

Full wwPDB X-ray Structure Validation Report (i)

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:	7XHP
:	Structure of a Glucose 6-Phosphate Dehydrogenase from Zymomonas mobilis
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:	2022-04-09
:	2.78 Å(reported)
	: : : :

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

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

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

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain				
1	А	493	49%	36%	6% 9%		
1	В	493	2% 42%	42%	9% 6%		
1	С	493	37%	29% •	30%		
1	D	493	.%	29% •	27%		
1	Е	493	2% 4 5%	39%	6% 10%		
1	F	493	2% 49%	41%	7% •		



Mol	Chain	Length	Quality of chain			
1	G	493	46%	40%	9%	6%
1	Н	493	53%	39%	•	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26350 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	451	Total	С	Ν	0	S	0	0	0
1	A	401	3319	2106	565	638	10	0	0	0
1	В	461	Total	С	Ν	0	S	0	0	0
1	D	401	3513	2235	601	666	11	0	0	0
1	С	345	Total	С	Ν	0	S	0	0	0
1		040	2684	1716	468	493	7	0	0	0
1	П	361	Total	С	Ν	0	S	0	0	0
1	D	501	2750	1749	486	508	7	0	0	0
1	F	446	Total	С	Ν	0	S	0	0	0
1	Ľ	440	3324	2116	567	631	10	0	0	
1	Б	480	Total	С	Ν	0	S	0	0	0
1	Г	400	3628	2305	620	692	11	0	0	0
1	С	465	Total	С	Ν	0	S	0	0	0
1	G	405	3521	2243	598	669	11	0	0	0
1	и	474	Total	С	Ν	0	S	0	0	0
	п	4/4	3499	2224	591	674	10	U	0	0

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

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	17	Total O 17 17	0	0
2	В	12	Total O 12 12	0	0
2	С	11	Total O 11 11	0	0
2	D	10	Total O 10 10	0	0
2	Е	8	Total O 8 8	0	0
2	F	22	TotalO2222	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	19	Total O 19 19	0	0
2	Н	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glucose 6-Phosphate Dehydrogenase

A474 L475 L475 A478 N483 V483 V483 V484 L486 L486 L486 L486 L486 H1S H1S H1S H1S H1S H1S

• Molecule 1: Glucose 6-Phosphate Dehydrogenase

Chain F: 49% 41% 7%

• Molecule 1: Glucose 6-Phosphate Dehydrogenase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	80.61Å 101.07Å 321.07Å	Denesiter
a, b, c, α , β , γ	90.00° 90.02° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	78.18 - 2.78	Depositor
Resolution (A)	$85.53 \ - \ 2.78$	EDS
% Data completeness	90.8 (78.18-2.78)	Depositor
(in resolution range)	89.4 (85.53-2.78)	EDS
R _{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.73 (at 2.77 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.233 , 0.289	Depositor
Π, Π_{free}	0.247 , 0.287	DCC
R_{free} test set	5876 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	56.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 79.6	EDS
L-test for twinning ²	$< L > = 0.35, < L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 118119 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	26350	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.80% 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)

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

Mal	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/3390	0.69	0/4634	
1	В	0.51	0/3586	0.74	0/4881	
1	С	0.38	0/2744	0.65	0/3733	
1	D	0.41	0/2817	0.67	0/3844	
1	Е	0.49	0/3396	0.71	0/4637	
1	F	0.46	0/3706	0.69	0/5049	
1	G	0.47	0/3594	0.73	1/4894~(0.0%)	
1	Н	0.40	0/3575	0.65	0/4886	
All	All	0.45	0/26808	0.69	1/36558~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	469	PRO	N-CA-CB	5.88	110.36	103.30

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	3319	0	3109	155	0
1	В	3513	0	3417	209	0
1	С	2684	0	2635	128	0
1	D	2750	0	2611	155	0

0 0	Southeast from proceeder pagem					
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	3324	0	3150	176	0
1	F	3628	0	3471	191	0
1	G	3521	0	3377	212	0
1	Н	3499	0	3273	181	0
2	А	17	0	0	2	0
2	В	12	0	0	0	0
2	С	11	0	0	4	0
2	D	10	0	0	0	0
2	Е	8	0	0	1	0
2	F	22	0	0	5	0
2	G	19	0	0	1	0
2	Н	13	0	0	1	0
All	All	26350	0	25043	1326	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 26.

All (1326) 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:F:8:MET:HG2	1:F:111:ALA:HB3	1.43	1.00
1:H:100:ALA:HB2	1:H:133:LEU:HD11	1.45	0.96
1:B:215:GLY:HA3	1:B:335:ARG:HH11	1.32	0.95
1:G:125:ILE:HG21	1:G:160:VAL:HA	1.49	0.94
1:G:6:SER:HA	1:G:39:LEU:HD13	1.49	0.93
1:A:13:SER:HA	1:A:18:SER:HB2	1.50	0.93
1:H:285:TYR:HB3	1:H:298:TYR:HB2	1.51	0.92
1:G:125:ILE:HG12	1:G:160:VAL:HG13	1.52	0.92
1:G:340:ARG:HG3	1:G:373:PRO:HD2	1.51	0.90
1:C:411:ARG:HD2	1:D:385:GLU:HG2	1.53	0.90
1:F:147:GLY:HA3	1:F:153:SER:HB2	1.54	0.89
1:G:216:LEU:HD23	1:G:334:LYS:HD2	1.54	0.89
1:A:271:ILE:HB	1:A:448:ILE:HG12	1.57	0.87
1:H:143:GLU:HG2	1:H:172:ILE:HB	1.56	0.87
1:F:319:ASP:HB3	1:G:352:HIS:HE1	1.41	0.86
1:H:272:ASN:HB3	1:H:275:THR:HG23	1.60	0.84
1:A:224:ASP:HA	1:A:308:THR:HG21	1.61	0.82
1:A:233:VAL:HA	1:A:237:ILE:HG13	1.60	0.82
1:E:22:LEU:HA	1:E:25:SER:HB3	1.61	0.82
1:E:166:GLU:HA	1:E:169:VAL:HG12	1.60	0.82
1:F:419:ARG:HE	1:F:431:LEU:HD11	1.45	0.81

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:354:ILE:HB	1:D:252:MET:HG2	1.60	0.81
1:G:6:SER:HA	1:G:39:LEU:CD1	2.10	0.81
1:E:211:ALA:HB1	1:E:336:LEU:HB2	1.63	0.81
1:E:283:GLY:H	1:E:311:PHE:HB3	1.43	0.79
1:D:220:ILE:HG12	1:D:302:LEU:HD21	1.62	0.79
1:A:452:TRP:HB2	1:A:457:MET:HB2	1.65	0.79
1:A:476:VAL:HB	1:A:481:VAL:HB	1.65	0.79
1:F:216:LEU:HD12	1:F:220:ILE:HD13	1.65	0.78
1:C:411:ARG:HG3	1:D:386:PRO:HD2	1.66	0.77
1:G:5:VAL:HG11	1:G:111:ALA:HB2	1.66	0.77
1:C:296:ALA:HB3	1:C:301:GLU:HG3	1.66	0.77
1:G:14:THR:CG2	1:G:45:SER:OG	2.33	0.77
1:C:452:TRP:HB2	1:C:457:MET:HB2	1.66	0.77
1:A:39:LEU:HD11	1:A:41:ILE:HG12	1.66	0.76
1:G:207:GLN:HE22	1:G:484:TYR:H	1.31	0.76
1:G:216:LEU:HD12	1:G:220:ILE:HG23	1.70	0.74
1:H:224:ASP:O	1:H:308:THR:HG21	1.88	0.74
1:F:166:GLU:OE1	1:F:171:ARG:NH2	2.21	0.74
1:G:331:ARG:NH2	2:G:501:HOH:O	2.20	0.74
1:H:77:ALA:HA	1:H:80:LEU:HB2	1.68	0.74
1:G:14:THR:HG22	1:G:45:SER:OG	1.88	0.74
1:A:320:ASN:O	1:A:321:TRP:HB3	1.88	0.73
1:G:429:ALA:HB1	1:G:432:PHE:HD2	1.52	0.73
1:E:272:ASN:O	1:E:275:THR:N	2.20	0.73
1:G:176:LEU:HB3	1:G:431:LEU:HD22	1.69	0.73
1:A:284:GLN:NE2	1:A:308:THR:O	2.22	0.73
1:G:299:ILE:HD11	1:G:306:SER:HB3	1.71	0.73
1:B:45:SER:O	1:B:87:THR:HG23	1.88	0.73
1:F:271:ILE:HG23	1:F:275:THR:HB	1.70	0.73
1:C:154:ASP:HA	1:C:435:ARG:HH22	1.54	0.72
1:H:235:SER:O	1:H:239:GLN:HG2	1.88	0.72
1:E:388:LEU:HD22	1:F:419:ARG:HB2	1.69	0.72
1:E:422:LEU:HA	1:E:425:ILE:HD12	1.72	0.72
1:A:411:ARG:NH2	1:B:386:PRO:O	2.22	0.72
1:F:229:LEU:HD21	1:F:445:ILE:HD12	1.72	0.72
1:G:419:ARG:HG3	1:H:388:LEU:HD22	1.72	0.72
1:F:475:LEU:HD12	1:F:478:ARG:HH12	1.55	0.71
1:E:254:ALA:HB2	1:E:428:ASP:HB3	1.72	0.71
1:G:389:ASP:HB2	1:G:392:GLY:O	1.91	0.71
1:E:138:SER:OG	1:E:168:GLN:HB3	1.90	0.71
1:F:56:ASP:O	1:F:59:GLU:HB3	1.91	0.70

		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:210:VAL:HG22	1:D:341:SER:HB3	1.73	0.70	
1:B:8:MET:HB3	1:B:39:LEU:HD11	1.73	0.70	
1:G:258:ABG:HD2	1:G:430:THR:HA	1.73	0.70	
1.H.289.VAL.HA	1·H·294·GLU·HA	1.72	0.70	
1:B:385:GLU:HG3	1:B:386:PRO:HD2	1.72	0.70	
1:F:48:GLU:HA	1:F:87:THR:CB	2.20	0.70	
1:H:173:ASP:OD2	1:H:239:GLN:NE2	2.24	0.70	
1:E:271:ILE:HG22	1:E:276:VAL:HG22	1.72	0.70	
1:B:140:LEU:N	1:B:168:GLN:O	2.24	0.70	
1:F:299:ILE:HD11	1:F:306:SER:OG	1.90	0.70	
1:A:254:ALA:HA	1:A:430:THR:HG22	1.73	0.70	
1:B:111:ALA:HA	1:B:139:ARG:O	1.92	0.70	
1:B:287:ALA:HB2	1:B:297:GLY:N	2.07	0.70	
1:H:89:ASP:HB3	1:H:92:ASP:HB2	1.74	0.69	
1:B:369:ILE:HG12	1:B:377:ILE:HG23	1.73	0.69	
1:E:359:GLY:HA3	1:E:394:HIS:HD2	1.57	0.69	
1·A·321·TBP·HB2	1:D:352:HIS:HB3	1.75	0.69	
1:A:354:ILE:HD12	1·B·252·MET·HG2	1.74	0.69	
1:G:284:GLN:N	1:G:460:LYS:O	2.24	0.69	
1:A:113:TYR:OH	1:A:145:PRO:HD2	1.93	0.69	
1:A:13:SEB:HA	1:A:18:SEB:CB	2.23	0.68	
1:C:429:ALA:HB1	1:C:432:PHE:CD1	2.29	0.68	
1:H:284:GLN:HE21	1:H:298:TYR:HD2	1.42	0.68	
1:A:30:ASP:HA	1:A:33:GLY:O	1.94	0.68	
1:H:273:ASN:O	1:H:455:ASN:ND2	2.26	0.68	
1:B:337:PRO:HG2	1:B:467:TRP:CD1	2.27	0.68	
1:C:315:LYS:HE2	1:C:327:PRO:HB3	1.74	0.68	
1:A:384:LYS:HA	1:A:395:MET:HG2	1.76	0.68	
1:G:207:GLN:HE22	1:G:484:TYR:N	1.92	0.68	
1:H:365:ASN:ND2	1:H:380:SER:O	2.27	0.68	
1:G:146:LEU:O	1:G:156:ILE:HD12	1.93	0.67	
1:H:417:TYR:HA	1:H:420:LEU:HD12	1.77	0.67	
1:A:190:GLY:HA2	1:B:362:LEU:HD23	1.76	0.67	
1:B:473:ILE:HG12	1:G:289:VAL:HG21	1.77	0.67	
1:D:125:ILE:HD12	1:D:125:ILE:H	1.60	0.67	
1:E:385:GLU:H	1:E:395:MET:HA	1.59	0.67	
1:F:415:ILE:HG22	1:F:418:GLU:HG2	1.76	0.67	
1:A:7:THR:HG23	1:A:42:VAL:H	1.59	0.67	
1:B:43:CYS:HB2	1:B:85:TYR:HD1	1.58	0.67	
1:B:226:SER:O	1:B:230:ARG:HB2	1.95	0.66	
1:D:368:ARG:HH21	1:D:370:VAL:HG21	1.61	0.66	

	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:10:LEU:N	1:E:42:VAL:O	2.28	0.66
1:F:48:GLU:HA	1:F:87:THR:HB	1.77	0.66
1:F:337:PRO:HG2	1:F:467:TRP:CD1	2.30	0.66
1:G:276:VAL:HG21	1:G:452:TRP:HB3	1.76	0.66
1:B:55:ARG:HA	1:B:83:LEU:HD22	1.76	0.66
1:C:341:SER:N	1:C:372:GLN:O	2.28	0.66
1:H:258:ARG:NH1	1:H:432:PHE:O	2.29	0.66
1:H:251:HIS:ND1	1:H:253:GLU:OE2	2.29	0.66
1:A:44:THR:HA	1:A:86:ALA:O	1.96	0.66
1:E:139:ARG:HA	1:E:168:GLN:HA	1.77	0.66
1:E:170:TYR:CE2	1:E:424:LEU:HA	2.31	0.66
1:E:41:ILE:HG13	1:E:82:LYS:CB	2.26	0.66
1:G:112:ILE:HB	1:G:140:LEU:HG	1.76	0.66
1:G:140:LEU:O	1:G:170:TYR:N	2.21	0.65
1:G:337:PRO:HG2	1:G:467:TRP:CD1	2.30	0.65
1:F:259:ASP:OD1	1:F:434:ARG:NH2	2.23	0.65
1:A:359:GLY:HA3	1:A:393:ALA:O	1.97	0.65
1:G:284:GLN:NE2	1:G:308:THR:O	2.28	0.65
1:B:369:ILE:HG23	1:B:377:ILE:HG12	1.79	0.65
1:A:342:GLU:OE1	1:A:368:ARG:NH1	2.30	0.65
1:G:408:PHE:HB3	1:G:411:ARG:HG3	1.79	0.65
1:H:104:GLY:N	1:H:105:PRO:HD3	2.12	0.65
1:A:357:SER:HB2	1:A:392:GLY:HA2	1.78	0.65
1:H:21:MET:O	1:H:22:LEU:HD23	1.96	0.65
1:B:215:GLY:HA3	1:B:335:ARG:NH1	2.09	0.65
1:D:239:GLN:HG3	1:D:265:PHE:HZ	1.62	0.65
1:F:54:PHE:O	1:F:58:ALA:HB3	1.96	0.65
1:H:466:THR:HG23	1:H:468:GLY:H	1.62	0.65
1:C:411:ARG:HB3	1:D:386:PRO:HB2	1.78	0.64
1:A:21:MET:O	1:A:24:PRO:HD2	1.97	0.64
1:E:175:TYR:HA	1:E:178:LYS:HE2	1.79	0.64
1:G:171:ARG:O	1:G:433:VAL:N	2.20	0.64
1:B:188:ARG:NH1	1:B:243:LEU:O	2.31	0.64
1:B:295:VAL:HB	1:B:335:ARG:NH2	2.12	0.64
1:H:251:HIS:CD2	1:H:252:MET:H	2.16	0.64
1:F:14:THR:HG22	1:F:45:SER:HB2	1.79	0.64
1:G:26:LEU:HA	1:G:29:LEU:HD12	1.80	0.64
1:A:262:VAL:HG11	1:A:436:ASP:HB2	1.78	0.64
1:H:7:THR:HG23	1:H:103:CYS:SG	2.38	0.64
1:B:365:ASN:ND2	1:B:380:SER:O	2.31	0.64
1:C:277:ILE:HG12	1:C:455:ASN:HD22	1.61	0.64

	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:155:HIS:HA	1:F:158:ASP:HB2	1.79	0.64
1:G:6:SER:H	1:G:109:GLY:HA3	1.63	0.64
1:G:386:PRO:O	1:H:411:ARG:NH2	2.30	0.64
1:A:140:LEU:HD13	1:A:169:VAL:HG23	1.79	0.64
1:E:251:HIS:HD1	1:E:252:MET:H	1.46	0.64
1:G:148:GLN:O	1:G:230:ARG:NH1	2.30	0.63
1:E:211:ALA:O	1:E:339:ARG:HA	1.98	0.63
1:C:337:PRO:HG3	1:C:465:GLY:HA2	1.80	0.63
1:A:299:ILE:HG22	1:A:306:SER:H	1.64	0.63
1:F:201:LYS:HE2	1:G:201:LYS:O	1.99	0.63
1:G:154:ASP:HA	1:G:435:ARG:HH12	1.64	0.63
1:G:429:ALA:HB1	1:G:432:PHE:CD2	2.33	0.63
1:A:388:LEU:HD23	1:B:419:ARG:HA	1.81	0.63
1:B:436:ASP:N	1:B:436:ASP:OD1	2.25	0.63
1:F:96:PHE:HD2	1:F:127:GLY:HA3	1.63	0.63
1:G:258:ARG:NH2	1:G:432:PHE:O	2.32	0.63
1:A:191:ASN:HB2	1:A:194:PHE:CE2	2.33	0.63
1:F:212:GLU:HA	1:F:339:ARG:HA	1.80	0.63
1:H:99:ILE:HG13	1:H:100:ALA:N	2.13	0.63
1:B:154:ASP:CG	1:B:435:ARG:HH22	2.01	0.63
1:G:54:PHE:HA	1:G:57:PHE:HB3	1.81	0.63
1:H:235:SER:HG	1:H:236:HIS:HD1	1.47	0.63
1:A:128:LEU:O	1:A:132:GLY:N	2.31	0.62
1:C:277:ILE:HG12	1:C:455:ASN:ND2	2.13	0.62
1:A:285:TYR:HB3	1:A:298:TYR:HB2	1.81	0.62
1:H:378:GLN:HB2	1:H:399:TRP:CE3	2.35	0.62
1:C:250:ALA:O	1:D:352:HIS:NE2	2.31	0.62
1:E:21:MET:O	1:E:22:LEU:HB3	1.99	0.62
1:E:257:VAL:HG12	1:E:261:LYS:HD2	1.80	0.62
1:F:299:ILE:CD1	1:F:306:SER:OG	2.47	0.62
1:B:203:ILE:HG23	1:B:346:GLN:O	1.99	0.62
1:D:311:PHE:HE1	1:D:336:LEU:HD11	1.64	0.62
1:A:191:ASN:HB2	1:A:194:PHE:HE2	1.65	0.62
1:D:277:ILE:HG23	1:D:278:THR:HG23	1.82	0.62
1:F:110:ILE:CB	1:F:138:SER:HA	2.30	0.62
1:F:153:SER:HA	1:F:156:ILE:HD12	1.82	0.62
1:F:195:GLU:N	1:F:196:PRO:HD2	2.14	0.62
1:H:80:LEU:HD23	1:H:83:LEU:HD12	1.80	0.62
1:H:142:LEU:HB2	1:H:146:LEU:HD11	1.82	0.62
1:A:106:VAL:O	1:A:136:PRO:HG3	2.00	0.62
1:A:213:THR:HG23	1:A:214:VAL:HG13	1.82	0.62

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:256:ALA:O	1:F:260:GLU:HG2	2.00	0.62
1:E:474:ALA:O	1:E:478:ARG:N	2.28	0.61
1:F:233:VAL:HA	1:F:237:ILE:HB	1.80	0.61
1:H:109:GLY:HA2	1:H:137:THR:OG1	2.00	0.61
1:A:236:HIS:H	1:A:236:HIS:CD2	2.17	0.61
1:F:54:PHE:CD2	1:F:85:TYR:HB2	2.36	0.61
1:A:245:ALA:O	1:A:323:TRP:NE1	2.33	0.61
1:D:230:ARG:HD2	1:D:442:TRP:HZ3	1.65	0.61
1:E:341:SER:O	1:E:370:VAL:HA	2.01	0.61
1:H:320:ASN:OD1	1:H:323:TRP:N	2.27	0.61
1:E:41:ILE:HD12	1:E:83:LEU:HD23	1.83	0.61
1:H:273:ASN:O	1:H:276:VAL:HG12	2.00	0.61
1:A:18:SER:HA	1:A:22:LEU:HB2	1.82	0.61
1:B:10:LEU:HB3	1:B:42:VAL:O	2.00	0.61
1:F:134:ALA:HB1	1:F:163:VAL:HG21	1.83	0.61
1:G:146:LEU:HD12	1:G:438:VAL:HG13	1.82	0.61
1:B:170:TYR:HB3	1:B:432:PHE:CD2	2.36	0.60
1:F:215:GLY:HA2	1:F:334:LYS:HD2	1.83	0.60
1:B:50:ASP:HB2	1:B:53:GLY:H	1.64	0.60
1:B:249:PRO:HG3	1:B:257:VAL:HG22	1.82	0.60
1:H:128:LEU:HG	1:H:133:LEU:HB2	1.83	0.60
1:H:175:TYR:CD2	1:H:236:HIS:HB3	2.36	0.60
1:A:191:ASN:OD1	1:B:382:MET:N	2.32	0.60
1:E:203:ILE:HA	1:E:347:PHE:HA	1.83	0.60
1:H:18:SER:O	1:H:23:LEU:HB2	2.01	0.60
1:B:26:LEU:HG	1:B:61:ALA:O	2.01	0.60
1:B:262:VAL:HG21	1:B:436:ASP:HB2	1.82	0.60
1:G:122:GLU:HG2	1:G:159:ALA:HB3	1.82	0.60
1:A:114:LEU:HD23	1:A:121:PHE:HA	1.83	0.60
1:A:258:ARG:NH1	1:A:432:PHE:O	2.34	0.60
1:B:271:ILE:HB	1:B:448:ILE:HG12	1.83	0.60
1:B:460:LYS:HD3	1:B:469:PRO:HB2	1.83	0.60
1:F:85:TYR:CG	1:F:86:ALA:N	2.70	0.60
1:E:484:TYR:CE1	1:E:486:LEU:HB3	2.37	0.60
1:G:164:PHE:HB3	1:G:168:GLN:HB2	1.83	0.60
1:D:171:ARG:HE	1:D:438:VAL:HG11	1.67	0.60
1:A:288:GLY:HA3	1:A:463:VAL:HG13	1.83	0.60
1:C:166:GLU:OE2	1:C:171:ARG:NH2	2.34	0.60
1:D:436:ASP:OD1	1:D:436:ASP:N	2.34	0.60
1:H:378:GLN:HB2	1:H:399:TRP:HE3	1.65	0.60
1:E:178:LYS:HB2	1:E:181:VAL:HG23	1.84	0.60

	is as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:143:GLU:HB3	1:B:172:ILE:HD12	1.83	0.59
1:C:154:ASP:OD1	1:C:435:ARG:NH2	2.34	0.59
1:E:127:GLY:O	1:E:131:ALA:N	2.35	0.59
1:E:170:TYR:HB3	1:E:432:PHE:CD2	2.36	0.59
1:F:336:LEU:HD13	1:F:467:TRP:CZ3	2.36	0.59
1:G:5:VAL:HA	1:G:109:GLY:HA3	1.84	0.59
1:D:195:GLU:HA	1:D:198:TRP:HB2	1.84	0.59
1:E:400:LEU:HD23	1:F:402:LEU:HB3	1.84	0.59
1:H:355:PHE:C	1:H:357:SER:H	2.04	0.59
1:B:160:VAL:HG13	1:B:164:PHE:HD2	1.67	0.59
1:H:466:THR:O	1:H:467:TRP:HB2	2.02	0.59
1:A:363:GLN:HB2	1:A:382:MET:HE1	1.84	0.59
1:E:9:ILE:HB	1:E:112:ILE:HG23	1.85	0.59
1:F:205:HIS:HB3	1:F:327:PRO:HG2	1.83	0.59
1:G:281:VAL:O	1:G:312:VAL:HA	2.01	0.59
1:D:154:ASP:HA	1:D:157:ASN:HB2	1.85	0.59
1:D:284:GLN:HB3	1:D:461:THR:HA	1.84	0.59
1:G:230:ARG:HA	1:G:234:GLN:HB2	1.84	0.59
1:D:435:ARG:HA	1:D:438:VAL:HG22	1.85	0.59
1:D:404:LEU:HD22	1:D:408:PHE:HE2	1.67	0.59
1:H:197:LEU:O	1:H:203:ILE:HG13	2.03	0.59
1:B:117:SER:HB2	1:B:118:PRO:HD2	1.85	0.59
1:F:319:ASP:HB3	1:G:352:HIS:CE1	2.30	0.59
1:H:29:LEU:O	1:H:34:LEU:HB2	2.03	0.59
1:H:76:LYS:O	1:H:80:LEU:N	2.33	0.59
1:H:273:ASN:HA	1:H:451:GLY:CA	2.32	0.59
1:G:408:PHE:HB3	1:G:411:ARG:CG	2.32	0.58
1:A:175:TYR:HA	1:A:178:LYS:HD2	1.84	0.58
1:C:271:ILE:HG22	1:C:276:VAL:HG22	1.85	0.58
1:F:187:LEU:O	1:F:191:ASN:ND2	2.34	0.58
1:A:208:ILE:HG12	1:A:343:ILE:HG23	1.84	0.58
1:A:350:VAL:HG12	1:B:192:ALA:HB2	1.84	0.58
1:B:151:ALA:O	1:B:155:HIS:HB3	2.03	0.58
1:C:285:TYR:CE1	1:C:298:TYR:HB2	2.38	0.58
1:C:315:LYS:NZ	2:C:502:HOH:O	2.35	0.58
1:E:466:THR:O	1:E:467:TRP:HB2	2.03	0.58
1:D:362:LEU:HA	1:D:382:MET:HE2	1.86	0.58
1:A:258:ARG:HA	1:A:261:LYS:HD3	1.85	0.58
1:G:156:ILE:O	1:G:160:VAL:HG23	2.04	0.58
1:A:463:VAL:HB	1:A:466:THR:HG21	1.86	0.58
1:H:274:ASP:O	1:H:277:ILE:HG22	2.03	0.58

	lous page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1.G.153.SEB.OG	1.G.442.TRP.NE1	2.37	0.58
1:E:10:LEU:O	1:E:44:THR:N	2.37	0.58
1.E.10.LEU.HD23	1·E·43·CYS·HB3	1.86	0.58
1:D:487:GLU:HA	1:D:490:HIS:CE1	2.39	0.58
1:B:246:MET:HE2	1:B:249:PRO:HD3	1.85	0.58
1:G:280:THR:HG23	1:G:314:ILE:HG23	1.86	0.58
1:H:276:VAL:HG12	1:H:455:ASN:HD22	1.68	0.58
1:E:385:GLU:N	1:E:395:MET:HA	2.18	0.57
1:H:234:GLN:NE2	1:H:441:GLN:OE1	2.37	0.57
1:H:258:ARG:NH1	1:H:429:ALA:O	2.37	0.57
1:C:148:GLN:NE2	1:C:225:SER:O	2.37	0.57
1:D:483:TRP:HA	1:D:483:TRP:CE3	2.39	0.57
1:F:60:LYS:HB2	1:F:64:ARG:CZ	2.34	0.57
1:G:419:ARG:CG	1:H:388:LEU:HD22	2.34	0.57
1:H:156:ILE:HG13	1:H:157:ASN:N	2.18	0.57
1:B:242:ALA:HA	1:B:264:VAL:HG11	1.85	0.57
1:C:209:SER:HB2	1:C:331:ARG:NH2	2.20	0.57
1:A:165:SER:N	1:A:168:GLN:HG3	2.20	0.57
1:B:43:CYS:HB2	1:B:85:TYR:CD1	2.39	0.57
1:C:178:LYS:HB2	1:C:181:VAL:HG23	1.86	0.57
1:C:262:VAL:HG22	1:C:437:GLU:HG2	1.85	0.57
1:G:21:MET:C	1:G:24:PRO:HD2	2.25	0.57
1:B:412:LYS:HG2	1:B:413:ARG:H	1.69	0.57
1:C:226:SER:HA	1:C:230:ARG:HE	1.69	0.57
1:G:146:LEU:HD11	1:G:234:GLN:HE22	1.68	0.57
1:F:434:ARG:O	1:F:438:VAL:HG23	2.05	0.57
1:H:322:ARG:HG2	1:H:323:TRP:CD1	2.40	0.57
1:E:23:LEU:HB2	1:E:24:PRO:HD3	1.85	0.57
1:B:337:PRO:HD2	1:B:467:TRP:CD2	2.39	0.57
1:G:5:VAL:HG22	1:G:110:ILE:H	1.70	0.57
1:G:408:PHE:O	1:G:411:ARG:HB2	2.05	0.57
1:H:385:GLU:H	1:H:395:MET:HA	1.70	0.57
1:A:165:SER:H	1:A:168:GLN:HG3	1.70	0.57
1:B:336:LEU:HD13	1:B:467:TRP:HE3	1.68	0.57
1:D:449:ARG:HA	1:D:452:TRP:CD1	2.40	0.57
1:B:230:ARG:O	1:B:234:GLN:HG2	2.04	0.56
1:D:195:GLU:OE1	1:D:322:ARG:NH1	2.38	0.56
1:D:378:GLN:HB2	1:D:399:TRP:HE3	1.70	0.56
1:D:178:LYS:O	1:D:182:GLN:HG3	2.04	0.56
1:A:170:TYR:HE2	1:A:429:ALA:HB3	1.70	0.56
1:A:189:PHE:CD1	1:A:248:PRO:HB3	2.40	0.56

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:385:GLU:O	1:D:394:HIS:HB2	2.06	0.56
1:D:439:GLU:O	1:D:443:ILE:HG13	2.05	0.56
1:G:146:LEU:HD11	1:G:234:GLN:NE2	2.19	0.56
1:G:201:LYS:O	1:G:348:LYS:HD2	2.06	0.56
1:G:254:ALA:O	1:G:430:THR:HB	2.04	0.56
1:A:286:GLY:O	1:A:464:SER:OG	2.20	0.56
1:B:41:ILE:HD13	1:B:83:LEU:HD12	1.87	0.56
1:B:88:VAL:HG13	1:B:99:ILE:HD11	1.87	0.56
1:E:128:LEU:HG	1:E:164:PHE:HZ	1.71	0.56
1:F:146:LEU:HD12	1:F:234:GLN:HE22	1.71	0.56
1:G:210:VAL:HG11	1:G:232:MET:HE3	1.88	0.56
1:G:267:ALA:O	1:G:319:ASP:HB2	2.05	0.56
1:G:466:THR:O	1:G:467:TRP:HB2	2.03	0.56
1:B:158:ASP:O	1:B:162:LYS:HG2	2.05	0.56
1:B:170:TYR:HB3	1:B:432:PHE:CG	2.40	0.56
1:E:402:LEU:HB2	1:F:400:LEU:HA	1.88	0.56
1:A:197:LEU:O	1:A:202:GLY:HA3	2.06	0.56
1:B:259:ASP:O	1:B:262:VAL:HG12	2.05	0.56
1:C:368:ARG:HG2	1:C:378:GLN:HG3	1.86	0.56
1:E:212:GLU:HA	1:E:339:ARG:HG3	1.86	0.56
1:E:276:VAL:HG11	1:E:452:TRP:HB3	1.86	0.56
1:F:23:LEU:N	1:F:24:PRO:HD2	2.21	0.56
1:F:423:ASP:HB3	1:F:429:ALA:HB2	1.87	0.56
1:G:140:LEU:N	1:G:168:GLN:O	2.38	0.56
1:B:321:TRP:CD1	1:C:351:PRO:HG2	2.41	0.56
1:D:417:TYR:O	1:D:418:GLU:HG2	2.04	0.56
1:G:384:LYS:N	1:H:186:THR:HG21	2.21	0.56
1:D:265:PHE:HA	1:D:268:LEU:HD12	1.87	0.56
1:E:233:VAL:HA	1:E:237:ILE:HB	1.88	0.56
1:F:223:PHE:HE2	1:F:310:THR:HG22	1.70	0.56
1:F:296:ALA:O	1:F:335:ARG:NH2	2.38	0.56
1:G:452:TRP:HB2	1:G:457:MET:HB2	1.88	0.56
1:A:90:ILE:HA	1:A:96:PHE:CZ	2.41	0.56
1:E:435:ARG:NH2	1:E:439:GLU:HG3	2.21	0.56
1:G:238:LEU:HD23	1:G:441:GLN:HG2	1.87	0.56
1:B:290:SER:HB2	1:B:295:VAL:HG11	1.86	0.55
1:E:234:GLN:NE2	1:E:441:GLN:OE1	2.39	0.55
1:E:317:HIS:HB3	1:E:319:ASP:OD1	2.06	0.55
1:H:302:LEU:HD23	1:H:306:SER:HB2	1.86	0.55
1:C:191:ASN:OD1	1:D:382:MET:N	2.32	0.55
1:C:226:SER:CA	1:C:230:ARG:HE	2.19	0.55

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:44:THR:HG22	1:B:88:VAL:HG22	1.88	0.55
1:C:210:VAL:HG22	1:C:341:SER:HB3	1.88	0.55
1:D:148:GLN:O	1:D:230:ARG:NH1	2.39	0.55
1:D:285:TYR:N	1:D:310:THR:OG1	2.40	0.55
1:G:51:THR:O	1:G:85:TYR:HB3	2.07	0.55
1:G:419:ARG:O	1:G:419:ARG:HG2	2.07	0.55
1:A:273:ASN:HB3	1:A:451:GLY:HA2	1.87	0.55
1:E:258:ARG:NH1	1:E:434:ARG:HB2	2.22	0.55
1:G:6:SER:N	1:G:109:GLY:HA3	2.22	0.55
1:B:378:GLN:HB2	1:B:399:TRP:CE3	2.41	0.55
1:D:340:ARG:NH1	1:D:368:ARG:HH22	2.04	0.55
1:G:336:LEU:HD13	1:G:467:TRP:CZ3	2.41	0.55
1:H:49:TYR:O	1:H:85:TYR:CE1	2.60	0.55
1:D:128:LEU:HA	1:D:133:LEU:HD12	1.89	0.55
1:C:356:SER:HA	1:C:360:GLY:HA3	1.89	0.55
1:D:180:THR:OG1	1:D:371:LEU:HB2	2.07	0.55
1:H:18:SER:HB3	1:H:23:LEU:HD13	1.89	0.55
1:H:281:VAL:HG23	1:H:475:LEU:HD22	1.89	0.55
1:A:118:PRO:HA	1:A:121:PHE:CZ	2.42	0.55
1:D:281:VAL:HB	1:D:313:ALA:HB3	1.88	0.55
1:G:378:GLN:HB2	1:G:399:TRP:CE3	2.42	0.55
1:H:269:ARG:C	1:H:444:TRP:HE1	2.10	0.55
1:A:320:ASN:HD21	1:A:323:TRP:HD1	1.53	0.55
1:B:17:LEU:HD12	1:B:17:LEU:H	1.70	0.55
1:C:177:GLY:HA3	1:C:420:LEU:HD21	1.88	0.55
1:D:375:GLU:OE2	1:D:405:THR:HG23	2.07	0.55
1:E:122:GLU:HA	1:E:125:ILE:HD11	1.89	0.55
1:F:281:VAL:HG21	1:F:472:ALA:HA	1.89	0.55
1:G:112:ILE:O	1:G:140:LEU:HA	2.07	0.55
1:A:223:PHE:CE2	1:A:310:THR:HG22	2.42	0.54
1:F:198:TRP:HA	1:F:203:ILE:HD12	1.89	0.54
1:G:272:ASN:O	1:G:274:ASP:N	2.33	0.54
1:A:363:GLN:H	1:A:382:MET:CE	2.20	0.54
1:A:378:GLN:NE2	1:A:401:ASP:OD1	2.40	0.54
1:D:234:GLN:O	1:D:441:GLN:HG2	2.07	0.54
1:E:233:VAL:HG21	1:E:312:VAL:HG11	1.88	0.54
1:H:273:ASN:HB3	1:H:451:GLY:HA2	1.89	0.54
1:B:242:ALA:O	1:B:246:MET:N	2.38	0.54
1:D:141:ALA:HA	1:D:170:TYR:HB2	1.88	0.54
1:D:398:VAL:HG22	1:D:399:TRP:H	1.72	0.54
1:B:336:LEU:HD13	1:B:467:TRP:CE3	2.42	0.54

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:173:ASP:OD1	1:C:176:LEU:N	2.31	0.54
1:C:452:TRP:HD1	1:C:453:LYS:N	2.05	0.54
1:E:269:ARG:HB2	1:E:319:ASP:OD2	2.08	0.54
1:E:337:PRO:HD3	1:E:467:TRP:H	1.72	0.54
1:B:413:ARG:HD3	1:B:414:ARG:HH11	1.73	0.54
1:B:228:SER:H	1:B:309:GLU:HG2	1.72	0.54
1:B:281:VAL:HG23	1:B:475:LEU:HD12	1.89	0.54
1:C:251:HIS:NE2	1:D:356:SER:HB2	2.23	0.54
1:F:150:LEU:O	1:F:154:ASP:N	2.30	0.54
1:F:438:VAL:HG12	1:F:442:TRP:CD1	2.42	0.54
1:H:462:TYR:HB2	1:H:466:THR:HG21	1.90	0.54
1:F:437:GLU:O	1:F:441:GLN:N	2.32	0.54
1:G:126:ALA:HA	1:G:163:VAL:HG21	1.88	0.54
1:B:296:ALA:O	1:B:335:ARG:NH2	2.41	0.54
1:C:368:ARG:NH2	2:C:501:HOH:O	2.34	0.54
1:A:213:THR:O	1:A:335:ARG:HA	2.08	0.54
1:F:79:PHE:O	1:F:83:LEU:HD23	2.07	0.54
1:H:175:TYR:CE2	1:H:236:HIS:HB3	2.43	0.54
1:H:298:TYR:O	1:H:302:LEU:N	2.38	0.54
1:A:148:GLN:HG3	1:A:230:ARG:CZ	2.38	0.53
1:A:195:GLU:N	1:A:196:PRO:HD2	2.23	0.53
1:D:150:LEU:HD21	1:D:439:GLU:CG	2.38	0.53
1:E:140:LEU:N	1:E:168:GLN:O	2.39	0.53
1:E:229:LEU:O	1:E:234:GLN:N	2.37	0.53
1:H:117:SER:O	1:H:120:LEU:HB2	2.08	0.53
1:A:363:GLN:H	1:A:382:MET:HE1	1.72	0.53
1:C:281:VAL:HG12	1:C:311:PHE:HE2	1.74	0.53
1:C:370:VAL:N	1:C:376:THR:O	2.35	0.53
1:D:483:TRP:HA	1:D:483:TRP:HE3	1.74	0.53
1:E:181:VAL:HG22	1:E:371:LEU:HD22	1.89	0.53
1:E:362:LEU:HD13	1:F:190:GLY:HA2	1.90	0.53
1:F:444:TRP:O	1:F:448:ILE:HD13	2.08	0.53
1:H:11:PHE:HD1	1:H:113:TYR:O	1.90	0.53
1:A:375:GLU:H	1:A:405:THR:HG1	1.54	0.53
1:C:343:ILE:HG13	1:C:371:LEU:HD11	1.90	0.53
1:C:404:LEU:HB3	1:C:408:PHE:CE1	2.42	0.53
1:E:340:ARG:NE	1:E:342:GLU:OE2	2.41	0.53
1:H:436:ASP:OD1	1:H:436:ASP:N	2.39	0.53
1:B:213:THR:HG22	1:B:339:ARG:HB2	1.91	0.53
1:B:357:SER:O	1:B:358:SER:HB2	2.09	0.53
1:C:288:GLY:O	1:C:295:VAL:HG22	2.08	0.53

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:142:LEU:N	1:D:170:TYR:O	2.34	0.53
1:D:233:VAL:O	1:D:238:LEU:HB2	2.07	0.53
1:E:258:ARG:HD3	1:E:434:ARG:HD3	1.88	0.53
1:F:232:MET:HB3	1:F:237:ILE:HD12	1.90	0.53
1:F:262:VAL:HG11	1:F:436:ASP:HB2	1.90	0.53
1:F:289:VAL:HA	1:F:294:GLU:HA	1.91	0.53
1:G:276:VAL:CG2	1:G:452:TRP:HB3	2.39	0.53
1:H:50:ASP:H	1:H:53:GLY:HA3	1.74	0.53
1:A:229:LEU:HD12	1:A:312:VAL:HG11	1.90	0.53
1:D:284:GLN:HE21	1:D:461:THR:HG22	1.73	0.53
1:G:180:THR:HG21	1:G:375:GLU:HB3	1.90	0.53
1:G:339:ARG:O	1:G:373:PRO:HD3	2.08	0.53
1:H:229:LEU:O	1:H:233:VAL:HB	2.09	0.53
1:C:410:ASP:CG	1:C:411:ARG:HE	2.12	0.53
1:E:114:LEU:HB3	1:E:142:LEU:HD23	1.91	0.53
1:F:107:GLU:HA	1:F:137:THR:HG21	1.91	0.53
1:G:21:MET:O	1:G:24:PRO:HD2	2.08	0.53
1:G:165:SER:O	1:G:169:VAL:HG23	2.09	0.53
1:G:377:ILE:HB	1:G:402:LEU:HD23	1.90	0.53
1:G:380:SER:HB3	1:G:399:TRP:CZ2	2.44	0.53
1:A:39:LEU:HD21	1:A:41:ILE:HD11	1.90	0.53
1:C:284:GLN:NE2	1:C:298:TYR:HB3	2.23	0.53
1:C:419:ARG:HA	1:D:388:LEU:HD11	1.91	0.53
1:C:436:ASP:OD1	1:C:436:ASP:N	2.38	0.53
1:F:402:LEU:HA	2:F:502:HOH:O	2.08	0.53
1:C:270:PRO:HA	1:C:444:TRP:CD1	2.44	0.53
1:D:275:THR:HB	1:D:279:HIS:ND1	2.24	0.53
1:E:419:ARG:HD2	1:F:388:LEU:HG	1.90	0.53
1:H:85:TYR:CG	1:H:86:ALA:N	2.76	0.53
1:H:277:ILE:HG23	1:H:278:THR:HG23	1.91	0.53
1:D:346:GLN:HG3	1:D:366:LYS:HG2	1.90	0.52
1:E:390:ARG:O	1:E:394:HIS:CE1	2.63	0.52
1:G:5:VAL:HG22	1:G:110:ILE:N	2.24	0.52
1:G:207:GLN:NE2	1:G:484:TYR:H	2.04	0.52
1:B:466:THR:O	1:B:467:TRP:HB2	2.09	0.52
1:E:170:TYR:CE2	1:E:429:ALA:HB2	2.44	0.52
1:E:370:VAL:O	1:E:375:GLU:HA	2.08	0.52
1:E:435:ARG:O	1:E:439:GLU:N	2.34	0.52
1:F:296:ALA:O	1:F:335:ARG:NH1	2.42	0.52
1:G:154:ASP:OD1	1:G:435:ARG:NH2	2.42	0.52
1:H:150:LEU:O	1:H:154:ASP:N	2.26	0.52

	hi a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:215:GLY:HA2	1:H:285:TYR:HE2	1.75	0.52
1:H:230:ARG:CZ	1:H:449:ARG:HD3	2.40	0.52
1:A:383:VAL:HG23	1:B:183:ASN:HB2	1.91	0.52
1:B:381:ILE:HG13	1:B:398:VAL:HG23	1.91	0.52
1:B:437:GLU:O	1:B:441:GLN:N	2.36	0.52
1:E:436:ASP:OD1	1:E:437:GLU:N	2.43	0.52
1:F:486:LEU:HD23	1:F:487:GLU:H	1.74	0.52
1:H:232:MET:O	1:H:237:ILE:HG13	2.09	0.52
1:D:142:LEU:HD11	1:D:169:VAL:HG13	1.91	0.52
1:G:171:ARG:O	1:G:433:VAL:HG23	2.08	0.52
1:H:199:ASN:HA	1:H:322:ARG:HG3	1.90	0.52
1:B:309:GLU:HG2	1:B:309:GLU:O	2.09	0.52
1:C:183:ASN:O	1:C:187:LEU:N	2.35	0.52
1:D:153:SER:O	1:D:157:ASN:N	2.39	0.52
1:D:340:ARG:HH12	1:D:368:ARG:HH22	1.58	0.52
1:G:370:VAL:O	1:G:375:GLU:HA	2.09	0.52
1:F:170:TYR:HB3	1:F:432:PHE:CD1	2.44	0.52
1:G:54:PHE:O	1:G:58:ALA:N	2.40	0.52
1:G:213:THR:O	1:G:335:ARG:HA	2.10	0.52
1:G:473:ILE:O	1:G:476:VAL:HG23	2.09	0.52
1:H:235:SER:OG	1:H:236:HIS:N	2.43	0.52
1:B:434:ARG:O	1:B:438:VAL:HG23	2.10	0.52
1:B:476:VAL:HG21	1:B:483:TRP:NE1	2.24	0.52
1:C:334:LYS:O	1:C:462:TYR:OH	2.28	0.52
1:E:22:LEU:O	1:E:26:LEU:HD22	2.09	0.52
1:G:140:LEU:HD23	1:G:141:ALA:N	2.24	0.52
1:G:297:GLY:O	1:G:301:GLU:HG3	2.09	0.52
1:A:170:TYR:CE2	1:A:429:ALA:HB3	2.45	0.52
1:B:172:ILE:HG12	1:B:432:PHE:HE1	1.75	0.52
1:D:254:ALA:HA	1:D:430:THR:OG1	2.09	0.52
1:F:422:LEU:O	1:F:426:GLU:N	2.33	0.52
1:G:6:SER:O	1:G:39:LEU:HD12	2.10	0.52
1:A:209:SER:HB3	1:A:331:ARG:HE	1.74	0.52
1:B:327:PRO:HB2	1:B:329:TYR:CZ	2.44	0.52
1:D:378:GLN:HB2	1:D:399:TRP:CE3	2.45	0.52
1:G:235:SER:O	1:G:239:GLN:HG2	2.09	0.52
1:A:230:ARG:HG2	1:A:442:TRP:CZ3	2.44	0.52
1:E:199:ASN:OD1	1:E:199:ASN:N	2.42	0.52
1:F:112:ILE:HD13	1:F:133:LEU:HD11	1.90	0.52
1:F:315:LYS:HE2	1:F:317:HIS:CE1	2.45	0.52
1:B:188:ARG:HH12	1:B:246:MET:HG2	1.75	0.51

	to de pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:340:ARG:HH12	1:F:485:ASP:CG	2.14	0.51
1:F:438:VAL:HA	1:F:441:GLN:HB2	1.91	0.51
1:G:22:LEU:O	1:G:26:LEU:HD13	2.10	0.51
1:A:400:LEU:HD23	1:B:402:LEU:HB3	1.91	0.51
1:B:197:LEU:O	1:B:202:GLY:HA3	2.09	0.51
1:C:179:GLU:CD	1:D:386:PRO:HB3	2.31	0.51
1:D:230:ARG:HD2	1:D:442:TRP:CZ3	2.44	0.51
1:G:474:ALA:O	1:G:478:ARG:HG2	2.10	0.51
1:B:198:TRP:HA	1:B:203:ILE:HD11	1.92	0.51
1:E:193:LEU:HA	1:F:197:LEU:HD11	1.93	0.51
1:E:401:ASP:O	1:F:401:ASP:N	2.37	0.51
1:F:378:GLN:HA	1:F:400:LEU:O	2.10	0.51
1:H:233:VAL:HA	1:H:237:ILE:HB	1.92	0.51
1:D:445:ILE:O	1:D:449:ARG:HG3	2.11	0.51
1:D:490:HIS:C	1:D:490:HIS:CD2	2.84	0.51
1:E:154:ASP:OD1	1:E:435:ARG:NH1	2.44	0.51
1:E:382:MET:HE2	1:E:397:GLU:HA	1.92	0.51
1:F:452:TRP:HB2	1:F:457:MET:HE3	1.92	0.51
1:E:258:ARG:NH2	1:E:432:PHE:O	2.43	0.51
1:E:335:ARG:CB	1:E:462:TYR:HE1	2.23	0.51
1:F:340:ARG:HH11	1:F:340:ARG:HG2	1.76	0.51
1:G:170:TYR:HB3	1:G:432:PHE:CD1	2.45	0.51
1:H:180:THR:HG21	1:H:375:GLU:HG2	1.90	0.51
1:A:252:MET:HG2	1:B:354:ILE:O	2.10	0.51
1:D:312:VAL:HG12	1:D:332:THR:HG22	1.93	0.51
1:E:23:LEU:N	1:E:24:PRO:CD	2.74	0.51
1:A:320:ASN:ND2	1:A:323:TRP:HD1	2.09	0.51
1:C:174:HIS:H	1:C:236:HIS:HE1	1.58	0.51
1:E:362:LEU:HA	1:E:382:MET:SD	2.51	0.51
1:G:195:GLU:N	1:G:196:PRO:HD2	2.26	0.51
1:G:340:ARG:HG3	1:G:373:PRO:CD	2.31	0.51
1:G:452:TRP:O	1:G:456:SER:N	2.43	0.51
1:H:224:ASP:OD2	1:H:302:LEU:HD22	2.11	0.51
1:A:445:ILE:O	1:A:449:ARG:HG3	2.11	0.51
1:D:188:ARG:HH12	1:D:246:MET:HG3	1.75	0.51
1:D:272:ASN:HB2	1:D:275:THR:HG23	1.93	0.51
1:G:262:VAL:HG23	1:G:437:GLU:HG2	1.92	0.51
1:A:269:ARG:HE	1:A:317:HIS:HB2	1.76	0.51
1:D:158:ASP:O	1:D:162:LYS:HB2	2.11	0.51
1:D:223:PHE:HD1	1:D:298:TYR:HH	1.59	0.51
1:D:276:VAL:HG21	1:D:452:TRP:HB3	1.92	0.51

	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:335:ARG:HB3	1:B:464:SER:HB3	1.93	0.50
1:B:366:LYS:H	1:B:380:SER:HB2	1.76	0.50
1:C:238:LEU:HD12	1:C:441:GLN:HG2	1.92	0.50
1:A:258:ARG:NH2	1:A:429:ALA:O	2.44	0.50
1:B:29:LEU:HD21	1:B:32:ASP:HB2	1.93	0.50
1:C:148:GLN:HG2	1:C:230:ARG:NE	2.26	0.50
1:D:281:VAL:HG11	1:D:472:ALA:HB2	1.93	0.50
1:F:466:THR:O	1:F:467:TRP:HB2	2.11	0.50
1:H:165:SER:H	1:H:168:GLN:HG3	1.75	0.50
1:A:412:LYS:NZ	2:A:506:HOH:O	2.43	0.50
1:D:336:LEU:HD22	1:D:467:TRP:HA	1.93	0.50
1:E:133:LEU:HB3	1:E:164:PHE:HE1	1.77	0.50
1:E:390:ARG:O	1:E:394:HIS:HE1	1.93	0.50
1:E:408:PHE:CE1	1:F:385:GLU:HG3	2.46	0.50
1:G:179:GLU:HA	1:G:182:GLN:OE1	2.11	0.50
1:G:225:SER:O	1:G:230:ARG:NH2	2.26	0.50
1:H:30:ASP:HB2	1:H:35:LEU:HD12	1.93	0.50
1:A:184:LEU:HD12	1:A:243:LEU:HD12	1.93	0.50
1:B:185:LEU:HD13	1:B:189:PHE:HD2	1.76	0.50
1:B:333:GLY:HA3	1:B:336:LEU:HD11	1.94	0.50
1:D:170:TYR:HB3	1:D:432:PHE:CD2	2.47	0.50
1:F:96:PHE:CD2	1:F:127:GLY:HA3	2.46	0.50
1:F:385:GLU:H	1:F:395:MET:HA	1.76	0.50
1:G:141:ALA:HA	1:G:170:TYR:O	2.11	0.50
1:G:357:SER:HB3	1:G:392:GLY:HA2	1.93	0.50
1:H:30:ASP:HA	1:H:35:LEU:HB2	1.93	0.50
1:H:242:ALA:O	1:H:246:MET:HG2	2.11	0.50
1:B:139:ARG:HD3	1:B:170:TYR:HE2	1.76	0.50
1:D:435:ARG:HH21	1:D:436:ASP:HB3	1.76	0.50
1:E:259:ASP:OD1	1:E:434:ARG:NH2	2.43	0.50
1:E:402:LEU:HD12	1:E:403:SER:N	2.27	0.50
1:F:358:SER:HB3	1:F:392:GLY:HA3	1.92	0.50
1:G:18:SER:HA	1:G:22:LEU:HD12	1.92	0.50
1:A:423:ASP:HB3	1:A:429:ALA:HB1	1.93	0.50
1:C:462:TYR:HD2	1:C:466:THR:HB	1.76	0.50
1:E:386:PRO:HD3	1:F:408:PHE:CE1	2.47	0.50
1:E:449:ARG:HA	1:E:452:TRP:NE1	2.26	0.50
1:F:397:GLU:HG3	1:F:398:VAL:N	2.27	0.50
1:G:207:GLN:HG2	1:G:483:TRP:CZ3	2.47	0.50
1:G:302:LEU:HG	1:G:304:GLN:H	1.76	0.50
1:H:89:ASP:OD1	1:H:90:ILE:N	2.45	0.50

	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:11:PHE:HA	1:A:44:THR:O	2.12	0.50
1:B:239:GLN:O	1:B:243:LEU:HG	2.12	0.50
1:C:195:GLU:OE1	1:C:322:ARG:NH2	2.31	0.50
1:C:309:GLU:HG3	1:C:311:PHE:O	2.12	0.50
1:C:452:TRP:HB2	1:C:457:MET:CB	2.38	0.50
1:E:187:LEU:HA	1:E:191:ASN:ND2	2.26	0.50
1:H:284:GLN:NE2	1:H:298:TYR:HD2	2.08	0.50
1:D:247:GLU:OE1	1:D:322:ARG:NE	2.40	0.50
1:F:128:LEU:HD13	1:F:133:LEU:HG	1.92	0.50
1:G:5:VAL:HG22	1:G:109:GLY:CA	2.42	0.50
1:C:404:LEU:HB3	1:C:408:PHE:CD1	2.47	0.49
1:E:166:GLU:HA	1:E:169:VAL:CG1	2.35	0.49
1:F:234:GLN:HG3	1:F:442:TRP:CZ3	2.47	0.49
1:B:24:PRO:HB2	1:B:415:ILE:HG13	1.93	0.49
1:B:262:VAL:HG23	1:B:437:GLU:HG2	1.94	0.49
1:E:187:LEU:O	1:E:191:ASN:ND2	2.45	0.49
1:F:56:ASP:HA	1:F:59:GLU:HB3	1.94	0.49
1:A:230:ARG:HG2	1:A:442:TRP:HZ3	1.75	0.49
1:F:315:LYS:HE2	1:F:317:HIS:HE1	1.77	0.49
1:A:368:ARG:HB3	1:A:378:GLN:CG	2.43	0.49
1:B:149:ASP:OD1	1:B:152:SER:N	2.38	0.49
1:B:337:PRO:HD3	1:B:467:TRP:HA	1.95	0.49
1:B:413:ARG:NH1	1:B:414:ARG:HD2	2.27	0.49
1:F:128:LEU:O	1:F:131:ALA:HB3	2.11	0.49
1:H:77:ALA:O	1:H:81:ASN:N	2.44	0.49
1:A:121:PHE:O	1:A:125:ILE:HG12	2.12	0.49
1:B:462:TYR:CD1	1:B:469:PRO:HD3	2.47	0.49
1:D:210:VAL:O	1:D:332:THR:OG1	2.21	0.49
1:D:284:GLN:NE2	1:D:461:THR:HG22	2.28	0.49
1:F:486:LEU:O	1:F:487:GLU:HB2	2.11	0.49
1:G:191:ASN:ND2	1:H:382:MET:O	2.46	0.49
1:G:240:LEU:O	1:G:244:VAL:HG23	2.13	0.49
1:H:50:ASP:O	1:H:54:PHE:N	2.40	0.49
1:H:273:ASN:HA	1:H:451:GLY:HA2	1.94	0.49
1:C:297:GLY:O	1:C:301:GLU:HB2	2.13	0.49
1:D:150:LEU:HD21	1:D:439:GLU:HA	1.94	0.49
1:E:173:ASP:OD2	1:E:239:GLN:HG3	2.13	0.49
1:A:199:ASN:O	1:A:201:LYS:N	2.42	0.49
1:B:158:ASP:HA	1:B:161:LEU:HB2	1.94	0.49
1:B:237:ILE:HG21	1:B:330:ILE:HG23	1.93	0.49
1:C:309:GLU:O	1:C:309:GLU:HG2	2.10	0.49

	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:402:LEU:HD21	1:C:404:LEU:HD21	1.95	0.49
1:H:149:ASP:OD1	1:H:152:SER:N	2.35	0.49
1:D:128:LEU:HD23	1:D:133:LEU:HB3	1.94	0.49
1:D:237:ILE:O	1:D:241:VAL:HG23	2.12	0.49
1:D:284:GLN:N	1:D:460:LYS:O	2.45	0.49
1:D:378:GLN:HA	1:D:400:LEU:O	2.13	0.49
1:E:175:TYR:CD2	1:E:236:HIS:HB3	2.48	0.49
1:E:351:PRO:HG3	1:H:201:LYS:HZ1	1.77	0.49
1:G:26:LEU:HA	1:G:29:LEU:CD1	2.42	0.49
1:G:99:ILE:O	1:G:100:ALA:HB3	2.13	0.49
1:G:183:ASN:HD21	1:H:383:VAL:HG22	1.78	0.49
1:A:201:LYS:HB3	1:D:201:LYS:HD2	1.95	0.49
1:B:159:ALA:O	1:B:163:VAL:HG23	2.13	0.49
1:E:149:ASP:N	1:E:149:ASP:OD1	2.45	0.49
1:F:258:ARG:NH1	1:F:432:PHE:O	2.45	0.49
1:G:161:LEU:HA	1:G:164:PHE:O	2.12	0.49
1:A:13:SER:N	1:A:45:SER:OG	2.45	0.49
1:B:322:ARG:HG2	1:B:323:TRP:CD1	2.48	0.49
1:E:396:ARG:HG2	1:E:396:ARG:HH11	1.78	0.49
1:H:49:TYR:HB3	1:H:53:GLY:C	2.33	0.49
1:H:403:SER:O	1:H:407:VAL:HG23	2.13	0.49
1:A:118:PRO:HA	1:A:121:PHE:CE2	2.48	0.48
1:B:185:LEU:HD13	1:B:189:PHE:CD2	2.48	0.48
1:B:476:VAL:HG21	1:B:483:TRP:CD1	2.48	0.48
1:C:197:LEU:HD21	1:D:196:PRO:HG2	1.94	0.48
1:C:411:ARG:CG	1:D:386:PRO:HD2	2.38	0.48
1:D:150:LEU:HD23	1:D:442:TRP:HB2	1.94	0.48
1:D:486:LEU:O	1:D:490:HIS:HB3	2.12	0.48
1:F:48:GLU:HA	1:F:87:THR:HG21	1.95	0.48
1:F:171:ARG:NH2	1:F:434:ARG:HA	2.28	0.48
1:F:173:ASP:CG	1:F:236:HIS:HD1	2.16	0.48
1:F:209:SER:HA	1:F:331:ARG:O	2.13	0.48
1:G:172:ILE:HG12	1:G:432:PHE:CD1	2.48	0.48
1:B:152:SER:O	1:B:153:SER:C	2.51	0.48
1:D:309:GLU:HG2	1:D:309:GLU:O	2.13	0.48
1:E:337:PRO:HD2	1:E:467:TRP:HA	1.94	0.48
1:G:485:ASP:O	1:G:487:GLU:N	2.46	0.48
1:H:236:HIS:HD1	1:H:236:HIS:H	1.61	0.48
1:B:364:PRO:O	1:B:366:LYS:NZ	2.46	0.48
1:D:435:ARG:NH2	1:D:436:ASP:HB3	2.28	0.48
1:A:337:PRO:HD2	1:A:467:TRP:CE3	2.49	0.48

	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:121:PHE:O	1:B:125:ILE:HG12	2.13	0.48
1:B:442:TRP:O	1:B:446:ASP:N	2.24	0.48
1:C:404:LEU:O	1:C:408:PHE:N	2.44	0.48
1:D:148:GLN:O	1:D:148:GLN:HG2	2.11	0.48
1:E:343:ILE:O	1:E:368:ARG:HA	2.13	0.48
1:F:323:TRP:CZ3	1:F:326:VAL:HG11	2.48	0.48
1:H:195:GLU:N	1:H:196:PRO:HD2	2.29	0.48
1:B:379:ILE:O	1:B:399:TRP:HA	2.13	0.48
1:D:421:MET:SD	1:D:421:MET:N	2.86	0.48
1:D:488:HIS:HA	1:D:491:HIS:NE2	2.29	0.48
1:F:48:GLU:HA	1:F:87:THR:CG2	2.44	0.48
1:G:378:GLN:HB2	1:G:399:TRP:HE3	1.79	0.48
1:G:412:LYS:CB	1:G:414:ARG:HD2	2.43	0.48
1:H:8:MET:SD	1:H:111:ALA:HB3	2.53	0.48
1:H:271:ILE:HG21	1:H:276:VAL:HG23	1.96	0.48
1:F:10:LEU:HG	1:F:11:PHE:N	2.29	0.48
1:G:41:ILE:O	1:G:83:LEU:HA	2.14	0.48
1:G:149:ASP:HA	1:G:442:TRP:CZ3	2.48	0.48
1:A:147:GLY:O	1:A:442:TRP:CZ2	2.67	0.48
1:B:452:TRP:HB2	1:B:457:MET:HB2	1.95	0.48
1:C:175:TYR:OH	1:C:210:VAL:HG11	2.12	0.48
1:C:194:PHE:HB3	1:C:198:TRP:CZ3	2.49	0.48
1:D:188:ARG:NH1	1:D:246:MET:HG3	2.29	0.48
1:D:311:PHE:CD1	1:D:336:LEU:HD21	2.49	0.48
1:E:265:PHE:HA	1:E:268:LEU:HD12	1.96	0.48
1:C:369:ILE:HG12	1:C:377:ILE:HG23	1.95	0.48
1:D:141:ALA:HB1	1:D:172:ILE:HD11	1.96	0.48
1:D:385:GLU:HB3	1:D:394:HIS:HB3	1.94	0.48
1:E:408:PHE:CE1	1:F:396:ARG:HD2	2.49	0.48
1:G:18:SER:HA	1:G:22:LEU:HG	1.94	0.48
1:G:143:GLU:HG3	1:G:144:LYS:N	2.29	0.48
1:G:197:LEU:O	1:G:203:ILE:HG13	2.14	0.48
1:G:434:ARG:O	1:G:438:VAL:HG23	2.14	0.48
1:B:47:SER:HB2	1:B:85:TYR:OH	2.14	0.48
1:B:94:THR:C	1:B:96:PHE:H	2.16	0.48
1:C:316:ALA:N	1:C:328:PHE:O	2.27	0.48
1:D:195:GLU:OE2	1:D:322:ARG:NH2	2.47	0.48
1:D:197:LEU:O	1:D:202:GLY:HA3	2.14	0.48
1:G:5:VAL:CA	1:G:109:GLY:HA3	2.44	0.48
1:G:11:PHE:HB3	1:G:115:SER:OG	2.14	0.48
1:H:233:VAL:O	1:H:238:LEU:HG	2.14	0.48

	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:242:ALA:HB1	1:H:261:LYS:HG2	1.95	0.48
1:H:297:GLY:O	1:H:301:GLU:N	2.46	0.48
1:B:99:ILE:O	1:B:102:LEU:HB2	2.14	0.47
1:C:209:SER:O	1:C:341:SER:HA	2.14	0.47
1:C:242:ALA:O	1:C:246:MET:HG2	2.14	0.47
1:D:172:ILE:HG12	1:D:432:PHE:CE2	2.49	0.47
1:E:400:LEU:HA	1:F:402:LEU:HB2	1.95	0.47
1:H:171:ARG:HH12	1:H:435:ARG:HA	1.79	0.47
1:A:283:GLY:HA2	1:A:460:LYS:O	2.14	0.47
1:A:356:SER:HB2	1:B:251:HIS:CE1	2.49	0.47
1:E:259:ASP:O	1:E:262:VAL:HG12	2.14	0.47
1:F:90:ILE:HA	1:F:96:PHE:CZ	2.49	0.47
1:F:288:GLY:HA3	1:F:464:SER:HB2	1.95	0.47
1:F:438:VAL:HG12	1:F:442:TRP:NE1	2.29	0.47
1:G:122:GLU:HG2	1:G:159:ALA:CB	2.44	0.47
1:A:385:GLU:HG3	1:B:408:PHE:CE1	2.49	0.47
1:B:41:ILE:CG2	1:B:83:LEU:HG	2.45	0.47
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.77	0.47
1:B:331:ARG:NH2	1:B:467:TRP:HB3	2.29	0.47
1:C:204:ASP:N	1:C:346:GLN:O	2.41	0.47
1:E:9:ILE:HA	1:E:42:VAL:O	2.15	0.47
1:E:229:LEU:HA	1:E:233:VAL:HB	1.95	0.47
1:E:452:TRP:HA	1:E:455:ASN:HB2	1.97	0.47
1:E:475:LEU:N	2:E:502:HOH:O	2.48	0.47
1:F:315:LYS:HB2	1:F:475:LEU:HD11	1.96	0.47
1:G:439:GLU:O	1:G:443:ILE:HG13	2.14	0.47
1:A:302:LEU:HD23	1:A:304:GLN:H	1.79	0.47
1:B:204:ASP:OD1	1:B:349:PRO:HD3	2.15	0.47
1:B:321:TRP:O	1:C:351:PRO:HB2	2.14	0.47
1:E:143:GLU:HG2	1:E:172:ILE:HB	1.95	0.47
1:F:337:PRO:HG2	1:F:467:TRP:CG	2.49	0.47
1:B:58:ALA:CB	1:B:83:LEU:HD21	2.45	0.47
1:D:281:VAL:HG13	1:D:471:THR:HG23	1.96	0.47
1:E:351:PRO:HB2	1:H:321:TRP:O	2.15	0.47
1:F:23:LEU:HD12	1:F:23:LEU:HA	1.73	0.47
1:F:171:ARG:NE	1:F:433:VAL:O	2.47	0.47
1:G:302:LEU:HD21	1:G:304:GLN:HB2	1.96	0.47
1:B:322:ARG:HE	1:B:322:ARG:HB2	1.45	0.47
1:F:282:THR:HB	1:F:459:PRO:HA	1.95	0.47
1:G:282:THR:HG21	1:G:309:GLU:HG2	1.96	0.47
1:A:211:ALA:HB3	1:A:340:ARG:H	1.79	0.47

	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:381:ILE:HD13	1:A:400:LEU:HD11	1.97	0.47
1:D:245:ALA:HB3	1:D:264:VAL:HG13	1.97	0.47
1:D:284:GLN:HE22	1:D:299:ILE:CD1	2.28	0.47
1:D:284:GLN:HE22	1:D:299:ILE:HD11	1.80	0.47
1:D:408:PHE:O	1:D:411:ARG:HB2	2.15	0.47
1:F:54:PHE:CE2	1:F:85:TYR:HB2	2.49	0.47
1:F:150:LEU:HD11	1:F:439:GLU:HG2	1.97	0.47
1:G:288:GLY:HA3	1:G:464:SER:H	1.80	0.47
1:H:118:PRO:O	1:H:119:SER:OG	2.29	0.47
1:A:180:THR:CG2	1:A:375:GLU:HG2	2.45	0.47
1:A:368:ARG:O	1:A:377:ILE:HA	2.15	0.47
1:B:11:PHE:HB2	1:B:113:TYR:O	2.15	0.47
1:D:366:LYS:H	1:D:380:SER:HB3	1.80	0.47
1:E:185:LEU:N	1:E:185:LEU:HD13	2.29	0.47
1:G:6:SER:OG	1:G:39:LEU:HA	2.14	0.47
1:G:43:CYS:HB2	1:G:85:TYR:CD1	2.50	0.47
1:H:11:PHE:O	1:H:115:SER:HB3	2.14	0.47
1:H:452:TRP:HA	1:H:455:ASN:HB2	1.97	0.47
1:A:198:TRP:HA	1:A:203:ILE:HD12	1.97	0.47
1:B:321:TRP:CE2	1:C:351:PRO:HD2	2.50	0.47
1:G:6:SER:CA	1:G:39:LEU:CD1	2.90	0.47
1:G:18:SER:HA	1:G:22:LEU:CG	2.44	0.47
1:G:337:PRO:HD2	1:G:467:TRP:CD2	2.50	0.47
1:B:335:ARG:O	1:B:465:GLY:N	2.48	0.47
1:E:272:ASN:O	1:E:276:VAL:HG23	2.15	0.47
1:F:14:THR:HG22	1:F:45:SER:CB	2.43	0.47
1:F:180:THR:HG21	1:F:371:LEU:O	2.15	0.47
1:F:246:MET:HE2	1:F:247:GLU:O	2.15	0.47
1:G:165:SER:O	1:G:169:VAL:N	2.48	0.47
1:H:153:SER:HG	1:H:442:TRP:HE1	1.62	0.47
1:B:253:GLU:O	1:B:257:VAL:HG23	2.15	0.46
1:B:285:TYR:CD1	1:B:335:ARG:HG3	2.50	0.46
1:C:222:TYR:O	1:C:226:SER:N	2.38	0.46
1:C:485:ASP:OD2	1:C:486:LEU:N	2.48	0.46
1:E:200:SER:N	1:E:322:ARG:O	2.48	0.46
1:E:258:ARG:NH2	1:E:429:ALA:O	2.40	0.46
1:G:45:SER:HB3	1:G:85:TYR:OH	2.14	0.46
1:G:114:LEU:HG	1:G:116:THR:CG2	2.45	0.46
1:H:51:THR:HB	1:H:84:PHE:HA	1.96	0.46
1:A:201:LYS:O	1:A:348:LYS:HD2	2.15	0.46
1:A:478:ARG:O	2:A:501:HOH:O	2.20	0.46

	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:216:LEU:HD22	1:B:334:LYS:HG2	1.97	0.46
1:C:258:ARG:HB3	1:C:434:ARG:NH1	2.31	0.46
1:C:275:THR:O	1:C:279:HIS:HB2	2.16	0.46
1:D:260:GLU:O	1:D:264:VAL:HG23	2.15	0.46
1:E:8:MET:HA	1:E:111:ALA:O	2.15	0.46
1:F:171:ARG:CZ	1:F:434:ARG:HA	2.45	0.46
1:G:357:SER:CB	1:G:392:GLY:HA2	2.45	0.46
1:H:143:GLU:HG3	1:H:417:TYR:OH	2.15	0.46
1:H:151:ALA:O	1:H:155:HIS:HB2	2.15	0.46
1:H:337:PRO:HG2	1:H:467:TRP:CD1	2.49	0.46
1:B:476:VAL:HB	1:B:481:VAL:HB	1.96	0.46
1:C:277:ILE:H	1:C:277:ILE:HG13	1.32	0.46
1:C:311:PHE:CE2	1:C:469:PRO:HD2	2.51	0.46
1:E:128:LEU:HD22	1:E:128:LEU:H	1.80	0.46
1:G:111:ALA:C	1:G:112:ILE:HG12	2.34	0.46
1:G:245:ALA:HA	1:G:323:TRP:CZ2	2.51	0.46
1:H:209:SER:HA	1:H:331:ARG:O	2.15	0.46
1:H:215:GLY:CA	1:H:285:TYR:HE2	2.28	0.46
1:A:90:ILE:HA	1:A:96:PHE:HZ	1.79	0.46
1:A:321:TRP:HA	1:D:352:HIS:HB2	1.96	0.46
1:B:26:LEU:HG	1:B:62:LEU:HA	1.98	0.46
1:B:26:LEU:CD2	1:B:62:LEU:HD12	2.45	0.46
1:B:180:THR:O	1:B:183:ASN:ND2	2.47	0.46
1:B:297:GLY:O	1:B:301:GLU:HG3	2.14	0.46
1:D:449:ARG:HA	1:D:452:TRP:NE1	2.31	0.46
1:E:385:GLU:HG3	1:E:396:ARG:HB2	1.98	0.46
1:F:224:ASP:O	1:F:308:THR:HG21	2.16	0.46
1:F:277:ILE:HG23	1:F:278:THR:HG22	1.96	0.46
1:G:258:ARG:NH1	1:G:429:ALA:O	2.48	0.46
1:C:144:LYS:HA	1:C:144:LYS:HD2	1.65	0.46
1:H:349:PRO:HD3	1:H:364:PRO:HB3	1.97	0.46
1:B:280:THR:HG22	1:B:314:ILE:HG23	1.98	0.46
1:B:340:ARG:HD2	1:B:368:ARG:NH2	2.31	0.46
1:E:165:SER:H	1:E:168:GLN:HB2	1.80	0.46
1:F:446:ASP:O	1:F:450:GLU:HG3	2.15	0.46
1:F:470:ILE:HA	1:F:473:ILE:HD12	1.97	0.46
1:H:13:SER:OG	1:H:43:CYS:HB3	2.16	0.46
1:H:148:GLN:O	1:H:230:ARG:CZ	2.64	0.46
1:H:434:ARG:NH2	1:H:436:ASP:OD2	2.46	0.46
1:C:239:GLN:O	1:C:243:LEU:HG	2.16	0.46
1:C:282:THR:HB	1:C:459:PRO:HB3	1.98	0.46

	to do pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:487:GLU:HA	1:D:490:HIS:CD2	2.50	0.46
1:G:204:ASP:OD2	1:G:349:PRO:HD3	2.15	0.46
1:G:271:ILE:HA	1:G:275:THR:HB	1.98	0.46
1:B:385:GLU:OE1	1:B:396:ARG:HB2	2.16	0.46
1:C:245:ALA:HA	1:C:323:TRP:CZ2	2.51	0.46
1:D:311:PHE:HB2	1:D:462:TYR:HE2	1.79	0.46
1:E:10:LEU:HB3	1:E:43:CYS:HA	1.97	0.46
1:E:355:PHE:CZ	1:F:189:PHE:HB2	2.51	0.46
1:G:90:ILE:H	1:G:90:ILE:HG12	1.40	0.46
1:G:378:GLN:HA	1:G:400:LEU:O	2.16	0.46
1:B:10:LEU:C	1:B:11:PHE:HD1	2.18	0.46
1:B:378:GLN:HB2	1:B:399:TRP:HE3	1.79	0.46
1:C:188:ARG:NH2	1:C:246:MET:O	2.23	0.46
1:E:283:GLY:N	1:E:311:PHE:HB3	2.20	0.46
1:E:336:LEU:HB3	1:E:467:TRP:CE3	2.51	0.46
1:F:51:THR:HG22	1:F:85:TYR:HB3	1.98	0.46
1:F:172:ILE:HG12	1:F:432:PHE:HE1	1.81	0.46
1:G:183:ASN:ND2	1:H:383:VAL:HG22	2.31	0.46
1:A:24:PRO:O	1:A:25:SER:C	2.53	0.46
1:B:376:THR:HG23	1:B:402:LEU:O	2.16	0.46
1:C:422:LEU:HD22	1:D:388:LEU:HD22	1.97	0.46
1:D:157:ASN:OD1	1:D:171:ARG:NH2	2.49	0.46
1:F:134:ALA:CB	1:F:163:VAL:HG21	2.45	0.46
1:F:140:LEU:HB3	1:F:168:GLN:O	2.16	0.46
1:G:376:THR:HG23	1:G:402:LEU:O	2.16	0.46
1:H:455:ASN:HB3	1:H:457:MET:HG3	1.98	0.46
1:E:201:LYS:HA	1:E:348:LYS:NZ	2.30	0.45
1:E:202:GLY:CA	1:E:348:LYS:HB2	2.46	0.45
1:E:272:ASN:HB3	1:E:275:THR:HG23	1.98	0.45
1:F:178:LYS:NZ	1:F:178:LYS:HA	2.30	0.45
1:G:43:CYS:HB2	1:G:85:TYR:HD1	1.81	0.45
1:G:216:LEU:HD22	1:G:223:PHE:CD1	2.51	0.45
1:G:258:ARG:HD3	1:G:434:ARG:NH1	2.31	0.45
1:H:142:LEU:CB	1:H:146:LEU:HD11	2.45	0.45
1:H:370:VAL:HG13	1:H:372:GLN:O	2.16	0.45
1:A:474:ALA:O	1:A:478:ARG:HG2	2.15	0.45
1:B:26:LEU:HD22	1:B:26:LEU:O	2.15	0.45
1:B:191:ASN:HB2	1:B:194:PHE:HD2	1.80	0.45
1:B:340:ARG:HD2	1:B:368:ARG:HH21	1.81	0.45
1:C:174:HIS:CD2	1:C:236:HIS:CE1	3.03	0.45
1:C:209:SER:HB2	1:C:331:ARG:HH21	1.82	0.45

	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:272:ASN:C	1:E:276:VAL:HG23	2.36	0.45
1:E:367:LEU:HD12	1:E:378:GLN:O	2.16	0.45
1:F:452:TRP:CB	1:F:457:MET:HE3	2.46	0.45
1:B:166:GLU:CD	1:B:171:ARG:HH12	2.17	0.45
1:B:281:VAL:HG21	1:B:472:ALA:HA	1.98	0.45
1:C:226:SER:HB3	1:C:230:ARG:HB2	1.98	0.45
1:C:365:ASN:HA	1:C:380:SER:OG	2.15	0.45
1:F:13:SER:HB3	1:F:44:THR:O	2.15	0.45
1:F:18:SER:O	1:F:23:LEU:HB2	2.16	0.45
1:C:237:ILE:O	1:C:241:VAL:HG23	2.16	0.45
1:E:337:PRO:HD3	1:E:467:TRP:N	2.32	0.45
1:E:358:SER:HB3	1:E:391:ASN:O	2.16	0.45
1:F:213:THR:OG1	1:F:339:ARG:HB2	2.17	0.45
1:H:311:PHE:HB2	1:H:462:TYR:HE2	1.81	0.45
1:B:157:ASN:O	1:B:161:LEU:HG	2.17	0.45
1:B:320:ASN:HD21	1:B:322:ARG:HB3	1.81	0.45
1:D:208:ILE:HG21	1:D:237:ILE:HG23	1.99	0.45
1:G:197:LEU:HD21	1:H:196:PRO:HG3	1.99	0.45
1:H:269:ARG:O	1:H:444:TRP:NE1	2.44	0.45
1:B:26:LEU:HD23	1:B:62:LEU:HD12	1.97	0.45
1:B:81:ASN:ND2	1:B:81:ASN:H	2.15	0.45
1:D:157:ASN:O	1:D:161:LEU:HB2	2.17	0.45
1:E:8:MET:HG3	1:E:111:ALA:HB3	1.98	0.45
1:F:198:TRP:CD1	1:F:323:TRP:HZ2	2.34	0.45
1:F:285:TYR:CD1	1:F:310:THR:HG21	2.51	0.45
1:G:476:VAL:HB	1:G:481:VAL:O	2.17	0.45
1:B:251:HIS:HD2	1:B:252:MET:H	1.65	0.45
1:D:215:GLY:C	1:D:217:GLU:H	2.20	0.45
1:E:272:ASN:O	1:E:276:VAL:N	2.48	0.45
1:G:283:GLY:HA2	1:G:460:LYS:H	1.81	0.45
1:H:49:TYR:O	1:H:85:TYR:CD1	2.70	0.45
1:H:170:TYR:CE2	1:H:424:LEU:HA	2.52	0.45
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.68	0.45
1:B:122:GLU:O	1:B:126:ALA:N	2.49	0.45
1:D:158:ASP:O	1:D:162:LYS:N	2.49	0.45
1:E:274:ASP:OD1	1:E:274:ASP:N	2.49	0.45
1:F:133:LEU:HD22	1:F:133:LEU:HA	1.77	0.45
1:H:230:ARG:NH2	1:H:449:ARG:HD3	2.32	0.45
1:A:273:ASN:HA	1:A:276:VAL:HG12	1.99	0.45
1:B:93:PRO:HA	1:B:96:PHE:CD2	2.52	0.45
1:C:281:VAL:HG11	1:C:472:ALA:HB2	1.99	0.45

	to de pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:368:ARG:O	1:C:378:GLN:N	2.38	0.45	
1:E:11:PHE:HA	1:E:44:THR:O	2.17	0.45	
1:E:331:ARG:CZ	1:E:483:TRP:HB3	2.47	0.45	
1:G:337:PRO:HG3	1:G:465:GLY:HA2	1.98	0.45	
1:B:140:LEU:HB3	1:B:169:VAL:HA	1.99	0.45	
1:E:254:ALA:HB2	1:E:428:ASP:CB	2.42	0.45	
1:F:60:LYS:HB3	1:F:60:LYS:HE2	1.75	0.45	
1:G:143:GLU:HB3	1:G:172:ILE:HB	1.99	0.45	
1:H:141:ALA:HB1	1:H:172:ILE:HD11	1.98	0.45	
1:C:146:LEU:H	1:C:146:LEU:HG	1.48	0.44	
1:D:309:GLU:H	1:D:309:GLU:CD	2.20	0.44	
1:E:254:ALA:CB	1:E:428:ASP:HB3	2.43	0.44	
1:E:351:PRO:HD2	1:H:321:TRP:CE2	2.52	0.44	
1:F:185:LEU:HD23	1:F:185:LEU:HA	1.70	0.44	
1:A:11:PHE:O	1:A:45:SER:HA	2.17	0.44	
1:A:321:TRP:O	1:A:321:TRP:CD1	2.70	0.44	
1:E:195:GLU:N	1:E:196:PRO:HD2	2.32	0.44	
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.84	0.44	
1:A:466:THR:O	1:A:467:TRP:HB2	2.16	0.44	
1:B:57:PHE:O	1:B:60:LYS:HG3	2.18	0.44	
1:B:310:THR:O	1:B:334:LYS:HB2	2.17	0.44	
1:C:191:ASN:CG	1:D:382:MET:H	2.18	0.44	
1:C:223:PHE:CZ	1:C:310:THR:HG22	2.51	0.44	
1:D:146:LEU:HD23	1:D:171:ARG:NH1	2.33	0.44	
1:E:475:LEU:HA	1:E:478:ARG:HB2	1.99	0.44	
1:G:246:MET:HA	1:G:264:VAL:HG21	1.99	0.44	
1:H:9:ILE:HB	1:H:112:ILE:HG23	1.98	0.44	
1:H:262:VAL:HG21	1:H:434:ARG:HH21	1.82	0.44	
1:B:195:GLU:N	1:B:196:PRO:HD2	2.33	0.44	
1:B:350:VAL:HG21	1:B:362:LEU:HD22	1.99	0.44	
1:B:429:ALA:HB3	1:B:432:PHE:HD2	1.83	0.44	
1:C:171:ARG:HD2	1:C:433:VAL:HB	1.99	0.44	
1:D:170:TYR:CD2	1:D:424:LEU:HD13	2.53	0.44	
1:D:408:PHE:HB3	1:D:411:ARG:HG3	2.00	0.44	
1:E:140:LEU:HD22	1:E:164:PHE:CE2	2.52	0.44	
1:E:408:PHE:CZ	1:F:385:GLU:HG3	2.53	0.44	
1:E:423:ASP:HA	1:E:426:GLU:O	2.17	0.44	
1:G:150:LEU:HB2	1:G:442:TRP:HB3	2.00	0.44	
1:G:216:LEU:H	1:G:216:LEU:HG	1.54	0.44	
1:A:194:PHE:HB3	1:A:198:TRP:CZ3	2.53	0.44	
1:A:355:PHE:CZ	1:B:189:PHE:HB2	2.53	0.44	

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:378:GLN:HG3	1:A:399:TRP:CE3	2.52	0.44
1:C:210:VAL:HG13	1:C:341:SER:OG	2.18	0.44
1:C:280:THR:HA	1:C:313:ALA:O	2.17	0.44
1:E:153:SER:O	1:E:157:ASN:HB2	2.18	0.44
1:E:362:LEU:CD1	1:F:190:GLY:HA2	2.47	0.44
1:F:9:ILE:HA	1:F:42:VAL:O	2.18	0.44
1:G:6:SER:HB3	1:G:105:PRO:HG2	1.99	0.44
1:G:251:HIS:NE2	1:H:356:SER:HB2	2.33	0.44
1:H:230:ARG:NH1	2:H:502:HOH:O	2.51	0.44
1:A:116:THR:O	1:A:121:PHE:HE1	2.01	0.44
1:B:287:ALA:HB2	1:B:297:GLY:H	1.81	0.44
1:C:365:ASN:ND2	1:C:381:ILE:HA	2.32	0.44
1:C:398:VAL:HG22	1:C:399:TRP:H	1.82	0.44
1:E:251:HIS:ND1	1:F:354:ILE:O	2.50	0.44
1:E:287:ALA:HB1	1:E:296:ALA:HB1	1.99	0.44
1:G:452:TRP:HD1	1:G:453:LYS:N	2.16	0.44
1:H:370:VAL:O	1:H:375:GLU:HA	2.17	0.44
1:C:368:ARG:N	1:C:378:GLN:O	2.31	0.44
1:D:488:HIS:O	1:D:489:HIS:HB3	2.18	0.44
1:E:151:ALA:O	1:E:155:HIS:HB2	2.17	0.44
1:E:407:VAL:HG21	1:F:398:VAL:HG21	1.99	0.44
1:F:216:LEU:H	1:F:334:LYS:HD2	1.83	0.44
1:F:288:GLY:O	1:F:294:GLU:HG3	2.16	0.44
1:G:337:PRO:HG3	1:G:465:GLY:O	2.18	0.44
1:B:51:THR:OG1	1:B:52:ASP:N	2.51	0.44
1:C:299:ILE:C	1:C:301:GLU:H	2.20	0.44
1:F:181:VAL:O	1:F:184:LEU:HB2	2.18	0.44
1:G:6:SER:H	1:G:109:GLY:CA	2.28	0.44
1:H:200:SER:N	1:H:322:ARG:O	2.50	0.44
1:A:209:SER:HA	1:A:331:ARG:O	2.18	0.44
1:D:284:GLN:O	1:D:462:TYR:N	2.35	0.44
1:E:107:GLU:H	1:E:107:GLU:HG2	1.37	0.44
1:F:10:LEU:O	1:F:11:PHE:HD1	2.01	0.44
1:G:379:ILE:O	1:G:399:TRP:HA	2.18	0.44
1:A:237:ILE:O	1:A:241:VAL:HG23	2.17	0.43
1:A:265:PHE:HA	1:A:268:LEU:HG	2.00	0.43
1:B:423:ASP:O	1:B:427:GLY:O	2.36	0.43
1:D:258:ARG:HH21	1:D:432:PHE:HB2	1.83	0.43
1:E:475:LEU:HA	1:E:475:LEU:HD23	1.75	0.43
1:F:288:GLY:CA	1:F:464:SER:HB2	2.48	0.43
1:H:271:ILE:CG2	1:H:276:VAL:HG23	2.48	0.43

	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:321:TRP:CD1	1:A:321:TRP:C	2.91	0.43	
1:F:172:ILE:HG12	1:F:432:PHE:CE1	2.53	0.43	
1:G:18:SER:HA	1:G:22:LEU:CD1	2.47	0.43	
1:H:171:ARG:NH1	1:H:435:ARG:HA	2.33	0.43	
1:A:318:VAL:HB	1:A:323:TRP:HB2	2.00	0.43	
1:B:173:ASP:HB3	1:B:176:LEU:HB2	2.00	0.43	
1:C:449:ARG:HA	1:C:452:TRP:NE1	2.33	0.43	
1:D:275:THR:O	1:D:279:HIS:HB2	2.18	0.43	
1:F:346:GLN:HG3	1:F:366:LYS:HG2	2.00	0.43	
1:B:85:TYR:O	1:B:86:ALA:HB3	2.17	0.43	
1:C:466:THR:HG22	1:C:466:THR:O	2.18	0.43	
1:D:242:ALA:HB1	1:D:261:LYS:HB3	2.00	0.43	
1:E:239:GLN:O	1:E:243:LEU:HG	2.18	0.43	
1:E:295:VAL:HG23	1:E:295:VAL:O	2.19	0.43	
1:F:60:LYS:HB2	1:F:64:ARG:NH2	2.33	0.43	
1:F:396:ARG:NH2	2:F:503:HOH:O	2.51	0.43	
1:G:101:ASP:N	1:G:101:ASP:OD1	2.51	0.43	
1:G:385:GLU:HG3	1:G:386:PRO:HD2	2.01	0.43	
1:B:138:SER:O	1:B:168:GLN:HG2	2.18	0.43	
1:B:213:THR:HA	1:B:336:LEU:O	2.19	0.43	
1:B:333:GLY:HA3	1:B:336:LEU:CD1	2.48	0.43	
1:C:472:ALA:O	1:C:483:TRP:NE1	2.36	0.43	
1:D:175:TYR:CD1	1:D:178:LYS:HE2	2.53	0.43	
1:D:272:ASN:N	1:D:275:THR:OG1	2.52	0.43	
1:E:376:THR:HG22	1:E:402:LEU:O	2.18	0.43	
1:E:434:ARG:O	1:E:438:VAL:HG23	2.18	0.43	
1:G:7:THR:O	1:G:111:ALA:N	2.49	0.43	
1:H:172:ILE:HG12	1:H:432:PHE:CE2	2.52	0.43	
1:D:242:ALA:HA	1:D:264:VAL:HG11	2.01	0.43	
1:E:272:ASN:N	1:E:275:THR:OG1	2.43	0.43	
1:F:210:VAL:HG21	1:F:237:ILE:HG12	2.01	0.43	
1:F:213:THR:HG23	1:F:339:ARG:N	2.33	0.43	
1:H:180:THR:CG2	1:H:375:GLU:HG2	2.48	0.43	
1:H:355:PHE:C	1:H:357:SER:N	2.71	0.43	
1:A:180:THR:HG22	1:A:375:GLU:HG2	2.00	0.43	
1:A:289:VAL:HA	1:A:294:GLU:HA	2.01	0.43	
1:A:363:GLN:CB	1:A:382:MET:HE1	2.49	0.43	
1:A:378:GLN:HG3	1:A:399:TRP:CZ3	2.53	0.43	
1:B:41:ILE:HG21	1:B:83:LEU:HG	2.01	0.43	
1:C:270:PRO:HA	1:C:444:TRP:HD1	1.82	0.43	
1:D:171:ARG:NE	1:D:438:VAL:HG11	2.32	0.43	

Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:F:385:GLU:OE2	1:F:396:ABG:HB2	2.17	0.43		
1:G:157:ASN:O	1:G:161:LEU:HG	2.19	0.43		
1:G:358:SER:N	1:G:392:GLY:HA3	2.34	0.43		
1:G:368:ARG:HG2	1:G:378:GLN:HE21	1.84	0.43		
1:H:8:MET:HA	1:H:111:ALA:O	2.17	0.43		
1:H:112:ILE:N	1:H:139:ARG:O	2.51	0.43		
1:A:211:ALA:HB1	1:A:338:ALA:O	2.18	0.43		
1:A:379:ILE:HD11	1:B:400:LEU:HD13	2.00	0.43		
1:F:177:GLY:O	1:F:416:ALA:HA	2.18	0.43		
1:H:45:SER:O	1:H:87:THR:HA	2.19	0.43		
1:H:171:ARG:O	1:H:433:VAL:HG23	2.19	0.43		
1:H:423:ASP:O	1:H:426:GLU:O	2.35	0.43		
1:B:246:MET:HE3	1:B:247:GLU:O	2.19	0.43		
1:C:316:ALA:HB3	1:C:328:PHE:HB2	2.00	0.43		
1:D:415:ILE:O	1:D:418:GLU:HG3	2.19	0.43		
1:F:302:LEU:HD12	2:F:506:HOH:O	2.19	0.43		
1:A:419:ARG:HD3	1:B:388:LEU:HD23	2.00	0.43		
1:B:331:ARG:HH21	1:B:467:TRP:HB3	1.84	0.43		
1:B:449:ARG:O	1:B:452:TRP:CD1	2.72	0.43		
1:C:176:LEU:HD21	1:C:239:GLN:HB3	2.01	0.43		
1:D:403:SER:O	1:D:407:VAL:HG23	2.18	0.43		
1:F:139:ARG:HG2	2:F:519:HOH:O	2.19	0.43		
1:G:23:LEU:N	1:G:24:PRO:CD	2.82	0.43		
1:G:251:HIS:CG	1:G:252:MET:H	2.37	0.43		
1:H:299:ILE:HD12	1:H:306:SER:H	1.83	0.43		
1:A:444:TRP:O	1:A:448:ILE:HG13	2.18	0.42		
1:B:347:PHE:HB2	1:B:365:ASN:O	2.18	0.42		
1:C:195:GLU:N	1:C:196:PRO:HD2	2.33	0.42		
1:G:5:VAL:CG1	1:G:111:ALA:HB2	2.44	0.42		
1:H:234:GLN:HG3	1:H:445:ILE:HG13	2.01	0.42		
1:H:323:TRP:HZ3	1:H:326:VAL:HG11	1.84	0.42		
1:H:329:TYR:OH	1:H:479:ASP:OD2	2.34	0.42		
1:H:452:TRP:HB2	1:H:457:MET:HB2	2.00	0.42		
1:A:45:SER:HB2	1:A:85:TYR:HE1	1.84	0.42		
1:B:92:ASP:C	1:B:94:THR:H	2.22	0.42		
1:B:354:ILE:H	1:B:354:ILE:HG12	1.45	0.42		
1:B:399:TRP:CZ2	1:B:484:TYR:HE2	2.37	0.42		
1:C:166:GLU:OE2	1:C:435:ARG:HB2	2.19	0.42		
1:D:173:ASP:HB3	1:D:176:LEU:HD12	2.00	0.42		
1:D:239:GLN:NE2	1:D:433:VAL:HG13	2.34	0.42		
1:E:81:ASN:OD1	1:E:81:ASN:N	2.51	0.42		

	A la C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:378:GLN:HB3	1:F:401:ASP:HA	2.01	0.42	
1:G:191:ASN:CG	1:H:382:MET:H	2.19	0.42	
1:G:276:VAL:HG23	1:G:280:THR:OG1	2.19	0.42	
1:G:419:ARG:NH2	1:H:389:ASP:HB2	2.34	0.42	
1:H:172:ILE:HG23	1:H:420:LEU:HD22	2.01	0.42	
1:H:385:GLU:N	1:H:395:MET:HA	2.32	0.42	
1:A:191:ASN:CG	1:B:382:MET:H	2.21	0.42	
1:A:232:MET:HE2	1:A:232:MET:HB3	1.74	0.42	
1:B:347:PHE:N	1:B:365:ASN:O	2.51	0.42	
1:D:140:LEU:HD11	1:D:142:LEU:HG	2.01	0.42	
1:E:40:ARG:HA	1:E:82:LYS:HA	2.00	0.42	
1:E:175:TYR:CE2	1:E:236:HIS:HB3	2.53	0.42	
1:E:277:ILE:HD12	1:E:277:ILE:HA	1.83	0.42	
1:F:43:CYS:N	1:F:84:PHE:O	2.41	0.42	
1:H:8:MET:SD	1:H:111:ALA:O	2.77	0.42	
1:A:318:VAL:HB	1:A:323:TRP:CB	2.48	0.42	
1:B:157:ASN:O	1:B:161:LEU:N	2.41	0.42	
1:C:153:SER:O	1:C:157:ASN:HB2	2.19	0.42	
1:D:246:MET:HE3	1:D:260:GLU:HB2	2.01	0.42	
1:G:395:MET:SD	1:H:186:THR:HG23	2.60	0.42	
1:H:234:GLN:CG	1:H:445:ILE:HG13	2.49	0.42	
1:A:340:ARG:HG2	1:A:373:PRO:HD3	2.02	0.42	
1:B:181:VAL:HA	1:B:184:LEU:HG	2.00	0.42	
1:C:308:THR:N	2:C:506:HOH:O	2.53	0.42	
1:D:204:ASP:O	1:D:326:VAL:HG13	2.19	0.42	
1:D:335:ARG:O	1:D:462:TYR:HE1	2.02	0.42	
1:E:199:ASN:OD1	1:E:201:LYS:O	2.36	0.42	
1:F:114:LEU:HB2	1:F:142:LEU:HD23	2.01	0.42	
1:F:198:TRP:CD1	1:F:323:TRP:CZ2	3.08	0.42	
1:F:238:LEU:HD23	1:F:238:LEU:HA	1.64	0.42	
1:H:35:LEU:HD23	1:H:35:LEU:HA	1.90	0.42	
1:H:150:LEU:O	1:H:154:ASP:HB2	2.18	0.42	
1:D:254:ALA:HB1	1:D:429:ALA:O	2.19	0.42	
1:E:125:ILE:HA	1:E:128:LEU:HD23	2.02	0.42	
1:F:128:LEU:CD1	1:F:133:LEU:HG	2.49	0.42	
1:F:147:GLY:O	1:F:442:TRP:CH2	2.72	0.42	
1:F:311:PHE:CD2	1:F:333:GLY:HA3	2.54	0.42	
1:A:237:ILE:HG21	1:A:330:ILE:CG2	2.50	0.42	
1:B:23:LEU:HD22	1:B:23:LEU:HA	1.77	0.42	
1:B:26:LEU:HD13	1:B:26:LEU:C	2.40	0.42	
1:B:268:LEU:HD22	1:B:444:TRP:CZ2	2.54	0.42	

		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:337:PRO:HD3	1:B:467:TRP:N	2.35	0.42
1:C:264:VAL:O	1:C:267:ALA:N	2.51	0.42
1:D:150:LEU:CD2	1:D:439:GLU:HA	2.50	0.42
1:E:80:LEU:HD13	1:E:80:LEU:HA	1.75	0.42
1:E:171:ARG:HB2	1:E:433:VAL:O	2.20	0.42
1:E:392:GLY:O	1:E:394:HIS:CE1	2.72	0.42
1:F:85:TYR:CD2	1:F:86:ALA:N	2.87	0.42
1:F:302:LEU:HG	1:F:304:GLN:H	1.85	0.42
1:F:403:SER:N	2:F:502:HOH:O	2.42	0.42
1:F:449:ARG:HA	1:F:452:TRP:NE1	2.34	0.42
1:G:169:VAL:O	1:G:170:TYR:HD1	2.02	0.42
1:G:404:LEU:HD22	1:G:408:PHE:HE2	1.85	0.42
1:H:50:ASP:C	1:H:53:GLY:H	2.23	0.42
1:A:475:LEU:HD12	1:A:478:ARG:HH21	1.84	0.42
1:B:211:ALA:HB1	1:B:338:ALA:O	2.20	0.42
1:B:307:ASP:O	1:B:459:PRO:HG3	2.19	0.42
1:B:476:VAL:HG21	1:B:483:TRP:HE1	1.83	0.42
1:D:379:ILE:HB	1:D:400:LEU:HD12	2.02	0.42
1:E:284:GLN:HA	1:E:310:THR:OG1	2.20	0.42
1:E:342:GLU:HA	1:E:369:ILE:O	2.20	0.42
1:F:72:ASN:HB2	1:F:75:ALA:HB3	2.01	0.42
1:H:176:LEU:HA	1:H:176:LEU:HD23	1.77	0.42
1:A:99:ILE:H	1:A:99:ILE:HG12	1.36	0.42
1:B:26:LEU:HD21	1:B:30:ASP:HB3	2.02	0.42
1:B:161:LEU:HA	1:B:164:PHE:O	2.19	0.42
1:B:245:ALA:HA	1:B:323:TRP:HE1	1.85	0.42
1:C:154:ASP:HA	1:C:435:ARG:NH2	2.30	0.42
1:C:414:ARG:NH2	2:C:505:HOH:O	2.52	0.42
1:E:178:LYS:HB2	1:E:181:VAL:CG2	2.48	0.42
1:G:226:SER:OG	1:G:230:ARG:HB2	2.20	0.42
1:G:438:VAL:HG12	1:G:442:TRP:HD1	1.85	0.42
1:H:285:TYR:CB	1:H:298:TYR:HB2	2.37	0.42
1:A:164:PHE:HB3	1:A:168:GLN:HB2	2.01	0.42
1:B:485:ASP:OD1	1:B:486:LEU:N	2.52	0.42
1:C:279:HIS:HA	1:C:475:LEU:HD11	2.02	0.42
1:D:180:THR:HG21	1:D:375:GLU:HG2	2.00	0.42
1:G:146:LEU:HD11	1:G:234:GLN:OE1	2.20	0.42
1:G:463:VAL:HB	1:G:466:THR:HG23	2.01	0.42
1:D:232:MET:O	1:D:236:HIS:HB2	2.20	0.41
1:E:139:ARG:HA	1:E:168:GLN:CA	2.46	0.41
1:E:171:ARG:HB3	1:E:433:VAL:HB	2.03	0.41

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:388:LEU:HD13	1:F:419:ARG:HA	2.01	0.41
1:E:478:ARG:HD2	1:E:478:ARG:HA	1.77	0.41
1:F:21:MET:O	1:F:24:PRO:HG2	2.19	0.41
1:F:118:PRO:O	1:F:119:SER:HB2	2.20	0.41
1:F:423:ASP:HB3	1:F:429:ALA:CB	2.49	0.41
1:G:295:VAL:HB	1:G:335:ARG:HH12	1.85	0.41
1:C:253:GLU:O	1:C:257:VAL:HG23	2.20	0.41
1:G:484:TYR:CE2	1:G:486:LEU:HA	2.56	0.41
1:H:335:ARG:O	1:H:462:TYR:HE1	2.03	0.41
1:H:383:VAL:HB	1:H:398:VAL:HG11	2.02	0.41
1:B:50:ASP:OD2	1:B:50:ASP:N	2.53	0.41
1:C:404:LEU:CD2	1:D:383:VAL:HG21	2.51	0.41
1:D:142:LEU:HD12	1:D:170:TYR:O	2.20	0.41
1:E:383:VAL:HG21	1:F:404:LEU:HD22	2.01	0.41
1:F:215:GLY:HA2	1:F:334:LYS:CD	2.49	0.41
1:G:38:ASP:OD1	1:G:38:ASP:N	2.53	0.41
1:H:41:ILE:HB	1:H:83:LEU:HD23	2.02	0.41
1:H:150:LEU:HD11	1:H:439:GLU:HG3	2.01	0.41
1:A:419:ARG:HD3	1:B:388:LEU:HB3	2.02	0.41
1:B:320:ASN:ND2	1:B:322:ARG:H	2.19	0.41
1:B:354:ILE:HD11	1:C:321:TRP:CE3	2.56	0.41
1:C:207:GLN:HB2	1:C:344:VAL:HB	2.02	0.41
1:C:368:ARG:HB3	1:C:399:TRP:HZ3	1.85	0.41
1:D:448:ILE:HG22	1:D:452:TRP:HD1	1.85	0.41
1:F:210:VAL:HB	1:F:332:THR:HB	2.03	0.41
1:F:229:LEU:HD12	1:F:312:VAL:HG21	2.02	0.41
1:G:43:CYS:HB3	1:G:54:PHE:CE2	2.55	0.41
1:G:161:LEU:HD22	1:G:165:SER:HA	2.03	0.41
1:H:238:LEU:HA	1:H:238:LEU:HD23	1.75	0.41
1:A:201:LYS:H	1:A:201:LYS:HG2	1.68	0.41
1:B:411:ARG:HA	1:B:411:ARG:HD3	1.85	0.41
1:E:287:ALA:CB	1:E:296:ALA:HB1	2.50	0.41
1:G:288:GLY:HA3	1:G:463:VAL:HG13	2.02	0.41
1:G:337:PRO:HD2	1:G:467:TRP:CG	2.56	0.41
1:G:452:TRP:HB2	1:G:457:MET:HG3	2.03	0.41
1:H:371:LEU:H	1:H:371:LEU:HG	1.70	0.41
1:A:149:ASP:HB2	1:A:152:SER:OG	2.21	0.41
1:E:272:ASN:OD1	1:E:273:ASN:N	2.54	0.41
1:E:414:ARG:HA	1:E:414:ARG:HD2	1.97	0.41
1:F:232:MET:O	1:F:236:HIS:HB2	2.20	0.41
1:G:173:ASP:OD2	1:G:235:SER:HB2	2.20	0.41

	A h o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:H:212:GLU:HB2	1:H:333:GLY:O	2.21	0.41	
1:A:321:TRP:HA	1:D:352:HIS:CB	2.50	0.41	
1:A:368:ARG:HB3	1:A:378:GLN:HG2	2.02	0.41	
1:A:384:LYS:H	1:B:183:ASN:HB2	1.85	0.41	
1:B:9:ILE:HG23	1:B:42:VAL:HG11	2.02	0.41	
1:B:26:LEU:CD2	1:B:30:ASP:HB3	2.50	0.41	
1:B:172:ILE:HG12	1:B:432:PHE:CE1	2.55	0.41	
1:C:187:LEU:HD13	1:C:377:ILE:HD13	2.03	0.41	
1:C:452:TRP:CD1	1:C:453:LYS:N	2.88	0.41	
1:D:487:GLU:HA	1:D:490:HIS:NE2	2.35	0.41	
1:E:166:GLU:CA	1:E:169:VAL:HG12	2.43	0.41	
1:F:17:LEU:HD22	1:F:17:LEU:HA	1.75	0.41	
1:F:154:ASP:O	1:F:158:ASP:N	2.43	0.41	
1:G:368:ARG:HB3	1:G:378:GLN:HG3	2.03	0.41	
1:H:285:TYR:N	1:H:310:THR:OG1	2.54	0.41	
1:A:242:ALA:HB2	1:A:265:PHE:CZ	2.56	0.41	
1:C:433:VAL:HG12	1:C:437:GLU:HB2	2.01	0.41	
1:D:311:PHE:CD1	1:D:333:GLY:HA3	2.56	0.41	
1:F:343:ILE:O	1:F:368:ARG:HA	2.20	0.41	
1:F:358:SER:CB	1:F:392:GLY:HA3	2.50	0.41	
1:G:183:ASN:HD21	1:H:383:VAL:CG2	2.33	0.41	
1:G:423:ASP:HB2	1:G:432:PHE:HE2	1.85	0.41	
1:H:276:VAL:HG11	1:H:451:GLY:C	2.41	0.41	
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.82	0.41	
1:A:189:PHE:CE1	1:A:248:PRO:HB3	2.56	0.41	
1:A:322:ARG:HG2	1:A:323:TRP:CD1	2.56	0.41	
1:A:355:PHE:CD2	1:B:252:MET:HG3	2.56	0.41	
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.83	0.41	
1:B:200:SER:HA	1:B:326:VAL:HG21	2.03	0.41	
1:B:251:HIS:CD2	1:B:252:MET:H	2.39	0.41	
1:B:259:ASP:OD1	1:B:434:ARG:NH1	2.44	0.41	
1:B:422:LEU:HD23	1:B:423:ASP:N	2.36	0.41	
1:C:238:LEU:HD23	1:C:238:LEU:HA	1.91	0.41	
1:C:340:ARG:HA	1:C:373:PRO:HD3	2.03	0.41	
1:D:150:LEU:HD23	1:D:150:LEU:HA	1.84	0.41	
1:D:245:ALA:HA	1:D:323:TRP:NE1	2.36	0.41	
1:D:302:LEU:HD23	1:D:302:LEU:HA	1.86	0.41	
1:D:488:HIS:H	1:D:488:HIS:CD2	2.38	0.41	
1:E:40:ARG:CB	1:E:84:PHE:HE2	2.34	0.41	
1:E:164:PHE:HA	1:E:168:GLN:OE1	2.21	0.41	
1:E:212:GLU:HB3	1:E:214:VAL:HG22	2.02	0.41	

		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:230:ARG:CZ	1:E:449:ARG:HD3	2.51	0.41	
1:F:41:ILE:HG22	1:F:43:CYS:SG	2.61	0.41	
1:F:60:LYS:H	1:F:60:LYS:HG2	1.36	0.41	
1:F:434:ARG:NE	1:F:436:ASP:OD2	2.54	0.41	
1:G:114:LEU:HA	1:G:114:LEU:HD12	1.81	0.41	
1:H:37:ASP:OD1	1:H:37:ASP:N	2.52	0.41	
1:H:273:ASN:CA	1:H:451:GLY:HA2	2.50	0.41	
1:H:433:VAL:HG12	1:H:437:GLU:HB2	2.03	0.41	
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.77	0.41	
1:B:180:THR:HA	1:B:183:ASN:HD22	1.86	0.41	
1:B:333:GLY:HA3	1:B:336:LEU:HG	2.03	0.41	
1:E:176:LEU:HA	1:E:176:LEU:HD12	1.89	0.41	
1:F:41:ILE:O	1:F:84:PHE:N	2.51	0.41	
1:F:83:LEU:HA	1:F:83:LEU:HD22	1.86	0.41	
1:F:133:LEU:HD13	1:F:138:SER:HB3	2.02	0.41	
1:F:173:ASP:OD2	1:F:235:SER:HB2	2.21	0.41	
1:F:408:PHE:HD1	1:F:411:ARG:HD3	1.85	0.41	
1:G:446:ASP:O	1:G:450:GLU:HB2	2.20	0.41	
1:H:223:PHE:CE1	1:H:310:THR:HG22	2.56	0.41	
1:B:10:LEU:HG	1:B:11:PHE:N	2.34	0.40	
1:B:213:THR:HG22	1:B:339:ARG:CB	2.51	0.40	
1:B:452:TRP:CD1	1:B:452:TRP:C	2.95	0.40	
1:C:357:SER:OG	1:C:358:SER:N	2.54	0.40	
1:F:167:LYS:H	1:F:167:LYS:HG3	1.68	0.40	
1:F:171:ARG:O	1:F:433:VAL:HG23	2.22	0.40	
1:G:5:VAL:HG11	1:G:111:ALA:CB	2.45	0.40	
1:G:227:GLY:O	1:G:231:ASP:HB2	2.21	0.40	
1:H:146:LEU:HB3	1:H:156:ILE:HD11	2.03	0.40	
1:H:316:ALA:N	1:H:328:PHE:O	2.53	0.40	
1:A:162:LYS:H	1:A:162:LYS:HG2	1.45	0.40	
1:A:462:TYR:CD1	1:A:469:PRO:HD3	2.56	0.40	
1:C:183:ASN:ND2	1:D:383:VAL:HG23	2.35	0.40	
1:C:288:GLY:H	1:C:295:VAL:HG22	1.86	0.40	
1:D:126:ALA:O	1:D:130:GLN:HB2	2.21	0.40	
1:E:128:LEU:HD12	1:E:133:LEU:HD13	2.03	0.40	
1:E:232:MET:HE3	1:E:232:MET:HB3	1.95	0.40	
1:F:64:ARG:HA	1:F:64:ARG:HD3	1.49	0.40	
1:G:130:GLN:HE21	1:G:130:GLN:HB2	1.58	0.40	
1:G:209:SER:HB2	1:G:483:TRP:CZ3	2.56	0.40	
1:G:299:ILE:HD13	1:G:299:ILE:HA	1.76	0.40	
1:H:8:MET:CE	1:H:424:LEU:HD21	2.51	0.40	

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:368:ARG:HB3	1:A:378:GLN:HG3	2.03	0.40	
1:A:379:ILE:O	1:A:399:TRP:HA	2.22	0.40	
1:A:394:HIS:C	1:A:395:MET:HG3	2.42	0.40	
1:B:348:LYS:HA	1:B:349:PRO:HD3	1.89	0.40	
1:C:230:ARG:O	1:C:234:GLN:HB3	2.21	0.40	
1:D:285:TYR:HB2	1:D:310:THR:HG21	2.03	0.40	
1:E:7:THR:HB	1:E:110:ILE:CB	2.52	0.40	
1:E:142:LEU:HB3	1:E:146:LEU:HD21	2.04	0.40	
1:E:352:HIS:HB3	1:H:321:TRP:HA	2.04	0.40	
1:F:26:LEU:HB3	1:F:79:PHE:CE1	2.56	0.40	
1:F:118:PRO:HA	1:F:121:PHE:HE2	1.86	0.40	
1:G:299:ILE:O	1:G:303:GLY:N	2.43	0.40	
1:H:51:THR:HA	1:H:85:TYR:H	1.86	0.40	
1:H:89:ASP:OD1	1:H:91:THR:OG1	2.39	0.40	
1:H:344:VAL:HG21	1:H:484:TYR:CD2	2.57	0.40	
1:H:345:VAL:O	1:H:366:LYS:HA	2.22	0.40	
1:B:370:VAL:HG23	1:B:376:THR:HB	2.04	0.40	
1:F:139:ARG:NH1	1:F:424:LEU:O	2.55	0.40	
1:G:16:ASP:OD2	1:G:17:LEU:HG	2.21	0.40	
1:G:357:SER:OG	1:G:392:GLY:HA2	2.21	0.40	
1:G:405:THR:O	1:G:409:LYS:HA	2.22	0.40	
1:A:385:GLU:HG3	1:B:408:PHE:HE1	1.85	0.40	
1:A:457:MET:HE3	1:A:457:MET:HB3	1.95	0.40	
1:B:58:ALA:HB2	1:B:83:LEU:HD21	2.02	0.40	
1:D:239:GLN:HE22	1:D:433:VAL:HG13	1.86	0.40	
1:D:442:TRP:HA	1:D:445:ILE:HB	2.03	0.40	
1:E:484:TYR:CZ	1:E:486:LEU:O	2.75	0.40	
1:F:157:ASN:HB2	1:F:435:ARG:HH21	1.85	0.40	
1:F:200:SER:N	1:F:322:ARG:O	2.53	0.40	
1:G:34:LEU:HD22	1:G:34:LEU:HA	1.75	0.40	
1:G:271:ILE:HG23	1:G:275:THR:HB	2.03	0.40	
1:G:282:THR:HB	1:G:309:GLU:HB3	2.04	0.40	
1:G:380:SER:HB3	1:G:399:TRP:CE2	2.57	0.40	
1:H:271:ILE:HB	1:H:448:ILE:HG12	2.02	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	Percen	tiles
1	А	447/493~(91%)	415~(93%)	32~(7%)	0	100	100
1	В	455/493~(92%)	425~(93%)	30~(7%)	0	100	100
1	С	341/493~(69%)	310~(91%)	31 (9%)	0	100	100
1	D	357/493~(72%)	327~(92%)	30 (8%)	0	100	100
1	Е	440/493~(89%)	396~(90%)	44 (10%)	0	100	100
1	F	478/493~(97%)	440 (92%)	38~(8%)	0	100	100
1	G	459/493~(93%)	421 (92%)	38~(8%)	0	100	100
1	Н	470/493~(95%)	431 (92%)	39(8%)	0	100	100
All	All	3447/3944~(87%)	3165~(92%)	282 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	330/417~(79%)	263 (80%)	67 (20%)	1 3
1	В	366/417~(88%)	289 (79%)	77 (21%)	1 3
1	С	280/417~(67%)	238~(85%)	42 (15%)	3 8
1	D	278/417~(67%)	241 (87%)	37~(13%)	4 11
1	Ε	336/417~(81%)	264 (79%)	72 (21%)	1 2
1	F	370/417~(89%)	307~(83%)	63~(17%)	2 5

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	361/417~(87%)	288~(80%)	73~(20%)	1 3
1	Н	348/417~(84%)	309~(89%)	39~(11%)	6 16
All	All	2669/3336~(80%)	2199 (82%)	470 (18%)	2 5

All (470) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	14	THR
1	А	17	LEU
1	А	18	SER
1	А	25	SER
1	А	27	TYR
1	А	30	ASP
1	А	38	ASP
1	А	39	LEU
1	А	80	LEU
1	А	91	THR
1	А	94	THR
1	А	99	ILE
1	А	103	CYS
1	А	106	VAL
1	А	116	THR
1	А	117	SER
1	А	128	LEU
1	А	133	LEU
1	А	140	LEU
1	А	143	GLU
1	А	146	LEU
1	А	148	GLN
1	А	150	LEU
1	А	154	ASP
1	А	168	GLN
1	А	169	VAL
1	А	171	ARG
1	А	174	HIS
1	А	189	PHE
1	А	193	LEU
1	А	204	ASP
1	A	212	GLU
1	А	224	ASP
1	А	226	SER

Mol	Chain	Res	Type
1	А	228	SER
1	А	232	MET
1	А	236	HIS
1	А	237	ILE
1	А	277	ILE
1	А	278	THR
1	А	282	THR
1	А	285	TYR
1	А	289	VAL
1	А	302	LEU
1	А	321	TRP
1	А	330	ILE
1	А	346	GLN
1	А	354	ILE
1	A	357	SER
1	А	366	LYS
1	А	371	LEU
1	А	380	SER
1	А	382	MET
1	А	383	VAL
1	А	401	ASP
1	А	403	SER
1	А	412	LYS
1	А	419	ARG
1	А	421	MET
1	А	428	ASP
1	А	434	ARG
1	А	435	ARG
1	A	436	ASP
1	А	450	GLU
1	А	452	TRP
1	A	485	ASP
1	А	486	LEU
1	В	8	MET
1	В	10	LEU
1	В	13	SER
1	В	14	THR
1	В	16	ASP
1	В	17	LEU
1	В	18	SER
1	В	21	MET
1	В	23	LEU

Mol	Chain	Res	Type
1	В	27	TYR
1	В	30	ASP
1	В	37	ASP
1	В	38	ASP
1	В	39	LEU
1	В	43	CYS
1	В	44	THR
1	В	45	SER
1	В	46	ARG
1	В	50	ASP
1	В	52	ASP
1	В	60	LYS
1	В	80	LEU
1	В	81	ASN
1	В	88	VAL
1	В	101	ASP
1	В	102	LEU
1	В	114	LEU
1	В	116	THR
1	В	119	SER
1	В	122	GLU
1	В	128	LEU
1	В	148	GLN
1	В	149	ASP
1	В	150	LEU
1	В	152	SER
1	В	155	HIS
1	В	160	VAL
1	В	162	LYS
1	В	163	VAL
1	В	183	ASN
1	В	199	ASN
1	В	201	LYS
1	В	213	THR
1	В	220	ILE
1	В	225	SER
1	В	226	SER
1	В	228	SER
1	В	231	ASP
1	В	236	HIS
1	В	237	ILE
1	В	251	HIS

Mol	Chain	Res	Type
1	В	255	ASN
1	В	262	VAL
1	В	266	ARG
1	В	290	SER
1	В	307	ASP
1	В	320	ASN
1	В	322	ARG
1	В	331	ARG
1	В	354	ILE
1	В	356	SER
1	В	366	LYS
1	В	370	VAL
1	В	378	GLN
1	В	388	LEU
1	В	401	ASP
1	В	405	THR
1	В	410	ASP
1	В	411	ARG
1	В	413	ARG
1	В	414	ARG
1	В	422	LEU
1	В	428	ASP
1	В	436	ASP
1	В	452	TRP
1	В	464	SER
1	В	478	ARG
1	С	142	LEU
1	С	144	LYS
1	С	146	LEU
1	С	153	SER
1	С	154	ASP
1	С	155	HIS
1	С	163	VAL
1	С	174	HIS
1	С	176	LEU
1	С	199	ASN
1	С	220	ILE
1	С	235	SER
1	С	274	ASP
1	С	277	ILE
1	С	278	THR
1	С	280	THR

Mol	Chain	Res	Type
1	С	282	THR
1	С	307	ASP
1	С	309	GLU
1	С	331	ARG
1	С	334	LYS
1	С	335	ARG
1	С	353	SER
1	С	354	ILE
1	С	355	PHE
1	С	357	SER
1	С	358	SER
1	С	366	LYS
1	C	368	ARG
1	С	371	LEU
1	С	380	SER
1	С	401	ASP
1	С	413	ARG
1	С	414	ARG
1	С	415	ILE
1	С	423	ASP
1	С	424	LEU
1	С	426	GLU
1	С	436	ASP
1	С	452	TRP
1	С	461	THR
1	С	478	ARG
1	D	140	LEU
1	D	142	LEU
1	D	143	GLU
1	D	146	LEU
1	D	148	GLN
1	D	149	ASP
1	D	150	LEU
1	D	153	SER
1	D	154	ASP
1	D	156	ILE
1	D	161	LEU
1	D	162	LYS
1	D	183	ASN
1	D	199	ASN
1	D	203	ILE
1	D	228	SER

Mol	Chain	Res	Type
1	D	231	ASP
1	D	285	TYR
1	D	309	GLU
1	D	350	VAL
1	D	354	ILE
1	D	355	PHE
1	D	368	ARG
1	D	374	ASP
1	D	378	GLN
1	D	388	LEU
1	D	389	ASP
1	D	405	THR
1	D	425	ILE
1	D	428	ASP
1	D	435	ARG
1	D	463	VAL
1	D	471	THR
1	D	483	TRP
1	D	485	ASP
1	D	490	HIS
1	D	491	HIS
1	Е	16	ASP
1	Е	17	LEU
1	Е	22	LEU
1	Е	23	LEU
1	Е	25	SER
1	Е	26	LEU
1	Е	38	ASP
1	Е	43	CYS
1	Ε	80	LEU
1	E	81	ASN
1	E	83	LEU
1	E	87	THR
1	E	88	VAL
1	E	94	THR
1	Е	96	PHE
1	E	99	ILE
1	Е	101	ASP
1	Е	103	CYS
1	E	107	GLU
1	Е	112	ILE
1	Е	120	LEU

Mol	Chain	Res	Type
1	Е	121	PHE
1	Е	125	ILE
1	Е	128	LEU
1	Е	143	GLU
1	Е	171	ARG
1	Е	174	HIS
1	Е	184	LEU
1	Е	185	LEU
1	Е	187	LEU
1	Е	193	LEU
1	Е	197	LEU
1	Е	200	SER
1	Е	209	SER
1	Е	213	THR
1	Е	220	ILE
1	E	224	ASP
1	Е	228	SER
1	Е	253	GLU
1	Е	259	ASP
1	Ε	262	VAL
1	Е	273	ASN
1	Е	274	ASP
1	Ε	279	HIS
1	Е	299	ILE
1	Ε	302	LEU
1	Е	309	GLU
1	Е	320	ASN
1	Ε	334	LYS
1	E	355	PHE
1	E	356	SER
1	E	358	SER
1	E	363	GLN
1	E	366	LYS
1	E	374	ASP
1	Е	376	THR
1	E	377	ILE
1	E	379	ILE
1	Е	380	SER
1	E	385	GLU
1	E	389	ASP
1	E	397	GLU
1	Е	403	SER

Mol	Chain	Res	Type
1	Е	405	THR
1	Е	411	ARG
1	Е	415	ILE
1	Е	417	TYR
1	Е	435	ARG
1	Е	452	TRP
1	Е	460	LYS
1	Е	466	THR
1	Е	485	ASP
1	F	10	LEU
1	F	14	THR
1	F	16	ASP
1	F	17	LEU
1	F	23	LEU
1	F	25	SER
1	F	26	LEU
1	F	54	PHE
1	F	57	PHE
1	F	59	GLU
1	F	60	LYS
1	F	62	LEU
1	F	63	ASP
1	F	64	ARG
1	F	69	ASP
1	F	70	ARG
1	F	83	LEU
1	F	87	THR
1	F	103	CYS
1	F	106	VAL
1	F	115	SER
1	F	116	THR
1	F	121	PHE
1	F	130	GLN
1	F	133	LEU
1	F	137	THR
1	F	143	GLU
1	F	146	LEU
1	F	154	ASP
1	F	161	LEU
1	F	178	LYS
1	F	183	ASN
1	F	198	TRP

Mol	Chain	Res	Type
1	F	200	SER
1	F	201	LYS
1	F	213	THR
1	F	214	VAL
1	F	226	SER
1	F	231	ASP
1	F	278	THR
1	F	282	THR
1	F	332	THR
1	F	342	GLU
1	F	355	PHE
1	F	356	SER
1	F	358	SER
1	F	389	ASP
1	F	400	LEU
1	F	407	VAL
1	F	410	ASP
1	F	414	ARG
1	F	415	ILE
1	F	418	GLU
1	F	420	LEU
1	F	436	ASP
1	F	449	ARG
1	F	452	TRP
1	F	467	TRP
1	F	470	ILE
1	F	482	THR
1	F	485	ASP
1	F	486	LEU
1	F	487	GLU
1	G	5	VAL
1	G	11	PHE
1	G	13	SER
1	G	20	ARG
1	G	21	MET
1	G	23	LEU
1	G	34	LEU
1	G	35	LEU
1	G	52	ASP
1	G	57	PHE
1	G	60	LYS
1	G	76	LYS

Mol	Chain	Res	Type
1	G	90	ILE
1	G	99	ILE
1	G	102	LEU
1	G	106	VAL
1	G	112	ILE
1	G	116	THR
1	G	117	SER
1	G	119	SER
1	G	122	GLU
1	G	125	ILE
1	G	128	LEU
1	G	130	GLN
1	G	142	LEU
1	G	144	LYS
1	G	150	LEU
1	G	154	ASP
1	G	162	LYS
1	G	171	ARG
1	G	174	HIS
1	G	200	SER
1	G	207	GLN
1	G	214	VAL
1	G	216	LEU
1	G	220	ILE
1	G	226	SER
1	G	228	SER
1	G	232	MET
1	G	262	VAL
1	G	280	THR
1	G	290	SER
1	G	299	ILE
1	G	307	ASP
1	G	308	THR
1	G	309	GLU
1	G	330	ILE
1	G	340	ARG
1	G	355	PHE
1	G	356	SER
1	G	357	SER
1	G	358	SER
1	G	365	ASN
1	G	388	LEU

Mol	Chain	Res	Type
1	G	401	ASP
1	G	403	SER
1	G	405	THR
1	G	410	ASP
1	G	415	ILE
1	G	419	ARG
1	G	421	MET
1	G	423	ASP
1	G	430	THR
1	G	452	TRP
1	G	466	THR
1	G	467	TRP
1	G	470	ILE
1	G	471	THR
1	G	473	ILE
1	G	476	VAL
1	G	485	ASP
1	G	486	LEU
1	G	487	GLU
1	Н	17	LEU
1	Н	18	SER
1	Н	25	SER
1	Н	37	ASP
1	Н	45	SER
1	Н	46	ARG
1	Н	50	ASP
1	Н	91	THR
1	Н	92	ASP
1	Н	99	ILE
1	Н	114	LEU
1	Н	137	THR
1	Н	142	LEU
1	Н	143	GLU
1	Н	148	GLN
1	Н	149	ASP
1	Н	153	SER
1	Н	168	GLN
1	Н	171	ARG
1	Н	174	HIS
1	Н	183	ASN
1	Н	214	VAL
1	Н	220	ILE

\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	Н	224	ASP
1	Н	225	SER
1	Н	273	ASN
1	Н	276	VAL
1	Н	285	TYR
1	Н	290	SER
1	Н	341	SER
1	Н	343	ILE
1	Н	358	SER
1	Н	366	LYS
1	Н	374	ASP
1	Н	383	VAL
1	Н	400	LEU
1	Н	452	TRP
1	Н	478	ARG
1	Н	482	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	81	ASN
1	А	236	HIS
1	В	81	ASN
1	В	183	ASN
1	В	284	GLN
1	С	148	GLN
1	С	174	HIS
1	С	236	HIS
1	С	346	GLN
1	С	455	ASN
1	D	234	GLN
1	D	284	GLN
1	D	394	HIS
1	D	441	GLN
1	D	488	HIS
1	D	490	HIS
1	Е	148	GLN
1	Е	157	ASN
1	Е	234	GLN
1	Е	304	GLN
1	Е	394	HIS
1	Е	441	GLN

Mol	Chain	Res	Type
1	F	234	GLN
1	F	239	GLN
1	F	273	ASN
1	F	317	HIS
1	G	130	GLN
1	G	205	HIS
1	G	207	GLN
1	G	284	GLN
1	G	352	HIS
1	G	365	ASN
1	G	378	GLN
1	Н	191	ASN
1	Н	234	GLN
1	Н	365	ASN
1	Н	441	GLN
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)

There are no ligands in this entry.

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	451/493~(91%)	0.10	9 (1%) 65 61	34, 51, 95, 109	0
1	В	461/493~(93%)	0.02	8 (1%) 70 67	31, 48, 88, 114	0
1	С	345/493~(69%)	0.15	12 (3%) 44 38	37, 58, 73, 85	0
1	D	361/493~(73%)	0.06	7 (1%) 66 63	40, 58, 72, 83	0
1	Ε	446/493~(90%)	0.09	10 (2%) 62 57	36, 61, 83, 94	0
1	F	480/493~(97%)	0.13	12 (2%) 57 52	33, 59, 82, 98	0
1	G	465/493~(94%)	0.07	10 (2%) 62 57	32, 48, 85, 105	0
1	Н	474/493~(96%)	-0.08	1 (0%) 95 95	30, 47, 65, 79	0
All	All	3483/3944 (88%)	0.06	69 (1%) 65 61	30, 54, 83, 114	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	214	VAL	6.9
1	А	10	LEU	5.3
1	Е	142	LEU	4.6
1	D	215	GLY	4.6
1	В	35	LEU	4.5
1	В	34	LEU	4.4
1	С	289	VAL	4.1
1	F	10	LEU	3.9
1	Е	213	THR	3.8
1	D	308	THR	3.7
1	F	392	GLY	3.6
1	D	226	SER	3.6
1	А	96	PHE	3.6
1	Е	223	PHE	3.5
1	G	110	ILE	3.5
1	В	99	ILE	3.5

Mol	Chain	Res	Type	RSRZ
1	В	102	LEU	3.3
1	С	302	LEU	3.3
1	G	43	CYS	3.2
1	В	96	PHE	3.2
1	С	409	LYS	3.1
1	В	113	TYR	3.0
1	Е	454	ALA	3.0
1	С	222	TYR	3.0
1	А	83	LEU	3.0
1	С	227	GLY	3.0
1	F	85	TYR	2.9
1	F	62	LEU	2.8
1	G	85	TYR	2.8
1	F	420	LEU	2.8
1	D	223	PHE	2.7
1	F	112	ILE	2.7
1	Е	388	LEU	2.7
1	А	90	ILE	2.7
1	Е	215	GLY	2.6
1	А	102	LEU	2.6
1	Е	46	ARG	2.6
1	G	160	VAL	2.5
1	С	360	GLY	2.5
1	Н	103	CYS	2.5
1	F	286	GLY	2.5
1	В	281	VAL	2.5
1	Е	291	GLY	2.5
1	F	141	ALA	2.4
1	А	134	ALA	2.3
1	F	96	PHE	2.3
1	А	110	ILE	2.3
1	А	169	VAL	2.3
1	С	286	GLY	2.2
1	С	214	VAL	2.2
1	F	417	TYR	2.2
1	G	10	LEU	2.2
1	G	80	LEU	2.2
1	D	302	LEU	2.1
1	С	216	LEU	2.1
1	G	13	SER	2.1
1	G	223	PHE	2.1
1	Е	88	VAL	2.1

	U	1	10	
Mol	Chain	\mathbf{Res}	Type	RSRZ
1	F	335	ARG	2.1
1	G	11	PHE	2.1
1	D	402	LEU	2.1
1	С	332	THR	2.1
1	F	161	LEU	2.0
1	G	420	LEU	2.0
1	С	403	SER	2.0
1	D	310	THR	2.0
1	С	416	ALA	2.0
1	А	469	PRO	2.0
1	В	233	VAL	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

