

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7XHL
Title	:	Complex structure of a Glucose 6-Phosphate Dehydrogenase from Zymomonas
		mobilis
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Deposited on	:	2022-04-08
Resolution	:	3.25 Å(reported)

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

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

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	Quali	ty of chain	
1	А	487	% 41%	47%	11% •
1	В	487	4%	43%	12% •
1	С	487	3% 56%	34%	5% 5%
1	D	487	2% 46%	45%	7% •
1	Е	487	44%	45%	9% •
1	F	487	46%	40%	8% 5%



Mol	Chain	Length	Qua	ality of chain	
1	G	487	.% 44%	49%	7%
1	Н	487	.% • 44%	46%	9% •

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	NMN	А	501	-	-	Х	-
2	NMN	В	501	-	-	Х	Х



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	499	Total	С	Ν	0	S	0	0	0
1	A	402	3712	2357	647	698	10	0	0	0
1	В	470	Total	С	Ν	0	S	0	0	0
	D	419	3625	2294	633	689	9	0	0	0
1	С	463	Total	С	Ν	0	S	0	Ο	0
1	U	405	3027	1896	552	573	6	0	0	0
1	л	470	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	D	415	3545	2250	606	679	10	0	0	0
1	F	476	Total	С	Ν	Ο	\mathbf{S}	0	0	0
T	Ľ	470	3587	2276	621	681	9	0	0	0
1	F	462	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	402	3378	2135	600	634	9	0	0	0
1	C	485	Total	С	Ν	0	\mathbf{S}	0	0	0
1	G	405	3735	2366	649	710	10	0	0	0
1	Ц	481	Total	С	Ν	0	S	0	0	0
	11	401	3679	2336	634	699	10	0	0	0

• Molecule 1 is a protein called Glucose 6-Phosphate Dehydrogenase.

• Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula: $C_{11}H_{16}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	Δ	1	Total	С	Ν	0	Р	0	0	
2	Π	T	22	11	2	8	1	0	0	
9	В	1	1 Total		Ν	0	Р	0	0	
	D		22	11	2	8	1	0	0	
0	F	1	Total	С	Ν	0	Р	0	0	
	Ľ	L	22	11	2	8	1	0	0	
0	С	1	Total	С	Ν	Ο	Р	0	0	
	G		22	11	2	8	1	U	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.















112 113









420

341

PDB EIN DATA BANK







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	80.32Å 342.33Å 103.36Å	Deneriten
a, b, c, α , β , γ	90.00° 92.66° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	78.11 - 3.25	Depositor
Resolution (A)	88.41 - 3.25	EDS
% Data completeness	98.8 (78.11-3.25)	Depositor
(in resolution range)	$83.3 \ (88.41 - 3.25)$	EDS
R _{merge}	0.15	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.80 (at 3.26 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.237 , 0.297	Depositor
Π, Π_{free}	0.250 , 0.283	DCC
R_{free} test set	4294 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	66.7	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 66.9	EDS
L-test for twinning ²	$< L >=0.39, < L^2>=0.21$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
Reported twinning fraction	0.200 for h,-k,-l	Depositor
Outliers	0 of 86165 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28376	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.54% 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: NMN

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	Mol Chain		lengths	Bond angles		
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.56	0/3790	0.79	0/5146	
1	В	0.55	0/3696	0.82	0/5028	
1	С	0.53	0/3079	0.78	0/4224	
1	D	0.55	0/3620	0.81	0/4945	
1	Е	0.56	0/3660	0.80	0/4983	
1	F	0.58	0/3444	0.81	0/4692	
1	G	0.52	0/3810	0.78	0/5173	
1	Н	0.54	0/3754	0.79	0/5104	
All	All	0.55	0/28853	0.80	0/39295	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3712	0	3640	246	0
1	В	3625	0	3513	271	0
1	С	3027	0	2453	157	0
1	D	3545	0	3326	204	0
1	Е	3587	0	3445	257	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3378	0	3145	213	0
1	G	3735	0	3668	223	0
1	Н	3679	0	3590	268	0
2	А	22	0	14	16	0
2	В	22	0	14	7	0
2	Е	22	0	14	4	0
2	G	22	0	14	5	0
All	All	28376	0	26836	1754	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 32.

All (1754) 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:E:54:PHE:CD2	1:E:84:PHE:HA	1.76	1.21
1:E:54:PHE:CE2	1:E:84:PHE:HA	1.84	1.13
1:A:144:LYS:HE3	2:A:501:NMN:C6	1.78	1.12
1:E:54:PHE:HE2	1:E:84:PHE:CB	1.63	1.11
1:E:54:PHE:HE2	1:E:84:PHE:HB3	1.10	1.10
1:E:54:PHE:CE2	1:E:84:PHE:HB3	1.91	1.05
1:E:54:PHE:CE2	1:E:84:PHE:CA	2.40	1.05
1:B:144:LYS:HE2	2:B:501:NMN:HC6	1.38	1.03
1:A:144:LYS:HE3	2:A:501:NMN:C5	1.90	1.00
1:C:211:ALA:HB3	1:C:340:ARG:H	1.28	0.97
1:D:476:VAL:HG22	1:D:481:VAL:HG13	1.47	0.96
1:E:474:ALA:HA	1:E:477:GLU:HB2	1.48	0.95
1:E:40:ARG:HB3	1:E:84:PHE:HE2	1.30	0.94
1:G:400:LEU:HD23	1:H:402:LEU:HB3	1.51	0.92
1:E:54:PHE:CE2	1:E:84:PHE:CB	2.50	0.92
1:E:54:PHE:HE2	1:E:84:PHE:CA	1.77	0.92
1:G:18:SER:HA	1:G:22:LEU:HB2	1.49	0.92
1:C:237:ILE:HA	1:C:240:LEU:HD12	1.52	0.92
1:A:45:SER:HB3	1:A:85:TYR:HE2	1.32	0.91
1:D:229:LEU:HA	1:D:233:VAL:HG12	1.50	0.91
1:A:419:ARG:HG2	1:B:388:LEU:HD22	1.52	0.90
1:D:8:MET:HG3	1:D:111:ALA:HB3	1.50	0.90
1:F:25:ALA:HA	1:F:415:ILE:HD13	1.51	0.90
1:F:144:LYS:HG3	1:F:145:PRO:HD3	1.54	0.88
2:B:501:NMN:H5R1	2:B:501:NMN:HC2	1.55	0.87
1:G:388:LEU:HA	1:H:419:ARG:HE	1.40	0.87



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:238:LEU:HD23	1:E:441:GLN:HG2	1.57	0.87
1:G:384:LYS:HB2	1:H:186:THR:HG21	1.56	0.86
1:E:476:VAL:HG22	1:E:481:VAL:HG23	1.56	0.86
1:F:275:THR:HG22	1:F:279:HIS:HD2	1.40	0.86
1:E:20:ARG:HA	1:E:65:PHE:CE2	2.11	0.85
1:F:262:VAL:HG22	1:F:437:GLU:HG3	1.58	0.85
1:G:271:ILE:HG13	1:G:448:ILE:HG13	1.58	0.85
1:H:99:ILE:HB	1:H:133:LEU:HD11	1.59	0.84
1:B:198:TRP:HH2	1:B:367:LEU:HD23	1.40	0.84
1:B:452:TRP:HB2	1:B:457:MET:HB2	1.58	0.84
1:A:257:VAL:HG12	1:A:261:LYS:HD2	1.60	0.84
1:G:95:GLN:O	1:G:98:LYS:HG3	1.78	0.84
1:E:233:VAL:O	1:E:238:LEU:HD13	1.78	0.84
1:D:54:PHE:HE2	1:D:83:LEU:HD12	1.40	0.83
1:E:12:GLY:HA2	1:E:46:ARG:HG2	1.59	0.83
1:E:340:ARG:HG2	1:E:372:GLN:HG2	1.60	0.83
1:A:411:ARG:HD3	1:B:386:PRO:HD2	1.61	0.83
1:C:463:VAL:O	1:C:466:THR:HG22	1.77	0.83
1:E:54:PHE:HD2	1:E:84:PHE:HA	1.42	0.82
1:A:479:ASP:HB2	1:A:481:VAL:HG12	1.62	0.82
1:C:154:ASP:HA	1:C:435:ARG:NH2	1.95	0.81
1:E:369:ILE:HG23	1:E:377:ILE:HG12	1.58	0.81
1:E:273:ASN:HA	1:E:451:GLY:CA	2.10	0.81
1:G:281:VAL:HB	1:G:313:ALA:HB3	1.62	0.81
1:G:233:VAL:HG21	1:G:312:VAL:HG11	1.62	0.81
1:H:359:GLY:O	1:H:394:HIS:HD2	1.63	0.81
1:F:114:LEU:HD13	1:F:140:LEU:HD21	1.63	0.80
1:G:17:LEU:HD22	2:G:501:NMN:C2	2.11	0.80
1:B:216:LEU:H	1:B:216:LEU:HD22	1.45	0.80
1:B:229:LEU:HA	1:B:233:VAL:HG13	1.64	0.80
1:B:144:LYS:HG3	1:B:145:PRO:HD3	1.63	0.79
1:A:45:SER:HB3	1:A:85:TYR:CE2	2.16	0.79
1:C:180:THR:HG21	1:C:371:LEU:HA	1.63	0.79
1:A:125:ILE:HA	1:A:128:LEU:HD12	1.65	0.79
1:C:381:ILE:HD11	1:C:400:LEU:HG	1.64	0.79
1:B:97:GLY:HA2	1:B:131:ALA:HB1	1.64	0.79
1:E:144:LYS:HG3	1:E:145:PRO:HD3	1.61	0.79
1:F:242:ALA:HA	1:F:264:VAL:HG21	1.65	0.78
1:F:306:SER:HB2	1:F:308:THR:HG22	1.66	0.78
1:A:17:LEU:HD22	2:A:501:NMN:H5R2	1.63	0.78
1:A:48:GLU:HB3	1:A:49:TYR:CD1	2.18	0.78



	• • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:466:THR:HG23	1:G:289:VAL:HG22	1.66	0.78
1:G:408:PHE:HE1	1:H:385:GLU:HG2	1.47	0.78
1:A:50:ASP:HA	1:A:85:TYR:CE1	2.19	0.78
1:B:429:ALA:HA	1:B:432:PHE:CD1	2.19	0.77
1:H:476:VAL:HG22	1:H:481:VAL:HG22	1.66	0.77
1:E:370:VAL:HB	1:E:372:GLN:HG3	1.64	0.77
1:D:229:LEU:HA	1:D:233:VAL:CG1	2.14	0.77
1:H:285:TYR:CD1	1:H:335:ARG:HG3	2.20	0.77
1:E:452:TRP:HB2	1:E:457:MET:HB2	1.67	0.77
1:B:88:VAL:HG13	1:B:95:GLN:HB3	1.66	0.77
1:D:312:VAL:HG12	1:D:332:THR:HG22	1.67	0.77
1:G:340:ARG:HA	1:G:373:PRO:HG3	1.67	0.76
1:G:389:ASP:H	1:H:419:ARG:HH21	1.32	0.76
1:H:203:ILE:HD11	1:H:345:VAL:HG13	1.66	0.76
1:A:216:LEU:HD12	1:A:219:ARG:HB2	1.68	0.76
1:D:54:PHE:CE2	1:D:83:LEU:HD12	2.20	0.76
1:B:5:VAL:HG22	1:B:109:GLY:HA3	1.68	0.76
1:B:216:LEU:HB2	1:B:220:ILE:HG23	1.66	0.76
1:G:144:LYS:HB3	1:G:145:PRO:HD3	1.66	0.76
1:A:46:ARG:H	1:A:46:ARG:HD3	1.51	0.76
1:F:10:LEU:HB3	1:F:42:VAL:O	1.85	0.76
1:G:125:ILE:HD12	1:G:160:VAL:HG22	1.66	0.76
1:E:40:ARG:HG3	1:E:105:PRO:HG2	1.66	0.76
1:E:337:PRO:HD2	1:E:467:TRP:CE3	2.21	0.76
1:F:23:LEU:HA	1:F:26:LEU:HD12	1.68	0.76
1:A:377:ILE:HG13	1:A:404:LEU:HD11	1.66	0.75
1:H:30:ASP:HA	1:H:35:LEU:HD11	1.67	0.75
1:A:49:TYR:HB3	1:A:54:PHE:HB2	1.69	0.75
1:E:449:ARG:HA	1:E:452:TRP:CE2	2.21	0.75
1:H:114:LEU:HD13	1:H:140:LEU:HD11	1.68	0.75
1:B:381:ILE:HG13	1:B:398:VAL:HG23	1.67	0.75
1:G:175:TYR:HA	1:G:178:LYS:HD2	1.68	0.75
1:D:23:LEU:HA	1:D:26:LEU:HD12	1.67	0.75
1:E:17:LEU:HB3	2:E:501:NMN:O2P	1.87	0.75
1:C:199:ASN:HB2	1:C:201:LYS:O	1.86	0.75
1:F:112:ILE:HD11	1:F:138:SER:HB2	1.67	0.75
1:E:207:GLN:HG2	1:E:329:TYR:HB2	1.68	0.74
1:B:265:PHE:HE2	1:B:437:GLU:HG2	1.51	0.74
1:H:216:LEU:HD22	1:H:223:PHE:HB2	1.69	0.74
1:B:215:GLY:HA2	1:B:334:LYS:HE3	1.70	0.74
1:D:255:ASN:O	1:D:259:ASP:N	2.20	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:365:ASN:ND2	1:F:380:SER:O	2.20	0.74
1:E:273:ASN:HA	1:E:451:GLY:HA3	1.70	0.73
1:B:258:ARG:HD2	1:B:434:ARG:HB2	1.68	0.73
1:G:222:TYR:OH	2:G:501:NMN:H2RC	1.87	0.73
1:E:9:ILE:HD13	1:E:112:ILE:HG12	1.69	0.73
1:D:152:SER:O	1:D:156:ILE:HG12	1.89	0.73
1:C:381:ILE:HD12	1:C:398:VAL:HG13	1.71	0.73
1:C:13:SER:HA	1:C:18:SER:CB	2.20	0.72
1:C:337:PRO:HG2	1:C:467:TRP:CE2	2.25	0.72
1:C:400:LEU:HD23	1:D:402:LEU:HB3	1.71	0.72
1:E:40:ARG:HB3	1:E:84:PHE:CE2	2.20	0.72
1:B:110:ILE:O	1:B:138:SER:HA	1.90	0.72
1:E:135:GLY:CA	1:E:138:SER:HB2	2.19	0.72
1:H:203:ILE:HG21	1:H:323:TRP:HZ3	1.55	0.72
1:F:408:PHE:HB3	1:F:411:ARG:HB2	1.72	0.72
1:G:271:ILE:HD11	1:G:444:TRP:O	1.88	0.72
1:B:27:TYR:OH	1:B:71:LEU:HA	1.90	0.71
1:H:233:VAL:O	1:H:238:LEU:HB2	1.90	0.71
1:H:439:GLU:O	1:H:443:ILE:HG13	1.90	0.71
1:G:66:VAL:HG11	1:G:71:LEU:HD13	1.71	0.71
1:A:193:LEU:HA	1:B:197:LEU:HD11	1.71	0.71
1:G:269:ARG:HB3	1:G:317:HIS:HB2	1.73	0.71
1:A:386:PRO:HD2	1:B:408:PHE:CE1	2.26	0.71
1:E:73:ASP:HA	1:E:76:LYS:HD3	1.73	0.71
1:H:265:PHE:HE2	1:H:437:GLU:HB3	1.56	0.71
1:G:118:SER:CB	1:G:146:LEU:HA	2.21	0.71
1:B:312:VAL:HG12	1:B:332:THR:HG22	1.73	0.70
1:C:376:THR:HG22	1:C:403:SER:HA	1.73	0.70
1:A:6:SER:O	1:A:39:LEU:HA	1.91	0.70
1:E:52:ASP:N	1:E:87:THR:HG1	1.89	0.70
1:G:40:ARG:HB3	1:G:84:PHE:CE2	2.26	0.70
1:H:462:TYR:HB2	1:H:466:THR:HG21	1.73	0.70
1:C:18:SER:HA	1:C:23:LEU:H	1.57	0.70
1:C:183:ASN:HB2	1:D:384:LYS:H	1.57	0.70
1:D:77:ALA:HA	1:D:80:LEU:HD12	1.74	0.70
1:F:70:ARG:HH21	1:F:415:ILE:HD12	1.56	0.70
1:H:203:ILE:HA	1:H:347:PHE:HA	1.73	0.70
1:A:165:SER:OG	1:A:167:LYS:NZ	2.24	0.70
1:D:7:THR:O	1:D:110:ILE:HA	1.92	0.70
1:E:54:PHE:CD2	1:E:84:PHE:CA	2.61	0.70
1:F:229:LEU:O	1:F:233:VAL:HG22	1.91	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:190:GLY:HA2	1:D:362:LEU:HD11	1.73	0.69
1:G:6:SER:HB2	1:G:109:GLY:C	2.12	0.69
1:E:166:GLU:HA	1:E:169:VAL:HG22	1.74	0.69
1:B:90:ILE:HA	1:B:96:PHE:CZ	2.27	0.69
1:B:170:TYR:CE2	1:B:429:ALA:HB2	2.27	0.69
1:E:340:ARG:HA	1:E:372:GLN:HB3	1.73	0.69
1:F:114:LEU:HD22	1:F:140:LEU:HD11	1.73	0.69
1:D:302:LEU:HD22	1:D:306:SER:HB2	1.73	0.69
1:A:118:SER:HA	1:A:121:PHE:CD2	2.28	0.69
1:B:97:GLY:HA2	1:B:131:ALA:CB	2.21	0.69
1:E:22:LEU:HD23	1:E:421:LEU:HD11	1.73	0.69
1:A:204:ASP:OD2	1:A:346:GLN:NE2	2.25	0.69
1:H:375:GLU:HB3	1:H:404:LEU:HB2	1.74	0.69
1:B:143:GLU:HB3	1:B:145:PRO:HD2	1.72	0.69
1:D:339:ARG:O	1:D:373:PRO:HD3	1.92	0.69
1:E:165:SER:O	1:E:169:VAL:HG13	1.93	0.69
1:B:422:LEU:O	1:B:426:GLU:HG2	1.93	0.69
1:B:29:LEU:HD22	1:B:422:LEU:HD13	1.75	0.69
1:F:281:VAL:HB	1:F:313:ALA:HB3	1.73	0.68
1:E:63:ASP:HA	1:E:71:LEU:HD21	1.74	0.68
1:F:275:THR:HG22	1:F:279:HIS:CD2	2.25	0.68
1:E:197:LEU:HD11	1:F:193:LEU:HA	1.73	0.68
1:E:213:THR:HG23	1:E:336:LEU:O	1.94	0.68
1:E:283:GLY:HA2	1:E:460:LYS:O	1.93	0.68
1:H:7:THR:OG1	1:H:104:GLY:HA3	1.93	0.68
1:H:339:ARG:O	1:H:373:PRO:HD3	1.93	0.68
1:B:197:LEU:HB3	1:B:347:PHE:CE1	2.28	0.68
1:A:435:ARG:O	1:A:439:GLU:HG2	1.94	0.68
1:F:9:ILE:HA	1:F:42:VAL:HB	1.76	0.68
1:H:476:VAL:HG13	1:H:481:VAL:O	1.94	0.68
1:G:341:SER:H	1:G:373:PRO:HD3	1.59	0.67
1:B:29:LEU:HB3	1:B:35:LEU:HG	1.75	0.67
1:G:197:LEU:O	1:G:202:GLY:HA3	1.94	0.67
1:B:215:GLY:N	1:B:335:ARG:HD2	2.10	0.67
1:E:166:GLU:O	1:E:169:VAL:HG22	1.94	0.67
1:A:26:LEU:HA	1:A:29:LEU:HD12	1.77	0.67
1:B:170:TYR:HB3	1:B:432:PHE:CD2	2.30	0.67
1:G:203:ILE:HA	1:G:347:PHE:HA	1.77	0.67
1:A:146:LEU:O	1:A:153:SER:HB3	1.95	0.67
1:A:17:LEU:HB2	2:A:501:NMN:O7	1.95	0.66
1:H:114:LEU:HB3	1:H:121:PHE:CE1	2.30	0.66



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:143:GLU:HG3	2:A:501:NMN:O4R	1.95	0.66
1:D:18:SER:HA	1:D:22:LEU:HB2	1.75	0.66
1:F:245:ALA:HA	1:F:323:TRP:CZ2	2.30	0.66
1:H:156:ILE:O	1:H:160:VAL:HG23	1.95	0.66
1:G:37:ASP:HA	1:G:82:LYS:HE2	1.77	0.66
1:E:56:ASP:O	1:E:59:GLU:N	2.28	0.66
1:C:183:ASN:OD1	1:D:383:VAL:HG23	1.95	0.66
1:A:224:ASP:O	1:A:308:THR:HG21	1.96	0.66
1:E:265:PHE:HA	1:E:268:LEU:HD12	1.76	0.66
1:A:55:ARG:HB3	1:A:80:LEU:CD2	2.26	0.66
1:E:341:SER:H	1:E:372:GLN:HB3	1.60	0.66
1:G:11:PHE:CZ	1:G:128:LEU:HD21	2.30	0.66
1:B:27:TYR:CD2	1:B:66:VAL:HG21	2.31	0.66
1:F:200:SER:HA	1:F:326:VAL:HG21	1.78	0.65
1:H:169:VAL:HG11	1:H:171:ARG:CZ	2.26	0.65
1:A:140:LEU:HD12	1:A:164:PHE:CD2	2.31	0.65
1:A:207:GLN:HG2	1:A:329:TYR:HB2	1.78	0.65
1:F:112:ILE:HB	1:F:140:LEU:HD23	1.78	0.65
1:G:259:ASP:OD1	1:G:434:ARG:NH1	2.29	0.65
1:A:387:GLY:HA3	1:A:394:HIS:CE1	2.30	0.65
1:B:13:SER:HA	1:B:18:SER:CB	2.27	0.65
1:G:18:SER:HA	1:G:22:LEU:CB	2.24	0.65
1:H:216:LEU:HD22	1:H:223:PHE:CB	2.27	0.65
1:G:25:ALA:HB1	1:G:418:GLU:HG3	1.77	0.65
1:A:411:ARG:CD	1:B:386:PRO:HD2	2.27	0.65
1:E:122:GLU:HA	1:E:125:ILE:HD12	1.77	0.65
1:A:423:ASP:O	1:A:427:GLY:N	2.30	0.65
1:B:265:PHE:CE2	1:B:437:GLU:HG2	2.32	0.65
1:D:117:SER:H	1:D:120:LEU:HD12	1.61	0.65
1:E:110:ILE:O	1:E:138:SER:HA	1.97	0.65
1:A:115:ALA:O	2:A:501:NMN:H4RC	1.97	0.65
1:C:25:ALA:HB2	1:C:415:ILE:HD12	1.77	0.65
1:F:9:ILE:HB	1:F:112:ILE:HA	1.79	0.65
1:A:419:ARG:O	1:A:422:LEU:HD23	1.97	0.65
1:A:450:GLU:HA	1:A:453:LYS:HD2	1.76	0.65
1:E:21:MET:O	1:E:22:LEU:HB2	1.97	0.65
1:B:237:ILE:HG21	1:B:330:ILE:HG23	1.80	0.64
1:D:378:GLN:HB2	1:D:399:TRP:CE3	2.32	0.64
1:C:277:ILE:HG23	1:C:278:THR:HG23	1.78	0.64
1:B:3:ASN:HB3	1:B:139:ARG:HH21	1.62	0.64
1:B:337:PRO:HD3	1:B:467:TRP:H	1.62	0.64



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:7:THR:O	1:C:110:ILE:HA	1.98	0.64
1:D:233:VAL:HA	1:D:237:ILE:HB	1.80	0.64
1:E:113:TYR:HA	1:E:141:ALA:HB3	1.77	0.64
1:C:282:THR:O	1:C:469:PRO:HG3	1.97	0.64
1:D:40:ARG:NH1	1:D:102:LEU:O	2.30	0.64
1:E:246:MET:HE3	1:E:249:PRO:HD3	1.79	0.64
1:F:128:LEU:O	1:F:133:LEU:HB3	1.97	0.64
1:H:80:LEU:HA	1:H:83:LEU:HD12	1.78	0.64
1:F:128:LEU:HA	1:F:131:ALA:HB3	1.78	0.64
1:B:5:VAL:HA	1:B:109:GLY:H	1.63	0.64
1:B:229:LEU:HB2	1:B:312:VAL:HG21	1.79	0.64
1:E:281:VAL:HG11	1:E:472:ALA:HB2	1.80	0.64
1:F:58:ALA:O	1:F:62:LEU:HB2	1.97	0.64
1:H:29:LEU:HA	1:H:34:LEU:HD12	1.80	0.64
1:B:161:LEU:HD21	1:B:435:ARG:HE	1.63	0.64
1:E:340:ARG:HG2	1:E:372:GLN:CG	2.28	0.64
1:B:112:ILE:HD11	1:B:138:SER:HB3	1.79	0.63
1:B:449:ARG:HA	1:B:452:TRP:CE2	2.34	0.63
1:C:462:TYR:CD1	1:C:468:GLY:HA2	2.34	0.63
1:D:262:VAL:HG22	1:D:437:GLU:HG3	1.80	0.63
1:F:161:LEU:HG	1:F:166:GLU:HB2	1.79	0.63
1:G:166:GLU:HA	1:G:169:VAL:HG22	1.80	0.63
1:H:169:VAL:C	1:H:170:TYR:HD1	2.01	0.63
1:G:389:ASP:H	1:H:419:ARG:NH2	1.95	0.63
1:E:370:VAL:HB	1:E:372:GLN:CG	2.29	0.63
1:H:255:ASN:HA	1:H:434:ARG:NH1	2.13	0.63
1:H:277:ILE:HG23	1:H:278:THR:HG23	1.81	0.63
1:E:372:GLN:HB2	1:E:373:PRO:HD2	1.79	0.63
1:G:112:ILE:HG13	1:G:139:ARG:O	1.98	0.63
1:D:462:TYR:HB2	1:D:466:THR:CG2	2.28	0.63
1:H:254:ALA:HB2	1:H:430:THR:HB	1.80	0.63
1:E:372:GLN:NE2	1:E:374:ASP:OD2	2.29	0.63
1:E:462:TYR:HD2	1:E:466:THR:HG22	1.64	0.63
1:G:408:PHE:CE1	1:H:385:GLU:HG2	2.33	0.63
1:B:70:ARG:NH1	1:B:414:ARG:HB2	2.14	0.63
1:F:419:ARG:HE	1:F:431:LEU:HD11	1.62	0.63
1:A:24:PRO:HB3	1:A:66:VAL:HG22	1.80	0.63
1:G:167:LYS:HG3	1:G:168:GLN:HG3	1.81	0.63
1:H:204:ASP:HB3	1:H:346:GLN:HE21	1.64	0.63
1:A:342:GLU:OE2	1:A:368:ARG:NH1	2.32	0.62
1:A:389:ASP:H	1:B:419:ARG:NH1	1.97	0.62



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:143:GLU:OE1	2:G:501:NMN:HC6	1.98	0.62
1:G:203:ILE:HG23	1:G:347:PHE:CD1	2.33	0.62
1:A:434:ARG:HB3	1:A:436:ASP:OD1	1.98	0.62
1:B:29:LEU:HD21	1:B:418:GLU:HB2	1.81	0.62
1:B:382:MET:HA	1:B:397:GLU:HA	1.81	0.62
1:C:121:PHE:O	1:C:125:ILE:N	2.28	0.62
1:H:462:TYR:HB2	1:H:466:THR:CG2	2.29	0.62
1:B:118:SER:HA	1:B:121:PHE:CD2	2.35	0.62
1:E:26:LEU:HB3	1:E:79:PHE:CE1	2.34	0.62
1:G:245:ALA:HA	1:G:323:TRP:CZ2	2.34	0.62
1:G:402:LEU:HB3	1:H:400:LEU:HD23	1.81	0.62
1:C:111:ALA:HB1	1:C:139:ARG:CB	2.29	0.62
1:C:438:VAL:HA	1:C:441:GLN:HE21	1.65	0.62
1:F:62:LEU:O	1:F:66:VAL:HB	1.99	0.62
1:F:398:VAL:HG22	1:F:399:TRP:H	1.64	0.62
1:G:139:ARG:HD3	1:G:170:TYR:CZ	2.35	0.62
1:H:75:ALA:HA	1:H:78:LYS:HD2	1.81	0.62
1:H:175:TYR:CD2	1:H:236:HIS:HB3	2.35	0.62
1:A:29:LEU:HA	1:A:34:LEU:HD12	1.82	0.62
1:E:273:ASN:HA	1:E:451:GLY:HA2	1.82	0.62
1:G:118:SER:HB3	1:G:146:LEU:HA	1.80	0.62
1:H:55:ARG:HB3	1:H:80:LEU:HG	1.81	0.62
1:B:202:GLY:O	1:B:347:PHE:HD1	1.83	0.62
1:E:277:ILE:HD11	1:E:455:ASN:CB	2.30	0.62
1:H:170:TYR:HE2	1:H:424:LEU:HA	1.64	0.62
1:A:226:SER:HB2	1:A:230:ARG:HB2	1.81	0.62
1:A:164:PHE:HD1	1:A:168:GLN:OE1	1.82	0.61
1:A:425:ILE:HG12	1:A:426:GLU:N	2.15	0.61
1:B:19:GLN:HE21	1:B:20:ARG:HG3	1.63	0.61
1:B:27:TYR:CE2	1:B:66:VAL:HG21	2.35	0.61
1:D:462:TYR:HB2	1:D:466:THR:HG21	1.82	0.61
1:G:422:LEU:O	1:G:426:GLU:HG3	1.98	0.61
1:B:226:SER:HA	1:B:230:ARG:HE	1.64	0.61
1:C:265:PHE:HE2	1:C:437:GLU:HG2	1.65	0.61
1:G:388:LEU:HD22	1:H:419:ARG:HD3	1.82	0.61
1:A:448:ILE:HD11	1:A:452:TRP:CZ2	2.35	0.61
1:B:209:SER:O	1:B:341:SER:HA	2.01	0.61
1:C:194:PHE:HB3	1:C:198:TRP:CZ3	2.35	0.61
1:E:419:ARG:HD2	1:F:388:LEU:HA	1.82	0.61
1:G:125:ILE:HA	1:G:128:LEU:HD12	1.81	0.61
1:G:386:PRO:HG3	1:H:408:PHE:HB3	1.81	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:224:ASP:O	1:H:308:THR:HG21	2.00	0.61
1:H:406:ASP:HA	1:H:409:LYS:HD2	1.81	0.61
1:B:180:THR:HG21	1:B:371:LEU:HA	1.82	0.61
1:F:27:TYR:HB2	1:F:79:PHE:CE2	2.36	0.61
1:F:269:ARG:NH2	1:F:319:ASP:OD1	2.33	0.61
1:D:283:GLY:HA2	1:D:460:LYS:O	2.00	0.61
1:E:66:VAL:HG13	1:E:71:LEU:HD22	1.81	0.61
1:D:143:GLU:HG2	1:D:172:ILE:HG23	1.81	0.61
1:H:112:ILE:N	1:H:139:ARG:O	2.23	0.61
1:H:210:VAL:HB	1:H:237:ILE:HD11	1.82	0.61
1:E:415:ILE:O	1:E:418:GLU:HB2	1.99	0.61
1:H:45:SER:O	1:H:46:ARG:HB3	2.00	0.61
1:D:209:SER:HA	1:D:331:ARG:O	2.00	0.61
1:F:282:THR:O	1:F:469:PRO:HG3	2.00	0.61
1:G:370:VAL:CG1	1:G:373:PRO:HG2	2.31	0.61
1:B:198:TRP:CH2	1:B:367:LEU:HD23	2.30	0.61
1:F:229:LEU:HD13	1:F:312:VAL:HG21	1.83	0.61
1:A:175:TYR:HA	1:A:178:LYS:HD2	1.82	0.61
1:C:200:SER:HA	1:C:326:VAL:CG2	2.31	0.61
1:C:284:GLN:HG3	1:C:310:THR:HG23	1.82	0.61
1:E:452:TRP:O	1:E:456:SER:N	2.34	0.61
1:H:170:TYR:HB3	1:H:432:PHE:CD1	2.36	0.61
1:D:213:THR:HG22	1:D:336:LEU:O	2.01	0.60
1:E:12:GLY:HA2	1:E:46:ARG:CG	2.30	0.60
1:E:193:LEU:HD23	1:E:193:LEU:H	1.65	0.60
1:G:139:ARG:HA	1:G:168:GLN:O	2.01	0.60
1:B:349:PRO:HG3	1:B:364:PRO:HG3	1.83	0.60
1:H:71:LEU:HD21	1:H:76:LYS:HD3	1.83	0.60
1:H:99:ILE:HB	1:H:133:LEU:CD1	2.31	0.60
1:H:295:VAL:HB	1:H:335:ARG:NH2	2.15	0.60
1:B:246:MET:HA	1:B:264:VAL:HG21	1.83	0.60
1:H:170:TYR:CE2	1:H:424:LEU:HA	2.36	0.60
1:H:460:LYS:HD3	1:H:471:THR:HG23	1.83	0.60
1:A:54:PHE:O	1:A:57:PHE:N	2.34	0.60
1:A:122:GLU:HA	1:A:125:ILE:HD12	1.82	0.60
1:C:479:ASP:HB2	1:C:481:VAL:HG12	1.84	0.60
1:A:90:ILE:HA	1:A:96:PHE:CZ	2.37	0.60
1:C:311:PHE:CD1	1:C:469:PRO:HD2	2.37	0.60
1:H:195:GLU:OE2	1:H:322:ARG:NH1	2.30	0.60
1:B:24:PRO:O	1:B:27:TYR:HB3	2.01	0.60
1:F:41:ILE:HB	1:F:83:LEU:HA	1.84	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:11:PHE:HZ	1:G:128:LEU:HD21	1.66	0.60
1:G:26:LEU:HA	1:G:29:LEU:HD12	1.83	0.60
1:G:18:SER:CA	1:G:22:LEU:HB2	2.27	0.60
1:A:40:ARG:CB	1:A:84:PHE:HE2	2.15	0.60
1:A:176:LEU:HD11	1:A:239:GLN:OE1	2.01	0.60
1:D:5:VAL:HG11	1:D:111:ALA:HB2	1.82	0.60
1:E:135:GLY:HA2	1:E:138:SER:HB2	1.83	0.60
1:B:125:ILE:HG23	1:B:163:VAL:HG11	1.82	0.60
1:F:378:GLN:HA	1:F:400:LEU:O	2.02	0.60
1:G:122:GLU:OE1	1:G:155:HIS:NE2	2.35	0.60
1:H:114:LEU:HB3	1:H:121:PHE:HE1	1.66	0.60
1:B:377:ILE:HD12	1:B:404:LEU:HD21	1.82	0.60
1:D:289:VAL:HA	1:D:294:GLU:HA	1.84	0.60
1:B:339:ARG:O	1:B:373:PRO:HD3	2.01	0.59
1:D:172:ILE:HD11	1:D:420:LEU:HD13	1.83	0.59
1:F:216:LEU:HD13	1:F:220:ILE:HG23	1.83	0.59
1:F:67:ALA:HB3	1:F:70:ARG:HG3	1.84	0.59
1:H:272:ASN:HB3	1:H:275:THR:HG23	1.83	0.59
1:A:283:GLY:HA2	1:A:460:LYS:O	2.02	0.59
1:B:451:GLY:O	1:B:455:ASN:HB2	2.02	0.59
1:F:340:ARG:HD2	1:F:368:ARG:NH2	2.16	0.59
1:D:118:SER:HA	1:D:121:PHE:CD2	2.36	0.59
1:E:135:GLY:HA3	1:E:138:SER:HB2	1.83	0.59
1:G:415:ILE:HG22	1:G:417:HIS:H	1.68	0.59
1:A:143:GLU:OE1	2:A:501:NMN:HC6	2.03	0.59
1:C:258:ARG:HD2	1:C:434:ARG:HB2	1.83	0.59
1:E:215:GLY:HA3	1:E:335:ARG:HH11	1.66	0.59
1:G:354:ILE:HG13	1:H:252:MET:HG2	1.84	0.59
1:G:40:ARG:HB3	1:G:84:PHE:HE2	1.68	0.59
1:B:216:LEU:HD13	1:B:334:LYS:HE2	1.84	0.59
1:H:203:ILE:HG21	1:H:323:TRP:CZ3	2.38	0.59
1:C:462:TYR:CG	1:C:468:GLY:HA2	2.38	0.58
1:E:29:LEU:HD13	1:E:422:LEU:HG	1.84	0.58
1:A:96:PHE:CG	1:A:127:GLY:HA3	2.39	0.58
1:C:200:SER:N	1:C:322:ARG:O	2.37	0.58
1:H:213:THR:HA	1:H:336:LEU:O	2.03	0.58
1:A:237:ILE:HG21	1:A:330:ILE:HG23	1.83	0.58
1:D:30:ASP:OD2	1:D:79:PHE:HB2	2.03	0.58
1:A:150:LEU:HB2	1:A:442:TRP:HB3	1.86	0.58
1:H:129:LYS:HA	1:H:134:ALA:CB	2.33	0.58
1:H:216:LEU:CD2	1:H:223:PHE:HB2	2.32	0.58



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:282:THR:OG1	1:D:459:PRO:HA	2.02	0.58
1:E:92:ASP:HB2	1:E:95:GLN:CD	2.23	0.58
1:E:322:ARG:HD2	1:E:323:TRP:NE1	2.19	0.58
1:F:216:LEU:HD11	1:F:285:TYR:HE2	1.68	0.58
1:H:265:PHE:CE2	1:H:437:GLU:HB3	2.39	0.58
1:D:116:THR:HB	1:D:120:LEU:HD12	1.86	0.58
1:G:191:ASN:HB3	1:H:365:ASN:HD21	1.69	0.58
1:A:156:ILE:O	1:A:160:VAL:HG23	2.03	0.58
1:A:372:GLN:HG2	1:A:373:PRO:HA	1.85	0.58
1:D:44:THR:HB	1:D:99:ILE:HD11	1.85	0.58
1:E:342:GLU:HB3	1:E:370:VAL:HG12	1.86	0.58
1:G:5:VAL:HA	1:G:425:ILE:O	2.04	0.58
1:A:229:LEU:O	1:A:233:VAL:HB	2.04	0.58
1:G:23:LEU:N	1:G:24:PRO:HD2	2.18	0.58
1:H:329:TYR:CE2	1:H:481:VAL:HG11	2.38	0.58
1:A:382:MET:HB2	1:B:191:ASN:OD1	2.03	0.58
1:B:93:PRO:HA	1:B:96:PHE:HD1	1.69	0.58
1:D:43:CYS:O	1:D:85:TYR:HA	2.04	0.58
1:E:18:SER:O	1:E:23:LEU:HB2	2.03	0.58
1:G:178:LYS:HB2	1:G:181:VAL:HG23	1.86	0.58
1:F:29:LEU:HG	1:F:418:GLU:HB3	1.85	0.57
1:A:198:TRP:HH2	1:A:367:LEU:HD23	1.68	0.57
1:A:385:GLU:HB2	1:A:396:ARG:HG3	1.86	0.57
1:D:310:THR:O	1:D:333:GLY:HA2	2.04	0.57
1:E:346:GLN:HG2	1:E:364:PRO:HB2	1.86	0.57
1:F:133:LEU:HG	1:F:164:PHE:CZ	2.39	0.57
1:A:235:SER:O	1:A:239:GLN:HG2	2.04	0.57
1:B:171:ARG:NH1	1:B:434:ARG:HA	2.19	0.57
1:C:175:TYR:O	1:C:178:LYS:N	2.32	0.57
1:C:289:VAL:HA	1:C:294:GLU:HA	1.85	0.57
1:D:368:ARG:HB3	1:D:378:GLN:HG3	1.86	0.57
1:E:146:LEU:HD11	1:E:438:VAL:HG11	1.86	0.57
1:G:44:THR:HB	1:G:86:ALA:O	2.04	0.57
1:C:154:ASP:HA	1:C:435:ARG:HH21	1.70	0.57
1:E:8:MET:HA	1:E:111:ALA:O	2.03	0.57
1:E:54:PHE:CD2	1:E:85:TYR:N	2.71	0.57
1:F:96:PHE:CG	1:F:127:GLY:HA3	2.39	0.57
1:B:429:ALA:HA	1:B:432:PHE:HD1	1.70	0.57
1:E:40:ARG:HG3	1:E:105:PRO:CG	2.32	0.57
1:E:281:VAL:HG21	1:E:472:ALA:HA	1.85	0.57
1:C:341:SER:H	1:C:373:PRO:HG2	1.69	0.57



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:16:ASP:O	1:E:19:GLN:HG2	2.05	0.57
1:E:345:VAL:O	1:E:366:LYS:HA	2.04	0.57
1:A:383:VAL:HG21	1:B:404:LEU:HD11	1.87	0.57
1:C:188:ARG:HH22	1:C:322:ARG:HH12	1.53	0.57
1:D:37:ASP:N	1:D:37:ASP:OD1	2.35	0.57
1:F:286:GLY:O	1:F:297:GLY:HA2	2.05	0.57
1:H:41:ILE:HD13	1:H:79:PHE:HE1	1.70	0.57
1:H:176:LEU:HD12	1:H:431:LEU:O	2.05	0.57
1:H:271:ILE:HG21	1:H:276:VAL:HG23	1.85	0.57
1:B:215:GLY:CA	1:B:335:ARG:HD2	2.34	0.57
1:C:229:LEU:HD21	1:C:445:ILE:HG23	1.86	0.57
1:E:223:PHE:HZ	1:E:310:THR:HA	1.68	0.57
1:H:209:SER:O	1:H:341:SER:HA	2.04	0.57
1:C:184:LEU:O	1:C:188:ARG:N	2.31	0.57
1:C:200:SER:HA	1:C:326:VAL:HG23	1.87	0.57
1:D:25:ALA:HA	1:D:418:GLU:HG2	1.87	0.57
1:E:8:MET:HG3	1:E:9:ILE:N	2.18	0.57
1:E:156:ILE:HG12	1:E:157:ASN:N	2.19	0.57
1:F:40:ARG:HA	1:F:84:PHE:HD2	1.70	0.57
1:H:230:ARG:HE	1:H:449:ARG:NE	2.02	0.57
1:E:69:ASP:OD1	1:E:70:ARG:HG3	2.04	0.56
1:E:306:SER:OG	1:E:308:THR:HG23	2.04	0.56
1:H:462:TYR:CD1	1:H:469:PRO:HD3	2.40	0.56
1:B:70:ARG:HH11	1:B:414:ARG:HB2	1.67	0.56
1:E:161:LEU:HA	1:E:164:PHE:O	2.04	0.56
1:E:417:HIS:HA	1:E:420:LEU:HB2	1.86	0.56
1:A:400:LEU:HB3	1:B:400:LEU:HB3	1.86	0.56
1:A:463:VAL:O	1:A:466:THR:HG22	2.06	0.56
1:B:20:ARG:HG2	1:B:65:PHE:CZ	2.40	0.56
1:D:247:GLU:HB2	1:D:260:GLU:OE1	2.05	0.56
1:E:334:LYS:O	1:E:462:TYR:OH	2.23	0.56
1:F:258:ARG:O	1:F:262:VAL:HG23	2.04	0.56
1:H:80:LEU:HD12	1:H:83:LEU:HD12	1.86	0.56
1:H:199:ASN:O	1:H:203:ILE:HG22	2.05	0.56
1:H:285:TYR:OH	1:H:301:GLU:OE1	2.23	0.56
1:E:313:ALA:O	1:E:314:ILE:HG13	2.05	0.56
1:H:320:ASN:O	1:H:324:HIS:HB2	2.06	0.56
2:A:501:NMN:C5R	2:A:501:NMN:HC2	2.36	0.56
1:B:423:ASP:OD1	1:B:428:ASP:HB2	2.06	0.56
1:B:452:TRP:O	1:B:456:SER:N	2.39	0.56
1:D:282:THR:HB	1:D:459:PRO:HB3	1.86	0.56



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:142:LEU:HD12	1:G:171:ARG:HG2	1.86	0.56
1:H:153:SER:HA	1:H:156:ILE:HD12	1.88	0.56
1:H:475:LEU:HD12	1:H:478:ARG:HH21	1.70	0.56
1:A:188:ARG:NH1	1:A:243:LEU:O	2.38	0.56
1:C:75:ALA:O	1:C:79:PHE:N	2.33	0.56
1:D:129:LYS:HA	1:D:134:ALA:HB3	1.86	0.56
1:G:315:LYS:HE3	1:G:327:PRO:HB3	1.87	0.56
1:H:285:TYR:HD2	1:H:310:THR:HG21	1.71	0.56
1:A:152:SER:O	1:A:156:ILE:HG23	2.05	0.56
1:A:458:LYS:HE3	1:A:459:PRO:HD2	1.86	0.56
1:B:36:ALA:HB3	1:B:39:LEU:HD12	1.88	0.56
1:B:46:ARG:HG3	1:B:120:LEU:HD23	1.87	0.56
1:B:423:ASP:O	1:B:427:GLY:N	2.38	0.56
1:F:144:LYS:HG3	1:F:145:PRO:CD	2.32	0.56
1:F:302:LEU:HG	1:F:303:GLY:H	1.71	0.56
1:H:349:PRO:HG3	1:H:364:PRO:HG3	1.87	0.56
1:A:212:GLU:O	1:A:336:LEU:N	2.35	0.56
1:B:216:LEU:HB3	1:B:219:ARG:HG3	1.86	0.56
1:C:423:ASP:HB3	1:C:430:THR:HG23	1.88	0.56
1:G:272:ASN:HB2	1:G:275:THR:HG23	1.88	0.56
1:G:370:VAL:HG12	1:G:373:PRO:HG2	1.86	0.56
1:E:160:VAL:HG12	1:E:161:LEU:HD12	1.86	0.56
1:A:366:LYS:HB2	1:A:380:SER:OG	2.06	0.56
1:B:9:ILE:HB	1:B:112:ILE:HA	1.88	0.56
1:B:229:LEU:HD23	1:B:230:ARG:HG2	1.87	0.56
1:B:298:TYR:HE2	1:B:308:THR:HB	1.71	0.56
1:D:55:ARG:HD3	1:D:80:LEU:O	2.06	0.56
1:D:202:GLY:O	1:D:347:PHE:HD1	1.89	0.56
1:B:237:ILE:HA	1:B:240:LEU:HD12	1.88	0.55
1:D:197:LEU:O	1:D:203:ILE:HG13	2.06	0.55
1:F:255:ASN:HA	1:F:258:ARG:HB2	1.88	0.55
1:G:378:GLN:HG3	1:G:399:TRP:CE3	2.40	0.55
1:G:474:ALA:O	1:G:478:ARG:HG2	2.05	0.55
1:H:175:TYR:CD1	1:H:236:HIS:HD2	2.24	0.55
1:E:90:ILE:HG13	1:E:120:LEU:HD23	1.88	0.55
1:H:216:LEU:HB2	1:H:220:ILE:HG23	1.88	0.55
1:C:148:GLN:H	1:C:152:SER:CB	2.18	0.55
1:F:10:LEU:HD12	1:F:11:PHE:H	1.72	0.55
1:H:340:ARG:HA	1:H:373:PRO:HD3	1.87	0.55
1:B:105:PRO:HG2	1:B:108:LYS:CB	2.36	0.55
1:B:193:LEU:HG	1:B:194:PHE:N	2.20	0.55



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:313:ALA:HA	1:B:330:ILE:O	2.06	0.55
1:D:128:LEU:HG	1:D:133:LEU:HD12	1.87	0.55
1:D:463:VAL:O	1:D:466:THR:HB	2.07	0.55
1:E:472:ALA:O	1:E:474:ALA:N	2.39	0.55
1:G:26:LEU:HD21	1:G:421:LEU:HD22	1.88	0.55
1:B:5:VAL:HG22	1:B:109:GLY:CA	2.36	0.55
1:D:7:THR:HB	1:D:109:GLY:O	2.07	0.55
1:E:366:LYS:H	1:E:380:SER:HB2	1.70	0.55
1:A:76:LYS:O	1:A:80:LEU:HD12	2.07	0.55
1:A:262:VAL:HG22	1:A:437:GLU:HG3	1.88	0.55
1:D:309:GLU:HB3	1:D:311:PHE:O	2.06	0.55
1:E:112:ILE:HD11	1:E:138:SER:HB3	1.88	0.55
1:E:125:ILE:HA	1:E:128:LEU:HD12	1.89	0.55
1:F:11:PHE:HA	1:F:44:THR:HB	1.87	0.55
1:G:186:THR:HA	1:H:355:PHE:CZ	2.41	0.55
1:B:246:MET:HE3	1:B:260:GLU:HB2	1.89	0.55
1:C:381:ILE:CD1	1:C:400:LEU:HG	2.37	0.55
1:D:403:SER:O	1:D:407:VAL:HG23	2.05	0.55
1:F:184:LEU:O	1:F:187:LEU:HB3	2.06	0.55
1:F:353:SER:HB3	1:F:356:SER:HB3	1.89	0.55
1:F:473:ILE:O	1:F:476:VAL:HG12	2.06	0.55
1:G:144:LYS:HD3	1:G:236:HIS:CE1	2.41	0.55
1:H:337:PRO:HG2	1:H:467:TRP:CG	2.41	0.55
1:A:144:LYS:CE	2:A:501:NMN:C5	2.76	0.55
1:B:125:ILE:CG2	1:B:163:VAL:HG21	2.36	0.55
1:E:364:PRO:O	1:E:366:LYS:NZ	2.37	0.55
1:H:136:PRO:O	1:H:137:THR:HG22	2.07	0.55
1:H:139:ARG:NH2	1:H:427:GLY:HA3	2.22	0.55
1:C:340:ARG:HA	1:C:373:PRO:HG2	1.88	0.55
1:E:239:GLN:NE2	1:E:441:GLN:HE22	2.05	0.55
1:E:285:TYR:CD1	1:E:335:ARG:HG3	2.42	0.55
1:G:388:LEU:HA	1:H:419:ARG:NE	2.17	0.55
1:A:55:ARG:HB3	1:A:80:LEU:HD22	1.89	0.55
1:A:180:THR:HG21	1:A:371:LEU:HA	1.89	0.55
1:B:117:SER:HB3	1:B:120:LEU:HD22	1.88	0.55
1:B:66:VAL:HG11	1:B:71:LEU:HD13	1.88	0.54
1:E:135:GLY:N	1:E:136:PRO:HD3	2.22	0.54
1:G:118:SER:HB2	1:G:146:LEU:HA	1.89	0.54
1:G:337:PRO:HD2	1:G:467:TRP:CD2	2.42	0.54
1:H:219:ARG:HB3	1:H:222:TYR:HD1	1.71	0.54
1:B:135:GLY:H	1:B:138:SER:HB2	1.72	0.54



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:148:GLN:HB3	1:B:230:ARG:CZ	2.37	0.54
1:E:419:ARG:HB2	1:F:388:LEU:HD22	1.88	0.54
1:A:345:VAL:O	1:A:366:LYS:HA	2.07	0.54
1:C:265:PHE:CE2	1:C:437:GLU:HG2	2.42	0.54
1:D:156:ILE:O	1:D:160:VAL:HG23	2.07	0.54
1:D:219:ARG:O	1:D:223:PHE:N	2.39	0.54
1:D:232:MET:O	1:D:236:HIS:HB2	2.07	0.54
1:D:435:ARG:O	1:D:439:GLU:HG2	2.07	0.54
1:G:283:GLY:HA2	1:G:460:LYS:O	2.06	0.54
1:A:29:LEU:HG	1:A:418:GLU:HG2	1.90	0.54
1:E:209:SER:HB2	1:E:342:GLU:HG3	1.88	0.54
1:F:128:LEU:HB3	1:F:133:LEU:CB	2.38	0.54
1:F:212:GLU:HA	1:F:339:ARG:HA	1.89	0.54
1:A:268:LEU:HD21	1:A:316:ALA:HB1	1.89	0.54
1:E:419:ARG:O	1:E:419:ARG:HG3	2.06	0.54
1:H:46:ARG:O	1:H:46:ARG:HG3	2.06	0.54
1:B:198:TRP:HA	1:B:203:ILE:HD11	1.90	0.54
1:C:278:THR:OG1	1:C:279:HIS:ND1	2.40	0.54
1:D:253:GLU:HB2	1:D:256:ALA:HB3	1.90	0.54
1:E:56:ASP:O	1:E:58:ALA:N	2.41	0.54
1:F:204:ASP:HB3	1:F:346:GLN:HG2	1.89	0.54
1:G:203:ILE:HG22	1:G:346:GLN:O	2.07	0.54
1:A:148:GLN:HG2	1:A:149:ASP:N	2.23	0.54
1:A:352:HIS:HB3	1:D:321:TRP:HA	1.89	0.54
1:E:171:ARG:HD3	1:E:438:VAL:HG21	1.90	0.54
1:F:311:PHE:CZ	1:F:313:ALA:HB2	2.43	0.54
1:A:17:LEU:HB2	2:A:501:NMN:C7	2.38	0.54
1:A:140:LEU:HD12	1:A:164:PHE:HD2	1.72	0.54
1:C:7:THR:HA	1:C:40:ARG:O	2.08	0.54
1:C:319:ASP:HB3	1:C:324:HIS:ND1	2.22	0.54
1:D:112:ILE:HD13	1:D:128:LEU:CD2	2.37	0.54
1:F:337:PRO:HG2	1:F:467:TRP:CD1	2.42	0.54
1:G:236:HIS:O	1:G:240:LEU:HD13	2.07	0.54
1:H:207:GLN:HG2	1:H:329:TYR:HB2	1.90	0.54
1:B:3:ASN:HB2	1:B:5:VAL:HG23	1.89	0.54
1:B:5:VAL:HA	1:B:109:GLY:N	2.22	0.54
1:D:61:ALA:HA	1:D:64:ARG:HG2	1.89	0.54
1:E:56:ASP:O	1:E:57:PHE:C	2.46	0.54
1:E:161:LEU:HG	1:E:164:PHE:O	2.08	0.54
1:E:164:PHE:HD2	1:E:168:GLN:HB2	1.72	0.54
1:F:8:MET:HG2	1:F:41:ILE:HG23	1.90	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:240:LEU:O	1:F:244:VAL:HG23	2.08	0.54
1:F:415:ILE:HG22	1:F:417:HIS:H	1.73	0.54
1:A:76:LYS:C	1:A:80:LEU:HD12	2.28	0.54
1:A:195:GLU:HA	1:A:198:TRP:HB2	1.90	0.54
1:B:161:LEU:CD2	1:B:435:ARG:HE	2.21	0.54
1:B:228:SER:H	1:B:309:GLU:HG2	1.72	0.54
1:A:143:GLU:HG3	2:A:501:NMN:C1R	2.38	0.53
1:A:386:PRO:HD2	1:B:408:PHE:CD1	2.43	0.53
1:D:224:ASP:O	1:D:308:THR:HG21	2.08	0.53
1:E:54:PHE:CE2	1:E:85:TYR:N	2.76	0.53
1:F:210:VAL:O	1:F:332:THR:HA	2.07	0.53
1:G:93:PRO:O	1:G:96:PHE:HB2	2.08	0.53
1:H:203:ILE:HD13	1:H:323:TRP:CZ3	2.43	0.53
1:A:17:LEU:CD2	2:A:501:NMN:H5R2	2.35	0.53
1:A:90:ILE:H	1:A:90:ILE:HD13	1.72	0.53
1:A:351:PRO:HD2	1:D:321:TRP:CZ2	2.43	0.53
1:E:475:LEU:HG	1:E:478:ARG:HH21	1.73	0.53
1:G:9:ILE:HG23	1:G:42:VAL:HB	1.90	0.53
1:H:42:VAL:HA	1:H:84:PHE:O	2.07	0.53
1:A:143:GLU:OE1	2:A:501:NMN:C6	2.55	0.53
1:B:58:ALA:O	1:B:62:LEU:N	2.34	0.53
1:C:354:ILE:O	1:D:252:MET:HG2	2.08	0.53
1:D:226:SER:O	1:D:230:ARG:HB2	2.08	0.53
1:F:27:TYR:HD1	1:F:79:PHE:CD2	2.26	0.53
1:F:142:LEU:N	1:F:170:TYR:O	2.42	0.53
1:G:146:LEU:HD23	1:G:146:LEU:H	1.73	0.53
1:H:336:LEU:HD22	1:H:467:TRP:CE3	2.43	0.53
1:A:475:LEU:HD12	1:A:478:ARG:HH21	1.71	0.53
1:C:58:ALA:O	1:C:62:LEU:N	2.36	0.53
1:C:378:GLN:HA	1:C:400:LEU:O	2.09	0.53
1:D:336:LEU:HD13	1:D:467:TRP:CZ3	2.44	0.53
1:E:30:ASP:O	1:E:33:GLY:N	2.35	0.53
1:G:208:ILE:HG23	1:G:343:ILE:HG12	1.89	0.53
1:H:479:ASP:HB2	1:H:481:VAL:HG12	1.91	0.53
1:C:259:ASP:OD1	1:C:434:ARG:NH2	2.34	0.53
1:E:370:VAL:HG22	1:E:376:THR:O	2.09	0.53
1:G:284:GLN:HA	1:G:309:GLU:O	2.09	0.53
1:A:309:GLU:C	1:A:311:PHE:H	2.11	0.53
1:D:49:TYR:CD2	1:D:54:PHE:HA	2.43	0.53
1:D:175:TYR:O	1:D:176:LEU:HB2	2.09	0.53
1:D:254:ALA:O	1:D:258:ARG:HG3	2.09	0.53



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:283:GLY:O	1:B:309:GLU:HA	2.09	0.53
1:B:287:ALA:O	1:B:463:VAL:HG23	2.09	0.53
1:E:6:SER:HA	1:E:109:GLY:O	2.08	0.53
1:F:128:LEU:HB3	1:F:133:LEU:HD13	1.90	0.53
1:F:289:VAL:HA	1:F:294:GLU:HA	1.90	0.53
2:A:501:NMN:HC2	2:A:501:NMN:H5R1	1.90	0.53
1:C:197:LEU:HD21	1:D:193:LEU:HA	1.91	0.53
1:D:30:ASP:CG	1:D:79:PHE:HB2	2.29	0.53
1:F:27:TYR:HB2	1:F:62:LEU:HD21	1.91	0.53
1:F:27:TYR:CE2	1:F:71:LEU:HA	2.43	0.53
1:G:118:SER:CB	1:G:147:GLY:H	2.22	0.53
1:C:436:ASP:HA	1:C:439:GLU:OE2	2.08	0.53
1:E:161:LEU:HD21	1:E:166:GLU:HB2	1.90	0.53
1:F:45:SER:O	1:F:46:ARG:C	2.46	0.53
1:F:188:ARG:NH2	1:F:322:ARG:HH12	2.07	0.53
1:A:401:ASP:O	1:B:400:LEU:HA	2.09	0.53
1:D:205:HIS:CD2	1:D:481:VAL:HG21	2.44	0.53
1:G:434:ARG:NH2	1:G:436:ASP:OD2	2.35	0.53
1:H:203:ILE:HD13	1:H:323:TRP:HZ3	1.74	0.53
1:A:128:LEU:HB3	1:A:133:LEU:HB2	1.91	0.52
1:A:242:ALA:O	1:A:246:MET:HB3	2.09	0.52
1:B:222:TYR:OH	2:B:501:NMN:H2RC	2.09	0.52
1:C:129:LYS:CB	1:C:134:ALA:HB2	2.39	0.52
1:E:40:ARG:HG3	1:E:105:PRO:CD	2.39	0.52
1:F:302:LEU:HD23	1:F:304:GLN:O	2.09	0.52
1:A:205:HIS:NE2	1:A:481:VAL:HG23	2.24	0.52
1:B:462:TYR:CD2	1:B:469:PRO:HD3	2.44	0.52
1:C:466:THR:OG1	1:C:467:TRP:N	2.40	0.52
1:F:415:ILE:N	1:F:418:GLU:OE1	2.43	0.52
1:H:167:LYS:O	1:H:170:TYR:HE1	1.91	0.52
1:A:93:PRO:HA	1:A:96:PHE:CD1	2.44	0.52
1:A:134:ALA:HA	1:A:164:PHE:CZ	2.43	0.52
1:B:70:ARG:HD2	1:B:414:ARG:HE	1.75	0.52
1:B:144:LYS:CE	2:B:501:NMN:HC6	2.27	0.52
1:H:175:TYR:CE1	1:H:236:HIS:HD2	2.27	0.52
1:A:242:ALA:HA	1:A:264:VAL:HG11	1.91	0.52
1:B:307:ASP:OD2	1:B:458:LYS:HD2	2.10	0.52
1:D:67:ALA:HB3	1:D:70:ARG:HG2	1.91	0.52
1:A:386:PRO:HG2	1:B:411:ARG:HG3	1.90	0.52
1:G:100:ALA:O	1:G:103:CYS:HB2	2.10	0.52
1:G:233:VAL:HG22	1:G:237:ILE:HD12	1.91	0.52



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:55:ARG:HB3	1:A:80:LEU:HD23	1.91	0.52
1:B:378:GLN:HB2	1:B:399:TRP:CE3	2.45	0.52
1:D:113:TYR:OH	1:D:143:GLU:HB2	2.10	0.52
1:F:150:LEU:HD22	1:F:443:ILE:HD13	1.91	0.52
1:F:245:ALA:HA	1:F:323:TRP:HZ2	1.72	0.52
1:G:79:PHE:O	1:G:83:LEU:HD13	2.09	0.52
1:H:7:THR:O	1:H:110:ILE:HA	2.09	0.52
1:H:172:ILE:HG23	1:H:420:LEU:HD13	1.91	0.52
1:H:202:GLY:O	1:H:347:PHE:HD1	1.93	0.52
1:A:48:GLU:HB3	1:A:49:TYR:CE1	2.44	0.52
1:E:177:GLY:HA3	1:E:420:LEU:HD21	1.92	0.52
1:F:322:ARG:HD2	1:F:323:TRP:NE1	2.24	0.52
1:A:183:ASN:O	1:A:186:THR:N	2.42	0.52
1:A:320:ASN:HD21	1:A:323:TRP:HD1	1.55	0.52
1:G:327:PRO:HB2	1:G:329:TYR:CE2	2.45	0.52
1:D:142:LEU:O	1:D:172:ILE:HG22	2.10	0.52
1:F:484:TYR:OH	1:F:486:LEU:HD23	2.10	0.52
1:A:242:ALA:HB2	1:A:265:PHE:CE1	2.45	0.52
1:D:287:ALA:O	1:D:463:VAL:HG13	2.10	0.52
1:F:476:VAL:HG13	1:F:477:GLU:N	2.24	0.52
1:G:5:VAL:O	1:G:425:ILE:HG23	2.09	0.52
1:C:286:GLY:C	1:C:297:GLY:HA2	2.29	0.51
1:C:409:LYS:HE2	1:C:409:LYS:HA	1.91	0.51
1:F:70:ARG:HH22	1:F:418:GLU:CD	2.14	0.51
1:F:176:LEU:HD21	1:F:239:GLN:HB3	1.93	0.51
1:G:185:LEU:HD22	1:G:189:PHE:CE2	2.45	0.51
1:G:271:ILE:HG13	1:G:448:ILE:CG1	2.37	0.51
1:A:96:PHE:CD2	1:A:127:GLY:HA3	2.44	0.51
1:B:153:SER:O	1:B:156:ILE:HG12	2.11	0.51
1:C:412:LYS:C	1:C:414:ARG:H	2.13	0.51
1:D:281:VAL:HG11	1:D:472:ALA:HB2	1.91	0.51
1:D:462:TYR:CD1	1:D:468:GLY:HA2	2.46	0.51
1:E:160:VAL:O	1:E:164:PHE:HB2	2.10	0.51
1:F:177:GLY:HA3	1:F:420:LEU:HD11	1.90	0.51
1:H:232:MET:HB2	1:H:332:THR:HG21	1.91	0.51
1:H:329:TYR:HB3	1:H:483:TRP:CH2	2.45	0.51
1:D:23:LEU:HD23	1:D:26:LEU:HD12	1.91	0.51
1:G:156:ILE:O	1:G:160:VAL:HG23	2.11	0.51
1:G:166:GLU:O	1:G:169:VAL:HG22	2.09	0.51
1:B:307:ASP:O	1:B:459:PRO:HG3	2.11	0.51
1:E:29:LEU:HD21	1:E:418:GLU:O	2.11	0.51



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:376:THR:HG23	1:E:402:LEU:O	2.10	0.51
1:F:284:GLN:HB2	1:F:459:PRO:HB2	1.91	0.51
1:A:486:LEU:O	1:A:487:GLU:HB2	2.09	0.51
1:D:337:PRO:HG2	1:D:467:TRP:CD1	2.46	0.51
1:G:75:ALA:HA	1:G:78:LYS:HD2	1.92	0.51
1:A:369:ILE:HG23	1:A:377:ILE:HG12	1.92	0.51
1:B:96:PHE:CD1	1:B:127:GLY:HA3	2.45	0.51
1:B:257:VAL:O	1:B:261:LYS:HG3	2.11	0.51
1:D:449:ARG:HA	1:D:452:TRP:CD1	2.45	0.51
1:E:276:VAL:HG11	1:E:452:TRP:CA	2.41	0.51
1:F:276:VAL:HA	1:F:280:THR:HG23	1.92	0.51
1:A:371:LEU:H	1:A:371:LEU:HD12	1.76	0.51
1:A:386:PRO:HA	1:B:179:GLU:OE2	2.11	0.51
1:C:314:ILE:HB	1:C:330:ILE:HD12	1.91	0.51
1:F:7:THR:O	1:F:111:ALA:N	2.43	0.51
1:H:35:LEU:HD13	1:H:82:LYS:HE2	1.91	0.51
1:H:237:ILE:HG21	1:H:330:ILE:HG23	1.92	0.51
1:A:268:LEU:HD23	1:A:317:HIS:O	2.11	0.51
1:D:154:ASP:HA	1:D:435:ARG:HH12	1.76	0.51
1:D:193:LEU:O	1:D:196:PRO:HG2	2.11	0.51
1:F:226:SER:O	1:F:230:ARG:HB3	2.11	0.51
1:F:316:ALA:N	1:F:328:PHE:O	2.40	0.51
1:G:271:ILE:HD13	1:G:271:ILE:H	1.76	0.51
1:G:385:GLU:CG	1:G:386:PRO:HD2	2.40	0.51
1:A:138:SER:HB2	1:A:164:PHE:CE1	2.46	0.51
1:A:188:ARG:NH1	1:A:246:MET:HG2	2.25	0.51
1:B:62:LEU:O	1:B:66:VAL:HG12	2.10	0.51
1:C:59:GLU:HA	1:C:62:LEU:HB2	1.91	0.51
1:C:452:TRP:HD1	1:C:453:LYS:N	2.09	0.51
1:D:118:SER:HA	1:D:121:PHE:CG	2.45	0.51
1:E:216:LEU:HD23	1:E:334:LYS:HD2	1.92	0.51
1:E:466:THR:O	1:E:468:GLY:N	2.38	0.51
1:G:452:TRP:HA	1:G:457:MET:HG3	1.92	0.51
1:H:5:VAL:HG13	1:H:109:GLY:C	2.31	0.51
1:H:359:GLY:HA3	1:H:393:ALA:O	2.11	0.51
1:B:262:VAL:HG21	1:B:436:ASP:OD2	2.10	0.51
1:D:85:TYR:CG	1:D:86:ALA:N	2.79	0.51
1:F:213:THR:HA	1:F:336:LEU:O	2.11	0.51
1:G:234:GLN:HG2	1:G:445:ILE:HG13	1.92	0.51
1:G:379:ILE:O	1:G:399:TRP:HA	2.11	0.51
1:G:381:ILE:HB	1:H:191:ASN:ND2	2.26	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:223:PHE:CE2	1:A:310:THR:HG22	2.46	0.50
1:E:166:GLU:CA	1:E:169:VAL:HG22	2.40	0.50
1:F:302:LEU:HG	1:F:303:GLY:N	2.25	0.50
1:G:43:CYS:O	1:G:85:TYR:HA	2.11	0.50
1:H:24:PRO:HA	1:H:62:LEU:HD23	1.93	0.50
1:A:144:LYS:HB3	2:A:501:NMN:HC6	1.94	0.50
1:A:183:ASN:O	1:A:184:LEU:C	2.49	0.50
1:C:205:HIS:HB3	1:C:327:PRO:HG2	1.93	0.50
1:D:327:PRO:HB2	1:D:329:TYR:CZ	2.46	0.50
1:F:470:ILE:O	1:F:473:ILE:N	2.44	0.50
1:A:154:ASP:HA	1:A:157:ASN:HB2	1.93	0.50
1:B:11:PHE:O	1:B:115:ALA:HB3	2.11	0.50
1:B:23:LEU:N	1:B:24:PRO:HD2	2.25	0.50
1:E:52:ASP:N	1:E:87:THR:OG1	2.44	0.50
1:E:135:GLY:HA2	1:E:138:SER:CB	2.42	0.50
1:G:17:LEU:HD22	2:G:501:NMN:N1	2.25	0.50
1:G:281:VAL:HG11	1:G:472:ALA:HB2	1.92	0.50
1:B:198:TRP:CH2	1:B:345:VAL:HG21	2.46	0.50
1:E:419:ARG:HA	1:F:388:LEU:HD22	1.93	0.50
1:G:337:PRO:HD3	1:G:467:TRP:HA	1.94	0.50
1:B:79:PHE:O	1:B:83:LEU:HD22	2.11	0.50
1:B:337:PRO:HD2	1:B:467:TRP:CE3	2.47	0.50
1:C:171:ARG:O	1:C:432:PHE:HD1	1.93	0.50
1:C:195:GLU:N	1:C:196:PRO:HD2	2.26	0.50
1:D:17:LEU:HD12	1:D:21:MET:HB2	1.93	0.50
1:D:262:VAL:CG2	1:D:437:GLU:HG3	2.41	0.50
1:E:25:ALA:HA	1:E:418:GLU:HG3	1.93	0.50
1:G:322:ARG:HD2	1:G:323:TRP:NE1	2.26	0.50
1:H:170:TYR:OH	1:H:427:GLY:HA2	2.12	0.50
1:A:52:ASP:OD1	1:A:84:PHE:HA	2.12	0.50
1:E:176:LEU:HA	1:E:181:VAL:HG11	1.94	0.50
1:E:186:THR:HA	1:F:355:PHE:CZ	2.47	0.50
1:G:337:PRO:HG3	1:G:465:GLY:O	2.12	0.50
1:A:213:THR:O	1:A:290:SER:OG	2.27	0.50
1:B:135:GLY:C	1:B:137:THR:N	2.61	0.50
1:D:199:ASN:O	1:D:203:ILE:HB	2.12	0.50
1:E:276:VAL:HG22	1:E:280:THR:HG21	1.92	0.50
1:F:343:ILE:O	1:F:368:ARG:HA	2.11	0.50
1:G:183:ASN:OD1	1:H:383:VAL:HG23	2.12	0.50
1:H:449:ARG:O	1:H:453:LYS:HG2	2.11	0.50
1:B:3:ASN:HB2	1:B:5:VAL:CG2	2.41	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:197:LEU:O	1:B:203:ILE:HG13	2.11	0.50
1:B:198:TRP:CZ2	1:B:345:VAL:HG21	2.47	0.50
1:B:273:ASN:O	1:B:455:ASN:ND2	2.45	0.50
1:F:27:TYR:HE2	1:F:71:LEU:HA	1.77	0.50
1:B:51:THR:C	1:B:53:GLY:H	2.15	0.50
1:D:254:ALA:HA	1:D:430:THR:HG22	1.93	0.50
1:D:276:VAL:HG22	1:D:280:THR:HG21	1.94	0.50
1:E:112:ILE:HB	1:E:140:LEU:HD23	1.93	0.50
1:E:203:ILE:HA	1:E:347:PHE:HA	1.93	0.50
1:E:238:LEU:HD23	1:E:441:GLN:CG	2.35	0.50
1:F:351:PRO:O	1:G:324:HIS:HB3	2.12	0.50
1:H:127:GLY:O	1:H:131:ALA:N	2.44	0.50
1:A:383:VAL:HG23	1:B:183:ASN:OD1	2.11	0.49
1:C:191:ASN:HD21	1:D:382:MET:H	1.59	0.49
1:D:462:TYR:CE1	1:D:468:GLY:HA2	2.46	0.49
1:E:101:ASP:HA	1:E:104:GLY:O	2.12	0.49
1:F:271:ILE:HG13	1:F:448:ILE:HG12	1.93	0.49
1:H:99:ILE:O	1:H:100:ALA:HB3	2.11	0.49
1:H:148:GLN:O	1:H:230:ARG:HD3	2.12	0.49
1:H:276:VAL:HG22	1:H:280:THR:OG1	2.12	0.49
1:H:285:TYR:N	1:H:310:THR:OG1	2.44	0.49
1:A:202:GLY:C	1:A:348:LYS:H	2.16	0.49
1:D:246:MET:HE1	1:D:249:PRO:HD3	1.94	0.49
1:E:27:TYR:HB2	1:E:62:LEU:HD11	1.94	0.49
1:F:172:ILE:HG12	1:F:432:PHE:CE2	2.47	0.49
1:G:365:ASN:ND2	1:H:191:ASN:OD1	2.44	0.49
1:H:258:ARG:HA	1:H:261:LYS:HD2	1.94	0.49
1:H:423:ASP:HB3	1:H:428:ASP:OD2	2.13	0.49
1:H:460:LYS:HD3	1:H:471:THR:CG2	2.43	0.49
1:A:118:SER:O	1:A:121:PHE:HB2	2.11	0.49
1:A:445:ILE:O	1:A:448:ILE:HG23	2.12	0.49
1:B:415:ILE:HG22	1:B:418:GLU:HG2	1.93	0.49
1:B:417:HIS:O	1:B:421:LEU:HG	2.13	0.49
1:E:45:SER:HB3	1:E:85:TYR:OH	2.12	0.49
1:E:183:ASN:O	1:E:186:THR:N	2.46	0.49
1:E:370:VAL:CG2	1:E:376:THR:H	2.25	0.49
1:F:112:ILE:HG21	1:F:128:LEU:HD13	1.93	0.49
1:H:99:ILE:HD12	1:H:133:LEU:HG	1.94	0.49
1:A:237:ILE:HG21	1:A:330:ILE:CG2	2.42	0.49
1:A:442:TRP:HA	1:A:442:TRP:CE3	2.47	0.49
1:C:337:PRO:HD3	1:C:466:THR:O	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:18:SER:O	1:H:23:LEU:HG	2.13	0.49
1:H:288:GLY:O	1:H:295:VAL:N	2.26	0.49
1:A:449:ARG:HH11	1:A:453:LYS:HZ1	1.59	0.49
1:C:433:VAL:HG12	1:C:438:VAL:HG23	1.94	0.49
1:E:203:ILE:HG12	1:E:347:PHE:CD1	2.48	0.49
1:F:121:PHE:O	1:F:125:ILE:HG13	2.11	0.49
1:F:283:GLY:O	1:F:309:GLU:HA	2.13	0.49
1:B:3:ASN:HB3	1:B:139:ARG:NH2	2.26	0.49
1:B:53:GLY:O	1:B:57:PHE:N	2.43	0.49
1:C:203:ILE:O	1:C:348:LYS:NZ	2.44	0.49
1:D:290:SER:H	1:D:295:VAL:HG13	1.78	0.49
1:D:385:GLU:HB3	1:D:394:HIS:O	2.13	0.49
1:E:183:ASN:O	1:E:184:LEU:C	2.51	0.49
1:E:276:VAL:HG11	1:E:452:TRP:N	2.28	0.49
1:E:277:ILE:HD11	1:E:455:ASN:HB3	1.93	0.49
1:H:334:LYS:O	1:H:335:ARG:HB2	2.13	0.49
1:H:378:GLN:HG3	1:H:399:TRP:CZ3	2.48	0.49
1:A:273:ASN:HA	1:A:451:GLY:HA2	1.95	0.49
1:B:139:ARG:NH1	1:B:427:GLY:HA2	2.28	0.49
1:B:476:VAL:HB	1:B:481:VAL:O	2.12	0.49
1:D:27:TYR:CE2	1:D:66:VAL:HG11	2.48	0.49
1:D:272:ASN:H	1:D:275:THR:HB	1.77	0.49
1:D:422:LEU:HD23	1:D:422:LEU:O	2.12	0.49
1:F:261:LYS:HB3	1:F:261:LYS:HE3	1.57	0.49
1:G:179:GLU:OE1	1:H:386:PRO:HA	2.12	0.49
1:H:359:GLY:O	1:H:394:HIS:CD2	2.54	0.49
1:B:216:LEU:HD13	1:B:334:LYS:CE	2.43	0.49
1:B:229:LEU:HG	1:B:445:ILE:HD11	1.93	0.49
1:B:470:ILE:O	1:B:473:ILE:HG12	2.12	0.49
1:C:367:LEU:HD13	1:C:379:ILE:HG12	1.95	0.49
1:D:444:TRP:O	1:D:448:ILE:HG13	2.13	0.49
1:E:226:SER:HA	1:E:230:ARG:NH1	2.27	0.49
1:F:197:LEU:O	1:F:202:GLY:HA3	2.13	0.49
1:F:408:PHE:CD1	1:F:411:ARG:HD3	2.48	0.49
1:C:285:TYR:CD1	1:C:335:ARG:HG3	2.48	0.49
1:D:114:LEU:HD21	1:D:121:PHE:CG	2.47	0.49
1:E:7:THR:O	1:E:8:MET:HB3	2.11	0.49
1:F:144:LYS:HD3	1:F:236:HIS:CE1	2.47	0.49
1:F:423:ASP:O	1:F:427:GLY:N	2.45	0.49
1:H:258:ARG:NH1	1:H:429:ALA:O	2.46	0.49
1:B:29:LEU:CD2	1:B:418:GLU:HB2	2.43	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:195:GLU:OE2	1:D:322:ARG:NH1	2.27	0.49
1:E:29:LEU:HG	1:E:418:GLU:HG2	1.95	0.49
1:E:377:ILE:C	1:E:378:GLN:HG3	2.33	0.49
1:F:112:ILE:HD12	1:F:139:ARG:C	2.34	0.49
1:G:64:ARG:HB2	1:G:64:ARG:HH11	1.78	0.49
1:G:149:ASP:OD1	1:G:149:ASP:N	2.43	0.49
1:H:429:ALA:HA	1:H:432:PHE:HD2	1.77	0.49
1:B:211:ALA:HB3	1:B:340:ARG:H	1.76	0.48
1:B:315:LYS:HE2	1:B:317:HIS:NE2	2.28	0.48
1:C:268:LEU:HD23	1:C:318:VAL:HG22	1.94	0.48
1:C:415:ILE:HB	1:C:418:GLU:HG3	1.95	0.48
1:D:114:LEU:HD23	1:D:142:LEU:HD23	1.95	0.48
1:D:199:ASN:OD1	1:D:201:LYS:O	2.31	0.48
1:H:227:GLY:O	1:H:231:ASP:HB2	2.13	0.48
1:C:86:ALA:O	1:C:87:THR:C	2.50	0.48
1:C:362:LEU:HD23	1:C:362:LEU:HA	1.70	0.48
1:D:45:SER:HB3	1:D:85:TYR:HE2	1.77	0.48
1:D:336:LEU:HD13	1:D:467:TRP:HZ3	1.77	0.48
1:E:315:LYS:HG3	1:E:329:TYR:CE1	2.48	0.48
1:F:262:VAL:HG22	1:F:437:GLU:CG	2.39	0.48
1:G:434:ARG:HH21	1:G:436:ASP:CG	2.15	0.48
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.67	0.48
1:E:69:ASP:OD1	1:E:70:ARG:N	2.45	0.48
1:E:247:GLU:HG2	1:E:248:PRO:HD2	1.95	0.48
1:E:273:ASN:CB	1:E:451:GLY:HA2	2.43	0.48
1:F:150:LEU:HD22	1:F:443:ILE:CD1	2.44	0.48
1:G:185:LEU:HD22	1:G:189:PHE:HE2	1.79	0.48
1:H:282:THR:HG23	1:H:309:GLU:HB3	1.95	0.48
1:A:164:PHE:CD1	1:A:168:GLN:OE1	2.65	0.48
1:A:168:GLN:HA	1:A:170:TYR:HE1	1.78	0.48
1:D:342:GLU:HA	1:D:370:VAL:HA	1.95	0.48
1:D:472:ALA:O	1:D:475:LEU:N	2.44	0.48
1:E:188:ARG:HD3	1:E:243:LEU:O	2.14	0.48
1:E:384:LYS:HG2	1:E:385:GLU:O	2.13	0.48
1:H:286:GLY:N	1:H:462:TYR:O	2.42	0.48
1:A:321:TRP:CH2	1:D:350:VAL:HB	2.48	0.48
1:A:409:LYS:HG2	1:A:410:ASP:N	2.28	0.48
1:E:306:SER:HG	1:E:308:THR:HG23	1.78	0.48
1:F:200:SER:HA	1:F:326:VAL:CG2	2.43	0.48
1:G:178:LYS:HB2	1:G:181:VAL:CG2	2.44	0.48
1:H:80:LEU:O	1:H:83:LEU:HB2	2.14	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:436:ASP:HA	1:B:439:GLU:OE2	2.13	0.48
1:E:309:GLU:O	1:E:311:PHE:N	2.41	0.48
1:E:337:PRO:HD2	1:E:467:TRP:CZ3	2.48	0.48
1:F:198:TRP:HH2	1:F:367:LEU:CD2	2.26	0.48
1:G:40:ARG:HD3	1:G:84:PHE:CE2	2.49	0.48
1:G:296:ALA:O	1:G:335:ARG:NH1	2.33	0.48
1:A:203:ILE:O	1:A:348:LYS:HE3	2.14	0.48
1:A:316:ALA:HB3	1:A:328:PHE:HB2	1.96	0.48
1:C:340:ARG:HA	1:C:373:PRO:CG	2.44	0.48
1:D:67:ALA:HB3	1:D:70:ARG:CG	2.44	0.48
1:E:189:PHE:CE1	1:E:248:PRO:HD3	2.49	0.48
1:E:313:ALA:C	1:E:314:ILE:HG13	2.33	0.48
1:E:352:HIS:CE1	1:F:250:ALA:O	2.67	0.48
1:F:188:ARG:HH22	1:F:322:ARG:HH12	1.61	0.48
1:H:99:ILE:HG21	1:H:131:ALA:O	2.13	0.48
1:B:12:GLY:HA3	1:B:115:ALA:O	2.14	0.48
1:B:233:VAL:HG22	1:B:445:ILE:HD11	1.96	0.48
1:C:395:MET:HE2	1:C:395:MET:HB2	1.61	0.48
1:E:193:LEU:H	1:E:193:LEU:CD2	2.27	0.48
1:E:415:ILE:HG23	1:E:418:GLU:OE2	2.13	0.48
1:F:207:GLN:O	1:F:343:ILE:HA	2.13	0.48
1:H:167:LYS:HE3	1:H:168:GLN:HG2	1.95	0.48
1:A:20:ARG:O	1:A:24:PRO:HG2	2.14	0.48
1:A:210:VAL:O	1:A:332:THR:HA	2.14	0.48
1:A:412:LYS:HG2	1:A:414:ARG:HG3	1.96	0.48
1:B:197:LEU:HD13	1:B:347:PHE:CD1	2.49	0.48
1:B:309:GLU:HB2	1:B:311:PHE:O	2.14	0.48
1:D:249:PRO:HG3	1:D:257:VAL:HG22	1.96	0.48
1:D:271:ILE:HG22	1:D:276:VAL:HG23	1.95	0.48
1:E:261:LYS:O	1:E:264:VAL:HB	2.14	0.48
1:G:211:ALA:HB3	1:G:340:ARG:N	2.29	0.48
1:H:8:MET:O	1:H:41:ILE:HA	2.14	0.48
1:A:114:LEU:HB3	1:A:121:PHE:CE1	2.48	0.48
1:D:106:VAL:O	1:D:109:GLY:N	2.47	0.48
1:F:204:ASP:CB	1:F:346:GLN:HG2	2.44	0.48
1:F:379:ILE:O	1:F:399:TRP:HA	2.14	0.48
1:H:433:VAL:HG12	1:H:434:ARG:H	1.78	0.48
1:A:54:PHE:CE1	1:A:85:TYR:HB2	2.48	0.47
1:B:193:LEU:O	1:B:196:PRO:HD2	2.12	0.47
1:B:378:GLN:HB2	1:B:399:TRP:HE3	1.78	0.47
1:E:52:ASP:HB3	1:E:85:TYR:HE2	1.78	0.47


		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:320:ASN:HD21	1:E:322:ARG:HB3	1.79	0.47
1:F:148:GLN:HG3	1:F:149:ASP:OD1	2.13	0.47
1:F:281:VAL:HG12	1:F:311:PHE:HE1	1.79	0.47
1:H:10:LEU:O	1:H:43:CYS:HA	2.14	0.47
1:B:93:PRO:HA	1:B:96:PHE:CD1	2.49	0.47
1:B:166:GLU:CD	1:B:171:ARG:HH22	2.17	0.47
1:B:200:SER:N	1:B:322:ARG:O	2.47	0.47
1:E:215:GLY:HA3	1:E:335:ARG:NH1	2.29	0.47
1:E:476:VAL:HG13	1:E:481:VAL:O	2.14	0.47
1:F:11:PHE:CE2	1:F:44:THR:HG21	2.49	0.47
1:G:335:ARG:HD2	1:G:464:SER:OG	2.14	0.47
1:H:211:ALA:O	1:H:339:ARG:HA	2.14	0.47
1:A:90:ILE:HA	1:A:96:PHE:HZ	1.79	0.47
1:B:144:LYS:HE2	2:B:501:NMN:C6	2.27	0.47
1:C:255:ASN:OD1	1:C:434:ARG:NH1	2.47	0.47
1:F:117:SER:H	1:F:120:LEU:HB2	1.79	0.47
1:F:172:ILE:HG12	1:F:432:PHE:HE2	1.80	0.47
1:G:337:PRO:CD	1:G:467:TRP:HA	2.44	0.47
1:H:178:LYS:O	1:H:182:GLN:HG3	2.15	0.47
1:B:43:CYS:HB2	1:B:84:PHE:O	2.15	0.47
1:B:217:GLU:O	1:B:220:ILE:HG12	2.15	0.47
1:G:213:THR:HG22	1:G:336:LEU:O	2.14	0.47
1:G:230:ARG:HA	1:G:234:GLN:HB2	1.96	0.47
1:G:289:VAL:HG13	1:G:292:GLY:O	2.15	0.47
1:H:237:ILE:HD12	1:H:332:THR:HB	1.96	0.47
1:H:285:TYR:CD2	1:H:310:THR:HG21	2.48	0.47
1:A:88:VAL:HG22	1:A:98:LYS:HD2	1.96	0.47
1:A:419:ARG:O	1:A:419:ARG:HD2	2.15	0.47
1:A:469:PRO:HB2	1:A:471:THR:OG1	2.14	0.47
1:B:121:PHE:HZ	1:B:143:GLU:HB2	1.80	0.47
1:B:142:LEU:O	1:B:172:ILE:HB	2.14	0.47
1:C:210:VAL:O	1:C:332:THR:HA	2.14	0.47
1:C:285:TYR:H	1:C:310:THR:HG21	1.79	0.47
1:D:284:GLN:CB	1:D:461:THR:HG22	2.45	0.47
1:E:143:GLU:HB3	2:E:501:NMN:H1RC	1.95	0.47
1:G:214:VAL:O	1:G:334:LYS:HB3	2.13	0.47
1:G:337:PRO:HG2	1:G:467:TRP:CD1	2.50	0.47
1:G:365:ASN:ND2	1:G:380:SER:O	2.48	0.47
1:H:460:LYS:HZ3	1:H:470:ILE:HG13	1.79	0.47
1:A:126:ALA:O	1:A:129:LYS:HG3	2.14	0.47
1:A:339:ARG:O	1:A:373:PRO:HD3	2.15	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:30:ASP:HA	1:B:35:LEU:HB2	1.96	0.47
1:C:229:LEU:O	1:C:233:VAL:HG12	2.14	0.47
1:C:345:VAL:O	1:C:366:LYS:HA	2.14	0.47
1:D:195:GLU:HA	1:D:198:TRP:HB2	1.96	0.47
1:E:246:MET:CE	1:E:249:PRO:HD3	2.44	0.47
1:H:14:THR:HB	1:H:45:SER:OG	2.14	0.47
1:A:214:VAL:O	1:A:335:ARG:N	2.46	0.47
1:A:431:LEU:C	1:A:432:PHE:CD2	2.88	0.47
1:B:3:ASN:HB3	1:B:425:ILE:O	2.15	0.47
1:B:201:LYS:HB3	1:C:201:LYS:HE3	1.96	0.47
1:B:329:TYR:CZ	1:B:481:VAL:HG11	2.49	0.47
1:B:428:ASP:O	1:B:429:ALA:HB3	2.15	0.47
1:C:212:GLU:HA	1:C:339:ARG:CB	2.45	0.47
1:C:226:SER:O	1:C:230:ARG:HB2	2.14	0.47
1:C:261:LYS:HE2	1:C:437:GLU:OE2	2.15	0.47
1:C:386:PRO:HD2	1:D:411:ARG:NH1	2.29	0.47
1:D:50:ASP:OD1	1:D:52:ASP:HB2	2.15	0.47
1:E:287:ALA:O	1:E:463:VAL:HG13	2.14	0.47
1:E:472:ALA:O	1:E:475:LEU:N	2.43	0.47
1:H:20:ARG:HH11	1:H:65:PHE:HE1	1.62	0.47
1:H:337:PRO:HG2	1:H:467:TRP:CD1	2.50	0.47
1:H:378:GLN:HA	1:H:400:LEU:O	2.14	0.47
1:H:415:ILE:HB	1:H:418:GLU:HG3	1.95	0.47
1:C:154:ASP:HA	1:C:435:ARG:HH22	1.76	0.47
1:C:285:TYR:CG	1:C:335:ARG:HG3	2.50	0.47
1:E:354:ILE:O	1:F:251:HIS:CD2	2.67	0.47
1:F:19:GLN:HA	1:F:23:LEU:HD12	1.96	0.47
1:B:3:ASN:CB	1:B:139:ARG:HH21	2.26	0.47
1:B:78:LYS:HB2	1:B:78:LYS:HE2	1.71	0.47
1:B:353:SER:C	1:B:355:PHE:H	2.16	0.47
1:C:242:ALA:HB2	1:C:265:PHE:CE1	2.50	0.47
1:E:213:THR:HA	1:E:336:LEU:H	1.79	0.47
1:E:341:SER:N	1:E:372:GLN:HB3	2.28	0.47
1:G:138:SER:O	1:G:168:GLN:HB3	2.14	0.47
1:H:78:LYS:HA	1:H:81:ASN:ND2	2.30	0.47
1:H:120:LEU:HD23	1:H:120:LEU:HA	1.77	0.47
1:H:198:TRP:CH2	1:H:345:VAL:HG21	2.50	0.47
1:H:284:GLN:HB2	1:H:459:PRO:HB2	1.97	0.47
1:A:15:GLY:N	1:A:46:ARG:HH12	2.13	0.47
1:A:135:GLY:N	1:A:164:PHE:CE1	2.82	0.47
1:B:143:GLU:O	1:B:146:LEU:HD23	2.15	0.47



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:402:LEU:HD12	1:B:403:SER:H	1.80	0.47
1:F:196:PRO:C	1:F:199:ASN:HD21	2.18	0.47
1:H:272:ASN:N	1:H:275:THR:OG1	2.48	0.47
1:A:7:THR:HG21	1:A:104:GLY:N	2.30	0.46
1:A:13:SER:HB2	1:A:43:CYS:HB3	1.96	0.46
1:C:262:VAL:HG22	1:C:437:GLU:HA	1.97	0.46
1:D:130:GLN:H	1:D:130:GLN:HG2	1.35	0.46
1:F:260:GLU:HA	1:F:263:LYS:HD3	1.97	0.46
1:F:322:ARG:HD2	1:F:323:TRP:CE2	2.49	0.46
1:G:191:ASN:HB3	1:H:365:ASN:ND2	2.29	0.46
1:G:377:ILE:HG22	1:H:400:LEU:HD21	1.97	0.46
1:H:26:LEU:HD21	1:H:421:LEU:HD22	1.97	0.46
1:H:272:ASN:CB	1:H:275:THR:HG23	2.44	0.46
1:A:258:ARG:O	1:A:261:LYS:N	2.48	0.46
1:B:474:ALA:HA	1:B:477:GLU:HB2	1.97	0.46
1:D:417:HIS:O	1:D:421:LEU:HD23	2.16	0.46
1:D:437:GLU:O	1:D:441:GLN:HG3	2.16	0.46
1:E:185:LEU:O	1:F:355:PHE:HZ	1.97	0.46
1:E:203:ILE:HG12	1:E:347:PHE:CE1	2.50	0.46
1:F:140:LEU:HB2	1:F:164:PHE:CE1	2.51	0.46
1:G:44:THR:HB	1:G:99:ILE:HD11	1.96	0.46
1:G:235:SER:O	1:G:239:GLN:N	2.40	0.46
1:G:245:ALA:O	1:G:323:TRP:NE1	2.43	0.46
1:G:417:HIS:HA	1:G:420:LEU:HD12	1.97	0.46
1:H:329:TYR:CZ	1:H:481:VAL:HG11	2.49	0.46
1:A:320:ASN:O	1:A:324:HIS:HB2	2.15	0.46
1:B:5:VAL:HG13	1:B:109:GLY:O	2.14	0.46
1:B:361:ILE:HG12	1:B:382:MET:HE1	1.97	0.46
1:B:463:VAL:HG11	1:G:294:GLU:HG3	1.97	0.46
1:E:236:HIS:O	1:E:239:GLN:N	2.45	0.46
1:E:388:LEU:HD21	1:F:414:ARG:NE	2.31	0.46
1:F:216:LEU:H	1:F:216:LEU:HG	1.49	0.46
1:F:438:VAL:CG1	1:F:442:TRP:HD1	2.29	0.46
1:G:6:SER:HB2	1:G:109:GLY:CA	2.45	0.46
1:G:166:GLU:CD	1:G:171:ARG:HH22	2.19	0.46
1:H:4:THR:HA	1:H:425:ILE:O	2.16	0.46
1:H:30:ASP:HA	1:H:35:LEU:CD1	2.41	0.46
1:H:60:LYS:HD3	1:H:60:LYS:HA	1.60	0.46
1:H:385:GLU:OE1	1:H:396:ARG:HD3	2.15	0.46
1:H:419:ARG:O	1:H:422:LEU:N	2.47	0.46
1:A:7:THR:HG21	1:A:104:GLY:H	1.81	0.46



	A + O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:214:VAL:O	1:D:334:LYS:HB3	2.15	0.46
1:G:249:PRO:HB2	1:G:251:HIS:O	2.16	0.46
1:H:293:LYS:HD3	1:H:293:LYS:HA	1.45	0.46
1:B:216:LEU:HD13	1:B:334:LYS:NZ	2.30	0.46
1:B:227:GLY:H	1:B:230:ARG:HG3	1.81	0.46
1:C:25:ALA:HB1	1:C:418:GLU:CG	2.46	0.46
1:C:250:ALA:O	1:D:354:ILE:HG22	2.16	0.46
1:C:431:LEU:HD12	1:C:431:LEU:O	2.14	0.46
1:D:7:THR:CG2	1:D:104:GLY:H	2.29	0.46
1:E:20:ARG:HA	1:E:65:PHE:CD2	2.48	0.46
1:E:52:ASP:HB3	1:E:85:TYR:CE2	2.50	0.46
1:E:299:ILE:O	1:E:302:LEU:O	2.34	0.46
1:F:262:VAL:HG13	1:F:437:GLU:HA	1.98	0.46
1:G:309:GLU:HB2	1:G:311:PHE:H	1.80	0.46
1:H:466:THR:O	1:H:467:TRP:HB2	2.15	0.46
1:B:113:TYR:HE2	1:B:172:ILE:HG13	1.81	0.46
1:B:148:GLN:HB3	1:B:230:ARG:NH2	2.30	0.46
1:C:48:GLU:CB	1:C:87:THR:HA	2.46	0.46
1:C:242:ALA:HB1	1:C:261:LYS:HG2	1.98	0.46
1:D:152:SER:O	1:D:156:ILE:N	2.34	0.46
1:E:355:PHE:CZ	1:F:186:THR:HA	2.50	0.46
1:F:28:GLY:HA3	1:F:70:ARG:NH2	2.30	0.46
1:F:208:ILE:HG23	1:F:343:ILE:HG12	1.96	0.46
1:F:415:ILE:O	1:F:418:GLU:HG3	2.16	0.46
1:G:187:LEU:HG	1:G:194:PHE:CE2	2.51	0.46
1:G:197:LEU:C	1:G:199:ASN:H	2.19	0.46
1:A:11:PHE:CE1	1:A:128:LEU:HD21	2.50	0.46
1:A:285:TYR:CD2	1:A:298:TYR:HB2	2.50	0.46
1:A:340:ARG:NH1	1:A:342:GLU:OE1	2.49	0.46
1:A:389:ASP:H	1:B:419:ARG:HH12	1.64	0.46
1:B:63:ASP:HA	1:B:71:LEU:HD21	1.98	0.46
1:C:183:ASN:HB2	1:D:384:LYS:N	2.27	0.46
1:C:386:PRO:HA	1:D:179:GLU:HG3	1.98	0.46
1:D:98:LYS:HA	1:D:101:ASP:OD2	2.15	0.46
1:G:70:ARG:NH1	1:G:413:ARG:O	2.49	0.46
1:G:86:ALA:O	1:G:99:ILE:HD11	2.16	0.46
1:H:197:LEU:O	1:H:199:ASN:N	2.47	0.46
1:H:210:VAL:O	1:H:332:THR:HA	2.16	0.46
1:A:157:ASN:HB3	1:A:435:ARG:HE	1.80	0.46
1:B:172:ILE:HD11	1:B:432:PHE:CE2	2.51	0.46
1:C:417:HIS:O	1:C:418:GLU:C	2.54	0.46



	1	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:276:VAL:HG13	1:E:457:MET:SD	2.56	0.46
1:F:297:GLY:O	1:F:301:GLU:N	2.48	0.46
1:G:15:GLY:O	1:G:19:GLN:HG3	2.16	0.46
1:G:412:LYS:HG2	1:G:414:ARG:HG2	1.98	0.46
1:H:176:LEU:CD1	1:H:431:LEU:O	2.63	0.46
1:A:7:THR:HG21	1:A:104:GLY:CA	2.46	0.46
1:A:20:ARG:HB3	1:A:65:PHE:CE1	2.50	0.46
1:A:146:LEU:HD22	1:A:438:VAL:HG11	1.98	0.46
1:A:247:GLU:HB2	1:A:260:GLU:OE1	2.16	0.46
1:A:378:GLN:HA	1:A:400:LEU:O	2.15	0.46
1:B:215:GLY:H	1:B:335:ARG:HD2	1.81	0.46
1:C:230:ARG:HD3	1:C:442:TRP:HH2	1.81	0.46
1:E:23:LEU:H	1:E:24:PRO:CD	2.29	0.46
1:E:355:PHE:HE2	1:F:190:GLY:HA2	1.81	0.46
1:F:16:ASP:HA	1:F:19:GLN:CG	2.45	0.46
1:G:6:SER:HB2	1:G:109:GLY:HA3	1.97	0.46
1:G:55:ARG:HD3	1:G:80:LEU:HB3	1.98	0.46
1:G:366:LYS:HE2	1:G:366:LYS:HB2	1.38	0.46
1:H:263:LYS:HB3	1:H:263:LYS:HE2	1.63	0.46
1:H:415:ILE:HD12	1:H:415:ILE:N	2.31	0.46
1:A:17:LEU:HD13	2:A:501:NMN:C3	2.46	0.46
1:C:360:GLY:N	1:C:394:HIS:HA	2.31	0.46
1:E:367:LEU:HG	1:E:369:ILE:HD11	1.97	0.46
1:E:370:VAL:HG23	1:E:376:THR:H	1.81	0.46
1:F:16:ASP:O	1:F:17:LEU:C	2.54	0.46
1:G:37:ASP:HA	1:G:82:LYS:CE	2.43	0.46
1:G:148:GLN:N	1:G:152:SER:OG	2.42	0.46
1:H:21:MET:C	1:H:24:PRO:HD2	2.37	0.46
1:H:161:LEU:HA	1:H:164:PHE:O	2.15	0.46
1:A:315:LYS:HD2	1:A:478:ARG:NH2	2.31	0.45
1:F:198:TRP:HH2	1:F:367:LEU:HD23	1.80	0.45
1:F:211:ALA:O	1:F:339:ARG:HA	2.16	0.45
1:G:340:ARG:HA	1:G:373:PRO:CG	2.41	0.45
1:H:172:ILE:HG12	1:H:432:PHE:HE1	1.81	0.45
1:B:14:THR:HG23	1:B:45:SER:HB2	1.97	0.45
1:B:380:SER:HB2	1:B:399:TRP:CE2	2.51	0.45
1:C:283:GLY:HA2	1:C:460:LYS:O	2.16	0.45
1:C:341:SER:H	1:C:373:PRO:CG	2.29	0.45
1:D:322:ARG:HD2	1:D:323:TRP:NE1	2.31	0.45
1:E:143:GLU:OE1	2:E:501:NMN:HC6	2.14	0.45
1:E:269:ARG:HB3	1:E:317:HIS:HB2	1.98	0.45



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:455:ASN:O	1:E:456:SER:HB2	2.16	0.45
1:G:11:PHE:HB2	1:G:114:LEU:HA	1.97	0.45
1:A:444:TRP:O	1:A:448:ILE:HG22	2.16	0.45
1:B:90:ILE:HD13	1:B:90:ILE:H	1.80	0.45
1:D:11:PHE:HB2	1:D:113:TYR:O	2.15	0.45
1:E:97:GLY:HA2	1:E:131:ALA:HB1	1.98	0.45
1:E:473:ILE:O	1:E:477:GLU:HG3	2.17	0.45
1:F:188:ARG:HH22	1:F:322:ARG:NH1	2.14	0.45
1:F:398:VAL:HG22	1:F:399:TRP:N	2.31	0.45
1:G:80:LEU:O	1:G:83:LEU:HB2	2.17	0.45
1:G:240:LEU:O	1:G:244:VAL:HG23	2.16	0.45
1:H:175:TYR:CD1	1:H:236:HIS:CD2	3.04	0.45
1:H:378:GLN:HB2	1:H:399:TRP:HE3	1.81	0.45
1:A:188:ARG:HH12	1:A:246:MET:HG2	1.81	0.45
1:A:258:ARG:HA	1:A:261:LYS:HD3	1.99	0.45
1:C:320:ASN:OD1	1:C:323:TRP:N	2.47	0.45
1:D:173:ASP:OD1	1:D:235:SER:HB2	2.16	0.45
1:D:302:LEU:CD2	1:D:306:SER:HB2	2.43	0.45
1:E:166:GLU:HA	1:E:169:VAL:CG2	2.44	0.45
1:E:350:VAL:HG13	1:E:362:LEU:CD2	2.47	0.45
1:F:261:LYS:O	1:F:264:VAL:HG13	2.16	0.45
1:H:76:LYS:HB3	1:H:76:LYS:HE3	1.80	0.45
1:A:32:ASP:HB2	1:A:34:LEU:HG	1.99	0.45
1:A:195:GLU:N	1:A:196:PRO:HD2	2.32	0.45
1:B:229:LEU:O	1:B:233:VAL:HG22	2.16	0.45
1:C:220:ILE:O	1:C:224:ASP:N	2.46	0.45
1:D:393:ALA:C	1:D:394:HIS:HD1	2.18	0.45
1:D:462:TYR:HB2	1:D:466:THR:HG22	1.98	0.45
1:E:377:ILE:HG13	1:E:404:LEU:HD21	1.99	0.45
1:F:449:ARG:HA	1:F:452:TRP:CE2	2.51	0.45
1:A:118:SER:HA	1:A:121:PHE:CG	2.51	0.45
1:B:166:GLU:O	1:B:169:VAL:HG22	2.17	0.45
1:B:198:TRP:HA	1:B:203:ILE:CD1	2.46	0.45
1:B:309:GLU:HG2	1:B:309:GLU:O	2.16	0.45
1:C:96:PHE:CB	1:C:131:ALA:HB3	2.47	0.45
1:D:114:LEU:HD21	1:D:121:PHE:CD1	2.52	0.45
1:E:229:LEU:HA	1:E:233:VAL:HG23	1.97	0.45
1:E:416:ALA:O	1:E:417:HIS:HB2	2.17	0.45
1:F:233:VAL:HG23	1:F:445:ILE:HD11	1.97	0.45
1:F:324:HIS:HB3	1:G:351:PRO:O	2.17	0.45
1:C:194:PHE:HB3	1:C:198:TRP:CE3	2.52	0.45



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:285:TYR:CB	1:C:335:ARG:HB2	2.47	0.45
1:D:27:TYR:CD2	1:D:66:VAL:HG11	2.52	0.45
1:E:23:LEU:N	1:E:24:PRO:CD	2.80	0.45
1:F:279:HIS:CE1	1:F:315:LYS:HD3	2.52	0.45
1:F:344:VAL:HG22	1:F:368:ARG:HG3	1.99	0.45
1:G:88:VAL:CB	1:G:95:GLN:HB2	2.46	0.45
1:G:271:ILE:CG1	1:G:448:ILE:HG13	2.37	0.45
1:H:30:ASP:HB2	1:H:35:LEU:HD11	1.98	0.45
1:H:198:TRP:O	1:H:322:ARG:HD3	2.16	0.45
1:A:99:ILE:O	1:A:102:LEU:HB2	2.17	0.45
1:A:144:LYS:N	1:A:145:PRO:HD2	2.32	0.45
1:A:273:ASN:HA	1:A:451:GLY:CA	2.47	0.45
1:D:29:LEU:HD23	1:D:34:LEU:HD12	1.97	0.45
1:D:205:HIS:NE2	1:D:481:VAL:HG21	2.32	0.45
1:F:62:LEU:O	1:F:66:VAL:N	2.49	0.45
1:F:242:ALA:CA	1:F:264:VAL:HG21	2.43	0.45
1:H:84:PHE:HB3	1:H:102:LEU:CB	2.47	0.45
1:H:211:ALA:HA	1:H:336:LEU:CD1	2.47	0.45
1:H:271:ILE:CG2	1:H:276:VAL:HG23	2.46	0.45
1:A:198:TRP:O	1:A:322:ARG:HD3	2.16	0.45
1:A:219:ARG:HB3	1:A:222:TYR:CZ	2.52	0.45
1:B:34:LEU:HB3	1:B:422:LEU:HD21	1.98	0.45
1:B:139:ARG:HH12	1:B:427:GLY:HA2	1.82	0.45
1:B:293:LYS:HE2	1:B:293:LYS:HB2	1.61	0.45
1:C:337:PRO:HG2	1:C:467:TRP:NE1	2.32	0.45
1:E:171:ARG:O	1:E:433:VAL:N	2.47	0.45
1:F:8:MET:CE	1:F:10:LEU:HB2	2.46	0.45
1:F:416:ALA:O	1:F:420:LEU:HD12	2.16	0.45
1:G:474:ALA:HA	1:G:477:GLU:HB2	1.98	0.45
1:H:269:ARG:O	1:H:444:TRP:NE1	2.43	0.45
1:A:283:GLY:O	1:A:309:GLU:O	2.35	0.45
1:A:381:ILE:HD13	1:A:400:LEU:HD11	1.98	0.45
1:C:271:ILE:HA	1:C:275:THR:HB	1.99	0.45
1:F:8:MET:HB3	1:F:40:ARG:O	2.17	0.45
1:F:26:LEU:HB2	1:F:79:PHE:HZ	1.82	0.45
1:F:219:ARG:HB3	1:F:222:TYR:CZ	2.52	0.45
1:F:233:VAL:O	1:F:238:LEU:HD13	2.17	0.45
1:G:284:GLN:HB2	1:G:459:PRO:HB2	1.97	0.45
1:A:354:ILE:O	1:B:251:HIS:HA	2.16	0.44
1:D:449:ARG:HA	1:D:452:TRP:NE1	2.33	0.44
1:F:96:PHE:CZ	1:F:124:ALA:HA	2.52	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:183:ASN:O	1:F:187:LEU:N	2.45	0.44
1:G:242:ALA:HA	1:G:264:VAL:HG11	2.00	0.44
1:G:382:MET:N	1:H:191:ASN:HD21	2.15	0.44
1:H:372:GLN:HG2	1:H:373:PRO:HA	1.99	0.44
1:A:51:THR:O	1:A:54:PHE:HB3	2.16	0.44
1:A:233:VAL:O	1:A:238:LEU:HG	2.16	0.44
1:A:285:TYR:CD1	1:A:335:ARG:HG3	2.52	0.44
1:B:255:ASN:O	1:B:259:ASP:N	2.43	0.44
1:C:286:GLY:O	1:C:464:SER:OG	2.31	0.44
1:D:299:ILE:HD12	1:D:304:GLN:O	2.18	0.44
1:E:204:ASP:HB2	1:E:347:PHE:O	2.17	0.44
1:E:415:ILE:HG12	1:E:418:GLU:HG3	2.00	0.44
1:G:382:MET:H	1:H:191:ASN:HD21	1.65	0.44
1:A:363:GLN:HA	1:A:364:PRO:HD3	1.86	0.44
1:B:165:SER:O	1:B:169:VAL:HG13	2.17	0.44
1:D:51:THR:O	1:D:55:ARG:HG3	2.16	0.44
1:D:298:TYR:CZ	1:D:302:LEU:HD13	2.52	0.44
1:D:467:TRP:HA	1:D:467:TRP:CE3	2.53	0.44
1:E:157:ASN:HA	1:E:160:VAL:HB	1.99	0.44
1:F:445:ILE:HA	1:F:448:ILE:HD12	1.99	0.44
1:G:247:GLU:HB2	1:G:260:GLU:OE1	2.17	0.44
1:G:381:ILE:HB	1:H:191:ASN:HD21	1.80	0.44
1:G:429:ALA:HA	1:G:432:PHE:CD1	2.52	0.44
1:H:422:LEU:O	1:H:426:GLU:HG2	2.17	0.44
1:H:475:LEU:HA	1:H:478:ARG:HE	1.81	0.44
1:B:75:ALA:O	1:B:78:LYS:HG3	2.17	0.44
1:C:359:GLY:HA3	1:C:393:ALA:O	2.17	0.44
1:D:64:ARG:HG3	1:D:65:PHE:CD2	2.52	0.44
1:D:378:GLN:HB2	1:D:399:TRP:HE3	1.82	0.44
1:E:26:LEU:HD13	1:E:41:ILE:HD12	2.00	0.44
1:E:156:ILE:O	1:E:160:VAL:N	2.49	0.44
1:E:340:ARG:CA	1:E:372:GLN:HB3	2.44	0.44
1:F:23:LEU:HB2	1:F:24:PRO:HD3	2.00	0.44
1:F:61:ALA:HA	1:F:64:ARG:HE	1.83	0.44
1:F:233:VAL:HA	1:F:237:ILE:HB	1.99	0.44
1:G:154:ASP:O	1:G:158:ASP:N	2.37	0.44
1:G:203:ILE:HG21	1:G:345:VAL:CG1	2.48	0.44
1:G:234:GLN:HA	1:G:445:ILE:HD11	2.00	0.44
1:H:96:PHE:C	1:H:98:LYS:H	2.21	0.44
1:H:237:ILE:O	1:H:241:VAL:HG23	2.17	0.44
1:H:460:LYS:NZ	1:H:470:ILE:HG13	2.33	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:7:THR:HG21	1:A:104:GLY:HA2	1.99	0.44
1:A:172:ILE:HG12	1:A:432:PHE:CE1	2.52	0.44
1:A:423:ASP:HA	1:A:426:GLU:HB2	1.99	0.44
1:A:433:VAL:CG1	1:A:437:GLU:HB3	2.47	0.44
1:B:189:PHE:CE1	1:B:248:PRO:HG3	2.53	0.44
1:B:222:TYR:HE1	2:B:501:NMN:H2RO	1.58	0.44
1:F:217:GLU:H	1:F:217:GLU:HG2	1.60	0.44
1:G:121:PHE:O	1:G:125:ILE:HG13	2.16	0.44
1:G:385:GLU:HG2	1:G:386:PRO:HD2	1.99	0.44
1:H:158:ASP:C	1:H:160:VAL:H	2.21	0.44
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.58	0.44
1:B:203:ILE:HD13	1:B:345:VAL:CG1	2.48	0.44
1:B:352:HIS:HB3	1:C:321:TRP:HA	1.99	0.44
1:B:361:ILE:HB	1:B:363:GLN:HG2	1.99	0.44
1:B:411:ARG:HA	1:B:411:ARG:HD2	1.76	0.44
1:B:412:LYS:C	1:B:414:ARG:HH22	2.21	0.44
1:D:100:ALA:HB2	1:D:131:ALA:HB1	1.99	0.44
1:E:127:GLY:O	1:E:131:ALA:N	2.50	0.44
1:F:229:LEU:HG	1:F:445:ILE:HD11	1.99	0.44
1:F:246:MET:HE3	1:F:260:GLU:HB2	2.00	0.44
1:G:420:LEU:O	1:G:423:ASP:HB2	2.17	0.44
1:H:170:TYR:HB3	1:H:432:PHE:CG	2.52	0.44
1:H:245:ALA:HA	1:H:323:TRP:HE1	1.83	0.44
1:H:254:ALA:HB2	1:H:430:THR:CB	2.47	0.44
1:A:14:THR:HG23	1:A:45:SER:OG	2.18	0.44
1:B:246:MET:HA	1:B:264:VAL:CG2	2.48	0.44
1:E:220:ILE:H	1:E:220:ILE:HG12	1.38	0.44
1:E:398:VAL:HG22	1:E:399:TRP:H	1.82	0.44
1:F:171:ARG:HB2	1:F:433:VAL:HB	1.99	0.44
1:F:220:ILE:H	1:F:220:ILE:HG12	1.51	0.44
1:G:302:LEU:HG	1:G:304:GLN:HG2	2.00	0.44
1:H:142:LEU:HB2	1:H:171:ARG:HA	2.00	0.44
1:H:148:GLN:NE2	1:H:149:ASP:OD1	2.51	0.44
1:A:202:GLY:O	1:A:348:LYS:N	2.47	0.44
1:A:298:TYR:HE2	1:A:306:SER:OG	2.01	0.44
1:A:394:HIS:H	1:A:394:HIS:CD2	2.35	0.44
1:B:20:ARG:HG2	1:B:65:PHE:CE1	2.52	0.44
1:B:290:SER:HB3	1:B:295:VAL:HG11	2.00	0.44
1:B:352:HIS:HD2	1:B:354:ILE:CG2	2.30	0.44
1:B:376:THR:HG23	1:B:402:LEU:O	2.17	0.44
1:D:234:GLN:HG3	1:D:442:TRP:CZ3	2.53	0.44



	1 5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:116:THR:H	1:E:121:PHE:HE1	1.64	0.44
1:F:282:THR:OG1	1:F:459:PRO:HA	2.18	0.44
1:F:337:PRO:HG2	1:F:467:TRP:NE1	2.33	0.44
1:G:11:PHE:O	1:G:115:ALA:HB3	2.18	0.44
1:G:386:PRO:HD3	1:H:408:PHE:CD2	2.53	0.44
1:G:388:LEU:CD2	1:H:419:ARG:HD3	2.48	0.44
1:H:180:THR:CG2	1:H:371:LEU:HA	2.48	0.44
1:A:293:LYS:HA	1:A:293:LYS:HD3	1.85	0.44
1:B:14:THR:HG21	1:B:47:SER:O	2.18	0.44
1:B:114:LEU:HD21	1:B:140:LEU:HD11	1.99	0.44
1:B:285:TYR:N	1:B:310:THR:OG1	2.51	0.44
1:D:11:PHE:CD1	1:D:113:TYR:O	2.71	0.44
1:E:157:ASN:O	1:E:158:ASP:C	2.56	0.44
1:E:214:VAL:O	1:E:334:LYS:HD3	2.18	0.44
1:E:448:ILE:H	1:E:448:ILE:HG13	1.57	0.44
1:F:14:THR:HG21	1:F:46:ARG:C	2.37	0.44
1:H:212:GLU:O	1:H:336:LEU:N	2.49	0.44
1:A:281:VAL:HG11	1:A:472:ALA:HB2	1.99	0.43
1:B:415:ILE:HG22	1:B:418:GLU:CD	2.37	0.43
1:C:253:GLU:O	1:C:257:VAL:HG23	2.18	0.43
1:D:268:LEU:HD21	1:D:316:ALA:HB1	1.99	0.43
1:E:350:VAL:HG13	1:E:362:LEU:HD21	1.98	0.43
1:G:144:LYS:HD2	1:G:231:ASP:O	2.18	0.43
1:H:170:TYR:HA	1:H:432:PHE:HB3	2.00	0.43
1:H:219:ARG:HB3	1:H:222:TYR:CD1	2.51	0.43
1:A:80:LEU:HA	1:A:83:LEU:HD12	2.00	0.43
1:A:289:VAL:HA	1:A:293:LYS:O	2.18	0.43
1:A:365:ASN:C	1:A:366:LYS:HG3	2.39	0.43
1:A:439:GLU:O	1:A:443:ILE:HG22	2.18	0.43
1:C:315:LYS:HE2	1:C:327:PRO:HB3	2.01	0.43
1:C:438:VAL:HA	1:C:441:GLN:NE2	2.31	0.43
1:D:202:GLY:CA	1:D:348:LYS:HB2	2.49	0.43
1:F:21:MET:C	1:F:24:PRO:HD2	2.37	0.43
1:F:128:LEU:C	1:F:133:LEU:HB3	2.38	0.43
1:G:39:LEU:O	1:G:82:LYS:HD3	2.18	0.43
1:G:167:LYS:HG3	1:G:168:GLN:N	2.33	0.43
1:H:165:SER:H	1:H:168:GLN:HG3	1.83	0.43
1:H:449:ARG:HA	1:H:452:TRP:HB2	2.00	0.43
1:B:89:ASP:OD2	1:B:91:THR:HB	2.18	0.43
1:B:215:GLY:H	1:B:335:ARG:NE	2.16	0.43
1:C:193:LEU:H	1:C:193:LEU:HG	1.43	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:435:ARG:HH11	1:C:439:GLU:CD	2.20	0.43
1:D:4:THR:HA	1:D:425:ILE:O	2.19	0.43
1:D:377:ILE:HB	1:D:402:LEU:HD23	1.99	0.43
1:E:65:PHE:O	1:E:66:VAL:C	2.57	0.43
1:E:107:GLU:O	1:E:108:LYS:C	2.56	0.43
1:E:211:ALA:HB3	1:E:340:ARG:H	1.83	0.43
1:E:456:SER:O	1:E:457:MET:C	2.56	0.43
1:G:147:GLY:HA3	1:G:152:SER:OG	2.18	0.43
1:H:235:SER:HG	1:H:236:HIS:H	1.66	0.43
1:B:13:SER:HA	1:B:18:SER:HB2	1.98	0.43
1:B:415:ILE:HG22	1:B:418:GLU:CG	2.48	0.43
1:B:475:LEU:HD12	1:B:478:ARG:HE	1.83	0.43
1:C:62:LEU:HD12	1:C:76:LYS:HA	1.99	0.43
1:C:258:ARG:HE	1:C:434:ARG:HD3	1.83	0.43
1:C:388:LEU:HA	1:D:419:ARG:HD2	2.00	0.43
1:D:36:ALA:O	1:D:39:LEU:HB2	2.18	0.43
1:D:128:LEU:HD23	1:D:133:LEU:HB2	1.99	0.43
1:E:16:ASP:HA	1:E:19:GLN:CD	2.39	0.43
1:F:277:ILE:H	1:F:277:ILE:HG13	1.61	0.43
1:G:211:ALA:HB1	1:G:338:ALA:O	2.18	0.43
1:H:149:ASP:HB2	1:H:446:ASP:OD2	2.18	0.43
1:A:34:LEU:HD11	1:A:414:ARG:HH22	1.83	0.43
1:A:92:ASP:HB3	1:A:95:GLN:NE2	2.34	0.43
1:A:321:TRP:CZ2	1:D:351:PRO:HD2	2.53	0.43
1:B:10:LEU:HB3	1:B:42:VAL:O	2.19	0.43
1:B:216:LEU:HB2	1:B:220:ILE:CG2	2.43	0.43
1:B:420:LEU:HD23	1:B:431:LEU:HD13	1.99	0.43
1:C:223:PHE:HE2	1:C:228:SER:HA	1.83	0.43
1:D:146:LEU:HD12	1:D:146:LEU:O	2.18	0.43
1:D:340:ARG:HH11	1:D:368:ARG:HH22	1.66	0.43
1:D:370:VAL:O	1:D:375:GLU:HA	2.18	0.43
1:F:40:ARG:HA	1:F:84:PHE:CD2	2.51	0.43
1:G:254:ALA:HB2	1:G:430:THR:HG22	1.99	0.43
1:G:404:LEU:HD21	1:H:383:VAL:HG21	2.00	0.43
1:H:5:VAL:HA	1:H:109:GLY:HA3	2.01	0.43
1:H:50:ASP:O	1:H:51:THR:C	2.57	0.43
1:H:460:LYS:NZ	1:H:471:THR:HG23	2.33	0.43
1:H:476:VAL:HG22	1:H:481:VAL:CG2	2.42	0.43
1:B:215:GLY:HA3	1:B:335:ARG:HD2	2.00	0.43
1:B:311:PHE:HB2	1:B:462:TYR:OH	2.19	0.43
1:G:450:GLU:O	1:G:453:LYS:N	2.50	0.43



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:118:SER:HA	1:H:121:PHE:CD2	2.53	0.43
1:H:129:LYS:HA	1:H:134:ALA:HB3	1.99	0.43
1:H:313:ALA:HA	1:H:330:ILE:O	2.18	0.43
1:A:29:LEU:HD23	1:A:34:LEU:HD12	2.01	0.43
1:B:70:ARG:HH11	1:B:414:ARG:CB	2.30	0.43
1:B:177:GLY:HA3	1:B:420:LEU:HD11	2.00	0.43
1:B:240:LEU:O	1:B:244:VAL:HG23	2.18	0.43
1:D:185:LEU:HD22	1:D:185:LEU:HA	1.76	0.43
1:E:41:ILE:HB	1:E:83:LEU:HD12	2.00	0.43
1:E:89:ASP:H	1:E:95:GLN:HG3	1.83	0.43
1:E:229:LEU:HB2	1:E:312:VAL:HG11	2.01	0.43
1:E:299:ILE:HD13	1:E:299:ILE:HA	1.82	0.43
1:G:17:LEU:HG	1:G:22:LEU:CD2	2.48	0.43
1:G:67:ALA:O	1:G:71:LEU:HB2	2.18	0.43
1:G:118:SER:HB3	1:G:145:PRO:O	2.18	0.43
1:H:24:PRO:HA	1:H:62:LEU:CD2	2.49	0.43
1:H:64:ARG:H	1:H:64:ARG:HG3	1.56	0.43
1:H:384:LYS:HE2	1:H:384:LYS:HB3	1.71	0.43
1:A:114:LEU:HD23	1:A:121:PHE:CD1	2.53	0.43
1:B:3:ASN:H	1:B:3:ASN:HD22	1.66	0.43
1:B:259:ASP:HA	1:B:434:ARG:HH22	1.84	0.43
1:D:24:PRO:HA	1:D:66:VAL:HG22	2.00	0.43
1:D:203:ILE:HG12	1:D:347:PHE:CD1	2.54	0.43
1:E:342:GLU:HA	1:E:370:VAL:HA	2.00	0.43
1:F:8:MET:N	1:F:40:ARG:O	2.43	0.43
1:F:27:TYR:OH	1:F:75:ALA:HB3	2.18	0.43
1:F:149:ASP:HA	1:F:446:ASP:OD1	2.18	0.43
1:G:161:LEU:HA	1:G:164:PHE:O	2.18	0.43
1:H:139:ARG:NH1	1:H:425:ILE:O	2.47	0.43
1:H:415:ILE:HG22	1:H:417:HIS:H	1.84	0.43
1:A:25:ALA:HB1	1:A:418:GLU:HG3	2.00	0.43
1:A:216:LEU:HD13	1:A:216:LEU:HA	1.87	0.43
1:A:265:PHE:HE2	1:A:437:GLU:HG2	1.83	0.43
1:A:350:VAL:HA	1:B:192:ALA:HB2	2.01	0.43
1:B:385:GLU:HG2	1:B:396:ARG:HB2	2.01	0.43
1:C:25:ALA:HB1	1:C:418:GLU:HG2	2.01	0.43
1:G:183:ASN:CG	1:H:383:VAL:HG23	2.39	0.43
1:H:285:TYR:CE1	1:H:335:ARG:HG3	2.53	0.43
1:A:300:ASP:OD1	1:A:300:ASP:N	2.52	0.43
1:B:272:ASN:HB3	1:B:273:ASN:H	1.62	0.43
1:B:361:ILE:HG12	1:B:361:ILE:H	1.50	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:315:LYS:HG2	1:C:329:TYR:CE1	2.54	0.43	
1:D:110:ILE:O	1:D:138:SER:HA	2.19	0.43	
1:D:176:LEU:HA	1:D:181:VAL:HG11	2.00	0.43	
1:D:466:THR:O	1:D:467:TRP:HB2	2.18	0.43	
1:E:40:ARG:HG3	1:E:105:PRO:HD2	2.01	0.43	
1:G:392:GLY:HA3	1:G:394:HIS:NE2	2.33	0.43	
1:H:172:ILE:HG12	1:H:432:PHE:CE1	2.54	0.43	
1:A:66:VAL:HB	1:A:71:LEU:HD22	1.99	0.42	
1:A:389:ASP:N	1:A:389:ASP:OD1	2.52	0.42	
1:D:79:PHE:O	1:D:83:LEU:HD23	2.19	0.42	
1:E:100:ALA:O	1:E:104:GLY:N	2.44	0.42	
1:E:139:ARG:HD3	1:E:170:TYR:CZ	2.54	0.42	
1:E:161:LEU:C	1:E:163:VAL:N	2.72	0.42	
1:E:282:THR:HG22	1:E:283:GLY:H	1.83	0.42	
1:F:219:ARG:HD2	1:F:222:TYR:CE2	2.54	0.42	
1:G:273:ASN:O	1:G:276:VAL:HG12	2.19	0.42	
1:A:54:PHE:O	1:A:57:PHE:HB3	2.19	0.42	
1:A:176:LEU:HD21	1:A:239:GLN:HB3	2.00	0.42	
1:C:77:ALA:HA	1:C:80:LEU:HD12	2.00	0.42	
1:D:45:SER:HB3	1:D:85:TYR:CE2	2.55	0.42	
1:D:269:ARG:N	1:D:317:HIS:O	2.44	0.42	
1:F:39:LEU:HD23	1:F:40:ARG:H	1.83	0.42	
1:G:237:ILE:HG21	1:G:330:ILE:HG23	2.00	0.42	
1:H:152:SER:O	1:H:156:ILE:HG13	2.19	0.42	
1:A:186:THR:HG21	1:B:384:LYS:N	2.35	0.42	
1:B:9:ILE:HG12	1:B:111:ALA:O	2.18	0.42	
1:D:121:PHE:O	1:D:125:ILE:HG13	2.18	0.42	
1:E:272:ASN:H	1:E:275:THR:HB	1.84	0.42	
1:F:9:ILE:O	1:F:113:TYR:N	2.48	0.42	
1:F:113:TYR:CE1	1:F:115:ALA:HB2	2.54	0.42	
1:F:148:GLN:HA	1:F:230:ARG:HD3	2.01	0.42	
1:G:176:LEU:HD23	1:G:176:LEU:HA	1.80	0.42	
1:G:252:MET:HG2	1:H:354:ILE:HD12	2.02	0.42	
1:H:224:ASP:HA	1:H:298:TYR:HH	1.85	0.42	
1:H:235:SER:HG	1:H:236:HIS:CE1	2.29	0.42	
1:A:229:LEU:HG	1:A:230:ARG:N	2.34	0.42	
1:B:215:GLY:CA	1:B:334:LYS:HE3	2.45	0.42	
1:B:242:ALA:O	1:B:246:MET:N	2.49	0.42	
1:C:215:GLY:HA2	1:C:335:ARG:HG2	2.01	0.42	
1:C:285:TYR:HB2	1:C:335:ARG:HB2	2.01	0.42	
1:E:273:ASN:CA	1:E:451:GLY:HA2	2.48	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:422:LEU:HA	1:E:425:ILE:HD12	2.02	0.42
1:F:315:LYS:HE2	1:F:327:PRO:HB3	2.00	0.42
1:B:216:LEU:H	1:B:216:LEU:CD2	2.23	0.42
1:B:216:LEU:HD13	1:B:334:LYS:HZ1	1.84	0.42
1:B:421:LEU:O	1:B:422:LEU:C	2.58	0.42
1:B:451:GLY:O	1:B:455:ASN:N	2.50	0.42
1:C:75:ALA:HA	1:C:78:LYS:CB	2.49	0.42
1:C:350:VAL:HG12	1:D:192:ALA:HB2	2.01	0.42
1:D:5:VAL:HG21	1:D:111:ALA:N	2.35	0.42
1:D:62:LEU:HA	1:D:66:VAL:HG23	2.02	0.42
1:D:85:TYR:CD1	1:D:86:ALA:N	2.87	0.42
1:E:385:GLU:HB2	1:E:394:HIS:O	2.18	0.42
1:E:438:VAL:O	1:E:441:GLN:HB2	2.18	0.42
1:G:234:GLN:OE1	1:G:441:GLN:HB3	2.19	0.42
1:G:283:GLY:O	1:G:309:GLU:O	2.37	0.42
1:H:314:ILE:O	1:H:329:TYR:HA	2.19	0.42
1:H:449:ARG:NH1	1:H:453:LYS:NZ	2.68	0.42
1:A:54:PHE:C	1:A:56:ASP:N	2.72	0.42
1:B:23:LEU:HD22	1:B:23:LEU:HA	1.82	0.42
1:C:348:LYS:HA	1:C:349:PRO:HD3	1.86	0.42
1:C:375:GLU:HB3	1:C:404:LEU:CB	2.48	0.42
1:D:269:ARG:HB2	1:D:317:HIS:HB2	2.02	0.42
1:F:152:SER:OG	1:F:153:SER:N	2.53	0.42
1:G:187:LEU:HG	1:G:194:PHE:HE2	1.85	0.42
1:A:153:SER:O	1:A:156:ILE:HG12	2.19	0.42
1:A:388:LEU:HD22	1:B:419:ARG:CG	2.49	0.42
1:A:476:VAL:HG22	1:A:481:VAL:HG22	2.02	0.42
1:B:255:ASN:O	1:B:434:ARG:NH1	2.51	0.42
1:C:76:LYS:HE3	1:C:76:LYS:HB2	1.66	0.42
1:D:56:ASP:O	1:D:60:LYS:HG3	2.19	0.42
1:E:258:ARG:NH1	1:E:432:PHE:O	2.53	0.42
1:F:70:ARG:NH2	1:F:415:ILE:HD12	2.30	0.42
1:F:188:ARG:NH2	1:F:322:ARG:NH1	2.68	0.42
1:F:238:LEU:HD23	1:F:441:GLN:HG2	2.01	0.42
1:G:277:ILE:H	1:G:277:ILE:HD13	1.84	0.42
1:A:129:LYS:HB2	1:A:129:LYS:HE2	1.42	0.42
1:C:188:ARG:NH2	1:C:322:ARG:HH12	2.16	0.42
1:C:197:LEU:O	1:C:199:ASN:N	2.53	0.42
1:C:230:ARG:HD3	1:C:442:TRP:CH2	2.54	0.42
1:D:25:ALA:CB	1:D:418:GLU:HG2	2.49	0.42
1:D:138:SER:O	1:D:164:PHE:HE2	2.03	0.42



	• • • • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:452:TRP:HB2	1:D:457:MET:SD	2.60	0.42	
1:E:372:GLN:HG3	1:E:372:GLN:H	1.45	0.42	
1:E:419:ARG:CB	1:F:388:LEU:HD22	2.50	0.42	
1:F:142:LEU:HB2	1:F:171:ARG:HA	2.02	0.42	
1:F:226:SER:HA	1:F:230:ARG:HH11	1.85	0.42	
1:G:162:LYS:HE3	1:G:162:LYS:HB3	1.51	0.42	
1:H:284:GLN:NE2	1:H:298:TYR:HD2	2.17	0.42	
1:B:3:ASN:H	1:B:3:ASN:ND2	2.18	0.42	
1:B:197:LEU:HB3	1:B:347:PHE:HE1	1.80	0.42	
1:C:186:THR:HG21	1:D:395:MET:HG2	2.02	0.42	
1:C:236:HIS:O	1:C:240:LEU:HG	2.20	0.42	
1:D:246:MET:CE	1:D:249:PRO:HD3	2.50	0.42	
1:D:247:GLU:OE2	1:D:322:ARG:NE	2.53	0.42	
1:D:436:ASP:HA	1:D:439:GLU:OE2	2.19	0.42	
1:F:476:VAL:CG1	1:F:477:GLU:N	2.83	0.42	
1:G:5:VAL:O	1:G:425:ILE:CG2	2.67	0.42	
1:H:113:TYR:CE1	1:H:115:ALA:HB2	2.55	0.42	
1:H:420:LEU:O	1:H:432:PHE:HZ	2.03	0.42	
1:A:18:SER:HA	1:A:22:LEU:HB2	2.02	0.42	
1:A:55:ARG:NH1	1:A:81:ASN:HA	2.35	0.42	
1:A:114:LEU:C	1:A:116:THR:H	2.21	0.42	
1:B:92:ASP:HB3	1:B:95:GLN:NE2	2.34	0.42	
1:B:197:LEU:HB3	1:B:347:PHE:CD1	2.54	0.42	
1:B:204:ASP:O	1:B:205:HIS:HB3	2.20	0.42	
1:B:223:PHE:O	1:B:225:SER:N	2.53	0.42	
1:B:432:PHE:CD1	1:B:432:PHE:N	2.87	0.42	
1:D:5:VAL:HG12	1:D:425:ILE:HA	2.02	0.42	
1:D:48:GLU:HA	1:D:87:THR:OG1	2.20	0.42	
1:D:449:ARG:O	1:D:453:LYS:N	2.44	0.42	
1:E:385:GLU:OE2	1:E:396:ARG:HG3	2.20	0.42	
1:E:422:LEU:HA	1:E:422:LEU:HD23	1.78	0.42	
1:G:144:LYS:HD3	1:G:236:HIS:NE2	2.35	0.42	
1:G:411:ARG:NH1	1:G:411:ARG:H	2.17	0.42	
1:H:38:ASP:HA	1:H:40:ARG:HH21	1.85	0.42	
1:H:99:ILE:CB	1:H:133:LEU:HD11	2.40	0.42	
1:B:90:ILE:HG13	1:B:120:LEU:HG	2.02	0.41	
1:B:222:TYR:CE2	2:B:501:NMN:O3P	2.73	0.41	
1:B:418:GLU:HG2	1:B:418:GLU:H	1.65	0.41	
1:D:5:VAL:HG23	1:D:109:GLY:C	2.40	0.41	
1:D:439:GLU:HG2	1:D:439:GLU:H	1.69	0.41	
1:E:382:MET:HE2	1:E:382:MET:HB3	1.81	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:29:LEU:CG	1:F:418:GLU:HB3	2.50	0.41
1:A:29:LEU:HB3	1:A:35:LEU:HG	2.02	0.41
1:A:179:GLU:HG3	1:B:386:PRO:HB3	2.02	0.41
1:B:160:VAL:O	1:B:164:PHE:N	2.42	0.41
1:B:234:GLN:O	1:B:441:GLN:NE2	2.53	0.41
1:B:415:ILE:HG23	1:B:417:HIS:H	1.85	0.41
1:C:274:ASP:O	1:C:277:ILE:HG22	2.20	0.41
1:C:435:ARG:NH1	1:C:439:GLU:OE1	2.53	0.41
1:D:11:PHE:CE1	1:D:112:ILE:HG23	2.55	0.41
1:D:128:LEU:O	1:D:132:GLY:N	2.51	0.41
1:E:19:GLN:HB2	1:E:61:ALA:HB1	2.02	0.41
1:F:237:ILE:HG21	1:F:330:ILE:HG23	2.01	0.41
1:G:174:HIS:CD2	1:G:236:HIS:NE2	2.88	0.41
1:G:258:ARG:HD2	1:G:434:ARG:HB2	2.01	0.41
1:G:311:PHE:CZ	1:G:469:PRO:HD2	2.55	0.41
1:G:436:ASP:HA	1:G:439:GLU:HG2	2.03	0.41
1:H:48:GLU:HA	1:H:87:THR:OG1	2.20	0.41
1:H:183:ASN:HA	1:H:186:THR:HG23	2.01	0.41
1:H:315:LYS:HE3	1:H:327:PRO:HB3	2.01	0.41
1:H:354:ILE:HG13	1:H:355:PHE:N	2.35	0.41
1:A:85:TYR:CD1	1:A:85:TYR:C	2.94	0.41
1:A:90:ILE:HG13	1:A:120:LEU:HG	2.02	0.41
1:A:439:GLU:HG2	1:A:439:GLU:H	1.60	0.41
1:A:457:MET:HE3	1:A:457:MET:HB3	1.72	0.41
1:B:15:GLY:C	1:B:17:LEU:H	2.23	0.41
1:B:322:ARG:HD2	1:B:323:TRP:NE1	2.36	0.41
1:G:318:VAL:HB	1:G:323:TRP:CB	2.49	0.41
1:H:236:HIS:ND1	1:H:236:HIS:N	2.67	0.41
1:H:282:THR:CG2	1:H:309:GLU:HB3	2.51	0.41
1:H:425:ILE:H	1:H:425:ILE:HG12	1.61	0.41
1:A:149:ASP:OD1	1:A:152:SER:HB3	2.20	0.41
1:C:205:HIS:CB	1:C:327:PRO:HG2	2.50	0.41
1:C:216:LEU:N	1:C:285:TYR:OH	2.43	0.41
1:C:258:ARG:O	1:C:262:VAL:HG23	2.20	0.41
1:D:70:ARG:HG2	1:D:70:ARG:H	1.58	0.41
1:D:417:HIS:HB3	1:D:421:LEU:HD23	2.03	0.41
1:E:116:THR:O	1:E:117:SER:HB3	2.19	0.41
1:F:127:GLY:O	1:F:131:ALA:N	2.53	0.41
1:G:258:ARG:HA	1:G:261:LYS:HG3	2.01	0.41
1:H:204:ASP:CB	1:H:346:GLN:HE21	2.32	0.41
1:A:281:VAL:HG11	1:A:472:ALA:N	2.35	0.41



	1.5	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:398:VAL:HG22	1:A:399:TRP:H	1.86	0.41	
1:B:113:TYR:CD2	1:B:141:ALA:HB3	2.55	0.41	
1:C:360:GLY:HA2	1:C:395:MET:H	1.86	0.41	
1:C:360:GLY:HA3	1:C:395:MET:HE2	2.03	0.41	
1:C:370:VAL:HG11	1:C:374:ASP:OD1	2.20	0.41	
1:D:25:ALA:CA	1:D:418:GLU:HG2	2.50	0.41	
1:E:116:THR:HB	1:E:120:LEU:HD22	2.03	0.41	
1:E:400:LEU:HB3	1:F:400:LEU:HB3	2.03	0.41	
1:F:39:LEU:HD23	1:F:40:ARG:N	2.36	0.41	
1:F:270:PRO:HA	1:F:444:TRP:CD1	2.56	0.41	
1:G:44:THR:CB	1:G:86:ALA:O	2.67	0.41	
1:H:51:THR:HA	1:H:85:TYR:CB	2.50	0.41	
1:H:254:ALA:O	1:H:255:ASN:HB2	2.20	0.41	
1:H:256:ALA:HA	1:H:259:ASP:HB2	2.03	0.41	
1:H:289:VAL:HG23	1:H:293:LYS:N	2.35	0.41	
1:H:343:ILE:HD11	1:H:371:LEU:HD11	2.02	0.41	
1:A:245:ALA:HA	1:A:323:TRP:CZ2	2.55	0.41	
1:C:186:THR:O	1:C:190:GLY:N	2.39	0.41	
1:C:237:ILE:O	1:C:240:LEU:N	2.53	0.41	
1:D:57:PHE:HA	1:D:60:LYS:HD2	2.03	0.41	
1:F:233:VAL:O	1:F:238:LEU:HB2	2.20	0.41	
1:F:259:ASP:O	1:F:263:LYS:HG3	2.20	0.41	
1:F:476:VAL:CG2	1:F:481:VAL:HG13	2.50	0.41	
1:G:271:ILE:HD13	1:G:271:ILE:N	2.36	0.41	
1:G:340:ARG:NH2	1:G:467:TRP:HZ2	2.18	0.41	
1:H:220:ILE:HG22	1:H:298:TYR:HE1	1.85	0.41	
1:H:476:VAL:O	1:H:481:VAL:HG13	2.21	0.41	
1:A:281:VAL:HG22	1:A:471:THR:HB	2.03	0.41	
1:B:144:LYS:N	1:B:145:PRO:CD	2.84	0.41	
1:C:228:SER:HB2	1:C:309:GLU:O	2.20	0.41	
1:D:102:LEU:HD12	1:D:102:LEU:HA	1.75	0.41	
1:E:209:SER:HB2	1:E:342:GLU:CG	2.50	0.41	
1:E:321:TRP:CE2	1:H:351:PRO:HD2	2.55	0.41	
1:F:314:ILE:HB	1:F:330:ILE:HD12	2.03	0.41	
1:B:34:LEU:O	1:B:422:LEU:HD11	2.21	0.41	
1:D:42:VAL:HG13	1:D:102:LEU:HD23	2.01	0.41	
1:D:466:THR:O	1:D:466:THR:HG23	2.20	0.41	
1:E:26:LEU:HA	1:E:26:LEU:HD23	1.79	0.41	
1:E:195:GLU:HA	1:E:198:TRP:HB2	2.02	0.41	
1:G:302:LEU:HD23	1:G:306:SER:CB	2.51	0.41	
1:H:154:ASP:OD1	1:H:435:ARG:NH2	2.53	0.41	



			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:20:ARG:HB3	1:A:65:PHE:CZ	2.56	0.41
1:A:58:ALA:O	1:A:61:ALA:HB3	2.21	0.41
1:A:309:GLU:HB3	1:A:311:PHE:O	2.21	0.41
1:B:62:LEU:O	1:B:63:ASP:C	2.60	0.41
1:B:262:VAL:HG22	1:B:437:GLU:HA	2.02	0.41
1:B:323:TRP:HZ3	1:B:326:VAL:HG11	1.86	0.41
1:B:415:ILE:HG23	1:B:417:HIS:N	2.36	0.41
1:C:13:SER:O	1:C:18:SER:O	2.39	0.41
1:C:457:MET:HE3	1:C:457:MET:HB3	1.91	0.41
1:D:336:LEU:HD23	1:D:336:LEU:HA	1.73	0.41
1:D:393:ALA:C	1:D:394:HIS:ND1	2.74	0.41
1:E:26:LEU:HB3	1:E:79:PHE:HE1	1.82	0.41
1:E:112:ILE:CD1	1:E:138:SER:HB3	2.51	0.41
1:E:226:SER:O	1:E:230:ARG:HB2	2.21	0.41
1:E:233:VAL:HG22	1:E:237:ILE:HD12	2.01	0.41
1:E:238:LEU:HB3	1:E:441:GLN:HE21	1.85	0.41
1:F:78:LYS:O	1:F:82:LYS:N	2.45	0.41
1:F:112:ILE:HD12	1:F:139:ARG:O	2.20	0.41
1:F:279:HIS:ND1	1:F:315:LYS:HB3	2.36	0.41
1:F:365:ASN:HA	1:F:380:SER:HB2	2.03	0.41
1:G:180:THR:HG23	1:G:375:GLU:HG2	2.02	0.41
1:G:271:ILE:HG12	1:G:271:ILE:O	2.21	0.41
1:H:185:LEU:HD22	1:H:185:LEU:HA	1.78	0.41
1:H:240:LEU:HD21	1:H:371:LEU:HD12	2.03	0.41
1:H:456:SER:HB3	1:H:458:LYS:HE2	2.02	0.41
1:A:92:ASP:HB3	1:A:95:GLN:HE21	1.86	0.41
1:B:191:ASN:HB3	1:B:193:LEU:HD23	2.03	0.41
1:B:219:ARG:HB3	1:B:222:TYR:CE2	2.55	0.41
1:B:246:MET:HE3	1:B:246:MET:HB2	1.92	0.41
1:C:216:LEU:HD13	1:C:216:LEU:HA	1.76	0.41
1:D:121:PHE:CD1	1:D:121:PHE:N	2.89	0.41
1:D:206:VAL:HG22	1:D:345:VAL:HG13	2.03	0.41
1:F:16:ASP:O	1:F:20:ARG:N	2.47	0.41
1:F:470:ILE:O	1:F:471:THR:C	2.59	0.41
1:G:129:LYS:HA	1:G:134:ALA:HB2	2.03	0.41
1:H:41:ILE:HD13	1:H:79:PHE:CE1	2.53	0.41
1:H:309:GLU:CD	1:H:309:GLU:H	2.24	0.41
1:H:435:ARG:HD3	1:H:435:ARG:O	2.21	0.41
1:A:128:LEU:CD2	1:A:133:LEU:HD12	2.51	0.40
1:A:180:THR:HG23	1:A:375:GLU:HB3	2.01	0.40
1:E:29:LEU:HD11	1:E:418:GLU:O	2.21	0.40



	1.5	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:89:ASP:HB3	1:E:95:GLN:HE21	1.86	0.40	
1:E:117:SER:HA	2:E:501:NMN:O3R	2.21	0.40	
1:E:475:LEU:O	1:E:478:ARG:HG2	2.19	0.40	
1:F:203:ILE:HG23	1:F:346:GLN:O	2.21	0.40	
1:G:253:GLU:HB3	1:G:256:ALA:HB3	2.02	0.40	
1:G:376:THR:HG22	1:G:377:ILE:N	2.36	0.40	
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.70	0.40	
1:C:26:LEU:O	1:C:29:LEU:N	2.50	0.40	
1:D:11:PHE:O	1:D:115:ALA:HB3	2.21	0.40	
1:E:200:SER:N	1:E:322:ARG:O	2.54	0.40	
1:F:8:MET:HE3	1:F:10:LEU:HB2	2.03	0.40	
1:G:37:ASP:O	1:G:40:ARG:NH2	2.54	0.40	
1:G:146:LEU:HD23	1:G:146:LEU:N	2.35	0.40	
1:G:238:LEU:HA	1:G:238:LEU:HD12	1.68	0.40	
1:G:470:ILE:H	1:G:470:ILE:HG12	1.69	0.40	
1:A:197:LEU:HD22	1:A:202:GLY:HA3	2.03	0.40	
1:A:387:GLY:HA3	1:A:394:HIS:HE1	1.83	0.40	
1:B:10:LEU:HD12	1:B:11:PHE:H	1.87	0.40	
1:B:74:ASP:O	1:B:75:ALA:C	2.60	0.40	
1:B:192:ALA:O	1:B:196:PRO:HD3	2.21	0.40	
1:B:311:PHE:CE1	1:B:469:PRO:HD2	2.56	0.40	
1:B:352:HIS:CD2	1:B:354:ILE:HG22	2.56	0.40	
1:D:269:ARG:CB	1:D:317:HIS:HB2	2.51	0.40	
1:G:144:LYS:HE2	2:G:501:NMN:C5	2.51	0.40	
1:G:268:LEU:HD23	1:G:268:LEU:HA	1.83	0.40	
1:G:382:MET:H	1:H:191:ASN:ND2	2.19	0.40	
1:H:5:VAL:HG22	1:H:109:GLY:CA	2.51	0.40	
1:H:30:ASP:CA	1:H:35:LEU:HD11	2.43	0.40	
1:H:112:ILE:O	1:H:140:LEU:HA	2.21	0.40	
1:H:299:ILE:H	1:H:299:ILE:HG12	1.60	0.40	
1:A:209:SER:O	1:A:341:SER:HA	2.20	0.40	
1:A:260:GLU:O	1:A:264:VAL:HG23	2.22	0.40	
1:C:448:ILE:HG22	1:C:452:TRP:CE3	2.56	0.40	
1:C:452:TRP:CD1	1:C:452:TRP:C	2.95	0.40	
1:F:16:ASP:HA	1:F:19:GLN:HE21	1.86	0.40	
1:F:419:ARG:CZ	1:F:431:LEU:HD21	2.51	0.40	
1:G:5:VAL:O	1:G:6:SER:CB	2.69	0.40	
1:G:21:MET:HB3	1:G:417:HIS:ND1	2.37	0.40	
1:G:388:LEU:CD1	1:H:34:LEU:HD13	2.52	0.40	
1:H:419:ARG:HG3	1:H:431:LEU:CD1	2.52	0.40	
1:H:435:ARG:HD3	1:H:435:ARG:C	2.42	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:TYR:CE2	1:A:481:VAL:HG11	2.57	0.40
1:C:435:ARG:NH1	1:C:439:GLU:CD	2.75	0.40
1:D:5:VAL:HG23	1:D:109:GLY:O	2.21	0.40
1:D:378:GLN:HB3	1:D:401:ASP:OD1	2.22	0.40
1:E:25:ALA:HA	1:E:418:GLU:CG	2.51	0.40
1:H:180:THR:HG21	1:H:371:LEU:HA	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	А	480/487~(99%)	446 (93%)	34 (7%)	0	100	100
1	В	473/487~(97%)	438 (93%)	35~(7%)	0	100	100
1	С	457/487~(94%)	408 (89%)	49 (11%)	0	100	100
1	D	475/487 (98%)	430 (90%)	45 (10%)	0	100	100
1	Е	470/487~(96%)	423 (90%)	45 (10%)	2(0%)	34	67
1	F	452/487~(93%)	413 (91%)	39 (9%)	0	100	100
1	G	483/487~(99%)	453 (94%)	30 (6%)	0	100	100
1	Н	477/487~(98%)	431 (90%)	46 (10%)	0	100	100
All	All	3767/3896~(97%)	3442 (91%)	323 (9%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	57	PHE
1	Е	117	SER



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	386/409~(94%)	304 (79%)	82 (21%)	1 4
1	В	372/409~(91%)	301 (81%)	71 (19%)	1 6
1	\mathbf{C}	214/409~(52%)	182 (85%)	32~(15%)	3 12
1	D	352/409~(86%)	295 (84%)	57 (16%)	2 10
1	Ε	364/409~(89%)	294 (81%)	70 (19%)	1 6
1	\mathbf{F}	321/409~(78%)	263~(82%)	58 (18%)	1 7
1	G	392/409~(96%)	320~(82%)	72 (18%)	1 7
1	Н	383/409~(94%)	317 (83%)	66 (17%)	2 9
All	All	2784/3272 (85%)	2276 (82%)	508 (18%)	1 7

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	THR
1	А	16	ASP
1	А	17	LEU
1	А	18	SER
1	А	19	GLN
1	А	20	ARG
1	А	37	ASP
1	А	38	ASP
1	А	39	LEU
1	А	43	CYS
1	А	44	THR
1	А	45	SER
1	А	48	GLU
1	А	54	PHE
1	А	56	ASP
1	А	69	ASP
1	А	71	LEU
1	А	87	THR
1	А	90	ILE



Mol	Chain	Res	Type
1	А	91	THR
1	А	94	THR
1	А	116	THR
1	А	117	SER
1	А	129	LYS
1	А	133	LEU
1	А	138	SER
1	А	143	GLU
1	А	144	LYS
1	А	146	LEU
1	А	153	SER
1	А	156	ILE
1	А	170	TYR
1	А	180	THR
1	А	183	ASN
1	А	198	TRP
1	А	216	LEU
1	А	217	GLU
1	А	219	ARG
1	А	220	ILE
1	А	222	TYR
1	А	224	ASP
1	А	225	SER
1	А	228	SER
1	А	229	LEU
1	А	240	LEU
1	А	269	ARG
1	А	271	ILE
1	А	274	ASP
1	А	277	ILE
1	А	284	GLN
1	А	285	TYR
1	A	299	ILE
1	А	300	ASP
1	A	304	GLN
1	A	308	THR
1	А	309	GLU
1	A	348	LYS
1	А	355	PHE
1	A	357	SER
1	А	369	ILE
1	А	374	ASP



Mol	Chain	Res	Type
1	А	384	LYS
1	А	389	ASP
1	А	394	HIS
1	А	405	THR
1	А	409	LYS
1	А	412	LYS
1	А	413	ARG
1	А	414	ARG
1	А	419	ARG
1	А	422	LEU
1	А	425	ILE
1	А	426	GLU
1	А	431	LEU
1	А	439	GLU
1	A	448	ILE
1	А	449	ARG
1	А	450	GLU
1	А	458	LYS
1	А	471	THR
1	А	475	LEU
1	А	476	VAL
1	В	6	SER
1	В	8	MET
1	В	19	GLN
1	В	21	MET
1	В	22	LEU
1	В	23	LEU
1	В	39	LEU
1	В	43	CYS
1	В	46	ARG
1	В	47	SER
1	В	50	ASP
1	В	69	ASP
1	В	78	LYS
1	В	80	LEU
1	В	83	LEU
1	В	90	ILE
1	В	94	THR
1	В	95	GLN
1	В	98	LYS
1	В	118	SER
1	В	120	LEU



Mol	Chain	Res	Type
1	В	139	ARG
1	В	140	LEU
1	В	143	GLU
1	В	144	LYS
1	В	148	GLN
1	В	153	SER
1	В	156	ILE
1	В	161	LEU
1	В	164	PHE
1	В	169	VAL
1	В	191	ASN
1	В	193	LEU
1	В	198	TRP
1	В	200	SER
1	В	201	LYS
1	В	204	ASP
1	В	216	LEU
1	В	217	GLU
1	В	219	ARG
1	В	220	ILE
1	В	222	TYR
1	В	229	LEU
1	В	233	VAL
1	В	302	LEU
1	В	304	GLN
1	В	307	ASP
1	В	331	ARG
1	В	332	THR
1	В	356	SER
1	В	361	ILE
1	В	378	GLN
1	В	380	SER
1	В	382	MET
1	В	384	LYS
1	В	396	ARG
1	В	411	ARG
1	В	414	ARG
1	В	415	ILE
1	В	417	HIS
1	В	419	ARG
1	В	423	ASP
1	В	425	ILE



Mol	Chain	Res	Type
1	В	431	LEU
1	В	445	ILE
1	В	449	ARG
1	В	452	TRP
1	В	453	LYS
1	В	455	ASN
1	В	456	SER
1	В	477	GLU
1	С	62	LEU
1	С	76	LYS
1	С	80	LEU
1	С	98	LYS
1	С	183	ASN
1	С	193	LEU
1	С	197	LEU
1	С	198	TRP
1	С	201	LYS
1	С	216	LEU
1	С	224	ASP
1	С	228	SER
1	С	229	LEU
1	С	302	LEU
1	С	307	ASP
1	С	309	GLU
1	С	312	VAL
1	С	315	LYS
1	С	335	ARG
1	С	357	SER
1	С	362	LEU
1	С	366	LYS
1	С	378	GLN
1	С	380	SER
1	С	381	ILE
1	C	384	LYS
1	С	388	LEU
1	С	395	MET
1	С	419	ARG
1	С	449	ARG
1	С	452	TRP
1	C	461	THR
1	D	4	THR
1	D	6	SER



Mol	Chain	Res	Type
1	D	17	LEU
1	D	44	THR
1	D	49	TYR
1	D	50	ASP
1	D	51	THR
1	D	57	PHE
1	D	64	ARG
1	D	69	ASP
1	D	70	ARG
1	D	73	ASP
1	D	102	LEU
1	D	125	ILE
1	D	130	GLN
1	D	138	SER
1	D	139	ARG
1	D	143	GLU
1	D	155	HIS
1	D	166	GLU
1	D	171	ARG
1	D	172	ILE
1	D	174	HIS
1	D	178	LYS
1	D	183	ASN
1	D	185	LEU
1	D	187	LEU
1	D	198	TRP
1	D	228	SER
1	D	229	LEU
1	D	231	ASP
1	D	268	LEU
1	D	269	ARG
1	D	274	ASP
1	D	276	VAL
1	D	277	ILE
1	D	289	VAL
1	D	295	VAL
1	D	299	ILE
1	D	302	LEU
1	D	362	LEU
1	D	367	LEU
1	D	370	VAL
1	D	371	LEU



Mol	Chain	Res	Type
1	D	375	GLU
1	D	376	THR
1	D	380	SER
1	D	402	LEU
1	D	408	PHE
1	D	424	LEU
1	D	430	THR
1	D	433	VAL
1	D	435	ARG
1	D	436	ASP
1	D	452	TRP
1	D	466	THR
1	D	467	TRP
1	Е	7	THR
1	Е	8	MET
1	E	16	ASP
1	Е	17	LEU
1	Е	19	GLN
1	Е	21	MET
1	Е	23	LEU
1	Е	39	LEU
1	Е	41	ILE
1	Е	42	VAL
1	Е	56	ASP
1	Е	59	GLU
1	Ε	63	ASP
1	Е	71	LEU
1	Е	72	ASN
1	E	78	LYS
1	Е	80	LEU
1	Е	83	LEU
1	E	87	THR
1	Е	88	VAL
1	E	95	GLN
1	Е	98	LYS
1	E	117	SER
1	E	118	SER
1	E	122	GLU
1	E	133	LEU
1	Е	140	LEU
1	E	146	LEU
1	Е	150	LEU



Mol	Chain	Res	Type
1	Е	156	ILE
1	Е	164	PHE
1	Е	165	SER
1	Е	214	VAL
1	Е	216	LEU
1	Е	220	ILE
1	Е	224	ASP
1	Е	229	LEU
1	Е	268	LEU
1	Е	269	ARG
1	Е	274	ASP
1	Е	276	VAL
1	Е	277	ILE
1	Е	289	VAL
1	Е	290	SER
1	Е	335	ARG
1	Е	339	ARG
1	Е	352	HIS
1	Е	356	SER
1	Е	371	LEU
1	Е	372	GLN
1	Е	374	ASP
1	Е	388	LEU
1	Е	404	LEU
1	Е	405	THR
1	Е	407	VAL
1	Е	410	ASP
1	Е	411	ARG
1	Е	414	ARG
1	Е	415	ILE
1	Е	419	ARG
1	Е	426	GLU
1	Е	428	ASP
1	Е	433	VAL
1	Е	435	ARG
1	Е	443	ILE
1	Е	445	ILE
1	Е	448	ILE
1	Е	475	LEU
1	E	476	VAL
1	Е	478	ARG
1	F	14	THR



Mol	Chain	Res	Type
1	F	16	ASP
1	F	21	MET
1	F	30	ASP
1	F	39	LEU
1	F	46	ARG
1	F	62	LEU
1	F	64	ARG
1	F	79	PHE
1	F	83	LEU
1	F	93	PRO
1	F	98	LYS
1	F	112	ILE
1	F	133	LEU
1	F	138	SER
1	F	140	LEU
1	F	142	LEU
1	F	164	PHE
1	F	165	SER
1	F	168	GLN
1	F	198	TRP
1	F	199	ASN
1	F	213	THR
1	F	214	VAL
1	F	216	LEU
1	F	217	GLU
1	F	220	ILE
1	F	222	TYR
1	F	224	ASP
1	F	234	GLN
1	F	243	LEU
1	F	261	LYS
1	F	263	LYS
1	F	264	VAL
1	F	273	ASN
1	F	274	ASP
1	F	275	THR
1	F	278	THR
1	F	308	THR
1	F	311	PHE
1	F	339	ARG
1	F	345	VAL
1	F	346	GLN



Mol	Chain	Res	Type
1	F	355	PHE
1	F	411	ARG
1	F	413	ARG
1	F	414	ARG
1	F	418	GLU
1	F	419	ARG
1	F	423	ASP
1	F	426	GLU
1	F	431	LEU
1	F	445	ILE
1	F	449	ARG
1	F	450	GLU
1	F	452	TRP
1	F	461	THR
1	F	466	THR
1	G	3	ASN
1	G	5	VAL
1	G	6	SER
1	G	13	SER
1	G	22	LEU
1	G	30	ASP
1	G	39	LEU
1	G	40	ARG
1	G	42	VAL
1	G	51	THR
1	G	52	ASP
1	G	57	PHE
1	G	59	GLU
1	G	60	LYS
1	G	64	ARG
1	G	69	ASP
1	G	70	ARG
1	G	72	ASN
1	G	74	ASP
1	G	81	ASN
1	G	87	THR
1	G	90	ILE
1	G	95	GLN
1	G	101	ASP
1	G	102	LEU
1	G	148	GLN
1	G	161	LEU



Mol	Chain	Res	Type
1	G	162	LYS
1	G	163	VAL
1	G	188	ARG
1	G	191	ASN
1	G	193	LEU
1	G	197	LEU
1	G	198	TRP
1	G	200	SER
1	G	203	ILE
1	G	219	ARG
1	G	231	ASP
1	G	261	LYS
1	G	263	LYS
1	G	264	VAL
1	G	271	ILE
1	G	274	ASP
1	G	275	THR
1	G	277	ILE
1	G	279	HIS
1	G	293	LYS
1	G	304	GLN
1	G	309	GLU
1	G	312	VAL
1	G	334	LYS
1	G	355	PHE
1	G	357	SER
1	G	362	LEU
1	G	363	GLN
1	G	366	LYS
1	G	371	LEU
1	G	383	VAL
1	G	388	LEU
1	G	394	HIS
1	G	397	GLU
1	G	410	ASP
1	G	411	ARG
1	G	413	ARG
1	G	414	ARG
1	G	457	MET
1	G	466	THR
1	G	471	THR
1	G	473	ILE



Mol	Chain	Res	Type
1	G	477	GLU
1	G	478	ARG
1	G	479	ASP
1	Н	8	MET
1	Н	16	ASP
1	Н	17	LEU
1	Н	18	SER
1	Н	30	ASP
1	Н	34	LEU
1	Н	35	LEU
1	Н	38	ASP
1	Н	40	ARG
1	Н	43	CYS
1	Н	46	ARG
1	Н	49	TYR
1	Н	54	PHE
1	Н	57	PHE
1	Н	59	GLU
1	Н	60	LYS
1	Н	62	LEU
1	Н	64	ARG
1	Н	71	LEU
1	Н	73	ASP
1	Н	74	ASP
1	Н	76	LYS
1	Н	78	LYS
1	Н	80	LEU
1	Н	99	ILE
1	Н	133	LEU
1	Н	155	HIS
1	Н	156	ILE
1	H	165	SER
1	Н	167	LYS
1	H	185	LEU
1	Н	186	THR
1	Н	187	LEU
1	Н	220	ILE
1	Н	222	TYR
1	Н	236	HIS
1	Н	274	ASP
1	Н	276	VAL
1	Н	289	VAL



Mol	Chain	Res	Type
1	Н	290	SER
1	Н	293	LYS
1	Н	334	LYS
1	Н	335	ARG
1	Н	339	ARG
1	Н	356	SER
1	Н	374	ASP
1	Н	375	GLU
1	Н	385	GLU
1	Н	388	LEU
1	Н	402	LEU
1	Н	403	SER
1	Н	405	THR
1	Н	422	LEU
1	Н	423	ASP
1	Н	424	LEU
1	Н	425	ILE
1	Н	426	GLU
1	Н	430	THR
1	Н	466	THR
1	Н	473	ILE
1	Н	475	LEU
1	Н	476	VAL
1	Н	477	GLU
1	Н	481	VAL
1	Н	486	LEU
1	Н	487	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	174	HIS
1	А	394	HIS
1	А	441	GLN
1	В	19	GLN
1	В	81	ASN
1	В	199	ASN
1	В	205	HIS
1	В	352	HIS
1	С	207	GLN
1	D	157	ASN
1	D	174	HIS



Mol	Chain	Res	Type
1	D	205	HIS
1	D	378	GLN
1	Е	346	GLN
1	Е	417	HIS
1	Е	441	GLN
1	F	72	ASN
1	F	207	GLN
1	F	234	GLN
1	F	279	HIS
1	F	346	GLN
1	F	363	GLN
1	G	3	ASN
1	G	19	GLN
1	G	81	ASN
1	G	168	GLN
1	G	174	HIS
1	G	284	GLN
1	Н	19	GLN
1	Н	346	GLN
1	Н	394	HIS
1	Н	455	ASN

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tune Chain Dec		Tiple	Bond lengths			Bond angles			
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NMN	В	501	-	22,23,23	0.91	2 (9%)	30,34,34	1.07	3 (10%)
2	NMN	G	501	-	22,23,23	0.88	1 (4%)	30,34,34	1.14	3 (10%)
2	NMN	Е	501	-	22,23,23	0.81	2 (9%)	30,34,34	1.09	3 (10%)
2	NMN	А	501	-	22,23,23	0.86	1 (4%)	30,34,34	1.18	4 (13%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	NMN	В	501	-	-	2/14/30/30	0/2/2/2
2	NMN	G	501	-	-	1/14/30/30	0/2/2/2
2	NMN	Е	501	-	-	6/14/30/30	0/2/2/2
2	NMN	А	501	-	-	2/14/30/30	0/2/2/2

All (6) bond length outliers are listed be	low:
--------------------------------------------	------

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	501	NMN	O4R-C1R	2.87	1.45	1.41
2	В	501	NMN	C2-N1	2.51	1.38	1.35
2	G	501	NMN	C2-N1	2.40	1.37	1.35
2	Е	501	NMN	C2-N1	2.36	1.37	1.35
2	А	501	NMN	O4R-C1R	2.35	1.44	1.41
2	Е	501	NMN	O4R-C1R	2.13	1.44	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	G	501	NMN	O3R-C3R-C2R	-3.81	99.49	111.82
2	В	501	NMN	C6-N1-C2	-3.02	119.22	121.97
2	Е	501	NMN	C3-C2-N1	-2.87	117.63	120.43
2	Е	501	NMN	C2-C3-C4	2.60	121.21	118.26
2	А	501	NMN	C6-N1-C2	-2.43	119.76	121.97
2	А	501	NMN	C2-C3-C7	-2.29	112.83	119.46
2	Е	501	NMN	C3R-C2R-C1R	-2.29	97.54	100.98



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	NMN	C2-C3-C4	2.18	120.73	118.26
2	В	501	NMN	O4R-C4R-C3R	-2.14	100.89	105.11
2	G	501	NMN	O2R-C2R-C1R	-2.08	103.19	110.85
2	В	501	NMN	C2R-C3R-C4R	-2.06	98.63	102.64
2	G	501	NMN	C6-N1-C2	-2.05	120.10	121.97
2	А	501	NMN	C4-C3-C7	2.02	126.44	121.04

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	В	501	NMN	O4R-C1R-N1-C2
2	Е	501	NMN	O4R-C1R-N1-C2
2	Е	501	NMN	O4R-C1R-N1-C6
2	Е	501	NMN	C2R-C1R-N1-C2
2	Е	501	NMN	C2R-C1R-N1-C6
2	А	501	NMN	C3R-C4R-C5R-O5R
2	А	501	NMN	O4R-C4R-C5R-O5R
2	G	501	NMN	C4R-C5R-O5R-P
2	Е	501	NMN	O4R-C4R-C5R-O5R
2	Е	501	NMN	C3R-C4R-C5R-O5R
2	В	501	NMN	O4R-C4R-C5R-O5R

All (11) torsion outliers are listed below:

There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	501	NMN	7	0
2	G	501	NMN	5	0
2	Е	501	NMN	4	0
2	А	501	NMN	16	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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.


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)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	482/487~(98%)	0.13	7 (1%) 73 71	31, 65, 96, 135	0
1	В	479/487~(98%)	0.20	18 (3%) 40 37	26, 63, 129, 151	0
1	С	463/487~(95%)	0.12	14 (3%) 50 48	49, 95, 152, 209	0
1	D	479/487~(98%)	0.15	12 (2%) 57 53	48, 83, 113, 166	0
1	E	476/487~(97%)	0.19	12 (2%) 57 53	40, 81, 116, 139	0
1	F	462/487~(94%)	0.40	36 (7%) 13 12	42, 82, 173, 204	0
1	G	485/487~(99%)	0.10	4 (0%) 86 86	27, 64, 103, 142	0
1	Н	481/487~(98%)	0.10	3 (0%) 89 89	33, 68, 106, 137	0
All	All	3807/3896~(97%)	0.17	106 (2%) 53 50	26, 76, 130, 209	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	133	LEU	6.7
1	С	14	THR	6.3
1	В	75	ALA	5.1
1	А	109	GLY	5.1
1	С	25	ALA	4.7
1	F	116	THR	4.7
1	Ε	115	ALA	4.7
1	Е	116	THR	4.6
1	F	84	PHE	4.4
1	В	79	PHE	4.4
1	F	72	ASN	3.9
1	F	11	PHE	3.8
1	F	103	CYS	3.7
1	В	417	HIS	3.6
1	А	360	GLY	3.6
1	В	39	LEU	3.5

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Mol	Chain	Res	Type	RSRZ	
1	Е	103	CYS	3.4	
1	G	79	PHE	3.4	
1	В	6	SER	3.4	
1	F	73	ASP	3.3	
1	В	8	MET	3.3	
1	D	386	PRO	3.3	
1	D	284	GLN	3.3	
1	А	359	GLY	3.3	
1	F	68	SER	3.3	
1	А	137	THR	3.2	
1	В	416	ALA	3.2	
1	F	115	ALA	3.2	
1	F	435	ARG	3.2	
1	F	330	ILE	3.1	
1	F	132	GLY	3.1	
1	F	234	GLN	3.0	
1	F	137	THR	3.0	
1	F	424	LEU	3.0	
1	F	83	LEU	3.0	
1	Н	184	LEU	2.9	
1	F	65	PHE	2.9	
1	F	96	PHE	2.9	
1	Е	75	ALA	2.9	
1	С	91	THR	2.9	
1	F	312	VAL	2.8	
1	В	111	ALA	2.8	
1	А	422	LEU	2.8	
1	D	96	PHE	2.8	
1	Е	90	ILE	2.7	
1	F	34	LEU	2.7	
1	F	138	SER	2.7	
1	F	305	PRO	2.7	
1	С	314	ILE	2.7	
1	D	229	LEU	2.6	
1	D	362	LEU	2.5	
1	Е	74	ASP	2.5	
1	F	166	GLU	2.5	
1	F	79	PHE	2.5	
1	F	304	GLN	2.5	
1	С	391	ASN	2.5	
1	F	101	ASP	2.5	
1	F	426	GLU	2.5	

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Mol	Chain	Res	Type	RSRZ
1	Е	131	ALA	2.4
1	С	332	THR	2.4
1	D	442	TRP	2.4
1	F	369	ILE	2.4
1	С	128	LEU	2.4
1	В	98	LYS	2.4
1	G	99	ILE	2.4
1	В	452	TRP	2.3
1	D	332	THR	2.3
1	Е	40	ARG	2.3
1	D	333	GLY	2.3
1	В	65	PHE	2.3
1	В	83	LEU	2.3
1	G	30	ASP	2.3
1	С	83	LEU	2.3
1	С	330	ILE	2.3
1	Н	85	TYR	2.2
1	С	86	ALA	2.2
1	F	8	MET	2.2
1	А	7	THR	2.2
1	С	80	LEU	2.2
1	В	87	THR	2.2
1	D	289	VAL	2.2
1	F	415	ILE	2.1
1	F	95	GLN	2.1
1	D	63	ASP	2.1
1	С	221	GLY	2.1
1	F	45	SER	2.1
1	D	111	ALA	2.1
1	В	146	LEU	2.1
1	F	433	VAL	2.1
1	F	53	GLY	2.1
1	F	343	ILE	2.1
1	В	97	GLY	2.1
1	Е	63	ASP	2.1
1	Е	393	ALA	2.1
1	Е	100	ALA	2.0
1	В	424	LEU	2.0
1	A	424	LEU	2.0
1	В	7	THR	2.0
1	С	311	PHE	2.0
1	F	69	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	В	88	VAL	2.0
1	Н	49	TYR	2.0
1	С	138	SER	2.0
1	Е	448	ILE	2.0
1	G	308	THR	2.0
1	D	62	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	NMN	В	501	22/22	0.75	0.43	87,100,104,172	0
2	NMN	Е	501	22/22	0.85	0.23	76,88,102,162	0
2	NMN	А	501	22/22	0.89	0.24	66,73,78,87	0
2	NMN	G	501	22/22	0.91	0.23	59,71,81,92	0

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.

