Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 11:54 PM EDT

PDB ID	:	1TED
Title	:	Crystal structure of a type III polyketide synthase PKS18 from Mycobacterium tuberculosis
Authors	:	Sankaranarayanan, R.; Shanmugam, V.M.; Rukmini, R.
Deposited on	:	2004-05-25
Resolution	:	2.25 Å(reported)

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

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

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

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

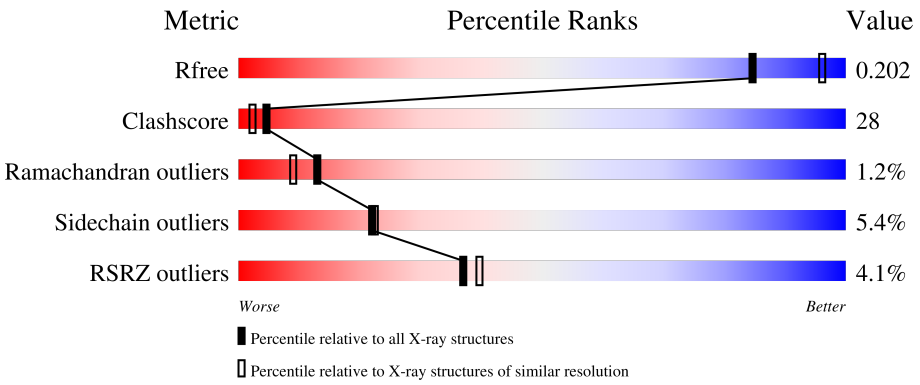
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	A	393	3% 58% 33% • 6%
1	B	393	2% 52% 35% • 9%
1	C	393	3% 57% 35% • • 6%
1	D	393	6% 55% 32% • 9%

2 Entry composition (i)

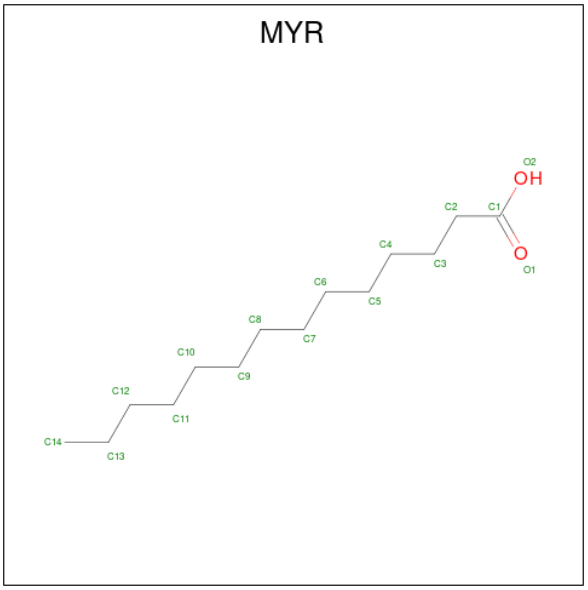
There are 3 unique types of molecules in this entry. The entry contains 12026 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 pks18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2745	1743	474	514	14	0	0	0
1	B	359	2683	1702	464	503	14	0	0	0
1	C	368	2745	1743	474	514	14	0	0	0
1	D	359	2683	1702	464	503	14	0	0	0

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	16	14	2	0	0
2	B	1	16	14	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	C	1	16	14	2	0	0
			Total	C	O		
2	D	1	16	14	2	0	0

- Molecule 3 is water.

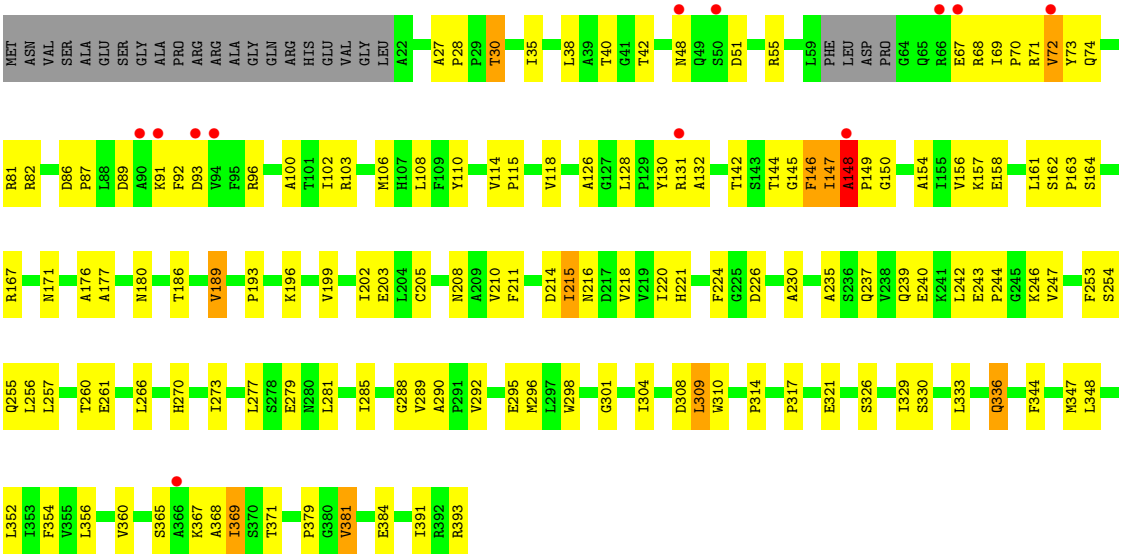
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	302	302	302	0	0
			Total	O		
3	B	236	236	236	0	0
			Total	O		
3	C	303	303	303	0	0
			Total	O		
3	D	265	265	265	0	0

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.

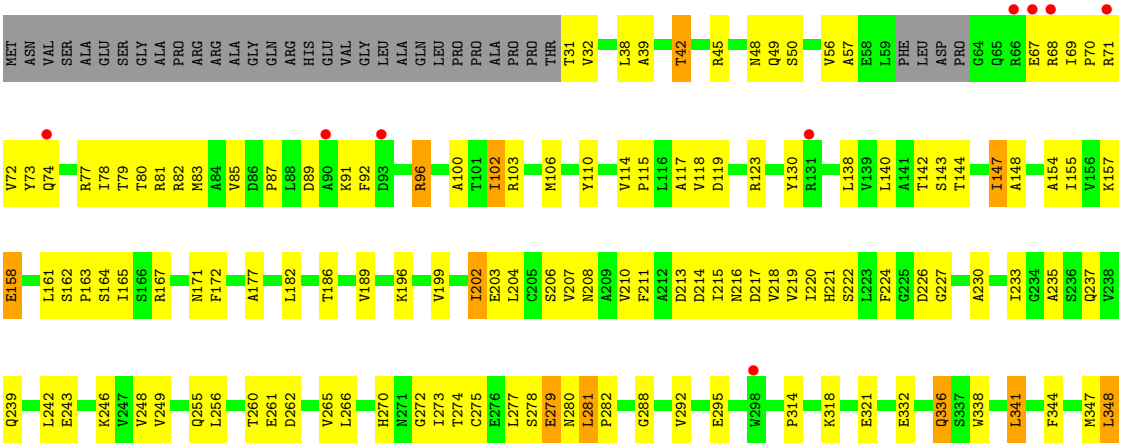
- Molecule 1: pks18

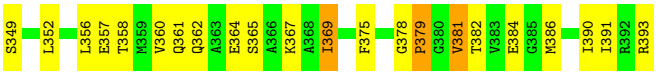
Chain A:



- Molecule 1: pks18

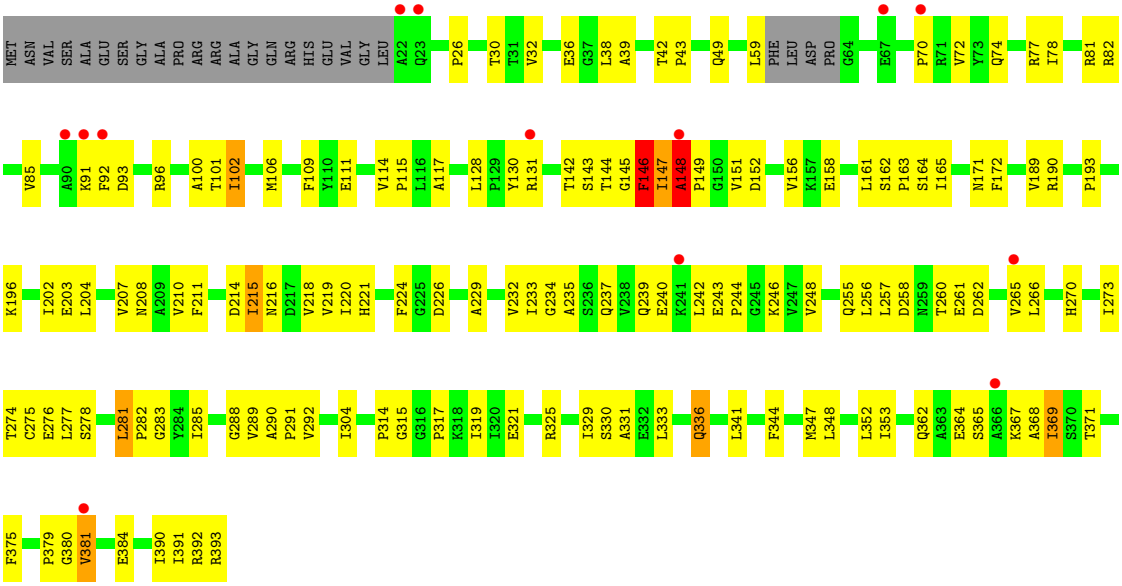
Chain B:





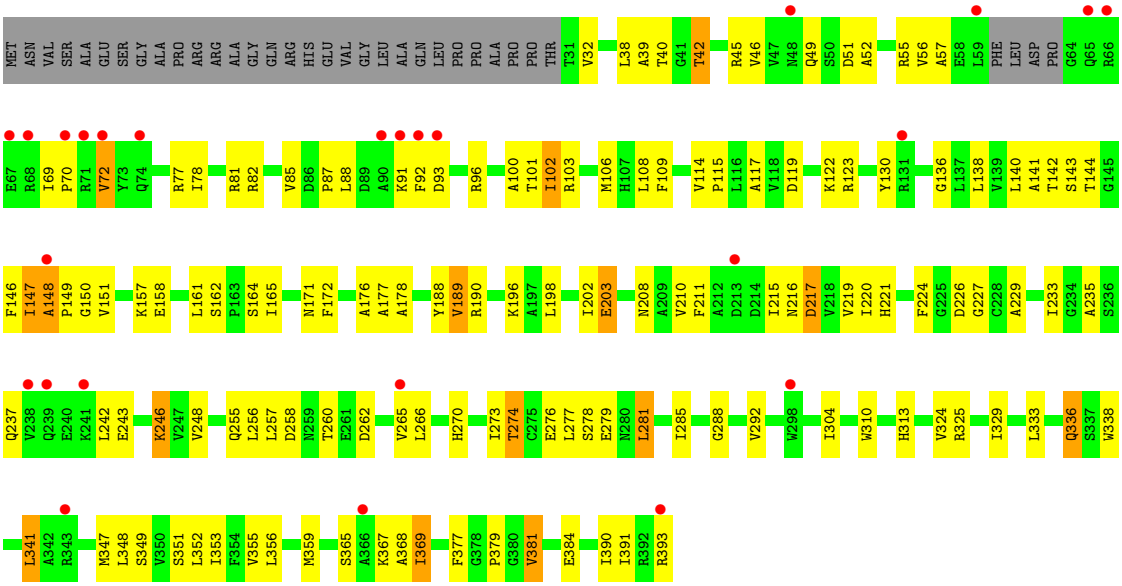
• Molecule 1: pks18

Chain C:



• Molecule 1: pks18

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.91Å 80.65Å 99.61Å 108.23° 92.97° 103.69°	Depositor
Resolution (Å)	24.87 – 2.25 24.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.0 (24.87-2.25) 95.1 (24.87-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.265 0.202 , 0.202	Depositor DCC
R_{free} test set	3889 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12026	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MYR

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	0.37	0/2793	0.67	1/3804 (0.0%)
1	B	0.37	0/2727	0.65	0/3709
1	C	0.37	0/2793	0.66	1/3804 (0.0%)
1	D	0.36	0/2727	0.64	0/3709
All	All	0.37	0/11040	0.66	2/15026 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	148	ALA	C-N-CD	5.90	140.79	128.40
1	A	148	ALA	C-N-CD	5.86	140.69	128.40

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	2745	0	2776	163	0
1	B	2683	0	2712	169	0
1	C	2745	0	2776	179	0
1	D	2683	0	2712	176	0
2	A	16	0	27	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	27	5	0
2	C	16	0	27	5	0
2	D	16	0	27	6	0
3	A	302	0	0	17	0
3	B	236	0	0	12	0
3	C	303	0	0	15	0
3	D	265	0	0	19	0
All	All	12026	0	11084	623	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 28.

All (623) 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:D:203:GLU:HG2	1:D:348:LEU:HB2	1.33	1.09
1:B:203:GLU:HG2	1:B:348:LEU:HB2	1.34	1.08
1:C:344:PHE:HB3	1:C:347:MET:HE3	1.37	1.05
1:D:215:ILE:HD12	1:D:215:ILE:H	1.17	1.04
1:A:148:ALA:HB2	1:B:266:LEU:H	1.21	1.03
1:C:266:LEU:H	1:D:148:ALA:HB2	1.23	0.99
1:D:336:GLN:H	1:D:336:GLN:HE21	1.12	0.98
1:C:203:GLU:HG2	1:C:348:LEU:HB2	1.44	0.98
1:D:49:GLN:HE22	1:D:81:ARG:HH21	1.03	0.98
1:A:210:VAL:H	1:A:221:HIS:HE1	1.11	0.97
1:D:100:ALA:H	1:D:270:HIS:HD2	1.02	0.96
1:C:242:LEU:HB2	1:C:391:ILE:HD12	1.49	0.94
1:A:203:GLU:HG2	1:A:348:LEU:HB2	1.47	0.94
1:C:266:LEU:H	1:D:148:ALA:CB	1.79	0.93
1:C:210:VAL:H	1:C:221:HIS:HE1	1.15	0.92
1:C:49:GLN:HE22	1:C:81:ARG:HH21	1.16	0.91
1:D:100:ALA:H	1:D:270:HIS:CD2	1.89	0.90
1:B:189:VAL:HG13	1:B:235:ALA:HB2	1.52	0.89
1:C:266:LEU:N	1:D:148:ALA:HB2	1.87	0.89
1:B:216:ASN:HD21	1:B:277:LEU:H	1.19	0.89
1:D:210:VAL:H	1:D:221:HIS:HE1	1.20	0.89
1:A:242:LEU:HB2	1:A:391:ILE:HD12	1.56	0.88
1:D:189:VAL:HG13	1:D:235:ALA:HB2	1.55	0.86
1:D:208:ASN:HD22	1:D:273:ILE:H	1.24	0.86
1:B:71:ARG:O	1:B:74:GLN:HG2	1.75	0.86
1:A:148:ALA:CB	1:B:266:LEU:H	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HB2	1:C:391:ILE:CD1	2.05	0.85
1:B:210:VAL:H	1:B:221:HIS:HE1	1.24	0.85
1:B:336:GLN:H	1:B:336:GLN:HE21	1.26	0.83
1:C:189:VAL:HG13	1:C:235:ALA:HB2	1.61	0.82
1:C:226:ASP:O	1:C:347:MET:HE2	1.79	0.82
1:D:49:GLN:NE2	1:D:81:ARG:HH21	1.77	0.82
1:B:83:MET:HG2	1:B:206:SER:HB3	1.60	0.81
1:B:142:THR:HG22	1:B:144:THR:H	1.45	0.81
1:C:142:THR:HG22	1:C:144:THR:H	1.44	0.81
1:D:161:LEU:HB3	1:D:165:ILE:HD12	1.63	0.81
1:D:215:ILE:H	1:D:215:ILE:CD1	1.93	0.80
1:A:148:ALA:HB2	1:B:266:LEU:N	1.96	0.80
1:B:100:ALA:H	1:B:270:HIS:HD2	1.28	0.80
1:B:49:GLN:HE22	1:B:81:ARG:HH21	1.29	0.80
1:C:208:ASN:ND2	1:C:273:ILE:H	1.80	0.79
1:A:106:MET:SD	1:A:145:GLY:O	2.41	0.79
1:B:249:VAL:HG13	1:B:386:MET:HE2	1.64	0.79
1:A:193:PRO:HG3	3:A:3273:HOH:O	1.81	0.79
1:B:221:HIS:HA	2:B:3046:MYR:H61	1.65	0.79
1:B:161:LEU:HB3	1:B:165:ILE:HD12	1.64	0.78
1:A:210:VAL:H	1:A:221:HIS:CE1	2.01	0.78
1:B:140:LEU:HD21	1:B:202:ILE:HD11	1.64	0.78
1:C:102:ILE:HD12	1:C:102:ILE:N	1.98	0.78
1:C:210:VAL:H	1:C:221:HIS:CE1	2.00	0.78
1:D:87:PRO:HG3	2:D:3048:MYR:H21	1.65	0.78
1:A:142:THR:HG22	1:A:144:THR:H	1.48	0.78
1:C:379:PRO:C	1:C:381:VAL:H	1.84	0.78
1:B:211:PHE:H	1:B:221:HIS:CE1	2.02	0.77
1:D:148:ALA:HB1	1:D:149:PRO:HD3	1.64	0.77
1:C:161:LEU:HB3	1:C:165:ILE:HD12	1.66	0.77
1:D:216:ASN:HD21	1:D:277:LEU:H	1.32	0.77
1:C:148:ALA:HB2	1:D:265:VAL:HG13	1.65	0.77
1:B:208:ASN:HD22	1:B:273:ILE:H	1.33	0.76
1:C:100:ALA:H	1:C:270:HIS:HD2	1.33	0.76
1:D:142:THR:HG22	1:D:144:THR:H	1.51	0.76
1:D:336:GLN:H	1:D:336:GLN:NE2	1.83	0.75
1:D:210:VAL:H	1:D:221:HIS:CE1	2.03	0.75
1:D:162:SER:HB3	1:D:165:ILE:HG13	1.69	0.75
1:C:142:THR:HG23	1:C:202:ILE:O	1.86	0.75
1:D:49:GLN:HG2	3:D:3112:HOH:O	1.87	0.74
1:D:100:ALA:N	1:D:270:HIS:HD2	1.82	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASN:HD22	1:C:273:ILE:H	1.35	0.74
1:A:221:HIS:HA	2:A:3045:MYR:H61	1.70	0.74
1:A:92:PHE:HB3	1:A:96:ARG:HD3	1.69	0.74
1:A:336:GLN:H	1:A:336:GLN:HE21	1.34	0.74
1:C:102:ILE:HD12	1:C:102:ILE:H	1.48	0.74
1:B:379:PRO:C	1:B:381:VAL:H	1.87	0.74
1:A:114:VAL:HB	1:A:115:PRO:HD3	1.70	0.73
1:A:270:HIS:N	1:B:102:ILE:HD11	2.02	0.73
1:A:100:ALA:H	1:A:270:HIS:HD2	1.35	0.73
1:D:226:ASP:O	1:D:347:MET:HE2	1.88	0.73
1:C:49:GLN:NE2	1:C:81:ARG:HH21	1.86	0.73
1:A:208:ASN:ND2	1:A:273:ILE:H	1.86	0.73
1:A:379:PRO:C	1:A:381:VAL:H	1.89	0.73
1:C:329:ILE:CG2	1:C:333:LEU:HD12	2.18	0.72
1:C:148:ALA:HB1	1:D:265:VAL:HA	1.72	0.72
1:D:242:LEU:HB2	1:D:391:ILE:HD12	1.71	0.72
1:A:216:ASN:HD21	1:A:277:LEU:H	1.36	0.72
1:C:221:HIS:HA	2:C:3047:MYR:H61	1.70	0.72
1:C:255:GLN:HE21	1:D:164:SER:HB3	1.55	0.72
1:D:208:ASN:ND2	1:D:273:ILE:H	1.85	0.72
1:C:148:ALA:CB	1:D:266:LEU:H	2.02	0.72
1:D:257:LEU:HD12	1:D:381:VAL:HG12	1.71	0.72
1:B:208:ASN:ND2	1:B:273:ILE:H	1.86	0.72
1:B:242:LEU:HB2	1:B:391:ILE:CD1	2.20	0.72
1:D:379:PRO:C	1:D:381:VAL:H	1.93	0.72
1:B:162:SER:HB3	1:B:165:ILE:HG13	1.72	0.71
1:C:270:HIS:N	1:D:102:ILE:HD11	2.05	0.71
1:A:216:ASN:ND2	1:A:277:LEU:H	1.89	0.71
1:B:114:VAL:HB	1:B:115:PRO:HD3	1.72	0.70
1:B:92:PHE:HB3	1:B:96:ARG:HH11	1.56	0.70
1:D:78:ILE:HG12	1:D:341:LEU:HD22	1.71	0.70
1:A:242:LEU:HB2	1:A:391:ILE:CD1	2.20	0.70
1:C:148:ALA:HB2	1:D:266:LEU:H	1.58	0.69
1:C:106:MET:SD	1:C:145:GLY:O	2.51	0.69
1:D:242:LEU:HB2	1:D:391:ILE:CD1	2.22	0.69
1:C:147:ILE:O	1:C:148:ALA:O	2.09	0.69
1:A:261:GLU:HG3	1:B:157:LYS:HZ1	1.58	0.69
1:B:42:THR:HG21	1:B:82:ARG:HG3	1.74	0.69
1:B:336:GLN:H	1:B:336:GLN:NE2	1.90	0.69
1:C:362:GLN:HG3	3:C:3103:HOH:O	1.91	0.69
1:A:148:ALA:HB1	1:A:149:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:HD3	3:B:3158:HOH:O	1.91	0.69
1:C:344:PHE:HB3	1:C:347:MET:CE	2.20	0.69
1:D:88:LEU:HD12	3:D:3122:HOH:O	1.92	0.68
1:D:233:ILE:HD12	1:D:233:ILE:N	2.08	0.68
1:C:148:ALA:CB	1:D:265:VAL:HG13	2.23	0.68
1:A:38:LEU:CD1	1:A:356:LEU:HD12	2.24	0.68
1:A:69:ILE:HB	1:A:70:PRO:HD3	1.74	0.68
1:A:261:GLU:HG3	1:B:157:LYS:NZ	2.09	0.68
1:C:151:VAL:HG11	1:C:202:ILE:CD1	2.24	0.68
1:B:321:GLU:HG3	3:B:3190:HOH:O	1.93	0.68
1:D:148:ALA:CB	1:D:149:PRO:CD	2.71	0.68
1:B:71:ARG:HG3	3:B:3250:HOH:O	1.94	0.68
1:B:100:ALA:H	1:B:270:HIS:CD2	2.11	0.68
1:D:215:ILE:HD12	1:D:215:ILE:N	2.02	0.68
1:B:274:THR:HG22	1:B:275:CYS:N	2.10	0.67
1:C:329:ILE:HG22	1:C:330:SER:N	2.07	0.67
1:B:266:LEU:HD22	2:B:3046:MYR:H141	1.77	0.67
1:C:216:ASN:HD21	1:C:277:LEU:H	1.41	0.67
1:B:78:ILE:HG12	1:B:341:LEU:HD22	1.76	0.67
1:C:171:ASN:HD22	1:D:171:ASN:HB2	1.56	0.67
1:D:257:LEU:HD12	1:D:381:VAL:CG1	2.25	0.67
1:D:148:ALA:CB	1:D:149:PRO:HD3	2.24	0.67
1:A:40:THR:HG23	1:A:354:PHE:CZ	2.30	0.66
1:A:329:ILE:HG23	1:A:333:LEU:HD12	1.76	0.66
1:A:208:ASN:HD22	1:A:273:ILE:H	1.42	0.66
1:B:57:ALA:HA	1:B:69:ILE:HD12	1.77	0.66
1:B:242:LEU:HB2	1:B:391:ILE:HD13	1.77	0.66
1:B:186:THR:HG22	3:B:3053:HOH:O	1.95	0.66
1:D:151:VAL:HG11	1:D:202:ILE:CD1	2.25	0.66
1:A:336:GLN:H	1:A:336:GLN:NE2	1.94	0.66
1:A:142:THR:HG23	1:A:202:ILE:O	1.96	0.66
1:B:214:ASP:OD1	1:B:217:ASP:HB2	1.96	0.66
1:C:270:HIS:CA	1:D:102:ILE:HD11	2.26	0.66
1:D:49:GLN:HE22	1:D:81:ARG:NH2	1.86	0.66
1:A:186:THR:HG22	3:A:3072:HOH:O	1.96	0.65
1:C:171:ASN:HB2	1:D:171:ASN:HD22	1.59	0.65
1:B:42:THR:CG2	1:B:82:ARG:HG3	2.27	0.65
1:C:237:GLN:HE22	1:C:239:GLN:HG3	1.59	0.65
1:C:365:SER:OG	1:C:367:LYS:HG2	1.96	0.65
1:C:214:ASP:HB2	3:C:3065:HOH:O	1.97	0.65
1:A:72:VAL:HG22	1:A:72:VAL:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:HB	1:B:70:PRO:HD3	1.77	0.65
1:A:211:PHE:H	1:A:221:HIS:CE1	2.15	0.64
1:B:142:THR:HG23	1:B:202:ILE:O	1.97	0.64
1:A:171:ASN:HD22	1:B:171:ASN:HB2	1.63	0.64
1:B:161:LEU:HB3	1:B:165:ILE:CD1	2.28	0.64
1:A:308:ASP:O	1:A:309:LEU:HB2	1.98	0.64
1:A:68:ARG:O	1:A:72:VAL:HG12	1.98	0.64
1:D:274:THR:HG23	3:D:3103:HOH:O	1.96	0.64
1:A:255:GLN:HG3	1:A:292:VAL:HG13	1.80	0.64
1:B:239:GLN:HE22	1:C:330:SER:HA	1.61	0.64
1:B:274:THR:HG22	1:B:275:CYS:H	1.63	0.64
1:B:379:PRO:C	1:B:381:VAL:N	2.51	0.63
1:A:27:ALA:HB3	1:C:325:ARG:HD3	1.81	0.63
1:A:164:SER:HB3	1:B:255:GLN:HE21	1.62	0.63
1:B:365:SER:OG	1:B:367:LYS:HG2	1.99	0.63
1:C:162:SER:HB3	1:C:165:ILE:HG13	1.81	0.63
1:A:81:ARG:HG2	3:A:3059:HOH:O	1.99	0.63
1:B:220:ILE:HG13	1:B:221:HIS:HD2	1.64	0.62
1:C:148:ALA:HB1	1:C:149:PRO:HD2	1.81	0.62
1:C:314:PRO:HB2	1:C:341:LEU:HB2	1.81	0.62
1:A:301:GLY:N	1:C:215:ILE:HD11	2.14	0.62
1:A:148:ALA:HB1	1:B:265:VAL:HA	1.81	0.62
1:D:224:PHE:HB2	2:D:3048:MYR:H62	1.82	0.62
1:C:49:GLN:HE22	1:C:81:ARG:NH2	1.94	0.62
1:C:255:GLN:HG2	3:C:3282:HOH:O	2.00	0.62
1:A:148:ALA:CB	1:A:149:PRO:CD	2.78	0.61
1:D:42:THR:CG2	1:D:82:ARG:HG3	2.30	0.61
1:C:265:VAL:HA	1:D:148:ALA:HB1	1.81	0.61
1:A:91:LYS:HG3	1:A:92:PHE:H	1.64	0.61
1:A:243:GLU:HG2	3:A:3142:HOH:O	1.98	0.61
1:C:148:ALA:HB1	1:C:149:PRO:CD	2.30	0.61
1:C:288:GLY:O	1:C:292:VAL:HG23	2.01	0.61
1:D:119:ASP:O	1:D:123:ARG:HG3	2.01	0.61
1:D:81:ARG:HG2	3:D:3112:HOH:O	1.99	0.61
1:B:314:PRO:HG2	3:B:3085:HOH:O	2.01	0.61
1:C:100:ALA:H	1:C:270:HIS:CD2	2.18	0.61
1:A:226:ASP:O	1:A:347:MET:HE2	2.00	0.60
1:D:365:SER:OG	1:D:367:LYS:HG2	2.02	0.60
1:C:148:ALA:CB	1:C:149:PRO:HD2	2.32	0.60
1:A:91:LYS:HG3	1:A:92:PHE:N	2.17	0.60
1:A:189:VAL:HG13	1:A:235:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:H	1:B:221:HIS:CE1	2.13	0.60
1:D:38:LEU:HD23	1:D:39:ALA:N	2.16	0.60
1:D:260:THR:OG1	1:D:381:VAL:HB	2.01	0.60
1:B:102:ILE:HD12	1:B:103:ARG:H	1.66	0.60
1:C:315:GLY:C	1:C:319:ILE:HD12	2.21	0.60
1:C:244:PRO:HG3	1:C:393:ARG:HA	1.83	0.59
1:A:270:HIS:CA	1:B:102:ILE:HD11	2.33	0.59
1:C:93:ASP:HA	1:C:96:ARG:HD3	1.85	0.59
1:C:243:GLU:HG2	3:C:3089:HOH:O	2.02	0.59
1:C:270:HIS:HA	1:D:102:ILE:HD11	1.85	0.59
1:D:146:PHE:HE1	1:D:171:ASN:HB3	1.67	0.59
1:A:100:ALA:H	1:A:270:HIS:CD2	2.19	0.59
1:A:317:PRO:O	1:A:321:GLU:HB2	2.03	0.59
1:A:329:ILE:CG2	1:A:333:LEU:HD12	2.32	0.59
1:D:176:ALA:HB3	3:D:3157:HOH:O	2.02	0.59
1:D:211:PHE:H	1:D:221:HIS:CE1	2.21	0.59
1:A:308:ASP:O	1:A:371:THR:O	2.21	0.59
1:B:352:LEU:HB2	3:B:3227:HOH:O	2.02	0.59
1:C:336:GLN:H	1:C:336:GLN:NE2	2.00	0.59
1:A:110:TYR:HD1	1:A:147:ILE:HD13	1.68	0.58
1:D:52:ALA:O	1:D:56:VAL:HG23	2.03	0.58
1:B:91:LYS:HG3	1:B:92:PHE:H	1.68	0.58
1:D:336:GLN:HE21	1:D:336:GLN:N	1.92	0.58
1:A:301:GLY:CA	1:C:215:ILE:HD11	2.34	0.58
1:C:148:ALA:HB2	1:D:266:LEU:N	2.19	0.58
1:D:162:SER:HB3	1:D:165:ILE:CG1	2.34	0.58
1:D:162:SER:H	1:D:165:ILE:HD11	1.67	0.58
1:D:243:GLU:HG3	1:D:246:LYS:HD3	1.84	0.58
1:A:118:VAL:HG11	1:A:158:GLU:HG2	1.85	0.58
1:D:178:ALA:HB3	3:D:3055:HOH:O	2.04	0.58
1:C:32:VAL:HG11	1:C:248:VAL:HG13	1.85	0.58
1:B:260:THR:OG1	1:B:381:VAL:HB	2.04	0.58
1:C:59:LEU:HD22	1:C:96:ARG:NH2	2.18	0.58
1:D:161:LEU:HB3	1:D:165:ILE:CD1	2.31	0.58
1:D:57:ALA:HA	1:D:69:ILE:HD12	1.86	0.57
1:B:68:ARG:O	1:B:71:ARG:HB2	2.05	0.57
1:C:211:PHE:H	1:C:221:HIS:CE1	2.23	0.57
1:D:42:THR:HG21	1:D:82:ARG:HG3	1.84	0.57
1:B:32:VAL:HG13	1:B:248:VAL:HG13	1.85	0.57
1:D:46:VAL:HG22	1:D:82:ARG:NE	2.20	0.56
1:A:157:LYS:HZ1	1:B:261:GLU:HG3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ASP:O	1:D:278:SER:HB2	2.04	0.56
1:C:38:LEU:HD23	1:C:39:ALA:N	2.20	0.56
1:C:102:ILE:HG13	1:C:270:HIS:O	2.05	0.56
1:B:119:ASP:OD2	1:B:123:ARG:NH2	2.38	0.56
1:C:147:ILE:N	1:C:147:ILE:HD12	2.20	0.56
1:B:274:THR:HG23	3:B:3064:HOH:O	2.06	0.56
1:A:308:ASP:O	1:A:309:LEU:CB	2.54	0.56
1:B:102:ILE:HG13	1:B:270:HIS:O	2.06	0.56
1:C:148:ALA:CB	1:C:149:PRO:CD	2.84	0.56
1:C:36:GLU:OE2	1:C:234:GLY:HA3	2.06	0.56
1:A:257:LEU:HD12	1:A:381:VAL:HG12	1.88	0.56
1:A:344:PHE:HB3	1:A:347:MET:CE	2.36	0.56
1:B:85:VAL:HG13	1:B:92:PHE:CE2	2.41	0.56
1:B:226:ASP:O	1:B:347:MET:HE3	2.06	0.55
1:D:92:PHE:HB3	1:D:96:ARG:HD3	1.88	0.55
1:D:265:VAL:HB	1:D:276:GLU:HB2	1.88	0.55
1:A:86:ASP:HB3	1:A:89:ASP:HB2	1.87	0.55
1:C:151:VAL:HG11	1:C:202:ILE:HD11	1.88	0.55
1:C:111:GLU:HG3	3:C:3297:HOH:O	2.05	0.55
1:C:329:ILE:CG2	1:C:330:SER:N	2.69	0.55
1:B:32:VAL:CG1	1:B:248:VAL:HG13	2.37	0.55
1:C:114:VAL:HB	1:C:115:PRO:HD3	1.87	0.55
1:B:216:ASN:HD21	1:B:277:LEU:N	1.95	0.55
1:D:221:HIS:HA	2:D:3048:MYR:H72	1.89	0.55
1:A:288:GLY:O	1:A:292:VAL:HG23	2.07	0.55
1:B:67:GLU:O	1:B:70:PRO:HD2	2.07	0.54
1:A:220:ILE:HG13	1:A:224:PHE:CZ	2.41	0.54
1:B:57:ALA:HA	1:B:69:ILE:CD1	2.36	0.54
1:A:379:PRO:C	1:A:381:VAL:N	2.60	0.54
1:C:229:ALA:HB1	1:C:353:ILE:HG21	1.89	0.54
1:B:280:ASN:N	1:B:280:ASN:HD22	2.03	0.54
1:A:237:GLN:O	1:A:240:GLU:HG2	2.08	0.54
1:D:142:THR:HG22	1:D:143:SER:N	2.21	0.54
1:B:239:GLN:NE2	1:C:330:SER:HA	2.23	0.54
1:A:171:ASN:HB2	1:B:171:ASN:HD22	1.72	0.54
1:C:232:VAL:C	1:C:233:ILE:HD12	2.28	0.54
1:A:285:ILE:O	1:A:289:VAL:HG23	2.09	0.54
1:B:87:PRO:HG3	2:B:3046:MYR:H22	1.89	0.53
1:B:211:PHE:H	1:B:221:HIS:HE1	1.51	0.53
1:C:117:ALA:HB2	1:C:202:ILE:CD1	2.39	0.53
1:B:182:LEU:HD21	1:B:386:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:GLU:HG3	3:C:3346:HOH:O	2.08	0.53
1:A:126:ALA:HB3	3:A:3106:HOH:O	2.08	0.53
1:D:148:ALA:HB1	1:D:149:PRO:CD	2.37	0.53
1:A:154:ALA:O	1:A:158:GLU:HB2	2.08	0.53
1:A:157:LYS:NZ	1:B:261:GLU:HG3	2.23	0.53
1:A:177:ALA:HA	1:A:180:ASN:HD22	1.74	0.53
1:C:274:THR:HG22	1:C:275:CYS:N	2.24	0.53
1:D:51:ASP:O	1:D:55:ARG:HG3	2.09	0.53
1:C:38:LEU:HD23	1:C:38:LEU:C	2.29	0.53
1:D:138:LEU:HD13	1:D:198:LEU:HD23	1.90	0.53
1:A:261:GLU:HB2	3:A:3086:HOH:O	2.08	0.53
1:B:38:LEU:C	1:B:38:LEU:HD23	2.29	0.53
1:C:193:PRO:HG3	3:C:3085:HOH:O	2.09	0.52
1:A:347:MET:HE3	3:A:3070:HOH:O	2.10	0.52
1:C:102:ILE:O	1:C:106:MET:HG2	2.09	0.52
1:D:313:HIS:CE1	1:D:351:SER:HB2	2.44	0.52
1:A:42:THR:OG1	1:A:82:ARG:HG3	2.09	0.52
1:C:261:GLU:HG3	1:D:157:LYS:NZ	2.23	0.52
1:C:274:THR:HG22	1:C:275:CYS:H	1.73	0.52
1:D:243:GLU:CG	1:D:246:LYS:HD3	2.40	0.52
1:D:45:ARG:HD2	3:D:3246:HOH:O	2.09	0.52
1:A:148:ALA:CB	1:A:149:PRO:HD3	2.37	0.52
1:D:148:ALA:HB3	1:D:149:PRO:CD	2.40	0.52
1:D:177:ALA:HB3	1:D:349:SER:HB3	1.91	0.52
1:A:254:SER:O	1:B:164:SER:HA	2.09	0.52
1:B:91:LYS:HG3	1:B:92:PHE:N	2.25	0.52
1:D:258:ASP:O	1:D:260:THR:HG23	2.09	0.52
1:C:304:ILE:HG23	1:C:329:ILE:HD11	1.91	0.52
1:B:49:GLN:NE2	1:B:81:ARG:HH21	2.04	0.52
1:C:275:CYS:HB2	2:C:3047:MYR:H131	1.91	0.52
1:D:142:THR:HG23	1:D:202:ILE:O	2.10	0.52
1:A:295:GLU:HA	1:A:295:GLU:OE1	2.10	0.52
1:B:79:THR:HG22	1:B:80:THR:HG23	1.92	0.52
1:B:242:LEU:HD12	1:B:391:ILE:HD11	1.91	0.52
1:D:32:VAL:CG1	1:D:248:VAL:HG13	2.40	0.52
1:B:215:ILE:O	1:B:219:VAL:HG23	2.10	0.51
1:C:336:GLN:H	1:C:336:GLN:HE21	1.58	0.51
1:A:344:PHE:HB3	1:A:347:MET:HE3	1.93	0.51
1:C:161:LEU:HB3	1:C:165:ILE:CD1	2.39	0.51
1:C:257:LEU:HD12	1:C:381:VAL:CG1	2.40	0.51
1:A:72:VAL:HG11	1:A:218:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:HG2	3:B:3115:HOH:O	2.09	0.51
1:A:257:LEU:HD12	1:A:381:VAL:CG1	2.40	0.51
1:B:203:GLU:HG2	1:B:348:LEU:CB	2.23	0.51
1:B:336:GLN:HE21	1:B:336:GLN:N	2.03	0.51
1:B:77:ARG:HD3	1:B:338:TRP:CZ3	2.46	0.51
1:B:130:TYR:CE1	1:B:196:LYS:HE3	2.45	0.51
1:D:102:ILE:HG13	1:D:270:HIS:O	2.10	0.51
1:D:220:ILE:HD11	1:D:277:LEU:HD12	1.93	0.51
1:B:177:ALA:HB3	1:B:349:SER:HB3	1.93	0.51
1:B:243:GLU:HG2	3:B:3141:HOH:O	2.10	0.51
1:D:229:ALA:HB1	1:D:353:ILE:HG21	1.93	0.51
1:A:30:THR:OG1	1:C:283:GLY:HA2	2.11	0.51
1:A:72:VAL:HG11	1:A:218:VAL:CG1	2.41	0.51
1:A:128:LEU:HG	1:A:130:TYR:CE2	2.46	0.51
1:A:214:ASP:HB2	3:A:3049:HOH:O	2.10	0.51
1:D:77:ARG:HD3	1:D:338:TRP:CZ3	2.46	0.51
1:D:122:LYS:HE2	3:D:3132:HOH:O	2.11	0.51
1:B:226:ASP:O	1:B:347:MET:CE	2.59	0.51
1:C:102:ILE:H	1:C:102:ILE:CD1	2.13	0.50
1:D:32:VAL:HG13	3:D:3245:HOH:O	2.10	0.50
1:D:210:VAL:N	1:D:221:HIS:HE1	2.00	0.50
1:C:102:ILE:HD11	1:D:270:HIS:CA	2.41	0.50
1:C:148:ALA:N	1:D:266:LEU:O	2.45	0.50
1:A:110:TYR:CD1	1:A:147:ILE:HD13	2.46	0.50
1:A:102:ILE:O	1:A:106:MET:HG2	2.11	0.50
1:A:304:ILE:HG13	3:A:3078:HOH:O	2.11	0.50
1:A:329:ILE:CG2	1:A:330:SER:N	2.73	0.50
1:B:38:LEU:HD23	1:B:39:ALA:N	2.26	0.50
1:B:318:LYS:HA	1:B:321:GLU:HB3	1.92	0.50
1:C:273:ILE:HG22	2:C:3047:MYR:H122	1.94	0.50
1:B:199:VAL:O	1:B:230:ALA:HA	2.11	0.50
1:D:114:VAL:HB	1:D:115:PRO:HD3	1.94	0.50
1:B:214:ASP:O	1:B:218:VAL:HG23	2.12	0.50
1:C:102:ILE:HD11	1:D:270:HIS:HB3	1.94	0.50
1:C:368:ALA:O	1:C:369:ILE:HB	2.12	0.50
1:D:279:GLU:H	1:D:279:GLU:CD	2.14	0.50
1:C:148:ALA:O	1:C:149:PRO:C	2.46	0.50
1:C:152:ASP:O	1:C:156:VAL:HG23	2.12	0.50
1:D:379:PRO:C	1:D:381:VAL:N	2.63	0.50
1:A:40:THR:HG23	1:A:354:PHE:CE1	2.46	0.49
1:A:314:PRO:HG2	3:A:3174:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:PRO:O	1:B:381:VAL:N	2.45	0.49
1:C:93:ASP:O	1:C:96:ARG:HG2	2.11	0.49
1:B:162:SER:HB3	1:B:165:ILE:CG1	2.42	0.49
1:C:221:HIS:NE2	2:C:3047:MYR:H72	2.27	0.49
1:D:136:GLY:HA3	1:D:188:TYR:OH	2.12	0.49
1:A:147:ILE:O	1:A:148:ALA:O	2.30	0.49
1:C:146:PHE:CD1	1:C:146:PHE:N	2.81	0.49
1:A:304:ILE:HG22	1:A:329:ILE:HD11	1.93	0.49
1:A:356:LEU:O	1:A:360:VAL:HG23	2.13	0.49
1:C:190:ARG:HD3	3:C:3077:HOH:O	2.12	0.49
1:C:233:ILE:HD12	1:C:233:ILE:N	2.27	0.49
1:C:304:ILE:CG2	1:C:329:ILE:HD11	2.43	0.49
1:A:221:HIS:CD2	2:A:3045:MYR:H72	2.48	0.49
1:D:102:ILE:HD12	1:D:103:ARG:H	1.77	0.49
1:D:221:HIS:HA	2:D:3048:MYR:C7	2.43	0.49
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.77	0.49
1:B:110:TYR:O	1:B:114:VAL:HG23	2.13	0.49
1:B:227:GLY:HA3	1:B:347:MET:HE2	1.94	0.49
1:C:148:ALA:HB2	1:D:265:VAL:CG1	2.40	0.49
1:A:210:VAL:N	1:A:221:HIS:HE1	1.95	0.49
1:D:72:VAL:O	1:D:72:VAL:HG22	2.13	0.49
1:D:162:SER:O	1:D:165:ILE:HG13	2.12	0.48
1:B:224:PHE:CD1	1:B:224:PHE:N	2.81	0.48
1:C:210:VAL:N	1:C:221:HIS:HE1	1.97	0.48
1:C:260:THR:OG1	1:C:381:VAL:HB	2.12	0.48
1:C:380:GLY:H	1:D:149:PRO:HG3	1.78	0.48
1:D:69:ILE:HB	1:D:70:PRO:HD3	1.94	0.48
1:D:217:ASP:O	1:D:221:HIS:HD2	1.96	0.48
1:C:171:ASN:HB2	1:D:171:ASN:HB2	1.94	0.48
1:B:77:ARG:HD3	1:B:338:TRP:HZ3	1.79	0.48
1:B:89:ASP:OD1	1:B:91:LYS:HG2	2.14	0.48
1:C:215:ILE:O	1:C:219:VAL:HG23	2.14	0.48
1:A:38:LEU:HD23	1:A:38:LEU:C	2.34	0.48
1:A:301:GLY:H	1:C:215:ILE:HD11	1.77	0.48
1:B:216:ASN:ND2	1:B:277:LEU:H	2.00	0.48
3:A:3057:HOH:O	1:B:102:ILE:HD12	2.14	0.48
1:A:365:SER:OG	1:A:367:LYS:HG2	2.12	0.48
1:B:221:HIS:CD2	2:B:3046:MYR:H72	2.48	0.48
1:D:329:ILE:HB	1:D:333:LEU:HD12	1.96	0.48
1:B:288:GLY:O	1:B:292:VAL:HG23	2.14	0.47
1:B:357:GLU:O	1:B:361:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLN:HG3	3:B:3145:HOH:O	2.13	0.47
1:C:203:GLU:HG2	1:C:348:LEU:CB	2.32	0.47
1:D:109:PHE:CZ	1:D:142:THR:HG21	2.48	0.47
1:A:224:PHE:CD1	1:A:224:PHE:N	2.80	0.47
1:A:148:ALA:O	1:A:149:PRO:C	2.49	0.47
1:C:102:ILE:HD11	1:D:270:HIS:HA	1.97	0.47
1:C:215:ILE:HD12	1:C:215:ILE:H	1.78	0.47
1:D:130:TYR:CE1	1:D:196:LYS:HE3	2.49	0.47
1:B:182:LEU:HD23	1:B:386:MET:HE3	1.95	0.47
1:D:101:THR:HG22	3:D:3264:HOH:O	2.13	0.47
1:B:237:GLN:HE22	1:C:331:ALA:CB	2.28	0.47
1:C:77:ARG:HG3	1:C:317:PRO:HB3	1.95	0.47
1:A:220:ILE:HG13	1:A:224:PHE:CE2	2.50	0.47
1:C:164:SER:HB3	1:D:255:GLN:HE21	1.80	0.47
1:A:71:ARG:C	1:A:73:TYR:H	2.18	0.46
1:C:102:ILE:HG13	1:C:270:HIS:C	2.36	0.46
1:B:92:PHE:HB3	1:B:96:ARG:NH1	2.27	0.46
1:C:189:VAL:HG13	1:C:235:ALA:CB	2.40	0.46
1:A:253:PHE:CD2	1:A:296:MET:HG3	2.50	0.46
1:C:93:ASP:HA	1:C:96:ARG:CD	2.43	0.46
1:C:315:GLY:HA3	1:C:319:ILE:HD12	1.97	0.46
1:A:35:ILE:HB	1:A:247:VAL:HB	1.97	0.46
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.31	0.46
1:D:208:ASN:HB2	2:D:3048:MYR:H101	1.98	0.46
1:D:356:LEU:HD13	1:D:356:LEU:O	2.15	0.46
1:D:288:GLY:O	1:D:292:VAL:HG23	2.16	0.46
1:A:266:LEU:HB2	1:B:148:ALA:HB3	1.98	0.46
1:B:102:ILE:HG23	1:B:272:GLY:N	2.31	0.46
1:B:274:THR:CG2	1:B:275:CYS:N	2.78	0.46
1:A:368:ALA:O	1:A:369:ILE:HB	2.15	0.46
1:B:249:VAL:HG13	1:B:386:MET:CE	2.41	0.46
1:D:176:ALA:HB1	1:D:384:GLU:HG3	1.97	0.46
1:C:203:GLU:HG3	1:C:348:LEU:HD22	1.97	0.46
1:D:40:THR:O	1:D:123:ARG:NH2	2.36	0.46
1:D:227:GLY:HA3	1:D:347:MET:CE	2.46	0.46
1:B:92:PHE:CD1	1:B:96:ARG:NH1	2.84	0.46
1:A:70:PRO:O	1:A:74:GLN:HG2	2.16	0.45
1:A:279:GLU:HG2	3:A:3112:HOH:O	2.14	0.45
1:A:344:PHE:CD1	1:A:347:MET:HE1	2.50	0.45
1:B:182:LEU:CD2	1:B:386:MET:HE1	2.46	0.45
1:C:109:PHE:CZ	1:C:142:THR:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:HD12	1:B:233:ILE:N	2.30	0.45
1:D:92:PHE:HB3	1:D:96:ARG:HH11	1.81	0.45
1:A:220:ILE:HG22	1:A:221:HIS:CD2	2.51	0.45
1:C:102:ILE:HD11	1:D:270:HIS:CB	2.46	0.45
1:A:87:PRO:HG3	2:A:3045:MYR:C2	2.46	0.45
1:C:142:THR:HG22	1:C:143:SER:N	2.31	0.45
1:D:57:ALA:HA	1:D:69:ILE:CD1	2.45	0.45
1:A:38:LEU:HD12	1:A:356:LEU:HD12	1.98	0.45
1:A:131:ARG:HH11	1:A:132:ALA:H	1.64	0.45
1:A:176:ALA:HB1	1:A:384:GLU:HB3	1.99	0.45
1:B:358:THR:O	1:B:362:GLN:HG2	2.15	0.45
1:C:375:PHE:HA	1:C:384:GLU:O	2.17	0.45
1:D:49:GLN:HG3	1:D:78:ILE:O	2.17	0.45
1:D:87:PRO:CG	2:D:3048:MYR:H21	2.40	0.45
1:D:102:ILE:O	1:D:106:MET:HG2	2.15	0.45
1:C:255:GLN:HG3	1:C:292:VAL:HG13	1.98	0.45
1:A:87:PRO:HG3	2:A:3045:MYR:H21	1.98	0.45
1:A:260:THR:OG1	1:A:381:VAL:HB	2.16	0.45
1:A:301:GLY:HA2	1:C:215:ILE:HD11	1.99	0.45
1:B:196:LYS:NZ	3:B:3168:HOH:O	2.50	0.45
1:B:239:GLN:NE2	3:B:3159:HOH:O	2.49	0.45
1:B:280:ASN:N	1:B:280:ASN:ND2	2.65	0.45
1:C:145:GLY:O	1:C:146:PHE:CB	2.64	0.45
1:A:199:VAL:O	1:A:230:ALA:HA	2.17	0.45
1:C:26:PRO:HG3	1:D:237:GLN:HG2	1.99	0.45
1:A:164:SER:HB3	1:B:255:GLN:NE2	2.31	0.44
1:A:304:ILE:CG2	1:A:329:ILE:HD11	2.47	0.44
1:A:167:ARG:NH2	1:B:382:THR:HG21	2.32	0.44
1:C:148:ALA:CB	1:D:265:VAL:HA	2.45	0.44
1:D:140:LEU:HD21	1:D:202:ILE:HD11	1.98	0.44
1:B:56:VAL:HG12	1:B:69:ILE:HD13	1.99	0.44
1:B:81:ARG:HH22	1:B:222:SER:HA	1.81	0.44
1:C:315:GLY:CA	1:C:319:ILE:HD12	2.47	0.44
1:D:368:ALA:O	1:D:369:ILE:HB	2.16	0.44
1:C:266:LEU:HD22	2:C:3047:MYR:H141	1.99	0.44
1:D:147:ILE:HD13	1:D:150:GLY:HA2	1.99	0.44
1:D:224:PHE:CD1	1:D:224:PHE:N	2.86	0.44
1:A:148:ALA:HB3	1:A:149:PRO:CD	2.48	0.44
1:B:182:LEU:HD23	1:B:386:MET:CE	2.48	0.44
1:B:237:GLN:HE22	1:C:331:ALA:HB2	1.82	0.44
1:D:85:VAL:HG13	1:D:92:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ILE:O	1:D:148:ALA:O	2.36	0.44
1:D:211:PHE:HA	3:D:3191:HOH:O	2.17	0.44
1:A:298:TRP:CZ3	1:C:215:ILE:HG23	2.53	0.44
1:B:117:ALA:HB1	1:B:155:ILE:HD11	1.99	0.44
1:B:142:THR:O	1:B:171:ASN:HA	2.17	0.44
1:A:242:LEU:HD12	1:A:391:ILE:HD11	2.00	0.44
1:A:368:ALA:O	3:A:3124:HOH:O	2.21	0.44
1:C:70:PRO:O	1:C:74:GLN:HG2	2.18	0.44
1:C:379:PRO:C	1:C:381:VAL:N	2.58	0.44
1:A:144:THR:HG22	2:A:3045:MYR:H121	1.98	0.43
1:A:176:ALA:HB1	1:A:384:GLU:CB	2.48	0.43
1:B:262:ASP:O	1:B:278:SER:HB2	2.18	0.43
3:A:3328:HOH:O	1:B:164:SER:HB3	2.17	0.43
1:A:67:GLU:O	1:A:70:PRO:HD2	2.18	0.43
1:B:114:VAL:O	1:B:118:VAL:HG23	2.17	0.43
1:C:329:ILE:CG2	1:C:330:SER:H	2.31	0.43
1:A:38:LEU:HD11	1:A:356:LEU:HD12	2.00	0.43
1:A:145:GLY:O	1:A:146:PHE:CB	2.66	0.43
1:A:156:VAL:HG13	1:A:161:LEU:HB2	2.00	0.43
1:A:270:HIS:HA	1:B:102:ILE:HD11	1.99	0.43
1:A:329:ILE:HG22	1:A:330:SER:N	2.31	0.43
1:C:32:VAL:HG11	1:C:248:VAL:CG1	2.47	0.43
1:C:274:THR:HG23	3:C:3059:HOH:O	2.18	0.43
1:D:355:VAL:O	1:D:359:MET:HG3	2.18	0.43
1:C:369:ILE:HA	1:C:390:ILE:O	2.19	0.43
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.92	0.43
1:A:148:ALA:O	1:A:150:GLY:N	2.52	0.43
1:A:224:PHE:N	1:A:224:PHE:HD1	2.16	0.43
1:B:162:SER:HA	1:B:163:PRO:HD3	1.85	0.43
1:D:277:LEU:HD22	1:D:281:LEU:HD12	2.00	0.43
1:C:128:LEU:HD22	3:C:3075:HOH:O	2.18	0.43
1:C:224:PHE:N	1:C:224:PHE:CD1	2.87	0.43
1:A:131:ARG:HD2	1:A:131:ARG:HA	1.92	0.43
1:C:42:THR:HG21	1:C:82:ARG:HG3	2.00	0.43
1:C:49:GLN:HG3	1:C:78:ILE:O	2.18	0.43
1:C:265:VAL:HA	1:D:148:ALA:CB	2.48	0.43
1:A:48:ASN:HB3	1:A:51:ASP:OD2	2.19	0.43
1:A:205:CYS:HB3	2:A:3045:MYR:H52	2.01	0.43
1:C:261:GLU:HG3	1:D:157:LYS:HZ1	1.84	0.43
1:C:285:ILE:O	1:C:289:VAL:HG23	2.18	0.43
1:D:369:ILE:HA	1:D:390:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:HB3	1:B:83:MET:O	2.18	0.43
1:B:102:ILE:O	1:B:106:MET:HG2	2.19	0.43
1:B:249:VAL:HG22	1:B:386:MET:HE1	2.01	0.43
1:B:378:GLY:O	1:B:381:VAL:HA	2.19	0.43
1:C:380:GLY:O	1:C:381:VAL:HB	2.19	0.43
1:D:82:ARG:NH2	3:D:3155:HOH:O	2.41	0.43
1:D:324:VAL:HG13	1:D:329:ILE:HG13	2.00	0.43
1:D:325:ARG:NH2	3:D:3192:HOH:O	2.51	0.42
1:A:237:GLN:OE1	1:A:239:GLN:HB2	2.18	0.42
1:C:43:PRO:HA	3:C:3097:HOH:O	2.18	0.42
1:D:215:ILE:O	1:D:219:VAL:HG23	2.19	0.42
1:A:244:PRO:HG3	1:A:393:ARG:HA	2.01	0.42
1:B:48:ASN:OD1	1:B:50:SER:HB2	2.20	0.42
1:B:85:VAL:O	1:B:87:PRO:HD3	2.19	0.42
1:B:279:GLU:H	1:B:279:GLU:CD	2.17	0.42
1:C:368:ALA:HA	1:C:392:ARG:HB2	2.01	0.42
1:B:154:ALA:O	1:B:158:GLU:HB2	2.20	0.42
1:D:217:ASP:O	1:D:221:HIS:CD2	2.73	0.42
1:D:393:ARG:HB2	3:D:3186:HOH:O	2.19	0.42
1:A:142:THR:O	1:A:171:ASN:HA	2.19	0.42
1:A:189:VAL:HG13	1:A:235:ALA:N	2.35	0.42
1:A:239:GLN:NE2	3:A:3274:HOH:O	2.42	0.42
1:D:87:PRO:HB2	1:D:211:PHE:HE1	1.83	0.42
1:D:117:ALA:HB2	1:D:202:ILE:HD13	2.02	0.42
1:A:336:GLN:HB2	3:A:3076:HOH:O	2.20	0.42
1:B:81:ARG:NH2	1:B:222:SER:HA	2.35	0.42
1:B:224:PHE:N	1:B:224:PHE:HD1	2.17	0.42
1:A:148:ALA:CB	1:B:265:VAL:HA	2.48	0.42
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.85	0.42
1:B:138:LEU:HB3	1:B:167:ARG:HG2	2.01	0.42
1:B:274:THR:CG2	1:B:275:CYS:H	2.31	0.42
1:C:72:VAL:HG11	1:C:218:VAL:HG12	2.00	0.42
1:D:72:VAL:O	1:D:72:VAL:HG13	2.19	0.42
1:B:102:ILE:HG23	1:B:272:GLY:H	1.84	0.42
1:B:375:PHE:HA	1:B:384:GLU:O	2.20	0.41
1:C:220:ILE:HG13	1:C:224:PHE:CZ	2.55	0.41
1:A:290:ALA:HB2	1:A:326:SER:O	2.20	0.41
1:B:369:ILE:HA	1:B:390:ILE:O	2.19	0.41
1:C:117:ALA:HB2	1:C:202:ILE:HD13	2.02	0.41
1:A:157:LYS:HZ2	1:B:261:GLU:CD	2.23	0.41
1:B:265:VAL:O	1:B:275:CYS:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLN:OE1	1:C:239:GLN:HB2	2.19	0.41
1:C:265:VAL:HB	1:C:276:GLU:HB2	2.03	0.41
1:A:51:ASP:O	1:A:55:ARG:HG3	2.21	0.41
1:A:130:TYR:CE1	1:A:196:LYS:HE3	2.54	0.41
1:A:162:SER:HA	1:A:163:PRO:HD3	1.94	0.41
1:B:162:SER:H	1:B:165:ILE:HD11	1.84	0.41
1:C:362:GLN:HG3	1:C:362:GLN:O	2.19	0.41
1:D:142:THR:O	1:D:171:ASN:HA	2.21	0.41
1:D:227:GLY:HA3	1:D:347:MET:HE1	2.02	0.41
1:D:274:THR:HG21	3:D:3312:HOH:O	2.20	0.41
1:D:285:ILE:HG23	1:D:377:PHE:CZ	2.54	0.41
1:D:336:GLN:HB2	3:D:3137:HOH:O	2.19	0.41
1:A:102:ILE:HG23	1:A:103:ARG:N	2.35	0.41
1:A:215:ILE:HD12	3:A:3049:HOH:O	2.20	0.41
1:C:102:ILE:HD13	1:D:270:HIS:N	2.35	0.41
1:C:142:THR:O	1:C:171:ASN:HA	2.21	0.41
1:C:317:PRO:O	1:C:321:GLU:HB2	2.21	0.41
1:D:45:ARG:HB2	1:D:45:ARG:NH1	2.36	0.41
1:D:140:LEU:HD13	1:D:141:ALA:N	2.36	0.41
1:D:162:SER:H	1:D:165:ILE:CD1	2.33	0.41
1:A:220:ILE:HG22	1:A:221:HIS:HD2	1.84	0.41
1:B:81:ARG:HA	1:B:344:PHE:HA	2.02	0.41
1:C:130:TYR:CZ	1:C:196:LYS:HE3	2.56	0.41
1:D:196:LYS:NZ	3:D:3294:HOH:O	2.53	0.41
1:A:304:ILE:HG23	1:A:310:TRP:CZ2	2.56	0.41
1:B:68:ARG:O	1:B:71:ARG:N	2.51	0.41
1:B:142:THR:HG22	1:B:143:SER:N	2.36	0.41
1:C:266:LEU:N	1:D:148:ALA:CB	2.59	0.41
1:D:151:VAL:HG11	1:D:202:ILE:HD11	2.00	0.41
1:D:243:GLU:HG2	3:D:3149:HOH:O	2.19	0.41
1:D:304:ILE:HG23	1:D:310:TRP:CZ2	2.56	0.41
1:D:190:ARG:HD3	3:D:3058:HOH:O	2.21	0.41
1:A:237:GLN:HB3	1:A:240:GLU:HG2	2.02	0.41
1:B:102:ILE:HD12	1:B:102:ILE:N	2.36	0.41
1:B:147:ILE:HD12	1:B:147:ILE:O	2.20	0.41
1:B:221:HIS:NE2	2:B:3046:MYR:H72	2.35	0.41
1:B:348:LEU:HB3	1:B:349:SER:H	1.70	0.41
1:B:356:LEU:HD13	1:B:360:VAL:HG23	2.01	0.41
1:C:101:THR:HA	3:C:3167:HOH:O	2.19	0.41
1:C:162:SER:HB3	1:C:165:ILE:CG1	2.48	0.41
1:C:215:ILE:HD12	1:C:215:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ASP:O	1:C:278:SER:HB2	2.21	0.41
1:C:281:LEU:N	1:C:282:PRO:HD2	2.36	0.41
1:D:130:TYR:CZ	1:D:196:LYS:HE3	2.56	0.41
1:D:147:ILE:H	1:D:147:ILE:HD12	1.86	0.41
1:D:352:LEU:HD12	1:D:352:LEU:HA	1.91	0.41
1:A:91:LYS:CG	1:A:92:PHE:N	2.84	0.41
1:C:162:SER:HA	1:C:163:PRO:HD3	1.98	0.41
1:A:146:PHE:C	1:A:147:ILE:HG13	2.38	0.40
1:B:281:LEU:HB3	1:B:282:PRO:CD	2.51	0.40
1:C:72:VAL:HG11	1:C:218:VAL:CG1	2.51	0.40
1:B:72:VAL:HG13	1:B:73:TYR:HD1	1.85	0.40
1:C:91:LYS:HG3	1:C:92:PHE:N	2.36	0.40
1:C:131:ARG:HG3	3:C:3111:HOH:O	2.21	0.40
1:C:266:LEU:O	1:D:148:ALA:HB2	2.22	0.40
1:D:91:LYS:HG3	1:D:92:PHE:N	2.37	0.40
1:C:371:THR:HB	3:C:3203:HOH:O	2.21	0.40
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.94	0.40
1:C:290:ALA:HB3	1:C:291:PRO:CD	2.51	0.40
1:D:49:GLN:NE2	1:D:81:ARG:NH2	2.56	0.40
1:D:55:ARG:HB2	1:D:88:LEU:HD13	2.02	0.40
1:A:27:ALA:HA	1:A:28:PRO:HD3	1.91	0.40
1:B:140:LEU:CD2	1:B:202:ILE:HD11	2.43	0.40
1:C:352:LEU:HB2	3:C:3083:HOH:O	2.20	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	364/393 (93%)	346 (95%)	12 (3%)	6 (2%)	9 5
1	B	355/393 (90%)	336 (95%)	16 (4%)	3 (1%)	19 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	364/393 (93%)	345 (95%)	15 (4%)	4 (1%)	14	10
1	D	355/393 (90%)	332 (94%)	19 (5%)	4 (1%)	14	10
All	All	1438/1572 (92%)	1359 (94%)	62 (4%)	17 (1%)	13	9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	C	148	ALA
1	D	148	ALA
1	A	72	VAL
1	D	72	VAL
1	A	146	PHE
1	A	369	ILE
1	C	146	PHE
1	B	369	ILE
1	C	381	VAL
1	B	381	VAL
1	C	369	ILE
1	D	369	ILE
1	D	381	VAL
1	A	309	LEU
1	A	381	VAL
1	B	379	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/316 (93%)	284 (97%)	9 (3%)	40	49
1	B	286/316 (90%)	265 (93%)	21 (7%)	14	12
1	C	293/316 (93%)	277 (94%)	16 (6%)	21	21
1	D	286/316 (90%)	270 (94%)	16 (6%)	21	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1158/1264 (92%)	1096 (95%)	62 (5%)	22 22

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	93	ASP
1	A	147	ILE
1	A	189	VAL
1	A	215	ILE
1	A	246	LYS
1	A	256	LEU
1	A	281	LEU
1	A	336	GLN
1	B	31	THR
1	B	42	THR
1	B	96	ARG
1	B	102	ILE
1	B	147	ILE
1	B	158	GLU
1	B	172	PHE
1	B	202	ILE
1	B	204	LEU
1	B	207	VAL
1	B	213	ASP
1	B	246	LYS
1	B	256	LEU
1	B	279	GLU
1	B	281	LEU
1	B	332	GLU
1	B	336	GLN
1	B	341	LEU
1	B	348	LEU
1	B	364	GLU
1	B	393	ARG
1	C	30	THR
1	C	85	VAL
1	C	102	ILE
1	C	146	PHE
1	C	147	ILE
1	C	158	GLU
1	C	172	PHE

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Mol	Chain	Res	Type
1	C	204	LEU
1	C	207	VAL
1	C	215	ILE
1	C	246	LYS
1	C	256	LEU
1	C	258	ASP
1	C	281	LEU
1	C	336	GLN
1	C	364	GLU
1	D	42	THR
1	D	93	ASP
1	D	102	ILE
1	D	108	LEU
1	D	147	ILE
1	D	158	GLU
1	D	172	PHE
1	D	189	VAL
1	D	203	GLU
1	D	217	ASP
1	D	246	LYS
1	D	256	LEU
1	D	274	THR
1	D	281	LEU
1	D	336	GLN
1	D	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	180	ASN
1	A	192	HIS
1	A	208	ASN
1	A	216	ASN
1	A	221	HIS
1	A	239	GLN
1	A	270	HIS
1	A	280	ASN
1	A	300	ASN
1	A	336	GLN
1	B	49	GLN
1	B	171	ASN

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Mol	Chain	Res	Type
1	B	180	ASN
1	B	192	HIS
1	B	208	ASN
1	B	216	ASN
1	B	221	HIS
1	B	237	GLN
1	B	239	GLN
1	B	255	GLN
1	B	270	HIS
1	B	280	ASN
1	B	336	GLN
1	C	49	GLN
1	C	171	ASN
1	C	180	ASN
1	C	208	ASN
1	C	216	ASN
1	C	221	HIS
1	C	255	GLN
1	C	270	HIS
1	C	280	ASN
1	C	300	ASN
1	C	336	GLN
1	D	49	GLN
1	D	171	ASN
1	D	208	ASN
1	D	216	ASN
1	D	221	HIS
1	D	255	GLN
1	D	269	ASN
1	D	270	HIS
1	D	280	ASN
1	D	300	ASN
1	D	313	HIS
1	D	336	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MYR	A	3045	-	15,15,15	0.70	1 (6%)	15,15,15	0.90	0
2	MYR	C	3047	-	15,15,15	0.73	1 (6%)	15,15,15	0.90	1 (6%)
2	MYR	B	3046	-	15,15,15	0.70	1 (6%)	15,15,15	0.88	0
2	MYR	D	3048	-	15,15,15	0.76	1 (6%)	15,15,15	0.92	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	3045	-	-	2/13/13/13	-
2	MYR	C	3047	-	-	2/13/13/13	-
2	MYR	B	3046	-	-	2/13/13/13	-
2	MYR	D	3048	-	-	2/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3048	MYR	O2-C1	-2.29	1.23	1.30
2	C	3047	MYR	O2-C1	-2.22	1.23	1.30
2	A	3045	MYR	O2-C1	-2.10	1.23	1.30
2	B	3046	MYR	O2-C1	-2.08	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3048	MYR	O2-C1-C2	2.04	120.59	114.03
2	C	3047	MYR	O2-C1-C2	2.02	120.52	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3048	MYR	O2-C1-C2-C3
2	A	3045	MYR	O1-C1-C2-C3
2	A	3045	MYR	O2-C1-C2-C3
2	C	3047	MYR	O1-C1-C2-C3
2	D	3048	MYR	O1-C1-C2-C3
2	C	3047	MYR	O2-C1-C2-C3
2	B	3046	MYR	O1-C1-C2-C3
2	B	3046	MYR	O2-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3045	MYR	6	0
2	C	3047	MYR	5	0
2	B	3046	MYR	5	0
2	D	3048	MYR	6	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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	368/393 (93%)	-0.19	12 (3%)	46	48	22, 31, 57, 78	7 (1%)
1	B	359/393 (91%)	-0.14	9 (2%)	57	60	23, 33, 59, 89	7 (1%)
1	C	368/393 (93%)	-0.15	13 (3%)	44	46	22, 31, 54, 75	7 (1%)
1	D	359/393 (91%)	-0.04	25 (6%)	16	17	23, 34, 64, 93	7 (1%)
All	All	1454/1572 (92%)	-0.13	59 (4%)	37	40	22, 32, 59, 93	28 (1%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	ALA	5.7
1	D	67	GLU	5.2
1	B	68	ARG	4.3
1	D	65	GLN	4.0
1	A	66	ARG	3.9
1	B	71	ARG	3.9
1	D	71	ARG	3.7
1	D	48	ASN	3.7
1	D	68	ARG	3.7
1	B	298	TRP	3.5
1	D	298	TRP	3.4
1	D	70	PRO	3.4
1	B	131	ARG	3.2
1	D	91	LYS	3.2
1	A	90	ALA	3.2
1	C	366	ALA	3.1
1	D	131	ARG	3.1
1	D	72	VAL	3.1
1	D	92	PHE	3.1
1	C	91	LYS	2.9
1	D	74	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	94	VAL	2.8
1	A	67	GLU	2.8
1	B	67	GLU	2.8
1	C	148	ALA	2.8
1	A	93	ASP	2.7
1	C	67	GLU	2.7
1	C	23	GLN	2.7
1	D	241	LYS	2.7
1	B	90	ALA	2.6
1	D	66	ARG	2.6
1	A	91	LYS	2.6
1	A	72	VAL	2.6
1	C	265	VAL	2.6
1	A	366	ALA	2.4
1	A	48	ASN	2.4
1	D	59	LEU	2.4
1	C	241	LYS	2.4
1	C	92	PHE	2.3
1	C	131	ARG	2.3
1	D	93	ASP	2.2
1	B	66	ARG	2.2
1	A	148	ALA	2.2
1	A	50	SER	2.2
1	D	366	ALA	2.2
1	D	238	VAL	2.2
1	D	213	ASP	2.2
1	C	90	ALA	2.2
1	D	343	ARG	2.1
1	A	131	ARG	2.1
1	C	22	ALA	2.1
1	C	381	VAL	2.1
1	D	239	GLN	2.1
1	D	265	VAL	2.1
1	C	70	PRO	2.1
1	B	74	GLN	2.0
1	D	148	ALA	2.0
1	B	93	ASP	2.0
1	D	393	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MYR	D	3048	16/16	0.81	0.41	41,46,55,56	0
2	MYR	C	3047	16/16	0.82	0.39	38,44,58,59	0
2	MYR	B	3046	16/16	0.82	0.33	37,45,60,61	0
2	MYR	A	3045	16/16	0.90	0.33	37,40,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.