



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:11 pm GMT

PDB ID : 3A73
Title : Crystal Structure Analysis of Human serum albumin complexed with delta 12-prostaglandin J2
Authors : Ito, S.
Deposited on : 2009-09-11
Resolution : 2.19 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

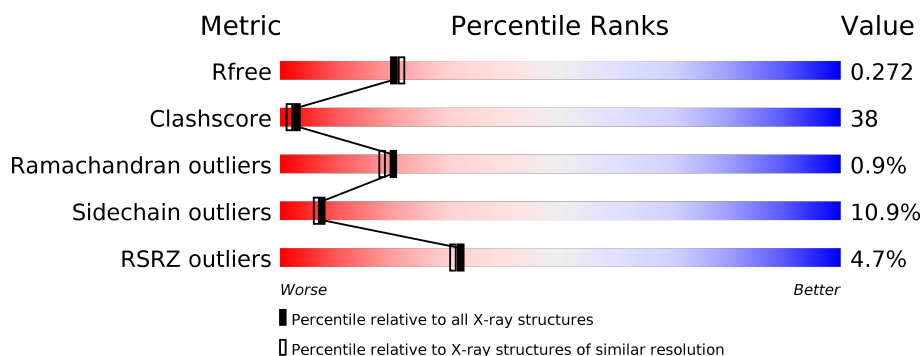
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 ≥ 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	585	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>35%</div> <div>5%</div> </div> </div>
1	B	585	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>38%</div> <div>7%</div> </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
2	MYR	A	1003	-	-	-	X
2	MYR	A	1004	-	-	X	-
2	MYR	A	1006	-	-	-	X
2	MYR	B	1002	-	-	-	X
2	MYR	B	1005	-	-	X	-
3	PJ2	A	1011	-	-	X	X
3	PJ2	A	1012	-	-	X	-
3	PJ2	B	1011	-	-	X	-

2 Entry composition [i](#)

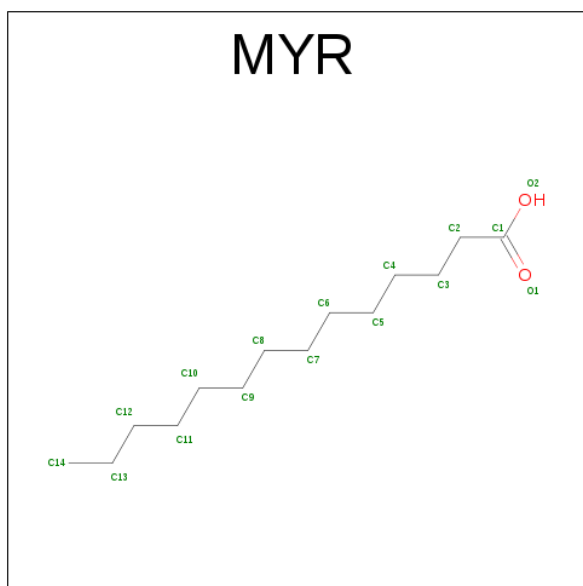
There are 4 unique types of molecules in this entry. The entry contains 9690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4580	2894	775	870	41			
1	B	576	Total	C	N	O	S	0	0	0
			4580	2894	775	870	41			

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



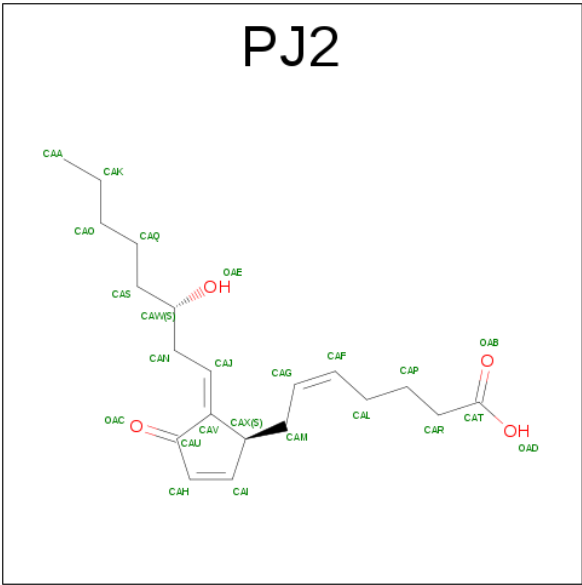
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C 12 12	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C 12 12	0	0

- Molecule 3 is (5Z,12Z,15S)-15-HYDROXY-11-OXOPROSTA-5,9,12-TRIEN-1-OIC ACID (three-letter code: PJ2) (formula: C₂₀H₃₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 24 20 4	0	0
3	A	1	Total C O 24 20 4	0	0
3	B	1	Total C O 24 20 4	0	0

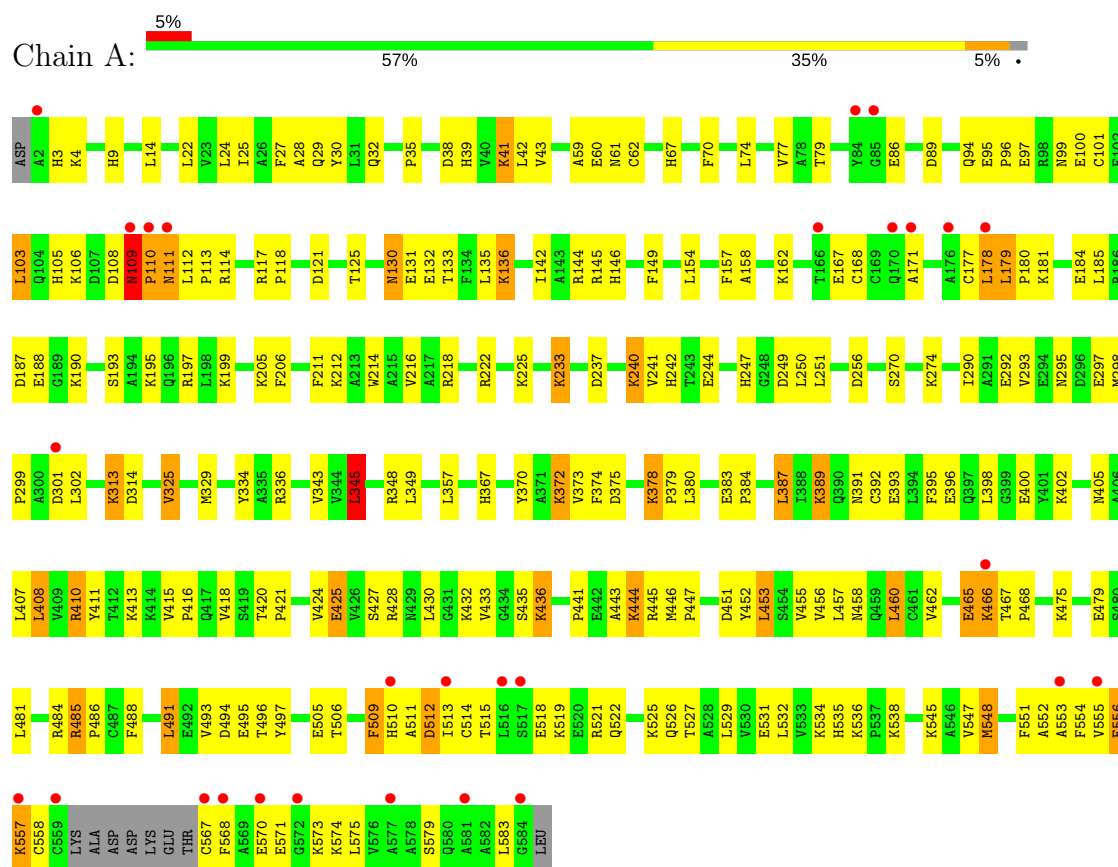
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	139	Total 139	O 139	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Serum albumin



• Molecule 1: Serum albumin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.06Å 92.05Å 94.66Å 74.80° 89.53° 80.21°	Depositor
Resolution (Å)	35.00 – 2.19 35.08 – 2.19	Depositor EDS
% Data completeness (in resolution range)	91.3 (35.00-2.19) 73.7 (35.08-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.229 , 0.291 0.241 , 0.272	Depositor DCC
R_{free} test set	2871 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.095 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, PJ2

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	0.91	1/4669 (0.0%)	0.91	4/6297 (0.1%)
1	B	0.89	4/4669 (0.1%)	0.88	3/6297 (0.0%)
All	All	0.90	5/9338 (0.1%)	0.89	7/12594 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	VAL	CB-CG2	5.47	1.64	1.52
1	B	371	ALA	CA-CB	5.46	1.64	1.52
1	B	348	ARG	C-N	-5.35	1.21	1.34
1	B	341	TYR	CD1-CE1	5.20	1.47	1.39
1	B	91	CYS	CB-SG	-5.18	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ALA	N-CA-C	5.90	126.94	111.00
1	A	336	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	171	ALA	N-CA-CB	-5.80	101.98	110.10
1	B	42	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	345	LEU	CB-CG-CD2	5.44	120.24	111.00
1	B	472	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	106	LYS	CB-CA-C	-5.25	99.90	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4580	0	4504	329	0
1	B	4580	0	4503	354	0
2	A	92	0	155	30	0
2	B	92	0	155	40	0
3	A	48	0	58	39	0
3	B	24	0	28	26	0
4	A	135	0	0	10	0
4	B	139	0	0	15	0
All	All	9690	0	9403	706	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 38.

All (706) 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:A:146:HIS:CE1	3:A:1012:PJ2:HAI	1.39	1.57
1:A:146:HIS:CE1	3:A:1012:PJ2:CAI	2.01	1.40
1:A:142:ILE:CD1	3:A:1011:PJ2:HAAA	1.53	1.35
1:B:117:ARG:HD2	3:B:1011:PJ2:CAH	1.59	1.32
1:B:117:ARG:CG	3:B:1011:PJ2:HAH	1.61	1.30
1:B:117:ARG:CD	3:B:1011:PJ2:HAH	1.60	1.29
3:A:1011:PJ2:CAP	3:A:1012:PJ2:OAC	1.80	1.26
3:A:1011:PJ2:HAP	3:A:1012:PJ2:OAC	1.07	1.20
1:A:142:ILE:HD13	3:A:1011:PJ2:CAA	1.73	1.19
3:A:1012:PJ2:HALA	3:A:1012:PJ2:OAD	1.44	1.15
1:B:117:ARG:CD	3:B:1011:PJ2:CAH	2.21	1.14
1:B:117:ARG:HG3	3:B:1011:PJ2:HAH	1.27	1.14
1:A:556:GLU:HB3	1:A:557:LYS:CE	1.79	1.12
1:B:505:GLU:O	1:B:508:THR:HG22	1.46	1.12
1:A:114:ARG:HD2	3:A:1012:PJ2:HAAB	1.31	1.12
1:B:460:LEU:HD21	2:B:1004:MYR:H131	1.20	1.11
1:B:298:MET:CE	1:B:337:ARG:HA	1.80	1.10
1:A:443:ALA:O	1:A:444:LYS:HE2	1.51	1.09
1:A:425:GLU:OE1	1:A:425:GLU:CA	1.99	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:O	1:B:433:VAL:HG12	1.51	1.08
1:B:210:ALA:HB1	2:B:1006:MYR:H121	1.13	1.07
1:A:485:ARG:HD2	2:A:1003:MYR:H32	1.35	1.06
1:B:274:LYS:HE3	1:B:294:GLU:OE2	1.56	1.06
1:A:556:GLU:HB3	1:A:557:LYS:HE3	1.11	1.05
1:A:458:ASN:HA	1:A:484:ARG:NH1	1.71	1.05
1:A:547:VAL:HG21	1:A:583:LEU:HD11	1.39	1.05
1:B:557:LYS:HD2	1:B:557:LYS:O	1.55	1.05
1:A:466:LYS:HA	1:A:466:LYS:HE3	1.31	1.04
1:B:117:ARG:HD2	3:B:1011:PJ2:HAH	1.19	1.04
1:B:13:ASP:OD2	1:B:13:ASP:C	1.96	1.04
1:B:35:PRO:HG2	1:B:38:ASP:OD1	1.58	1.03
1:A:481:LEU:HD12	1:A:481:LEU:O	1.56	1.03
1:B:394:LEU:O	1:B:394:LEU:HD23	1.56	1.03
1:B:348:ARG:HD3	4:B:710:HOH:O	1.56	1.03
1:B:567:CYS:HB2	1:B:571:GLU:CG	1.90	1.02
1:A:205:LYS:NZ	1:A:206:PHE:CE2	2.28	1.01
1:A:211:PHE:CE1	1:A:242:HIS:CD2	2.49	1.00
1:A:556:GLU:HA	1:A:556:GLU:OE1	1.58	1.00
1:B:394:LEU:HD21	1:B:398:LEU:HD22	1.42	1.00
3:A:1011:PJ2:HAP	3:A:1012:PJ2:CAU	1.91	1.00
1:A:108:ASP:C	1:A:110:PRO:CD	2.30	0.99
1:A:108:ASP:C	1:A:110:PRO:HD3	1.82	0.99
1:B:551:PHE:O	1:B:554:PHE:HB3	1.62	0.99
1:A:142:ILE:HD13	3:A:1011:PJ2:HAAA	0.99	0.98
1:A:556:GLU:CB	1:A:557:LYS:HE3	1.92	0.98
1:A:444:LYS:HE3	4:A:648:HOH:O	1.64	0.97
1:A:146:HIS:NE2	3:A:1012:PJ2:CAH	2.28	0.97
1:B:117:ARG:CG	3:B:1011:PJ2:CAH	2.44	0.96
3:B:1011:PJ2:HAOA	3:B:1011:PJ2:OAE	1.63	0.95
1:B:199:LYS:HG2	1:B:242:HIS:NE2	1.81	0.95
1:B:117:ARG:HH11	1:B:179:LEU:HG	1.30	0.95
1:A:110:PRO:O	1:A:111:ASN:HB2	1.66	0.95
1:B:298:MET:HE1	1:B:337:ARG:HA	1.48	0.95
1:A:218:ARG:NH1	1:A:222:ARG:HE	1.65	0.94
1:A:552:ALA:HA	1:A:555:VAL:CG2	1.97	0.94
1:B:173:ASP:HB3	1:B:176:ALA:CB	1.96	0.94
1:A:525:LYS:HE2	2:A:1005:MYR:O2	1.66	0.94
1:A:108:ASP:O	1:A:110:PRO:HD2	1.68	0.94
1:A:251:LEU:HD21	2:A:1002:MYR:H112	1.48	0.94
1:A:415:VAL:HG23	1:A:415:VAL:O	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASN:HD21	1:B:410:ARG:HH12	1.00	0.94
1:B:567:CYS:HB2	1:B:571:GLU:HG3	1.46	0.94
1:B:210:ALA:HB1	2:B:1006:MYR:C12	1.97	0.94
1:A:391:ASN:HD21	1:A:410:ARG:HH12	1.15	0.94
1:B:210:ALA:CB	2:B:1006:MYR:H121	1.98	0.93
1:A:298:MET:CE	1:A:302:LEU:HD12	1.99	0.93
1:B:298:MET:HE3	1:B:337:ARG:HA	1.52	0.92
1:B:466:LYS:C	1:B:468:PRO:HD3	1.88	0.92
1:B:428:ARG:HH21	1:B:526:GLN:HE22	1.16	0.92
1:B:173:ASP:HB3	1:B:176:ALA:HB3	1.51	0.91
1:A:142:ILE:HG12	3:A:1011:PJ2:HALA	1.51	0.91
1:A:167:GLU:HG2	1:A:181:LYS:HE3	1.49	0.91
1:B:117:ARG:CD	3:B:1011:PJ2:CAI	2.49	0.90
1:B:117:ARG:HD2	3:B:1011:PJ2:CAI	2.02	0.90
1:B:394:LEU:HD23	1:B:394:LEU:C	1.90	0.89
1:B:238:LEU:HD23	1:B:238:LEU:C	1.93	0.89
1:B:382:GLU:HG3	1:B:386:ASN:ND2	1.87	0.88
1:A:425:GLU:OE1	1:A:425:GLU:HA	1.04	0.88
3:A:1011:PJ2:CAR	3:A:1012:PJ2:OAC	2.21	0.88
1:B:460:LEU:HD21	2:B:1004:MYR:C13	2.02	0.88
1:B:95:GLU:HB3	1:B:96:PRO:HD3	1.56	0.88
1:B:511:ALA:HA	1:B:568:PHE:CE1	2.10	0.87
1:A:146:HIS:HE1	3:A:1012:PJ2:HAI	1.05	0.87
1:A:428:ARG:HH22	1:A:522:GLN:HE21	1.21	0.86
1:B:433:VAL:CG1	2:B:1003:MYR:H122	2.05	0.86
1:B:408:LEU:HD21	1:B:526:GLN:HB3	1.54	0.86
1:A:554:PHE:CD2	1:A:575:LEU:CD2	2.58	0.86
1:A:372:LYS:CG	1:A:375:ASP:OD2	2.24	0.85
1:A:142:ILE:HG12	3:A:1011:PJ2:CAL	2.07	0.85
1:B:551:PHE:CG	2:B:1005:MYR:H72	2.11	0.85
1:B:500:LYS:HE3	1:B:501:GLU:H	1.39	0.85
1:A:86:GLU:OE1	1:A:105:HIS:HE1	1.57	0.85
1:B:500:LYS:HA	1:B:500:LYS:HE3	1.58	0.85
1:A:458:ASN:CA	1:A:484:ARG:NH1	2.39	0.84
1:A:112:LEU:HD12	1:A:145:ARG:CG	2.07	0.84
1:B:356:THR:HG21	1:B:373:VAL:HG21	1.60	0.84
1:A:130:ASN:C	1:A:130:ASN:HD22	1.81	0.84
1:A:444:LYS:CE	4:A:648:HOH:O	2.21	0.84
1:A:142:ILE:CD1	3:A:1011:PJ2:CAA	2.44	0.84
1:A:415:VAL:HG21	2:A:1004:MYR:H121	1.59	0.84
1:A:392:CYS:O	1:A:396:GLU:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.60	0.83
1:A:211:PHE:CZ	1:A:242:HIS:CD2	2.65	0.83
1:A:467:THR:N	1:A:468:PRO:HD3	1.94	0.83
1:B:178:LEU:HD13	1:B:182:LEU:HD11	1.60	0.83
1:A:146:HIS:NE2	3:A:1012:PJ2:CAX	2.41	0.82
1:B:435:SER:O	1:B:439:LYS:HD3	1.79	0.82
1:A:131:GLU:OE1	1:A:162:LYS:HE3	1.80	0.82
1:A:222:ARG:NH2	2:A:1007:MYR:H92	1.95	0.81
1:B:391:ASN:ND2	1:B:410:ARG:HH12	1.78	0.81
1:B:178:LEU:CD1	1:B:182:LEU:HD11	2.10	0.81
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.63	0.81
1:A:552:ALA:HA	1:A:555:VAL:HG22	1.60	0.80
1:A:158:ALA:HB2	3:A:1011:PJ2:HAO	1.63	0.80
1:B:178:LEU:HD13	1:B:182:LEU:CD1	2.11	0.80
1:B:6:GLU:HG2	4:B:650:HOH:O	1.80	0.80
1:A:94:GLN:HE21	1:A:94:GLN:HA	1.45	0.80
1:A:95:GLU:OE1	1:A:99:ASN:HB2	1.82	0.80
1:B:117:ARG:HG3	3:B:1011:PJ2:CAH	2.07	0.79
3:B:1011:PJ2:CAO	3:B:1011:PJ2:OAE	2.29	0.79
1:B:291:ALA:HA	2:B:1007:MYR:H102	1.63	0.79
1:B:394:LEU:CD2	1:B:398:LEU:HD22	2.12	0.79
1:A:418:VAL:HG21	2:A:1004:MYR:H142	1.64	0.79
1:B:117:ARG:HD3	3:B:1011:PJ2:HAI	1.65	0.78
1:B:138:TYR:CD2	3:B:1011:PJ2:HAW	2.18	0.78
1:A:556:GLU:OE1	1:A:556:GLU:CA	2.30	0.78
1:A:205:LYS:NZ	1:A:206:PHE:CZ	2.50	0.78
1:B:502:PHE:HB2	1:B:535:HIS:CE1	2.18	0.78
1:A:400:GLU:OE2	1:A:435:SER:CB	2.32	0.78
1:B:567:CYS:HB2	1:B:571:GLU:HG2	1.65	0.78
1:B:500:LYS:HE3	1:B:501:GLU:N	1.97	0.78
1:A:389:LYS:O	1:A:393:GLU:HG3	1.83	0.77
1:B:298:MET:HE1	1:B:337:ARG:CA	2.14	0.77
1:B:466:LYS:O	1:B:468:PRO:HD3	1.82	0.77
1:A:112:LEU:HD12	1:A:145:ARG:HG3	1.66	0.77
1:A:432:LYS:O	1:A:436:LYS:HG2	1.85	0.77
1:B:244:GLU:HG3	1:B:256:ASP:OD1	1.84	0.77
1:A:554:PHE:CD2	1:A:575:LEU:HD22	2.18	0.77
1:B:391:ASN:HD21	1:B:410:ARG:NH1	1.81	0.77
1:A:222:ARG:HD3	1:A:295:ASN:ND2	2.00	0.76
1:A:428:ARG:HH21	1:A:526:GLN:HE22	1.33	0.76
1:B:356:THR:HG21	1:B:373:VAL:CG2	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LYS:HE3	1:A:237:ASP:OD1	1.85	0.76
3:A:1011:PJ2:HARA	3:A:1012:PJ2:OAC	1.86	0.76
1:A:553:ALA:O	1:A:557:LYS:HD2	1.85	0.76
1:A:567:CYS:HB2	1:A:571:GLU:HG3	1.68	0.76
1:A:372:LYS:HG3	1:A:375:ASP:OD2	1.86	0.76
1:B:500:LYS:CE	1:B:501:GLU:N	2.49	0.76
1:A:453:LEU:O	1:A:457:LEU:HG	1.85	0.75
1:A:554:PHE:CG	1:A:575:LEU:HD22	2.21	0.75
1:A:86:GLU:CD	1:A:105:HIS:HE1	1.90	0.75
1:B:440:HIS:HB3	1:B:444:LYS:HB3	1.68	0.75
1:B:537:PRO:HG2	1:B:538:LYS:HD3	1.67	0.75
1:B:394:LEU:CD2	1:B:394:LEU:C	2.54	0.75
1:A:408:LEU:HD13	1:A:427:SER:OG	1.86	0.74
1:B:117:ARG:NH1	1:B:179:LEU:HG	2.02	0.74
3:A:1012:PJ2:CAL	3:A:1012:PJ2:OAD	2.30	0.74
1:B:500:LYS:CE	1:B:501:GLU:H	2.00	0.74
1:A:142:ILE:CG1	3:A:1011:PJ2:HALA	2.18	0.74
1:B:394:LEU:HD21	1:B:398:LEU:CD2	2.16	0.74
1:A:458:ASN:HA	1:A:484:ARG:HH12	1.53	0.74
1:A:552:ALA:O	1:A:556:GLU:HB2	1.87	0.74
1:B:95:GLU:CB	1:B:96:PRO:HD3	2.17	0.74
1:A:108:ASP:O	1:A:110:PRO:CD	2.31	0.73
1:B:74:LEU:O	1:B:77:VAL:HG22	1.88	0.73
1:A:485:ARG:HD3	2:A:1003:MYR:O1	1.88	0.73
1:A:372:LYS:HG2	1:A:375:ASP:OD2	1.88	0.73
1:A:109:ASN:O	1:A:111:ASN:N	2.22	0.73
1:A:35:PRO:HD2	1:A:38:ASP:OD1	1.88	0.73
1:B:518:GLU:O	1:B:522:GLN:HG2	1.87	0.72
1:B:428:ARG:HH21	1:B:526:GLN:NE2	1.86	0.72
1:B:94:GLN:HE21	1:B:94:GLN:HA	1.53	0.72
1:B:222:ARG:HD3	1:B:295:ASN:ND2	2.05	0.72
1:A:391:ASN:ND2	1:A:410:ARG:HH12	1.86	0.72
1:B:222:ARG:HD3	1:B:295:ASN:HD22	1.52	0.72
1:B:274:LYS:CE	1:B:294:GLU:OE2	2.36	0.72
1:A:112:LEU:HD12	1:A:145:ARG:HG2	1.72	0.72
1:B:518:GLU:HA	1:B:518:GLU:OE2	1.90	0.71
1:A:552:ALA:CA	1:A:555:VAL:HG22	2.20	0.71
1:B:488:PHE:HA	1:B:491:LEU:CD2	2.21	0.71
1:A:222:ARG:HD3	1:A:295:ASN:HD22	1.56	0.71
1:B:173:ASP:HB3	1:B:176:ALA:HB2	1.71	0.71
1:B:347:LEU:HD13	2:B:1006:MYR:H131	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1012:PJ2:HANA	3:A:1012:PJ2:HAM	1.74	0.70
1:B:466:LYS:O	1:B:468:PRO:CD	2.40	0.70
1:A:108:ASP:C	1:A:110:PRO:HD2	2.06	0.70
1:A:400:GLU:OE2	1:A:435:SER:HB2	1.91	0.70
1:B:509:PHE:HD2	1:B:524:LYS:HZ1	1.39	0.70
1:A:488:PHE:HB3	2:A:1004:MYR:H72	1.74	0.69
1:A:513:ILE:HG12	1:A:521:ARG:HG3	1.73	0.69
1:B:174:LYS:HE2	4:B:701:HOH:O	1.91	0.69
1:B:77:VAL:CG2	1:B:80:LEU:HD13	2.22	0.69
1:A:112:LEU:CD1	1:A:145:ARG:HG3	2.21	0.69
1:B:238:LEU:HD23	1:B:238:LEU:O	1.92	0.69
1:A:485:ARG:CD	2:A:1003:MYR:H32	2.18	0.69
1:A:430:LEU:O	1:A:433:VAL:CG1	2.41	0.69
1:A:521:ARG:O	1:A:525:LYS:HG3	1.93	0.69
1:B:187:ASP:O	1:B:190:LYS:HB3	1.92	0.69
1:B:554:PHE:O	1:B:558:CYS:HB2	1.91	0.69
1:A:481:LEU:CD1	1:A:481:LEU:O	2.40	0.69
1:B:204:GLN:HB3	4:B:645:HOH:O	1.93	0.68
1:B:156:PHE:CZ	1:B:285:GLU:HG2	2.27	0.68
1:B:502:PHE:HB2	1:B:535:HIS:NE2	2.07	0.68
1:A:109:ASN:N	1:A:110:PRO:CD	2.54	0.68
1:A:525:LYS:CE	2:A:1005:MYR:O2	2.39	0.68
1:A:458:ASN:CA	1:A:484:ARG:HH11	2.05	0.68
1:A:430:LEU:HA	1:A:433:VAL:HG12	1.73	0.68
1:B:420:THR:HB	1:B:421:PRO:HD3	1.77	0.67
1:B:522:GLN:O	1:B:526:GLN:HG3	1.94	0.67
1:B:382:GLU:HG2	1:B:383:GLU:N	2.06	0.67
1:B:117:ARG:HH11	1:B:179:LEU:CG	2.06	0.67
1:B:408:LEU:HD13	1:B:427:SER:CB	2.25	0.67
1:B:433:VAL:CG1	2:B:1003:MYR:C12	2.72	0.67
1:B:532:LEU:HD11	1:B:583:LEU:HD11	1.76	0.67
1:A:233:LYS:HG2	4:A:599:HOH:O	1.95	0.67
1:A:510:HIS:O	1:A:568:PHE:CE1	2.47	0.67
1:A:86:GLU:CD	1:A:105:HIS:CE1	2.68	0.66
1:B:536:LYS:HD2	1:B:583:LEU:HB3	1.77	0.66
1:A:130:ASN:ND2	1:A:133:THR:H	1.93	0.66
1:A:240:LYS:NZ	1:A:244:GLU:CD	2.49	0.66
1:A:488:PHE:HA	1:A:491:LEU:HD22	1.78	0.66
1:A:551:PHE:O	1:A:555:VAL:HG22	1.94	0.66
1:B:419:SER:HB2	1:B:421:PRO:HD2	1.78	0.66
1:A:206:PHE:HA	4:A:636:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:HG22	2:B:1002:MYR:H121	1.78	0.66
1:B:237:ASP:O	1:B:241:VAL:HG13	1.94	0.66
1:B:500:LYS:HE3	1:B:500:LYS:CA	2.26	0.66
1:B:199:LYS:CG	1:B:242:HIS:NE2	2.58	0.66
1:B:13:ASP:OD2	1:B:14:LEU:N	2.29	0.66
1:B:235:VAL:O	1:B:239:THR:HG23	1.94	0.65
1:A:108:ASP:OD1	1:A:108:ASP:O	2.13	0.65
1:B:142:ILE:HD12	3:B:1011:PJ2:HAR	1.77	0.65
1:A:511:ALA:HA	1:A:568:PHE:CZ	2.30	0.65
1:B:509:PHE:HD2	1:B:524:LYS:NZ	1.94	0.65
1:B:567:CYS:CB	1:B:571:GLU:HG2	2.26	0.65
1:A:41:LYS:HE3	1:A:42:LEU:HD23	1.79	0.64
1:B:130:ASN:ND2	1:B:133:THR:H	1.94	0.64
1:B:168:CYS:SG	1:B:181:LYS:HE2	2.37	0.64
1:A:375:ASP:O	1:A:378:LYS:HB2	1.97	0.64
1:B:120:VAL:HG11	1:B:174:LYS:HB3	1.80	0.64
1:A:465:GLU:O	1:A:466:LYS:HB2	1.98	0.64
1:B:174:LYS:CE	4:B:701:HOH:O	2.46	0.64
1:A:552:ALA:HA	1:A:555:VAL:HG21	1.80	0.64
1:A:430:LEU:O	1:A:433:VAL:HG12	1.98	0.64
1:B:513:ILE:HA	1:B:516:LEU:CD2	2.27	0.64
1:B:394:LEU:HD22	1:B:403:PHE:CD1	2.33	0.64
1:B:382:GLU:HG3	1:B:386:ASN:HD21	1.63	0.63
1:B:298:MET:CE	1:B:337:ARG:CA	2.68	0.63
1:B:408:LEU:HD13	1:B:427:SER:HB3	1.80	0.63
1:A:30:TYR:CZ	1:A:106:LYS:HE3	2.33	0.63
1:A:466:LYS:CA	1:A:466:LYS:HE3	2.20	0.63
1:B:27:PHE:C	1:B:39:HIS:HE1	2.01	0.63
1:B:433:VAL:HG13	2:B:1003:MYR:H122	1.78	0.63
1:A:244:GLU:HG3	1:A:256:ASP:OD1	1.99	0.63
1:B:212:LYS:HG2	1:B:239:THR:HG21	1.80	0.63
1:B:117:ARG:HD3	3:B:1011:PJ2:CAI	2.23	0.63
1:A:467:THR:N	1:A:468:PRO:CD	2.62	0.62
1:B:27:PHE:O	1:B:39:HIS:HE1	1.82	0.62
1:B:415:VAL:O	1:B:415:VAL:HG23	1.97	0.62
1:B:348:ARG:CD	4:B:710:HOH:O	2.28	0.62
1:A:556:GLU:CB	1:A:557:LYS:CE	2.65	0.62
1:B:342:SER:OG	1:B:345:LEU:HB2	1.99	0.62
1:B:570:GLU:HA	1:B:573:LYS:HG3	1.81	0.62
1:A:94:GLN:NE2	1:A:94:GLN:HA	2.14	0.62
1:B:488:PHE:HA	1:B:491:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:VAL:O	1:B:580:GLN:HG3	1.99	0.62
1:B:484:ARG:HH21	1:B:484:ARG:CB	2.12	0.62
1:A:408:LEU:HD13	1:A:427:SER:CB	2.30	0.62
1:B:510:HIS:HB2	1:B:512:ASP:OD1	1.99	0.62
1:A:510:HIS:HB2	1:A:512:ASP:OD2	1.99	0.62
1:B:433:VAL:HG11	2:B:1003:MYR:C12	2.30	0.62
1:A:177:CYS:O	1:A:181:LYS:HG3	2.00	0.61
1:A:216:VAL:HG21	2:A:1006:MYR:O1	2.00	0.61
1:A:509:PHE:N	1:A:509:PHE:CD1	2.66	0.61
1:A:95:GLU:O	1:A:96:PRO:C	2.38	0.61
1:B:556:GLU:CD	1:B:557:LYS:N	2.54	0.61
1:B:77:VAL:HG21	1:B:80:LEU:HD13	1.81	0.61
1:B:66:LEU:CD1	2:B:1002:MYR:H143	2.30	0.61
1:B:13:ASP:OD2	1:B:13:ASP:O	2.18	0.61
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.82	0.61
1:A:131:GLU:O	1:A:135:LEU:HD22	2.01	0.61
1:B:484:ARG:HH21	1:B:484:ARG:CG	2.13	0.61
1:A:535:HIS:O	1:A:536:LYS:HD3	2.01	0.61
1:A:218:ARG:HH22	1:A:295:ASN:HD21	1.49	0.61
1:A:554:PHE:O	1:A:558:CYS:HB2	2.00	0.61
1:B:497:TYR:O	1:B:499:PRO:HD3	2.01	0.61
1:B:95:GLU:CB	1:B:96:PRO:CD	2.79	0.61
1:B:281:LYS:HB3	1:B:282:PRO:HD2	1.83	0.60
1:B:394:LEU:HD22	1:B:403:PHE:HD1	1.66	0.60
1:A:430:LEU:HA	1:A:433:VAL:CG1	2.31	0.60
1:B:218:ARG:CZ	1:B:222:ARG:HE	2.14	0.60
1:B:218:ARG:HH22	1:B:295:ASN:HD21	1.49	0.60
1:B:238:LEU:C	1:B:238:LEU:CD2	2.70	0.60
1:A:466:LYS:HA	1:A:466:LYS:CE	2.18	0.59
1:A:14:LEU:HD11	2:A:1002:MYR:H72	1.84	0.59
1:B:509:PHE:CD2	1:B:524:LYS:NZ	2.70	0.59
1:A:556:GLU:CG	1:A:557:LYS:HE3	2.32	0.59
1:B:199:LYS:HG2	1:B:242:HIS:CE1	2.36	0.59
1:B:500:LYS:HE2	1:B:501:GLU:N	2.17	0.59
1:A:428:ARG:HH22	1:A:522:GLN:NE2	1.95	0.59
1:B:22:LEU:HD13	2:B:1002:MYR:H72	1.84	0.59
1:B:484:ARG:HH21	1:B:484:ARG:HB2	1.68	0.59
2:A:1004:MYR:H61	2:A:1004:MYR:C2	2.20	0.59
1:B:283:LEU:O	1:B:283:LEU:HD23	2.02	0.59
1:B:459:GLN:HG2	1:B:459:GLN:O	2.01	0.59
1:B:353:TYR:O	1:B:356:THR:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD11	2:B:1002:MYR:H143	1.85	0.59
1:A:372:LYS:HG2	1:A:375:ASP:HB2	1.85	0.59
1:A:458:ASN:CB	1:A:484:ARG:NH1	2.66	0.58
1:A:553:ALA:HA	1:A:557:LYS:NZ	2.18	0.58
1:B:513:ILE:HA	1:B:516:LEU:HD21	1.84	0.58
1:A:481:LEU:HD12	1:A:481:LEU:C	2.17	0.58
1:B:536:LYS:HD2	1:B:583:LEU:O	2.03	0.58
1:B:95:GLU:HB3	1:B:96:PRO:CD	2.30	0.58
1:A:108:ASP:CA	1:A:110:PRO:HD3	2.34	0.58
1:B:127:PHE:CE1	1:B:165:PHE:HB3	2.39	0.58
1:B:387:LEU:HD12	1:B:390:GLN:NE2	2.18	0.58
1:B:378:LYS:CB	1:B:379:PRO:HD3	2.33	0.57
2:A:1004:MYR:H22	2:A:1004:MYR:H61	1.85	0.57
1:A:130:ASN:HD21	1:A:133:THR:H	1.52	0.57
1:A:462:VAL:O	1:A:465:GLU:HG3	2.04	0.57
1:A:485:ARG:HD2	2:A:1003:MYR:C3	2.24	0.57
1:B:204:GLN:OE1	1:B:204:GLN:HA	2.04	0.57
1:A:109:ASN:O	1:A:110:PRO:C	2.41	0.57
1:A:167:GLU:CG	1:A:177:CYS:SG	2.92	0.57
1:A:211:PHE:CE1	1:A:242:HIS:NE2	2.71	0.57
1:A:519:LYS:O	1:A:522:GLN:HB2	2.05	0.57
1:B:179:LEU:CB	1:B:180:PRO:HD3	2.34	0.57
1:B:160:ARG:NH1	1:B:188:GLU:OE1	2.38	0.57
1:A:430:LEU:O	1:A:433:VAL:HG13	2.04	0.57
1:B:235:VAL:O	1:B:239:THR:CG2	2.53	0.57
1:B:567:CYS:CB	1:B:571:GLU:CG	2.75	0.57
1:A:553:ALA:HA	1:A:557:LYS:HZ2	1.70	0.57
1:A:131:GLU:O	1:A:135:LEU:CD2	2.53	0.56
1:A:30:TYR:CE2	1:A:106:LYS:HE3	2.40	0.56
1:A:372:LYS:HG2	1:A:375:ASP:CG	2.26	0.56
1:A:416:PRO:O	1:A:534:LYS:HE2	2.06	0.56
1:B:557:LYS:CD	1:B:557:LYS:O	2.43	0.56
1:A:298:MET:HE1	1:A:302:LEU:HD12	1.82	0.56
1:A:465:GLU:OE2	1:A:466:LYS:HG2	2.06	0.56
1:B:101:CYS:O	1:B:105:HIS:HD2	1.89	0.56
1:A:552:ALA:CA	1:A:555:VAL:CG2	2.76	0.56
1:B:516:LEU:HB3	1:B:520:GLU:HB2	1.87	0.56
1:A:131:GLU:HG2	1:A:135:LEU:CD2	2.35	0.56
1:A:460:LEU:HD11	2:A:1004:MYR:H141	1.88	0.56
1:B:142:ILE:CD1	3:B:1011:PJ2:HAR	2.35	0.56
1:B:291:ALA:HA	2:B:1007:MYR:H82	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.88	0.56
1:B:286:LYS:O	1:B:290:ILE:HG13	2.06	0.56
1:A:391:ASN:HD21	1:A:410:ARG:NH1	1.94	0.55
1:B:258:ALA:CB	1:B:283:LEU:HD21	2.36	0.55
1:A:28:ALA:HA	1:A:39:HIS:CE1	2.42	0.55
1:B:10:ARG:NH2	1:B:255:ASP:OD1	2.32	0.55
1:A:199:LYS:HB3	1:A:242:HIS:HE1	1.70	0.55
1:B:433:VAL:HG11	2:B:1003:MYR:H122	1.86	0.55
1:A:167:GLU:HG3	1:A:177:CYS:SG	2.47	0.55
1:B:130:ASN:HD22	1:B:130:ASN:C	2.11	0.55
1:B:557:LYS:HD2	1:B:557:LYS:C	2.25	0.55
1:A:86:GLU:OE1	1:A:105:HIS:CE1	2.50	0.55
3:A:1012:PJ2:CAM	3:A:1012:PJ2:HANA	2.37	0.54
1:B:532:LEU:HD13	2:B:1005:MYR:H121	1.87	0.54
1:B:420:THR:N	1:B:421:PRO:CD	2.70	0.54
1:B:113:PRO:O	1:B:145:ARG:NH1	2.32	0.54
1:A:548:MET:HG2	2:A:1005:MYR:H51	1.88	0.54
3:B:1011:PJ2:CAN	3:B:1011:PJ2:OAC	2.55	0.54
1:A:512:ASP:O	1:A:515:THR:N	2.33	0.54
1:A:557:LYS:H	1:A:557:LYS:HD2	1.72	0.54
1:B:387:LEU:HD12	1:B:390:GLN:HE21	1.71	0.54
1:B:510:HIS:O	1:B:513:ILE:HG22	2.08	0.54
1:B:77:VAL:HG23	1:B:80:LEU:HB2	1.88	0.54
1:B:90:CYS:O	1:B:98:ARG:HG3	2.07	0.54
1:A:400:GLU:OE2	1:A:435:SER:HB3	2.08	0.54
1:B:179:LEU:CB	1:B:180:PRO:CD	2.85	0.54
1:B:383:GLU:OE1	1:B:485:ARG:NH1	2.36	0.54
1:B:179:LEU:HB3	1:B:180:PRO:HD3	1.88	0.54
1:B:556:GLU:OE1	1:B:557:LYS:HA	2.08	0.54
1:B:511:ALA:CA	1:B:568:PHE:CE1	2.89	0.54
1:A:142:ILE:CD1	3:A:1011:PJ2:HALA	2.38	0.54
1:A:250:LEU:HD23	2:A:1002:MYR:H121	1.89	0.53
1:A:60:GLU:O	1:A:61:ASN:HB2	2.08	0.53
1:A:430:LEU:CA	1:A:433:VAL:HG12	2.38	0.53
1:B:101:CYS:O	1:B:105:HIS:CD2	2.61	0.53
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.89	0.53
1:B:291:ALA:CA	2:B:1007:MYR:H102	2.37	0.53
1:B:231:VAL:O	1:B:235:VAL:HG13	2.08	0.53
1:A:79:THR:HG22	1:B:515:THR:HB	1.89	0.53
1:A:240:LYS:HZ1	1:A:244:GLU:CD	2.10	0.53
1:B:94:GLN:HE21	1:B:94:GLN:CA	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:CE1	1:A:188:GLU:OE2	2.62	0.53
1:A:458:ASN:N	1:A:484:ARG:HH11	2.06	0.53
1:A:579:SER:O	1:A:583:LEU:HD12	2.09	0.53
1:B:35:PRO:CG	1:B:38:ASP:OD1	2.44	0.53
1:A:177:CYS:SG	1:A:181:LYS:HE2	2.49	0.53
1:A:199:LYS:HB3	1:A:242:HIS:CE1	2.44	0.53
1:A:457:LEU:O	1:A:460:LEU:HB3	2.08	0.53
1:B:173:ASP:O	1:B:176:ALA:N	2.41	0.53
1:B:460:LEU:CD2	2:B:1004:MYR:C14	2.87	0.53
1:A:117:ARG:NH2	1:A:179:LEU:HD12	2.23	0.52
1:B:547:VAL:HA	4:B:622:HOH:O	2.09	0.52
1:A:110:PRO:O	1:A:111:ASN:CB	2.46	0.52
1:A:420:THR:HB	1:A:421:PRO:HD3	1.90	0.52
1:A:131:GLU:OE1	1:A:162:LYS:CE	2.53	0.52
1:B:433:VAL:HG13	2:B:1003:MYR:C12	2.39	0.52
1:A:460:LEU:HD11	2:A:1004:MYR:C14	2.40	0.52
1:A:511:ALA:O	1:A:514:CYS:SG	2.68	0.52
1:A:378:LYS:CB	1:A:379:PRO:HD3	2.40	0.52
1:A:571:GLU:O	1:A:575:LEU:N	2.43	0.52
1:A:553:ALA:O	1:A:557:LYS:CD	2.56	0.52
1:A:380:LEU:O	1:A:384:PRO:HD2	2.11	0.52
1:B:27:PHE:C	1:B:39:HIS:CE1	2.82	0.52
1:A:114:ARG:HD2	3:A:1012:PJ2:CAA	2.21	0.51
1:A:551:PHE:CE2	1:A:555:VAL:HG11	2.45	0.51
1:A:552:ALA:O	1:A:555:VAL:HG23	2.10	0.51
1:B:222:ARG:HA	1:B:295:ASN:HD22	1.75	0.51
1:B:240:LYS:HD2	4:B:661:HOH:O	2.09	0.51
1:A:22:LEU:HD13	2:A:1002:MYR:H71	1.92	0.51
1:A:117:ARG:HG2	1:A:118:PRO:O	2.10	0.51
1:A:551:PHE:CG	2:A:1005:MYR:H72	2.45	0.51
1:B:218:ARG:CZ	1:B:222:ARG:NE	2.73	0.51
1:A:383:GLU:OE1	1:A:387:LEU:HD22	2.10	0.51
1:B:507:PHE:CG	2:B:1005:MYR:H132	2.46	0.51
1:B:114:ARG:HD2	1:B:114:ARG:N	2.25	0.51
1:A:298:MET:HE2	1:A:302:LEU:HD12	1.86	0.51
1:A:458:ASN:CB	1:A:484:ARG:HH12	2.24	0.51
1:B:173:ASP:O	1:B:174:LYS:C	2.49	0.51
1:B:11:PHE:CZ	1:B:16:GLU:HB2	2.45	0.51
1:B:178:LEU:HD13	1:B:182:LEU:HD12	1.89	0.51
1:A:554:PHE:CD2	1:A:575:LEU:HD23	2.43	0.51
1:A:67:HIS:HE1	1:A:249:ASP:OD1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:HD3	2:B:1003:MYR:O1	2.11	0.51
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.40	0.51
1:A:372:LYS:HE2	1:A:375:ASP:HB2	1.92	0.51
1:A:420:THR:HG21	1:A:527:THR:HG23	1.92	0.51
1:A:413:LYS:HB3	1:A:493:VAL:HG22	1.92	0.51
1:B:424:VAL:O	1:B:428:ARG:HG3	2.11	0.51
1:A:571:GLU:O	1:A:574:LYS:N	2.44	0.50
1:A:95:GLU:O	1:A:95:GLU:OE1	2.29	0.50
1:B:536:LYS:HG3	1:B:583:LEU:HD13	1.93	0.50
1:A:240:LYS:NZ	1:A:244:GLU:OE1	2.45	0.50
1:B:173:ASP:CB	1:B:176:ALA:HB2	2.40	0.50
1:A:86:GLU:HG3	1:A:105:HIS:CE1	2.46	0.50
1:B:250:LEU:O	1:B:250:LEU:HD12	2.12	0.50
1:B:418:VAL:HG21	2:B:1004:MYR:H121	1.93	0.50
1:B:484:ARG:NH2	4:B:626:HOH:O	2.37	0.50
1:A:222:ARG:HG3	1:A:222:ARG:NH2	2.27	0.50
1:B:28:ALA:HA	1:B:39:HIS:CE1	2.47	0.50
1:B:558:CYS:SG	1:B:567:CYS:O	2.69	0.50
1:A:411:TYR:HB3	2:A:1004:MYR:H112	1.94	0.50
1:B:60:GLU:O	1:B:61:ASN:HB2	2.12	0.50
1:B:553:ALA:O	1:B:557:LYS:HB3	2.11	0.50
1:A:205:LYS:HB3	1:A:205:LYS:NZ	2.26	0.50
1:B:449:ALA:O	1:B:453:LEU:HB2	2.11	0.50
1:B:509:PHE:CE1	1:B:551:PHE:HE1	2.30	0.50
1:B:555:VAL:HG23	1:B:556:GLU:N	2.26	0.50
1:A:372:LYS:HG2	1:A:375:ASP:CB	2.42	0.49
1:A:444:LYS:HE2	4:A:648:HOH:O	2.00	0.49
1:A:466:LYS:C	1:A:468:PRO:HD3	2.32	0.49
1:A:554:PHE:CB	1:A:575:LEU:HD22	2.42	0.49
1:B:250:LEU:HD12	1:B:250:LEU:C	2.31	0.49
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.78	0.49
1:B:123:MET:SD	3:B:1011:PJ2:OAC	2.69	0.49
1:A:416:PRO:HB2	1:A:497:TYR:CE2	2.47	0.49
1:B:433:VAL:HG13	1:B:434:GLY:N	2.27	0.49
1:A:548:MET:HG2	2:A:1005:MYR:C5	2.42	0.49
1:A:556:GLU:HB3	1:A:557:LYS:CD	2.41	0.49
1:B:258:ALA:HB1	1:B:283:LEU:HD21	1.94	0.49
1:B:281:LYS:HB3	1:B:282:PRO:CD	2.43	0.49
1:B:500:LYS:CA	1:B:500:LYS:CE	2.91	0.49
1:B:298:MET:HE1	1:B:337:ARG:CB	2.42	0.49
1:A:86:GLU:O	1:A:89:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HD11	3:A:1011:PJ2:HAAA	1.77	0.48
1:B:551:PHE:CD2	2:B:1005:MYR:H72	2.48	0.48
3:B:1011:PJ2:OAC	3:B:1011:PJ2:HAN	2.14	0.48
1:B:458:ASN:O	1:B:462:VAL:HG23	2.13	0.48
1:B:555:VAL:CG2	1:B:556:GLU:N	2.77	0.48
1:B:130:ASN:HD22	1:B:133:THR:H	1.59	0.48
1:B:453:LEU:O	1:B:457:LEU:HG	2.14	0.48
1:A:452:TYR:O	1:A:456:VAL:HG23	2.13	0.48
1:A:415:VAL:CG2	2:A:1004:MYR:H121	2.39	0.48
1:A:167:GLU:HG2	1:A:177:CYS:SG	2.53	0.48
1:A:411:TYR:O	1:A:415:VAL:HG22	2.13	0.48
1:B:312:SER:O	1:B:315:VAL:HG23	2.14	0.48
1:B:446:MET:N	1:B:447:PRO:CD	2.77	0.48
1:B:467:THR:N	1:B:468:PRO:HD3	2.25	0.48
1:A:132:GLU:O	1:A:136:LYS:HB2	2.13	0.48
1:B:481:LEU:HD23	2:B:1006:MYR:H143	1.95	0.48
1:B:205:LYS:HG2	1:B:206:PHE:CE2	2.49	0.48
1:A:552:ALA:C	1:A:555:VAL:HG22	2.35	0.48
1:B:405:ASN:N	1:B:405:ASN:HD22	2.11	0.48
1:B:460:LEU:HD21	2:B:1004:MYR:C14	2.43	0.48
1:A:408:LEU:HD11	1:A:424:VAL:HA	1.96	0.47
1:B:356:THR:HG21	1:B:373:VAL:HG23	1.95	0.47
3:A:1012:PJ2:HAS	3:A:1012:PJ2:HAM	1.95	0.47
1:A:117:ARG:NH2	1:A:179:LEU:CD1	2.77	0.47
1:B:353:TYR:O	1:B:356:THR:CG2	2.62	0.47
1:A:130:ASN:C	1:A:130:ASN:ND2	2.55	0.47
1:A:218:ARG:NH1	1:A:222:ARG:NE	2.47	0.47
1:B:212:LYS:O	1:B:216:VAL:HG23	2.13	0.47
1:B:294:GLU:HB2	4:B:700:HOH:O	2.14	0.47
1:B:380:LEU:O	1:B:384:PRO:HD2	2.13	0.47
1:B:433:VAL:HG11	2:B:1003:MYR:H121	1.94	0.47
1:B:146:HIS:N	1:B:147:PRO:CD	2.78	0.47
1:B:378:LYS:CB	1:B:379:PRO:CD	2.93	0.47
1:B:536:LYS:HE2	4:B:687:HOH:O	2.14	0.47
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.96	0.47
1:A:405:ASN:ND2	1:A:526:GLN:HG2	2.30	0.47
1:B:546:ALA:HA	1:B:549:ASP:HB2	1.97	0.47
1:B:117:ARG:CD	3:B:1011:PJ2:HAI	2.24	0.47
1:B:423:LEU:O	1:B:427:SER:HB2	2.13	0.47
1:A:177:CYS:SG	1:A:181:LYS:CE	3.03	0.47
1:A:142:ILE:HG23	3:A:1011:PJ2:HAPA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:HG3	1:A:222:ARG:HH21	1.80	0.47
1:A:372:LYS:O	1:A:372:LYS:HG2	2.15	0.47
1:B:100:GLU:OE2	1:B:247:HIS:HE1	1.97	0.47
1:B:485:ARG:N	1:B:486:PRO:HD2	2.30	0.47
1:A:142:ILE:HG12	3:A:1011:PJ2:CAP	2.45	0.47
1:A:86:GLU:CG	1:A:105:HIS:CE1	2.98	0.47
1:A:494:ASP:OD1	1:A:496:THR:N	2.44	0.47
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.96	0.47
1:B:513:ILE:O	1:B:516:LEU:HD22	2.15	0.47
1:A:103:LEU:HA	1:A:103:LEU:HD12	1.67	0.46
1:B:161:TYR:OH	3:B:1011:PJ2:HAP	2.16	0.46
1:B:6:GLU:HG3	1:B:66:LEU:HD23	1.96	0.46
1:B:382:GLU:CG	1:B:386:ASN:ND2	2.70	0.46
1:B:426:VAL:HG23	1:B:427:SER:N	2.30	0.46
1:B:485:ARG:N	1:B:486:PRO:CD	2.77	0.46
3:A:1011:PJ2:HAS	3:A:1011:PJ2:HAK	1.11	0.46
1:A:458:ASN:CA	1:A:484:ARG:HH12	2.19	0.46
1:A:545:LYS:HE3	1:A:545:LYS:HB2	1.63	0.46
1:B:73:LYS:HA	1:B:73:LYS:HD2	1.77	0.46
1:A:168:CYS:SG	1:A:181:LYS:CE	3.03	0.46
1:A:218:ARG:HH12	1:A:222:ARG:HE	1.56	0.46
1:B:488:PHE:HB3	2:B:1004:MYR:H51	1.97	0.46
1:B:525:LYS:HE2	2:B:1005:MYR:O2	2.15	0.46
1:A:325:VAL:O	1:A:329:MET:HG3	2.15	0.46
1:B:551:PHE:CD1	2:B:1005:MYR:H72	2.49	0.46
1:B:211:PHE:HE2	1:B:238:LEU:CD2	2.29	0.46
1:B:484:ARG:HG2	1:B:484:ARG:O	2.15	0.46
1:A:158:ALA:HA	3:A:1011:PJ2:HASA	1.97	0.46
1:B:401:TYR:OH	1:B:525:LYS:HD3	2.16	0.46
1:B:94:GLN:CA	1:B:94:GLN:NE2	2.78	0.46
1:A:136:LYS:HA	1:A:136:LYS:HD2	1.67	0.45
1:A:557:LYS:HD2	1:A:557:LYS:N	2.30	0.45
1:B:156:PHE:CE2	1:B:285:GLU:HG2	2.52	0.45
3:A:1012:PJ2:HASA	3:A:1012:PJ2:HAKA	1.81	0.45
1:A:121:ASP:O	1:A:125:THR:OG1	2.20	0.45
1:A:556:GLU:CB	1:A:557:LYS:HZ2	2.29	0.45
1:A:131:GLU:HG2	1:A:135:LEU:HD23	1.97	0.45
1:B:3:HIS:CE1	1:B:9:HIS:CE1	3.05	0.45
2:A:1004:MYR:H22	2:A:1004:MYR:C6	2.43	0.45
1:B:186:ARG:O	1:B:190:LYS:HB2	2.17	0.45
1:B:551:PHE:CG	2:B:1005:MYR:C7	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1004:MYR:H31	2:A:1004:MYR:H61	1.24	0.45
1:A:146:HIS:NE2	3:A:1012:PJ2:HAX	2.29	0.45
1:B:178:LEU:HD11	1:B:182:LEU:HD11	1.92	0.45
1:B:505:GLU:OE2	1:B:508:THR:HG21	2.17	0.45
1:B:95:GLU:HG3	1:B:96:PRO:HD3	1.98	0.45
1:B:484:ARG:HG3	1:B:484:ARG:NH2	2.32	0.45
1:A:446:MET:HB3	1:A:447:PRO:HD3	1.99	0.45
1:B:218:ARG:NH2	1:B:222:ARG:HE	2.15	0.45
1:B:416:PRO:HD2	1:B:417:GLN:HE22	1.82	0.45
1:B:179:LEU:HA	1:B:179:LEU:HD12	1.73	0.45
2:A:1004:MYR:H111	2:A:1004:MYR:H81	1.43	0.44
1:A:484:ARG:CZ	4:A:679:HOH:O	2.64	0.44
1:A:505:GLU:N	1:A:505:GLU:OE2	2.50	0.44
1:A:513:ILE:CG1	1:A:521:ARG:HG3	2.44	0.44
1:A:556:GLU:HG3	1:A:557:LYS:HE3	1.98	0.44
1:A:74:LEU:O	1:A:77:VAL:HG13	2.17	0.44
1:B:178:LEU:HD22	1:B:182:LEU:HG	1.99	0.44
1:B:94:GLN:HA	1:B:94:GLN:NE2	2.27	0.44
1:A:222:ARG:HH22	2:A:1007:MYR:H92	1.80	0.44
1:B:95:GLU:CG	1:B:96:PRO:HD3	2.47	0.44
1:B:416:PRO:O	1:B:534:LYS:HE2	2.17	0.44
1:A:130:ASN:O	1:A:130:ASN:ND2	2.49	0.44
1:A:149:PHE:CE2	1:A:193:SER:HB2	2.53	0.44
1:B:466:LYS:O	1:B:468:PRO:HD2	2.16	0.44
1:A:179:LEU:HD13	1:A:179:LEU:HA	1.47	0.44
1:A:432:LYS:O	1:A:436:LYS:CG	2.62	0.44
1:B:428:ARG:NH2	1:B:526:GLN:HE22	1.99	0.44
1:B:66:LEU:HD12	2:B:1002:MYR:H143	1.98	0.44
1:A:177:CYS:O	1:A:181:LYS:HE2	2.18	0.44
1:B:460:LEU:CD2	2:B:1004:MYR:C13	2.87	0.44
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.53	0.43
1:A:348:ARG:NE	4:A:607:HOH:O	2.43	0.43
1:B:298:MET:HE2	1:B:302:LEU:HD12	1.99	0.43
1:B:525:LYS:HB3	2:B:1005:MYR:C4	2.47	0.43
1:B:555:VAL:O	1:B:559:CYS:SG	2.76	0.43
1:B:158:ALA:HA	3:B:1011:PJ2:HAK	1.99	0.43
1:B:378:LYS:HB2	1:B:379:PRO:CD	2.38	0.43
1:A:441:PRO:O	1:A:445:ARG:HG3	2.18	0.43
1:A:100:GLU:OE1	1:A:247:HIS:HE1	2.01	0.43
1:A:112:LEU:CD1	1:A:145:ARG:CG	2.84	0.43
1:A:67:HIS:CE1	1:A:249:ASP:OD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASN:N	4:B:700:HOH:O	2.32	0.43
1:B:484:ARG:NH2	1:B:484:ARG:CG	2.76	0.43
1:A:506:THR:CG2	1:A:531:GLU:HG3	2.49	0.43
1:A:521:ARG:HG2	1:A:525:LYS:HD2	2.00	0.43
1:A:94:GLN:NE2	1:A:94:GLN:CA	2.79	0.43
1:B:23:VAL:HG12	1:B:43:VAL:HG22	2.01	0.43
1:B:401:TYR:OH	2:B:1005:MYR:H32	2.19	0.43
2:A:1007:MYR:H71	2:A:1007:MYR:H102	1.38	0.43
1:A:168:CYS:HB3	1:A:177:CYS:HB3	1.93	0.43
1:A:372:LYS:CE	1:A:375:ASP:HB2	2.48	0.43
1:A:24:LEU:HB2	1:A:43:VAL:HG21	1.99	0.43
1:B:394:LEU:HA	1:B:397:GLN:HG2	2.01	0.43
1:B:484:ARG:HH21	1:B:484:ARG:HG3	1.82	0.43
1:B:506:THR:HG21	1:B:531:GLU:HB3	2.01	0.43
1:A:408:LEU:CD1	1:A:427:SER:OG	2.62	0.43
1:A:95:GLU:OE1	1:A:99:ASN:CB	2.60	0.43
1:A:96:PRO:HD2	1:A:97:GLU:OE2	2.19	0.43
1:B:455:VAL:O	1:B:456:VAL:C	2.56	0.43
1:B:80:LEU:HD11	1:B:87:MET:CE	2.48	0.43
1:A:395:PHE:CD2	1:A:395:PHE:C	2.92	0.43
1:B:138:TYR:HB3	3:B:1011:PJ2:HAQA	2.01	0.43
1:A:112:LEU:HD11	1:A:144:ARG:HG3	2.01	0.43
1:B:127:PHE:CE1	1:B:165:PHE:CB	3.02	0.43
1:B:76:THR:O	1:B:77:VAL:C	2.58	0.43
1:B:117:ARG:HH11	1:B:179:LEU:CD1	2.32	0.42
1:B:258:ALA:HB2	1:B:283:LEU:HD21	2.00	0.42
1:A:178:LEU:C	1:A:180:PRO:HD2	2.40	0.42
1:A:506:THR:HG21	1:A:531:GLU:HB3	2.01	0.42
1:A:538:LYS:N	4:A:649:HOH:O	2.37	0.42
1:B:297:GLU:CD	4:B:639:HOH:O	2.58	0.42
1:B:574:LYS:O	1:B:575:LEU:C	2.57	0.42
1:B:95:GLU:C	1:B:95:GLU:CD	2.78	0.42
1:B:551:PHE:CD1	2:B:1005:MYR:H92	2.55	0.42
1:B:274:LYS:HE2	1:B:295:ASN:O	2.19	0.42
1:A:114:ARG:HH21	3:A:1012:PJ2:HAO	1.84	0.42
1:A:187:ASP:OD2	1:A:432:LYS:HE2	2.19	0.42
1:A:345:LEU:HD22	1:A:349:LEU:HG	2.02	0.42
1:A:432:LYS:O	1:A:436:LYS:HD3	2.19	0.42
1:A:94:GLN:CA	1:A:94:GLN:HE21	2.14	0.42
2:B:1004:MYR:H52	2:B:1004:MYR:H21	1.12	0.42
1:B:557:LYS:HE3	1:B:557:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASN:ND2	1:B:133:THR:HB	2.35	0.42
1:A:158:ALA:CB	3:A:1011:PJ2:HAQ	2.49	0.42
3:A:1012:PJ2:CAM	3:A:1012:PJ2:HAS	2.50	0.42
1:A:100:GLU:OE1	1:A:247:HIS:CE1	2.73	0.42
1:B:174:LYS:NZ	4:B:701:HOH:O	2.27	0.42
1:A:32:GLN:O	1:A:144:ARG:HD2	2.20	0.42
1:B:130:ASN:ND2	1:B:133:THR:CB	2.83	0.42
1:B:187:ASP:O	1:B:188:GLU:C	2.58	0.42
1:B:375:ASP:O	1:B:378:LYS:HB2	2.19	0.42
1:B:420:THR:OG1	1:B:531:GLU:OE1	2.32	0.42
1:B:138:TYR:CB	3:B:1011:PJ2:HAQA	2.50	0.42
1:B:32:GLN:O	1:B:144:ARG:HD2	2.20	0.42
1:B:441:PRO:O	1:B:445:ARG:HG3	2.20	0.42
1:A:142:ILE:HD12	3:A:1011:PJ2:HAAA	1.80	0.41
1:A:240:LYS:HG2	4:A:661:HOH:O	2.20	0.41
1:A:430:LEU:C	1:A:433:VAL:HG12	2.40	0.41
1:B:3:HIS:CD2	1:B:9:HIS:CD2	3.08	0.41
1:B:72:ASP:O	1:B:76:THR:HG23	2.20	0.41
1:A:101:CYS:O	1:A:105:HIS:HD2	2.02	0.41
1:A:405:ASN:HD21	1:A:526:GLN:HG2	1.85	0.41
1:A:27:PHE:CZ	1:A:70:PHE:CD1	3.08	0.41
1:B:313:LYS:HB2	1:B:313:LYS:HE3	1.54	0.41
1:A:212:LYS:O	1:A:216:VAL:HG23	2.21	0.41
1:A:274:LYS:NZ	1:A:297:GLU:OE1	2.36	0.41
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.51	0.41
1:A:3:HIS:CD2	1:A:9:HIS:CD2	3.08	0.41
1:B:556:GLU:C	1:B:558:CYS:H	2.23	0.41
1:B:572:GLY:O	1:B:573:LYS:C	2.59	0.41
1:A:114:ARG:CD	3:A:1012:PJ2:HAAB	2.23	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.87	0.41
1:A:420:THR:O	1:A:424:VAL:HG23	2.20	0.41
1:B:433:VAL:CG1	1:B:434:GLY:N	2.84	0.41
1:A:551:PHE:CD2	1:A:551:PHE:C	2.94	0.41
1:B:525:LYS:HB3	2:B:1005:MYR:H41	2.03	0.41
1:B:211:PHE:CE1	1:B:242:HIS:ND1	2.89	0.41
1:B:403:PHE:O	1:B:407:LEU:HG	2.21	0.41
1:A:27:PHE:C	1:A:39:HIS:HE1	2.23	0.41
1:B:66:LEU:HA	1:B:66:LEU:HD13	1.33	0.41
1:B:94:GLN:HB2	1:B:95:GLU:H	1.63	0.41
1:A:290:ILE:O	1:A:293:VAL:HG12	2.20	0.41
1:A:35:PRO:HA	4:A:587:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:THR:HG23	1:A:531:GLU:HG3	2.02	0.41
1:B:25:ILE:O	1:B:29:GLN:HG3	2.21	0.41
1:A:402:LYS:HE2	1:A:402:LYS:HB3	1.95	0.41
1:B:114:ARG:CD	1:B:114:ARG:N	2.84	0.41
1:B:3:HIS:NE2	1:B:9:HIS:NE2	2.69	0.41
1:A:211:PHE:CD1	1:A:242:HIS:CD2	3.04	0.41
1:A:525:LYS:NZ	2:A:1005:MYR:O2	2.54	0.41
1:A:59:ALA:O	1:A:62:CYS:HB2	2.20	0.41
1:B:103:LEU:HD12	4:B:718:HOH:O	2.21	0.41
1:B:430:LEU:HA	1:B:430:LEU:HD23	1.77	0.41
1:B:570:GLU:C	1:B:572:GLY:N	2.73	0.41
1:A:313:LYS:HG2	1:A:314:ASP:N	2.36	0.41
1:A:415:VAL:CG2	1:A:415:VAL:O	2.42	0.41
1:A:458:ASN:CG	1:A:484:ARG:HH12	2.24	0.41
1:A:512:ASP:O	1:A:513:ILE:C	2.59	0.40
1:A:529:LEU:O	1:A:532:LEU:HB3	2.21	0.40
1:B:537:PRO:HG2	1:B:538:LYS:CD	2.45	0.40
1:A:408:LEU:HD21	1:A:526:GLN:HB3	2.03	0.40
1:B:138:TYR:CD2	3:B:1011:PJ2:CAW	2.98	0.40
1:B:225:LYS:HG2	1:B:299:PRO:HG3	2.03	0.40
1:B:298:MET:CE	1:B:337:ARG:CG	3.00	0.40
1:B:80:LEU:HD23	1:B:88:ALA:HA	2.04	0.40
1:B:93:LYS:O	1:B:94:GLN:O	2.39	0.40
1:A:142:ILE:HD13	3:A:1011:PJ2:HAAB	1.87	0.40
1:A:179:LEU:N	1:A:180:PRO:HD2	2.36	0.40
1:A:25:ILE:O	1:A:29:GLN:HG3	2.21	0.40
1:A:367:HIS:HA	1:A:370:TYR:CE1	2.56	0.40
1:B:127:PHE:CD1	1:B:165:PHE:HB3	2.57	0.40
1:A:113:PRO:O	1:A:114:ARG:C	2.59	0.40
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.77	0.40
1:B:413:LYS:HB3	1:B:493:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	572/585 (98%)	532 (93%)	35 (6%)	5 (1%)	20	18
1	B	572/585 (98%)	532 (93%)	35 (6%)	5 (1%)	20	18
All	All	1144/1170 (98%)	1064 (93%)	70 (6%)	10 (1%)	20	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	PRO
1	B	94	GLN
1	A	111	ASN
1	B	95	GLU
1	A	479	GLU
1	A	109	ASN
1	A	378	LYS
1	B	378	LYS
1	B	467	THR
1	B	469	VAL

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	503/511 (98%)	452 (90%)	51 (10%)	9	8
1	B	503/511 (98%)	444 (88%)	59 (12%)	6	5
All	All	1006/1022 (98%)	896 (89%)	110 (11%)	7	6

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	41	LYS
1	A	103	LEU

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	130	ASN
1	A	136	LYS
1	A	154	LEU
1	A	178	LEU
1	A	179	LEU
1	A	184	GLU
1	A	185	LEU
1	A	190	LYS
1	A	195	LYS
1	A	197	ARG
1	A	233	LYS
1	A	240	LYS
1	A	270	SER
1	A	292	GLU
1	A	301	ASP
1	A	313	LYS
1	A	334	TYR
1	A	345	LEU
1	A	357	LEU
1	A	372	LYS
1	A	387	LEU
1	A	389	LYS
1	A	398	LEU
1	A	407	LEU
1	A	408	LEU
1	A	410	ARG
1	A	425	GLU
1	A	436	LYS
1	A	444	LYS
1	A	451	ASP
1	A	453	LEU
1	A	455	VAL
1	A	460	LEU
1	A	465	GLU
1	A	466	LYS
1	A	475	LYS
1	A	485	ARG
1	A	491	LEU
1	A	495	GLU
1	A	509	PHE
1	A	512	ASP

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Mol	Chain	Res	Type
1	A	518	GLU
1	A	548	MET
1	A	556	GLU
1	A	557	LYS
1	A	570	GLU
1	A	573	LYS
1	B	13	ASP
1	B	48	GLU
1	B	60	GLU
1	B	66	LEU
1	B	94	GLN
1	B	103	LEU
1	B	107	ASP
1	B	117	ARG
1	B	130	ASN
1	B	135	LEU
1	B	140	TYR
1	B	156	PHE
1	B	170	GLN
1	B	178	LEU
1	B	179	LEU
1	B	185	LEU
1	B	190	LYS
1	B	197	ARG
1	B	202	SER
1	B	235	VAL
1	B	239	THR
1	B	240	LYS
1	B	241	VAL
1	B	252	GLU
1	B	262	LYS
1	B	276	LYS
1	B	280	GLU
1	B	313	LYS
1	B	334	TYR
1	B	345	LEU
1	B	351	LYS
1	B	357	LEU
1	B	382	GLU
1	B	387	LEU
1	B	394	LEU
1	B	398	LEU

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Mol	Chain	Res	Type
1	B	408	LEU
1	B	410	ARG
1	B	413	LYS
1	B	417	GLN
1	B	419	SER
1	B	439	LYS
1	B	451	ASP
1	B	453	LEU
1	B	467	THR
1	B	482	VAL
1	B	484	ARG
1	B	485	ARG
1	B	491	LEU
1	B	495	GLU
1	B	500	LYS
1	B	516	LEU
1	B	518	GLU
1	B	522	GLN
1	B	538	LYS
1	B	541	LYS
1	B	545	LYS
1	B	556	GLU
1	B	557	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	39	HIS
1	A	44	ASN
1	A	67	HIS
1	A	94	GLN
1	A	105	HIS
1	A	109	ASN
1	A	128	HIS
1	A	130	ASN
1	A	242	HIS
1	A	247	HIS
1	A	295	ASN
1	A	367	HIS
1	A	385	GLN
1	A	391	ASN

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Mol	Chain	Res	Type
1	A	405	ASN
1	A	417	GLN
1	A	429	ASN
1	A	440	HIS
1	A	522	GLN
1	A	526	GLN
1	A	580	GLN
1	B	39	HIS
1	B	44	ASN
1	B	67	HIS
1	B	94	GLN
1	B	99	ASN
1	B	105	HIS
1	B	128	HIS
1	B	130	ASN
1	B	295	ASN
1	B	385	GLN
1	B	386	ASN
1	B	390	GLN
1	B	391	ASN
1	B	405	ASN
1	B	417	GLN
1	B	429	ASN
1	B	526	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	1002	-	12,15,15	0.38	0	11,15,15	0.62	0
2	MYR	A	1003	-	12,15,15	0.74	0	11,15,15	1.10	2 (18%)
2	MYR	A	1004	-	12,15,15	0.30	0	11,15,15	1.56	2 (18%)
2	MYR	A	1005	-	12,15,15	0.34	0	11,15,15	0.93	0
2	MYR	A	1006	-	12,15,15	0.32	0	11,15,15	1.29	1 (9%)
2	MYR	A	1007	-	11,11,15	0.33	0	10,10,15	0.69	0
3	PJ2	A	1011	-	18,24,24	2.50	5 (27%)	18,29,29	2.98	5 (27%)
3	PJ2	A	1012	1	18,24,24	1.93	4 (22%)	18,29,29	1.71	2 (11%)
2	MYR	B	1002	-	12,15,15	0.48	0	11,15,15	0.57	0
2	MYR	B	1003	-	12,15,15	0.54	0	11,15,15	0.59	0
2	MYR	B	1004	-	12,15,15	0.39	0	11,15,15	1.36	2 (18%)
2	MYR	B	1005	-	12,15,15	0.46	0	11,15,15	0.50	0
2	MYR	B	1006	-	12,15,15	0.55	0	11,15,15	0.51	0
2	MYR	B	1007	-	11,11,15	0.27	0	10,10,15	0.74	0
3	PJ2	B	1011	-	18,24,24	2.22	6 (33%)	18,29,29	2.67	6 (33%)

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	1002	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1003	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1004	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1005	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1006	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1007	-	-	0/9/9/13	0/0/0/0
3	PJ2	A	1011	-	-	0/17/32/32	0/1/1/1
3	PJ2	A	1012	1	-	0/17/32/32	0/1/1/1
2	MYR	B	1002	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1003	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1004	-	-	0/11/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	B	1005	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1006	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1007	-	-	0/9/9/13	0/0/0/0
3	PJ2	B	1011	-	-	0/17/32/32	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1011	PJ2	CAN-CAJ	-5.80	1.38	1.50
3	A	1012	PJ2	CAN-CAJ	-5.50	1.39	1.50
3	B	1011	PJ2	CAM-CAG	-4.92	1.34	1.50
3	B	1011	PJ2	CAN-CAJ	-4.57	1.41	1.50
3	A	1012	PJ2	CAM-CAG	-3.83	1.37	1.50
3	A	1011	PJ2	CAN-CAW	-3.41	1.47	1.53
3	A	1011	PJ2	CAM-CAG	-3.34	1.39	1.50
3	B	1011	PJ2	CAM-CAX	-2.76	1.48	1.54
3	A	1012	PJ2	CAL-CAF	-2.37	1.37	1.50
3	A	1011	PJ2	CAL-CAF	-2.33	1.38	1.50
3	B	1011	PJ2	OAE-CAW	-2.31	1.36	1.43
3	B	1011	PJ2	CAL-CAF	-2.04	1.39	1.50
3	A	1012	PJ2	CAJ-CAV	3.61	1.38	1.33
3	B	1011	PJ2	CAJ-CAV	4.37	1.39	1.33
3	A	1011	PJ2	CAJ-CAV	6.36	1.41	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1011	PJ2	OAC-CAU-CAV	-7.65	119.50	127.14
3	A	1011	PJ2	CAN-CAJ-CAV	-5.63	119.12	126.45
3	A	1011	PJ2	OAC-CAU-CAV	-4.36	122.79	127.14
2	A	1004	MYR	C5-C4-C3	-3.41	96.89	114.45
2	B	1004	MYR	C4-C3-C2	-3.31	100.53	113.70
2	A	1006	MYR	C4-C3-C2	-3.18	101.08	113.70
2	A	1004	MYR	C6-C5-C4	-3.00	98.97	114.45
3	B	1011	PJ2	CAM-CAG-CAF	-2.95	117.37	126.29
2	B	1004	MYR	C5-C4-C3	-2.56	101.28	114.45
3	A	1011	PJ2	CAO-CAQ-CAS	-2.40	105.11	113.63
3	A	1012	PJ2	OAC-CAU-CAV	-2.32	124.82	127.14
3	B	1011	PJ2	OAE-CAW-CAS	-2.29	102.96	109.26
2	A	1003	MYR	C6-C5-C4	2.02	124.86	114.45
3	B	1011	PJ2	CAR-CAP-CAL	2.39	117.37	113.16
3	B	1011	PJ2	CAI-CAH-CAU	2.40	112.24	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	MYR	C4-C3-C2	2.81	124.87	113.70
3	A	1011	PJ2	CAI-CAH-CAU	2.84	112.67	109.86
3	B	1011	PJ2	CAH-CAU-CAV	5.53	111.05	106.63
3	A	1012	PJ2	CAH-CAU-CAV	6.12	111.52	106.63
3	A	1011	PJ2	CAH-CAU-CAV	8.82	113.69	106.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 135 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	MYR	4	0
2	A	1003	MYR	4	0
2	A	1004	MYR	12	0
2	A	1005	MYR	6	0
2	A	1006	MYR	1	0
2	A	1007	MYR	3	0
3	A	1011	PJ2	22	0
3	A	1012	PJ2	22	0
2	B	1002	MYR	5	0
2	B	1003	MYR	8	0
2	B	1004	MYR	8	0
2	B	1005	MYR	11	0
2	B	1006	MYR	5	0
2	B	1007	MYR	3	0
3	B	1011	PJ2	26	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, 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	576/585 (98%)	0.37	28 (4%) 30 29	19, 29, 37, 44	0
1	B	576/585 (98%)	0.43	26 (4%) 34 32	19, 30, 38, 44	0
All	All	1152/1170 (98%)	0.40	54 (4%) 32 31	19, 29, 37, 44	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	CYS	8.1
1	B	557	LYS	5.7
1	A	176	ALA	5.2
1	A	567	CYS	5.1
1	A	581	ALA	4.7
1	A	570	GLU	4.5
1	A	516	LEU	4.4
1	A	568	PHE	4.2
1	B	568	PHE	4.2
1	A	584	GLY	4.1
1	B	466	LYS	4.1
1	A	301	ASP	4.0
1	B	498	VAL	3.8
1	B	172	ALA	3.7
1	B	515	THR	3.7
1	A	510	HIS	3.6
1	B	570	GLU	3.6
1	A	517	SER	3.6
1	B	513	ILE	3.5
1	B	516	LEU	3.4
1	B	567	CYS	3.3
1	A	111	ASN	3.3
1	B	465	GLU	3.2
1	A	2	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	84	TYR	3.1
1	A	110	PRO	3.1
1	B	569	ALA	3.1
1	B	467	THR	2.9
1	B	558	CYS	2.9
1	B	511	ALA	2.8
1	A	109	ASN	2.8
1	A	572	GLY	2.8
1	A	555	VAL	2.6
1	B	540	THR	2.6
1	B	174	LYS	2.5
1	B	175	ALA	2.5
1	A	85	GLY	2.5
1	A	178	LEU	2.5
1	B	481	LEU	2.5
1	A	171	ALA	2.4
1	A	557	LYS	2.4
1	A	466	LYS	2.4
1	B	2	ALA	2.3
1	A	513	ILE	2.3
1	B	95	GLU	2.3
1	B	501	GLU	2.2
1	B	166	THR	2.1
1	B	582	ALA	2.1
1	A	170	GLN	2.1
1	B	94	GLN	2.1
1	A	577	ALA	2.1
1	A	559	CYS	2.1
1	A	166	THR	2.0
1	A	553	ALA	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	PJ2	A	1011	24/24	0.71	0.27	3.45	50,65,71,72	0
2	MYR	A	1006	16/16	0.76	0.21	2.83	44,53,59,60	0
2	MYR	A	1003	16/16	0.80	0.19	2.62	37,50,58,59	0
2	MYR	B	1002	16/16	0.83	0.18	2.25	40,49,56,56	0
3	PJ2	B	1011	24/24	0.73	0.20	1.82	46,61,65,65	0
2	MYR	B	1007	12/16	0.88	0.19	1.66	49,55,59,60	0
2	MYR	A	1002	16/16	0.85	0.17	1.51	37,48,62,62	0
2	MYR	B	1005	16/16	0.83	0.19	1.31	52,56,56,57	0
2	MYR	B	1003	16/16	0.89	0.14	0.66	33,40,47,48	0
2	MYR	B	1006	16/16	0.80	0.16	0.40	46,54,57,58	0
3	PJ2	A	1012	24/24	0.75	0.23	0.28	65,74,78,79	0
2	MYR	B	1004	16/16	0.89	0.15	0.14	45,49,53,55	0
2	MYR	A	1004	16/16	0.88	0.14	0.14	43,49,57,58	0
2	MYR	A	1005	16/16	0.88	0.16	0.04	43,48,57,59	0
2	MYR	A	1007	12/16	0.86	0.14	-0.14	52,53,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.