1:B:613:ILE:CD1	2.06	0.84
1:B:508:LEU:HD21	1:B:510:ILE:HD11	1.56	0.84
1:B:745:LEU:HD13	1:B:747:LEU:HD11	1.57	0.83
1:C:1028:ARG:O	1:C:1032:ILE:HG22	1.78	0.83
1:C:305:THR:HG21	1:C:329:TYR:CD1	2.12	0.83
1:C:771:LEU:HD12	1:C:927:TYR:HE2	1.44	0.83
1:B:465:ARG:NH2	1:B:864:GLU:OE2	2.12	0.83
1:B:379:VAL:HG12	1:B:380:ASP:N	1.93	0.83
1:C:610:ARG:HH11	1:C:610:ARG:HB3	1.43	0.82
1:C:834:VAL:HG12	1:C:835:GLY:H	1.43	0.82
1:B:103:TYR:HB2	1:B:176:PHE:CD2	2.15	0.82
1:B:198:LEU:HD12	1:B:198:LEU:H	1.44	0.81
1:B:381:GLU:O	1:B:384:ARG:HG2	1.79	0.81
1:B:32:ARG:H	1:B:32:ARG:HD3	1.44	0.81
1:B:58:ARG:H	1:B:61:GLN:HE21	1.29	0.81
1:C:609:SER:O	1:C:613:ILE:HD13	1.80	0.81
1:C:39:GLU:H	1:C:39:GLU:CD	1.81	0.81
1:C:58:ARG:H	1:C:61:GLN:HE21	1.29	0.81
1:C:413:ASP:OD1	1:C:414:VAL:HG13	1.80	0.81
1:B:403:VAL:O	1:B:404:MET:HB3	1.77	0.80
1:C:784:ASN:ND2	1:C:959:SER:H	1.80	0.80
1:C:305:THR:HG22	1:C:306:ALA:H	1.45	0.80
1:C:134:ILE:HD13	1:C:135:GLY:N	1.96	0.80
1:C:628:VAL:HG11	1:C:640:ALA:HB2	1.63	0.80
1:C:58:ARG:HB2	1:C:61:GLN:NE2	1.97	0.79
1:B:369:VAL:HG21	1:B:393:ILE:CG2	2.12	0.79
1:B:470:ASP:O	1:B:472:GLU:HB2	1.82	0.79
1:B:921:GLY:O	1:B:925:GLU:HG2	1.83	0.79
1:C:560:ILE:HG13	1:C:561:THR:H	1.48	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:555:HIS:HA	1:B:639:ILE:CD1	2.12	0.79
1:C:824:ILE:HG23	1:C:852:PRO:HG3	1.64	0.79
1:C:470:ASP:O	1:C:472:GLU:N	2.16	0.79
1:B:224:THR:HG22	1:B:245:GLY:O	1.82	0.78
1:B:256:ASP:HB3	1:B:474:LYS:HD3	1.65	0.78
1:C:610:ARG:HB3	1:C:610:ARG:NH1	1.98	0.78
1:B:492:ARG:HG3	1:B:492:ARG:HH11	1.49	0.78
1:C:1010:VAL:O	1:C:1014:ALA:HB2	1.83	0.78
1:B:470:ASP:O	1:B:472:GLU:N	2.17	0.78
1:B:719:LEU:HD11	1:B:1019:GLU:HA	1.66	0.78
1:C:921:GLY:O	1:C:925:GLU:HG2	1.84	0.78
1:C:357:THR:HB	1:C:360:ASP:HB2	1.66	0.78
1:C:58:ARG:HB2	1:C:61:GLN:HE21	1.49	0.78
1:B:95:LEU:HD13	1:B:100:LYS:HD3	1.65	0.77
1:C:301:ILE:HD12	1:C:301:ILE:H	1.49	0.77
1:B:163:THR:HG21	1:B:186:ALA:HB1	1.67	0.77
1:B:390:GLU:C	1:B:392:HIS:N	2.27	0.77
1:C:85:THR:HB	2:C:2055:ANP:O1A	1.84	0.77
1:C:797:ILE:HG23	1:C:876:HIS:ND1	2.00	0.77
1:C:103:TYR:HB2	1:C:176:PHE:CD2	2.19	0.77
1:B:56:GLU:OE1	1:B:57:PRO:HD2	1.83	0.77
1:B:709:ARG:HG2	1:B:710:ASN:H	1.49	0.77
1:B:768:ARG:NH1	1:B:768:ARG:HB3	2.00	0.77
1:B:608:ASN:HD22	1:B:610:ARG:HH11	1.33	0.76
1:B:1043:LEU:HD23	1:B:1046:MET:HE2	1.67	0.76
1:B:22:ILE:O	1:B:576:PRO:HD2	1.86	0.76
1:C:992:LYS:HE2	1:C:992:LYS:HA	1.66	0.76
1:C:396:VAL:HG11	1:C:399:ILE:HB	1.66	0.76
1:C:712:SER:HB2	1:C:986:ARG:HH11	1.49	0.76
1:C:436:THR:HG23	1:C:447:GLY:HA3	1.68	0.76
1:C:848:ARG:HB2	1:C:887:PHE:CD2	2.21	0.76
1:C:712:SER:HB2	1:C:986:ARG:NH1	2.01	0.75
1:B:387:PRO:C	1:B:389:VAL:N	2.37	0.75
1:B:626:VAL:HB	1:B:653:VAL:HG22	1.69	0.75
1:B:279:ILE:HG22	1:B:281:TYR:CE1	2.22	0.75
1:B:687:ARG:HA	1:B:1029:MET:CE	2.17	0.75
1:C:414:VAL:HG12	1:C:424:PRO:HD3	1.68	0.75
1:B:58:ARG:HB2	1:B:61:GLN:HE21	1.50	0.75
1:B:436:THR:HG23	1:B:447:GLY:HA3	1.69	0.75
1:B:391:ARG:O	1:B:391:ARG:HD3	1.86	0.75
1:C:720:VAL:HG13	1:C:961:ILE:HD11	1.68	0.75



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:763:GLU:HG3	1:B:900:LYS:HG2	1.69	0.74
1:C:50:PHE:CD2	1:C:57:PRO:HG3	2.22	0.74
1:B:703:TRP:CD1	1:B:709:ARG:HA	2.21	0.74
1:B:32:ARG:H	1:B:32:ARG:CD	1.98	0.74
1:B:560:ILE:HD12	1:B:579:ALA:HB2	1.70	0.74
1:C:975:THR:HG22	1:C:979:ILE:HG13	1.67	0.74
1:C:787:LEU:HD13	1:C:789:PHE:CE2	2.23	0.74
1:C:1029:MET:O	1:C:1032:ILE:HG23	1.87	0.74
1:B:192:LYS:HB3	1:B:196:LYS:HE3	1.70	0.74
1:B:774:TYR:CZ	1:B:886:ARG:HG3	2.22	0.74
1:B:873:ARG:H	1:B:876:HIS:HD2	1.35	0.74
1:C:922:ARG:HH21	1:C:922:ARG:HG3	1.51	0.74
1:B:384:ARG:HB3	1:B:384:ARG:NH1	2.03	0.73
1:B:103:TYR:HE1	1:B:161:THR:HG23	1.53	0.73
1:B:397:ARG:HA	1:B:400:LEU:HD12	1.68	0.73
1:C:303:ILE:HG12	1:C:304:VAL:H	1.52	0.73
1:B:476:ILE:HG22	1:B:478:GLU:OE2	1.89	0.73
1:C:790:SER:HA	1:C:958:GLN:HE22	1.53	0.73
1:C:438:ARG:O	1:C:444:LEU:HD12	1.87	0.73
1:B:735:ARG:HA	1:B:950:VAL:O	1.88	0.73
1:B:784:ASN:HD22	1:B:959:SER:N	1.86	0.73
1:B:370:LYS:O	1:B:373:ALA:HB3	1.88	0.73
1:B:262:GLU:HG2	1:B:454:ASP:OD2	1.89	0.72
1:C:241:ASN:O	1:C:530:LYS:HD2	1.89	0.72
1:B:413:ASP:OD1	1:B:414:VAL:HG13	1.88	0.72
1:C:784:ASN:HD22	1:C:959:SER:H	1.37	0.72
1:B:529:VAL:HG12	1:B:530:LYS:N	2.05	0.72
1:B:608:ASN:HD22	1:B:610:ARG:NH1	1.87	0.72
1:B:904:ILE:HD12	1:B:904:ILE:O	1.89	0.72
1:C:135:GLY:HA3	1:C:156:PHE:CE1	2.24	0.72
1:C:875:GLU:O	1:C:878:ALA:HB3	1.90	0.72
1:B:70:ARG:HH21	1:B:618:LYS:HD2	1.53	0.72
1:B:271:LEU:HD23	1:B:481:PHE:HZ	1.53	0.72
1:B:690:GLU:OE2	1:B:715:ARG:NH1	2.23	0.72
1:C:608:ASN:HD22	1:C:610:ARG:NH1	1.88	0.72
1:B:1037:LEU:HD23	1:B:1038:ASP:N	2.04	0.72
1:B:390:GLU:C	1:B:392:HIS:H	1.83	0.72
1:C:181:VAL:HB	1:C:222:VAL:HG12	1.71	0.72
1:C:370:LYS:O	1:C:373:ALA:HB3	1.90	0.72
1:C:738:ALA:HA	1:C:947:VAL:HA	1.72	0.72
1:C:1007:ARG:HA	1:C:1010:VAL:HG12	1.70	0.72



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:376:TYR:O	1:B:377:ARG:HB3	1.90	0.72
1:B:212:TRP:O	1:B:213:VAL:HG13	1.90	0.71
1:B:895:PHE:H	1:B:895:PHE:HD2	1.38	0.71
1:B:1012:ARG:HH11	1:B:1012:ARG:HG2	1.54	0.71
1:B:58:ARG:H	1:B:61:GLN:NE2	1.87	0.71
1:B:736:LYS:O	1:B:737:ILE:HG22	1.89	0.71
1:B:540:ILE:HG13	1:B:541:PRO:CD	2.20	0.71
1:C:103:TYR:HB3	1:C:179:ILE:HG13	1.71	0.71
1:C:212:TRP:O	1:C:213:VAL:HG13	1.89	0.71
1:C:763:GLU:HG3	1:C:900:LYS:HG2	1.72	0.71
1:B:731:SER:O	1:B:951:PRO:HB3	1.90	0.71
1:C:490:GLU:O	1:C:493:ASP:HB3	1.89	0.71
1:B:58:ARG:HH21	1:B:83:GLY:N	1.89	0.71
1:B:821:GLY:HA3	1:B:848:ARG:HH22	1.56	0.71
1:B:787:LEU:HD13	1:B:789:PHE:CE2	2.26	0.70
1:C:163:THR:HG21	1:C:186:ALA:HB1	1.72	0.70
1:C:176:PHE:HB2	1:C:179:ILE:HD11	1.73	0.70
1:C:480:ASP:O	1:C:482:GLU:N	2.24	0.70
1:C:617:ARG:HA	1:C:647:LEU:HD22	1.72	0.70
1:B:884:PHE:CE2	1:B:888:MET:HG3	2.26	0.70
1:B:1009:LEU:HD22	1:B:1009:LEU:H	1.56	0.70
1:C:492:ARG:HG3	1:C:492:ARG:HH11	1.55	0.70
1:B:768:ARG:HB3	1:B:768:ARG:HH11	1.56	0.70
1:C:735:ARG:HA	1:C:950:VAL:O	1.91	0.70
1:B:361:ILE:HG22	1:B:397:ARG:HB3	1.73	0.70
1:B:480:ASP:O	1:B:482:GLU:N	2.25	0.70
1:C:360:ASP:O	1:C:362:ASP:N	2.25	0.70
1:B:438:ARG:O	1:B:444:LEU:HD12	1.92	0.69
1:B:618:LYS:O	1:B:621:HIS:HB3	1.91	0.69
1:B:687:ARG:HA	1:B:1029:MET:HE3	1.72	0.69
1:C:301:ILE:HG22	1:C:302:GLY:H	1.58	0.69
1:B:334:VAL:HG12	1:B:335:ARG:HG3	1.74	0.69
1:B:971:GLY:O	1:B:972:ARG:HD3	1.92	0.69
1:B:490:GLU:O	1:B:493:ASP:HB3	1.92	0.69
1:C:540:ILE:HG13	1:C:541:PRO:HD2	1.72	0.69
1:B:791:VAL:HG13	1:B:958:GLN:NE2	2.07	0.69
1:B:1037:LEU:HD23	1:B:1038:ASP:H	1.56	0.69
1:B:638:LYS:CB	1:B:684:GLN:HG3	2.21	0.69
1:C:244:ILE:HG22	1:C:245:GLY:H	1.55	0.69
1:C:608:ASN:HD22	1:C:610:ARG:HH11	1.37	0.69
1:C:747:LEU:N	1:C:747:LEU:HD12	2.07	0.69



	A (A (A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1012:ARG:O	1:C:1013:TYR:HB2	1.92	0.69
1:B:309:LYS:H	1:B:309:LYS:HD2	1.57	0.69
1:B:426:LEU:HD11	1:B:466:ALA:HA	1.74	0.69
1:C:39:GLU:HG2	1:C:70:ARG:HG2	1.73	0.69
1:C:379:VAL:HG12	1:C:380:ASP:N	2.04	0.69
1:B:305:THR:CG2	1:B:306:ALA:N	2.55	0.69
1:B:364:LEU:HD23	1:B:368:MET:SD	2.33	0.69
1:B:479:VAL:HG23	1:B:481:PHE:H	1.56	0.69
1:C:834:VAL:HG12	1:C:835:GLY:N	2.07	0.68
1:C:510:ILE:CD1	1:C:616:LEU:HD22	2.23	0.68
1:C:1001:LEU:O	1:C:1005:VAL:HG23	1.93	0.68
1:B:379:VAL:CG1	1:B:380:ASP:H	1.97	0.68
1:B:438:ARG:C	1:B:444:LEU:HD12	2.14	0.68
1:C:58:ARG:H	1:C:61:GLN:NE2	1.91	0.68
1:C:95:LEU:HD13	1:C:100:LYS:HD3	1.74	0.68
1:B:262:GLU:HG2	1:B:454:ASP:CG	2.13	0.68
1:B:617:ARG:HA	1:B:647:LEU:HD22	1.74	0.68
1:B:747:LEU:N	1:B:747:LEU:HD12	2.08	0.68
1:C:476:ILE:HG22	1:C:478:GLU:OE2	1.93	0.68
1:B:419:GLY:O	1:B:420:GLU:HB2	1.93	0.68
1:C:337:LEU:HD21	1:C:343:ILE:HD11	1.76	0.68
1:C:259:VAL:HG12	1:C:261:ASP:H	1.59	0.68
1:C:754:PHE:O	1:C:943:VAL:HG23	1.94	0.68
1:B:736:LYS:NZ	1:B:736:LYS:HA	2.08	0.68
1:C:257:VAL:HB	1:C:450:PHE:CD1	2.28	0.68
1:B:610:ARG:NH1	1:B:610:ARG:HB3	2.08	0.67
1:C:296:LYS:HA	1:C:301:ILE:HG12	1.76	0.67
1:C:305:THR:O	1:C:307:THR:N	2.27	0.67
1:C:873:ARG:H	1:C:876:HIS:HD2	1.41	0.67
1:B:916:ILE:HG22	1:B:932:VAL:HA	1.76	0.67
1:C:305:THR:HG21	1:C:329:TYR:HD1	1.60	0.67
1:B:248:ARG:HG3	1:B:249:ILE:N	2.08	0.67
1:B:616:LEU:HA	1:B:619:LEU:HD12	1.77	0.67
1:B:2:ILE:N	1:B:11:PRO:N	2.43	0.67
1:B:426:LEU:O	1:B:430:ILE:HD12	1.94	0.67
1:B:784:ASN:ND2	1:B:959:SER:N	2.42	0.67
1:C:303:ILE:HG12	1:C:304:VAL:N	2.09	0.67
1:C:858:VAL:HG21	1:C:880:TYR:CE1	2.30	0.67
1:B:305:THR:HG23	1:B:329:TYR:CE1	2.30	0.67
1:B:363:SER:O	1:B:364:LEU:HB2	1.95	0.67
1:B:834:VAL:HG12	1:B:835:GLY:H	1.60	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:304:VAL:O	1:B:305:THR:HB	1.95	0.66
1:C:3:PRO:O	1:C:11:PRO:N	2.28	0.66
1:C:735:ARG:HB3	1:C:949:SER:HB3	1.78	0.66
1:B:265:SER:O	1:B:267:LEU:N	2.28	0.66
1:B:791:VAL:HG13	1:B:958:GLN:HE21	1.61	0.66
1:B:809:TYR:CE2	1:B:811:ARG:HB2	2.31	0.66
1:C:376:TYR:O	1:C:377:ARG:CB	2.42	0.66
1:C:419:GLY:O	1:C:420:GLU:HB2	1.95	0.66
1:C:608:ASN:ND2	1:C:610:ARG:HH11	1.93	0.66
1:B:358:ILE:HD11	1:B:419:GLY:C	2.15	0.66
1:C:510:ILE:HD11	1:C:616:LEU:HD22	1.75	0.66
1:B:800:GLU:OE2	1:B:876:HIS:HE1	1.78	0.66
1:B:305:THR:HG22	1:B:306:ALA:N	2.11	0.66
1:B:749:HIS:CD2	1:B:751:GLU:HB2	2.30	0.66
1:C:694:ILE:HD13	1:C:715:ARG:NH2	2.10	0.66
1:C:904:ILE:HD12	1:C:904:ILE:O	1.96	0.66
1:B:855:ARG:O	1:B:859:GLN:HG3	1.96	0.66
1:C:736:LYS:C	1:C:737:ILE:HG23	2.17	0.66
1:B:872:LEU:HA	1:B:876:HIS:CD2	2.31	0.65
1:C:58:ARG:HH21	1:C:83:GLY:N	1.94	0.65
1:B:739:ILE:O	1:B:945:ALA:HA	1.96	0.65
1:B:85:THR:HB	2:B:2055:ANP:O1A	1.96	0.65
1:B:357:THR:HB	1:B:360:ASP:HB2	1.77	0.65
1:C:376:TYR:O	1:C:377:ARG:HB2	1.95	0.65
1:B:51:ARG:HA	1:B:55:GLY:O	1.96	0.65
1:C:700:GLN:HA	1:C:703:TRP:CE3	2.32	0.65
1:B:135:GLY:HA3	1:B:156:PHE:CD1	2.31	0.65
1:B:754:PHE:O	1:B:943:VAL:HG23	1.97	0.65
1:B:849:PRO:HD3	1:B:883:ILE:HG22	1.78	0.65
1:C:468:LEU:HD11	1:C:853:LEU:HD21	1.79	0.65
1:B:270:ILE:O	1:B:273:LYS:HB3	1.96	0.65
1:C:301:ILE:HD12	1:C:301:ILE:N	2.11	0.65
1:C:396:VAL:CG1	1:C:399:ILE:HB	2.27	0.65
1:C:756:LEU:O	1:C:940:THR:HG23	1.96	0.65
1:C:895:PHE:HB2	1:C:920:GLU:O	1.97	0.65
1:B:438:ARG:HG3	1:B:439:LEU:N	2.12	0.65
1:B:1010:VAL:O	1:B:1014:ALA:HB2	1.97	0.65
1:C:745:LEU:HD13	1:C:747:LEU:HD11	1.79	0.65
1:C:873:ARG:HB2	1:C:875:GLU:OE2	1.95	0.65
1:C:60:ILE:HD13	1:C:546:VAL:HG21	1.78	0.65
1:B:301:ILE:HG22	1:B:302:GLY:H	1.62	0.64



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:771:LEU:HD12	1:B:927:TYR:CE2	2.24	0.64
1:B:905:GLU:HG2	1:B:910:THR:HB	1.79	0.64
1:B:259:VAL:HG22	1:B:477:ASP:OD1	1.97	0.64
1:B:439:LEU:CD1	1:B:444:LEU:HD13	2.27	0.64
1:B:439:LEU:HD13	1:B:444:LEU:HD13	1.79	0.64
1:B:553:ILE:HB	1:B:612:ARG:HE	1.60	0.64
1:C:705:ARG:O	1:C:706:PHE:HB3	1.96	0.64
1:C:1002:GLY:O	1:C:1005:VAL:HB	1.96	0.64
1:B:254:VAL:HG22	1:B:436:THR:CG2	2.28	0.64
1:B:512:GLU:OE1	1:B:630:THR:HB	1.97	0.64
1:B:197:LEU:HA	1:B:200:LEU:HD12	1.80	0.64
1:C:254:VAL:HG22	1:C:436:THR:CG2	2.26	0.64
1:C:220:LEU:HD12	1:C:221:MET:H	1.62	0.64
1:C:756:LEU:O	1:C:940:THR:HA	1.98	0.64
1:C:109:SER:HB3	1:C:138:HIS:CD2	2.33	0.64
1:C:1037:LEU:HD23	1:C:1038:ASP:N	2.13	0.64
1:B:86:SER:N	2:B:2055:ANP:O1A	2.30	0.64
1:B:470:ASP:O	1:B:471:ILE:C	2.35	0.64
1:C:190:ALA:HB3	1:C:193:ASN:ND2	2.12	0.64
1:C:63:MET:HG2	1:C:63:MET:O	1.98	0.64
1:C:109:SER:HB3	1:C:138:HIS:HD2	1.62	0.64
1:C:224:THR:OG1	1:C:247:SER:HB3	1.98	0.64
1:B:529:VAL:CG1	1:B:530:LYS:N	2.61	0.64
1:B:706:PHE:CD1	1:B:706:PHE:O	2.51	0.64
1:B:738:ALA:HA	1:B:947:VAL:HA	1.79	0.64
1:C:573:ARG:O	1:C:574:PHE:HB2	1.97	0.64
1:B:50:PHE:CD2	1:B:57:PRO:HG3	2.33	0.63
1:C:194:VAL:O	1:C:198:LEU:HD12	1.97	0.63
1:C:718:THR:O	1:C:721:LEU:HB3	1.99	0.63
1:B:570:VAL:HG21	1:B:1047:TYR:OH	1.98	0.63
1:B:681:VAL:O	1:B:685:VAL:HG23	1.98	0.63
1:B:830:GLY:O	1:B:831:ASP:HB2	1.97	0.63
1:B:901:LYS:HG3	1:B:902:TYR:N	2.12	0.63
1:B:901:LYS:HG3	1:B:902:TYR:H	1.64	0.63
1:B:493:ASP:HA	1:B:496:ARG:NH2	2.14	0.63
1:B:883:ILE:HD12	1:B:883:ILE:H	1.62	0.63
1:B:709:ARG:O	1:B:710:ASN:HB2	1.98	0.63
1:C:248:ARG:C	1:C:249:ILE:HG12	2.18	0.63
1:B:1002:GLY:O	1:B:1005:VAL:HB	1.99	0.63
1:C:530:LYS:O	1:C:537:VAL:HG12	1.98	0.63
1:B:740:VAL:HG12	1:B:741:ARG:N	2.14	0.63



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:642:ASP:C	1:C:646:LEU:HD12	2.18	0.63
1:C:816:ARG:O	1:C:845:GLU:HG3	1.99	0.63
1:B:1042:ALA:O	1:B:1046:MET:HG3	1.98	0.63
1:C:267:LEU:O	1:C:270:ILE:HG22	1.99	0.63
1:C:560:ILE:HG13	1:C:561:THR:N	2.14	0.63
1:C:685:VAL:O	1:C:688:ARG:HB3	1.99	0.62
1:B:610:ARG:HH11	1:B:610:ARG:HB3	1.64	0.62
1:B:620:ALA:HB2	1:B:647:LEU:HD13	1.81	0.62
1:B:858:VAL:HG12	1:B:862:ILE:HD11	1.81	0.62
1:C:345:PHE:HA	1:C:436:THR:OG1	1.99	0.62
1:C:440:PHE:CD2	1:C:495:TYR:HA	2.34	0.62
1:C:735:ARG:O	1:C:949:SER:HA	1.99	0.62
1:B:55:GLY:O	1:B:57:PRO:HD3	2.00	0.62
1:B:103:TYR:HB3	1:B:179:ILE:HG12	1.81	0.62
1:B:207:LEU:N	1:B:207:LEU:HD23	2.14	0.62
1:B:472:GLU:OE2	1:B:472:GLU:HA	1.98	0.62
1:B:560:ILE:HD12	1:B:579:ALA:CB	2.29	0.62
1:C:895:PHE:H	1:C:895:PHE:HD2	1.48	0.62
1:B:426:LEU:HD12	1:B:465:ARG:HG3	1.80	0.62
1:B:1007:ARG:HA	1:B:1010:VAL:HG12	1.81	0.62
1:C:363:SER:O	1:C:364:LEU:HD12	2.00	0.62
1:C:398:GLU:HG3	1:C:399:ILE:HD12	1.81	0.62
1:C:855:ARG:HG3	1:C:877:PHE:HB3	1.81	0.62
1:B:267:LEU:O	1:B:270:ILE:HG22	1.99	0.62
1:C:883:ILE:HD12	1:C:883:ILE:H	1.63	0.62
1:B:384:ARG:O	1:B:387:PRO:HB3	1.99	0.62
1:C:37:PHE:HB2	1:C:621:HIS:CE1	2.34	0.62
1:C:849:PRO:HG2	1:C:884:PHE:HA	1.82	0.62
1:B:387:PRO:HB2	1:B:389:VAL:H	1.64	0.62
1:B:756:LEU:O	1:B:940:THR:HG23	2.00	0.62
1:C:154:ARG:HE	1:C:174:GLY:HA3	1.63	0.62
1:C:249:ILE:HG23	1:C:541:PRO:HG2	1.81	0.62
1:B:972:ARG:NH1	1:B:1026:GLU:HG3	2.14	0.62
1:B:194:VAL:O	1:B:195:ASP:C	2.36	0.61
1:C:1007:ARG:HA	1:C:1010:VAL:CG1	2.30	0.61
1:C:1010:VAL:HG13	1:C:1011:ARG:N	2.15	0.61
1:B:212:TRP:CZ2	1:B:235:LEU:HD11	2.35	0.61
1:B:721:LEU:O	1:B:725:ILE:HG12	2.01	0.61
1:B:904:ILE:HD12	1:B:911:ALA:H	1.65	0.61
1:B:975:THR:HG22	1:B:979:ILE:HG12	1.80	0.61
1:B:1009:LEU:HD22	1:B:1009:LEU:N	2.15	0.61



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:238:GLN:HG3	1:C:239:LEU:HD23	1.82	0.61
1:C:244:ILE:CG2	1:C:245:GLY:N	2.57	0.61
1:B:140:ARG:O	1:B:141:ILE:O	2.18	0.61
1:B:333:LEU:N	1:B:333:LEU:HD22	2.14	0.61
1:B:774:TYR:CE2	1:B:886:ARG:HG3	2.35	0.61
1:C:101:ARG:HH22	1:C:174:GLY:HA3	1.65	0.61
1:C:556:VAL:HB	1:C:613:ILE:CD1	2.29	0.61
1:B:190:ALA:HB3	1:B:193:ASN:ND2	2.16	0.61
1:B:314:LYS:HB3	1:B:320:ILE:HG12	1.82	0.61
1:B:1010:VAL:HG13	1:B:1011:ARG:N	2.15	0.61
1:B:1049:GLU:O	1:B:1052:SER:HB3	1.99	0.61
1:C:212:TRP:CZ2	1:C:235:LEU:HD11	2.35	0.61
1:C:740:VAL:HG12	1:C:741:ARG:N	2.16	0.61
1:B:393:ILE:HG22	1:B:397:ARG:NE	2.14	0.61
1:B:612:ARG:HG3	1:B:612:ARG:NH1	2.14	0.61
1:B:690:GLU:HG3	1:B:694:ILE:HG13	1.83	0.61
1:C:852:PRO:O	1:C:853:LEU:HD23	2.01	0.61
1:B:1009:LEU:H	1:B:1009:LEU:CD2	2.12	0.61
1:C:731:SER:O	1:C:951:PRO:HB3	2.00	0.61
1:B:968:ARG:HD2	1:B:1019:GLU:OE1	2.00	0.61
1:C:266:THR:O	1:C:267:LEU:HB2	1.99	0.61
1:B:1025:LEU:O	1:B:1025:LEU:HD23	2.01	0.61
1:C:61:GLN:HE22	2:C:2055:ANP:HN61	1.47	0.61
1:C:849:PRO:HD3	1:C:883:ILE:HG22	1.83	0.61
1:C:705:ARG:O	1:C:706:PHE:CB	2.49	0.61
1:B:176:PHE:HB2	1:B:179:ILE:HD11	1.83	0.60
1:B:849:PRO:HG2	1:B:884:PHE:HA	1.82	0.60
1:B:70:ARG:NH2	1:B:618:LYS:HD2	2.15	0.60
1:B:849:PRO:HD2	1:B:887:PHE:HD2	1.66	0.60
1:B:771:LEU:HB3	1:B:886:ARG:NH1	2.16	0.60
1:C:494:ARG:O	1:C:497:ARG:N	2.34	0.60
1:C:687:ARG:HA	1:C:1029:MET:CE	2.31	0.60
1:C:357:THR:HG22	1:C:358:ILE:N	2.16	0.60
1:B:63:MET:HG3	1:B:622:ASP:HB3	1.83	0.60
1:B:800:GLU:OE2	1:B:876:HIS:CE1	2.54	0.60
1:B:612:ARG:HG3	1:B:612:ARG:HH11	1.65	0.60
1:C:463:ILE:HD13	1:C:474:LYS:HG3	1.83	0.60
1:C:739:ILE:O	1:C:945:ALA:HA	2.01	0.60
1:B:709:ARG:HG3	1:B:709:ARG:HH11	1.66	0.60
1:B:735:ARG:O	1:B:949:SER:HA	2.02	0.60
1:B:301:ILE:HD12	1:B:301:ILE:N	2.14	0.60



	A la C	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:560:ILE:HG13	1:B:561:THR:H	1.66	0.60
1:C:518:ARG:O	1:C:522:ARG:HD2	2.02	0.60
1:C:203:PHE:CD1	1:C:239:LEU:HD12	2.37	0.60
1:C:532:LEU:O	1:C:534:GLY:N	2.35	0.60
1:B:415:VAL:HG12	1:B:422:ILE:HB	1.83	0.59
1:C:63:MET:CE	1:C:67:ARG:HH21	2.15	0.59
1:C:1012:ARG:C	1:C:1013:TYR:HD1	2.06	0.59
1:B:66:LYS:O	1:B:70:ARG:HG3	2.01	0.59
1:B:463:ILE:HD13	1:B:474:LYS:HG3	1.82	0.59
1:B:532:LEU:HD12	1:B:619:LEU:HD21	1.83	0.59
1:C:958:GLN:O	1:C:961:ILE:HG22	2.01	0.59
1:B:309:LYS:HD2	1:B:309:LYS:N	2.16	0.59
1:B:374:TYR:C	1:B:376:TYR:H	2.04	0.59
1:C:101:ARG:NH1	1:C:154:ARG:HA	2.17	0.59
1:B:260:ASN:ND2	1:B:260:ASN:O	2.35	0.59
1:B:339:LEU:HB2	1:B:343:ILE:HG12	1.85	0.59
1:B:471:ILE:HG22	1:B:471:ILE:O	2.01	0.59
1:C:56:GLU:OE1	1:C:57:PRO:HD2	2.03	0.59
1:C:609:SER:HA	1:C:612:ARG:NH1	2.17	0.59
1:B:107:PRO:HA	1:B:163:THR:HG22	1.84	0.59
1:B:257:VAL:HB	1:B:450:PHE:CD1	2.37	0.59
1:B:358:ILE:HD12	1:B:358:ILE:N	2.12	0.59
1:B:735:ARG:HB3	1:B:949:SER:CA	2.33	0.59
1:B:387:PRO:CB	1:B:389:VAL:H	2.16	0.59
1:B:664:ARG:O	1:B:668:GLU:HG3	2.03	0.59
1:C:339:LEU:HB2	1:C:343:ILE:HG13	1.85	0.59
1:C:771:LEU:HD12	1:C:927:TYR:CE2	2.33	0.59
1:B:735:ARG:HB3	1:B:949:SER:HB3	1.85	0.59
1:C:264:ILE:C	1:C:264:ILE:HD13	2.23	0.59
1:C:459:LEU:O	1:C:463:ILE:HG12	2.03	0.59
1:C:848:ARG:HG3	1:C:887:PHE:CE2	2.38	0.59
1:B:376:TYR:O	1:B:377:ARG:CB	2.50	0.58
1:C:514:PRO:O	1:C:517:ALA:HB3	2.03	0.58
1:B:692:ARG:HG2	1:B:692:ARG:HH21	1.68	0.58
1:B:358:ILE:HD11	1:B:419:GLY:O	2.04	0.58
1:C:561:THR:OG1	1:C:585:ARG:HD2	2.03	0.58
1:B:440:PHE:H	1:B:440:PHE:HD1	1.52	0.58
1:B:555:HIS:O	1:B:581:ILE:HD12	2.02	0.58
1:C:477:ASP:C	1:C:479:VAL:H	2.06	0.58
1:C:760:LEU:HD21	1:C:938:THR:HB	1.85	0.58
1:B:682:LYS:HD3	1:B:1039:TYR:CD2	2.39	0.58



	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:687:ARG:HA	1:C:1029:MET:HE1	1.86	0.58
1:C:737:ILE:HD13	1:C:950:VAL:HG21	1.84	0.58
1:B:103:TYR:HB2	1:B:176:PHE:CE2	2.38	0.58
1:B:271:LEU:HD23	1:B:481:PHE:CZ	2.38	0.58
1:B:309:LYS:HG2	1:B:310:GLY:H	1.67	0.58
1:B:608:ASN:ND2	1:B:610:ARG:HB2	2.19	0.58
1:B:717:GLN:OE1	1:B:982:ARG:HD3	2.02	0.58
1:B:49:PHE:CD2	1:B:94:PHE:HD1	2.21	0.58
1:B:135:GLY:HA3	1:B:156:PHE:CE1	2.37	0.58
1:B:402:LYS:HG2	1:B:403:VAL:HG13	1.84	0.58
1:B:613:ILE:HG21	1:B:646:LEU:HD22	1.86	0.58
1:C:808:THR:HG23	1:C:848:ARG:HE	1.67	0.58
1:B:60:ILE:HD12	1:B:506:PRO:HG3	1.86	0.58
1:B:164:GLN:HE21	1:B:164:GLN:C	2.07	0.58
1:B:608:ASN:ND2	1:B:610:ARG:HH11	2.00	0.58
1:B:608:ASN:HD21	1:B:610:ARG:HB2	1.69	0.58
1:B:766:GLU:HB3	1:B:768:ARG:HE	1.69	0.58
1:B:824:ILE:HG23	1:B:852:PRO:HG3	1.85	0.58
1:B:858:VAL:O	1:B:862:ILE:HG13	2.04	0.58
1:C:470:ASP:O	1:C:471:ILE:C	2.41	0.58
1:C:509:PHE:O	1:C:549:VAL:HA	2.03	0.58
1:C:664:ARG:O	1:C:668:GLU:HG3	2.04	0.58
1:C:983:LEU:HB3	1:C:989:VAL:HG23	1.84	0.58
1:B:93:LEU:HA	1:B:158:ILE:HD11	1.85	0.57
1:B:268:SER:O	1:B:272:GLU:HG2	2.03	0.57
1:B:387:PRO:HG2	1:B:389:VAL:HA	1.86	0.57
1:B:883:ILE:HD12	1:B:883:ILE:N	2.19	0.57
1:B:901:LYS:HA	1:B:914:GLU:HA	1.85	0.57
1:B:972:ARG:HB3	1:B:973:PRO:HD2	1.85	0.57
1:C:466:ALA:HB1	1:C:472:GLU:HG3	1.85	0.57
1:C:714:GLY:O	1:C:716:ALA:N	2.37	0.57
1:C:279:ILE:O	1:C:346:ALA:HA	2.05	0.57
1:C:305:THR:CG2	1:C:329:TYR:CD1	2.85	0.57
1:C:358:ILE:HD11	1:C:419:GLY:C	2.25	0.57
1:C:791:VAL:H	1:C:958:GLN:NE2	2.02	0.57
1:B:386:LEU:HD23	1:B:386:LEU:N	2.03	0.57
1:B:804:ASN:O	1:B:806:LEU:HG	2.04	0.57
1:B:972:ARG:HB3	1:B:973:PRO:CD	2.34	0.57
1:C:618:LYS:O	1:C:621:HIS:HB3	2.05	0.57
1:B:365:SER:OG	1:B:368:MET:HB2	2.05	0.57
1:C:32:ARG:HD2	1:C:32:ARG:N	2.18	0.57



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:492:ARG:HG3	1:C:492:ARG:NH1	2.18	0.57
1:B:194:VAL:O	1:B:197:LEU:N	2.34	0.57
1:B:612:ARG:HH11	1:B:612:ARG:CG	2.17	0.57
1:C:79:PRO:HG2	1:C:504:ILE:HD13	1.86	0.57
1:C:426:LEU:O	1:C:430:ILE:HD12	2.04	0.57
1:B:970:ILE:HD11	1:B:1019:GLU:HG3	1.87	0.57
1:C:3:PRO:O	1:C:4:VAL:CB	2.53	0.57
1:B:23:GLU:O	1:B:24:LYS:CB	2.51	0.57
1:B:362:ASP:O	1:B:397:ARG:NH1	2.38	0.57
1:B:518:ARG:O	1:B:522:ARG:HD3	2.04	0.57
1:C:58:ARG:HG2	1:C:502:ASP:HB2	1.87	0.57
1:C:259:VAL:HB	1:C:452:LEU:CD2	2.34	0.57
1:C:418:GLU:HG3	1:C:418:GLU:O	2.05	0.57
1:C:532:LEU:HD12	1:C:619:LEU:HD21	1.87	0.57
1:C:758:ILE:HG22	1:C:938:THR:OG1	2.05	0.57
1:C:824:ILE:HG23	1:C:852:PRO:CG	2.34	0.57
1:C:981:ASP:O	1:C:982:ARG:C	2.43	0.57
1:B:279:ILE:HG22	1:B:281:TYR:HE1	1.67	0.57
1:B:380:ASP:HB3	1:B:383:GLU:OE2	2.05	0.57
1:C:63:MET:HE1	1:C:67:ARG:HH21	1.70	0.57
1:C:93:LEU:HA	1:C:158:ILE:HD11	1.85	0.57
1:C:791:VAL:HG21	1:C:977:ALA:HA	1.85	0.57
1:C:968:ARG:HD2	1:C:1019:GLU:OE1	2.04	0.57
1:B:58:ARG:HB2	1:B:61:GLN:NE2	2.19	0.56
1:B:134:ILE:HD12	1:B:135:GLY:N	2.20	0.56
1:B:418:GLU:O	1:B:418:GLU:HG3	2.04	0.56
1:B:905:GLU:HA	1:B:910:THR:HA	1.87	0.56
1:C:374:TYR:C	1:C:376:TYR:H	2.07	0.56
1:C:638:LYS:HE2	1:C:642:ASP:OD2	2.05	0.56
1:C:743:PHE:C	1:C:745:LEU:H	2.08	0.56
1:B:510:ILE:CD1	1:B:616:LEU:HD22	2.36	0.56
1:B:706:PHE:O	1:B:706:PHE:HD1	1.88	0.56
1:B:957:THR:O	1:B:958:GLN:C	2.44	0.56
1:B:985:MET:CE	1:B:986:ARG:HH21	2.17	0.56
1:C:690:GLU:OE2	1:C:715:ARG:NH1	2.39	0.56
1:C:835:GLY:O	1:C:836:ARG:HB2	2.05	0.56
1:B:170:TYR:CZ	1:B:171:ARG:HG2	2.41	0.56
1:B:337:LEU:HD21	1:B:343:ILE:HD11	1.87	0.56
1:B:477:ASP:C	1:B:479:VAL:H	2.08	0.56
1:B:492:ARG:HG3	1:B:492:ARG:NH1	2.16	0.56
1:B:687:ARG:HA	1:B:1029:MET:HE1	1.87	0.56



A + 1	A 4 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:983:LEU:HB3	1:B:989:VAL:HG23	1.85	0.56
1:C:195:ASP:HA	1:C:198:LEU:HD13	1.87	0.56
1:C:207:LEU:N	1:C:207:LEU:HD23	2.21	0.56
1:C:703:TRP:CD1	1:C:709:ARG:HA	2.40	0.56
1:C:1012:ARG:O	1:C:1013:TYR:CB	2.52	0.56
1:B:76:ALA:HB2	1:B:221:MET:HE2	1.87	0.56
1:B:476:ILE:O	1:B:476:ILE:HG13	2.05	0.56
1:B:315:PHE:HB2	1:B:323:LEU:HD11	1.87	0.56
1:B:385:LEU:O	1:B:387:PRO:HD3	2.05	0.56
1:C:249:ILE:HD12	1:C:541:PRO:CG	2.36	0.56
1:B:497:ARG:O	1:B:500:GLU:HG2	2.05	0.56
1:B:767:LEU:O	1:B:767:LEU:HD23	2.05	0.56
1:C:322:HIS:O	1:C:323:LEU:HD12	2.05	0.56
1:C:358:ILE:HG23	1:C:404:MET:SD	2.45	0.56
1:B:834:VAL:HG12	1:B:835:GLY:N	2.20	0.56
1:C:787:LEU:HD13	1:C:789:PHE:HE2	1.69	0.56
1:C:830:GLY:O	1:C:831:ASP:HB2	2.05	0.56
1:B:93:LEU:O	1:B:97:LEU:HG	2.05	0.56
1:B:391:ARG:O	1:B:392:HIS:HB2	2.05	0.56
1:C:860:ARG:HH11	1:C:860:ARG:HB3	1.71	0.56
1:B:197:LEU:O	1:B:201:LEU:HD12	2.05	0.56
1:B:305:THR:HG23	1:B:329:TYR:CZ	2.40	0.56
1:B:791:VAL:HG21	1:B:977:ALA:HA	1.86	0.56
1:C:476:ILE:H	1:C:478:GLU:HG2	1.71	0.56
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.71	0.56
1:B:433:SER:O	1:B:436:THR:HG22	2.06	0.56
1:B:47:VAL:HG13	1:B:57:PRO:HG2	1.88	0.55
1:B:344:ARG:HH12	1:B:488:LEU:HD12	1.69	0.55
1:B:936:LEU:O	1:B:936:LEU:HD12	2.06	0.55
1:B:4:VAL:CB	1:B:32:ARG:HH21	2.19	0.55
1:B:179:ILE:O	1:B:220:LEU:HD12	2.05	0.55
1:B:305:THR:O	1:B:307:THR:N	2.40	0.55
1:C:426:LEU:HD11	1:C:466:ALA:CA	2.29	0.55
1:C:176:PHE:HB2	1:C:179:ILE:CD1	2.36	0.55
1:C:465:ARG:O	1:C:465:ARG:HD3	2.07	0.55
1:B:80:THR:HG21	1:B:438:ARG:NH1	2.21	0.55
1:B:559:LEU:HD11	1:B:689:ILE:HD13	1.88	0.55
1:C:63:MET:HG3	1:C:622:ASP:HB3	1.88	0.55
1:C:706:PHE:HD1	1:C:706:PHE:O	1.90	0.55
1:C:717:GLN:OE1	1:C:982:ARG:HD3	2.05	0.55
1:C:936:LEU:HD12	1:C:936:LEU:O	2.06	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:266:THR:O	1:B:267:LEU:HB2	2.05	0.55
1:B:555:HIS:HA	1:B:639:ILE:HD13	1.88	0.55
1:B:760:LEU:H	1:B:760:LEU:CD2	2.14	0.55
1:B:975:THR:HG22	1:B:979:ILE:CG1	2.36	0.55
1:B:79:PRO:HG2	1:B:504:ILE:HG21	1.88	0.55
1:B:692:ARG:HG2	1:B:692:ARG:NH2	2.21	0.55
1:B:961:ILE:HD13	1:B:961:ILE:O	2.06	0.55
1:C:274:LEU:HD22	1:C:450:PHE:HE2	1.70	0.55
1:C:508:LEU:HD21	1:C:510:ILE:HD11	1.88	0.55
1:C:757:THR:O	1:C:904:ILE:HA	2.06	0.55
1:C:784:ASN:HB3	1:C:959:SER:HB2	1.88	0.55
1:C:883:ILE:HD12	1:C:883:ILE:N	2.21	0.55
1:B:106:PHE:O	1:B:163:THR:N	2.39	0.55
1:B:608:ASN:ND2	1:B:610:ARG:CB	2.70	0.55
1:C:61:GLN:OE1	1:C:83:GLY:HA3	2.07	0.55
1:C:433:SER:O	1:C:436:THR:HG22	2.07	0.55
1:B:965:MET:HE1	1:B:980:VAL:HG23	1.88	0.55
1:C:235:LEU:O	1:C:239:LEU:HB2	2.07	0.55
1:C:540:ILE:HG13	1:C:541:PRO:CD	2.35	0.55
1:C:616:LEU:HA	1:C:619:LEU:HD12	1.89	0.55
1:C:774:TYR:CD2	1:C:886:ARG:HG2	2.42	0.55
1:C:848:ARG:CB	1:C:887:PHE:CD2	2.90	0.55
1:B:965:MET:CE	1:B:980:VAL:HG23	2.37	0.55
1:C:251:VAL:O	1:C:252:ARG:HB3	2.07	0.55
1:C:615:ALA:O	1:C:618:LYS:HB3	2.07	0.55
1:C:735:ARG:HB3	1:C:949:SER:CB	2.36	0.55
1:C:138:HIS:NE2	1:C:140:ARG:HB2	2.21	0.55
1:B:366:PRO:HA	1:B:393:ILE:HG12	1.87	0.54
1:B:376:TYR:OH	1:B:409:PRO:HD3	2.07	0.54
1:B:714:GLY:O	1:B:715:ARG:HB3	2.07	0.54
1:C:194:VAL:HG12	1:C:198:LEU:HD11	1.88	0.54
1:C:616:LEU:HD23	1:C:619:LEU:HD12	1.89	0.54
1:B:134:ILE:HD12	1:B:135:GLY:H	1.72	0.54
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.73	0.54
1:B:248:ARG:CG	1:B:249:ILE:N	2.70	0.54
1:B:570:VAL:O	1:B:571:ASN:HB2	2.08	0.54
1:C:47:VAL:HG12	1:C:51:ARG:NH1	2.22	0.54
1:C:198:LEU:O	1:C:201:LEU:N	2.37	0.54
1:B:153:LEU:O	1:B:154:ARG:HB2	2.07	0.54
1:B:416:VAL:HG13	1:B:417:ARG:N	2.22	0.54
1:B:736:LYS:HA	1:B:736:LYS:HZ3	1.71	0.54



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:801:LEU:HB3	1:B:807:ILE:CD1	2.38	0.54
1:C:3:PRO:HA	1:C:16:ASP:CB	2.38	0.54
1:B:61:GLN:NE2	2:B:2055:ANP:N6	2.40	0.54
1:B:64:TRP:O	1:B:67:ARG:HB2	2.07	0.54
1:B:638:LYS:HE2	1:B:642:ASP:OD2	2.07	0.54
1:B:749:HIS:HD2	1:B:751:GLU:HB2	1.72	0.54
1:B:849:PRO:HD2	1:B:887:PHE:CD2	2.42	0.54
1:B:972:ARG:CZ	1:B:1026:GLU:HG3	2.38	0.54
1:B:1051:LYS:C	1:B:1053:ILE:H	2.11	0.54
1:C:687:ARG:NH2	1:C:972:ARG:HB2	2.23	0.54
1:B:735:ARG:NH1	1:B:951:PRO:HG3	2.23	0.54
1:B:828:TYR:HD2	1:B:829:LEU:HD23	1.72	0.54
1:B:344:ARG:NH1	1:B:488:LEU:HD12	2.23	0.54
1:B:377:ARG:HG3	1:B:382:ILE:HG13	1.88	0.54
1:C:170:TYR:CZ	1:C:171:ARG:HG2	2.42	0.54
1:C:542:MET:O	1:C:544:LYS:N	2.40	0.54
1:B:1012:ARG:HH11	1:B:1012:ARG:CG	2.20	0.54
1:C:66:LYS:HD2	1:C:622:ASP:HA	1.88	0.54
1:B:194:VAL:HG12	1:B:195:ASP:N	2.22	0.54
1:B:708:ASN:C	1:B:708:ASN:HD22	2.11	0.54
1:B:809:TYR:CZ	1:B:811:ARG:HB2	2.43	0.54
1:C:330:TYR:O	1:C:333:LEU:HD23	2.08	0.54
1:C:351:CYS:HB3	1:C:462:PHE:CD1	2.43	0.54
1:C:556:VAL:HG23	1:C:557:VAL:HG13	1.89	0.54
1:C:970:ILE:HD11	1:C:1019:GLU:HG3	1.88	0.54
1:B:682:LYS:HD3	1:B:1039:TYR:HD2	1.73	0.54
1:B:700:GLN:HA	1:B:703:TRP:CE3	2.43	0.54
1:B:935:GLU:HG2	1:B:936:LEU:N	2.23	0.54
1:C:207:LEU:HG	1:C:208:LYS:N	2.23	0.54
1:C:381:GLU:O	1:C:384:ARG:HG2	2.08	0.54
1:C:468:LEU:HD22	1:C:468:LEU:H	1.73	0.54
1:B:465:ARG:HH22	1:B:864:GLU:CD	2.06	0.53
1:C:80:THR:HG21	1:C:438:ARG:NH1	2.23	0.53
1:C:305:THR:HG1	1:C:329:TYR:HB3	1.71	0.53
1:C:344:ARG:O	1:C:345:PHE:HB3	2.08	0.53
1:C:991:GLU:HG3	1:C:995:ARG:O	2.08	0.53
1:B:37:PHE:O	1:B:40:ASP:HB2	2.09	0.53
1:B:358:ILE:H	1:B:358:ILE:CD1	2.08	0.53
1:B:1022:THR:O	1:B:1026:GLU:HB2	2.08	0.53
1:C:824:ILE:CG2	1:C:852:PRO:HG3	2.36	0.53
1:C:860:ARG:HH11	1:C:860:ARG:CG	2.21	0.53



A + a 1	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:58:ARG:NH2	1:B:81:GLY:O	2.41	0.53
1:B:153:LEU:O	1:B:154:ARG:CB	2.56	0.53
1:B:854:THR:O	1:B:858:VAL:HG23	2.09	0.53
1:C:255:GLU:OE1	1:C:484:LEU:HD11	2.09	0.53
1:C:348:PHE:HZ	1:C:432:GLY:HA3	1.74	0.53
1:C:479:VAL:HG23	1:C:481:PHE:H	1.74	0.53
1:B:101:ARG:HA	1:B:157:LYS:O	2.07	0.53
1:B:256:ASP:CB	1:B:474:LYS:HD3	2.39	0.53
1:C:88:GLY:O	1:C:92:SER:HB2	2.09	0.53
1:B:361:ILE:CG2	1:B:397:ARG:HB3	2.38	0.53
1:C:683:ALA:O	1:C:687:ARG:HB2	2.07	0.53
1:C:1009:LEU:H	1:C:1009:LEU:HD22	1.72	0.53
1:B:981:ASP:O	1:B:982:ARG:C	2.46	0.53
1:C:859:GLN:O	1:C:863:GLN:HG2	2.09	0.53
1:B:399:ILE:O	1:B:403:VAL:HG22	2.08	0.53
1:C:164:GLN:C	1:C:164:GLN:HE21	2.13	0.53
1:C:468:LEU:HD22	1:C:468:LEU:N	2.24	0.53
1:C:609:SER:HA	1:C:612:ARG:HH11	1.73	0.53
1:C:715:ARG:HG2	1:C:716:ALA:N	2.24	0.53
1:C:736:LYS:HD2	1:C:736:LYS:N	2.23	0.53
1:B:720:VAL:HG13	1:B:961:ILE:HD11	1.92	0.52
1:B:1029:MET:O	1:B:1032:ILE:HG23	2.09	0.52
1:C:34:LEU:HD13	1:C:648:SER:HB3	1.91	0.52
1:C:736:LYS:O	1:C:737:ILE:HG23	2.09	0.52
1:C:935:GLU:HG2	1:C:936:LEU:N	2.22	0.52
1:B:207:LEU:O	1:B:210:LYS:HG3	2.09	0.52
1:B:555:HIS:HA	1:B:639:ILE:HD11	1.88	0.52
1:B:775:THR:O	1:B:776:THR:C	2.47	0.52
1:C:39:GLU:CD	1:C:39:GLU:N	2.58	0.52
1:C:463:ILE:O	1:C:466:ALA:HB3	2.09	0.52
1:B:895:PHE:N	1:B:895:PHE:CD2	2.77	0.52
1:C:869:VAL:HG21	1:C:872:LEU:HD12	1.91	0.52
1:C:981:ASP:O	1:C:984:PHE:N	2.42	0.52
1:B:74:PHE:CZ	1:B:221:MET:HG3	2.44	0.52
1:B:981:ASP:O	1:B:984:PHE:N	2.36	0.52
1:C:414:VAL:HG12	1:C:424:PRO:CD	2.39	0.52
1:B:314:LYS:CB	1:B:320:ILE:HG12	2.39	0.52
1:B:397:ARG:O	1:B:401:LYS:HG3	2.10	0.52
1:B:493:ASP:HA	1:B:496:ARG:CZ	2.39	0.52
1:C:107:PRO:HG3	1:C:183:ASP:HB3	1.91	0.52
1:C:314:LYS:HB3	1:C:320:ILE:HD13	1.92	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:818:SER:O	1:C:821:GLY:N	2.41	0.52
1:B:305:THR:HG23	1:B:329:TYR:CD1	2.44	0.52
1:B:309:LYS:HG2	1:B:310:GLY:N	2.25	0.52
1:B:466:ALA:HB1	1:B:472:GLU:HG3	1.90	0.52
1:C:364:LEU:HD22	1:C:368:MET:SD	2.50	0.52
1:C:425:ASP:OD2	1:C:428:THR:HB	2.09	0.52
1:C:446:LYS:HD3	1:C:447:GLY:H	1.73	0.52
1:C:628:VAL:HG21	1:C:640:ALA:HA	1.91	0.52
1:B:207:LEU:HD23	1:B:207:LEU:H	1.75	0.52
1:B:463:ILE:CD1	1:B:474:LYS:HG3	2.40	0.52
1:B:709:ARG:HG2	1:B:710:ASN:N	2.22	0.52
1:B:1028:ARG:O	1:B:1031:ALA:HB3	2.09	0.52
1:C:265:SER:O	1:C:267:LEU:N	2.42	0.52
1:C:276:THR:HA	1:C:322:HIS:CE1	2.45	0.52
1:C:296:LYS:HA	1:C:301:ILE:CG1	2.38	0.52
1:B:212:TRP:CH2	1:B:235:LEU:HD21	2.44	0.52
1:B:697:VAL:HG21	1:B:1050:ILE:HD12	1.92	0.52
1:B:1010:VAL:CG1	1:B:1011:ARG:N	2.73	0.52
1:B:1029:MET:HA	1:B:1032:ILE:CG2	2.40	0.52
1:C:712:SER:CB	1:C:986:ARG:HH11	2.22	0.52
1:B:291:ILE:O	1:B:294:SER:N	2.43	0.52
1:B:292:TYR:CD2	1:B:303:ILE:HB	2.44	0.52
1:B:760:LEU:HD22	1:B:938:THR:OG1	2.10	0.52
1:B:897:VAL:HG13	1:B:897:VAL:O	2.10	0.52
1:C:231:LYS:O	1:C:234:GLU:HB2	2.09	0.52
1:C:460:SER:O	1:C:463:ILE:HB	2.10	0.52
1:C:808:THR:CG2	1:C:848:ARG:NE	2.73	0.52
1:B:241:ASN:O	1:B:530:LYS:HD2	2.10	0.52
1:B:384:ARG:HH22	1:C:497:ARG:HD3	1.75	0.52
1:C:60:ILE:HD12	1:C:506:PRO:HG3	1.91	0.52
1:C:160:ILE:O	1:C:161:THR:HG22	2.10	0.52
1:C:464:GLU:O	1:C:467:LYS:HB2	2.10	0.52
1:B:182:ASP:O	1:B:223:SER:HB3	2.09	0.51
1:B:523:PHE:CE2	1:B:663:ARG:N	2.78	0.51
1:B:529:VAL:CG1	1:B:530:LYS:H	2.22	0.51
1:B:832:ASP:HA	1:B:893:ARG:HG3	1.91	0.51
1:C:873:ARG:N	1:C:876:HIS:HD2	2.09	0.51
1:B:124:GLU:C	1:B:125:LYS:HD2	2.30	0.51
1:B:653:VAL:HG12	1:B:653:VAL:O	2.09	0.51
1:C:113:ILE:HD11	1:C:138:HIS:CE1	2.44	0.51
1:C:117:GLU:HB3	1:C:121:LYS:NZ	2.25	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:135:GLY:HA3	1:C:156:PHE:CD1	2.45	0.51
1:C:498:ARG:NH1	2:C:2055:ANP:O1G	2.43	0.51
1:B:476:ILE:O	1:B:477:ASP:HB2	2.11	0.51
1:C:66:LYS:O	1:C:70:ARG:HG3	2.10	0.51
1:C:438:ARG:CG	1:C:439:LEU:N	2.74	0.51
1:C:709:ARG:O	1:C:710:ASN:HB2	2.10	0.51
1:B:553:ILE:HG22	1:B:553:ILE:O	2.11	0.51
1:B:832:ASP:O	1:B:893:ARG:HG3	2.09	0.51
1:C:58:ARG:HH21	1:C:83:GLY:H	1.58	0.51
1:B:14:GLY:HA2	1:B:21:GLU:O	2.10	0.51
1:B:573:ARG:O	1:B:574:PHE:HB2	2.10	0.51
1:B:910:THR:HG23	1:B:910:THR:O	2.10	0.51
1:C:872:LEU:HA	1:C:876:HIS:CD2	2.46	0.51
1:C:1051:LYS:C	1:C:1053:ILE:H	2.14	0.51
1:B:370:LYS:O	1:B:373:ALA:CB	2.55	0.51
1:B:581:ILE:HG22	1:B:582:LYS:N	2.26	0.51
1:C:22:ILE:O	1:C:575:VAL:HG13	2.11	0.51
1:C:637:GLU:HA	1:C:637:GLU:OE1	2.11	0.51
1:B:377:ARG:O	1:B:378:ASN:C	2.49	0.51
1:B:708:ASN:ND2	1:B:709:ARG:O	2.43	0.51
1:B:907:ASP:O	1:B:909:LYS:HG2	2.10	0.51
1:C:816:ARG:HA	1:C:838:TRP:O	2.11	0.51
1:B:43:LEU:O	1:B:46:PHE:N	2.44	0.51
1:B:170:TYR:CG	1:B:171:ARG:N	2.79	0.51
1:B:715:ARG:HG2	1:B:716:ALA:N	2.26	0.51
1:B:743:PHE:C	1:B:745:LEU:H	2.13	0.51
1:C:171:ARG:HG3	1:C:171:ARG:HH11	1.76	0.51
1:B:419:GLY:O	1:B:420:GLU:CB	2.58	0.51
1:B:757:THR:O	1:B:904:ILE:HA	2.11	0.51
1:B:784:ASN:HB3	1:B:959:SER:HB2	1.92	0.51
1:C:940:THR:HG22	1:C:940:THR:O	2.10	0.51
1:C:462:PHE:O	1:C:463:ILE:C	2.49	0.51
1:C:512:GLU:OE1	1:C:630:THR:HB	2.10	0.51
1:C:1053:ILE:HG13	1:C:1054:ASP:N	2.26	0.51
1:B:387:PRO:HB2	1:B:389:VAL:N	2.27	0.50
1:B:682:LYS:HB2	1:B:1032:ILE:HD11	1.93	0.50
1:C:532:LEU:O	1:C:533:ASP:C	2.49	0.50
1:C:719:LEU:HD21	1:C:1017:VAL:O	2.11	0.50
1:C:821:GLY:HA3	1:C:848:ARG:HH22	1.76	0.50
1:B:58:ARG:HH21	1:B:83:GLY:H	1.57	0.50
1:B:682:LYS:CB	1:B:1032:ILE:HD11	2.42	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:791:VAL:HG23	1:B:977:ALA:HB1	1.93	0.50
1:B:807:ILE:N	1:B:850:THR:HG23	2.26	0.50
1:C:352:PRO:O	1:C:425:ASP:HB3	2.11	0.50
1:C:466:ALA:HB1	1:C:472:GLU:CG	2.41	0.50
1:C:627:ILE:HD13	1:C:673:LEU:HD21	1.93	0.50
1:C:824:ILE:HD12	1:C:852:PRO:HD3	1.93	0.50
1:C:1017:VAL:O	1:C:1017:VAL:HG12	2.11	0.50
1:B:754:PHE:CE2	1:B:906:PHE:HB2	2.47	0.50
1:C:55:GLY:O	1:C:57:PRO:HD3	2.11	0.50
1:C:248:ARG:HG3	1:C:249:ILE:N	2.26	0.50
1:C:254:VAL:HG22	1:C:436:THR:HG23	1.92	0.50
1:C:258:ALA:HA	1:C:451:LEU:O	2.12	0.50
1:C:874:TRP:CG	1:C:875:GLU:N	2.79	0.50
1:B:1052:SER:O	1:B:1053:ILE:HG23	2.11	0.50
1:C:278:GLY:O	1:C:279:ILE:HD13	2.11	0.50
1:C:533:ASP:OD1	1:C:533:ASP:N	2.45	0.50
1:C:735:ARG:HB3	1:C:949:SER:CA	2.41	0.50
1:B:184:VAL:O	1:B:188:LEU:HG	2.12	0.50
1:B:736:LYS:HA	1:B:736:LYS:HZ2	1.76	0.50
1:C:52:LYS:NZ	1:C:126:ALA:HB3	2.27	0.50
1:C:105:ILE:HD12	1:C:181:VAL:HG22	1.93	0.50
1:C:570:VAL:O	1:C:571:ASN:HB2	2.12	0.50
1:B:95:LEU:HD13	1:B:100:LYS:CD	2.39	0.50
1:B:330:TYR:O	1:B:333:LEU:HD23	2.12	0.50
1:C:103:TYR:HE1	1:C:161:THR:HG23	1.76	0.50
1:C:490:GLU:O	1:C:493:ASP:N	2.42	0.50
1:C:662:THR:O	1:C:663:ARG:C	2.50	0.50
1:B:101:ARG:HH22	1:B:174:GLY:HA3	1.76	0.50
1:C:476:ILE:C	1:C:478:GLU:H	2.15	0.50
1:C:734:ARG:HB2	1:C:952:LYS:HA	1.93	0.50
1:C:947:VAL:O	1:C:948:LYS:HG3	2.11	0.50
1:B:344:ARG:NH1	1:B:488:LEU:HB2	2.27	0.50
1:C:329:TYR:O	1:C:332:THR:N	2.44	0.50
1:C:745:LEU:HD22	1:C:747:LEU:HD11	1.94	0.50
1:C:1012:ARG:C	1:C:1013:TYR:CD1	2.85	0.50
1:B:138:HIS:NE2	1:B:140:ARG:HB2	2.27	0.50
1:B:735:ARG:HB3	1:B:949:SER:CB	2.41	0.50
1:B:1050:ILE:O	1:B:1053:ILE:HG12	2.12	0.50
1:C:720:VAL:O	1:C:724:ILE:HG13	2.12	0.50
1:C:56:GLU:OE1	1:C:56:GLU:HA	2.12	0.49
1:C:58:ARG:N	1:C:61:GLN:HE21	2.04	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:775:THR:O	1:C:776:THR:C	2.50	0.49
1:C:791:VAL:H	1:C:958:GLN:HE22	1.58	0.49
1:B:128:VAL:HG12	1:B:130:THR:H	1.76	0.49
1:B:558:ASP:CG	1:B:688:ARG:HH21	2.15	0.49
1:C:106:PHE:CE2	1:C:115:ALA:HB2	2.48	0.49
1:C:747:LEU:HD12	1:C:747:LEU:H	1.77	0.49
1:C:760:LEU:CD2	1:C:938:THR:OG1	2.59	0.49
1:B:181:VAL:HB	1:B:222:VAL:HG12	1.94	0.49
1:B:254:VAL:HG22	1:B:436:THR:HG22	1.93	0.49
1:B:383:GLU:OE1	1:C:497:ARG:NH2	2.45	0.49
1:C:712:SER:HB3	1:C:986:ARG:HG3	1.93	0.49
1:B:465:ARG:HA	1:B:468:LEU:HD23	1.94	0.49
1:C:194:VAL:O	1:C:195:ASP:C	2.50	0.49
1:C:524:PHE:HB2	1:C:540:ILE:HG12	1.94	0.49
1:C:870:GLU:O	1:C:872:LEU:HG	2.12	0.49
1:B:397:ARG:O	1:B:400:LEU:HB2	2.13	0.49
1:B:518:ARG:HD3	1:B:538:TYR:OH	2.13	0.49
1:B:874:TRP:CG	1:B:875:GLU:N	2.80	0.49
1:C:43:LEU:C	1:C:43:LEU:HD23	2.33	0.49
1:C:760:LEU:HD23	1:C:938:THR:OG1	2.11	0.49
1:C:808:THR:HG23	1:C:848:ARG:NE	2.27	0.49
1:B:455:ASP:O	1:B:456:SER:C	2.51	0.49
1:C:61:GLN:NE2	2:C:2055:ANP:HN61	2.10	0.49
1:C:103:TYR:HB2	1:C:176:PHE:CE2	2.48	0.49
1:C:249:ILE:HD12	1:C:541:PRO:HG3	1.94	0.49
1:C:330:TYR:HA	1:C:333:LEU:HD23	1.94	0.49
1:B:298:LYS:O	1:B:299:PHE:CD1	2.65	0.49
1:B:304:VAL:O	1:B:305:THR:CB	2.60	0.49
1:B:532:LEU:O	1:B:533:ASP:C	2.49	0.49
1:B:802:PHE:CD1	1:B:809:TYR:HA	2.47	0.49
1:C:259:VAL:O	1:C:452:LEU:HA	2.13	0.49
1:C:968:ARG:HG2	1:C:968:ARG:HH11	1.77	0.49
1:B:195:ASP:HA	1:B:198:LEU:HD13	1.95	0.49
1:B:278:GLY:H	1:B:322:HIS:CD2	2.31	0.49
1:B:320:ILE:HD13	1:B:320:ILE:N	2.27	0.49
1:B:363:SER:O	1:B:364:LEU:CD1	2.60	0.49
1:B:825:ALA:HA	1:B:888:MET:HE1	1.94	0.49
1:B:985:MET:HE1	1:B:986:ARG:HH21	1.77	0.49
1:C:198:LEU:HB3	1:C:203:PHE:HB2	1.93	0.49
1:C:681:VAL:O	1:C:684:GLN:HB3	2.12	0.49
1:C:767:LEU:HD23	1:C:767:LEU:O	2.13	0.49



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:808:THR:CG2	1:C:848:ARG:HE	2.26	0.49
1:C:887:PHE:C	1:C:889:ALA:N	2.66	0.49
1:C:35:CYS:CB	1:C:650:CYS:N	2.76	0.49
1:C:103:TYR:HD1	1:C:159:VAL:O	1.96	0.49
1:C:337:LEU:HB3	1:C:435:ARG:HE	1.78	0.49
1:C:463:ILE:CD1	1:C:474:LYS:HG3	2.42	0.49
1:C:737:ILE:HA	1:C:747:LEU:O	2.13	0.49
1:C:834:VAL:HG21	1:C:893:ARG:HA	1.95	0.49
1:B:137:TYR:CD1	1:B:137:TYR:C	2.85	0.49
1:B:217:ARG:HD2	1:B:217:ARG:O	2.13	0.49
1:B:382:ILE:O	1:B:385:LEU:HB3	2.11	0.49
1:B:415:VAL:CG1	1:B:422:ILE:HB	2.43	0.49
1:B:469:TYR:O	1:B:470:ASP:C	2.51	0.49
1:B:760:LEU:HD23	1:B:760:LEU:N	2.16	0.49
1:B:774:TYR:CE1	1:B:886:ARG:HG3	2.48	0.49
1:B:821:GLY:HA3	1:B:848:ARG:NH2	2.27	0.49
1:B:31:LYS:N	1:B:32:ARG:NE	2.61	0.48
1:B:393:ILE:N	1:B:393:ILE:HD12	2.27	0.48
1:B:440:PHE:CD2	1:B:495:TYR:HA	2.47	0.48
1:B:1039:TYR:HA	1:B:1042:ALA:HB3	1.95	0.48
1:C:721:LEU:O	1:C:724:ILE:HB	2.12	0.48
1:B:712:SER:HB2	1:B:986:ARG:HH11	1.79	0.48
1:C:79:PRO:HG2	1:C:504:ILE:HG21	1.95	0.48
1:C:197:LEU:O	1:C:200:LEU:N	2.44	0.48
1:C:351:CYS:SG	1:C:451:LEU:HD21	2.53	0.48
1:C:518:ARG:HG2	1:C:538:TYR:CE2	2.48	0.48
1:C:736:LYS:C	1:C:737:ILE:CG2	2.81	0.48
1:C:745:LEU:HD22	1:C:747:LEU:CD1	2.43	0.48
1:C:756:LEU:HD13	1:C:757:THR:H	1.78	0.48
1:C:1007:ARG:CA	1:C:1010:VAL:HG12	2.40	0.48
1:B:100:LYS:HG2	1:B:177:ASP:CG	2.34	0.48
1:B:1007:ARG:HA	1:B:1010:VAL:CG1	2.42	0.48
1:C:613:ILE:HD12	1:C:613:ILE:N	2.28	0.48
1:C:784:ASN:CG	1:C:958:GLN:HB2	2.34	0.48
1:B:376:TYR:HE2	1:B:407:GLU:HB3	1.78	0.48
1:B:387:PRO:CG	1:B:389:VAL:HA	2.43	0.48
1:C:887:PHE:C	1:C:889:ALA:H	2.16	0.48
1:B:131:GLU:O	1:B:133:LEU:N	2.46	0.48
1:B:320:ILE:CG2	1:B:322:HIS:O	2.62	0.48
1:C:379:VAL:CG1	1:C:380:ASP:H	2.07	0.48
1:B:527:PRO:HB3	1:B:540:ILE:HB	1.95	0.48



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:735:ARG:HB3	1:B:949:SER:HA	1.94	0.48
1:B:857:ASP:O	1:B:861:LEU:HG	2.13	0.48
1:B:905:GLU:CG	1:B:910:THR:HB	2.42	0.48
1:C:207:LEU:HD23	1:C:207:LEU:H	1.77	0.48
1:C:365:SER:OG	1:C:368:MET:HB2	2.13	0.48
1:B:621:HIS:HD2	1:B:622:ASP:OD2	1.97	0.48
1:C:122:TYR:O	1:C:125:LYS:HD3	2.14	0.48
1:C:117:GLU:HB3	1:C:121:LYS:HZ3	1.77	0.48
1:C:274:LEU:HD23	1:C:345:PHE:CD2	2.49	0.48
1:C:358:ILE:HG23	1:C:404:MET:CE	2.44	0.48
1:C:725:ILE:C	1:C:727:ARG:H	2.17	0.48
1:B:102:CYS:C	1:B:176:PHE:HD2	2.16	0.48
1:B:697:VAL:HG21	1:B:1050:ILE:CD1	2.44	0.48
1:B:754:PHE:HE2	1:B:906:PHE:HB2	1.77	0.48
1:B:828:TYR:CD2	1:B:829:LEU:HD23	2.49	0.48
1:B:1000:LYS:O	1:B:1001:LEU:C	2.52	0.48
1:C:194:VAL:O	1:C:197:LEU:HB2	2.14	0.48
1:C:274:LEU:HD23	1:C:345:PHE:CE2	2.49	0.48
1:C:446:LYS:HD3	1:C:447:GLY:N	2.28	0.48
1:B:386:LEU:HD12	1:C:500:GLU:OE1	2.14	0.48
1:C:278:GLY:HA3	1:C:345:PHE:CZ	2.49	0.48
1:C:661:VAL:HG12	1:C:661:VAL:O	2.13	0.48
1:C:768:ARG:HG3	1:C:768:ARG:HH11	1.79	0.48
1:B:80:THR:HG21	1:B:438:ARG:HH11	1.78	0.47
1:B:975:THR:O	1:B:979:ILE:HG12	2.13	0.47
1:C:192:LYS:O	1:C:193:ASN:C	2.51	0.47
1:C:249:ILE:CG2	1:C:541:PRO:HG2	2.43	0.47
1:C:484:LEU:O	1:C:488:LEU:HG	2.14	0.47
1:B:374:TYR:O	1:B:375:LEU:HB2	2.14	0.47
1:B:609:SER:O	1:B:613:ILE:HG12	2.14	0.47
1:B:763:GLU:CD	1:B:900:LYS:HE2	2.35	0.47
1:B:816:ARG:HA	1:B:838:TRP:O	2.14	0.47
1:C:480:ASP:O	1:C:481:PHE:C	2.51	0.47
1:C:490:GLU:O	1:C:493:ASP:CB	2.60	0.47
1:C:754:PHE:HE2	1:C:906:PHE:HB2	1.78	0.47
1:B:272:GLU:HB2	1:B:299:PHE:CZ	2.50	0.47
1:B:685:VAL:O	1:B:688:ARG:HB3	2.14	0.47
1:B:740:VAL:CG1	1:B:741:ARG:N	2.78	0.47
1:C:610:ARG:HH11	1:C:610:ARG:CB	2.21	0.47
1:C:791:VAL:CG2	1:C:977:ALA:HA	2.43	0.47
1:B:154:ARG:CZ	1:B:174:GLY:HA2	2.45	0.47



A + a 1	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:333:LEU:N	1:B:333:LEU:CD2	2.76	0.47
1:B:758:ILE:HG22	1:B:938:THR:OG1	2.14	0.47
1:C:65:ALA:HA	1:C:91:MET:HE2	1.96	0.47
1:C:172:GLU:O	1:C:172:GLU:HG2	2.14	0.47
1:C:476:ILE:HG23	1:C:476:ILE:O	2.14	0.47
1:C:581:ILE:HG22	1:C:582:LYS:N	2.30	0.47
1:C:834:VAL:CG1	1:C:835:GLY:H	2.21	0.47
1:C:858:VAL:HG21	1:C:880:TYR:HE1	1.79	0.47
1:B:95:LEU:HB2	1:B:102:CYS:SG	2.54	0.47
1:B:462:PHE:O	1:B:463:ILE:C	2.51	0.47
1:B:468:LEU:N	1:B:468:LEU:HD22	2.29	0.47
1:B:705:ARG:HD3	1:B:1008:PHE:CE1	2.49	0.47
1:B:708:ASN:C	1:B:708:ASN:ND2	2.68	0.47
1:C:106:PHE:O	1:C:163:THR:N	2.44	0.47
1:C:301:ILE:N	1:C:301:ILE:CD1	2.76	0.47
1:C:716:ALA:O	1:C:720:VAL:HG23	2.14	0.47
1:C:957:THR:O	1:C:958:GLN:C	2.53	0.47
1:B:72:GLU:HB3	1:B:530:LYS:HZ1	1.78	0.47
1:C:140:ARG:O	1:C:141:ILE:O	2.32	0.47
1:B:279:ILE:HD11	1:B:315:PHE:CE1	2.48	0.47
1:B:394:ASP:HA	1:B:397:ARG:HG3	1.97	0.47
1:B:559:LEU:HD12	1:B:688:ARG:HG3	1.96	0.47
1:B:719:LEU:HD13	1:B:970:ILE:CD1	2.45	0.47
1:B:749:HIS:CG	1:B:906:PHE:HE2	2.32	0.47
1:B:972:ARG:NH1	1:B:1026:GLU:CG	2.78	0.47
1:C:71:LYS:HG2	1:C:219:CYS:HB3	1.97	0.47
1:C:105:ILE:CG2	1:C:163:THR:HA	2.44	0.47
1:C:123:ALA:C	1:C:125:LYS:H	2.18	0.47
1:C:170:TYR:CE2	1:C:171:ARG:HG2	2.50	0.47
1:C:201:LEU:O	1:C:217:ARG:HB2	2.14	0.47
1:C:260:ASN:O	1:C:260:ASN:ND2	2.48	0.47
1:C:283:ARG:NH2	1:C:453:GLU:OE2	2.47	0.47
1:C:544:LYS:O	1:C:545:TYR:CG	2.68	0.47
1:C:754:PHE:CE2	1:C:906:PHE:HB2	2.50	0.47
1:C:912:GLU:OE1	1:C:912:GLU:N	2.47	0.47
1:B:369:VAL:CG1	1:B:393:ILE:HG23	2.38	0.47
1:C:259:VAL:HB	1:C:452:LEU:HD22	1.96	0.47
1:C:363:SER:O	1:C:364:LEU:HB2	2.15	0.47
1:B:60:ILE:HG21	1:B:82:VAL:HG11	1.96	0.47
1:B:510:ILE:HD11	1:B:616:LEU:HD22	1.97	0.47
1:B:662:THR:O	1:B:663:ARG:C	2.53	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:807:ILE:CA	1:B:850:THR:HG23	2.45	0.47
1:C:95:LEU:HB2	1:C:102:CYS:SG	2.54	0.47
1:C:131:GLU:O	1:C:133:LEU:N	2.48	0.47
1:C:236:PHE:O	1:C:240:LEU:N	2.45	0.47
1:C:884:PHE:CE1	1:C:888:MET:HG3	2.49	0.47
1:B:271:LEU:C	1:B:273:LYS:H	2.19	0.47
1:B:271:LEU:CD2	1:B:481:PHE:HZ	2.24	0.47
1:B:370:LYS:O	1:B:373:ALA:N	2.48	0.47
1:B:440:PHE:CD1	1:B:440:PHE:N	2.83	0.47
1:B:276:THR:HA	1:B:322:HIS:CE1	2.50	0.46
1:B:470:ASP:O	1:B:472:GLU:CB	2.58	0.46
1:B:1037:LEU:CD2	1:B:1038:ASP:N	2.76	0.46
1:C:73:SER:HA	1:C:220:LEU:O	2.14	0.46
1:C:249:ILE:HD12	1:C:541:PRO:HG2	1.97	0.46
1:B:60:ILE:HD13	1:B:546:VAL:HG21	1.97	0.46
1:B:65:ALA:O	1:B:66:LYS:C	2.53	0.46
1:B:745:LEU:HD22	1:B:747:LEU:CD1	2.45	0.46
1:B:801:LEU:HD12	1:B:801:LEU:HA	1.63	0.46
1:C:137:TYR:CD1	1:C:137:TYR:C	2.88	0.46
1:C:179:ILE:O	1:C:220:LEU:HD12	2.14	0.46
1:C:439:LEU:CD1	1:C:444:LEU:HD13	2.44	0.46
1:C:544:LYS:HB3	1:C:545:TYR:CD1	2.50	0.46
1:C:873:ARG:H	1:C:876:HIS:CD2	2.28	0.46
1:B:103:TYR:CE1	1:B:161:THR:HG23	2.43	0.46
1:B:292:TYR:HD2	1:B:303:ILE:HB	1.80	0.46
1:B:492:ARG:NH1	1:B:492:ARG:CG	2.77	0.46
1:B:565:PHE:N	1:B:568:VAL:O	2.48	0.46
1:B:736:LYS:O	1:B:948:LYS:O	2.34	0.46
1:B:957:THR:O	1:B:959:SER:N	2.49	0.46
1:B:957:THR:HG22	1:B:995:ARG:HG2	1.97	0.46
1:C:154:ARG:NE	1:C:174:GLY:CA	2.78	0.46
1:C:1010:VAL:CG1	1:C:1011:ARG:N	2.77	0.46
1:B:58:ARG:N	1:B:61:GLN:HE21	2.06	0.46
1:B:301:ILE:N	1:B:301:ILE:CD1	2.76	0.46
1:B:385:LEU:O	1:B:387:PRO:CD	2.63	0.46
1:B:477:ASP:HA	1:B:479:VAL:HG13	1.97	0.46
1:B:720:VAL:O	1:B:723:TRP:N	2.48	0.46
1:C:314:LYS:HA	1:C:319:GLU:OE2	2.16	0.46
1:C:561:THR:CB	1:C:585:ARG:HH11	2.29	0.46
1:C:723:TRP:CZ3	1:C:964:MET:HG2	2.50	0.46
1:B:194:VAL:O	1:B:198:LEU:HD12	2.15	0.46



	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:387:PRO:HB2	1:B:389:VAL:CA	2.45	0.46
1:B:628:VAL:HG21	1:B:640:ALA:HA	1.97	0.46
1:B:873:ARG:N	1:B:876:HIS:HD2	2.09	0.46
1:C:682:LYS:HD3	1:C:1039:TYR:HD2	1.80	0.46
1:C:793:GLN:O	1:C:797:ILE:HG12	2.15	0.46
1:B:309:LYS:CG	1:B:310:GLY:H	2.27	0.46
1:B:544:LYS:HB3	1:B:545:TYR:CD1	2.51	0.46
1:B:906:PHE:O	1:B:907:ASP:C	2.54	0.46
1:B:983:LEU:HB3	1:B:989:VAL:CG2	2.45	0.46
1:C:212:TRP:CH2	1:C:235:LEU:HD21	2.50	0.46
1:C:756:LEU:HD22	1:C:906:PHE:HB3	1.97	0.46
1:B:301:ILE:O	1:B:320:ILE:HG23	2.16	0.46
1:B:330:TYR:CD1	1:B:337:LEU:HD12	2.51	0.46
1:C:52:LYS:HE3	1:C:125:LYS:O	2.16	0.46
1:C:67:ARG:HD3	1:C:74:PHE:CD2	2.51	0.46
1:C:259:VAL:HB	1:C:452:LEU:HD23	1.96	0.46
1:C:413:ASP:OD2	1:C:465:ARG:NH2	2.49	0.46
1:C:1009:LEU:HD22	1:C:1009:LEU:N	2.31	0.46
1:B:11:PRO:O	1:B:12:VAL:CB	2.64	0.46
1:B:720:VAL:O	1:B:722:GLY:N	2.49	0.46
1:B:775:THR:HG22	1:B:814:SER:O	2.15	0.46
1:B:834:VAL:CG2	1:B:893:ARG:HA	2.46	0.46
1:C:981:ASP:O	1:C:983:LEU:N	2.49	0.46
1:B:556:VAL:HG23	1:B:557:VAL:N	2.29	0.46
1:B:733:GLU:HB2	1:B:952:LYS:HB2	1.97	0.46
1:C:268:SER:O	1:C:272:GLU:HG2	2.16	0.46
1:C:510:ILE:HD13	1:C:616:LEU:HD22	1.98	0.46
1:C:542:MET:HE1	1:C:544:LYS:HB2	1.98	0.46
1:C:558:ASP:OD2	1:C:559:LEU:N	2.47	0.46
1:C:635:GLU:HG2	1:C:684:GLN:HE21	1.81	0.46
1:C:1029:MET:HA	1:C:1032:ILE:CG2	2.46	0.46
1:B:166:LEU:HD11	1:B:200:LEU:HD11	1.97	0.46
1:C:438:ARG:C	1:C:444:LEU:HD12	2.35	0.46
1:C:747:LEU:N	1:C:747:LEU:CD1	2.79	0.46
1:C:760:LEU:HD21	1:C:938:THR:CB	2.46	0.46
1:C:879:LEU:O	1:C:880:TYR:C	2.53	0.46
1:C:975:THR:HG22	1:C:979:ILE:CG1	2.42	0.46
1:B:187:ILE:HG23	1:B:193:ASN:HB3	1.98	0.45
1:B:267:LEU:O	1:B:270:ILE:N	2.48	0.45
1:B:322:HIS:C	1:B:323:LEU:HD12	2.35	0.45
1:B:386:LEU:N	1:B:386:LEU:CD2	2.73	0.45



A + a 1	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:832:ASP:HA	1:B:893:ARG:CD	2.46	0.45
1:B:907:ASP:C	1:B:909:LYS:H	2.20	0.45
1:C:134:ILE:HD13	1:C:134:ILE:C	2.36	0.45
1:C:380:ASP:HB3	1:C:383:GLU:OE2	2.16	0.45
1:B:363:SER:O	1:B:364:LEU:CB	2.62	0.45
1:B:714:GLY:O	1:B:716:ALA:N	2.49	0.45
1:B:816:ARG:O	1:B:845:GLU:HG3	2.17	0.45
1:C:363:SER:O	1:C:364:LEU:CB	2.64	0.45
1:C:758:ILE:HB	1:C:939:GLY:H	1.82	0.45
1:C:832:ASP:HA	1:C:893:ARG:CD	2.47	0.45
1:B:264:ILE:O	1:B:264:ILE:HG12	2.16	0.45
1:B:331:GLY:O	1:B:336:GLY:HA2	2.17	0.45
1:B:466:ALA:HB1	1:B:472:GLU:CG	2.46	0.45
1:B:754:PHE:CZ	1:B:907:ASP:HB2	2.51	0.45
1:C:87:PHE:O	1:C:88:GLY:C	2.54	0.45
1:C:253:ASN:OD1	1:C:446:LYS:HG2	2.17	0.45
1:C:257:VAL:HB	1:C:450:PHE:HD1	1.77	0.45
1:C:320:ILE:CG2	1:C:321:ASP:N	2.79	0.45
1:C:682:LYS:HD3	1:C:1039:TYR:CD2	2.52	0.45
1:C:725:ILE:HD13	1:C:1003:ILE:HG12	1.98	0.45
1:C:740:VAL:HG12	1:C:741:ARG:H	1.81	0.45
1:C:858:VAL:O	1:C:862:ILE:HG13	2.16	0.45
1:B:697:VAL:O	1:B:701:LYS:HG2	2.17	0.45
1:B:740:VAL:HG12	1:B:741:ARG:H	1.80	0.45
1:B:766:GLU:OE2	1:B:766:GLU:HA	2.16	0.45
1:C:508:LEU:HD13	1:C:619:LEU:HB3	1.99	0.45
1:C:1009:LEU:H	1:C:1009:LEU:CD2	2.29	0.45
1:B:52:LYS:HG2	1:B:125:LYS:HB3	1.99	0.45
1:B:134:ILE:HD11	1:B:160:ILE:HD12	1.97	0.45
1:B:315:PHE:CG	1:B:323:LEU:HD13	2.51	0.45
1:B:725:ILE:O	1:B:727:ARG:N	2.43	0.45
1:B:986:ARG:HA	1:B:986:ARG:HD3	1.66	0.45
1:C:63:MET:CE	1:C:67:ARG:NH2	2.79	0.45
1:C:194:VAL:O	1:C:197:LEU:N	2.41	0.45
1:C:261:ASP:CG	1:C:262:GLU:H	2.20	0.45
1:C:279:ILE:HD12	1:C:323:LEU:HB2	1.97	0.45
1:C:580:SER:HB3	1:C:584:CYS:SG	2.57	0.45
1:C:627:ILE:HA	1:C:654:LYS:O	2.15	0.45
1:B:257:VAL:HG21	1:B:450:PHE:CE1	2.51	0.45
1:B:279:ILE:HG12	1:B:343:ILE:CD1	2.47	0.45
1:B:440:PHE:HD1	1:B:440:PHE:N	2.15	0.45



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:853:LEU:HD13	1:B:861:LEU:HD12	1.98	0.45
1:C:43:LEU:HD23	1:C:47:VAL:HG23	1.99	0.45
1:C:64:TRP:O	1:C:65:ALA:C	2.55	0.45
1:C:341:GLU:OE2	1:C:496:ARG:HG2	2.16	0.45
1:C:583:ARG:HB3	1:C:608:ASN:CG	2.37	0.45
1:B:76:ALA:HB2	1:B:221:MET:CE	2.46	0.45
1:B:292:TYR:O	1:B:295:LEU:O	2.35	0.45
1:B:426:LEU:HD13	1:B:469:TYR:CD1	2.52	0.45
1:C:277:GLY:N	1:C:321:ASP:O	2.46	0.45
1:C:333:LEU:N	1:C:333:LEU:HD22	2.32	0.45
1:C:416:VAL:HG13	1:C:417:ARG:N	2.31	0.45
1:C:719:LEU:HD11	1:C:1019:GLU:HA	1.97	0.45
1:C:806:LEU:C	1:C:850:THR:HG23	2.36	0.45
1:B:100:LYS:O	1:B:177:ASP:OD1	2.35	0.45
1:B:374:TYR:C	1:B:376:TYR:N	2.70	0.45
1:B:712:SER:HB3	1:B:986:ARG:HG3	1.98	0.45
1:B:884:PHE:C	1:B:884:PHE:CD2	2.90	0.45
1:C:304:VAL:HB	1:C:305:THR:H	1.57	0.45
1:B:37:PHE:HB3	1:B:39:GLU:OE2	2.16	0.45
1:B:277:GLY:N	1:B:321:ASP:O	2.40	0.45
1:B:511:VAL:O	1:B:551:ALA:HA	2.16	0.45
1:B:791:VAL:CG2	1:B:977:ALA:HA	2.47	0.45
1:C:807:ILE:N	1:C:850:THR:HG23	2.31	0.45
1:B:248:ARG:CG	1:B:249:ILE:H	2.29	0.45
1:B:263:SER:OG	1:B:267:LEU:HB2	2.17	0.45
1:B:342:ARG:O	1:B:343:ILE:C	2.56	0.45
1:B:620:ALA:CB	1:B:647:LEU:HD13	2.46	0.45
1:C:254:VAL:HA	1:C:447:GLY:C	2.37	0.45
1:C:384:ARG:CZ	1:C:396:VAL:HB	2.47	0.45
1:C:584:CYS:O	1:C:585:ARG:HB2	2.16	0.45
1:C:790:SER:HA	1:C:958:GLN:NE2	2.28	0.45
1:C:986:ARG:HD3	1:C:986:ARG:HA	1.63	0.45
1:B:2:ILE:CA	1:B:11:PRO:N	2.80	0.44
1:B:89:LEU:HD12	1:B:118:THR:HG21	2.00	0.44
1:B:170:TYR:CE2	1:B:171:ARG:HG2	2.53	0.44
1:B:194:VAL:CG1	1:B:198:LEU:HD11	2.48	0.44
1:B:437:SER:HA	1:B:445:THR:OG1	2.17	0.44
1:B:438:ARG:HG3	1:B:439:LEU:H	1.81	0.44
1:B:860:ARG:O	1:B:863:GLN:N	2.50	0.44
1:C:98:LYS:O	1:C:99:GLY:C	2.54	0.44
1:C:358:ILE:HD11	1:C:419:GLY:O	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:887:PHE:O	1:C:889:ALA:N	2.50	0.44
1:B:212:TRP:C	1:B:213:VAL:HG22	2.38	0.44
1:B:303:ILE:HD13	1:B:304:VAL:N	2.32	0.44
1:B:693:TRP:O	1:B:697:VAL:HG23	2.18	0.44
1:B:699:SER:O	1:B:702:LEU:HB2	2.17	0.44
1:B:703:TRP:CH2	1:B:709:ARG:NH1	2.85	0.44
1:B:760:LEU:CD2	1:B:938:THR:OG1	2.65	0.44
1:C:640:ALA:HA	1:C:643:LEU:HD12	1.98	0.44
1:C:966:LYS:O	1:C:969:GLY:N	2.50	0.44
1:B:46:PHE:O	1:B:49:PHE:HB3	2.17	0.44
1:B:100:LYS:HG2	1:B:177:ASP:CB	2.47	0.44
1:B:377:ARG:HG3	1:B:382:ILE:CG1	2.46	0.44
1:B:381:GLU:OE1	1:B:381:GLU:N	2.51	0.44
1:B:480:ASP:O	1:B:481:PHE:C	2.55	0.44
1:B:689:ILE:H	1:B:689:ILE:HG12	1.64	0.44
1:B:725:ILE:C	1:B:727:ARG:H	2.21	0.44
1:B:1050:ILE:HG22	1:B:1051:LYS:N	2.33	0.44
1:C:86:SER:O	1:C:87:PHE:C	2.55	0.44
1:C:124:GLU:C	1:C:125:LYS:HD2	2.38	0.44
1:C:476:ILE:C	1:C:478:GLU:N	2.70	0.44
1:C:611:SER:O	1:C:615:ALA:N	2.50	0.44
1:C:739:ILE:HG22	1:C:740:VAL:O	2.17	0.44
1:C:1017:VAL:O	1:C:1017:VAL:CG1	2.66	0.44
1:C:54:VAL:HG12	1:C:55:GLY:N	2.32	0.44
1:C:252:ARG:NH2	1:C:256:ASP:OD1	2.50	0.44
1:C:553:ILE:HB	1:C:612:ARG:NE	2.32	0.44
1:C:991:GLU:HG3	1:C:995:ARG:C	2.38	0.44
1:B:700:GLN:O	1:B:703:TRP:N	2.40	0.44
1:B:791:VAL:H	1:B:958:GLN:HE22	1.65	0.44
1:C:43:LEU:O	1:C:46:PHE:N	2.50	0.44
1:C:494:ARG:O	1:C:495:TYR:C	2.56	0.44
1:C:529:VAL:HG12	1:C:530:LYS:N	2.33	0.44
1:C:854:THR:O	1:C:858:VAL:HG23	2.17	0.44
1:B:144:ARG:HG2	1:B:144:ARG:HH11	1.82	0.44
1:B:737:ILE:HD11	1:B:746:VAL:CG1	2.47	0.44
1:B:767:LEU:HA	1:B:895:PHE:O	2.18	0.44
1:B:873:ARG:H	1:B:876:HIS:CD2	2.25	0.44
1:B:1005:VAL:O	1:B:1009:LEU:HD23	2.17	0.44
1:C:138:HIS:O	1:C:140:ARG:N	2.50	0.44
1:C:254:VAL:HA	1:C:447:GLY:CA	2.48	0.44
1:C:617:ARG:HG3	1:C:647:LEU:HD23	1.99	0.44



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:774:TYR:CG	1:C:886:ARG:HG2	2.53	0.44
1:B:58:ARG:O	1:B:59:ALA:C	2.56	0.44
1:B:386:LEU:H	1:B:386:LEU:CD2	1.97	0.44
1:B:685:VAL:O	1:B:686:VAL:C	2.56	0.44
1:B:901:LYS:CG	1:B:902:TYR:N	2.79	0.44
1:C:95:LEU:HB3	1:C:100:LYS:HB3	1.99	0.44
1:C:252:ARG:CA	1:C:444:LEU:HD21	2.47	0.44
1:C:439:LEU:HD13	1:C:444:LEU:HD13	2.00	0.44
1:C:477:ASP:C	1:C:479:VAL:N	2.71	0.44
1:C:565:PHE:N	1:C:568:VAL:O	2.51	0.44
1:C:856:ASP:O	1:C:857:ASP:C	2.56	0.44
1:C:883:ILE:H	1:C:883:ILE:CD1	2.31	0.44
1:B:12:VAL:HA	1:B:19:SER:O	2.17	0.44
1:B:470:ASP:HB3	1:B:471:ILE:H	1.61	0.44
1:B:966:LYS:O	1:B:967:GLU:C	2.55	0.44
1:B:1029:MET:HA	1:B:1032:ILE:HG23	1.99	0.44
1:B:320:ILE:HG21	1:B:322:HIS:O	2.17	0.44
1:B:750:ASP:C	1:B:751:GLU:OE1	2.57	0.44
1:C:11:PRO:HA	1:C:16:ASP:CB	2.47	0.44
1:C:166:LEU:HD11	1:C:200:LEU:HD11	2.00	0.44
1:C:436:THR:HG23	1:C:436:THR:O	2.18	0.44
1:C:702:LEU:HD21	1:C:1009:LEU:HD21	1.99	0.44
1:B:31:LYS:N	1:B:32:ARG:CZ	2.81	0.43
1:B:119:ILE:O	1:B:120:ARG:C	2.55	0.43
1:B:546:VAL:O	1:B:546:VAL:HG12	2.17	0.43
1:B:736:LYS:NZ	1:B:736:LYS:CA	2.79	0.43
1:C:58:ARG:O	1:C:61:GLN:N	2.51	0.43
1:C:121:LYS:O	1:C:125:LYS:NZ	2.48	0.43
1:C:154:ARG:NE	1:C:174:GLY:HA3	2.33	0.43
1:C:768:ARG:HG3	1:C:768:ARG:NH1	2.31	0.43
1:C:1028:ARG:O	1:C:1031:ALA:HB3	2.17	0.43
1:B:38:PRO:C	1:B:40:ASP:H	2.20	0.43
1:B:366:PRO:CA	1:B:393:ILE:HG12	2.48	0.43
1:B:382:ILE:O	1:B:386:LEU:CD2	2.66	0.43
1:B:468:LEU:HD22	1:B:468:LEU:H	1.83	0.43
1:B:509:PHE:O	1:B:549:VAL:HA	2.17	0.43
1:B:832:ASP:CA	1:B:893:ARG:HG3	2.47	0.43
1:C:208:LYS:C	1:C:210:LYS:H	2.21	0.43
1:C:436:THR:HG23	1:C:447:GLY:CA	2.44	0.43
1:C:477:ASP:HA	1:C:479:VAL:HG13	1.99	0.43
1:C:609:SER:CB	1:C:612:ARG:NH1	2.81	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:740:VAL:CG1	1:C:741:ARG:N	2.80	0.43
1:B:314:LYS:HA	1:B:319:GLU:OE2	2.19	0.43
1:B:393:ILE:N	1:B:393:ILE:CD1	2.82	0.43
1:B:562:ASN:O	1:B:563:ARG:C	2.57	0.43
1:B:763:GLU:OE1	1:B:900:LYS:HE2	2.18	0.43
1:B:907:ASP:O	1:B:909:LYS:N	2.51	0.43
1:C:212:TRP:HB2	1:C:213:VAL:H	1.59	0.43
1:C:337:LEU:CD2	1:C:343:ILE:HD11	2.46	0.43
1:C:570:VAL:O	1:C:573:ARG:HB2	2.17	0.43
1:B:207:LEU:HG	1:B:208:LYS:N	2.33	0.43
1:B:291:ILE:O	1:B:292:TYR:C	2.56	0.43
1:B:518:ARG:HG2	1:B:522:ARG:CZ	2.48	0.43
1:B:638:LYS:HB2	1:B:684:GLN:CG	2.28	0.43
1:B:702:LEU:HD21	1:B:1009:LEU:HD21	1.99	0.43
1:B:756:LEU:O	1:B:940:THR:HA	2.18	0.43
1:B:832:ASP:HA	1:B:893:ARG:CG	2.48	0.43
1:B:947:VAL:O	1:B:948:LYS:HG3	2.19	0.43
1:C:125:LYS:O	1:C:126:ALA:HB3	2.19	0.43
1:C:276:THR:HG21	1:C:321:ASP:OD1	2.18	0.43
1:C:413:ASP:OD1	1:C:413:ASP:C	2.57	0.43
1:C:118:THR:HG22	1:C:122:TYR:CZ	2.54	0.43
1:C:274:LEU:HG	1:C:274:LEU:O	2.19	0.43
1:C:357:THR:CG2	1:C:358:ILE:N	2.81	0.43
1:C:666:ILE:O	1:C:667:LEU:C	2.56	0.43
1:C:706:PHE:O	1:C:708:ASN:N	2.52	0.43
1:C:824:ILE:HG23	1:C:852:PRO:CD	2.48	0.43
1:C:1012:ARG:O	1:C:1013:TYR:CD1	2.72	0.43
1:B:87:PHE:O	1:B:88:GLY:C	2.56	0.43
1:B:456:SER:O	1:B:457:GLU:C	2.57	0.43
1:C:13:CYS:O	1:C:20:LYS:HA	2.18	0.43
1:C:320:ILE:CG2	1:C:322:HIS:O	2.66	0.43
1:C:735:ARG:NH1	1:C:951:PRO:HG3	2.34	0.43
1:C:736:LYS:HB3	1:C:737:ILE:H	1.48	0.43
1:C:1000:LYS:O	1:C:1001:LEU:C	2.55	0.43
1:B:315:PHE:HA	1:B:320:ILE:HB	2.00	0.43
1:B:522:ARG:HA	1:B:525:GLY:O	2.19	0.43
1:B:628:VAL:HG13	1:B:630:THR:HG23	1.99	0.43
1:B:669:ALA:C	1:B:671:GLU:H	2.20	0.43
1:B:797:ILE:HG23	1:B:876:HIS:ND1	2.33	0.43
1:B:883:ILE:H	1:B:883:ILE:CD1	2.29	0.43
1:C:94:PHE:O	1:C:98:LYS:HD3	2.19	0.43



	A4 ama 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:109:SER:O	1:C:112:VAL:HB	2.17	0.43
1:C:236:PHE:HD1	1:C:244:ILE:HD11	1.83	0.43
1:C:259:VAL:N	1:C:451:LEU:O	2.46	0.43
1:C:427:ARG:HG3	1:C:427:ARG:HH11	1.83	0.43
1:C:613:ILE:CD1	1:C:613:ILE:H	2.31	0.43
1:C:719:LEU:HD13	1:C:970:ILE:HD13	2.00	0.43
1:C:991:GLU:O	1:C:992:LYS:HE2	2.18	0.43
1:B:101:ARG:NH1	1:B:154:ARG:HA	2.33	0.43
1:B:361:ILE:O	1:B:362:ASP:O	2.36	0.43
1:B:369:VAL:HG21	1:B:393:ILE:HG23	1.95	0.43
1:B:436:THR:HG23	1:B:447:GLY:CA	2.46	0.43
1:B:560:ILE:HG13	1:B:561:THR:N	2.32	0.43
1:C:35:CYS:HB2	1:C:648:SER:O	2.18	0.43
1:C:89:LEU:O	1:C:92:SER:HB3	2.18	0.43
1:C:706:PHE:O	1:C:706:PHE:CD1	2.70	0.43
1:B:60:ILE:CG2	1:B:82:VAL:HG11	2.49	0.43
1:B:103:TYR:HD1	1:B:159:VAL:O	2.02	0.43
1:B:304:VAL:HB	1:B:305:THR:H	1.63	0.43
1:B:377:ARG:O	1:B:379:VAL:O	2.37	0.43
1:B:426:LEU:O	1:B:427:ARG:C	2.57	0.43
1:B:477:ASP:C	1:B:479:VAL:N	2.73	0.43
1:B:694:ILE:H	1:B:694:ILE:HG12	1.60	0.43
1:B:743:PHE:N	1:B:743:PHE:CD1	2.86	0.43
1:B:856:ASP:O	1:B:857:ASP:C	2.57	0.43
1:C:160:ILE:C	1:C:161:THR:CG2	2.87	0.43
1:C:236:PHE:CD1	1:C:244:ILE:HD11	2.53	0.43
1:C:470:ASP:HB3	1:C:471:ILE:H	1.54	0.43
1:C:666:ILE:O	1:C:669:ALA:N	2.51	0.43
1:C:758:ILE:CG2	1:C:938:THR:HA	2.49	0.43
1:B:274:LEU:HD22	1:B:450:PHE:HE2	1.83	0.43
1:B:357:THR:HG22	1:B:358:ILE:N	2.34	0.43
1:B:360:ASP:O	1:B:361:ILE:C	2.57	0.43
1:B:374:TYR:O	1:B:376:TYR:N	2.52	0.43
1:B:440:PHE:CE2	1:B:442:GLY:HA3	2.54	0.43
1:B:505:LYS:O	1:B:545:TYR:HB3	2.19	0.43
1:C:22:ILE:CB	1:C:641:TRP:HH2	2.32	0.43
1:C:154:ARG:NH2	1:C:174:GLY:HA2	2.34	0.43
1:C:260:ASN:O	1:C:454:ASP:HA	2.18	0.43
1:C:296:LYS:O	1:C:301:ILE:HD11	2.18	0.43
1:C:305:THR:HG22	1:C:306:ALA:N	2.23	0.43
1:C:665:ALA:HA	1:C:668:GLU:OE2	2.19	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:766:GLU:HB3	1:C:768:ARG:HE	1.83	0.43	
1:C:887:PHE:C	1:C:887:PHE:CD1	2.93	0.43	
1:C:972:ARG:NH1	1:C:1026:GLU:HG3	2.34	0.43	
1:B:326:THR:HG1	1:B:329:TYR:HD2	1.66	0.42	
1:B:530:LYS:HB3	1:B:537:VAL:CG1	2.49	0.42	
1:B:936:LEU:O	1:B:936:LEU:CD1	2.67	0.42	
1:C:260:ASN:HA	1:C:453:GLU:O	2.19	0.42	
1:C:455:ASP:O	1:C:456:SER:C	2.57	0.42	
1:B:512:GLU:CD	1:B:630:THR:HB	2.39	0.42	
1:B:720:VAL:O	1:B:721:LEU:C	2.58	0.42	
1:B:753:GLU:HG3	1:B:754:PHE:N	2.34	0.42	
1:C:220:LEU:HD12	1:C:221:MET:N	2.33	0.42	
1:C:537:VAL:O	1:C:537:VAL:HG13	2.18	0.42	
1:C:942:ARG:H	1:C:942:ARG:HG2	1.64	0.42	
1:B:283:ARG:HG3	1:B:287:GLU:OE1	2.18	0.42	
1:B:296:LYS:HA	1:B:301:ILE:HG12	2.02	0.42	
1:B:544:LYS:O	1:B:545:TYR:CG	2.72	0.42	
1:B:774:TYR:OH	1:B:782:ASP:CB	2.67	0.42	
1:B:935:GLU:HG2	1:B:936:LEU:H	1.84	0.42	
1:C:697:VAL:O	1:C:700:GLN:HB3	2.20	0.42	
1:C:743:PHE:O	1:C:745:LEU:N	2.51	0.42	
1:C:829:LEU:O	1:C:830:GLY:O	2.37	0.42	
1:C:860:ARG:HH11	1:C:860:ARG:CB	2.30	0.42	
1:B:176:PHE:HB2	1:B:179:ILE:CD1	2.49	0.42	
1:B:305:THR:O	1:B:306:ALA:C	2.57	0.42	
1:B:834:VAL:HG21	1:B:893:ARG:HA	2.01	0.42	
1:C:63:MET:HG3	1:C:622:ASP:O	2.19	0.42	
1:C:170:TYR:CG	1:C:171:ARG:N	2.87	0.42	
1:C:315:PHE:HB2	1:C:323:LEU:HD11	2.00	0.42	
1:C:476:ILE:O	1:C:476:ILE:HG13	2.18	0.42	
1:C:583:ARG:O	1:C:583:ARG:HG2	2.19	0.42	
1:C:756:LEU:CD1	1:C:904:ILE:HB	2.49	0.42	
1:C:818:SER:O	1:C:819:ASP:C	2.58	0.42	
1:B:60:ILE:CD1	1:B:546:VAL:HG11	2.50	0.42	
1:B:396:VAL:O	1:B:400:LEU:HG	2.20	0.42	
1:B:720:VAL:C	1:B:722:GLY:N	2.73	0.42	
1:B:829:LEU:HB2	1:B:833:PHE:HB2	2.00	0.42	
1:B:853:LEU:O	1:B:854:THR:O	2.38	0.42	
1:C:101:ARG:HD3	1:C:176:PHE:CD1	2.54	0.42	
1:C:154:ARG:HE	1:C:174:GLY:CA	2.29	0.42	
1:C:557:VAL:C	1:C:581:ILE:HD11	2.40	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:658:PHE:CD1	1:C:658:PHE:N	2.87	0.42
1:B:444:LEU:O	1:B:445:THR:C	2.57	0.42
1:B:690:GLU:HG3	1:B:694:ILE:CG1	2.49	0.42
1:B:764:ARG:HD3	1:B:764:ARG:H	1.83	0.42
1:B:838:TRP:O	1:B:839:GLY:O	2.38	0.42
1:B:912:GLU:O	1:B:912:GLU:HG2	2.19	0.42
1:B:912:GLU:OE1	1:B:912:GLU:N	2.52	0.42
1:B:989:VAL:HG12	1:B:990:VAL:N	2.34	0.42
1:C:43:LEU:O	1:C:46:PHE:HB3	2.19	0.42
1:C:58:ARG:CB	1:C:61:GLN:HE21	2.27	0.42
1:C:148:ASN:N	1:C:148:ASN:ND2	2.67	0.42
1:C:638:LYS:CB	1:C:684:GLN:HG3	2.39	0.42
1:C:812:THR:CG2	1:C:847:ILE:HG13	2.49	0.42
1:C:857:ASP:O	1:C:861:LEU:HG	2.20	0.42
1:C:860:ARG:CG	1:C:860:ARG:NH1	2.82	0.42
1:C:1012:ARG:HB3	1:C:1012:ARG:NH1	2.34	0.42
1:B:58:ARG:CB	1:B:61:GLN:HE21	2.26	0.42
1:B:508:LEU:CD2	1:B:510:ILE:HD11	2.39	0.42
1:B:991:GLU:HG3	1:B:995:ARG:O	2.19	0.42
1:C:43:LEU:HD23	1:C:47:VAL:CG2	2.50	0.42
1:C:370:LYS:O	1:C:373:ALA:CB	2.63	0.42
1:C:530:LYS:HB3	1:C:537:VAL:CG1	2.50	0.42
1:C:557:VAL:O	1:C:581:ILE:HD11	2.20	0.42
1:C:570:VAL:HB	1:C:571:ASN:H	1.62	0.42
1:C:763:GLU:OE1	1:C:900:LYS:HE2	2.20	0.42
1:B:58:ARG:NH2	1:B:82:VAL:HA	2.35	0.42
1:B:153:LEU:O	1:B:154:ARG:HG3	2.19	0.42
1:B:175:HIS:C	1:B:176:PHE:CD1	2.93	0.42
1:B:192:LYS:O	1:B:193:ASN:C	2.58	0.42
1:B:391:ARG:HD3	1:B:391:ARG:C	2.34	0.42
1:B:426:LEU:HD11	1:B:466:ALA:CA	2.45	0.42
1:B:756:LEU:HD11	1:B:904:ILE:HB	2.02	0.42
1:B:756:LEU:HD13	1:B:757:THR:H	1.85	0.42
1:B:772:PRO:O	1:B:886:ARG:NH1	2.46	0.42
1:B:830:GLY:C	1:B:832:ASP:H	2.23	0.42
1:B:872:LEU:HD22	1:B:876:HIS:CG	2.55	0.42
1:C:187:ILE:HG23	1:C:193:ASN:HB3	2.02	0.42
1:C:283:ARG:HG3	1:C:287:GLU:OE1	2.20	0.42
1:C:305:THR:OG1	1:C:329:TYR:CB	2.52	0.42
1:C:318:GLY:HA2	1:C:342:ARG:HH11	1.85	0.42
1:C:351:CYS:HB3	1:C:462:PHE:CE1	2.55	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:123:ALA:C	1:B:125:LYS:H	2.22	0.42
1:B:341:GLU:OE2	1:B:496:ARG:HG2	2.19	0.42
1:B:494:ARG:O	1:B:497:ARG:N	2.53	0.42
1:B:533:ASP:OD1	1:B:534:GLY:N	2.44	0.42
1:B:708:ASN:C	1:B:709:ARG:O	2.55	0.42
1:B:709:ARG:HH11	1:B:709:ARG:CG	2.33	0.42
1:B:756:LEU:HD22	1:B:906:PHE:HB3	2.01	0.42
1:C:65:ALA:O	1:C:66:LYS:C	2.58	0.42
1:C:86:SER:N	2:C:2055:ANP:O1A	2.52	0.42
1:C:138:HIS:H	1:C:141:ILE:CD1	2.32	0.42
1:C:357:THR:HG22	1:C:358:ILE:H	1.85	0.42
1:C:374:TYR:O	1:C:376:TYR:N	2.53	0.42
1:C:469:TYR:O	1:C:470:ASP:C	2.58	0.42
1:C:480:ASP:OD1	1:C:483:LYS:HG3	2.19	0.42
1:C:879:LEU:O	1:C:881:ASP:N	2.52	0.42
1:B:58:ARG:HH21	1:B:82:VAL:HA	1.85	0.42
1:B:64:TRP:O	1:B:65:ALA:C	2.57	0.42
1:B:103:TYR:O	1:B:179:ILE:HA	2.19	0.42
1:B:258:ALA:O	1:B:476:ILE:HD12	2.19	0.42
1:B:906:PHE:N	1:B:906:PHE:CD1	2.88	0.42
1:B:1012:ARG:CG	1:B:1012:ARG:NH1	2.82	0.42
1:C:37:PHE:CD2	1:C:621:HIS:ND1	2.88	0.42
1:C:58:ARG:HE	1:C:82:VAL:HA	1.85	0.42
1:C:252:ARG:N	1:C:444:LEU:HD21	2.35	0.42
1:C:580:SER:OG	1:C:610:ARG:HB2	2.19	0.42
1:C:617:ARG:HG3	1:C:647:LEU:CD2	2.50	0.42
1:C:642:ASP:O	1:C:646:LEU:HD12	2.20	0.42
1:C:784:ASN:ND2	1:C:958:GLN:HB2	2.35	0.42
1:C:874:TRP:CD2	1:C:875:GLU:N	2.88	0.42
1:B:314:LYS:HG2	1:B:319:GLU:OE1	2.20	0.41
1:B:333:LEU:CD2	1:B:333:LEU:H	2.32	0.41
1:B:361:ILE:O	1:B:362:ASP:C	2.58	0.41
1:B:483:LYS:O	1:B:486:ARG:N	2.53	0.41
1:C:46:PHE:HA	1:C:94:PHE:CE1	2.54	0.41
1:C:198:LEU:HD12	1:C:198:LEU:N	2.21	0.41
1:C:272:GLU:OE1	1:C:322:HIS:CD2	2.73	0.41
1:C:480:ASP:O	1:C:483:LYS:N	2.51	0.41
1:C:540:ILE:HG13	1:C:541:PRO:N	2.35	0.41
1:C:608:ASN:ND2	1:C:610:ARG:CB	2.83	0.41
1:C:608:ASN:C	1:C:610:ARG:N	2.72	0.41
1:C:613:ILE:CD1	1:C:613:ILE:N	2.82	0.41



	A construction of the cons	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:687:ARG:HA	1:C:1029:MET:HE3	2.02	0.41
1:B:400:LEU:O	1:B:403:VAL:O	2.38	0.41
1:B:417:ARG:HB3	1:B:418:GLU:H	1.62	0.41
1:B:469:TYR:O	1:B:470:ASP:O	2.38	0.41
1:B:544:LYS:HE3	1:B:671:GLU:OE1	2.20	0.41
1:B:734:ARG:HB2	1:B:952:LYS:HA	2.02	0.41
1:B:934:ASN:HD22	1:B:935:GLU:H	1.68	0.41
1:C:374:TYR:C	1:C:376:TYR:N	2.73	0.41
1:C:440:PHE:CE2	1:C:495:TYR:HA	2.55	0.41
1:C:634:THR:HB	1:C:684:GLN:HB2	2.02	0.41
1:C:733:GLU:O	1:C:952:LYS:N	2.53	0.41
1:C:784:ASN:ND2	1:C:959:SER:N	2.59	0.41
1:B:393:ILE:HG22	1:B:397:ARG:CG	2.50	0.41
1:B:608:ASN:ND2	1:B:610:ARG:HB3	2.35	0.41
1:B:750:ASP:OD1	1:B:751:GLU:OE1	2.38	0.41
1:B:1038:ASP:C	1:B:1038:ASP:OD2	2.59	0.41
1:C:138:HIS:CE1	1:C:140:ARG:HB3	2.56	0.41
1:C:212:TRP:C	1:C:213:VAL:HG22	2.41	0.41
1:C:253:ASN:O	1:C:254:VAL:O	2.37	0.41
1:C:814:SER:OG	1:C:816:ARG:HB2	2.21	0.41
1:B:39:GLU:HG3	1:B:70:ARG:HG2	2.03	0.41
1:B:181:VAL:CG2	1:B:222:VAL:HG12	2.49	0.41
1:B:747:LEU:N	1:B:747:LEU:CD1	2.79	0.41
1:B:825:ALA:HA	1:B:888:MET:SD	2.60	0.41
1:B:881:ASP:OD1	1:B:882:LEU:HD12	2.19	0.41
1:C:377:ARG:O	1:C:378:ASN:C	2.57	0.41
1:C:472:GLU:OE2	1:C:472:GLU:HA	2.20	0.41
1:C:703:TRP:CH2	1:C:709:ARG:NH1	2.87	0.41
1:C:851:ARG:O	1:C:853:LEU:N	2.53	0.41
1:C:975:THR:O	1:C:976:TYR:C	2.57	0.41
1:C:984:PHE:CD1	1:C:989:VAL:HB	2.55	0.41
1:B:358:ILE:HG23	1:B:404:MET:SD	2.60	0.41
1:B:361:ILE:HD13	1:B:400:LEU:HB2	2.03	0.41
1:B:366:PRO:C	1:B:368:MET:H	2.23	0.41
1:B:674:ARG:HG3	1:B:674:ARG:HH11	1.85	0.41
1:B:784:ASN:ND2	1:B:958:GLN:HB2	2.35	0.41
1:C:285:GLY:O	1:C:288:ALA:HB3	2.19	0.41
1:C:320:ILE:HG22	1:C:321:ASP:N	2.36	0.41
1:C:958:GLN:O	1:C:962:ILE:HG12	2.21	0.41
1:C:965:MET:HB3	1:C:970:ILE:O	2.19	0.41
1:B:426:LEU:CD1	1:B:466:ALA:HA	2.48	0.41



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:756:LEU:CD1	1:B:904:ILE:HB	2.51	0.41
1:C:66:LYS:HB3	1:C:70:ARG:NH1	2.36	0.41
1:C:266:THR:O	1:C:267:LEU:CB	2.68	0.41
1:C:336:GLY:O	1:C:337:LEU:HB3	2.21	0.41
1:C:757:THR:O	1:C:904:ILE:HG22	2.20	0.41
1:C:830:GLY:C	1:C:832:ASP:H	2.23	0.41
1:C:1005:VAL:O	1:C:1006:PHE:C	2.58	0.41
1:B:38:PRO:O	1:B:40:ASP:N	2.54	0.41
1:B:254:VAL:HA	1:B:447:GLY:C	2.40	0.41
1:B:320:ILE:HG22	1:B:321:ASP:N	2.34	0.41
1:B:351:CYS:HA	1:B:451:LEU:HD11	2.03	0.41
1:B:558:ASP:OD2	1:B:559:LEU:N	2.49	0.41
1:B:687:ARG:NH2	1:B:1026:GLU:OE1	2.49	0.41
1:B:1002:GLY:O	1:B:1005:VAL:N	2.53	0.41
1:C:426:LEU:HD13	1:C:469:TYR:CD1	2.55	0.41
1:C:720:VAL:O	1:C:721:LEU:C	2.59	0.41
1:C:763:GLU:CD	1:C:900:LYS:HE2	2.41	0.41
1:C:790:SER:CA	1:C:958:GLN:HE22	2.28	0.41
1:C:1007:ARG:C	1:C:1010:VAL:HG12	2.41	0.41
1:B:106:PHE:CD1	1:B:182:ASP:HB2	2.56	0.41
1:B:109:SER:HB3	1:B:138:HIS:CD2	2.55	0.41
1:B:388:ALA:O	1:B:389:VAL:HB	2.21	0.41
1:B:628:VAL:HG11	1:B:640:ALA:HB2	2.02	0.41
1:B:712:SER:CB	1:B:986:ARG:HH11	2.34	0.41
1:B:822:GLN:HE21	1:B:822:GLN:HB3	1.65	0.41
1:B:1007:ARG:CA	1:B:1010:VAL:HG12	2.50	0.41
1:C:46:PHE:CZ	1:C:91:MET:HB2	2.56	0.41
1:C:76:ALA:N	1:C:222:VAL:O	2.52	0.41
1:C:112:VAL:HG21	1:C:162:THR:HG23	2.00	0.41
1:C:184:VAL:CG1	1:C:225:ALA:HA	2.50	0.41
1:C:382:ILE:O	1:C:386:LEU:CD2	2.68	0.41
1:C:413:ASP:CG	1:C:860:ARG:NH2	2.74	0.41
1:C:419:GLY:O	1:C:420:GLU:CB	2.65	0.41
1:C:691:ASP:O	1:C:695:GLY:HA3	2.20	0.41
1:C:810:HIS:O	1:C:847:ILE:HD11	2.21	0.41
1:B:140:ARG:HB3	1:B:141:ILE:H	1.63	0.41
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.36	0.41
1:B:330:TYR:HA	1:B:333:LEU:HD23	2.03	0.41
1:B:497:ARG:O	1:B:500:GLU:CG	2.68	0.41
1:B:545:TYR:CE1	1:B:670:LEU:HD13	2.56	0.41
1:B:556:VAL:HB	1:B:613:ILE:HD12	1.96	0.41



			Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:637:GLU:HG2	1:B:680:LEU:HB2	2.03	0.41
1:B:698:LEU:HD22	1:B:1009:LEU:HD12	2.03	0.41
1:B:745:LEU:CD1	1:B:747:LEU:HD11	2.41	0.41
1:B:849:PRO:CG	1:B:884:PHE:HA	2.47	0.41
1:B:870:GLU:O	1:B:872:LEU:HG	2.21	0.41
1:B:904:ILE:O	1:B:911:ALA:N	2.54	0.41
1:C:171:ARG:HG3	1:C:171:ARG:NH1	2.36	0.41
1:C:425:ASP:OD2	1:C:428:THR:CB	2.69	0.41
1:C:497:ARG:O	1:C:500:GLU:HB2	2.21	0.41
1:C:628:VAL:HG13	1:C:630:THR:HG23	2.02	0.41
1:C:681:VAL:O	1:C:685:VAL:HG23	2.20	0.41
1:C:791:VAL:HG11	1:C:980:VAL:HG11	2.01	0.41
1:C:1022:THR:O	1:C:1026:GLU:HB2	2.20	0.41
1:B:279:ILE:HD11	1:B:315:PHE:CZ	2.55	0.41
1:B:337:LEU:HB3	1:B:435:ARG:HE	1.85	0.41
1:B:365:SER:HA	1:B:366:PRO:HD3	1.82	0.41
1:B:581:ILE:HG22	1:B:582:LYS:H	1.86	0.41
1:B:791:VAL:HG23	1:B:977:ALA:CB	2.52	0.41
1:B:879:LEU:O	1:B:880:TYR:C	2.57	0.41
1:B:962:ILE:HD13	1:B:962:ILE:HA	1.87	0.41
1:C:68:ILE:C	1:C:70:ARG:H	2.24	0.41
1:C:167:SER:OG	1:C:193:ASN:OD1	2.37	0.41
1:C:440:PHE:HD1	1:C:440:PHE:H	1.68	0.41
1:C:624:GLU:HA	1:C:650:CYS:O	2.20	0.41
1:C:736:LYS:O	1:C:948:LYS:O	2.40	0.41
1:C:808:THR:HG21	1:C:848:ARG:NE	2.36	0.41
1:C:901:LYS:HA	1:C:914:GLU:HA	2.02	0.41
1:B:124:GLU:O	1:B:125:LYS:HD2	2.21	0.40
1:B:246:SER:OG	1:B:247:SER:N	2.54	0.40
1:B:279:ILE:CG2	1:B:281:TYR:CE1	2.98	0.40
1:B:323:LEU:HB3	1:B:330:TYR:OH	2.21	0.40
1:B:336:GLY:O	1:B:337:LEU:HB3	2.21	0.40
1:B:381:GLU:N	1:B:381:GLU:CD	2.74	0.40
1:B:403:VAL:O	1:B:404:MET:CB	2.58	0.40
1:B:413:ASP:O	1:B:424:PRO:HG2	2.21	0.40
1:B:754:PHE:CE2	1:B:907:ASP:N	2.90	0.40
1:B:985:MET:HE2	1:B:986:ARG:HH21	1.83	0.40
1:C:374:TYR:O	1:C:375:LEU:HB2	2.22	0.40
1:C:542:MET:CE	1:C:544:LYS:HB2	2.51	0.40
1:C:743:PHE:CD1	1:C:743:PHE:N	2.88	0.40
1:C:895:PHE:CD2	1:C:895:PHE:N	2.82	0.40



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:1018:SER:O	1:C:1021:ARG:N	2.54	0.40	
1:B:338:ASP:OD1	1:B:340:PRO:HD3	2.21	0.40	
1:B:377:ARG:O	1:B:377:ARG:HG2	2.21	0.40	
1:B:476:ILE:C	1:B:478:GLU:H	2.23	0.40	
1:B:637:GLU:HG2	1:B:680:LEU:HD12	2.04	0.40	
1:B:758:ILE:HB	1:B:938:THR:HA	2.03	0.40	
1:B:942:ARG:H	1:B:942:ARG:HG2	1.66	0.40	
1:B:991:GLU:O	1:B:992:LYS:HE2	2.21	0.40	
1:C:35:CYS:HB2	1:C:650:CYS:N	2.35	0.40	
1:C:289:GLU:O	1:C:293:GLU:OE2	2.40	0.40	
1:C:737:ILE:HG23	1:C:950:VAL:HG22	2.03	0.40	
1:B:152:ASN:O	1:B:152:ASN:ND2	2.55	0.40	
1:B:266:THR:O	1:B:267:LEU:CB	2.70	0.40	
1:B:276:THR:HA	1:B:322:HIS:NE2	2.37	0.40	
1:B:393:ILE:O	1:B:394:ASP:C	2.60	0.40	
1:B:433:SER:O	1:B:436:THR:CG2	2.68	0.40	
1:B:878:ALA:O	1:B:881:ASP:HB3	2.20	0.40	
1:C:278:GLY:HA2	1:C:345:PHE:O	2.21	0.40	
1:C:901:LYS:HG3	1:C:902:TYR:H	1.86	0.40	
1:C:1025:LEU:HD23	1:C:1025:LEU:O	2.21	0.40	
1:B:106:PHE:CE2	1:B:115:ALA:HB2	2.57	0.40	
1:B:387:PRO:CA	1:B:389:VAL:H	2.32	0.40	
1:B:438:ARG:O	1:B:444:LEU:HA	2.22	0.40	
1:B:1053:ILE:HG13	1:B:1054:ASP:N	2.35	0.40	
1:C:243:ASP:HB3	1:C:529:VAL:HB	2.02	0.40	
1:C:267:LEU:HD12	1:C:452:LEU:HD13	2.04	0.40	
1:C:296:LYS:HG3	1:C:301:ILE:HD13	2.04	0.40	
1:C:542:MET:HB2	1:C:543:GLN:HE21	1.87	0.40	
1:C:1007:ARG:O	1:C:1011:ARG:HG3	2.22	0.40	
1:C:1050:ILE:O	1:C:1053:ILE:HG12	2.22	0.40	
1:B:305:THR:CG2	1:B:329:TYR:CZ	3.05	0.40	
1:B:312:TYR:CE2	1:B:316:VAL:CG2	3.04	0.40	
1:B:496:ARG:HG3	1:B:496:ARG:HH11	1.86	0.40	
1:B:504:ILE:HG22	1:B:546:VAL:HG23	2.02	0.40	
1:C:170:TYR:HB3	1:C:196:LYS:HB3	2.03	0.40	
1:C:642:ASP:HB3	1:C:646:LEU:HD11	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	Perce	ntiles
1	В	1010/1054~(96%)	752 (74%)	177 (18%)	81 (8%)	1	6
1	С	987/1054~(94%)	696 (70%)	214 (22%)	77 (8%)	1	6
All	All	1997/2108~(95%)	1448 (72%)	391 (20%)	158 (8%)	1	6

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	3	PRO
1	В	5	VAL
1	В	12	VAL
1	В	24	LYS
1	В	32	ARG
1	В	128	VAL
1	В	141	ILE
1	В	154	ARG
1	В	213	VAL
1	В	266	THR
1	В	267	LEU
1	В	306	ALA
1	В	307	THR
1	В	361	ILE
1	В	362	ASP
1	В	364	LEU
1	В	387	PRO
1	В	420	GLU
1	В	445	THR
1	В	471	ILE
1	В	476	ILE
1	В	481	PHE
1	В	947	VAL
1	С	4	VAL
1	С	154	ARG



Mol	Chain	Res	Type
1	С	213	VAL
1	С	244	ILE
1	С	254	VAL
1	С	266	THR
1	С	267	LEU
1	С	305	THR
1	С	306	ALA
1	С	307	THR
1	С	361	ILE
1	С	362	ASP
1	С	364	LEU
1	С	379	VAL
1	С	420	GLU
1	С	471	ILE
1	С	481	PHE
1	С	533	ASP
1	С	543	GLN
1	С	580	SER
1	С	630	THR
1	С	707	ASN
1	С	737	ILE
1	С	947	VAL
1	В	130	THR
1	В	139	GLY
1	В	194	VAL
1	В	228	LYS
1	В	254	VAL
1	В	377	ARG
1	В	392	HIS
1	В	404	MET
1	В	419	GLY
1	В	470	ASP
1	В	502	ASP
1	В	533	ASP
1	В	709	ARG
1	В	736	LYS
1	В	737	ILE
1	В	830	GLY
1	В	838	TRP
1	В	854	THR
1	В	871	GLY
1	В	908	GLY



Mol	Chain	Res	Type
1	С	128	VAL
1	С	133	LEU
1	С	139	GLY
1	С	208	LYS
1	С	262	GLU
1	С	374	TYR
1	С	377	ARG
1	С	378	ASN
1	С	564	GLY
1	С	715	ARG
1	С	732	ARG
1	С	752	GLU
1	С	830	GLY
1	С	838	TRP
1	С	871	GLY
1	С	1013	TYR
1	В	173	LEU
1	В	378	ASN
1	В	455	ASP
1	В	456	SER
1	В	563	ARG
1	В	707	ASN
1	В	752	GLU
1	В	839	GLY
1	В	982	ARG
1	В	1052	SER
1	В	1053	ILE
1	С	76	ALA
1	С	130	THR
1	С	502	ASP
1	С	709	ARG
1	С	770	PRO
1	С	777	GLU
1	С	846	CYS
1	С	982	ARG
1	В	39	GLU
1	В	101	ARG
1	В	165	PHE
1	В	195	ASP
1	В	196	LYS
1	В	208	LYS
1	В	305	THR



Mol	Chain	Res	Type
1	В	374	TYR
1	В	411	ALA
1	В	417	ARG
1	В	721	LEU
1	В	726	ASP
1	В	805	GLY
1	С	101	ARG
1	С	141	ILE
1	С	249	ILE
1	С	283	ARG
1	С	417	ARG
1	С	456	SER
1	C	507	ALA
1	С	744	ASP
1	В	133	LEU
1	В	249	ILE
1	В	379	VAL
1	В	564	GLY
1	В	715	ARG
1	В	786	ILE
1	В	860	ARG
1	С	5	VAL
1	С	411	ALA
1	С	519	GLN
1	С	570	VAL
1	С	736	LYS
1	С	1053	ILE
1	В	706	PHE
1	В	735	ARG
1	С	12	VAL
1	С	153	LEU
1	C	173	LEU
1	С	194	VAL
1	C	$25\overline{2}$	ARG
1	С	337	LEU
1	C	470	ASP
1	С	842	GLY
1	С	54	VAL
1	С	666	ILE
1	В	842	GLY
1	С	83	GLY
1	В	570	VAL



Continued from previous page...

Mol	Chain	Res	Type
1	С	839	GLY
1	В	463	ILE
1	В	835	GLY
1	С	686	VAL
1	В	685	VAL
1	С	142	PRO
1	С	463	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	В	876/925~(95%)	782~(89%)	94 (11%)	6	27	
1	С	863/925~(93%)	773~(90%)	90 (10%)	7	28	
All	All	1739/1850~(94%)	1555~(89%)	184 (11%)	6	27	

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	32	ARG
1	В	34	LEU
1	В	42	LEU
1	В	53	CYS
1	В	56	GLU
1	1 B 57		PRO
1	В	60	ILE
1	В	71	LYS
1	В	77	THR
1	В	92	SER
1	В	120	ARG
1	В	131	GLU
1	В	134	ILE
1	В	140	ARG
1	В	150	MET
1	В	152	ASN



Mol	Chain	Res	Type
1	В	158	ILE
1	В	161	THR
1	В	164	GLN
1	В	204	HIS
1	В	212	TRP
1	В	213	VAL
1	В	224	THR
1	В	234	GLU
1	В	235	LEU
1	В	239	LEU
1	В	252	ARG
1	В	253	ASN
1	В	260	ASN
1	В	264	ILE
1	В	267	LEU
1	В	279	ILE
1	В	296	LYS
1	В	301	ILE
1	В	303	ILE
1	В	309	LYS
1	В	328	HIS
1	В	337	LEU
1	В	354	PHE
1	В	364	LEU
1	В	381	GLU
1	В	384	ARG
1	В	386	LEU
1	В	387	PRO
1	В	391	ARG
1	В	392	HIS
1	В	436	THR
1	В	438	ARG
1	В	440	PHE
1	В	467	LYS
1	В	470	ASP
1	В	472	GLU
1	В	479	VAL
1	В	494	ARG
1	В	518	ARG
1	В	542	MET
1	В	543	GLN
1	В	560	ILE



Mol	Chain	Res	Type
1	В	606	VAL
1	В	612	ARG
1	В	666	ILE
1	В	670	LEU
1	В	672	SER
1	В	691	ASP
1	В	705	ARG
1	В	708	ASN
1	В	724	ILE
1	В	736	LYS
1	В	742	ASP
1	В	745	LEU
1	В	747	LEU
1	В	751	GLU
1	В	756	LEU
1	В	760	LEU
1	В	764	ARG
1	В	767	LEU
1	В	768	ARG
1	В	777	GLU
1	В	791	VAL
1	В	796	GLN
1	В	801	LEU
1	В	811	ARG
1	В	848	ARG
1	В	886	ARG
1	В	895	PHE
1	В	934	ASN
1	В	936	LEU
1	В	938	THR
1	В	943	VAL
1	В	961	ILE
1	В	965	MET
1	В	1027	SER
1	В	1032	ILE
1	В	1050	ILE
1	C	32	ARG
1	С	34	LEU
1	C	39	GLU
1	C	53	CYS
1	С	60	ILE
1	С	71	LYS



Mol	Chain	Res	Type
1	С	77	THR
1	С	120	ARG
1	С	131	GLU
1	С	134	ILE
1	С	140	ARG
1	С	150	MET
1	С	152	ASN
1	С	154	ARG
1	С	161	THR
1	С	164	GLN
1	С	198	LEU
1	С	204	HIS
1	С	212	TRP
1	С	213	VAL
1	С	217	ARG
1	С	224	THR
1	С	232	LYS
1	С	234	GLU
1	С	235	LEU
1	С	249	ILE
1	С	252	ARG
1	С	253	ASN
1	С	260	ASN
1	С	264	ILE
1	С	267	LEU
1	С	295	LEU
1	С	301	ILE
1	С	305	THR
1	С	309	LYS
1	С	320	ILE
1	С	328	HIS
1	С	337	LEU
1	С	354	PHE
1	С	364	LEU
1	С	377	ARG
1	С	381	GLU
1	С	384	ARG
1	С	385	LEU
1	С	386	LEU
1	С	413	ASP
1	С	436	THR
1	С	440	PHE



Mol	Chain	Res	Type
1	С	465	ARG
1	С	533	ASP
1	C	543	GLN
1	C	606	VAL
1	C	691	ASP
1	С	705	ARG
1	С	708	ASN
1	С	709	ARG
1	С	736	LYS
1	С	737	ILE
1	С	742	ASP
1	С	745	LEU
1	С	747	LEU
1	С	750	ASP
1	С	753	GLU
1	С	756	LEU
1	С	760	LEU
1	С	767	LEU
1	С	768	ARG
1	С	774	TYR
1	С	782	ASP
1	С	791	VAL
1	С	796	GLN
1	С	801	LEU
1	С	811	ARG
1	С	823	ARG
1	С	848	ARG
1	С	860	ARG
1	С	873	ARG
1	С	875	GLU
1	С	886	ARG
1	С	895	PHE
1	С	922	ARG
1	С	934	ASN
1	С	936	LEU
1	C	938	THR
1	С	943	VAL
1	С	1012	ARG
1	С	1025	LEU
1	С	1032	ILE
1	С	1039	TYR
1	С	1050	ILE

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	61	GLN
1	В	148	ASN
1	В	152	ASN
1	В	164	GLN
1	В	193	ASN
1	В	253	ASN
1	В	260	ASN
1	В	322	HIS
1	В	431	GLN
1	В	519	GLN
1	В	543	GLN
1	В	566	HIS
1	В	608	ASN
1	В	621	HIS
1	В	708	ASN
1	В	710	ASN
1	В	784	ASN
1	В	804	ASN
1	В	822	GLN
1	В	876	HIS
1	В	934	ASN
1	В	958	GLN
1	В	963	GLN
1	С	61	GLN
1	С	148	ASN
1	С	152	ASN
1	С	164	GLN
1	С	175	HIS
1	С	253	ASN
1	С	260	ASN
1	С	431	GLN
1	С	519	GLN
1	С	543	GLN
1	С	608	ASN
1	С	621	HIS
1	С	708	ASN
1	С	710	ASN
1	С	784	ASN
1	С	793	GLN
1	С	804	ASN
1	С	822	GLN



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Mol	Chain	Res	Type
1	С	876	HIS
1	С	934	ASN
1	С	958	GLN
1	С	963	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol Tuno		Chain Bog		Tink	Bond lengths			Bond angles		
WIOI	туре	Unam	nes	LIUK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	ANP	В	2055	-	29,33,33	2.01	7 (24%)	31,52,52	2.32	10 (32%)
2	ANP	С	2055	-	29,33,33	2.42	9 (31%)	31,52,52	2.25	10 (32%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	В	2055	-	1/1/7/8	3/14/38/38	0/3/3/3
2	ANP	С	2055	-	-	5/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	С	2055	ANP	PB-O3A	7.85	1.69	1.59
2	В	2055	ANP	C2'-C1'	-4.92	1.46	1.53
2	С	2055	ANP	C2'-C1'	-4.50	1.46	1.53
2	В	2055	ANP	PB-O3A	4.34	1.64	1.59
2	В	2055	ANP	PB-O2B	-3.96	1.46	1.56
2	В	2055	ANP	PG-01G	3.75	1.52	1.46
2	С	2055	ANP	PB-O2B	-3.75	1.46	1.56
2	С	2055	ANP	PG-01G	3.65	1.51	1.46
2	С	2055	ANP	C2-N3	3.26	1.37	1.32
2	С	2055	ANP	PB-O1B	3.22	1.51	1.46
2	В	2055	ANP	PG-N3B	2.42	1.69	1.63
2	В	2055	ANP	C2-N3	2.40	1.36	1.32
2	С	2055	ANP	PG-N3B	2.36	1.69	1.63
2	С	2055	ANP	PB-N3B	-2.18	1.57	1.63
2	С	2055	ANP	C2-N1	2.14	1.37	1.33
2	В	2055	ANP	PB-O1B	2.12	1.49	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	2055	ANP	O1B-PB-N3B	-5.55	103.59	111.77
2	В	2055	ANP	O1B-PB-N3B	-5.46	103.73	111.77
2	В	2055	ANP	O1G-PG-N3B	-5.43	103.78	111.77
2	С	2055	ANP	O1G-PG-N3B	-5.36	103.87	111.77
2	В	2055	ANP	C3'-C2'-C1'	5.12	108.69	100.98
2	С	2055	ANP	O4'-C1'-C2'	-4.51	100.34	106.93
2	В	2055	ANP	O4'-C1'-C2'	-4.27	100.68	106.93
2	В	2055	ANP	O3A-PB-N3B	3.88	117.35	106.59
2	С	2055	ANP	O3A-PB-N3B	3.86	117.30	106.59
2	С	2055	ANP	C3'-C2'-C1'	3.54	106.31	100.98
2	С	2055	ANP	PB-O3A-PA	3.00	143.17	132.62
2	В	2055	ANP	PB-O3A-PA	2.89	142.78	132.62
2	В	2055	ANP	N3-C2-N1	-2.54	124.71	128.68
2	С	2055	ANP	N3-C2-N1	-2.49	124.79	128.68
2	С	2055	ANP	O4'-C4'-C3'	-2.28	100.60	105.11
2	С	2055	ANP	O2G-PG-O3G	2.18	113.43	107.64
2	C	2055	ANP	O3'-C3'-C4'	-2.13	104.88	111.05



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	2055	ANP	O3'-C3'-C4'	-2.13	104.88	111.05
2	В	2055	ANP	O2G-PG-O3G	2.12	113.29	107.64
2	В	2055	ANP	O3'-C3'-C2'	-2.07	105.12	111.82

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All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	В	2055	ANP	C2'

All (8) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	2055	ANP	PB-N3B-PG-O1G
2	В	2055	ANP	PA-O3A-PB-O1B
2	С	2055	ANP	PB-N3B-PG-O1G
2	С	2055	ANP	PA-O3A-PB-O1B
2	С	2055	ANP	PA-O3A-PB-O2B
2	С	2055	ANP	C3'-C4'-C5'-O5'
2	В	2055	ANP	PG-N3B-PB-O1B
2	С	2055	ANP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2055	ANP	5	0
2	С	2055	ANP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	С	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	15:GLY	C	16:ASP	N	13.42



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	В	1020/1054~(96%)	-0.31	15 (1%) 73 61	1, 38, 137, 192	0
1	С	1005/1054~(95%)	0.32	79 (7%) 12 6	24, 92, 160, 195	0
All	All	2025/2108~(96%)	0.00	94 (4%) 32 20	1, 68, 153, 195	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	942	ARG	7.8
1	С	140	ARG	6.4
1	С	139	GLY	6.2
1	С	380	ASP	5.5
1	С	907	ASP	5.5
1	С	381	GLU	5.4
1	С	311	ASP	5.2
1	С	940	THR	4.7
1	С	301	ILE	4.6
1	С	364	LEU	4.4
1	С	912	GLU	4.3
1	С	360	ASP	4.2
1	С	404	MET	4.2
1	С	914	GLU	4.2
1	С	359	GLU	4.2
1	С	755	ASP	4.2
1	С	583	ARG	4.1
1	С	204	HIS	3.9
1	С	303	ILE	3.8
1	С	933	LYS	3.8
1	В	742	ASP	3.6
1	С	732	ARG	3.5
1	С	399	ILE	3.5
1	С	743	PHE	3.4



Mol	Chain	Res	Type	RSRZ
1	С	945	ALA	3.4
1	С	953	VAL	3.4
1	С	943	VAL	3.3
1	В	734	ARG	3.3
1	С	398	GLU	3.2
1	С	304	VAL	3.2
1	В	937	PRO	3.2
1	С	138	HIS	3.2
1	С	366	PRO	3.1
1	С	903	SER	3.1
1	С	941	PHE	3.1
1	С	265	SER	3.1
1	В	942	ARG	3.0
1	С	407	GLU	3.0
1	С	929	ALA	3.0
1	С	769	THR	3.0
1	С	899	VAL	2.9
1	С	365	SER	2.9
1	С	418	GLU	2.9
1	С	831	ASP	2.9
1	В	376	TYR	2.9
1	С	212	TRP	2.9
1	С	764	ARG	2.9
1	В	388	ALA	2.8
1	С	385	LEU	2.8
1	С	142	PRO	2.7
1	С	998	PRO	2.7
1	С	136	TYR	2.7
1	С	376	TYR	2.6
1	С	897	VAL	2.6
1	В	144	ARG	2.6
1	С	891	GLN	2.6
1	С	310	GLY	2.4
1	С	309	LYS	2.4
1	С	292	TYR	2.4
1	В	393	ILE	2.4
1	C	931	TRP	2.4
1	В	944	LYS	2.4
1	С	930	VAL	2.4
1	С	750	ASP	2.3
1	В	753	GLU	2.3
1	В	212	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	С	829	LEU	2.3
1	С	286	GLU	2.3
1	В	741	ARG	2.3
1	С	367	GLN	2.3
1	С	149	PHE	2.3
1	С	767	LEU	2.3
1	С	323	LEU	2.2
1	В	739	ILE	2.2
1	С	146	LYS	2.2
1	С	915	ARG	2.2
1	С	756	LEU	2.2
1	В	1054	ASP	2.2
1	С	936	LEU	2.2
1	С	405	GLY	2.2
1	С	921	GLY	2.2
1	С	447	GLY	2.2
1	С	215	GLU	2.1
1	С	384	ARG	2.1
1	С	965	MET	2.1
1	В	760	LEU	2.1
1	С	1011	ARG	2.1
1	С	762	GLU	2.1
1	С	924	TYR	2.1
1	С	793	GLN	2.1
1	С	308	LYS	2.0
1	С	164	GLN	2.0
1	С	410	GLN	2.0
1	С	471	ILE	2.0

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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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	$\mathbf{Q}{<}0.9$
3	MG	С	2056	1/1	0.31	1.04	70,70,70,70	0
3	MG	В	2056	1/1	0.83	0.38	40,40,40,40	0
2	ANP	С	2055	31/31	0.88	0.23	$38,\!57,\!75,\!77$	0
2	ANP	В	2055	31/31	0.95	0.20	$24,\!34,\!69,\!77$	0

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.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

