

Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 01:12 am BST

PDB ID	:	2J7N
Title	:	Structure of the RNAi polymerase from Neurospora crassa
Authors	:	Salgado, P.S.; Koivunen, M.R.L.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.;
		Grimes, J.M.
Deposited on	:	2006-10-13
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain				
1	А	1022	62%	23%	6% • 9%		
1	В	1022	19%	24%	8% • 9%		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15945 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 RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	935	Total 7520	C 4814	N 1304	O 1368	S 34	0	0	1
1	В	932	Total 7498	C 4798	N 1300	O 1366	S 34	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	559	ALA	GLY	conflict	UNP Q9Y7G6
В	559	ALA	GLY	conflict	UNP Q9Y7G6

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mg 1 1	0	0
2	В	1	Total Mg 1 1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	В	1	Total 5	${ m C} { m 3}$	O 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	499	Total O 499 499	0	0
4	В	421	Total O 421 421	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: RNA-DEPENDENT RNA POLYMERASE





PR0 GUU VAL TTR ASP OLU VAL LEU VAL LEU CLY ASP PHE ASP PHE CLY TTR ASP TTR A TTR AS



19%			
Chain B:	57%	24%	8% • 9%
GLU SER ALA ALA ARG SER CLN VAL H390 CLN VAL H391 P392 V393 V393 V393 V395 A395	R397 R398 R399 R400 N400 P403 P405 P405 P405 F405 R404 R403 R410 A412 A413	1414 1417 1418 1418 1420 1420 1422 1423 1425 1426 1426 1426	K428 K429 D430 D430 L631 L631 D433 B634 B435 C437 C437 K439 K439 Y440
P442 P443 P443 P444 P446 P446 P449 P449 P449 P449 P449	1458 1459 1460 1460 1461 1460 1461 1465 1465 1465 1465 1465 1465 1465	144 /5 144 /5 144 77 144 78 144 84 148 26 148 26 16	4491 14492 14493 1494 1498 1498 1498 1498 1498 1498 1498
P506 T507 A503 P503 L511 L512 L512 P517 P517 P517 P517 P517 P517 P517 T526	R528 F530 F530 F530 653 1530 1533 1533 1545 F541 F544 F544 F544 F544 F544	P551 P553 V553 V554 V555 R555 Q557 Q555 A559 A560 A560 E53 V54	1565 9566 9566 1570 1570 1570 1581 1581 1585 15887 8585
C C C C C C C C C C C C C C C C C C C	LYS PRO 1607 1607 1601 1615 1615 1615 1620 1620 1620 1621 1621 1621 1622 1622	PHES PHES LYBE LYBE ARG SER SER PRO GLU CLU PRO CLU	VAL GLU G641 T643 T643 T643 M650 M650 R671 B73 R671 G673
L674 K678 K678 K679 F679 F679 F679 C711 C711 C7114 K713 M714 S715 S715 M715 M717	A719 K720 R721 1722 1723 P724 V725 D730 Q736 Q736 Q736 Q736 Q736 Q736 Q736 Q736	W7 46 D755 D755 D755 C69 E769 E769 V773 D774 M775	H176 H176 R177 R177 R177 R179 R179 R179 R179 R179
1821 1821 1824 1826 1826 8826 8826 8826 8826 8826 8826	K838 K838 K838 K841 K841 K842 K862 K862 <t< td=""><td>8870 885 885 885 885 885 885 885 885 885 88</td><td>1905 1906 1906 1907 1911 1912 1913 1923 1923 1923 1923 1923</td></t<>	8870 885 885 885 885 885 885 885 885 885 88	1905 1906 1906 1907 1911 1912 1913 1923 1923 1923 1923 1923
9338 8941 8945 8946 8946 8946 8948 8948 8948 8948 8948	L969 1966 1966 1966 1988 1988 1990 1990 1990 1990	ULULI V 1015 C1016 P1019 P1019 D1035 D1035 L1036 S1037 S1037	R1038 11040 K1041 K1042 K1042 K1048 S1058 91063 11065 T1065 Y1066
D1067 M1068 K1071 F1073 F1075 F1075 F1077 F1077 P1077 P1077 P1077 P1077 P1077 P1078 P10778 P1077	E1090 R102 K1102 L1107 V1110 V1111 V1115 V1115 V1115 V1115 V1115 V1115 V1115 V1115 V1115 V11120	11122 11122 11122 11122 11132 11133 11134 11135 11135 11135	C1138 C1138 A1140 L1141 L1141 S1142 M1147 M1148 K1148 S1150 D1151 S1152 W1153
L1164 G1155 G1156 G1156 G1156 E1158 P1163 P1163 P1163 P1164 P1166 L1166 L1166 L1166 L1166 A1171	R1172 P1173 P1173 P1176 P1176 P1176 P1176 F1176 F1180 F1182 F1182 F1182 A1186 A1186 A1186 A1186 A1186 A1186 A1186 A1186	M1169 M1190 D1191 E1192 E1195 D1195 A1196 A1196 A1196 D1196 P1200 D1200	A1204 81205 71207 71207 71207 81213 81214 81215 81215 81215 81216 81216 81218 81218 81218
81220 A1221 L1223 F1224 F1224 K1228 K1228 R1230 F1231 G1233 F1231 G1233 F1233 F1233 F1233 F1233 F1233	R1240 LEU V.A.C. LEU V.A.C. LYS ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	M1265 W1265 012 012 012 012 012 012 012 012 012 012	ALA ASN TYR ASP ASP S2282 K1284 T1285 E1289 R1296 N1299
11300 11301 11303 11303 11303 11303 11303 11303 11303 11315 11315 11315 11315 11315	G1326 B1327 Q1328 C1329 X1333 X1333 X1333 F1357 F1357 F1357 F1351 F1351 A1354 A1354	L1356 L1356 K1360 L1363 L1370 L1370 G1372 D1373	CLY SER CLU CLU FRO FRO FRO FRO FRO FRO FRO FRO FRO FRO



ASP ASP PHE ASP CLY CLY CLY CLY CLY CLY PHE CLY CLY ASN CLY ASN ASP TYR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	101.02Å 122.55Å 114.70Å	Depositor
a, b, c, α , β , γ	90.00° 108.90° 90.00°	Depositor
Bosolution(Å)	19.98 - 2.30	Depositor
Resolution (A)	19.97 - 2.30	EDS
% Data completeness	97.7 (19.98-2.30)	Depositor
(in resolution range)	97.7 (19.97-2.30)	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.46 (at 2.30 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
P. P.	0.217 , 0.264	Depositor
n, n_{free}	0.218 , 0.216	DCC
R_{free} test set	5728 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	45.5	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 52.0	EDS
L-test for $twinning^2$	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15945	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 27.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1432e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bo	ond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.89	10/7713~(0.1%)	0.76	10/10439~(0.1%)	
1	В	0.61	12/7689~(0.2%)	0.73	8/10407~(0.1%)	
All	All	0.77	22/15402~(0.1%)	0.74	18/20846~(0.1%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	16
1	В	0	16
All	All	0	32

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	434	GLU	CD-OE2	50.04	1.80	1.25
1	А	434	GLU	CD-OE1	25.38	1.53	1.25
1	А	432	GLU	CD-OE1	16.68	1.44	1.25
1	А	436	LEU	C-N	16.11	1.62	1.33
1	В	435	SER	CB-OG	-13.76	1.24	1.42
1	В	436	LEU	C-N	11.41	1.53	1.33
1	А	434	GLU	C-O	10.18	1.42	1.23
1	В	432	GLU	CD-OE1	10.04	1.36	1.25
1	В	411	GLU	CD-OE2	9.22	1.35	1.25
1	А	434	GLU	CG-CD	7.65	1.63	1.51
1	А	1257	ARG	CZ-NH1	7.48	1.42	1.33
1	В	434	GLU	C-N	6.85	1.49	1.34
1	B	434	GLU	C-O	6.59	1.35	1.23
1	А	436	LEU	C-O	6.49	1.35	1.23



2J7N

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	В	1219	SER	CB-OG	6.37	1.50	1.42
1	А	435	SER	CA-CB	-6.22	1.43	1.52
1	В	440	TYR	CG-CD1	6.07	1.47	1.39
1	В	405	PHE	CG-CD2	5.69	1.47	1.38
1	А	435	SER	CB-OG	-5.41	1.35	1.42
1	В	436	LEU	C-O	5.39	1.33	1.23
1	В	440	TYR	CE1-CZ	5.32	1.45	1.38
1	В	405	PHE	CE1-CZ	5.00	1.46	1.37

Continued from previous page...

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	434	GLU	OE1-CD-OE2	13.01	138.91	123.30
1	А	436	LEU	O-C-N	7.02	135.13	123.20
1	А	952	LEU	CA-CB-CG	6.91	131.20	115.30
1	А	1316	LYS	N-CA-C	-6.56	93.28	111.00
1	А	1283	LYS	N-CA-C	-6.52	93.40	111.00
1	А	432	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	В	398	LEU	CA-CB-CG	6.26	129.69	115.30
1	В	433	ASP	CB-CG-OD1	6.24	123.92	118.30
1	А	436	LEU	CA-C-N	-6.06	104.09	116.20
1	В	1139	GLY	N-CA-C	-5.88	98.41	113.10
1	В	1154	LEU	CA-CB-CG	5.67	128.33	115.30
1	В	839	VAL	CB-CA-C	-5.65	100.66	111.40
1	В	962	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	А	798	LEU	CA-CB-CG	5.53	128.01	115.30
1	В	433	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	В	952	LEU	CA-CB-CG	5.30	127.49	115.30
1	А	560	ALA	N-CA-C	5.21	125.06	111.00
1	А	459	ARG	N-CA-C	5.07	124.68	111.00

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1138	GLY	Peptide
1	А	1139	GLY	Peptide
1	А	1213	ILE	Peptide
1	А	1217	SER	Peptide
1	А	1220	SER	Peptide
1	А	1252	ASP	Peptide
1	А	1282	SER	Peptide



2J	7	Ν	

Mol	Chain	Res	Type	Group
1	А	1315	HIS	Peptide
1	А	456	THR	Peptide
1	А	504	ASN	Peptide
1	А	506	PRO	Peptide
1	А	545	SER	Peptide
1	А	547	SER	Peptide
1	А	555	SER	Peptide
1	А	559	ALA	Peptide
1	А	624	PRO	Peptide
1	В	1137	LEU	Peptide
1	В	1138	GLY	Peptide
1	В	1139	GLY	Peptide
1	В	1154	LEU	Peptide
1	В	1218	ARG	Peptide
1	В	1252	ASP	Peptide
1	В	1282	SER	Peptide
1	В	436	LEU	Mainchain
1	В	487	SER	Peptide
1	В	506	PRO	Peptide
1	В	545	SER	Peptide
1	В	547	SER	Peptide
1	В	552	PRO	Peptide
1	В	555	SER	Peptide
1	В	559	ALA	Peptide
1	В	641	GLN	Peptide

Continued from previous page...

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	7520	0	7468	365	1
1	В	7498	0	7440	401	1
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	В	5	0	5	1	0
4	А	499	0	0	20	2
4	В	421	0	0	22	2
All	All	15945	0	14913	757	3



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 25.

All (757) 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:431:LEU:CB	1:B:432:GLU:HB2	1.34	1.51
1:B:407:LYS:CB	1:B:408:TRP:HB3	1.41	1.51
1:A:641:GLN:CB	1:A:642:ARG:HB2	1.50	1.41
1:B:407:LYS:HB2	1:B:408:TRP:CB	1.47	1.41
1:B:431:LEU:HB3	1:B:432:GLU:CB	1.48	1.40
1:A:1184:ASN:N	1:A:1185:ALA:HB3	1.49	1.25
1:A:1193:GLU:HA	1:A:1194:ASP:O	1.37	1.25
1:B:462:ALA:HB3	1:B:463:PHE:O	1.29	1.24
1:A:399:ARG:CB	1:A:400:ASN:HB3	1.69	1.21
1:A:434:GLU:OE2	1:A:434:GLU:CD	1.80	1.19
1:A:1315:HIS:HB2	1:A:1316:LYS:CB	1.72	1.18
1:A:438:LEU:HA	1:A:439:LYS:CB	1.71	1.17
1:A:438:LEU:HA	1:A:439:LYS:HB3	1.18	1.15
1:A:465:GLY:HA2	1:A:466:LYS:HB2	1.29	1.15
1:B:418:TRP:CB	1:B:419:GLU:HB2	1.76	1.15
1:A:399:ARG:HD2	1:A:507:THR:HG22	1.23	1.14
1:A:641:GLN:HB2	1:A:642:ARG:CB	1.77	1.14
1:B:505:SER:CB	1:B:506:PRO:HD3	1.75	1.14
1:A:503:ASP:O	1:A:504:ASN:HB2	1.38	1.14
1:A:1210:PHE:O	1:A:1214:SER:HB2	1.47	1.14
1:A:393:VAL:HG23	1:A:394:VAL:HG23	1.14	1.13
1:B:461:ASP:N	1:B:462:ALA:HA	1.63	1.12
1:B:879:MET:HE3	1:B:885:PRO:HG3	1.25	1.12
1:A:439:LYS:HG3	1:A:440:TYR:H	1.06	1.11
1:A:1186:MET:H	1:A:1187:LYS:HB3	1.01	1.10
1:B:505:SER:HB2	1:B:506:PRO:CD	1.81	1.10
1:A:1315:HIS:CB	1:A:1316:LYS:HB2	1.81	1.10
1:B:459:ARG:N	1:B:460:LEU:HB2	1.67	1.10
1:A:723:ARG:HH11	1:A:723:ARG:HG2	0.99	1.07
1:A:439:LYS:HG3	1:A:440:TYR:N	1.65	1.07
1:A:1184:ASN:H	1:A:1185:ALA:CB	1.68	1.07
1:B:505:SER:HB3	1:B:506:PRO:HD3	1.32	1.06
1:A:412:ALA:HB1	1:A:413:PRO:HA	1.37	1.06
1:B:403:PRO:HA	1:B:404:LYS:HB2	1.28	1.06
1:A:438:LEU:CA	1:A:439:LYS:HB3	1.86	1.05
1:B:723:ARG:HH11	1:B:723:ARG:CG	1.70	1.05
1:B:829:SER:HA	1:B:832:LYS:HE3	1.05	1.04



	A l O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:418:TRP:HB3	1:B:419:GLU:HB2	1.04	1.04
1:A:1194:ASP:HB2	1:A:1195:GLY:HA2	1.36	1.02
1:B:1137:LEU:HB3	1:B:1138:GLY:HA3	1.37	1.02
1:B:545:SER:HA	1:B:546:THR:HG22	1.41	1.01
1:A:457:LEU:HB3	1:A:458:TYR:CB	1.90	1.01
1:B:505:SER:CB	1:B:506:PRO:CD	2.34	1.01
1:B:403:PRO:HA	1:B:404:LYS:CB	1.90	1.01
1:B:433:ASP:HB2	1:B:434:GLU:HB3	1.40	1.01
1:A:412:ALA:HB1	1:A:413:PRO:CA	1.90	1.00
1:B:450:VAL:H	1:B:451:THR:HB	1.27	0.99
1:B:723:ARG:HG2	1:B:723:ARG:NH1	1.65	0.99
1:A:399:ARG:HB3	1:A:400:ASN:CB	1.91	0.99
1:A:412:ALA:CB	1:A:413:PRO:HA	1.92	0.99
1:B:723:ARG:HH11	1:B:723:ARG:HG2	0.82	0.98
1:B:1188:ALA:N	1:B:1189:ALA:HB2	1.78	0.98
1:B:879:MET:HE3	1:B:885:PRO:CG	1.93	0.97
1:B:397:ARG:CG	1:B:397:ARG:HH21	1.77	0.96
1:B:460:LEU:N	1:B:461:ASP:HA	1.77	0.96
1:B:829:SER:CA	1:B:832:LYS:HE3	1.96	0.96
1:A:1220:SER:N	1:A:1221:ALA:HB3	1.80	0.96
1:A:399:ARG:HB3	1:A:400:ASN:HB3	0.96	0.96
1:A:624:PRO:HA	1:A:625:ASP:HB2	1.45	0.95
1:A:723:ARG:HG2	1:A:723:ARG:NH1	1.77	0.95
1:B:397:ARG:HH21	1:B:397:ARG:HG2	1.28	0.95
1:A:399:ARG:HE	1:A:399:ARG:HA	1.29	0.95
1:A:457:LEU:HB3	1:A:458:TYR:HB3	1.48	0.95
1:A:1186:MET:N	1:A:1187:LYS:HB3	1.83	0.94
1:B:451:THR:HB	1:B:452:ASP:HB2	1.49	0.94
1:A:1217:SER:CB	1:A:1221:ALA:HB2	1.97	0.94
1:B:452:ASP:O	1:B:454:TRP:N	2.00	0.94
1:A:1193:GLU:CA	1:A:1194:ASP:O	2.14	0.94
1:B:462:ALA:CB	1:B:463:PHE:O	2.15	0.93
1:B:418:TRP:HB3	1:B:419:GLU:CB	1.97	0.92
1:A:1194:ASP:CB	1:A:1195:GLY:HA2	1.98	0.92
1:B:403:PRO:CA	1:B:404:LYS:HB2	1.99	0.92
1:A:439:LYS:CG	1:A:440:TYR:N	2.33	0.91
1:A:1217:SER:OG	1:A:1221:ALA:HB2	1.70	0.91
1:B:1232:GLY:O	1:B:1236:LYS:HG3	1.72	0.90
1:A:1210:PHE:O	1:A:1214:SER:CB	2.21	0.89
1:A:395:ALA:HB1	1:A:396:ALA:HA	1.52	0.89
1:A:456:THR:HG22	1:A:457:LEU:HA	1.53	0.89



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:450:VAL:O	1:B:453:ILE:HB	1.73	0.88
1:A:393:VAL:H	1:A:394:VAL:C	1.77	0.88
1:A:399:ARG:CB	1:A:400:ASN:CB	2.48	0.87
1:A:838:PRO:HA	1:A:879:MET:HE1	1.55	0.87
1:A:1194:ASP:HB2	1:A:1195:GLY:CA	2.04	0.87
1:A:466:LYS:H	1:A:467:PRO:HA	1.39	0.87
1:B:1139:GLY:O	4:B:2339:HOH:O	1.90	0.87
1:A:1140:ALA:O	1:A:1141:LEU:O	1.94	0.86
1:B:451:THR:H	1:B:452:ASP:C	1.80	0.85
1:A:468:PHE:HA	1:A:469:PRO:O	1.76	0.85
1:A:559:ALA:CB	1:A:562:GLU:OE1	2.23	0.85
1:B:576:VAL:HG12	1:B:576:VAL:O	1.75	0.85
1:A:641:GLN:CB	1:A:642:ARG:CB	2.45	0.85
1:B:1112:GLY:O	1:B:1115:VAL:HG22	1.77	0.85
1:B:450:VAL:H	1:B:451:THR:CB	1.90	0.84
1:A:641:GLN:HB2	1:A:642:ARG:HB2	0.85	0.84
1:A:922:MET:HE1	1:A:1011:ASP:HB3	1.59	0.84
1:B:1137:LEU:HB3	1:B:1138:GLY:CA	2.08	0.84
1:A:879:MET:HE3	1:A:885:PRO:HG3	1.60	0.84
1:B:431:LEU:CB	1:B:432:GLU:CB	2.25	0.84
1:A:1217:SER:HB3	1:A:1221:ALA:HB2	1.59	0.84
1:A:723:ARG:HH11	1:A:723:ARG:CG	1.86	0.83
1:A:417:ALA:HB1	1:A:576:VAL:HG13	1.61	0.83
1:A:559:ALA:HB1	1:A:562:GLU:OE1	1.78	0.83
1:B:1134:ARG:O	4:B:2333:HOH:O	1.96	0.83
1:A:454:TRP:O	1:A:458:TYR:HB3	1.77	0.83
1:B:460:LEU:H	1:B:461:ASP:CA	1.92	0.83
1:A:457:LEU:HB3	1:A:458:TYR:HB2	1.60	0.83
1:B:463:PHE:HA	1:B:464:ARG:C	2.00	0.82
1:B:1041:LYS:O	1:B:1123:VAL:HG12	1.80	0.82
1:B:461:ASP:H	1:B:462:ALA:HA	1.43	0.81
1:A:423:LEU:HD11	1:A:458:TYR:CE1	2.16	0.81
1:A:438:LEU:CA	1:A:439:LYS:CB	2.52	0.81
1:B:418:TRP:CA	1:B:419:GLU:HB2	2.11	0.80
1:B:456:THR:N	1:B:457:LEU:O	2.14	0.80
1:A:1315:HIS:HB2	1:A:1316:LYS:HB2	0.85	0.80
1:B:460:LEU:N	1:B:461:ASP:CA	2.43	0.80
1:A:450:VAL:HG11	1:A:472:PRO:HD2	1.64	0.80
1:B:1218:ARG:N	1:B:1219:SER:HB3	1.95	0.80
1:B:1131:GLN:O	1:B:1135:GLU:HG3	1.82	0.80
1:B:829:SER:HA	1:B:832:LYS:CE	2.00	0.80



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:942:LYS:HD2	1:B:949:SER:OG	1.82	0.79
1:B:429:VAL:O	1:B:430:ASP:HB2	1.81	0.79
1:A:1186:MET:H	1:A:1187:LYS:CB	1.90	0.78
1:B:419:GLU:H	1:B:422:ARG:HB2	1.48	0.78
1:B:433:ASP:HA	1:B:434:GLU:HB2	1.64	0.78
1:B:460:LEU:HB3	1:B:462:ALA:HB2	1.64	0.78
1:B:1217:SER:HB3	1:B:1221:ALA:HB2	1.65	0.78
1:B:409:LEU:HD12	1:B:409:LEU:H	1.49	0.78
1:A:503:ASP:O	1:A:504:ASN:CB	2.25	0.78
1:B:460:LEU:H	1:B:461:ASP:HB3	1.49	0.78
1:A:1029:GLU:HB3	4:A:2359:HOH:O	1.82	0.78
1:B:407:LYS:CA	1:B:408:TRP:HB3	2.14	0.78
1:B:505:SER:HB2	1:B:506:PRO:HD2	1.62	0.77
1:A:453:ILE:O	1:A:454:TRP:HD1	1.66	0.77
1:A:828:PHE:CD1	1:A:1178:GLU:HG2	2.19	0.77
1:B:1137:LEU:CB	1:B:1138:GLY:HA3	2.14	0.77
1:A:393:VAL:HG23	1:A:394:VAL:CG2	2.07	0.77
1:A:412:ALA:HB2	4:A:2004:HOH:O	1.83	0.77
1:B:667:LYS:HE2	4:B:2033:HOH:O	1.85	0.77
1:A:1112:GLY:O	1:A:1115:VAL:HG22	1.84	0.77
1:B:431:LEU:HB2	1:B:432:GLU:HB2	1.61	0.77
1:B:459:ARG:CA	1:B:460:LEU:HB2	2.15	0.76
1:A:399:ARG:HB2	1:A:400:ASN:O	1.86	0.76
1:A:438:LEU:HA	1:A:439:LYS:HB2	1.66	0.76
1:B:390:HIS:CD2	1:B:566:GLN:HE22	2.02	0.76
1:B:714:MET:HE2	1:B:718:VAL:HG12	1.68	0.75
1:A:457:LEU:HD12	1:A:457:LEU:O	1.85	0.75
1:B:1269:THR:HG23	1:B:1270:PRO:HD2	1.67	0.75
1:A:829:SER:HA	1:A:832:LYS:HE3	1.68	0.75
1:B:836:ASN:HA	1:B:886:LYS:HD2	1.69	0.75
1:A:488:LYS:HG3	1:B:1373:ASP:N	2.01	0.75
1:A:796:LEU:HA	1:A:799:LEU:HD12	1.68	0.75
1:B:400:ASN:O	1:B:402:TRP:N	2.20	0.75
1:B:867:LEU:HD13	1:B:1326:GLY:HA3	1.66	0.75
1:A:576:VAL:O	1:A:576:VAL:HG12	1.86	0.75
1:A:423:LEU:HD21	1:A:458:TYR:HD1	1.52	0.74
1:B:879:MET:HE3	1:B:885:PRO:CD	2.17	0.74
1:B:433:ASP:HB2	1:B:434:GLU:CB	2.17	0.74
1:B:460:LEU:H	1:B:461:ASP:CB	2.00	0.74
1:B:723:ARG:HD3	1:B:730:ASP:C	2.08	0.74
1:B:801:VAL:HG23	4:B:2130:HOH:O	1.88	0.74



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:400:ASN:CG	1:B:401:ILE:N	2.40	0.74
1:B:879:MET:CE	1:B:885:PRO:CD	2.66	0.74
1:B:879:MET:CE	1:B:885:PRO:HD3	2.18	0.73
1:A:408:TRP:HZ3	1:A:431:LEU:O	1.71	0.73
1:A:1315:HIS:ND1	4:A:2470:HOH:O	2.21	0.73
1:B:456:THR:H	1:B:457:LEU:CB	2.00	0.73
1:A:393:VAL:CG2	1:A:394:VAL:HG23	2.08	0.73
1:B:1270:PRO:HG2	1:B:1289:GLU:HG3	1.69	0.73
1:A:1214:SER:HA	1:A:1217:SER:OG	1.89	0.72
1:A:879:MET:HE3	1:A:885:PRO:CG	2.20	0.72
1:B:1188:ALA:HB3	1:B:1189:ALA:HA	1.70	0.72
1:B:433:ASP:CB	1:B:434:GLU:HB3	2.18	0.72
1:A:465:GLY:CA	1:A:466:LYS:HB2	2.16	0.72
1:A:470:GLU:O	1:A:471:LYS:HB3	1.89	0.72
1:B:431:LEU:HB3	1:B:432:GLU:CA	2.19	0.72
1:A:705:GLU:OE2	1:A:1001:LYS:NZ	2.15	0.72
1:B:451:THR:CB	1:B:452:ASP:HB2	2.20	0.72
1:A:826:ARG:NH1	1:A:913:ARG:HH22	1.88	0.72
1:B:391:ALA:HB3	1:B:563:GLU:HG3	1.70	0.72
1:A:457:LEU:H	1:A:459:ARG:HB2	1.55	0.71
1:B:449:ASP:HB3	1:B:451:THR:HB	1.72	0.71
1:B:450:VAL:N	1:B:451:THR:CB	2.53	0.71
1:B:1139:GLY:HA3	1:B:1141:LEU:HB3	1.71	0.71
1:A:1253:PRO:HD2	1:A:1256:VAL:HB	1.72	0.71
1:A:457:LEU:N	1:A:459:ARG:HB2	2.06	0.71
1:B:398:LEU:HD13	1:B:510:LEU:HD23	1.71	0.70
1:A:879:MET:HE3	1:A:885:PRO:CD	2.22	0.70
1:B:435:SER:HB2	1:B:436:LEU:HB2	1.72	0.70
1:B:774:ASP:HB3	1:B:777:GLN:HG2	1.73	0.70
1:A:1184:ASN:N	1:A:1185:ALA:CB	2.41	0.70
1:B:576:VAL:O	1:B:576:VAL:CG1	2.40	0.70
1:B:626:VAL:O	1:B:626:VAL:HG13	1.91	0.70
1:B:842:ARG:HD2	4:B:2168:HOH:O	1.92	0.70
1:B:1269:THR:CG2	4:B:2377:HOH:O	2.39	0.70
1:B:1315:HIS:O	4:B:2386:HOH:O	2.09	0.70
1:A:465:GLY:HA2	1:A:466:LYS:CB	2.15	0.70
1:A:879:MET:CE	1:A:885:PRO:HD3	2.22	0.70
1:A:641:GLN:CA	1:A:642:ARG:HB2	2.21	0.69
1:A:395:ALA:HB1	1:A:396:ALA:CA	2.23	0.69
1:B:397:ARG:HG2	1:B:397:ARG:NH2	1.99	0.69
1:A:459:ARG:O	1:A:461:ASP:N	2.23	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:466:LYS:N	1:A:467:PRO:HA	2.06	0.69
1:A:1184:ASN:CA	1:A:1185:ALA:HB3	2.22	0.69
1:A:1344:ALA:HB1	1:B:1327:ARG:HD3	1.75	0.69
1:B:433:ASP:HA	1:B:434:GLU:CB	2.21	0.69
1:B:456:THR:H	1:B:457:LEU:HB2	1.57	0.69
1:A:1219:SER:C	1:A:1221:ALA:HB3	2.13	0.69
1:B:459:ARG:HB2	1:B:460:LEU:HD23	1.75	0.69
1:B:1337:THR:HG22	4:B:2395:HOH:O	1.93	0.69
1:B:491:ALA:HB1	1:B:532:PRO:HB3	1.75	0.68
1:A:408:TRP:CZ3	1:A:431:LEU:O	2.45	0.68
1:B:433:ASP:CA	1:B:434:GLU:CB	2.72	0.68
1:B:1304:LEU:O	1:B:1308:THR:CG2	2.41	0.68
1:B:461:ASP:N	1:B:462:ALA:CA	2.51	0.68
1:B:406:PRO:HB3	1:B:408:TRP:NE1	2.09	0.68
1:A:498:LEU:HD22	1:A:513:VAL:HG22	1.75	0.67
1:B:462:ALA:HB3	1:B:463:PHE:C	2.14	0.67
1:A:391:ALA:HB3	1:A:392:PRO:HA	1.75	0.67
1:B:546:THR:HG23	1:B:546:THR:O	1.94	0.67
1:A:412:ALA:HB1	1:A:413:PRO:C	2.14	0.67
1:B:424:PHE:HA	1:B:428:LYS:O	1.95	0.67
1:B:843:GLN:HG3	1:B:1363:THR:HG21	1.77	0.67
1:A:399:ARG:HB2	1:A:400:ASN:CB	2.23	0.67
1:B:1188:ALA:H	1:B:1189:ALA:HB2	1.59	0.67
1:B:1304:LEU:O	1:B:1308:THR:HG22	1.95	0.67
1:A:412:ALA:CB	1:A:413:PRO:CA	2.55	0.67
1:B:555:SER:HA	1:B:557:GLN:H	1.60	0.67
1:B:838:PRO:HA	1:B:879:MET:HE1	1.76	0.67
1:A:456:THR:O	1:A:459:ARG:HD2	1.95	0.67
1:A:397:ARG:O	1:A:398:LEU:HB2	1.93	0.66
1:B:547:SER:OG	1:B:548:PRO:HD3	1.95	0.66
1:A:453:ILE:O	1:A:454:TRP:CD1	2.48	0.66
1:A:828:PHE:CG	1:A:1178:GLU:HG2	2.29	0.66
1:B:403:PRO:HA	1:B:404:LYS:CG	2.25	0.66
1:B:456:THR:N	1:B:457:LEU:HB2	2.11	0.66
1:B:1159:PRO:HB3	1:B:1164:ASP:HB3	1.76	0.66
1:B:1217:SER:HB2	1:B:1218:ARG:C	2.16	0.66
1:B:505:SER:HB2	1:B:506:PRO:HD3	1.55	0.66
1:A:1217:SER:OG	1:A:1221:ALA:CB	2.44	0.66
1:B:408:TRP:HE3	1:B:408:TRP:O	1.78	0.66
1:B:509:PRO:O	1:B:510:LEU:HB3	1.96	0.66
1:A:1044:LYS:HD2	4:A:2207:HOH:O	1.96	0.65



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:399:ARG:NH2	4:A:2002:HOH:O	2.29	0.65
1:B:402:TRP:HB3	1:B:575:LEU:HD23	1.78	0.65
1:B:667:LYS:CE	4:B:2033:HOH:O	2.40	0.65
1:A:560:ALA:HB1	1:A:563:GLU:HB3	1.78	0.65
1:B:400:ASN:CG	1:B:401:ILE:H	1.98	0.65
1:A:418:TRP:CD1	1:A:518:LEU:HD13	2.32	0.65
1:A:836:ASN:OD1	1:A:886:LYS:HE3	1.96	0.65
1:B:462:ALA:H	1:B:463:PHE:C	1.99	0.65
1:B:450:VAL:HG12	1:B:451:THR:OG1	1.97	0.65
1:A:399:ARG:HD2	1:A:507:THR:CG2	2.13	0.65
1:B:429:VAL:HG21	1:B:463:PHE:CZ	2.32	0.65
1:B:443:SER:H	1:B:445:SER:N	1.95	0.65
1:B:406:PRO:HB3	1:B:408:TRP:CD1	2.32	0.65
1:B:879:MET:HE2	1:B:885:PRO:HD3	1.78	0.65
1:A:942:LYS:HG3	1:A:949:SER:OG	1.97	0.64
1:B:625:ASP:HB3	1:B:643:THR:CG2	2.27	0.64
1:A:796:LEU:HD12	1:A:797:GLN:N	2.12	0.64
1:B:461:ASP:O	1:B:464:ARG:HG3	1.97	0.64
1:A:1220:SER:N	1:A:1221:ALA:CB	2.58	0.64
1:B:429:VAL:O	1:B:430:ASP:CB	2.44	0.64
1:B:429:VAL:CG2	1:B:463:PHE:CZ	2.81	0.64
1:A:550:VAL:HG22	4:A:2058:HOH:O	1.96	0.63
1:B:394:VAL:HG21	1:B:560:ALA:HB1	1.80	0.63
1:B:444:TRP:H	1:B:453:ILE:HG13	1.63	0.63
1:B:405:PHE:CE2	1:B:409:LEU:HD13	2.33	0.63
1:B:450:VAL:N	1:B:451:THR:OG1	2.31	0.63
1:A:1180:GLU:OE1	1:A:1180:GLU:HA	1.99	0.63
1:A:605:LYS:HD2	1:A:605:LYS:H	1.63	0.62
1:B:1041:LYS:HB2	1:B:1123:VAL:HG13	1.80	0.62
1:A:423:LEU:HD11	1:A:458:TYR:HE1	1.63	0.62
1:A:565:ILE:HD13	1:A:1074:HIS:HA	1.81	0.62
1:B:836:ASN:OD1	1:B:886:LYS:HE3	1.98	0.62
1:A:1216:LYS:HE3	1:A:1216:LYS:HA	1.81	0.62
1:B:1203:LEU:O	1:B:1307:SER:HB2	2.00	0.62
1:A:626:VAL:N	1:A:627:PHE:HA	2.15	0.61
1:B:393:VAL:HG22	1:B:394:VAL:H	1.64	0.61
1:B:431:LEU:CA	1:B:432:GLU:HB2	2.27	0.61
1:B:431:LEU:CA	1:B:432:GLU:CB	2.79	0.61
1:B:516:LYS:HD3	1:B:517:PRO:HD2	1.83	0.61
1:A:1202:ASP:O	1:A:1205:SER:HB2	2.00	0.61
1:B:418:TRP:CD1	1:B:518:LEU:HD13	2.35	0.61



A + 1	A 4 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:390:HIS:CE1	1:A:566:GLN:HE22	2.18	0.61
1:A:879:MET:HE3	1:A:885:PRO:HD3	1.82	0.61
1:A:624:PRO:CA	1:A:625:ASP:HB2	2.27	0.61
1:A:408:TRP:CH2	1:A:438:LEU:HD13	2.36	0.60
1:A:457:LEU:O	1:A:460:LEU:HB2	2.01	0.60
1:B:460:LEU:HD12	1:B:462:ALA:HB1	1.82	0.60
1:A:412:ALA:HB3	1:A:413:PRO:HA	1.82	0.60
1:B:941:SER:HB2	4:B:2225:HOH:O	2.01	0.60
1:A:1207:TYR:CD2	1:A:1311:LYS:HG3	2.36	0.60
1:A:1300:THR:HA	1:A:1303:LEU:HD23	1.83	0.60
1:A:797:GLN:O	1:A:797:GLN:HG3	1.97	0.60
1:A:423:LEU:HD21	1:A:458:TYR:CD1	2.35	0.60
1:A:509:PRO:O	1:A:510:LEU:HB3	2.01	0.60
1:B:503:ASP:O	1:B:504:ASN:ND2	2.29	0.60
1:B:916:ARG:HH21	1:B:1019:PRO:CD	2.15	0.60
1:A:1186:MET:HB2	1:A:1187:LYS:HB2	1.82	0.60
1:B:393:VAL:O	1:B:394:VAL:HB	2.02	0.60
1:A:820:LEU:HD11	1:A:906:LEU:HD21	1.83	0.60
1:A:1184:ASN:CA	1:A:1185:ALA:CB	2.79	0.60
1:B:641:GLN:HB3	1:B:642:ARG:HG2	1.84	0.60
1:B:1207:TYR:HD1	1:B:1308:THR:HB	1.66	0.60
1:A:460:LEU:O	1:A:461:ASP:CB	2.49	0.60
1:A:922:MET:HE1	1:A:1011:ASP:CB	2.31	0.60
1:A:399:ARG:HA	1:A:399:ARG:NE	2.11	0.59
1:A:884:ASP:HB3	1:A:887:LYS:HB2	1.84	0.59
1:B:459:ARG:H	1:B:460:LEU:HB2	1.65	0.59
1:A:922:MET:HE2	1:A:1012:MET:C	2.23	0.59
1:B:428:LYS:O	1:B:429:VAL:HG23	2.02	0.59
1:A:453:ILE:O	1:A:453:ILE:HG22	2.02	0.59
1:A:393:VAL:N	1:A:394:VAL:O	2.25	0.59
1:A:491:ALA:HB1	1:A:532:PRO:HB3	1.84	0.59
1:A:1141:LEU:HD12	4:A:2421:HOH:O	2.02	0.59
1:A:835:LEU:HD13	1:A:841:PHE:CE1	2.38	0.58
1:A:723:ARG:NH1	1:A:724:ASP:OD1	2.33	0.58
1:B:671:ARG:HH22	1:B:1119:LYS:HZ2	1.51	0.58
1:B:879:MET:HE2	1:B:885:PRO:CD	2.32	0.58
1:B:1194:ASP:O	1:B:1196:ALA:N	2.35	0.58
1:B:1218:ARG:H	1:B:1219:SER:HB3	1.66	0.58
1:A:1285:ILE:O	1:A:1289:GLU:HB2	2.03	0.58
1:B:1042:LYS:HG2	1:B:1122:ILE:HG12	1.85	0.58
1:B:1147:MET:HA	1:B:1147:MET:CE	2.33	0.58



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:922:MET:CE	1:A:1012:MET:C	2.71	0.58
1:B:1227:LEU:HD13	1:B:1301:TRP:CZ2	2.38	0.58
1:B:1217:SER:HB2	1:B:1218:ARG:CA	2.34	0.58
1:B:417:ALA:O	1:B:421:THR:OG1	2.20	0.58
1:B:453:ILE:C	1:B:455:LYS:H	2.05	0.58
1:A:624:PRO:HA	1:A:625:ASP:CB	2.28	0.58
1:B:1333:LYS:O	1:B:1337:THR:HB	2.04	0.58
1:B:528:ARG:NH2	1:B:679:THR:O	2.37	0.57
1:B:723:ARG:CG	1:B:723:ARG:NH1	2.41	0.57
1:B:772:PHE:O	1:B:778:ARG:HD2	2.04	0.57
1:A:674:LEU:CD1	4:A:2095:HOH:O	2.53	0.57
1:A:509:PRO:O	1:A:510:LEU:CB	2.53	0.57
1:A:1259:ASN:O	1:A:1263:GLU:HG3	2.05	0.57
1:B:916:ARG:HH21	1:B:1019:PRO:HD3	1.69	0.57
1:A:820:LEU:CD1	1:A:906:LEU:HD21	2.35	0.57
1:A:1235:GLU:HG2	1:A:1313:TYR:CZ	2.39	0.57
1:B:400:ASN:O	1:B:401:ILE:HG12	2.05	0.57
1:A:439:LYS:HA	4:A:2013:HOH:O	2.04	0.57
1:A:861:VAL:HG13	1:A:873:GLU:HG2	1.86	0.57
1:A:456:THR:O	1:A:459:ARG:NH1	2.38	0.57
1:B:431:LEU:HB3	1:B:432:GLU:HB2	0.60	0.57
1:B:721:ARG:O	1:B:725:VAL:HG13	2.04	0.57
1:B:418:TRP:CA	1:B:419:GLU:CB	2.83	0.56
1:A:622:PHE:HA	1:A:642:ARG:O	2.05	0.56
1:A:879:MET:CE	1:A:885:PRO:CD	2.81	0.56
1:B:397:ARG:CG	1:B:397:ARG:NH2	2.49	0.56
1:B:589:GLY:H	1:B:611:ARG:HH21	1.53	0.56
1:B:419:GLU:H	1:B:422:ARG:CB	2.17	0.56
1:B:441:ASP:HB3	1:B:442:PRO:CA	2.36	0.56
1:B:450:VAL:CG1	1:B:451:THR:HA	2.35	0.56
1:A:454:TRP:O	1:A:458:TYR:CB	2.52	0.56
1:B:1285:ILE:HD12	1:B:1285:ILE:C	2.27	0.56
1:A:408:TRP:CD1	1:A:408:TRP:C	2.78	0.55
1:B:411:GLU:HG2	1:B:412:ALA:N	2.21	0.55
1:B:445:SER:O	1:B:446:THR:HG23	2.05	0.55
1:B:400:ASN:C	1:B:401:ILE:HG12	2.27	0.55
1:B:419:GLU:OE2	1:B:419:GLU:HA	2.07	0.55
1:A:1217:SER:OG	1:A:1221:ALA:N	2.40	0.55
1:B:1116:ASP:HB3	1:B:1120:GLN:HG2	1.87	0.55
1:B:1172:ARG:HB3	1:B:1173:PRO:HD3	1.88	0.55
1:B:1363:THR:O	1:B:1367:VAL:HG13	2.06	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1315:HIS:HB2	1:A:1316:LYS:CA	2.36	0.55
1:B:769:GLU:HG3	4:B:2030:HOH:O	2.07	0.55
1:B:397:ARG:HH21	1:B:397:ARG:HG3	1.69	0.55
1:B:533:ASP:OD1	1:B:642:ARG:NH2	2.39	0.55
1:B:1270:PRO:HG3	1:B:1301:TRP:CD2	2.41	0.55
1:B:1327:ARG:HD2	1:B:1331:TYR:OH	2.07	0.55
1:A:547:SER:HB2	1:A:548:PRO:CA	2.35	0.55
1:A:393:VAL:N	1:A:394:VAL:C	2.54	0.55
1:B:408:TRP:CE3	1:B:408:TRP:C	2.80	0.55
1:A:395:ALA:CB	1:A:396:ALA:HA	2.31	0.54
1:A:813:ARG:HD2	4:A:2227:HOH:O	2.07	0.54
1:B:456:THR:CA	1:B:457:LEU:HB2	2.37	0.54
1:A:1193:GLU:N	1:A:1194:ASP:O	2.40	0.54
1:A:399:ARG:CB	1:A:400:ASN:CA	2.85	0.54
1:B:433:ASP:CA	1:B:434:GLU:HB2	2.35	0.54
1:B:1024:GLY:HA3	4:B:2291:HOH:O	2.07	0.54
1:B:1217:SER:CB	1:B:1218:ARG:HA	2.36	0.54
1:A:899:GLN:HA	1:A:899:GLN:OE1	2.07	0.54
1:B:428:LYS:C	1:B:429:VAL:HG23	2.28	0.54
1:B:1036:LEU:HB3	1:B:1040:LEU:HD22	1.89	0.54
1:B:1269:THR:HG21	4:B:2377:HOH:O	2.03	0.54
1:A:466:LYS:HB3	1:A:467:PRO:O	2.08	0.54
1:B:433:ASP:CB	1:B:434:GLU:CB	2.83	0.54
1:B:1120:GLN:HA	1:B:1120:GLN:OE1	2.07	0.54
1:A:470:GLU:HB2	4:A:2020:HOH:O	2.06	0.54
1:A:1186:MET:N	1:A:1187:LYS:CB	2.60	0.54
1:B:1269:THR:HG23	1:B:1270:PRO:CD	2.35	0.54
1:B:451:THR:N	1:B:452:ASP:C	2.55	0.54
1:B:1165:TYR:O	1:B:1169:SER:HB2	2.08	0.53
1:A:942:LYS:CG	1:A:949:SER:OG	2.56	0.53
1:B:484:ASN:O	1:B:485:PHE:HB2	2.08	0.53
1:A:397:ARG:O	1:A:398:LEU:CB	2.56	0.53
1:A:723:ARG:NH1	1:A:723:ARG:CG	2.53	0.53
1:A:838:PRO:HA	1:A:879:MET:CE	2.31	0.53
1:A:438:LEU:CB	1:A:439:LYS:HB3	2.38	0.53
1:A:641:GLN:HB3	1:A:642:ARG:HB2	1.75	0.53
1:A:1210:PHE:O	1:A:1213:ILE:HG22	2.08	0.53
1:A:457:LEU:CB	1:A:458:TYR:CB	2.78	0.53
1:A:1213:ILE:O	1:A:1216:LYS:HB3	2.08	0.53
1:B:406:PRO:CB	1:B:408:TRP:CD1	2.92	0.53
1:B:860:ARG:HA	1:B:1354:ALA:HB2	1.90	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:391:ALA:HB1	1:A:393:VAL:HG22	1.90	0.53
1:A:793:GLY:HA2	1:A:914:VAL:H	1.73	0.53
1:B:1089:LYS:HA	1:B:1107:LEU:HD13	1.91	0.53
1:A:399:ARG:CD	1:A:507:THR:HG22	2.16	0.53
1:A:1315:HIS:H	1:A:1315:HIS:CD2	2.26	0.53
1:A:1343:GLY:HA3	1:B:860:ARG:HD2	1.91	0.53
1:B:1038:ARG:HG2	1:B:1038:ARG:O	2.09	0.53
1:A:555:SER:O	1:A:555:SER:OG	2.21	0.52
1:B:716:ARG:O	1:B:720:LYS:HG2	2.08	0.52
1:A:580:TRP:HB3	1:A:614:PHE:HB3	1.90	0.52
1:A:1146:PRO:HB3	1:A:1148:TYR:CE2	2.44	0.52
1:A:586:LYS:HG2	1:A:587:ASP:N	2.23	0.52
1:B:394:VAL:HG21	1:B:560:ALA:CB	2.39	0.52
1:B:466:LYS:O	1:B:468:PHE:N	2.43	0.52
1:A:883:PHE:CE2	1:A:1203:LEU:HD21	2.44	0.52
1:B:546:THR:HA	1:B:547:SER:HB3	1.92	0.52
1:A:417:ALA:CB	1:A:576:VAL:HG13	2.37	0.52
1:B:916:ARG:HD2	1:B:945:ASP:OD2	2.09	0.52
1:A:576:VAL:O	1:A:576:VAL:CG1	2.58	0.52
1:A:605:LYS:HD2	1:A:605:LYS:N	2.25	0.52
1:B:408:TRP:O	1:B:408:TRP:CE3	2.63	0.52
1:B:545:SER:HA	1:B:546:THR:CG2	2.29	0.52
1:A:774:ASP:OD1	1:A:776:HIS:N	2.43	0.52
1:B:452:ASP:HA	1:B:455:LYS:HB2	1.92	0.52
1:A:427:CYS:O	1:A:428:LYS:HB2	2.10	0.52
1:A:456:THR:HG22	1:A:457:LEU:CA	2.33	0.52
1:A:967:PHE:CD2	1:A:1031:PRO:HG3	2.45	0.52
1:B:829:SER:O	1:B:832:LYS:HG2	2.10	0.52
1:A:451:THR:OG1	1:A:471:LYS:HE3	2.09	0.51
1:A:458:TYR:CZ	1:A:465:GLY:O	2.64	0.51
1:A:1203:LEU:O	1:A:1307:SER:HB2	2.10	0.51
1:B:843:GLN:O	1:B:847:GLU:HG3	2.11	0.51
1:B:1303:LEU:HD13	4:B:2381:HOH:O	2.10	0.51
1:A:439:LYS:O	1:A:440:TYR:HB2	2.11	0.51
1:A:890:TYR:CE2	1:A:894:ILE:HD11	2.45	0.51
1:A:1189:ALA:HB1	1:A:1195:GLY:HA3	1.92	0.51
1:A:828:PHE:CG	1:A:1178:GLU:CG	2.93	0.51
1:A:1219:SER:CA	1:A:1221:ALA:HB3	2.41	0.51
1:B:406:PRO:CB	1:B:408:TRP:NE1	2.74	0.51
1:B:1088:TYR:CE1	1:B:1143:LEU:HD22	2.46	0.51
1:B:468:PHE:HB3	4:B:2007:HOH:O	2.10	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:622:PHE:HA	1:B:642:ARG:O	2.10	0.51
1:A:1194:ASP:OD2	1:A:1194:ASP:N	2.43	0.51
1:B:403:PRO:HA	1:B:404:LYS:HG2	1.91	0.51
1:B:450:VAL:HG12	1:B:451:THR:HA	1.92	0.51
1:B:552:PRO:N	1:B:553:VAL:HB	2.26	0.51
1:B:1189:ALA:O	1:B:1190:LYS:C	2.48	0.51
1:A:1312:LEU:O	1:A:1315:HIS:CD2	2.64	0.51
1:B:462:ALA:N	1:B:463:PHE:C	2.63	0.51
1:B:923:ILE:HB	1:B:990:ILE:HD13	1.92	0.51
1:B:1194:ASP:C	1:B:1196:ALA:H	2.13	0.51
1:A:534:ARG:HD2	1:A:642:ARG:HD2	1.92	0.51
1:A:839:VAL:HG13	1:B:1351:PHE:CZ	2.45	0.51
1:B:441:ASP:HB3	1:B:442:PRO:C	2.31	0.51
1:A:1129:TRP:CZ2	1:A:1133:ARG:HD3	2.46	0.51
1:B:411:GLU:O	1:B:412:ALA:HB3	2.11	0.51
1:B:449:ASP:O	1:B:477:PHE:CD2	2.63	0.51
1:B:456:THR:H	1:B:457:LEU:CA	2.23	0.51
1:B:1152:SER:O	1:B:1154:LEU:HD13	2.10	0.51
1:A:391:ALA:HB3	1:A:392:PRO:CA	2.40	0.50
1:A:1335:GLN:HE21	3:B:3375:GOL:H2	1.76	0.50
1:A:1352:MET:O	1:B:842:ARG:NH2	2.43	0.50
1:B:1140:ALA:O	1:B:1141:LEU:O	2.28	0.50
1:B:714:MET:CE	1:B:718:VAL:HG12	2.39	0.50
1:A:450:VAL:HG12	1:A:471:LYS:HE2	1.94	0.50
1:B:503:ASP:O	1:B:504:ASN:HB3	2.11	0.50
1:B:1038:ARG:HD2	1:B:1039:TYR:CE2	2.47	0.50
1:B:407:LYS:CB	1:B:408:TRP:CB	2.37	0.50
1:B:443:SER:HA	1:B:444:TRP:C	2.32	0.50
1:B:1304:LEU:O	1:B:1308:THR:HG23	2.10	0.50
1:A:705:GLU:HG2	1:A:998:PRO:HD2	1.93	0.50
1:B:497:VAL:HG23	1:B:539:LEU:HB2	1.93	0.50
1:B:1252:ASP:O	1:B:1252:ASP:OD2	2.30	0.50
1:A:400:ASN:C	1:A:400:ASN:OD1	2.50	0.50
1:A:1328:GLN:O	1:A:1332:ILE:HG13	2.12	0.50
1:A:558:PRO:O	1:A:559:ALA:C	2.50	0.49
1:B:509:PRO:O	1:B:510:LEU:CB	2.58	0.49
1:A:1186:MET:CA	1:A:1187:LYS:CB	2.90	0.49
1:B:1023:ASP:HB2	4:B:2285:HOH:O	2.11	0.49
1:A:457:LEU:CB	1:A:458:TYR:HB3	2.33	0.49
1:B:460:LEU:HD13	1:B:460:LEU:O	2.12	0.49
1:B:1194:ASP:CG	1:B:1195:GLY:H	2.15	0.49



	A construction of the cons	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:466:LYS:H	1:A:467:PRO:CA	2.18	0.49
1:B:470:GLU:O	1:B:471:LYS:HB3	2.12	0.49
1:A:904:ASP:HA	1:A:907:LYS:HE2	1.94	0.49
1:A:917:SER:HA	1:A:1015:VAL:O	2.12	0.49
1:A:667:LYS:HE2	1:A:1119:LYS:O	2.13	0.49
1:A:859:GLY:O	1:A:860:ARG:HB3	2.11	0.49
1:B:678:LYS:H	1:B:783:ARG:NH1	2.11	0.49
1:B:570:MET:O	1:B:570:MET:HG3	2.11	0.49
1:A:991:PHE:CD2	1:A:999:LEU:HB3	2.48	0.49
1:B:1200:ASP:OD1	1:B:1202:ASP:HB2	2.13	0.49
1:A:524:CYS:SG	1:A:527:THR:HG23	2.53	0.48
1:A:565:ILE:CD1	1:A:1074:HIS:HA	2.43	0.48
1:B:546:THR:HA	1:B:547:SER:CB	2.43	0.48
1:B:861:VAL:HG21	1:B:873:GLU:HG2	1.95	0.48
1:B:1112:GLY:O	1:B:1115:VAL:CG2	2.57	0.48
1:A:498:LEU:O	1:A:541:PRO:HD3	2.13	0.48
1:A:1300:THR:HA	1:A:1303:LEU:CD2	2.43	0.48
1:A:1317:SER:O	1:A:1321:VAL:HG12	2.13	0.48
1:B:1102:LYS:HG3	4:B:2324:HOH:O	2.13	0.48
1:A:458:TYR:CE2	1:A:465:GLY:O	2.67	0.48
1:B:453:ILE:C	1:B:455:LYS:N	2.67	0.48
1:B:551:PRO:C	1:B:553:VAL:HB	2.34	0.48
1:B:1195:GLY:O	1:B:1196:ALA:HB3	2.13	0.48
1:B:456:THR:HB	1:B:457:LEU:HB2	1.96	0.47
1:B:459:ARG:N	1:B:460:LEU:CB	2.58	0.47
1:A:456:THR:O	1:A:459:ARG:CD	2.62	0.47
1:B:454:TRP:HA	1:B:457:LEU:HD23	1.95	0.47
1:B:626:VAL:O	1:B:626:VAL:CG1	2.62	0.47
1:A:457:LEU:CB	1:A:458:TYR:HB2	2.40	0.47
1:A:900:LYS:HB2	1:A:900:LYS:HE3	1.58	0.47
1:A:1211:LYS:O	1:A:1214:SER:HB3	2.14	0.47
1:B:408:TRP:O	1:B:439:LYS:HG3	2.14	0.47
1:B:450:VAL:HG11	1:B:471:LYS:HG2	1.96	0.47
1:A:464:ARG:HD2	1:A:464:ARG:HA	1.70	0.47
1:A:791:SER:HB3	4:A:2214:HOH:O	2.13	0.47
1:B:424:PHE:HD2	1:B:430:ASP:H	1.62	0.47
1:B:448:ARG:HG2	1:B:478:VAL:HG22	1.97	0.47
1:B:529:ARG:HD3	1:B:776:HIS:CD2	2.49	0.47
1:A:458:TYR:N	1:A:459:ARG:C	2.68	0.47
1:A:721:ARG:O	1:A:725:VAL:HG13	2.15	0.47
1:A:723:ARG:NH2	1:B:947:GLU:HG2	2.30	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1186:MET:CB	1:A:1187:LYS:HB2	2.45	0.47
1:B:1119:LYS:HG3	1:B:1120:GLN:NE2	2.30	0.47
1:B:460:LEU:HD12	1:B:462:ALA:CB	2.45	0.47
1:B:1214:SER:HA	1:B:1217:SER:HA	1.96	0.47
1:A:774:ASP:OD1	1:A:774:ASP:C	2.53	0.47
1:A:1200:ASP:OD1	1:A:1202:ASP:HB2	2.15	0.47
1:A:464:ARG:HA	1:A:465:GLY:O	2.15	0.47
1:A:589:GLY:H	1:A:611:ARG:HH21	1.63	0.47
1:B:407:LYS:H	1:B:408:TRP:HD1	1.63	0.47
1:B:942:LYS:HD2	1:B:949:SER:CB	2.44	0.47
1:A:1217:SER:OG	1:A:1221:ALA:CA	2.64	0.46
1:A:1224:PHE:CE2	1:A:1228:LYS:HE3	2.50	0.46
1:B:1254:TYR:HB3	1:B:1255:PRO:HD3	1.97	0.46
1:A:444:TRP:CE2	1:A:453:ILE:HG23	2.50	0.46
1:A:466:LYS:N	1:A:467:PRO:CA	2.77	0.46
1:B:821:ILE:HG13	1:B:1170:ILE:HG23	1.97	0.46
1:A:395:ALA:HA	1:A:397:ARG:O	2.15	0.46
1:A:406:PRO:HG3	1:A:431:LEU:HB3	1.97	0.46
1:A:622:PHE:CD1	1:A:622:PHE:N	2.84	0.46
1:A:712:GLY:O	1:A:746:TRP:HA	2.16	0.46
1:A:1169:SER:O	1:A:1173:PRO:HG2	2.15	0.46
1:A:1182:PHE:N	1:A:1182:PHE:CD2	2.83	0.46
1:B:501:ASN:HD22	1:B:502:PRO:HD2	1.79	0.46
1:B:859:GLY:O	1:B:860:ARG:HB3	2.15	0.46
1:A:456:THR:C	1:A:459:ARG:HB2	2.36	0.46
1:A:458:TYR:H	1:A:459:ARG:C	2.19	0.46
1:B:433:ASP:OD2	1:B:438:LEU:HD11	2.16	0.46
1:B:447:ALA:HB3	1:B:453:ILE:HD11	1.98	0.46
1:B:503:ASP:HB3	1:B:504:ASN:H	1.45	0.46
1:B:459:ARG:HB2	1:B:460:LEU:HB2	1.98	0.46
1:A:723:ARG:HD3	1:A:730:ASP:C	2.36	0.46
1:B:1270:PRO:HG3	1:B:1301:TRP:CE3	2.50	0.46
1:A:456:THR:O	1:A:459:ARG:CZ	2.64	0.46
1:A:484:ASN:O	1:A:485:PHE:HB2	2.16	0.46
1:A:966:HIS:ND1	1:A:1089:LYS:HE3	2.31	0.46
1:B:459:ARG:CB	1:B:460:LEU:HB2	2.46	0.46
1:A:434:GLU:OE2	1:A:434:GLU:N	2.48	0.45
1:A:559:ALA:HB2	1:A:562:GLU:OE1	2.13	0.45
1:A:738:ARG:HD3	1:A:743:LYS:HG2	1.98	0.45
1:A:1185:ALA:H	1:A:1188:ALA:HB2	1.81	0.45
1:B:426:HIS:HA	1:B:427:CYS:HA	1.57	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:546:THR:O	1:B:546:THR:CG2	2.63	0.45
1:B:589:GLY:O	1:B:590:TYR:HB2	2.15	0.45
1:A:879:MET:HE2	1:A:885:PRO:HD3	1.95	0.45
1:B:462:ALA:H	1:B:464:ARG:N	2.15	0.45
1:B:503:ASP:O	1:B:504:ASN:CB	2.64	0.45
1:B:1041:LYS:HB2	1:B:1123:VAL:CG1	2.45	0.45
1:B:403:PRO:CB	1:B:404:LYS:HB2	2.45	0.45
1:B:457:LEU:HA	1:B:458:TYR:HA	1.58	0.45
1:B:839:VAL:HG22	4:B:2167:HOH:O	2.16	0.45
1:A:456:THR:O	1:A:459:ARG:HB2	2.16	0.45
1:A:1102:LYS:N	1:A:1103:PRO:HD2	2.32	0.45
1:B:557:GLN:HG3	1:B:557:GLN:O	2.17	0.45
1:B:610:GLU:HG3	1:B:1077:LEU:HD22	1.99	0.45
1:B:621:THR:HG22	1:B:622:PHE:CD2	2.52	0.45
1:A:399:ARG:HB2	1:A:400:ASN:CA	2.46	0.45
1:B:828:PHE:CD2	1:B:1178:GLU:HG2	2.51	0.45
1:A:1140:ALA:O	1:A:1141:LEU:C	2.54	0.45
1:B:826:ARG:NH1	1:B:826:ARG:HB3	2.32	0.45
1:B:966:HIS:ND1	1:B:1089:LYS:HE2	2.32	0.45
1:A:674:LEU:HD11	4:A:2095:HOH:O	2.17	0.45
1:A:952:LEU:HG	1:A:978:PHE:CD1	2.52	0.45
1:B:441:ASP:CB	1:B:442:PRO:HA	2.46	0.45
1:A:391:ALA:CB	1:A:393:VAL:HG22	2.47	0.44
1:A:394:VAL:HA	1:A:395:ALA:HA	1.76	0.44
1:A:396:ALA:HB1	1:A:399:ARG:CZ	2.48	0.44
1:B:400:ASN:OD1	1:B:401:ILE:N	2.39	0.44
1:B:447:ALA:CB	1:B:453:ILE:HD11	2.47	0.44
1:A:414:LEU:HD13	1:A:485:PHE:CZ	2.53	0.44
1:A:867:LEU:HD22	1:A:874:THR:HG23	1.99	0.44
1:A:1182:PHE:HA	1:A:1185:ALA:CB	2.47	0.44
1:B:551:PRO:HB2	1:B:553:VAL:HG11	1.99	0.44
1:B:861:VAL:CG2	1:B:873:GLU:HG2	2.48	0.44
1:B:407:LYS:HB2	1:B:408:TRP:HB3	0.56	0.44
1:B:451:THR:H	1:B:452:ASP:CA	2.31	0.44
1:A:883:PHE:CZ	1:A:1203:LEU:HD21	2.53	0.44
1:A:959:LEU:HD22	1:A:1021:ILE:HG22	2.00	0.44
1:A:1193:GLU:H	1:A:1194:ASP:C	2.20	0.44
1:B:475:ASP:OD1	1:B:476:VAL:N	2.51	0.44
1:B:1063:GLN:CB	4:B:2306:HOH:O	2.65	0.44
1:A:406:PRO:O	1:A:410:HIS:CD2	2.71	0.44
1:A:1134:ARG:HG3	4:A:2232:HOH:O	2.16	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:407:LYS:N	1:B:408:TRP:CD1	2.85	0.44
1:B:861:VAL:HG21	1:B:873:GLU:CG	2.47	0.44
1:A:839:VAL:HG22	4:A:2246:HOH:O	2.18	0.44
1:A:1190:LYS:HG3	1:A:1191:ASP:H	1.81	0.44
1:B:481:MET:HE3	4:B:2003:HOH:O	2.18	0.44
1:A:468:PHE:CA	1:A:469:PRO:O	2.56	0.44
1:A:1184:ASN:H	1:A:1185:ALA:HB3	0.71	0.44
1:B:1252:ASP:O	1:B:1252:ASP:CG	2.55	0.44
1:B:554:VAL:O	1:B:555:SER:C	2.55	0.44
1:B:737:GLY:C	1:B:738:ARG:HD2	2.38	0.44
1:A:624:PRO:CA	1:A:625:ASP:CB	2.93	0.44
1:A:931:GLU:OE2	1:A:994:LYS:NZ	2.51	0.44
1:B:443:SER:CA	1:B:444:TRP:C	2.85	0.44
1:B:841:PHE:HB3	1:B:879:MET:HE1	1.99	0.43
1:B:1217:SER:CB	1:B:1218:ARG:CA	2.94	0.43
1:A:947:GLU:H	1:A:947:GLU:HG2	1.65	0.43
1:A:1094:TYR:CE2	1:A:1146:PRO:HA	2.53	0.43
1:B:429:VAL:HG22	1:B:463:PHE:CE2	2.53	0.43
1:A:467:PRO:HB2	1:A:468:PHE:H	1.53	0.43
1:B:544:THR:HG21	1:B:1079:PRO:HD3	1.99	0.43
1:B:551:PRO:HA	1:B:552:PRO:HD3	1.67	0.43
1:B:916:ARG:HD3	4:B:2284:HOH:O	2.17	0.43
1:B:962:ARG:HD3	1:B:1011:ASP:HB3	2.00	0.43
1:B:1289:GLU:O	1:B:1299:ASN:ND2	2.51	0.43
1:B:772:PHE:O	1:B:778:ARG:CD	2.67	0.43
1:A:665:HIS:HE1	4:A:2366:HOH:O	2.00	0.43
1:A:905:THR:HG23	1:A:909:LYS:HD2	2.01	0.43
1:B:451:THR:N	1:B:452:ASP:CA	2.81	0.43
1:A:1299:ASN:O	1:A:1303:LEU:HD22	2.19	0.43
1:B:432:GLU:O	1:B:433:ASP:HB3	2.18	0.43
1:B:456:THR:O	1:B:456:THR:CG2	2.67	0.43
1:B:1073:PHE:O	1:B:1077:LEU:HG	2.18	0.43
1:B:428:LYS:O	1:B:429:VAL:CB	2.66	0.43
1:A:444:TRP:HZ2	1:A:456:THR:HG21	1.84	0.43
1:A:464:ARG:HA	1:A:465:GLY:C	2.38	0.43
1:A:835:LEU:HD13	1:A:841:PHE:CZ	2.54	0.43
1:B:451:THR:CA	1:B:452:ASP:HB2	2.49	0.43
1:B:498:LEU:O	1:B:541:PRO:HD3	2.19	0.43
1:B:900:LYS:HE3	1:B:900:LYS:HB2	1.64	0.43
1:B:1211:LYS:HE2	1:B:1211:LYS:HB3	1.86	0.43
1:A:852:ARG:O	1:A:856:VAL:HG23	2.19	0.43



	A h O	Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:420:VAL:C	1:B:422:ARG:H	2.22	0.43	
1:B:1075:PHE:O	1:B:1078:GLN:HG2	2.19	0.43	
1:A:444:TRP:CD1	1:A:453:ILE:HG23	2.53	0.43	
1:A:457:LEU:HD12	1:A:457:LEU:C	2.35	0.43	
1:A:547:SER:CB	1:A:548:PRO:CA	2.96	0.43	
1:A:740:GLY:HA3	1:A:772:PHE:CE2	2.54	0.43	
1:A:1344:ALA:HB1	1:B:1327:ARG:CD	2.48	0.43	
1:B:1143:LEU:HD12	1:B:1143:LEU:HA	1.81	0.43	
1:A:408:TRP:CH2	1:A:431:LEU:HD23	2.54	0.42	
1:B:423:LEU:HD21	1:B:458:TYR:HE2	1.84	0.42	
1:B:1139:GLY:HA2	1:B:1140:ALA:HB3	2.01	0.42	
1:A:399:ARG:HB2	1:A:400:ASN:C	2.38	0.42	
1:A:460:LEU:O	1:A:461:ASP:HB3	2.19	0.42	
1:A:654:LEU:HD12	4:A:2200:HOH:O	2.19	0.42	
1:A:1222:LEU:HD12	1:A:1222:LEU:HA	1.86	0.42	
1:B:459:ARG:HB2	1:B:460:LEU:CB	2.49	0.42	
1:B:1229:ASN:O	1:B:1233:GLU:HG3	2.19	0.42	
1:B:429:VAL:HG12	1:B:430:ASP:H	1.83	0.42	
1:B:530:PHE:CE2	1:B:650:MET:HG2	2.55	0.42	
1:B:580:TRP:HB3	1:B:614:PHE:HB3	1.99	0.42	
1:B:991:PHE:CD2	1:B:999:LEU:HB3	2.54	0.42	
1:A:419:GLU:OE1	1:A:422:ARG:HD3	2.20	0.42	
1:A:467:PRO:HG2	1:A:468:PHE:HD2	1.85	0.42	
1:A:1190:LYS:HG3	1:A:1191:ASP:N	2.34	0.42	
1:B:404:LYS:HA	1:B:404:LYS:HD3	1.76	0.42	
1:B:1187:LYS:HE2	1:B:1187:LYS:HB3	1.89	0.42	
1:A:454:TRP:HA	1:A:457:LEU:HD23	2.01	0.42	
1:A:547:SER:CB	1:A:548:PRO:HA	2.50	0.42	
1:B:667:LYS:HE2	1:B:667:LYS:HB2	1.56	0.42	
1:A:454:TRP:O	1:A:458:TYR:CG	2.72	0.42	
1:A:772:PHE:O	1:A:778:ARG:CD	2.67	0.42	
1:B:441:ASP:HB2	1:B:444:TRP:CG	2.54	0.42	
1:B:1224:PHE:CE2	1:B:1228:LYS:HE3	2.55	0.42	
1:A:426:HIS:HB3	1:A:469:PRO:HD3	2.02	0.42	
1:A:444:TRP:CD2	1:A:453:ILE:HG23	2.54	0.42	
1:B:1182:PHE:O	1:B:1186:MET:HG2	2.19	0.42	
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.90	0.42	
1:A:796:LEU:HA	1:A:799:LEU:CD1	2.46	0.42	
1:B:429:VAL:HG12	1:B:430:ASP:N	2.35	0.42	
1:A:456:THR:HG22	1:A:457:LEU:HD13	2.01	0.42	
1:A:705:GLU:HG2	1:A:998:PRO:CD	2.50	0.42	



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:441:ASP:CB	1:B:442:PRO:CA	2.96	0.42
1:B:455:LYS:C	1:B:457:LEU:O	2.58	0.42
1:B:555:SER:CA	1:B:557:GLN:H	2.32	0.42
1:B:712:GLY:O	1:B:746:TRP:HA	2.20	0.42
1:A:889:LYS:HG2	1:A:1198:PHE:CZ	2.55	0.41
1:A:966:HIS:ND1	1:A:1089:LYS:CE	2.83	0.41
1:A:1189:ALA:O	1:A:1190:LYS:C	2.59	0.41
1:A:1220:SER:H	1:A:1221:ALA:HB3	1.73	0.41
1:B:459:ARG:HB2	1:B:460:LEU:CD2	2.48	0.41
1:B:551:PRO:HB2	1:B:553:VAL:CG1	2.50	0.41
1:B:1075:PHE:HE2	1:B:1118:SER:HA	1.84	0.41
1:B:449:ASP:HB3	1:B:450:VAL:H	1.65	0.41
1:B:456:THR:H	1:B:457:LEU:C	2.24	0.41
1:B:907:LYS:HG3	1:B:1175:ILE:HD13	2.02	0.41
1:B:1153:TRP:NE1	1:B:1157:GLY:O	2.52	0.41
1:A:423:LEU:HD11	1:A:458:TYR:CD1	2.54	0.41
1:A:696:ASP:HB3	1:A:706:VAL:HG13	2.02	0.41
1:A:922:MET:HE3	1:A:1012:MET:CA	2.51	0.41
1:A:1182:PHE:HA	1:A:1185:ALA:HB1	2.01	0.41
1:A:1183:HIS:HA	1:A:1186:MET:HG3	2.03	0.41
1:A:1334:ALA:HB3	1:B:1347:LEU:HD13	2.01	0.41
1:B:407:LYS:CA	1:B:408:TRP:CB	2.92	0.41
1:B:565:ILE:HD13	1:B:1074:HIS:HA	2.03	0.41
1:B:722:ILE:O	1:B:726:LEU:HB2	2.20	0.41
1:A:514:LYS:HB3	1:A:514:LYS:HE3	1.88	0.41
1:A:581:ARG:NH1	4:A:2068:HOH:O	2.54	0.41
1:A:605:LYS:HA	1:A:606:PRO:HD3	1.88	0.41
1:B:393:VAL:O	1:B:394:VAL:CB	2.64	0.41
1:B:400:ASN:OD1	1:B:509:PRO:HB3	2.20	0.41
1:A:794:LEU:HD11	1:A:802:LEU:HD11	2.03	0.41
1:A:799:LEU:HB2	1:A:800:PRO:HD3	2.02	0.41
1:A:869:ASP:HB3	4:A:2264:HOH:O	2.21	0.41
1:A:1141:LEU:HD13	1:A:1141:LEU:HA	1.89	0.41
1:A:1146:PRO:CB	1:A:1148:TYR:CE2	3.04	0.41
1:B:428:LYS:O	1:B:429:VAL:CG2	2.68	0.41
1:B:441:ASP:HB3	1:B:442:PRO:O	2.20	0.41
1:B:458:TYR:HB3	1:B:463:PHE:O	2.21	0.41
1:B:462:ALA:HB1	1:B:463:PHE:CD2	2.56	0.41
1:B:1203:LEU:HG	1:B:1329:LEU:HD22	2.03	0.41
1:B:1218:ARG:N	1:B:1219:SER:CB	2.77	0.41
1:B:400:ASN:HD22	1:B:404:LYS:NZ	2.19	0.41



A 4 1	A +	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:429:VAL:HG22	1:B:463:PHE:CZ	2.55	0.41
1:A:1089:LYS:HB2	1:A:1107:LEU:HB3	2.03	0.40
1:B:457:LEU:H	1:B:459:ARG:HG2	1.86	0.40
1:B:775:LYS:HG2	4:B:2109:HOH:O	2.20	0.40
1:A:488:LYS:HE3	1:B:1371:GLU:O	2.22	0.40
1:A:1150:SER:HB2	4:A:2426:HOH:O	2.20	0.40
1:B:419:GLU:N	1:B:422:ARG:HB2	2.26	0.40
1:B:456:THR:O	1:B:459:ARG:HG2	2.21	0.40
1:B:1087:ASN:O	1:B:1091:ARG:HG3	2.21	0.40
1:A:454:TRP:O	1:A:458:TYR:CD1	2.75	0.40
1:A:648:SER:HA	1:A:1065:THR:HG21	2.03	0.40
1:B:391:ALA:HB3	1:B:563:GLU:CG	2.45	0.40
1:B:431:LEU:HD13	1:B:432:GLU:OE1	2.21	0.40
1:A:485:PHE:HB3	1:A:532:PRO:HB2	2.02	0.40
1:A:557:GLN:HE21	1:A:557:GLN:HB3	1.68	0.40
1:A:1265:TRP:CZ2	1:A:1325:ALA:HB2	2.56	0.40
1:B:449:ASP:O	1:B:450:VAL:HB	2.22	0.40
1:A:459:ARG:HB3	1:A:460:LEU:H	1.52	0.40
1:A:626:VAL:HG13	1:A:626:VAL:O	2.22	0.40
1:A:1207:TYR:CE2	1:A:1311:LYS:HG3	2.55	0.40
1:A:1220:SER:H	1:A:1221:ALA:CB	2.29	0.40
1:B:547:SER:CB	1:B:548:PRO:CD	2.99	0.40
1:B:699:SER:HA	1:B:700:PRO:HD3	1.98	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2389:HOH:O	4:B:2333:HOH:O[1_455]	1.90	0.30
1:A:1156:ARG:NH1	1:B:1126:GLU:OE2[1_455]	2.07	0.13
4:A:2109:HOH:O	4:B:2384:HOH:O[2_746]	2.16	0.04

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	n shows the r	number o	f residues	for which	the bac	ckbone confo	rmation	was
analysed, and the tota	al number of	residues.						
Mol Chain /	halved	Favou	$\mathbf{rod} \mid \mathbf{All}$		Intliare	Dorcontilo	ne l	

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	925/1022~(90%)	836~(90%)	51~(6%)	38~(4%)	3 1
1	В	922/1022~(90%)	811 (88%)	63~(7%)	48 (5%)	2 1
All	All	1847/2044~(90%)	1647 (89%)	114 (6%)	86 (5%)	2 1

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	399	ARG
1	А	412	ALA
1	А	439	LYS
1	А	440	TYR
1	А	459	ARG
1	А	460	LEU
1	А	466	LYS
1	А	467	PRO
1	А	504	ASN
1	А	510	LEU
1	А	547	SER
1	А	553	VAL
1	А	621	THR
1	А	625	ASP
1	А	642	ARG
1	А	1140	ALA
1	А	1141	LEU
1	А	1193	GLU
1	А	1194	ASP
1	В	401	ILE
1	В	406	PRO
1	В	411	GLU
1	В	419	GLU
1	В	429	VAL
1	В	430	ASP
1	В	432	GLU
1	В	434	GLU
1	В	446	THR
1	В	453	ILE
1	В	460	LEU
1	В	463	PHE
1	В	467	PRO
1	В	504	ASN



1 B 505 SER 1 B 547 SER 1 B 548 PRO 1 B 1141 LEU 1 B 1190 LYS 1 B 1217 SER 1 B 1219 SER 1 A 394 VAL 1 A 394 VAL 1 A 394 VAL 1 A 398 LEU 1 A 503 ASP 1 A 1185 ALA 1 A 1185 ALA 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 408 TRP 1 B 503 ASP 1 B 503 ASP 1 B <	Mol	Chain	Res	Type
1 B 547 SER 1 B 1141 LEU 1 B 1190 LYS 1 B 1217 SER 1 B 1219 SER 1 A 394 VAL 1 A 394 VAL 1 A 398 LEU 1 A 398 LEU 1 A 503 ASP 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1187 LYS 1 A 1214 SER 1 B 407 LYS 1 B 408 TRP 1 B 407 LYS 1 B 503 ASP 1 B 503 ASP 1 B	1	В	505	SER
1 B 548 PRO 1 B 1141 LEU 1 B 1217 SER 1 B 1217 SER 1 B 1219 SER 1 A 394 VAL 1 A 394 VAL 1 A 398 LEU 1 A 461 ASP 1 A 461 ASP 1 A 138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 B 407 LYS 1 B 431 LEU 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B <	1	В	547	SER
1 B 1141 LEU 1 B 1190 LYS 1 B 1217 SER 1 B 1219 SER 1 A 394 VAL 1 A 394 VAL 1 A 398 LEU 1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1187 LYS 1 A 1214 SER 1 B 407 LYS 1 B 431 LEU 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B	1	В	548	PRO
1 B 1190 LYS 1 B 1217 SER 1 B 1219 SER 1 A 394 VAL 1 A 394 VAL 1 A 398 LEU 1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 B 407 LYS 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B 1196 ALA 1 B	1	В	1141	LEU
1 B 1217 SER 1 B 1219 SER 1 A 394 VAL 1 A 398 LEU 1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1138 GLY 1 A 1138 GLY 1 A 1138 GLY 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 B 407 LYS 1 B 408 TRP 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B 10 LEU 1 B <	1	В	1190	LYS
1 B 1219 SER 1 A 394 VAL 1 A 398 LEU 1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 408 TRP 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B 559 ALA 1 B 1214 SER 1 A	1	В	1217	SER
1 A 394 VAL 1 A 398 LEU 1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 408 TRP 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 510 LEU 1 B 555 SER 1 B 1214 SER 1 A 1315 HIS 1 A 1315 HIS 1 A	1	В	1219	SER
1 A 398 LEU 1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 408 TRP 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B 1214 SER 1 A 1214 SER 1 <th>1</th> <th>А</th> <th>394</th> <th>VAL</th>	1	А	394	VAL
1 A 461 ASP 1 A 503 ASP 1 A 1138 GLY 1 A 1185 ALA 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 408 TRP 1 B 450 VAL 1 B 503 ASP 1 B 555 SER 1 B 1214 SER 1 A 1218 ARG 1 A 1218 ARG 1 </th <th>1</th> <th>А</th> <th>398</th> <th>LEU</th>	1	А	398	LEU
1 A 503 ASP 1 A 1138 GLY 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 510 LEU 1 B 555 SER 1 B 1214 SER 1 A 559 ALA 1 A 1218 ARG 1 B 114 ASP 1 B 1194 <	1	А	461	ASP
1 A 1138 GLY 1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 A 1316 LYS 1 B 407 LYS 1 B 408 TRP 1 B 431 LEU 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 510 LEU 1 B 555 SER 1 B 621 THR 1 B 1214 SER 1 A 559 ALA 1 A 1315 HIS 1 A 1315 HIS 1 B 404 LYS 1 B 1194 ASP 1 B 1194 ASP 1	1	А	503	ASP
1 A 1185 ALA 1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 407 LYS 1 B 408 TRP 1 B 431 LEU 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 510 LEU 1 B 555 SER 1 B 621 THR 1 B 1214 SER 1 B 1214 SER 1 A 559 ALA 1 A 1315 HIS 1 A 1315 HIS 1 B 1441 ASP 1 B 1189 ALA 1 B 1194 ASP 1<	1	А	1138	GLY
1 A 1187 LYS 1 A 1214 SER 1 A 1316 LYS 1 B 407 LYS 1 B 407 LYS 1 B 408 TRP 1 B 431 LEU 1 B 450 VAL 1 B 450 VAL 1 B 503 ASP 1 B 510 LEU 1 B 555 SER 1 B 621 THR 1 B 1214 SER 1 A 559 ALA 1 A 1218 ARG 1 A 1315 HIS 1 B 404 LYS 1 B 1189 ALA 1 B 1194 ASP 1 B 1194 ASP 1 A 469 PRO 1 <th>1</th> <th>А</th> <th>1185</th> <th>ALA</th>	1	А	1185	ALA
1A1214SER1A1316LYS1B407LYS1B408TRP1B431LEU1B450VAL1B451THR1B503ASP1B510LEU1B555SER1B621THR1B1214SER1B1214SER1A559ALA1A1315HIS1B404LYS1B1194ASP1B1194ASP1A469PRO1A471LYS1A488LYS1B1195GLY1B1205SER	1	А	1187	LYS
1A1316LYS1B407LYS1B408TRP1B431LEU1B450VAL1B451THR1B503ASP1B510LEU1B555SER1B621THR1B1214SER1B1214SER1A559ALA1A1315HIS1B404LYS1B1194ASP1B1194ASP1A469PRO1A471LYS1A488LYS1B1195GLY1B1205SER	1	А	1214	SER
1B 407 LYS1B 408 TRP1B 431 LEU1B 450 VAL1B 450 VAL1B 450 VAL1B 503 ASP1B 503 ASP1B 510 LEU1B 555 SER1B 621 THR1B 1214 SER1B 1214 SER1A 559 ALA1A 1218 ARG1A 1218 ARG1B 404 LYS1B 1194 ASP1B 1194 ASP1A 469 PRO1A 471 LYS1B 471 LYS1B 553 VAL1B 1195 GLY1B 1205 SER	1	А	1316	LYS
1B 408 TRP1B 431 LEU1B 450 VAL1B 451 THR1B 503 ASP1B 510 LEU1B 555 SER1B 621 THR1B 1214 SER1B 1214 SER1A 559 ALA1A 1218 ARG1A 1218 ARG1A 1218 ARG1B 404 LYS1B 1194 ASP1B 1194 ASP1A 458 TYR1A 469 PRO1A 471 LYS1B 471 LYS1B 553 VAL1B 1195 GLY1B 1205 SER	1	В	407	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	408	TRP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	431	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	450	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	451	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	503	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	510	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	555	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	621	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	1196	ALA
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	1214	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	559	ALA
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	1218	ARG
1 B 404 LYS 1 B 441 ASP 1 B 1189 ALA 1 B 1194 ASP 1 B 1194 ASP 1 A 458 TYR 1 A 469 PRO 1 A 469 PRO 1 A 471 LYS 1 A 471 LYS 1 B 471 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	А	1315	HIS
1 B 441 ASP 1 B 1189 ALA 1 B 1194 ASP 1 A 458 TYR 1 A 469 PRO 1 A 471 LYS 1 A 488 LYS 1 B 471 LYS 1 B 471 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	В	404	LYS
1 B 1189 ALA 1 B 1194 ASP 1 A 458 TYR 1 A 469 PRO 1 A 469 PRO 1 A 471 LYS 1 A 488 LYS 1 B 471 LYS 1 B 471 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	В	441	ASP
1 B 1194 ASP 1 A 458 TYR 1 A 469 PRO 1 A 471 LYS 1 A 488 LYS 1 B 471 LYS 1 B 471 LYS 1 B 471 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	В	1189	ALA
1 A 458 TYR 1 A 469 PRO 1 A 471 LYS 1 A 471 LYS 1 A 488 LYS 1 B 471 LYS 1 B 471 LYS 1 B 1205 GLY 1 B 1205 SER	1	В	1194	ASP
1 A 469 PRO 1 A 471 LYS 1 A 488 LYS 1 B 471 LYS 1 B 471 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	A	458	TYR
1 A 471 LYS 1 A 488 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	A	469	PRO
1 A 488 LYS 1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	A	471	LYS
1 B 471 LYS 1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	A	488	LYS
1 B 553 VAL 1 B 1195 GLY 1 B 1205 SER	1	В	471	LYS
1 B 1195 GLY 1 B 1205 SER	1	В	553	VAL
1 B 1205 SER	1	В	1195	GLY
	1	В	1205	SER



e entitudea ji enti preette ae pagem					
\mathbf{Mol}	Chain	Res	Type		
1	В	412	ALA		
1	В	418	TRP		
1	В	445	SER		
1	В	507	THR		
1	В	1140	ALA		
1	А	468	PHE		
1	В	392	PRO		
1	В	394	VAL		
1	А	453	ILE		
1	А	1253	PRO		
1	В	552	PRO		

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	Percer	ntiles
1	А	815/891~(92%)	748~(92%)	67~(8%)	11	14
1	В	812/891~(91%)	716 (88%)	96 (12%)	5	5
All	All	1627/1782~(91%)	1464 (90%)	163 (10%)	7	9

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	393	VAL
1	А	394	VAL
1	А	399	ARG
1	А	408	TRP
1	А	409	LEU
1	А	414	LEU
1	А	456	THR
1	А	457	LEU
1	А	458	TYR
1	А	482	THR
1	А	504	ASN
1	А	507	THR



Mol	Chain	Res	Type
1	А	515	LEU
1	A	518	
1	A	526	LEU
1	A	546	THR
1	A	547	SER
1	A	553	VAL
1	A	555	SER.
1	A	605	LYS
1	A	622	PHE
1	A	623	ARG
1	A	701	SER.
1	A	716	ARG
- 1	A	725	VAL
1	A	726	LEU
1	A	730	ASP
1	A	755	ASP
1	A	774	ASP
1	A	796	LEU
1	A	797	GLN
1	A	798	LEU
1	A	835	LEU
1	A	839	VAL
1	A	891	LEU
1	A	896	TRP
1	A	947	GLU
1	A	949	SER
1	A	952	LEU
1	A	953	LEU
1	A	955	ASP
1	A	959	LEU
1	А	999	LEU
1	A	1032	LEU
1	A	1056	THR
1	A	1134	ARG
1	A	1137	LEU
1	A	1141	LEU
1	A	1172	ARG
1	А	1182	PHE
1	A	1187	LYS
1	A	1193	GLU
1	A	1194	ASP
1	A	1203	LEU
-			



Mol	Chain	Res	Type
1	А	1211	LYS
1	А	1214	SER
1	А	1216	LYS
1	А	1217	SER
1	А	1218	ARG
1	А	1223	LEU
1	А	1235	GLU
1	А	1240	ARG
1	А	1269	THR
1	А	1282	SER
1	А	1303	LEU
1	А	1317	SER
1	А	1321	VAL
1	В	397	ARG
1	В	398	LEU
1	В	399	ARG
1	В	400	ASN
1	В	401	ILE
1	В	408	TRP
1	В	409	LEU
1	В	414	LEU
1	В	419	GLU
1	В	421	THR
1	В	425	MET
1	В	427	CYS
1	В	431	LEU
1	В	440	TYR
1	В	446	THR
1	В	449	ASP
1	В	450	VAL
1	B	451	THR
1	В	482	THR
1	В	487	SER
1	В	488	LYS
1	В	501	ASN
1	В	503	ASP
1	В	507	THR
1	В	518	LEU
1	В	526	LEU
1	В	544	THR
1	В	554	VAL
1	В	575	LEU



Mol	Chain	Res	Type
1	В	581	ARG
1	В	586	LYS
1	В	611	ARG
1	В	621	THR
1	В	623	ARG
1	В	674	LEU
1	В	720	LYS
1	В	721	ARG
1	В	723	ARG
1	В	725	VAL
1	В	726	LEU
1	В	769	GLU
1	В	775	LYS
1	В	790	LYS
1	В	796	LEU
1	В	824	LEU
1	В	835	LEU
1	В	839	VAL
1	В	849	TYR
1	В	861	VAL
1	В	867	LEU
1	В	870	SER
1	В	889	LYS
1	В	900	LYS
1	В	905	THR
1	В	910	LEU
1	В	916	ARG
1	В	947	GLU
1	В	948	GLU
1	В	952	LEU
1	В	953	LEU
1	В	955	ASP
1	В	959	LEU
1	В	999	LEU
1	В	1036	LEU
1	В	1040	LEU
1	В	1048	LYS
1	В	1058	SER
1	В	1067	ASP
1	В	1071	LYS
1	В	1102	LYS
1	В	1110	LEU



Mol	Chain	Res	Type
1	В	1133	ARG
1	В	1137	LEU
1	В	1143	LEU
1	В	1154	LEU
1	В	1156	ARG
1	В	1191	ASP
1	В	1203	LEU
1	В	1205	SER
1	В	1216	LYS
1	В	1217	SER
1	В	1223	LEU
1	В	1236	LYS
1	В	1269	THR
1	В	1282	SER
1	В	1283	LYS
1	В	1285	ILE
1	В	1303	LEU
1	В	1308	THR
1	В	1312	LEU
1	В	1315	HIS
1	В	1321	VAL
1	В	1337	THR
1	В	1347	LEU
1	В	1360	LYS
1	В	1370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	390	HIS
1	А	557	GLN
1	А	566	GLN
1	А	579	GLN
1	А	827	GLN
1	А	843	GLN
1	В	390	HIS
1	В	501	ASN
1	В	566	GLN
1	В	665	HIS
1	В	776	HIS
1	В	777	GLN
1	В	822	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	В	1113	ASN
1	В	1299	ASN
1	В	1315	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Bog	Link	ink Bond lengths			Bond angles		
Moi Typ	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	GOL	В	3375	-	3,4,5	0.28	0	1,4,5	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	В	3375	-	-	0/2/2/4	-



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	3375	GOL	1	0

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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	436:LEU	С	437:GLY	Ν	1.62



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	935/1022~(91%)	0.84	141 (15%)	2	3	39, 50, 65, 78	0
1	В	932/1022~(91%)	1.09	190 (20%)	1	1	38, 51, 64, 77	0
All	All	1867/2044~(91%)	0.96	331 (17%)	1	1	38, 51, 64, 78	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	590	TYR	12.7
1	В	1191	ASP	11.2
1	В	507	THR	10.2
1	В	466	LYS	9.5
1	А	626	VAL	9.2
1	А	1186	MET	9.1
1	В	460	LEU	9.0
1	А	604	PRO	8.8
1	В	1189	ALA	8.8
1	В	464	ARG	8.6
1	В	626	VAL	8.6
1	В	468	PHE	8.5
1	В	443	SER	8.0
1	А	1138	GLY	8.0
1	В	1190	LYS	7.9
1	В	1192	THR	7.9
1	В	459	ARG	7.6
1	А	627	PHE	7.3
1	А	589	GLY	7.2
1	В	1195	GLY	7.2
1	В	508	ALA	7.1
1	В	469	PRO	6.9
1	В	454	TRP	6.8
1	В	1184	ASN	6.5



|--|

Mol	Chain	Res	Type	RSRZ
1	В	607	ILE	6.2
1	В	1185	ALA	6.2
1	А	1141	LEU	6.1
1	В	428	LYS	6.1
1	В	546	THR	6.0
1	А	1218	ARG	5.9
1	А	457	LEU	5.9
1	А	1191	ASP	5.9
1	А	468	PHE	5.8
1	А	467	PRO	5.7
1	А	849	TYR	5.7
1	А	1254	TYR	5.6
1	В	512	LEU	5.6
1	В	1188	ALA	5.5
1	А	1187	LYS	5.5
1	А	1188	ALA	5.5
1	А	1222	LEU	5.4
1	В	488	LYS	5.4
1	В	589	GLY	5.4
1	А	1192	THR	5.3
1	В	1194	ASP	5.3
1	В	1154	LEU	5.3
1	А	1185	ALA	5.1
1	В	396	ALA	5.1
1	В	1156	ARG	5.0
1	В	436	LEU	4.8
1	А	1193	GLU	4.8
1	В	1252	ASP	4.7
1	А	399	ARG	4.6
1	В	1218	ARG	4.6
1	А	605	LYS	4.6
1	А	1372	GLY	4.6
1	А	420	VAL	4.6
1	А	458	TYR	4.6
1	А	559	ALA	4.5
1	А	1217	SER	4.5
1	А	558	PRO	4.5
1	В	425	MET	4.4
1	А	396	ALA	4.4
1	В	1254	TYR	4.3
1	А	1215	ASP	4.3
1	В	739	PHE	4.3



2J	[7N
$\Delta \mathbf{J}$	111

Mol	Chain	Res	Type	RSRZ
1	А	1166	LEU	4.3
1	А	1373	ASP	4.2
1	В	1140	ALA	4.2
1	А	466	LYS	4.2
1	В	1373	ASP	4.2
1	В	467	PRO	4.1
1	А	438	LEU	4.1
1	В	440	TYR	4.1
1	В	503	ASP	4.1
1	А	1189	ALA	4.1
1	В	429	VAL	4.1
1	В	1186	MET	4.0
1	В	780	LEU	4.0
1	В	1137	LEU	4.0
1	А	469	PRO	4.0
1	В	510	LEU	4.0
1	В	463	PHE	4.0
1	А	1304	LEU	4.0
1	В	620	ILE	4.0
1	А	409	LEU	4.0
1	А	588	ALA	4.0
1	В	449	ASP	4.0
1	В	1157	GLY	3.9
1	В	849	TYR	3.9
1	А	989	ILE	3.9
1	А	546	THR	3.9
1	А	1190	LYS	3.9
1	В	553	VAL	3.9
1	А	395	ALA	3.9
1	В	456	THR	3.8
1	В	947	GLU	3.8
1	В	520	PHE	3.8
1	В	623	ARG	3.8
1	А	547	SER	3.8
1	А	606	PRO	3.8
1	В	1015	VAL	3.8
1	В	439	LYS	3.8
1	В	989	ILE	3.8
1	В	1182	PHE	3.7
1	В	470	GLU	3.7
1	В	461	ASP	3.7
1	В	1138	GLY	3.7

Continued from previous page...



Mol	Chain	Res	Type	RSRZ
1	А	1315	HIS	3.7
1	А	464	ARG	3.7
1	В	1187	LYS	3.6
1	В	1166	LEU	3.6
1	А	641	GLN	3.6
1	А	1163	ILE	3.6
1	В	518	LEU	3.6
1	В	434	GLU	3.6
1	В	442	PRO	3.5
1	В	548	PRO	3.5
1	В	391	ALA	3.5
1	В	559	ALA	3.5
1	А	417	ALA	3.5
1	В	651	LEU	3.5
1	В	1151	ASP	3.5
1	А	759	ILE	3.5
1	В	588	ALA	3.5
1	А	1184	ASN	3.4
1	В	398	LEU	3.4
1	В	558	PRO	3.4
1	А	400	ASN	3.4
1	В	433	ASP	3.3
1	В	472	PRO	3.3
1	В	1193	GLU	3.3
1	А	620	ILE	3.3
1	А	1282	SER	3.3
1	В	545	SER	3.3
1	В	960	VAL	3.3
1	В	570	MET	3.3
1	А	1107	LEU	3.3
1	В	991	PHE	3.3
1	В	412	ALA	3.2
1	В	1107	LEU	3.2
1	A	463	PHE	3.2
1	В	413	PRO	3.2
1	В	505	SER	3.2
1	В	404	LYS	3.2
1	В	755	ASP	3.2
1	A	555	SER	3.2
1	B	971	ILE	3.2
1	В	511	TYR	3.1
1	A	960	VAL	3.1



Continued from previous page					
Mol	Chain	Res	Type	RSRZ	
1	В	1217	SER	3.1	
1	А	390	HIS	3.1	
1	В	1282	SER	3.1	
1	В	1216	LYS	3.1	
1	В	502	PRO	3.1	
1	А	923	ILE	3.1	
1	А	990	ILE	3.1	
1	В	390	HIS	3.0	
1	В	1257	ARG	3.0	
1	А	991	PHE	3.0	
1	В	1016	CYS	3.0	
1	А	570	MET	3.0	
1	В	563	GLU	3.0	
1	A	1015	VAL	3.0	
1	A	510	LEU	3.0	
1	А	701	SER	3.0	
1	А	1210	PHE	3.0	
1	В	437	GLY	3.0	
1	В	1065	THR	3.0	
1	В	1068	MET	3.0	
1	А	780	LEU	3.0	
1	В	448	ARG	3.0	
1	В	409	LEU	2.9	
1	В	432	GLU	2.9	
1	В	1222	LEU	2.9	
1	А	560	ALA	2.9	
1	В	625	ASP	2.9	
1	В	556	LYS	2.9	
1	В	1074	HIS	2.9	
1	В	455	LYS	2.9	
1	А	459	ARG	2.9	
1	В	458	TYR	2.9	
1	А	1140	ALA	2.9	
1	В	1219	SER	2.9	
1	А	1139	GLY	2.8	
1	В	494	LEU	2.8	
1	В	392	PRO	2.8	
1	В	1253	PRO	2.8	
1	В	547	SER	2.8	
1	В	1265	TRP	2.8	
1	В	1215	ASP	2.8	
1	А	1110	LEU	2.8	

A1110LEU2.8Continued on next page...



2.	J7	'N
<u></u>	1	ΤN

Mol	Chain	Res	Type	RSRZ
1	А	1162	ILE	2.8
1	В	501	ASN	2.8
1	В	418	TRP	2.8
1	А	999	LEU	2.7
1	А	1321	VAL	2.7
1	А	428	LYS	2.7
1	А	394	VAL	2.7
1	В	424	PHE	2.7
1	А	1068	MET	2.7
1	А	1211	LYS	2.7
1	В	1212	GLU	2.7
1	В	999	LEU	2.7
1	А	439	LYS	2.7
1	В	988	VAL	2.7
1	В	482	THR	2.7
1	В	1141	LEU	2.7
1	В	430	ASP	2.7
1	В	414	LEU	2.7
1	А	461	ASP	2.6
1	А	1237	GLU	2.6
1	В	399	ARG	2.6
1	В	1296	ARG	2.6
1	А	556	LYS	2.6
1	В	1132	LEU	2.6
1	В	506	PRO	2.6
1	А	423	LEU	2.6
1	В	1356	LEU	2.6
1	В	1063	GLN	2.6
1	А	850	SER	2.6
1	В	1177	LYS	2.6
1	А	506	PRO	2.6
1	А	541	PRO	2.6
1	А	959	LEU	2.6
1	А	1183	HIS	2.6
1	А	755	ASP	2.6
1	А	465	GLY	2.6
1	В	465	GLY	2.6
1	В	850	SER	2.5
1	А	802	LEU	2.5
1	А	1132	LEU	2.5
1	В	427	CYS	2.5
1	В	759	ILE	2.5



2.	J7	'N
<u></u>	1	ΤN

Mol	Chain	Res	Type	RSRZ
1	В	990	ILE	2.5
1	В	438	LEU	2.5
1	В	959	LEU	2.5
1	А	1316	LYS	2.5
1	А	391	ALA	2.5
1	А	421	THR	2.5
1	А	548	PRO	2.5
1	В	471	LYS	2.5
1	А	796	LEU	2.5
1	А	1137	LEU	2.5
1	В	1180	GLU	2.5
1	А	971	ILE	2.5
1	В	1139	GLY	2.5
1	А	511	TYR	2.5
1	В	924	ALA	2.4
1	А	739	PHE	2.4
1	A	801	VAL	2.4
1	А	1252	ASP	2.4
1	В	1309	ALA	2.4
1	В	938	GLY	2.4
1	А	946	GLU	2.4
1	В	1220	SER	2.4
1	В	1155	GLY	2.3
1	А	502	PRO	2.3
1	А	668	LEU	2.3
1	А	924	ALA	2.3
1	В	1223	LEU	2.3
1	A	416	VAL	2.3
1	В	492	VAL	2.3
1	А	1239	GLY	2.3
1	A	1120	GLN	2.3
1	A	424	PHE	2.3
1	А	642	ARG	2.3
1	A	540	ILE	2.3
1	В	1354	ALA	2.3
1	В	1064	THR	2.3
1	В	1133	ARG	2.3
1	А	1069	ILE	2.3
1	В	951	THR	2.2
1	А	448	ARG	2.2
1	A	623	ARG	2.2
1	А	1371	GLU	2.2



2.	17	Ν

Mol	Chain	Res	Type	RSRZ	
1	А	1285	ILE	2.2	
1	В	616	ALA	2.2	
1	В	1163	ILE	2.2	
1	А	507	THR	2.2	
1	В	740	GLY	2.2	
1	А	988	VAL	2.2	
1	А	799	LEU	2.2	
1	А	1236	LYS	2.2	
1	А	1116	ASP	2.2	
1	А	1032	LEU	2.2	
1	В	450	VAL	2.2	
1	В	395	ALA	2.2	
1	В	446	THR	2.2	
1	А	740	GLY	2.2	
1	В	1149	LYS	2.2	
1	В	1162	ILE	2.1	
1	В	457	LEU	2.1	
1	В	1236	LYS	2.1	
1	В	420	VAL	2.1	
1	В	735	VAL	2.1	
1	В	923	ILE	2.1	
1	В	1072	SER	2.1	
1	А	711	VAL	2.1	
1	В	435	SER	2.1	
1	А	746	TRP	2.1	
1	А	742	ALA	2.1	
1	А	951	THR	2.1	
1	А	1354	ALA	2.1	
1	A	672	ILE	2.1	
1	В	802	LEU	2.1	
1	В	1352	MET	2.1	
1	A	434	GLU	2.1	
1	В	711	VAL	2.1	
1	В	403	PRO	2.1	
1	В	714	MET	2.1	
1	A	937	VAL	2.1	
1	В	473	PRO	2.1	
1	В	509	PRO	2.1	
1	В	410	HIS	2.0	
1	А	820	LEU	2.0	
1	В	498	LEU	2.0	
1	В	912	ILE	2.0	



Mol	Chain	Res	Type	RSRZ
1	В	519	MET	2.0
1	А	703	THR	2.0
1	В	1150	SER	2.0
1	В	937	VAL	2.0
1	В	1183	HIS	2.0
1	В	1231	ILE	2.0
1	А	869	ASP	2.0
1	А	494	LEU	2.0
1	А	1021	ILE	2.0
1	В	672	ILE	2.0
1	В	1110	LEU	2.0
1	В	1143	LEU	2.0
1	В	1035	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	GOL	В	3375	5/6	0.89	0.21	66,67,67,67	0
2	MG	А	3374	1/1	0.95	0.05	50,50,50,50	0
2	MG	В	3374	1/1	0.98	0.10	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.

