



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:56 AM GMT

PDB ID : 3NL6  
Title : The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosynthesis of Eukaryotes  
Authors : Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2010-06-21  
Resolution : 2.61 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

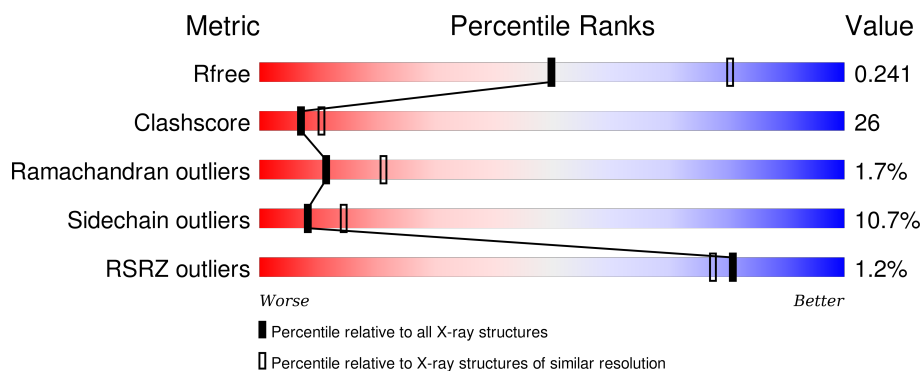
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	A	540	<div> <div></div> <div>53% 36% 6% . .</div> </div>
1	B	540	<div> <div></div> <div>55% 34% 6% 5%</div> </div>
1	C	540	<div> <div></div> <div>57% 33% 5% 5%</div> </div>

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
4	ACP	B	999	-	-	X	X
4	ACP	C	899	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

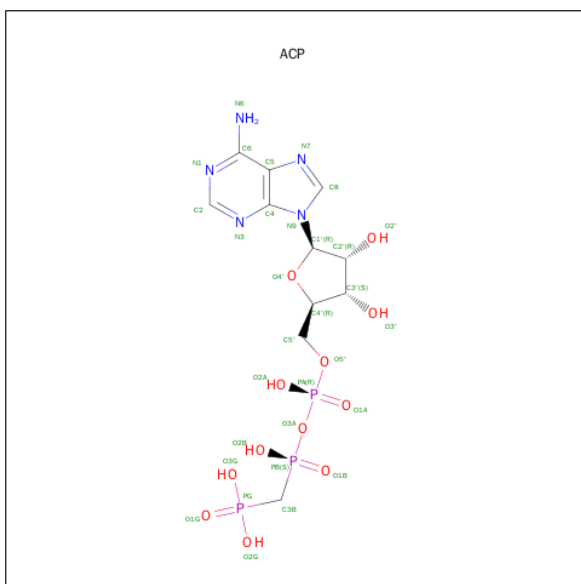
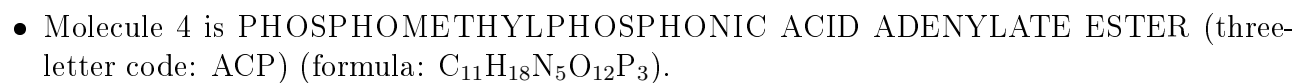
- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3862	2441	648	751	22			
1	B	514	Total	C	N	O	S	0	0	0
			3837	2426	646	743	22			
1	C	513	Total	C	N	O	S	0	0	0
			3817	2413	640	741	23			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMIN PHOSPHATE (three-letter code: TPS) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>4</sub>PS).

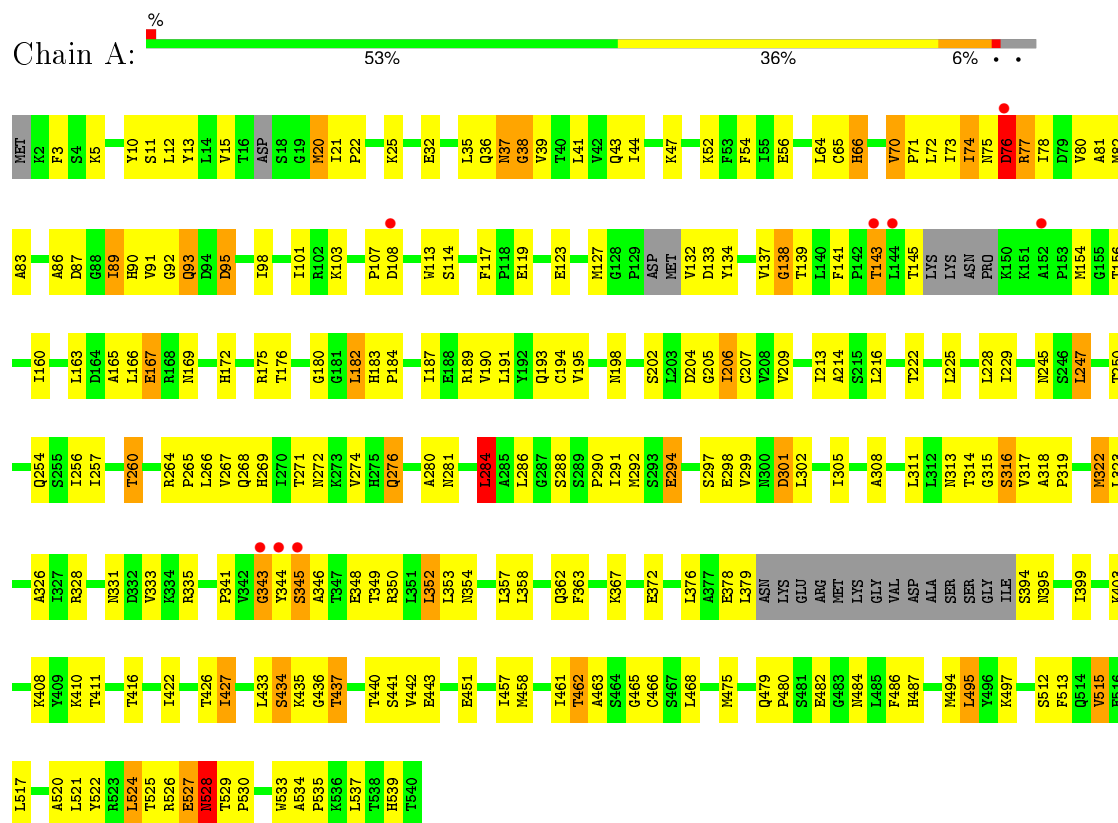


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

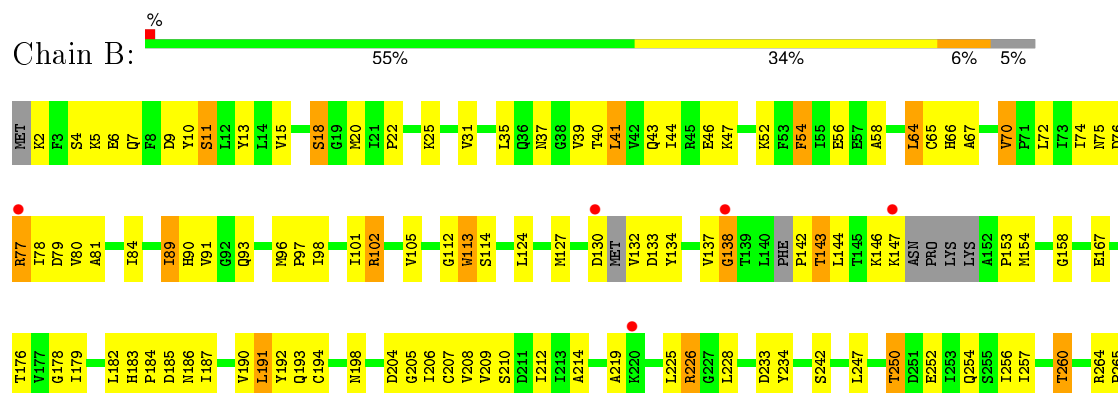
### 3 Residue-property plots

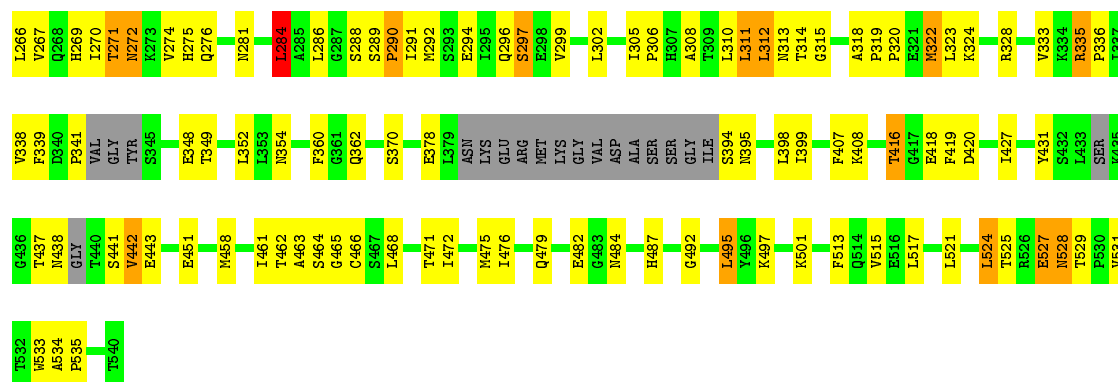
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Thiamine biosynthetic bifunctional enzyme

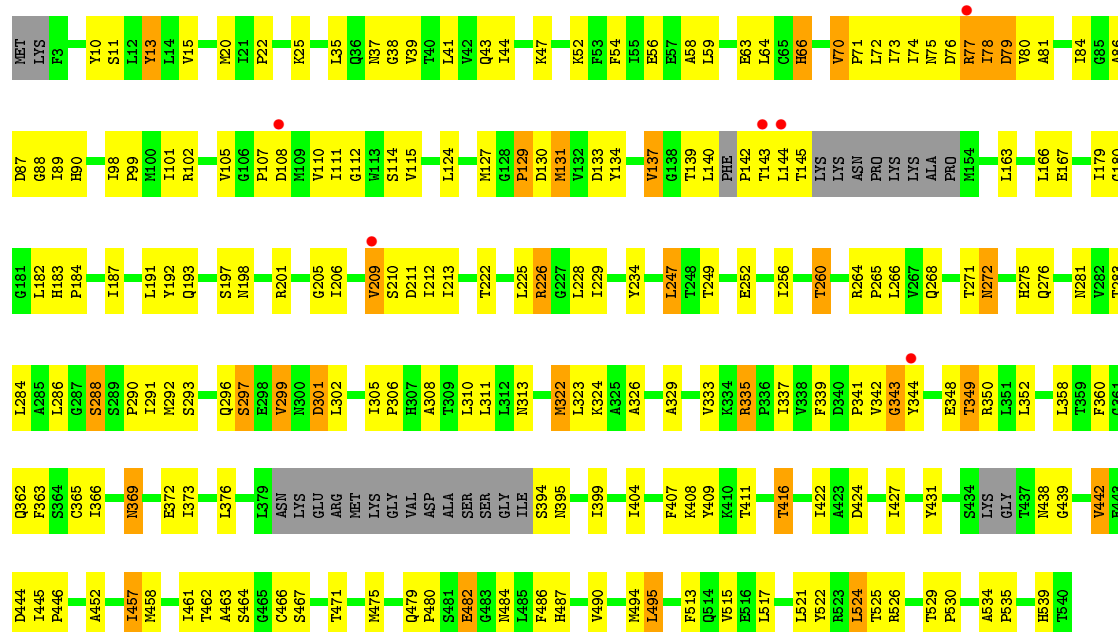


#### • Molecule 1: Thiamine biosynthetic bifunctional enzyme





• Molecule 1: Thiamine biosynthetic bifunctional enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.17Å 153.53Å 109.62Å 90.00° 117.99° 90.00°	Depositor
Resolution (Å)	39.00 – 2.61 48.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	88.4 (39.00-2.61) 88.4 (48.00-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.221 , 0.271 0.228 , 0.241	Depositor DCC
$R_{free}$ test set	3489 reflections (5.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 69154 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	1/3923 (0.0%)	0.64	5/5323 (0.1%)
1	B	0.38	0/3893	0.58	2/5275 (0.0%)
1	C	0.37	0/3876	0.58	0/5259
All	All	0.39	1/11692 (0.0%)	0.60	7/15857 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	CYS	CB-SG	-5.23	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	GLY	N-CA-C	13.99	148.08	113.10
1	A	39	VAL	N-CA-CB	-8.56	92.67	111.50
1	B	284	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	76	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	39	VAL	N-CA-C	-5.21	96.95	111.00
1	A	284	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	124	LEU	CA-CB-CG	5.01	126.82	115.30

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	A	3862	0	3853	214	0
1	B	3837	0	3852	200	0
1	C	3817	0	3806	214	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	21	0	16	2	0
3	B	22	0	16	6	0
3	C	22	0	16	8	0
4	A	31	0	14	7	0
4	B	31	0	14	10	0
4	C	31	0	14	4	0
All	All	11677	0	11601	613	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 (613) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:VAL:HB	1:C:209:VAL:CG2	1.36	1.49
1:C:15:VAL:CB	1:C:209:VAL:CG2	2.26	1.14
1:A:37:ASN:O	1:A:222:THR:HG22	1.45	1.14
1:C:15:VAL:HB	1:C:209:VAL:HG22	1.32	1.11
1:B:416:THR:OG1	4:B:999:ACP:O2A	1.65	1.09
1:C:15:VAL:O	1:C:209:VAL:HG22	1.54	1.08
1:A:76:ASP:OD1	1:A:95:ASP:OD2	1.72	1.06
1:A:265:PRO:HD2	1:A:288:SER:HB3	1.36	1.05
1:B:143:THR:OG1	3:B:2006:TPS:O1	1.74	1.05
1:A:195:VAL:HG12	1:A:202:SER:HB3	1.39	1.04
1:C:344:TYR:OH	1:C:376:LEU:HD23	1.58	1.02
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.24	1.02
1:A:341:PRO:HB2	1:A:344:TYR:CD2	1.96	1.00
1:C:15:VAL:HB	1:C:209:VAL:HG23	1.41	0.99
1:C:416:THR:HB	4:C:899:ACP:O3'	1.63	0.98
1:C:15:VAL:HB	1:C:209:VAL:HG21	1.43	0.97
1:A:74:ILE:HD13	1:A:81:ALA:HA	1.44	0.97
1:A:37:ASN:N	1:A:37:ASN:HD22	1.63	0.96
1:A:344:TYR:HB2	1:A:354:ASN:HD22	1.28	0.96
1:A:344:TYR:CB	1:A:354:ASN:ND2	2.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD23	1:A:38:GLY:O	1.62	0.95
1:C:15:VAL:CB	1:C:209:VAL:HG22	1.89	0.94
1:A:344:TYR:OH	1:A:376:LEU:HG	1.68	0.94
1:A:344:TYR:HB3	1:A:354:ASN:ND2	1.83	0.93
1:A:75:ASN:O	1:A:77:ARG:N	2.02	0.93
1:C:15:VAL:C	1:C:209:VAL:HG22	1.89	0.92
1:A:37:ASN:O	1:A:222:THR:CG2	2.17	0.92
1:B:416:THR:HB	4:B:999:ACP:H5'	1.51	0.92
1:B:497:LYS:NZ	4:B:999:ACP:O2'	2.04	0.91
1:C:78:ILE:O	1:C:81:ALA:N	2.04	0.91
1:C:15:VAL:CA	1:C:209:VAL:HG22	2.02	0.88
1:C:167:GLU:HG3	1:C:198:ASN:HD21	1.39	0.88
1:C:167:GLU:CG	1:C:198:ASN:HD21	1.88	0.87
1:B:416:THR:OG1	4:B:999:ACP:PA	2.34	0.86
1:C:339:PHE:CE2	1:C:341:PRO:HG3	2.12	0.85
1:A:299:VAL:HG11	1:A:326:ALA:HA	1.59	0.83
1:C:484:ASN:HD22	1:C:487:HIS:H	1.26	0.83
1:A:74:ILE:HD12	1:A:86:ALA:HB2	1.60	0.83
1:A:463:ALA:HB1	1:A:466:CYS:HB2	1.61	0.82
1:A:74:ILE:HD13	1:A:81:ALA:CA	2.09	0.82
1:A:484:ASN:HD22	1:A:487:HIS:H	1.24	0.81
1:A:497:LYS:NZ	4:A:799:ACP:O2'	2.12	0.81
1:A:204:ASP:OD1	1:A:434:SER:HB3	1.81	0.81
1:B:90:HIS:HD2	1:B:134:TYR:OH	1.64	0.81
1:A:266:LEU:HD11	1:A:291:ILE:HG13	1.62	0.80
1:C:15:VAL:O	1:C:209:VAL:HG13	1.81	0.80
1:B:527:GLU:O	1:B:529:THR:HG23	1.82	0.80
1:A:344:TYR:HB2	1:A:354:ASN:ND2	1.93	0.79
1:C:15:VAL:O	1:C:209:VAL:CG2	2.30	0.79
1:C:210:SER:OG	3:C:2002:TPS:O2	1.98	0.79
1:B:44:ILE:HG13	1:B:72:LEU:HD11	1.64	0.79
1:B:265:PRO:HD2	1:B:288:SER:HB3	1.65	0.78
1:A:78:ILE:HG13	1:A:89:ILE:HD12	1.65	0.78
1:A:463:ALA:HA	4:A:799:ACP:O1G	1.83	0.78
1:A:44:ILE:HG13	1:A:72:LEU:HD11	1.66	0.78
1:C:344:TYR:OH	1:C:376:LEU:CD2	2.32	0.77
1:B:484:ASN:HD22	1:B:487:HIS:H	1.30	0.77
1:C:344:TYR:CZ	1:C:376:LEU:HG	2.20	0.76
1:C:78:ILE:O	1:C:80:VAL:N	2.18	0.76
1:C:10:TYR:O	1:C:11:SER:OG	2.03	0.76
1:C:209:VAL:O	1:C:213:ILE:HB	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASN:O	1:A:539:HIS:HE1	1.69	0.75
1:C:44:ILE:HG13	1:C:72:LEU:HD11	1.69	0.75
1:A:167:GLU:HG2	1:A:198:ASN:HD21	1.52	0.75
1:C:127:MET:HB3	1:C:131:MET:HG3	1.68	0.74
1:C:35:LEU:HD22	1:C:70:VAL:HG11	1.68	0.74
1:C:143:THR:OG1	3:C:2002:TPS:O1	2.04	0.74
1:B:190:VAL:O	1:B:194:CYS:HB2	1.87	0.74
1:A:256:ILE:HG22	1:A:475:MET:HE3	1.69	0.73
1:B:167:GLU:CG	1:B:198:ASN:HD21	2.01	0.73
1:C:66:HIS:HE1	1:C:87:ASP:OD1	1.71	0.73
1:B:462:THR:H	1:C:281:ASN:HD21	1.36	0.73
1:B:308:ALA:O	1:B:335:ARG:HD3	1.88	0.73
1:A:465:GLY:H	4:A:799:ACP:H3B2	1.52	0.73
1:A:410:LYS:HE3	1:A:427:ILE:HD11	1.71	0.73
1:A:167:GLU:CG	1:A:198:ASN:HD21	2.01	0.72
1:C:129:PRO:O	1:C:131:MET:N	2.22	0.72
1:A:187:ILE:HG23	1:A:206:ILE:HD13	1.71	0.72
1:A:143:THR:OG1	3:A:2001:TPS:O1	2.07	0.72
1:A:76:ASP:O	1:A:77:ARG:CG	2.38	0.71
1:B:254:GLN:HG3	1:B:528:ASN:HD21	1.56	0.71
1:C:11:SER:H	1:C:205:GLY:HA3	1.55	0.71
1:B:90:HIS:HE1	1:B:114:SER:OG	1.74	0.70
1:B:77:ARG:CG	1:B:77:ARG:HH11	1.99	0.70
1:C:299:VAL:HG11	1:C:326:ALA:HA	1.73	0.70
1:A:74:ILE:CD1	1:A:81:ALA:HA	2.20	0.70
1:C:344:TYR:HB2	1:C:372:GLU:HG2	1.74	0.70
1:B:35:LEU:HA	1:B:39:VAL:HG12	1.73	0.69
1:B:58:ALA:HB1	1:B:84:ILE:HD13	1.73	0.69
1:B:416:THR:CB	4:B:999:ACP:H5'2	2.20	0.69
1:A:308:ALA:O	1:A:335:ARG:HD3	1.92	0.69
1:C:463:ALA:HA	4:C:899:ACP:O2G	1.93	0.69
1:A:416:THR:OG1	4:A:799:ACP:O2A	2.11	0.69
1:B:270:ILE:HD12	1:B:310:LEU:HD11	1.75	0.68
1:A:176:THR:O	1:A:204:ASP:HB2	1.92	0.68
1:A:74:ILE:HD12	1:A:86:ALA:CB	2.23	0.68
1:B:427:ILE:HG22	1:B:427:ILE:O	1.93	0.68
1:B:176:THR:O	1:B:204:ASP:HB2	1.93	0.68
1:A:280:ALA:O	1:A:284:LEU:HD22	1.93	0.68
1:A:37:ASN:ND2	1:A:37:ASN:N	2.33	0.67
1:C:308:ALA:O	1:C:335:ARG:HD3	1.94	0.67
1:C:422:ILE:HG22	1:C:486:PHE:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD23	1:B:39:VAL:HG13	1.76	0.66
1:B:18:SER:HB2	1:B:46:GLU:OE2	1.96	0.66
1:B:252:GLU:O	1:B:256:ILE:HG12	1.95	0.66
1:B:305:ILE:HG23	1:B:306:PRO:HD2	1.76	0.66
1:B:167:GLU:HG3	1:B:198:ASN:HD21	1.59	0.66
1:C:78:ILE:O	1:C:79:ASP:C	2.34	0.66
1:C:252:GLU:O	1:C:256:ILE:HG12	1.95	0.66
1:A:74:ILE:CG2	1:A:75:ASN:N	2.58	0.66
1:C:484:ASN:ND2	1:C:487:HIS:H	1.92	0.66
1:B:407:PHE:HE2	1:B:427:ILE:HD11	1.59	0.66
1:B:65:CYS:HB3	1:B:70:VAL:O	1.95	0.66
1:A:266:LEU:CD1	1:A:291:ILE:HG13	2.25	0.66
1:A:264:ARG:HG2	1:A:264:ARG:O	1.94	0.66
1:B:77:ARG:NH1	1:B:77:ARG:HG3	2.03	0.66
1:C:265:PRO:HD2	1:C:288:SER:HB3	1.78	0.65
1:A:76:ASP:O	1:A:77:ARG:HG3	1.96	0.65
1:A:344:TYR:CZ	1:A:376:LEU:HG	2.31	0.65
1:A:183:HIS:HB3	1:A:184:PRO:HD2	1.78	0.65
1:B:286:LEU:HD11	1:B:471:THR:HG23	1.77	0.65
1:C:342:VAL:O	1:C:344:TYR:N	2.30	0.65
1:C:35:LEU:CD2	1:C:70:VAL:HG11	2.26	0.65
1:A:15:VAL:HB	1:A:209:VAL:HG22	1.78	0.65
1:A:344:TYR:OH	1:A:372:GLU:O	2.11	0.65
1:B:521:LEU:O	1:B:525:THR:HG23	1.97	0.65
1:C:342:VAL:HG12	1:C:343:GLY:N	2.12	0.65
1:C:272:ASN:H	1:C:272:ASN:ND2	1.94	0.65
1:C:76:ASP:O	1:C:77:ARG:C	2.36	0.64
1:A:462:THR:H	1:B:281:ASN:HD21	1.45	0.64
1:B:78:ILE:HD11	1:B:101:ILE:HG12	1.80	0.64
1:B:146:LYS:O	1:B:147:LYS:HB2	1.97	0.64
1:A:298:GLU:OE1	1:C:350:ARG:HD2	1.98	0.64
1:A:341:PRO:O	1:A:344:TYR:HD2	1.81	0.64
1:B:266:LEU:HD11	1:B:291:ILE:CG1	2.28	0.64
1:A:145:THR:HB	3:A:2001:TPS:H72	1.79	0.64
1:C:283:THR:HG21	1:C:290:PRO:HB3	1.79	0.64
1:C:290:PRO:HB2	1:C:292:MET:HE1	1.80	0.63
1:C:286:LEU:HD11	1:C:471:THR:HG23	1.80	0.63
1:B:458:MET:HG2	1:B:513:PHE:HZ	1.63	0.63
1:C:268:GLN:OE1	1:C:302:LEU:HD23	1.99	0.62
1:B:254:GLN:HG3	1:B:528:ASN:ND2	2.14	0.62
1:B:78:ILE:CD1	1:B:101:ILE:HG12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ALA:HB1	1:C:466:CYS:HB2	1.81	0.62
1:A:77:ARG:HE	1:A:80:VAL:HG23	1.64	0.62
1:C:310:LEU:HB3	1:C:337:ILE:HG23	1.81	0.62
1:C:424:ASP:HB3	1:C:446:PRO:HG2	1.81	0.62
1:B:407:PHE:CE2	1:B:427:ILE:HD11	2.34	0.62
1:C:74:ILE:HD12	1:C:86:ALA:HB2	1.82	0.62
1:C:416:THR:OG1	4:C:899:ACP:O1A	2.17	0.62
1:C:167:GLU:HG2	1:C:198:ASN:HD21	1.65	0.62
1:C:193:GLN:NE2	1:C:362:GLN:HE22	1.97	0.61
1:B:266:LEU:HD11	1:B:291:ILE:HG13	1.82	0.61
1:A:257:ILE:HD11	1:A:533:TRP:HH2	1.65	0.61
1:C:90:HIS:HD2	1:C:134:TYR:OH	1.82	0.61
1:A:494:MET:HE3	1:A:535:PRO:HG2	1.81	0.61
1:B:534:ALA:N	1:B:535:PRO:HD2	2.16	0.61
1:B:22:PRO:HG2	1:B:25:LYS:HD3	1.82	0.61
1:B:471:THR:O	1:B:475:MET:HG2	2.01	0.61
1:A:484:ASN:ND2	1:A:487:HIS:H	1.98	0.60
1:C:534:ALA:N	1:C:535:PRO:HD2	2.15	0.60
1:C:101:ILE:O	1:C:105:VAL:HG22	2.01	0.60
1:B:418:GLU:HG2	1:B:419:PHE:CE1	2.35	0.60
1:A:143:THR:HG23	1:A:145:THR:H	1.66	0.60
1:C:110:VAL:HA	1:C:133:ASP:OD2	2.02	0.60
1:C:74:ILE:HD11	1:C:84:ILE:HD11	1.83	0.60
1:C:301:ASP:N	1:C:301:ASP:OD2	2.28	0.60
1:A:367:LYS:HE2	1:A:465:GLY:O	2.00	0.60
1:A:20:MET:HE1	1:A:213:ILE:HB	1.85	0.59
1:B:137:VAL:O	1:B:138:GLY:O	2.20	0.59
1:B:77:ARG:HB3	1:B:80:VAL:HB	1.83	0.59
1:C:90:HIS:HE1	1:C:114:SER:OG	1.83	0.59
1:A:267:VAL:HG12	1:A:269:HIS:CE1	2.37	0.59
1:C:107:PRO:O	1:C:108:ASP:HB2	2.03	0.59
1:C:344:TYR:CZ	1:C:376:LEU:CD2	2.86	0.59
1:C:89:ILE:HD11	1:C:101:ILE:HG21	1.84	0.59
1:A:297:SER:OG	1:C:349:THR:HG21	2.03	0.59
1:C:290:PRO:HB2	1:C:292:MET:CE	2.33	0.59
1:C:15:VAL:O	1:C:209:VAL:CG1	2.49	0.58
1:B:495:LEU:HD22	1:B:521:LEU:HD23	1.83	0.58
1:A:75:ASN:O	1:A:76:ASP:C	2.40	0.58
1:C:342:VAL:O	1:C:343:GLY:C	2.41	0.58
1:C:395:ASN:O	1:C:399:ILE:HG13	2.03	0.58
1:B:484:ASN:ND2	1:B:487:HIS:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:CE1	1:A:71:PRO:HD3	2.38	0.58
1:A:495:LEU:HD22	1:A:521:LEU:HD23	1.86	0.58
1:A:437:THR:CG2	1:A:440:THR:H	2.16	0.58
1:A:281:ASN:HD21	1:C:462:THR:H	1.52	0.58
1:B:281:ASN:HA	1:B:284:LEU:HD23	1.86	0.58
1:A:65:CYS:HB3	1:A:70:VAL:O	2.03	0.58
1:B:468:LEU:O	1:B:468:LEU:HD12	2.04	0.58
1:B:77:ARG:NH1	1:B:79:ASP:OD1	2.36	0.58
1:B:74:ILE:HD12	1:B:81:ALA:HA	1.85	0.58
1:C:124:LEU:HD23	1:C:124:LEU:C	2.24	0.58
1:C:422:ILE:HG22	1:C:486:PHE:CE1	2.39	0.58
1:C:305:ILE:HG23	1:C:306:PRO:HD2	1.86	0.58
1:A:349:THR:HG21	1:B:297:SER:HB2	1.84	0.58
1:B:78:ILE:HD13	1:B:101:ILE:HG23	1.86	0.58
1:C:52:LYS:O	1:C:56:GLU:HG3	2.04	0.58
1:A:89:ILE:HD11	1:A:101:ILE:HG21	1.86	0.58
1:A:521:LEU:O	1:A:525:THR:HG23	2.04	0.58
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.61	0.57
1:C:11:SER:O	1:C:229:ILE:HD13	2.04	0.57
1:A:89:ILE:HD11	1:A:101:ILE:CG2	2.34	0.57
1:B:322:MET:HG3	1:B:323:LEU:N	2.18	0.57
1:C:452:ALA:HB2	1:C:535:PRO:HA	1.86	0.57
1:B:322:MET:HE2	1:B:322:MET:O	2.04	0.57
1:C:344:TYR:CB	1:C:372:GLU:HG2	2.35	0.57
1:B:312:LEU:HD21	1:B:323:LEU:HD22	1.86	0.57
1:A:52:LYS:O	1:A:56:GLU:HG3	2.04	0.57
1:A:358:LEU:HD23	1:A:363:PHE:HE1	1.68	0.57
1:B:416:THR:HB	4:B:999:ACP:C5'	2.31	0.57
1:B:77:ARG:HG2	1:B:80:VAL:HG23	1.86	0.57
1:A:256:ILE:HG22	1:A:475:MET:CE	2.35	0.57
1:B:89:ILE:HD11	1:B:101:ILE:HG21	1.87	0.57
1:C:272:ASN:N	1:C:272:ASN:ND2	2.50	0.57
1:B:333:VAL:O	1:B:333:VAL:HG12	2.05	0.57
1:A:74:ILE:HG23	1:A:75:ASN:N	2.20	0.57
1:A:394:SER:OG	1:A:395:ASN:N	2.37	0.57
1:A:172:HIS:O	1:A:175:ARG:NH2	2.38	0.57
1:C:495:LEU:HD22	1:C:521:LEU:HD23	1.87	0.56
1:A:344:TYR:CD1	1:A:345:SER:N	2.73	0.56
1:A:422:ILE:HG22	1:A:486:PHE:HE1	1.69	0.56
1:A:462:THR:H	1:B:281:ASN:ND2	2.04	0.56
1:B:11:SER:HB3	1:B:226:ARG:NH2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:VAL:O	1:C:209:VAL:CB	2.54	0.56
1:C:76:ASP:O	1:C:78:ILE:N	2.39	0.56
1:B:101:ILE:O	1:B:105:VAL:HG22	2.06	0.56
1:C:322:MET:HG3	1:C:323:LEU:N	2.20	0.56
1:B:458:MET:HG2	1:B:513:PHE:CZ	2.40	0.55
1:C:183:HIS:HB3	1:C:184:PRO:HD2	1.88	0.55
1:A:190:VAL:O	1:A:194:CYS:HB2	2.06	0.55
1:A:341:PRO:HB2	1:A:344:TYR:HD2	1.66	0.55
1:C:90:HIS:NE2	3:C:2002:TPS:C2A	2.69	0.55
1:B:96:MET:HG2	1:B:97:PRO:HD2	1.88	0.55
1:C:35:LEU:HD23	1:C:39:VAL:HG12	1.86	0.55
1:A:76:ASP:OD1	1:A:95:ASP:CG	2.43	0.55
1:B:90:HIS:CD2	1:B:134:TYR:OH	2.54	0.54
1:C:37:ASN:O	1:C:222:THR:HG22	2.07	0.54
1:C:209:VAL:O	1:C:213:ILE:CB	2.55	0.54
1:B:302:LEU:HA	1:B:305:ILE:HD12	1.88	0.54
1:A:119:GLU:CD	1:A:119:GLU:H	2.10	0.54
1:B:13:TYR:CE1	1:B:41:LEU:HD13	2.42	0.54
1:C:15:VAL:CB	1:C:209:VAL:HG21	2.20	0.54
1:C:143:THR:HG23	1:C:145:THR:H	1.72	0.54
1:B:210:SER:CB	3:B:2006:TPS:O2	2.56	0.54
1:C:416:THR:HB	4:C:899:ACP:C3'	2.37	0.54
1:B:462:THR:HG22	1:C:281:ASN:HD21	1.73	0.54
1:A:344:TYR:OH	1:A:376:LEU:CG	2.51	0.54
1:B:142:PRO:HB3	1:B:153:PRO:HG2	1.90	0.54
1:C:458:MET:HG2	1:C:513:PHE:HZ	1.73	0.53
1:B:4:SER:OG	1:B:7:GLN:HG3	2.08	0.53
1:C:124:LEU:HA	1:C:127:MET:HE2	1.90	0.53
1:A:395:ASN:O	1:A:399:ILE:HG13	2.08	0.53
1:A:160:ILE:HD11	1:A:193:GLN:O	2.09	0.53
1:A:276:GLN:HE22	1:A:292:MET:HB3	1.72	0.53
1:B:311:LEU:HD23	1:B:338:VAL:HB	1.91	0.53
1:B:15:VAL:HG22	1:B:43:GLN:HB3	1.89	0.53
1:A:66:HIS:HE1	1:A:87:ASP:OD1	1.91	0.53
1:B:35:LEU:HD23	1:B:39:VAL:CG1	2.38	0.53
1:A:322:MET:HG3	1:A:323:LEU:N	2.22	0.53
1:A:265:PRO:O	1:A:288:SER:HB2	2.09	0.53
1:A:344:TYR:HB3	1:A:354:ASN:HD21	1.66	0.53
1:B:52:LYS:O	1:B:56:GLU:HG3	2.08	0.53
1:B:11:SER:CB	1:B:226:ARG:HH22	2.22	0.53
1:A:189:ARG:O	1:A:193:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:TYR:CD1	1:C:234:TYR:HD2	2.26	0.53
1:C:343:GLY:O	1:C:350:ARG:HD3	2.09	0.52
1:A:358:LEU:HD23	1:A:363:PHE:CE1	2.44	0.52
1:A:5:LYS:HE3	1:A:133:ASP:OD2	2.09	0.52
1:A:141:PHE:HE2	1:A:190:VAL:CG2	2.22	0.52
1:B:264:ARG:HG2	1:B:264:ARG:O	2.09	0.52
1:C:407:PHE:CD1	1:C:442:VAL:HG23	2.44	0.52
1:A:274:VAL:CG1	1:B:292:MET:HG3	2.39	0.52
1:C:344:TYR:CZ	1:C:376:LEU:CG	2.90	0.52
1:C:112:GLY:HA3	1:C:134:TYR:CZ	2.44	0.52
1:B:154:MET:HB2	1:B:158:GLY:HA3	1.91	0.52
1:B:22:PRO:CG	1:B:25:LYS:HD3	2.40	0.51
1:B:394:SER:OG	1:B:395:ASN:N	2.43	0.51
1:A:137:VAL:O	1:A:138:GLY:O	2.27	0.51
1:B:275:HIS:CG	1:B:275:HIS:O	2.63	0.51
1:A:341:PRO:HB2	1:A:344:TYR:CE2	2.45	0.51
1:B:191:LEU:HD13	1:B:206:ILE:HD11	1.93	0.51
1:B:90:HIS:NE2	3:B:2006:TPS:HM22	2.26	0.51
1:B:77:ARG:HG2	1:B:80:VAL:CG2	2.40	0.51
1:A:353:LEU:O	1:A:357:LEU:HG	2.11	0.51
1:A:344:TYR:HA	1:A:350:ARG:HB3	1.93	0.51
1:C:193:GLN:HE21	1:C:362:GLN:HE22	1.58	0.51
1:C:342:VAL:C	1:C:344:TYR:N	2.63	0.51
1:B:290:PRO:HB2	1:B:292:MET:CE	2.41	0.51
1:B:146:LYS:O	1:B:147:LYS:CB	2.58	0.51
1:B:313:ASN:ND2	1:B:466:CYS:SG	2.79	0.51
1:A:107:PRO:O	1:A:108:ASP:HB2	2.11	0.51
1:A:15:VAL:O	1:A:209:VAL:HG13	2.11	0.51
1:B:137:VAL:CG2	1:B:178:GLY:HA2	2.40	0.51
1:B:339:PHE:CE2	1:B:341:PRO:HG3	2.45	0.50
1:A:74:ILE:HD13	1:A:81:ALA:CB	2.41	0.50
1:C:187:ILE:HG23	1:C:206:ILE:CD1	2.41	0.50
1:C:458:MET:HG2	1:C:513:PHE:CZ	2.45	0.50
1:B:167:GLU:CG	1:B:198:ASN:ND2	2.73	0.50
1:C:140:LEU:O	1:C:142:PRO:HD3	2.12	0.50
1:B:10:TYR:O	1:B:205:GLY:HA3	2.12	0.50
1:B:296:GLN:O	1:B:299:VAL:HG22	2.10	0.50
1:C:266:LEU:HD11	1:C:291:ILE:HD11	1.93	0.50
1:C:167:GLU:CG	1:C:198:ASN:ND2	2.67	0.50
1:A:35:LEU:HD22	1:A:70:VAL:HG11	1.94	0.50
1:A:254:GLN:HG3	1:A:528:ASN:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HA	1:B:39:VAL:CG1	2.42	0.50
1:B:4:SER:HB2	1:B:6:GLU:OE2	2.12	0.50
1:B:370:SER:HB2	1:B:398:LEU:HD21	1.94	0.50
1:C:358:LEU:HD13	1:C:409:TYR:CE2	2.46	0.50
1:C:179:ILE:HD13	3:C:2002:TPS:C6A	2.41	0.50
1:B:274:VAL:HG13	1:C:292:MET:HG3	1.94	0.50
1:B:271:THR:HB	1:B:313:ASN:HB3	1.94	0.50
1:C:329:ALA:O	1:C:333:VAL:HG23	2.12	0.50
1:A:422:ILE:HG22	1:A:486:PHE:CE1	2.47	0.49
1:B:167:GLU:HG3	1:B:198:ASN:ND2	2.27	0.49
1:A:187:ILE:HG23	1:A:206:ILE:CD1	2.42	0.49
1:C:424:ASP:O	1:C:445:ILE:HB	2.12	0.49
1:A:290:PRO:HB2	1:A:292:MET:CE	2.41	0.49
1:A:74:ILE:CD1	1:A:86:ALA:HB2	2.37	0.49
1:C:342:VAL:CG1	1:C:343:GLY:N	2.76	0.49
1:A:98:ILE:HG21	1:A:132:VAL:HG23	1.94	0.49
1:B:416:THR:HA	1:B:420:ASP:OD1	2.13	0.49
1:A:281:ASN:HA	1:A:284:LEU:CD2	2.43	0.49
1:A:290:PRO:HB2	1:A:292:MET:HE2	1.95	0.49
1:A:93:GLN:NE2	1:A:114:SER:O	2.36	0.49
1:C:209:VAL:O	1:C:213:ILE:CG1	2.61	0.49
1:C:167:GLU:HG2	1:C:198:ASN:ND2	2.26	0.49
1:A:36:GLN:C	1:A:37:ASN:HD22	2.15	0.49
1:C:225:LEU:O	1:C:229:ILE:HG13	2.12	0.49
1:C:90:HIS:CD2	3:C:2002:TPS:CM2	2.96	0.49
1:B:37:ASN:ND2	1:B:219:ALA:HA	2.27	0.49
1:C:78:ILE:HG12	1:C:89:ILE:HD12	1.95	0.49
1:B:265:PRO:O	1:B:288:SER:HB2	2.13	0.49
1:B:130:ASP:O	1:B:132:VAL:N	2.46	0.49
1:A:167:GLU:HG2	1:A:198:ASN:ND2	2.24	0.49
1:B:395:ASN:O	1:B:399:ILE:HG13	2.12	0.49
1:B:314:THR:CG2	1:B:315:GLY:N	2.75	0.49
1:A:344:TYR:CB	1:A:354:ASN:HD22	1.95	0.49
1:B:167:GLU:HG2	1:B:198:ASN:HD21	1.74	0.49
1:A:344:TYR:O	1:A:346:ALA:N	2.40	0.48
1:B:324:LYS:HB2	1:B:360:PHE:CE1	2.48	0.48
1:C:275:HIS:O	1:C:275:HIS:CG	2.66	0.48
1:C:74:ILE:HD11	1:C:84:ILE:CD1	2.43	0.48
1:C:74:ILE:HD13	1:C:80:VAL:HG12	1.94	0.48
1:C:11:SER:HA	1:C:206:ILE:H	1.78	0.48
1:B:11:SER:CB	1:B:226:ARG:NH2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PHE:HE2	1:A:190:VAL:HG21	1.78	0.48
1:B:183:HIS:HB3	1:B:184:PRO:HD2	1.95	0.48
1:A:74:ILE:HG23	1:A:75:ASN:H	1.77	0.48
1:B:90:HIS:HD2	1:B:134:TYR:CZ	2.32	0.48
1:B:462:THR:HG22	1:C:281:ASN:ND2	2.28	0.48
1:B:437:THR:O	1:B:437:THR:HG23	2.13	0.48
1:A:74:ILE:HG21	1:A:77:ARG:O	2.14	0.48
1:C:482:GLU:H	1:C:482:GLU:CD	2.17	0.48
1:A:90:HIS:HD2	1:A:134:TYR:OH	1.96	0.48
1:C:342:VAL:HG12	1:C:343:GLY:H	1.79	0.48
1:A:294:GLU:HG2	1:A:318:ALA:HB2	1.95	0.48
1:C:11:SER:N	1:C:205:GLY:HA3	2.25	0.48
1:C:522:TYR:O	1:C:526:ARG:HD3	2.14	0.48
1:A:435:LYS:N	1:A:436:GLY:HA2	2.29	0.48
1:A:495:LEU:HD22	1:A:521:LEU:CD2	2.44	0.48
1:B:20:MET:HG3	1:B:214:ALA:HB2	1.95	0.48
1:B:5:LYS:HD3	1:B:133:ASP:CG	2.34	0.48
1:C:210:SER:O	1:C:212:ILE:N	2.47	0.47
1:B:274:VAL:CG1	1:C:292:MET:HG3	2.44	0.47
1:C:22:PRO:HG2	1:C:25:LYS:HB2	1.96	0.47
1:B:465:GLY:H	4:B:999:ACP:C3B	2.27	0.47
1:A:127:MET:HE3	1:A:132:VAL:HG23	1.96	0.47
1:A:267:VAL:CG1	1:A:269:HIS:CE1	2.97	0.47
1:B:13:TYR:CD1	1:B:41:LEU:HB3	2.48	0.47
1:B:22:PRO:O	1:B:25:LYS:HB2	2.14	0.47
1:A:20:MET:HE3	1:A:214:ALA:HB2	1.95	0.47
1:B:257:ILE:HD11	1:B:533:TRP:HH2	1.79	0.47
1:C:209:VAL:O	1:C:209:VAL:HG12	2.13	0.47
1:A:75:ASN:CG	1:A:76:ASP:H	2.17	0.47
1:C:407:PHE:CE2	1:C:427:ILE:HD11	2.49	0.47
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.65	0.47
1:B:318:ALA:HB1	1:B:322:MET:HG2	1.97	0.47
1:C:15:VAL:CG1	1:C:209:VAL:HG21	2.44	0.47
1:A:32:GLU:O	1:A:36:GLN:HG3	2.14	0.47
1:A:78:ILE:O	1:A:82:MET:HG3	2.14	0.47
1:A:167:GLU:HG3	1:A:198:ASN:HD21	1.78	0.47
1:C:13:TYR:CE1	1:C:43:GLN:HB2	2.49	0.47
1:B:98:ILE:HD11	1:B:113:TRP:CD1	2.50	0.47
1:A:399:ILE:O	1:A:403:LYS:HG3	2.15	0.47
1:C:124:LEU:HD23	1:C:124:LEU:O	2.15	0.47
1:B:256:ILE:HD12	1:B:479:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ALA:N	1:A:535:PRO:CD	2.78	0.47
1:C:534:ALA:N	1:C:535:PRO:CD	2.78	0.47
1:B:314:THR:HG21	1:B:354:ASN:HD21	1.80	0.47
1:A:163:LEU:HA	1:A:166:LEU:HD12	1.97	0.46
1:B:291:ILE:HD12	1:B:302:LEU:HG	1.97	0.46
1:B:97:PRO:O	1:B:101:ILE:HG13	2.15	0.46
1:A:41:LEU:CD1	1:A:71:PRO:HG2	2.46	0.46
1:C:291:ILE:HG22	1:C:293:SER:H	1.78	0.46
1:B:193:GLN:NE2	1:B:362:GLN:HE22	2.13	0.46
1:C:41:LEU:CD1	1:C:71:PRO:HG2	2.45	0.46
1:B:281:ASN:HA	1:B:284:LEU:CD2	2.45	0.46
1:B:419:PHE:N	1:B:419:PHE:CD1	2.83	0.46
1:A:77:ARG:HD3	1:A:80:VAL:HG21	1.98	0.46
1:A:344:TYR:CE2	1:A:372:GLU:HB3	2.50	0.46
1:C:256:ILE:O	1:C:260:THR:HG23	2.14	0.46
1:B:75:ASN:HA	1:B:76:ASP:HA	1.64	0.46
1:C:139:THR:HG23	1:C:180:GLY:HA3	1.98	0.46
1:B:465:GLY:H	4:B:999:ACP:H3B1	1.81	0.46
1:A:512:SER:HA	1:A:515:VAL:CG1	2.46	0.46
1:A:465:GLY:N	4:A:799:ACP:H3B2	2.26	0.46
1:B:35:LEU:CD1	1:B:64:LEU:HD22	2.46	0.46
1:C:276:GLN:HE22	1:C:292:MET:HB3	1.81	0.46
1:A:43:GLN:HA	1:A:73:ILE:O	2.15	0.46
1:C:11:SER:HA	1:C:205:GLY:HA2	1.97	0.46
1:A:138:GLY:HA3	1:A:154:MET:CE	2.45	0.46
1:C:495:LEU:HD11	1:C:525:THR:CG2	2.46	0.46
1:A:193:GLN:HE21	1:A:362:GLN:HE21	1.63	0.46
1:A:301:ASP:N	1:A:301:ASP:OD2	2.48	0.46
1:B:527:GLU:O	1:B:528:ASN:C	2.53	0.46
1:A:123:GLU:O	1:A:127:MET:HG3	2.15	0.46
1:B:15:VAL:O	1:B:209:VAL:HG22	2.16	0.46
1:A:47:LYS:NZ	1:A:76:ASP:OD2	2.39	0.45
1:B:482:GLU:H	1:B:482:GLU:CD	2.20	0.45
1:A:82:MET:O	1:A:83:ALA:C	2.55	0.45
1:A:191:LEU:HD13	1:A:206:ILE:HD11	1.97	0.45
1:A:534:ALA:N	1:A:535:PRO:HD2	2.31	0.45
1:A:20:MET:CE	1:A:213:ILE:HB	2.45	0.45
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.74	0.45
1:A:195:VAL:HG12	1:A:202:SER:CB	2.29	0.45
1:B:289:SER:HA	1:B:290:PRO:HD3	1.78	0.45
1:A:21:ILE:HG23	1:A:22:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:VAL:HG11	1:B:292:MET:HG3	1.98	0.45
1:B:269:HIS:HB2	1:B:292:MET:HE2	1.99	0.45
1:A:22:PRO:O	1:A:25:LYS:HB2	2.17	0.45
1:A:10:TYR:O	1:A:205:GLY:HA3	2.16	0.45
1:B:74:ILE:CD1	1:B:80:VAL:HG12	2.46	0.45
1:A:344:TYR:C	1:A:346:ALA:H	2.18	0.45
1:C:422:ILE:N	1:C:422:ILE:HD12	2.32	0.45
1:C:358:LEU:HD23	1:C:363:PHE:HE1	1.80	0.45
1:A:333:VAL:HG12	1:A:333:VAL:O	2.16	0.45
1:B:112:GLY:HA3	1:B:134:TYR:CZ	2.51	0.45
1:A:245:ASN:O	1:A:539:HIS:CE1	2.60	0.45
1:A:256:ILE:O	1:A:260:THR:HG22	2.17	0.45
1:A:269:HIS:HB2	1:A:292:MET:SD	2.56	0.45
1:A:254:GLN:HG3	1:A:528:ASN:HB2	1.99	0.45
1:C:247:LEU:HD21	1:C:539:HIS:CD2	2.52	0.45
1:B:20:MET:CG	1:B:214:ALA:HB2	2.47	0.45
1:A:268:GLN:OE1	1:A:302:LEU:HD23	2.17	0.45
1:C:11:SER:O	1:C:229:ILE:CD1	2.65	0.45
1:B:271:THR:CB	1:B:313:ASN:HB3	2.47	0.45
1:A:107:PRO:O	1:A:108:ASP:CB	2.65	0.45
1:B:427:ILE:CG2	1:B:427:ILE:O	2.65	0.45
1:B:418:GLU:HG2	1:B:419:PHE:CD1	2.52	0.45
1:A:286:LEU:HD21	1:A:521:LEU:HD22	1.99	0.45
1:A:457:ILE:HG23	1:A:513:PHE:CE1	2.51	0.45
1:A:441:SER:C	1:A:443:GLU:H	2.20	0.45
1:C:209:VAL:O	1:C:209:VAL:CG1	2.65	0.44
1:C:90:HIS:CD2	3:C:2002:TPS:HM22	2.52	0.44
1:B:137:VAL:HG22	1:B:178:GLY:HA2	1.99	0.44
1:A:92:GLY:H	1:A:95:ASP:HB2	1.83	0.44
1:C:187:ILE:HG23	1:C:206:ILE:HD12	1.99	0.44
1:C:13:TYR:HE1	1:C:43:GLN:HB2	1.82	0.44
1:A:229:ILE:HG23	1:A:433:LEU:HD11	1.98	0.44
1:B:305:ILE:HA	1:B:306:PRO:HD3	1.86	0.44
1:C:271:THR:HA	1:C:313:ASN:HB2	2.00	0.44
1:C:59:LEU:CD2	1:C:84:ILE:HB	2.47	0.44
1:A:426:THR:C	1:A:427:ILE:HG13	2.36	0.44
1:A:344:TYR:CG	1:A:345:SER:N	2.85	0.44
1:C:302:LEU:HA	1:C:305:ILE:HD12	1.99	0.44
1:B:290:PRO:HB2	1:B:292:MET:HE1	1.99	0.44
1:C:73:ILE:HA	1:C:88:GLY:O	2.17	0.44
1:B:90:HIS:CD2	3:B:2006:TPS:HM22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:MET:SD	4:A:799:ACP:H1'	2.57	0.44
1:C:358:LEU:HD23	1:C:363:PHE:CE1	2.53	0.44
1:C:212:ILE:HD11	1:C:225:LEU:HD12	1.99	0.44
1:B:462:THR:H	1:C:281:ASN:ND2	2.08	0.44
1:B:305:ILE:CG2	1:B:306:PRO:HD2	2.46	0.44
1:C:495:LEU:HD22	1:C:521:LEU:CD2	2.48	0.44
1:A:139:THR:HG23	1:A:180:GLY:HA3	1.99	0.44
1:B:534:ALA:N	1:B:535:PRO:CD	2.81	0.44
1:C:163:LEU:HD22	1:C:201:ARG:HD3	1.99	0.44
1:A:36:GLN:HB2	1:A:37:ASN:ND2	2.33	0.43
1:A:344:TYR:HA	1:A:350:ARG:CB	2.48	0.43
1:A:533:TRP:HB3	1:A:535:PRO:HD2	1.99	0.43
1:B:187:ILE:HG23	1:B:206:ILE:CD1	2.48	0.43
1:C:102:ARG:CZ	1:C:111:ILE:HD12	2.48	0.43
1:C:529:THR:N	1:C:530:PRO:HD3	2.32	0.43
1:B:192:TYR:HA	1:B:431:TYR:HB3	2.00	0.43
1:B:472:ILE:O	1:B:476:ILE:HG13	2.18	0.43
1:A:266:LEU:CD2	1:A:305:ILE:HD12	2.49	0.43
1:C:260:THR:HG21	1:C:475:MET:HA	2.00	0.43
1:C:107:PRO:O	1:C:108:ASP:CB	2.66	0.43
1:A:318:ALA:HA	1:A:319:PRO:HD3	1.74	0.43
1:B:208:VAL:HG21	1:B:212:ILE:HD12	2.00	0.43
1:A:528:ASN:C	1:A:530:PRO:HD3	2.38	0.43
1:C:438:ASN:HA	1:C:439:GLY:HA2	1.72	0.43
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.87	0.43
1:A:484:ASN:HD21	1:A:486:PHE:HB3	1.83	0.43
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.84	0.43
1:A:41:LEU:HD12	1:A:71:PRO:HG2	2.00	0.43
1:B:501:LYS:HA	1:B:501:LYS:HD2	1.79	0.43
1:B:441:SER:C	1:B:443:GLU:H	2.22	0.43
1:A:527:GLU:O	1:A:529:THR:N	2.51	0.43
1:A:416:THR:HB	4:A:799:ACP:H5'2	2.01	0.43
1:C:471:THR:O	1:C:475:MET:HG2	2.19	0.43
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.83	0.43
1:A:247:LEU:HG	1:A:537:LEU:HG	2.01	0.43
1:C:210:SER:C	1:C:212:ILE:N	2.72	0.43
1:B:13:TYR:CD2	1:B:207:CYS:SG	3.12	0.43
1:A:91:VAL:HB	1:A:95:ASP:HB2	2.01	0.43
1:A:276:GLN:HB3	1:A:276:GLN:HE21	1.59	0.43
1:C:404:ILE:HA	1:C:442:VAL:HG22	2.00	0.43
1:B:275:HIS:CD2	1:B:466:CYS:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASP:OD2	1:B:40:THR:HG21	2.18	0.43
1:B:102:ARG:HD3	1:B:102:ARG:HA	1.58	0.43
1:C:78:ILE:C	1:C:80:VAL:N	2.72	0.42
1:C:394:SER:OG	1:C:395:ASN:N	2.51	0.42
1:B:407:PHE:CD1	1:B:442:VAL:HG23	2.54	0.42
1:B:31:VAL:O	1:B:31:VAL:HG12	2.19	0.42
1:B:210:SER:N	3:B:2006:TPS:O2	2.45	0.42
1:B:167:GLU:HG2	1:B:198:ASN:ND2	2.33	0.42
1:B:46:GLU:HB2	1:B:54:PHE:CE2	2.54	0.42
1:A:494:MET:HB3	1:A:494:MET:HE3	1.91	0.42
1:B:179:ILE:HG13	1:B:207:CYS:HB3	2.02	0.42
1:B:127:MET:CE	1:B:132:VAL:HG23	2.49	0.42
1:C:369:ASN:O	1:C:373:ILE:HG12	2.19	0.42
1:A:343:GLY:N	1:A:372:GLU:OE2	2.51	0.42
1:C:75:ASN:ND2	1:C:76:ASP:OD2	2.53	0.42
1:B:58:ALA:CB	1:B:84:ILE:HD13	2.46	0.42
1:C:305:ILE:HA	1:C:306:PRO:HD3	1.86	0.42
1:A:117:PHE:HB3	1:A:119:GLU:OE1	2.19	0.42
1:B:271:THR:HA	1:B:313:ASN:HB3	2.01	0.42
1:A:331:ASN:HD22	1:A:331:ASN:HA	1.67	0.42
1:A:344:TYR:HE2	1:A:372:GLU:HB3	1.84	0.42
1:C:90:HIS:NE2	3:C:2002:TPS:HM22	2.35	0.42
1:B:35:LEU:CA	1:B:39:VAL:HG12	2.46	0.42
1:B:78:ILE:HD12	1:B:96:MET:SD	2.60	0.42
1:B:271:THR:OG1	1:B:272:ASN:N	2.52	0.42
1:B:234:TYR:HB2	1:B:431:TYR:HE1	1.83	0.42
1:A:315:GLY:O	1:A:316:SER:C	2.57	0.42
1:C:344:TYR:CE2	1:C:376:LEU:HD21	2.54	0.42
1:C:192:TYR:CD1	1:C:234:TYR:CD2	3.07	0.42
1:C:58:ALA:HB1	1:C:84:ILE:HD13	2.00	0.42
1:B:260:THR:O	1:B:265:PRO:HD3	2.20	0.42
1:C:90:HIS:NE2	3:C:2002:TPS:CM2	2.83	0.42
1:B:186:ASN:O	1:B:190:VAL:HG23	2.20	0.42
1:C:534:ALA:H	1:C:535:PRO:HD2	1.84	0.42
1:A:156:THR:HG21	1:A:193:GLN:HG3	2.01	0.42
1:C:192:TYR:HA	1:C:431:TYR:HB3	2.01	0.42
1:C:366:ILE:HD12	1:C:411:THR:HG21	2.01	0.42
1:A:520:ALA:O	1:A:524:LEU:HB2	2.19	0.42
1:B:187:ILE:CD1	1:B:225:LEU:HD22	2.50	0.42
1:A:352:LEU:HA	1:A:352:LEU:HD13	1.87	0.42
1:C:457:ILE:O	1:C:457:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:HG21	1:A:468:LEU:HD23	2.02	0.41
1:A:183:HIS:HB3	1:A:184:PRO:CD	2.48	0.41
1:A:349:THR:CG2	1:B:297:SER:HB2	2.48	0.41
1:A:522:TYR:O	1:A:526:ARG:HD3	2.20	0.41
1:B:76:ASP:CB	1:B:91:VAL:HG12	2.49	0.41
1:B:250:THR:HG21	1:B:531:VAL:CG2	2.49	0.41
1:A:378:GLU:O	1:A:379:LEU:C	2.59	0.41
1:A:479:GLN:HA	1:A:480:PRO:HD3	1.69	0.41
1:A:165:ALA:O	1:A:169:ASN:HB2	2.20	0.41
4:B:999:ACP:O5'	4:B:999:ACP:H8	2.21	0.41
1:B:210:SER:HB3	3:B:2006:TPS:O2	2.20	0.41
1:C:342:VAL:CG1	1:C:343:GLY:H	2.33	0.41
1:A:343:GLY:O	1:A:344:TYR:C	2.59	0.41
1:C:296:GLN:O	1:C:299:VAL:HG23	2.20	0.41
1:C:115:VAL:O	1:C:137:VAL:HA	2.19	0.41
1:A:314:THR:HG21	1:A:354:ASN:HD21	1.86	0.41
1:C:112:GLY:CA	1:C:134:TYR:CE2	3.03	0.41
1:A:281:ASN:HA	1:A:281:ASN:HD22	1.75	0.41
1:B:475:MET:HG3	1:B:492:GLY:HA2	2.01	0.41
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.80	0.41
1:C:20:MET:O	1:C:20:MET:HG2	2.20	0.41
1:C:249:THR:HG23	1:C:252:GLU:OE1	2.20	0.41
1:A:25:LYS:HE2	1:A:216:LEU:O	2.20	0.41
1:C:98:ILE:N	1:C:99:PRO:HD2	2.36	0.41
1:C:112:GLY:HA3	1:C:134:TYR:CE2	2.55	0.41
1:B:335:ARG:HA	1:B:336:PRO:HD3	1.82	0.41
1:C:247:LEU:HD22	1:C:539:HIS:NE2	2.36	0.41
1:B:234:TYR:HB2	1:B:431:TYR:CE1	2.56	0.41
1:C:74:ILE:HD12	1:C:86:ALA:CB	2.49	0.41
1:C:281:ASN:HA	1:C:284:LEU:HD23	2.02	0.41
1:A:191:LEU:HD11	1:A:433:LEU:HD21	2.02	0.41
1:C:286:LEU:CD2	1:C:525:THR:HG21	2.50	0.41
1:C:264:ARG:N	1:C:265:PRO:HD3	2.36	0.41
1:B:463:ALA:HB1	1:B:466:CYS:HB2	2.02	0.41
1:A:268:GLN:CD	1:A:302:LEU:HD23	2.40	0.41
1:C:38:GLY:HA3	1:C:226:ARG:HG3	2.02	0.41
1:A:271:THR:HA	1:A:313:ASN:HB2	2.01	0.41
1:B:319:PRO:HA	1:B:320:PRO:HD3	1.96	0.41
1:A:98:ILE:HD13	1:A:101:ILE:HD12	2.03	0.41
1:B:322:MET:HE2	1:B:322:MET:C	2.42	0.41
1:C:427:ILE:O	1:C:427:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.89	0.41
1:A:265:PRO:CD	1:A:288:SER:HB3	2.27	0.40
1:C:344:TYR:CE2	1:C:376:LEU:HG	2.56	0.40
1:B:226:ARG:HA	1:B:226:ARG:HD3	1.77	0.40
1:C:529:THR:HG22	1:C:529:THR:O	2.20	0.40
1:B:74:ILE:HD12	1:B:81:ALA:CA	2.51	0.40
1:A:10:TYR:O	1:A:11:SER:C	2.59	0.40
1:B:349:THR:CG2	1:C:297:SER:HB2	2.51	0.40
1:C:490:VAL:O	1:C:494:MET:HG2	2.20	0.40
1:C:187:ILE:HG12	1:C:206:ILE:HD13	2.03	0.40
1:C:479:GLN:HA	1:C:480:PRO:HD3	1.91	0.40
1:B:458:MET:SD	4:B:999:ACP:H1'	2.61	0.40
1:B:64:LEU:O	1:B:67:ALA:HB3	2.21	0.40
1:C:344:TYR:CE2	1:C:376:LEU:CD2	3.04	0.40
1:C:272:ASN:N	1:C:272:ASN:HD22	2.20	0.40
1:C:197:SER:O	1:C:442:VAL:HB	2.21	0.40
1:B:267:VAL:HG12	1:B:269:HIS:CE1	2.57	0.40
1:C:140:LEU:O	1:C:142:PRO:CD	2.69	0.40
1:C:324:LYS:HB2	1:C:360:PHE:CE1	2.56	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	Percentiles	
1	A	508/540 (94%)	458 (90%)	41 (8%)	9 (2%)	11	20
1	B	498/540 (92%)	459 (92%)	34 (7%)	5 (1%)	19	37
1	C	503/540 (93%)	448 (89%)	44 (9%)	11 (2%)	8	14
All	All	1509/1620 (93%)	1365 (90%)	119 (8%)	25 (2%)	11	21

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	A	343	GLY
1	B	138	GLY
1	B	528	ASN
1	C	77	ARG
1	C	79	ASP
1	C	130	ASP
1	A	138	GLY
1	A	316	SER
1	A	434	SER
1	C	247	LEU
1	C	343	GLY
1	A	77	ARG
1	A	345	SER
1	A	528	ASN
1	B	11	SER
1	C	211	ASP
1	B	290	PRO
1	C	129	PRO
1	C	131	MET
1	B	378	GLU
1	C	78	ILE
1	C	209	VAL
1	A	95	ASP
1	C	369	ASN

### 5.3.2 Protein sidechains ⓘ

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	A	418/449 (93%)	371 (89%)	47 (11%)	7	12
1	B	417/449 (93%)	368 (88%)	49 (12%)	6	11
1	C	412/449 (92%)	374 (91%)	38 (9%)	11	21
All	All	1247/1347 (93%)	1113 (89%)	134 (11%)	8	14

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	A	20	MET
1	A	37	ASN
1	A	54	PHE
1	A	64	LEU
1	A	66	HIS
1	A	70	VAL
1	A	74	ILE
1	A	89	ILE
1	A	93	GLN
1	A	103	LYS
1	A	113	TRP
1	A	143	THR
1	A	167	GLU
1	A	182	LEU
1	A	206	ILE
1	A	225	LEU
1	A	228	LEU
1	A	247	LEU
1	A	250	THR
1	A	260	THR
1	A	272	ASN
1	A	276	GLN
1	A	284	LEU
1	A	294	GLU
1	A	301	ASP
1	A	311	LEU
1	A	317	VAL
1	A	322	MET
1	A	328	ARG
1	A	348	GLU
1	A	352	LEU
1	A	408	LYS
1	A	411	THR
1	A	427	ILE
1	A	437	THR
1	A	442	VAL
1	A	451	GLU
1	A	461	ILE
1	A	462	THR
1	A	482	GLU
1	A	495	LEU
1	A	515	VAL

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Mol	Chain	Res	Type
1	A	517	LEU
1	A	524	LEU
1	A	527	GLU
1	A	528	ASN
1	B	2	LYS
1	B	18	SER
1	B	41	LEU
1	B	47	LYS
1	B	54	PHE
1	B	64	LEU
1	B	66	HIS
1	B	70	VAL
1	B	77	ARG
1	B	89	ILE
1	B	93	GLN
1	B	102	ARG
1	B	113	TRP
1	B	143	THR
1	B	182	LEU
1	B	185	ASP
1	B	191	LEU
1	B	226	ARG
1	B	228	LEU
1	B	233	ASP
1	B	242	SER
1	B	247	LEU
1	B	250	THR
1	B	260	THR
1	B	271	THR
1	B	272	ASN
1	B	276	GLN
1	B	284	LEU
1	B	294	GLU
1	B	297	SER
1	B	311	LEU
1	B	312	LEU
1	B	322	MET
1	B	328	ARG
1	B	335	ARG
1	B	348	GLU
1	B	352	LEU
1	B	408	LYS

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Mol	Chain	Res	Type
1	B	416	THR
1	B	438	ASN
1	B	442	VAL
1	B	451	GLU
1	B	461	ILE
1	B	464	SER
1	B	495	LEU
1	B	515	VAL
1	B	517	LEU
1	B	524	LEU
1	B	527	GLU
1	C	13	TYR
1	C	47	LYS
1	C	54	PHE
1	C	63	GLU
1	C	64	LEU
1	C	66	HIS
1	C	70	VAL
1	C	137	VAL
1	C	182	LEU
1	C	191	LEU
1	C	226	ARG
1	C	228	LEU
1	C	260	THR
1	C	272	ASN
1	C	288	SER
1	C	297	SER
1	C	299	VAL
1	C	301	ASP
1	C	311	LEU
1	C	322	MET
1	C	335	ARG
1	C	348	GLU
1	C	349	THR
1	C	352	LEU
1	C	365	CYS
1	C	408	LYS
1	C	416	THR
1	C	442	VAL
1	C	444	ASP
1	C	457	ILE
1	C	461	ILE

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Mol	Chain	Res	Type
1	C	464	SER
1	C	467	SER
1	C	482	GLU
1	C	495	LEU
1	C	515	VAL
1	C	517	LEU
1	C	524	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	66	HIS
1	A	75	ASN
1	A	90	HIS
1	A	169	ASN
1	A	193	GLN
1	A	276	GLN
1	A	281	ASN
1	A	313	ASN
1	A	355	ASN
1	A	484	ASN
1	A	539	HIS
1	B	37	ASN
1	B	66	HIS
1	B	90	HIS
1	B	93	GLN
1	B	169	ASN
1	B	183	HIS
1	B	193	GLN
1	B	272	ASN
1	B	276	GLN
1	B	281	ASN
1	B	355	ASN
1	B	479	GLN
1	B	484	ASN
1	C	66	HIS
1	C	75	ASN
1	C	90	HIS
1	C	93	GLN
1	C	193	GLN
1	C	272	ASN

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Mol	Chain	Res	Type
1	C	276	GLN
1	C	281	ASN
1	C	313	ASN
1	C	355	ASN
1	C	484	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	TPS	A	2001	-	13,22,23	7.18	6 (46%)	19,30,33	2.68	8 (42%)
4	ACP	A	799	2	25,33,33	3.37	12 (48%)	31,52,52	2.55	6 (19%)
3	TPS	B	2006	-	18,23,23	6.32	7 (38%)	25,33,33	1.91	8 (32%)
4	ACP	B	999	2	25,33,33	3.38	12 (48%)	31,52,52	2.56	6 (19%)
3	TPS	C	2002	-	18,23,23	6.25	8 (44%)	25,33,33	2.07	7 (28%)
4	ACP	C	899	2	25,33,33	3.36	12 (48%)	31,52,52	2.55	6 (19%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPS	A	2001	-	-	0/7/10/11	0/2/2/2
4	ACP	A	799	2	-	0/15/38/38	0/3/3/3
3	TPS	B	2006	-	-	0/10/11/11	0/2/2/2
4	ACP	B	999	2	-	0/15/38/38	0/3/3/3
3	TPS	C	2002	-	-	0/10/11/11	0/2/2/2
4	ACP	C	899	2	-	0/15/38/38	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	999	ACP	PB-O2B	-4.15	1.46	1.56
4	A	799	ACP	PB-O2B	-4.13	1.46	1.56
4	C	899	ACP	PB-O2B	-4.11	1.46	1.56
4	C	899	ACP	PG-O3G	-3.42	1.46	1.54
4	B	999	ACP	PG-O3G	-3.42	1.46	1.54
4	A	799	ACP	PG-O3G	-3.40	1.46	1.54
3	A	2001	TPS	C4A-N3A	-2.96	1.30	1.35
3	C	2002	TPS	C4A-N3A	-2.53	1.31	1.35
3	B	2006	TPS	C7A-N3	-2.35	1.44	1.48
3	C	2002	TPS	C6A-C5A	-2.08	1.32	1.37
3	A	2001	TPS	C6A-C5A	-2.05	1.33	1.37
4	C	899	ACP	C2-N1	2.01	1.37	1.33
4	B	999	ACP	C2-N1	2.07	1.37	1.33
4	A	799	ACP	C2-N1	2.07	1.37	1.33
3	A	2001	TPS	C2A-N3A	2.56	1.38	1.34
3	C	2002	TPS	C2A-N3A	2.74	1.39	1.34
3	C	2002	TPS	P1-O2	2.82	1.64	1.54
3	B	2006	TPS	P1-O3	2.84	1.64	1.54
3	B	2006	TPS	P1-O2	2.93	1.65	1.54
3	C	2002	TPS	P1-O3	3.19	1.66	1.54
3	B	2006	TPS	C2A-N3A	3.19	1.40	1.34
4	A	799	ACP	C6-N6	3.83	1.46	1.34
4	C	899	ACP	PA-O1A	3.84	1.65	1.51
4	C	899	ACP	C6-N6	3.84	1.46	1.34
4	B	999	ACP	C6-N6	3.84	1.46	1.34
4	A	799	ACP	PA-O1A	3.85	1.65	1.51
4	B	999	ACP	PA-O1A	3.86	1.65	1.51
3	C	2002	TPS	C2A-N1A	4.02	1.41	1.34
3	A	2001	TPS	C2A-N1A	4.15	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	899	ACP	PG-O2G	4.20	1.65	1.54
4	A	799	ACP	PG-O2G	4.21	1.65	1.54
4	B	999	ACP	PG-O2G	4.24	1.65	1.54
4	C	899	ACP	C2-N3	4.34	1.39	1.32
4	B	999	ACP	C8-N7	4.35	1.43	1.34
4	A	799	ACP	C8-N7	4.36	1.43	1.34
4	A	799	ACP	C2-N3	4.36	1.39	1.32
4	B	999	ACP	C2-N3	4.38	1.39	1.32
4	C	899	ACP	C8-N7	4.39	1.43	1.34
3	A	2001	TPS	C4A-N4A	4.42	1.45	1.34
4	C	899	ACP	O4'-C1'	4.59	1.47	1.41
4	B	999	ACP	O4'-C1'	4.62	1.47	1.41
4	A	799	ACP	O4'-C1'	4.69	1.47	1.41
3	B	2006	TPS	C4A-N4A	4.80	1.46	1.34
3	B	2006	TPS	C2A-N1A	4.81	1.42	1.34
3	C	2002	TPS	C4A-N4A	4.92	1.46	1.34
4	C	899	ACP	PB-O1B	5.10	1.64	1.51
4	A	799	ACP	PB-O1B	5.13	1.64	1.51
4	B	999	ACP	PB-O1B	5.14	1.64	1.51
4	C	899	ACP	PG-O1G	6.55	1.65	1.50
4	A	799	ACP	PG-O1G	6.59	1.65	1.50
4	B	999	ACP	PG-O1G	6.62	1.65	1.50
4	C	899	ACP	PB-O3A	7.61	1.67	1.58
4	A	799	ACP	PB-O3A	7.66	1.67	1.58
4	B	999	ACP	PB-O3A	7.67	1.67	1.58
3	A	2001	TPS	C4-N3	24.57	1.61	1.39
3	C	2002	TPS	C4-N3	24.73	1.61	1.39
3	B	2006	TPS	C4-N3	24.96	1.61	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	999	ACP	N3-C2-N1	-11.53	120.06	128.89
4	A	799	ACP	N3-C2-N1	-11.50	120.09	128.89
4	C	899	ACP	N3-C2-N1	-11.48	120.11	128.89
3	A	2001	TPS	C6-C5-C4	-8.22	120.20	127.56
3	C	2002	TPS	C6-C5-C4	-4.81	123.25	127.56
4	B	999	ACP	PA-O3A-PB	-4.68	119.58	132.73
4	A	799	ACP	PA-O3A-PB	-4.67	119.61	132.73
4	C	899	ACP	PA-O3A-PB	-4.67	119.62	132.73
3	A	2001	TPS	N1A-C2A-N3A	-3.22	119.64	125.60
3	B	2006	TPS	N1A-C2A-N3A	-2.88	120.28	125.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	TPS	N1A-C2A-N3A	-2.75	120.52	125.60
3	C	2002	TPS	CM4-C4-C5	-2.74	122.73	128.90
4	C	899	ACP	C2'-C1'-N9	-2.63	110.27	114.29
4	A	799	ACP	C2'-C1'-N9	-2.61	110.30	114.29
4	B	999	ACP	C2'-C1'-N9	-2.61	110.31	114.29
3	B	2006	TPS	C5A-C6A-N1A	-2.58	119.38	123.86
3	A	2001	TPS	CM4-C4-C5	-2.55	123.16	128.90
3	A	2001	TPS	C5A-C6A-N1A	-2.46	119.59	123.86
3	C	2002	TPS	C5A-C6A-N1A	-2.24	119.97	123.86
3	B	2006	TPS	O7-C7-C6	2.05	117.89	109.30
4	C	899	ACP	O4'-C4'-C5'	2.06	116.67	109.32
4	B	999	ACP	O4'-C4'-C5'	2.06	116.70	109.32
4	A	799	ACP	O4'-C4'-C5'	2.07	116.71	109.32
3	C	2002	TPS	C6A-N1A-C2A	2.16	119.55	115.77
4	B	999	ACP	O5'-C5'-C4'	2.26	117.46	109.12
4	A	799	ACP	O5'-C5'-C4'	2.27	117.50	109.12
4	C	899	ACP	O5'-C5'-C4'	2.29	117.56	109.12
3	B	2006	TPS	N4A-C4A-N3A	2.34	120.34	116.95
3	B	2006	TPS	C6A-N1A-C2A	2.39	119.95	115.77
3	B	2006	TPS	CM2-C2A-N1A	2.42	119.93	117.03
4	C	899	ACP	O3A-PA-O5'	2.49	109.54	102.94
4	B	999	ACP	O3A-PA-O5'	2.51	109.58	102.94
4	A	799	ACP	O3A-PA-O5'	2.51	109.59	102.94
3	A	2001	TPS	CM2-C2A-N1A	2.77	120.35	117.03
3	A	2001	TPS	C6A-N1A-C2A	2.77	120.61	115.77
3	A	2001	TPS	C6A-C5A-C4A	2.89	119.86	115.72
3	A	2001	TPS	C6-C5-S1	3.00	124.43	120.24
3	C	2002	TPS	C6A-C5A-C4A	3.67	120.98	115.72
3	B	2006	TPS	C6A-C5A-C4A	3.72	121.06	115.72
3	B	2006	TPS	C6-C5-S1	4.19	126.10	120.24
3	C	2002	TPS	C6-C5-S1	4.33	126.29	120.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	TPS	2	0
4	A	799	ACP	7	0
3	B	2006	TPS	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	ACP	10	0
3	C	2002	TPS	8	0
4	C	899	ACP	4	0

## 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	518/540 (95%)	-0.26	8 (1%) 76 71	23, 50, 70, 83	0
1	B	514/540 (95%)	-0.19	5 (0%) 84 81	24, 54, 74, 102	0
1	C	513/540 (95%)	-0.20	6 (1%) 81 77	20, 57, 79, 103	0
All	All	1545/1620 (95%)	-0.22	19 (1%) 81 77	20, 54, 75, 103	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	TYR	4.7
1	C	209	VAL	3.9
1	C	143	THR	3.6
1	A	76	ASP	3.5
1	C	344	TYR	3.4
1	C	77	ARG	3.3
1	B	138	GLY	3.3
1	A	144	LEU	2.9
1	A	343	GLY	2.8
1	C	108	ASP	2.5
1	B	220	LYS	2.4
1	B	77	ARG	2.3
1	A	345	SER	2.3
1	C	144	LEU	2.3
1	A	108	ASP	2.1
1	A	152	ALA	2.1
1	B	130	ASP	2.1
1	A	143	THR	2.0
1	B	147	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACP	B	999	31/31	0.73	0.26	3.44	74,104,138,149	0
4	ACP	C	899	31/31	0.82	0.25	2.87	80,102,137,174	0
4	ACP	A	799	31/31	0.85	0.23	1.78	81,96,127,132	0
2	MG	B	541	1/1	0.55	0.19	1.78	30,30,30,30	0
2	MG	C	541	1/1	0.78	0.13	0.66	30,30,30,30	0
3	TPS	B	2006	22/22	0.91	0.20	0.30	45,61,76,81	0
3	TPS	A	2001	21/22	0.95	0.17	0.17	45,56,75,98	0
3	TPS	C	2002	22/22	0.93	0.18	-0.00	56,71,95,107	0
2	MG	A	541	1/1	0.91	0.09	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.