Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:58 PM GMT

PDB ID	:	4DX7
Title	:	Transport of drugs by the multidrug transporter AcrB involves an access and a deep binding pocket that are separated by a switch-loop
Authors	:	Eicher, T.; Cha, H.; Seeger, M.A.; Brandstaetter, L.; El-Delik, J.; Bohnert, J.A.; Kern, W.V.; Verrey, F.; Gruetter, M.G.; Diederichs, K.; Pos, K.M.
Deposited on	:	2012-02-27
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

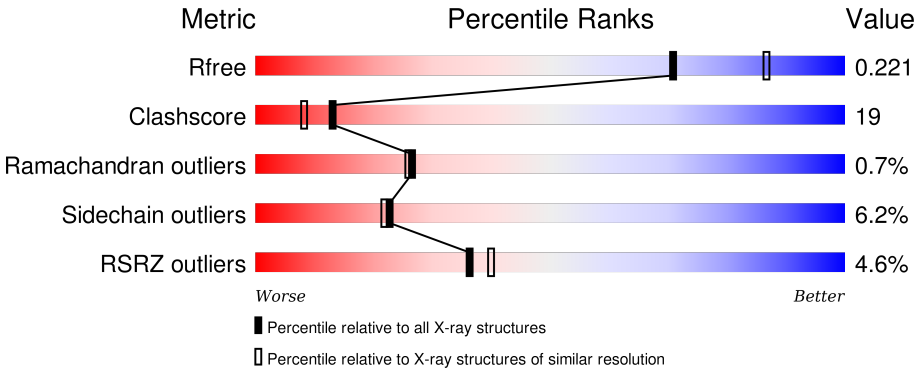
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	1057	5% 67% 26% 5%
1	B	1057	3% 74% 21%
1	C	1057	3% 76% 19%
2	D	169	2% 73% 17% 8%
2	E	169	19% 62% 25% 10%

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
3	LMT	A	1103	-	-	-	X
3	LMT	A	1104	-	-	-	X
3	LMT	B	1102	-	-	-	X
4	DM2	A	1105	-	-	X	-
4	DM2	B	1104	-	-	-	X
5	D12	A	1107	-	-	-	X
5	D12	B	1109	-	-	-	X
7	LMU	B	1103	-	-	-	X
8	GOL	B	1106	-	-	-	X
8	GOL	B	1107	-	-	-	X
8	GOL	C	1103	-	-	-	X
9	HEX	B	1108	-	-	-	X
9	HEX	C	1105	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28467 atoms, of which 273 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7927	5097	1311	1475	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	C	1036	Total	C	N	O	S	0	0	0
			7875	5067	1302	1462	44			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	EXPRESSION TAG	UNP P31224
A	1051	GLU	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
A	1054	HIS	-	EXPRESSION TAG	UNP P31224
A	1055	HIS	-	EXPRESSION TAG	UNP P31224
A	1056	HIS	-	EXPRESSION TAG	UNP P31224
A	1057	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	LEU	-	EXPRESSION TAG	UNP P31224
B	1051	GLU	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1054	HIS	-	EXPRESSION TAG	UNP P31224
B	1055	HIS	-	EXPRESSION TAG	UNP P31224
B	1056	HIS	-	EXPRESSION TAG	UNP P31224
B	1057	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	LEU	-	EXPRESSION TAG	UNP P31224
C	1051	GLU	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1054	HIS	-	EXPRESSION TAG	UNP P31224
C	1055	HIS	-	EXPRESSION TAG	UNP P31224
C	1056	HIS	-	EXPRESSION TAG	UNP P31224

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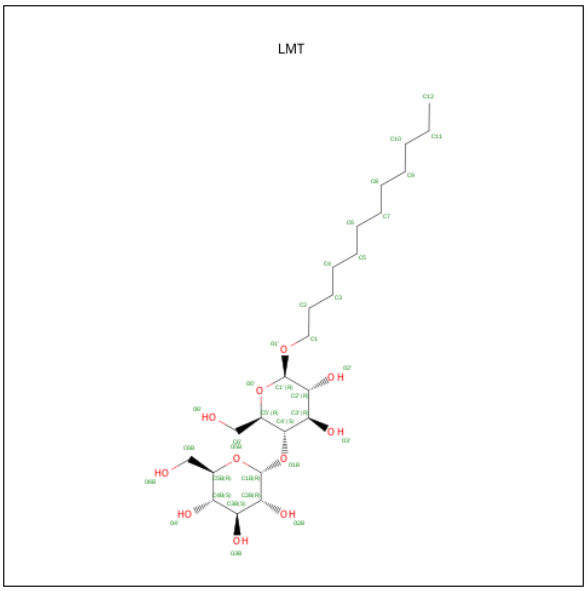
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

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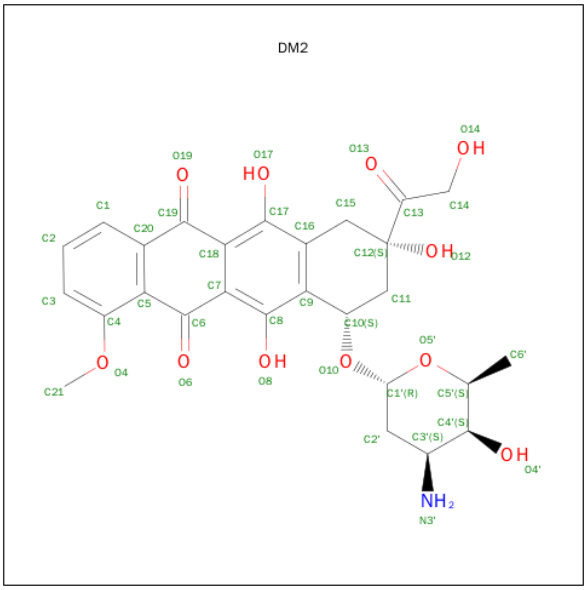
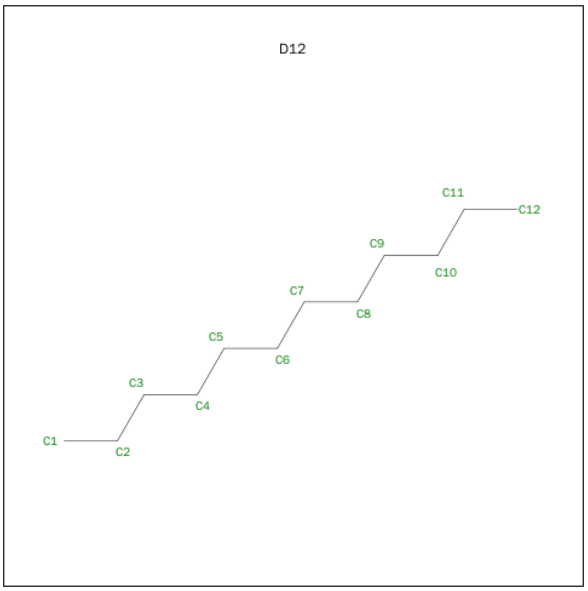
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 35 24 11	0	0

- Molecule 4 is DOXORUBICIN (three-letter code: DM2) (formula: $C_{27}H_{29}NO_{11}$).



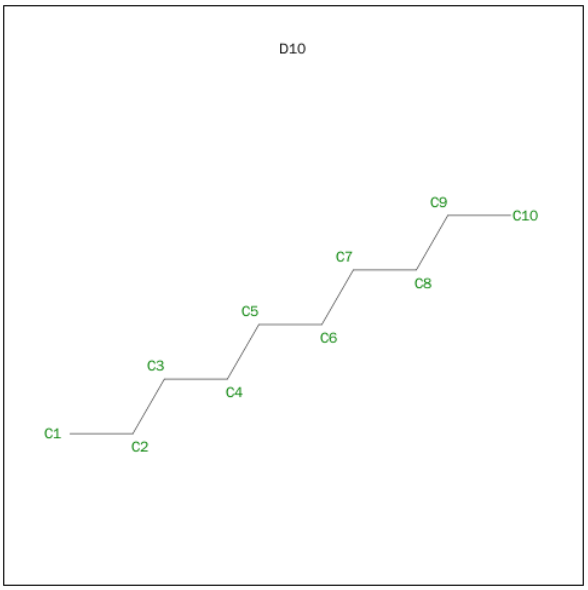
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 39 27 1 11	0	0
4	A	1	Total C H N O 68 27 29 1 11	0	0
4	B	1	Total C N O 39 27 1 11	0	0

- Molecule 5 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



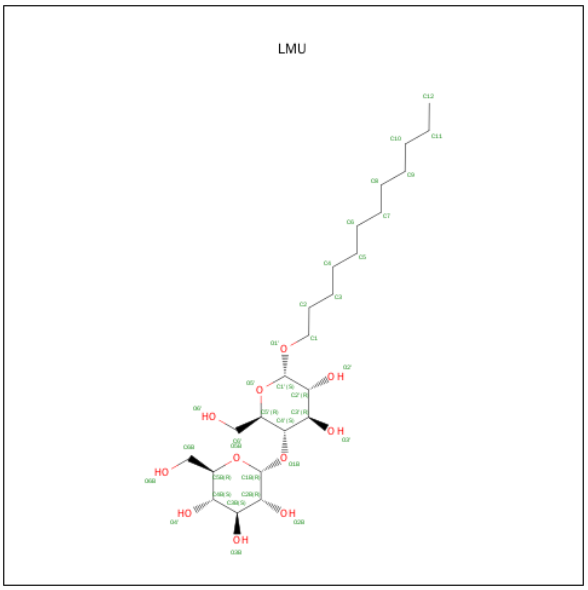
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H 38 12 26	0	0
5	B	1	Total C H 38 12 26	0	0
5	C	1	Total C H 38 12 26	0	0
5	C	1	Total C H 38 12 26	0	0

- Molecule 6 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



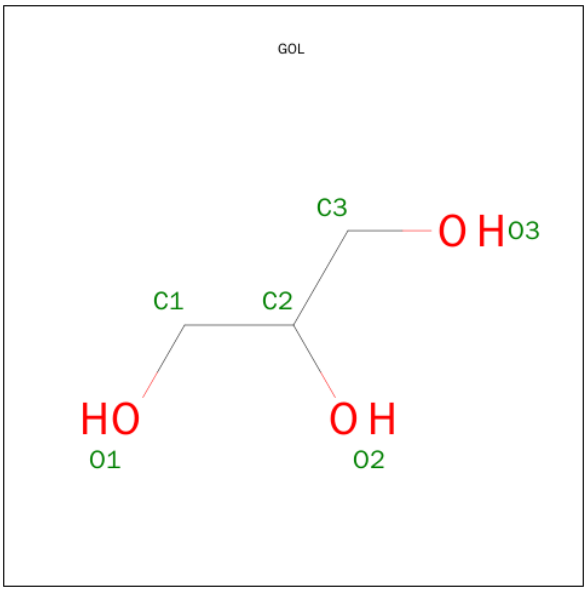
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H 32 10 22	0	0
6	A	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0

- Molecule 7 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



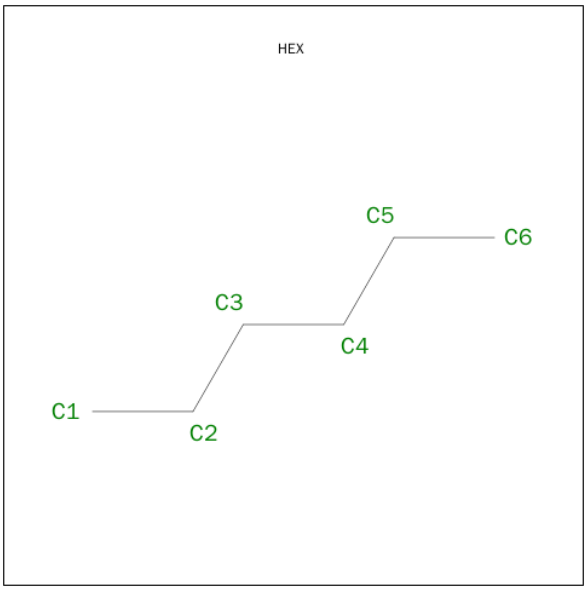
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 35 24 11	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			14	3	8	3		
8	B	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	H	0	0
			20	6	14		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	H	0	0
			20	6	14		

- Molecule 10 is water.

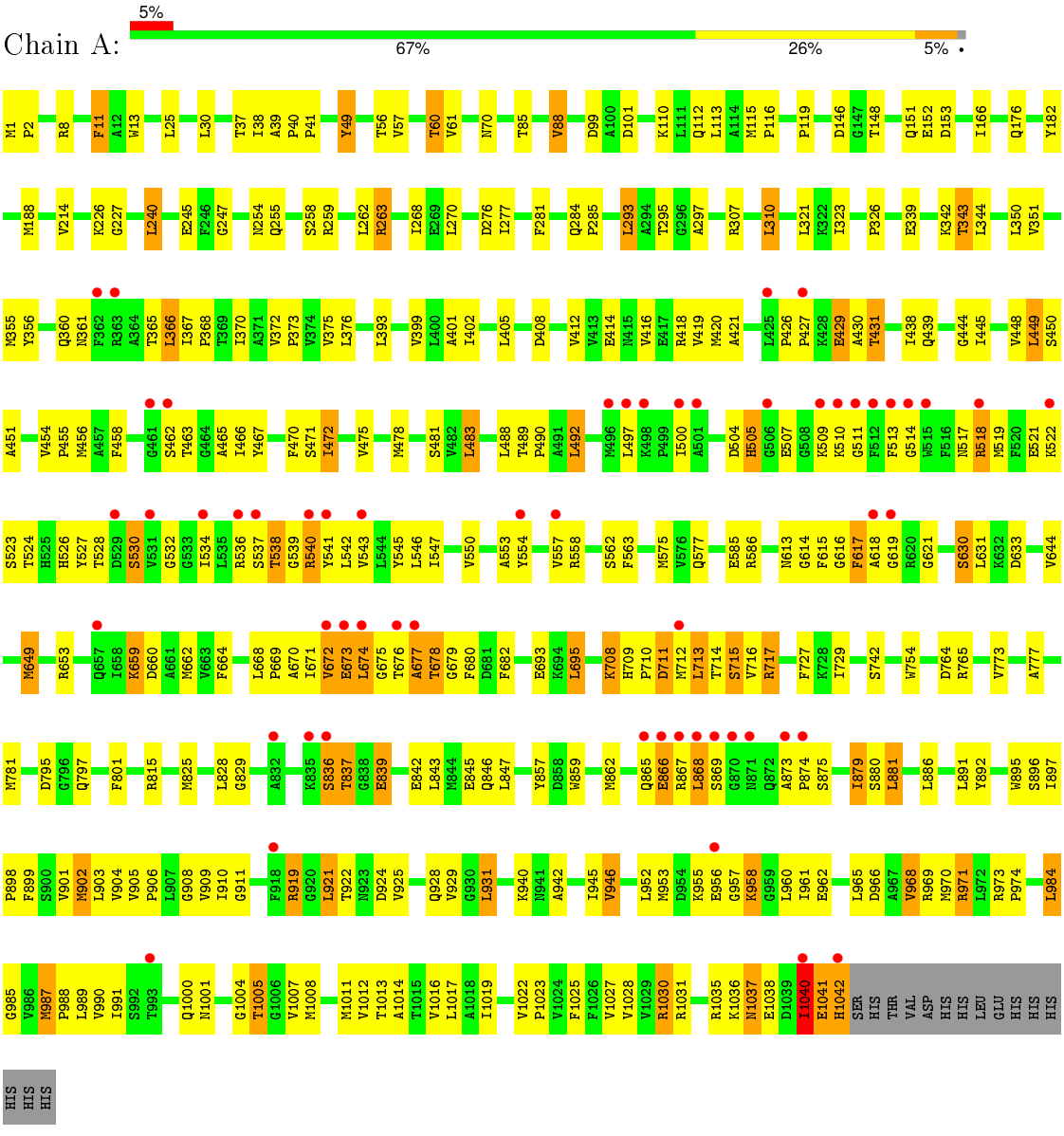
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	497	Total	O	0	0
			497	497		
10	B	494	Total	O	0	0
			494	494		
10	C	572	Total	O	0	0
			572	572		
10	D	81	Total	O	0	0
			81	81		
10	E	56	Total	O	0	0
			56	56		

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

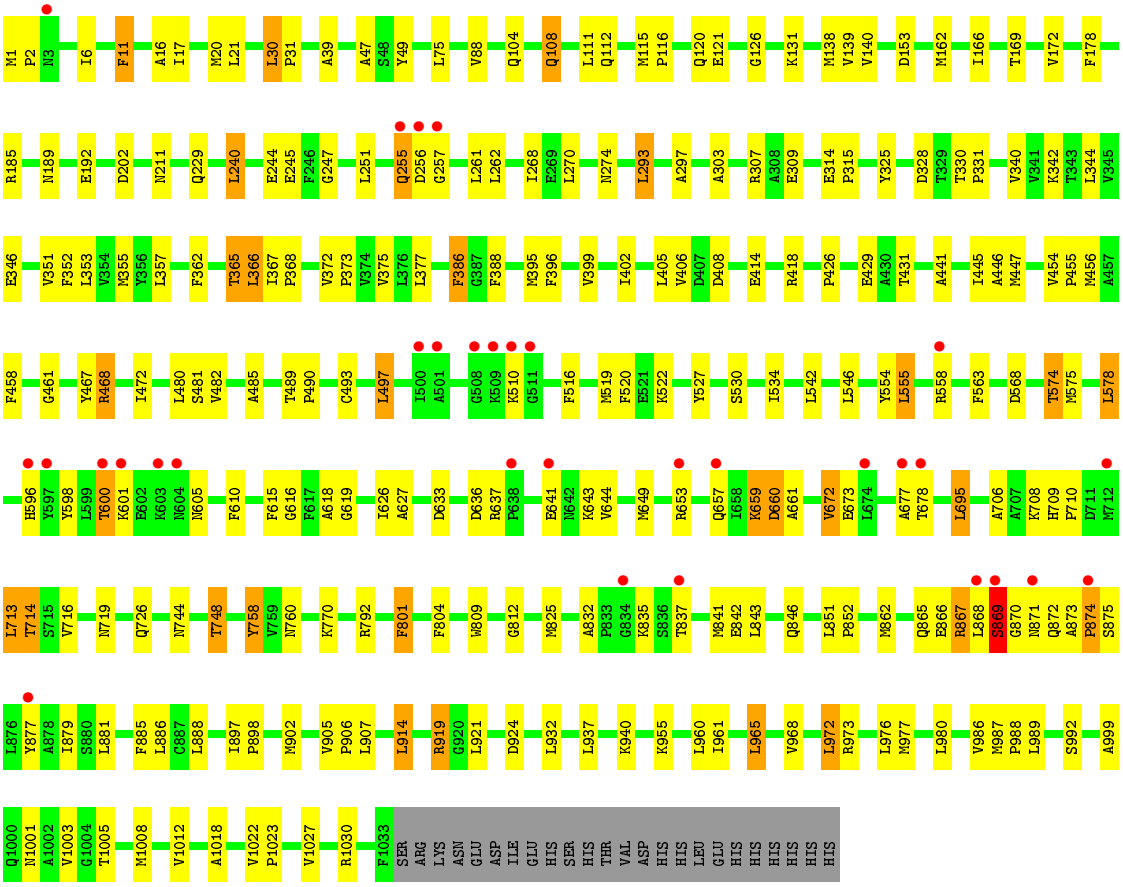
- Molecule 1: Acriflavine resistance protein B

Chain A:



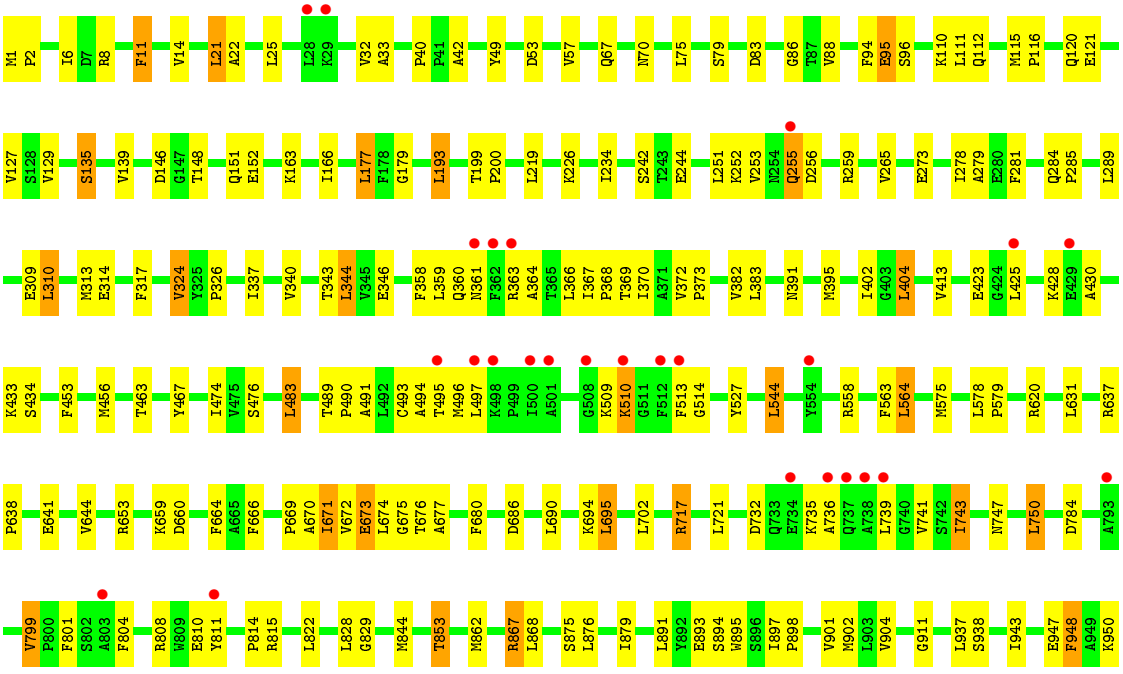
- Molecule 1: Acriflavine resistance protein B

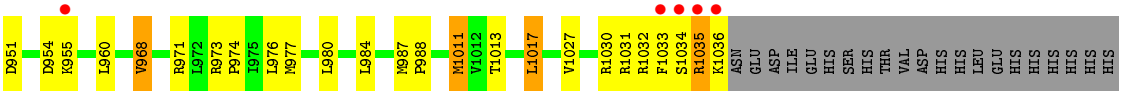
Chain B:



• Molecule 1: Acriflavine resistance protein B

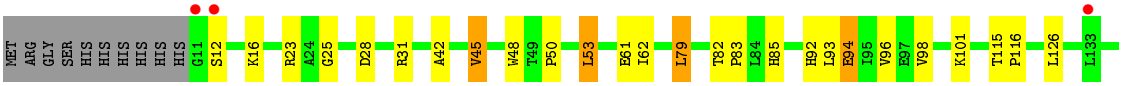
Chain C:





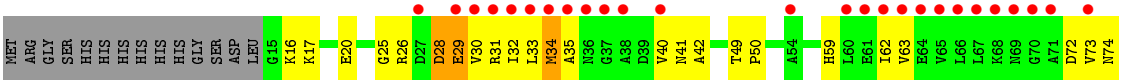
- Molecule 2: DARPIN

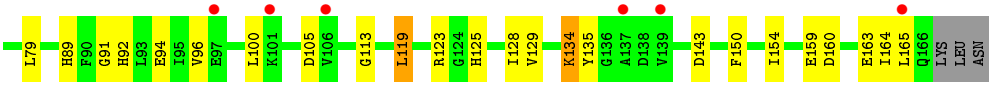
Chain D:



- Molecule 2: DARPIN

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.94Å 163.28Å 245.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.25 49.09 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.09-2.25) 99.5 (49.09-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.185 , 0.227 0.182 , 0.221	Depositor DCC
R_{free} test set	13724 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 274585 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28467	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, D10, D12, LMT, HEX, LMU, DM2

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	0/8078	0.53	1/10968 (0.0%)
1	B	0.37	0/7999	0.53	0/10863
1	C	0.39	0/8025	0.54	0/10896
2	D	0.35	0/1196	0.48	0/1626
2	E	0.32	0/1170	0.45	0/1591
All	All	0.37	0/26468	0.53	1/35944 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	VAL	CB-CA-C	-5.32	101.29	111.40

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	7927	0	8072	451	0
1	B	7849	0	8001	238	0
1	C	7875	0	8032	232	0
2	D	1177	0	1159	23	0
2	E	1151	0	1136	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	140	0	184	28	0
3	B	70	0	92	14	0
3	C	35	0	46	1	0
4	A	78	29	58	43	0
4	B	39	0	29	9	0
5	A	12	26	26	3	0
5	B	12	26	26	0	0
5	C	24	52	52	2	0
6	A	20	44	44	2	0
6	B	10	22	22	1	0
6	C	10	22	22	0	0
7	B	35	0	46	4	0
8	B	12	16	16	1	0
8	C	6	8	8	1	0
9	B	6	14	14	0	0
9	C	6	14	14	0	0
10	A	497	0	0	25	0
10	B	494	0	0	20	0
10	C	572	0	0	29	0
10	D	81	0	0	1	0
10	E	56	0	0	4	0
All	All	28194	273	27099	1016	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 19.

All (1016) 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:867:ARG:N	1:A:868:LEU:HB2	1.40	1.33
1:C:509:LYS:CA	1:C:510:LYS:HB2	1.72	1.20
1:A:146:ASP:HB2	10:A:1514:HOH:O	1.45	1.14
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.33	1.11
1:A:866:GLU:HG2	1:A:867:ARG:HA	1.21	1.11
1:A:617:PHE:HB2	4:A:1105:DM2:H142	1.15	1.10
1:C:673:GLU:N	1:C:673:GLU:OE2	1.84	1.09
1:A:671:ILE:O	1:A:674:LEU:HB2	1.54	1.08
1:A:867:ARG:N	1:A:868:LEU:CB	2.16	1.07
1:A:919:ARG:HH11	1:A:919:ARG:HG3	1.18	1.07
1:C:509:LYS:HA	1:C:510:LYS:HB2	1.10	1.07
1:B:414:GLU:HG3	1:B:977:MET:CE	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ARG:H	1:A:868:LEU:CB	1.68	1.05
1:C:244:GLU:N	1:C:244:GLU:OE1	1.90	1.05
3:A:1103:LMT:H3'	3:A:1103:LMT:O2B	1.55	1.04
1:A:537:SER:HB2	1:A:540:ARG:HD3	1.39	1.03
1:A:866:GLU:OE2	1:A:866:GLU:N	1.90	1.03
4:A:1105:DM2:H2'2	4:A:1105:DM2:H6'3	1.41	1.03
1:A:987:MET:CE	1:A:987:MET:HA	1.88	1.03
1:A:1031:ARG:NH1	1:A:1038:GLU:OE1	1.91	1.02
1:A:676:THR:HB	4:A:1105:DM2:C21	1.88	1.01
1:A:866:GLU:HG2	1:A:867:ARG:CA	1.89	1.01
1:C:70:ASN:O	1:C:110:LYS:NZ	1.95	1.00
1:B:919:ARG:HG2	1:B:919:ARG:HH11	1.22	1.00
1:A:987:MET:HE2	1:A:987:MET:CA	1.90	1.00
2:D:94:GLU:N	2:D:94:GLU:OE1	1.94	0.99
1:A:540:ARG:HD2	1:A:540:ARG:H	1.27	0.99
1:A:919:ARG:CG	1:A:919:ARG:HH11	1.74	0.99
1:C:527:TYR:CE2	1:C:968:VAL:HG13	1.99	0.98
1:B:748:THR:HG21	10:B:1536:HOH:O	1.62	0.98
1:A:672:VAL:HG22	1:A:673:GLU:H	1.28	0.97
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.44	0.97
1:A:866:GLU:C	1:A:868:LEU:HB2	1.83	0.97
1:A:1041:GLU:HG3	1:A:1042:HIS:H	1.27	0.96
1:C:671:ILE:H	1:C:862:MET:HE1	1.26	0.96
1:A:507:GLU:HG2	1:A:518:ARG:HD2	1.45	0.96
1:A:987:MET:HA	1:A:987:MET:HE2	0.98	0.95
1:C:671:ILE:HD11	1:C:674:LEU:CD1	1.96	0.95
1:A:671:ILE:H	1:A:674:LEU:HD12	1.29	0.95
1:A:866:GLU:CG	1:A:867:ARG:HA	1.98	0.94
1:A:617:PHE:HB2	4:A:1105:DM2:C14	1.98	0.93
1:A:987:MET:HE1	1:A:1008:MET:CE	1.99	0.93
1:A:676:THR:HB	4:A:1105:DM2:H211	1.50	0.92
1:C:509:LYS:HA	1:C:510:LYS:CB	1.99	0.92
1:A:1041:GLU:CG	1:A:1042:HIS:H	1.82	0.92
1:B:108:GLN:CG	1:C:112:GLN:HG3	2.00	0.92
2:E:31:ARG:NH2	10:E:204:HOH:O	2.03	0.91
1:A:966:ASP:O	1:A:970:MET:HG3	1.69	0.91
1:A:674:LEU:HB3	1:A:675:GLY:CA	1.99	0.91
1:A:867:ARG:H	1:A:868:LEU:CG	1.83	0.91
1:A:616:GLY:O	1:A:618:ALA:N	2.04	0.91
1:A:990:VAL:HG11	1:A:1008:MET:HE2	1.54	0.90
4:B:1104:DM2:O6	4:B:1104:DM2:H212	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LYS:HD3	1:A:659:LYS:N	1.87	0.89
1:A:865:GLN:HA	1:A:866:GLU:C	1.92	0.89
1:A:1041:GLU:HG3	1:A:1042:HIS:N	1.88	0.89
1:A:393:LEU:HD22	1:A:470:PHE:CE1	2.08	0.88
1:A:255:GLN:OE1	1:A:255:GLN:N	2.05	0.88
1:B:875:SER:HB3	3:B:1101:LMT:H6'2	1.54	0.88
1:A:355:MET:HA	1:A:355:MET:HE2	1.55	0.88
1:A:546:LEU:O	1:A:550:VAL:HG23	1.73	0.87
4:A:1105:DM2:O8	4:A:1105:DM2:H2'1	1.74	0.87
1:A:674:LEU:HB3	1:A:675:GLY:HA2	1.54	0.87
1:B:244:GLU:N	1:B:244:GLU:OE2	2.07	0.87
4:A:1106:DM2:N3'	10:A:1609:HOH:O	2.06	0.87
1:A:537:SER:CB	1:A:540:ARG:HD3	2.04	0.87
3:A:1103:LMT:H6'1	1:C:8:ARG:HH21	1.40	0.86
1:A:534:ILE:HG23	1:A:541:TYR:CZ	2.10	0.86
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.38	0.86
1:C:671:ILE:CD1	1:C:674:LEU:HG	2.06	0.86
1:C:53:ASP:O	1:C:57:VAL:HG23	1.74	0.86
1:B:660:ASP:N	10:B:1560:HOH:O	2.07	0.86
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.36	0.85
1:A:867:ARG:H	1:A:868:LEU:HB2	1.28	0.85
1:B:673:GLU:N	1:B:673:GLU:OE2	2.09	0.84
1:A:586:ARG:NH2	1:A:660:ASP:HB2	1.91	0.84
1:A:672:VAL:CG2	1:A:673:GLU:N	2.39	0.84
1:A:659:LYS:HD3	1:A:659:LYS:H	1.42	0.84
1:B:527:TYR:OH	1:B:968:VAL:CG1	2.26	0.84
1:C:1:MET:N	10:C:1705:HOH:O	2.08	0.84
1:C:42:ALA:O	10:C:1274:HOH:O	1.96	0.84
1:A:507:GLU:HG2	1:A:518:ARG:CD	2.07	0.84
1:A:672:VAL:CG2	1:A:673:GLU:H	1.91	0.83
3:B:1101:LMT:O2'	3:B:1101:LMT:H22	1.78	0.83
1:C:735:LYS:O	1:C:739:LEU:HD13	1.77	0.83
1:A:1:MET:N	10:A:1259:HOH:O	2.08	0.83
1:A:713:LEU:HD22	1:A:843:LEU:HD23	1.60	0.82
2:E:31:ARG:HH11	2:E:31:ARG:HG2	1.44	0.82
1:A:674:LEU:CB	1:A:675:GLY:HA2	2.09	0.82
1:C:309:GLU:HG3	1:C:313:MET:CE	2.10	0.82
1:C:1011:MET:CE	1:C:1011:MET:HA	2.10	0.82
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.60	0.82
1:C:1033:PHE:O	1:C:1034:SER:OG	1.95	0.82
1:C:509:LYS:CB	1:C:510:LYS:HB2	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.81	0.81
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.61	0.81
1:A:676:THR:HB	4:A:1105:DM2:H213	1.61	0.81
1:C:671:ILE:HD11	1:C:674:LEU:CG	2.11	0.81
1:A:356:TYR:HA	1:A:365:THR:HG21	1.60	0.81
1:C:423:GLU:OE1	1:C:433:LYS:NZ	2.14	0.81
1:B:919:ARG:CG	1:B:919:ARG:HH11	1.92	0.80
1:C:255:GLN:HE21	1:C:256:ASP:N	1.78	0.80
1:C:671:ILE:HD11	1:C:674:LEU:HG	1.62	0.80
1:A:717:ARG:HH12	4:A:1105:DM2:C1	1.95	0.79
2:D:94:GLU:CD	2:D:94:GLU:H	1.84	0.79
1:C:671:ILE:N	1:C:862:MET:HE1	1.97	0.79
1:C:309:GLU:HG3	1:C:313:MET:HE2	1.62	0.79
2:E:34:MET:HA	2:E:34:MET:HE2	1.65	0.79
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.13	0.79
1:B:527:TYR:CE2	1:B:968:VAL:HG12	2.18	0.79
1:A:866:GLU:N	1:A:867:ARG:HB2	1.98	0.78
1:C:509:LYS:CA	1:C:510:LYS:CB	2.53	0.78
2:E:34:MET:CE	2:E:34:MET:HA	2.13	0.78
2:E:28:ASP:O	2:E:31:ARG:N	2.14	0.78
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.65	0.78
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.64	0.78
1:C:163:LYS:HE2	10:C:1769:HOH:O	1.83	0.78
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.63	0.78
1:A:527:TYR:OH	1:A:1019:ILE:O	2.01	0.78
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.65	0.78
1:A:966:ASP:OD1	1:A:969:ARG:NH1	2.17	0.78
1:C:255:GLN:NE2	1:C:256:ASP:H	1.82	0.77
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.67	0.77
1:A:815:ARG:NH1	10:A:1658:HOH:O	2.10	0.77
1:B:255:GLN:OE1	1:B:255:GLN:N	2.16	0.77
1:B:987:MET:HG3	1:B:1008:MET:CE	2.15	0.77
1:C:67:GLN:OE1	10:C:1665:HOH:O	2.02	0.77
2:E:16:LYS:NZ	2:E:20:GLU:OE1	2.16	0.77
1:A:866:GLU:HG2	1:A:867:ARG:CB	2.15	0.77
1:A:57:VAL:CG1	1:A:88:VAL:CG2	2.63	0.77
1:A:987:MET:HE1	1:A:1008:MET:SD	2.25	0.77
1:A:919:ARG:NH1	1:A:919:ARG:HG3	1.89	0.76
1:C:244:GLU:H	1:C:244:GLU:CD	1.89	0.76
1:B:919:ARG:HD3	1:B:1005:THR:HG21	1.66	0.76
1:C:360:GLN:HG2	1:C:513:PHE:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1102:LMT:H5B	3:B:1102:LMT:H6E	1.67	0.76
1:A:867:ARG:H	1:A:868:LEU:CD2	1.99	0.76
4:B:1104:DM2:H2'2	4:B:1104:DM2:H6'3	1.66	0.76
1:B:744:ASN:O	1:B:748:THR:HG23	1.85	0.75
1:A:38:ILE:C	1:A:38:ILE:HD12	2.07	0.75
1:B:16:ALA:O	1:B:20:MET:HG3	1.85	0.75
1:B:869:SER:OG	10:B:1483:HOH:O	2.04	0.75
1:A:867:ARG:HG2	1:A:867:ARG:O	1.84	0.75
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.67	0.75
1:C:255:GLN:HE21	1:C:256:ASP:H	1.31	0.75
1:A:717:ARG:HH22	4:A:1105:DM2:C2	2.00	0.75
3:A:1101:LMT:O4'	3:B:1101:LMT:H2B	1.87	0.75
1:A:507:GLU:CG	1:A:518:ARG:HD2	2.17	0.74
1:C:259:ARG:NH2	10:C:1499:HOH:O	2.17	0.74
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.68	0.74
1:A:987:MET:CE	1:A:1008:MET:SD	2.76	0.74
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.69	0.74
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.67	0.74
1:A:537:SER:HB2	1:A:540:ARG:CD	2.15	0.74
1:C:146:ASP:OD2	1:C:148:THR:OG1	2.04	0.74
4:A:1106:DM2:O4'	10:A:1564:HOH:O	2.05	0.74
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.70	0.74
1:A:456:MET:HG3	1:A:471:SER:OG	1.88	0.74
2:E:26:ARG:O	2:E:30:VAL:HG23	1.88	0.74
1:A:1012:VAL:O	1:A:1016:VAL:HG22	1.88	0.74
1:A:875:SER:O	1:A:879:ILE:HG23	1.88	0.74
1:C:875:SER:O	1:C:879:ILE:HG22	1.87	0.73
1:A:1016:VAL:HG23	1:A:1017:LEU:HD13	1.70	0.73
1:C:151:GLN:NE2	1:C:279:ALA:O	2.21	0.73
1:B:637:ARG:O	1:B:643:LYS:HE3	1.88	0.73
1:B:414:GLU:CG	1:B:977:MET:HE1	2.19	0.73
1:C:671:ILE:HG23	1:C:862:MET:HE3	1.71	0.73
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.70	0.73
1:A:393:LEU:HD22	1:A:470:PHE:HE1	1.53	0.73
1:C:259:ARG:NH2	10:C:1489:HOH:O	1.82	0.73
1:A:563:PHE:O	1:A:924:ASP:HB2	1.88	0.73
1:A:467:TYR:OH	1:A:928:GLN:OE1	2.06	0.73
1:A:942:ALA:O	1:A:946:VAL:HG13	1.87	0.73
1:C:671:ILE:HG13	1:C:671:ILE:O	1.87	0.72
1:A:659:LYS:CD	1:A:659:LYS:H	1.99	0.72
1:B:362:PHE:O	1:B:365:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TYR:HE2	1:B:968:VAL:HG12	1.53	0.72
1:A:717:ARG:NH1	4:A:1105:DM2:C1	2.52	0.72
1:C:867:ARG:HG2	1:C:867:ARG:NH1	2.04	0.72
3:B:1102:LMT:H5B	3:B:1102:LMT:C6'	2.19	0.72
1:B:554:TYR:CE1	1:B:558:ARG:NE	2.55	0.72
1:C:273:GLU:O	8:C:1103:GOL:O2	2.07	0.72
1:C:1011:MET:HA	1:C:1011:MET:HE3	1.70	0.72
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.90	0.72
1:A:717:ARG:NH1	4:A:1105:DM2:H1	2.04	0.71
1:C:815:ARG:NH2	10:C:1596:HOH:O	2.14	0.71
1:B:414:GLU:HG3	1:B:977:MET:HE3	1.70	0.71
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.71	0.71
1:C:135:SER:HB3	1:C:672:VAL:O	1.89	0.71
1:B:414:GLU:CG	1:B:977:MET:CE	2.66	0.71
1:A:356:TYR:HA	1:A:365:THR:CG2	2.20	0.71
1:C:346:GLU:OE1	10:C:1581:HOH:O	2.09	0.70
1:A:797:GLN:OE1	10:A:1570:HOH:O	2.08	0.70
1:A:709:HIS:N	1:A:710:PRO:HD3	2.06	0.70
2:E:150:PHE:CZ	2:E:154:ILE:HD11	2.27	0.70
1:C:21:LEU:HD12	1:C:22:ALA:N	2.07	0.70
1:A:617:PHE:CB	4:A:1105:DM2:H142	2.09	0.69
1:A:928:GLN:HE21	3:A:1102:LMT:H22	1.57	0.69
1:B:153:ASP:OD1	10:B:1674:HOH:O	2.10	0.69
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.73	0.69
1:B:600:THR:HG22	1:B:601:LYS:N	2.06	0.69
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.73	0.69
1:A:255:GLN:CD	1:A:255:GLN:H	1.94	0.69
1:B:1018:ALA:O	1:B:1022:VAL:HG13	1.92	0.69
1:A:867:ARG:H	1:A:868:LEU:HD23	1.57	0.69
1:A:528:THR:CG2	1:A:969:ARG:HB3	2.23	0.69
4:B:1104:DM2:O19	10:B:1692:HOH:O	2.11	0.69
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.74	0.69
1:C:867:ARG:NH1	10:C:1700:HOH:O	2.11	0.68
1:A:540:ARG:HG2	1:A:541:TYR:CD1	2.27	0.68
2:D:45:VAL:HG22	10:D:248:HOH:O	1.92	0.68
1:B:672:VAL:CG1	7:B:1103:LMU:H61	2.23	0.68
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.23	0.68
1:C:509:LYS:CB	1:C:510:LYS:CB	2.71	0.68
1:A:259:ARG:NE	10:A:1533:HOH:O	2.24	0.68
1:B:871:ASN:O	3:B:1101:LMT:O6B	2.11	0.68
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:ARG:HH12	1:A:1038:GLU:CD	1.97	0.67
1:B:352:PHE:CE1	1:B:365:THR:CG2	2.77	0.67
1:C:815:ARG:NE	10:C:1596:HOH:O	2.17	0.67
1:A:534:ILE:HG23	1:A:541:TYR:CE1	2.29	0.67
1:B:672:VAL:HG11	7:B:1103:LMU:H61	1.76	0.67
1:C:430:ALA:O	1:C:434:SER:OG	2.13	0.67
1:B:636:ASP:O	10:B:1691:HOH:O	2.12	0.67
1:A:509:LYS:O	1:A:514:GLY:HA3	1.94	0.67
1:A:444:GLY:CA	3:A:1103:LMT:H12	2.24	0.67
1:A:765:ARG:NH2	10:A:1680:HOH:O	2.26	0.67
1:A:795:ASP:OD1	1:A:797:GLN:HG3	1.94	0.67
1:A:987:MET:O	1:A:990:VAL:HG22	1.95	0.67
1:B:596:HIS:O	1:B:600:THR:HB	1.93	0.67
1:A:891:LEU:HD13	3:A:1103:LMT:H11	1.77	0.66
1:A:1035:ARG:C	1:A:1036:LYS:HD3	2.15	0.66
1:A:585:GLU:OE2	10:A:1654:HOH:O	2.12	0.66
1:B:846:GLN:OE1	10:B:1588:HOH:O	2.13	0.66
1:C:671:ILE:HG23	1:C:862:MET:CE	2.25	0.66
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.77	0.66
2:E:25:GLY:HA2	2:E:62:ILE:CD1	2.25	0.66
1:A:539:GLY:O	1:A:543:VAL:HG23	1.96	0.66
1:B:527:TYR:OH	1:B:968:VAL:HG11	1.94	0.66
1:A:360:GLN:HG2	1:A:513:PHE:CD2	2.31	0.66
1:A:1042:HIS:ND1	1:A:1042:HIS:O	2.29	0.66
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.76	0.66
4:A:1105:DM2:H6'3	4:A:1105:DM2:C2'	2.22	0.66
1:A:674:LEU:HB3	1:A:675:GLY:O	1.95	0.66
1:A:1035:ARG:HG3	1:A:1036:LYS:NZ	2.10	0.66
1:B:386:PHE:HB3	1:B:388:PHE:CD2	2.31	0.66
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.15	0.66
1:A:662:MET:HB3	1:A:664:PHE:HE2	1.59	0.66
1:A:412:VAL:HG11	1:A:489:THR:HG22	1.78	0.66
1:A:112:GLN:HG2	1:B:112:GLN:OE1	1.96	0.65
1:B:973:ARG:HG2	1:B:977:MET:CE	2.26	0.65
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.78	0.65
1:A:617:PHE:CG	4:A:1106:DM2:H1	2.32	0.65
1:C:253:VAL:HG12	1:C:259:ARG:HG2	1.79	0.65
1:A:70:ASN:O	1:A:110:LYS:HE3	1.96	0.65
1:C:671:ILE:HG12	1:C:862:MET:SD	2.37	0.65
1:A:507:GLU:HG2	1:A:518:ARG:NE	2.11	0.65
1:C:344:LEU:HD21	1:C:402:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:ASP:O	2:E:163:GLU:HG2	1.97	0.65
1:B:960:LEU:CD2	1:B:1027:VAL:HG22	2.27	0.65
1:B:600:THR:HG22	1:B:601:LYS:HG3	1.79	0.65
1:B:555:LEU:HD21	1:B:914:LEU:CD1	2.27	0.65
1:B:961:ILE:HG22	1:B:965:LEU:CD2	2.27	0.65
1:A:519:MET:O	1:A:523:SER:OG	2.13	0.64
1:A:901:VAL:O	1:A:904:VAL:HG22	1.97	0.64
1:A:891:LEU:CD1	3:A:1103:LMT:H11	2.27	0.64
1:A:562:SER:OG	1:A:922:THR:HG21	1.97	0.64
1:C:509:LYS:HB3	1:C:510:LYS:HB3	1.79	0.64
1:C:670:ALA:HA	10:C:1332:HOH:O	1.96	0.64
1:C:360:GLN:HG2	1:C:513:PHE:CG	2.32	0.64
2:E:17:LYS:O	10:E:233:HOH:O	2.14	0.64
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.31	0.64
1:C:867:ARG:NH2	10:C:1700:HOH:O	2.23	0.64
1:C:1035:ARG:HA	1:C:1036:LYS:HG3	1.78	0.64
1:A:8:ARG:HH12	5:A:1107:D12:H111	1.62	0.64
1:B:677:ALA:O	1:B:678:THR:OG1	2.08	0.64
1:A:361:ASN:ND2	10:A:1267:HOH:O	2.31	0.64
1:A:881:LEU:HD12	3:A:1102:LMT:H121	1.80	0.64
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.28	0.64
2:E:125:HIS:O	2:E:129:VAL:HG23	1.98	0.64
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.80	0.64
1:A:444:GLY:HA3	3:A:1103:LMT:H12	1.80	0.64
1:A:693:GLU:OE1	1:A:693:GLU:N	2.30	0.64
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.78	0.64
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.33	0.63
1:B:309:GLU:OE1	10:B:1337:HOH:O	2.15	0.63
1:B:229:GLN:O	10:B:1455:HOH:O	2.15	0.63
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.80	0.63
1:C:1013:THR:O	1:C:1017:LEU:HB2	1.97	0.63
1:C:193:LEU:HD13	1:C:265:VAL:HB	1.80	0.63
1:A:965:LEU:O	1:A:969:ARG:HG2	1.98	0.63
3:A:1103:LMT:H3'	3:A:1103:LMT:H2O1	1.64	0.63
3:A:1102:LMT:H5B	3:A:1102:LMT:H6D	1.80	0.63
3:C:1101:LMT:O3'	10:C:1540:HOH:O	2.11	0.63
1:C:366:LEU:HD23	1:C:496:MET:HE1	1.81	0.63
1:A:355:MET:CE	1:A:355:MET:HA	2.27	0.63
4:B:1104:DM2:C2'	4:B:1104:DM2:H6'3	2.29	0.62
1:B:999:ALA:O	1:B:1003:VAL:HG12	1.98	0.62
1:A:115:MET:HB2	1:A:116:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:MET:CE	2:E:40:VAL:HG12	2.30	0.62
1:C:808:ARG:NH1	10:C:1749:HOH:O	2.20	0.62
1:C:360:GLN:HG2	1:C:513:PHE:CE2	2.34	0.62
1:A:865:GLN:CA	1:A:866:GLU:C	2.66	0.61
1:C:671:ILE:CG1	1:C:671:ILE:O	2.48	0.61
1:C:115:MET:N	1:C:116:PRO:HD2	2.14	0.61
1:C:1035:ARG:HA	1:C:1036:LYS:CB	2.31	0.61
1:A:454:VAL:HB	1:A:455:PRO:HD3	1.83	0.61
7:B:1103:LMU:H21	7:B:1103:LMU:O5'	2.01	0.61
1:B:426:PRO:HD2	1:B:429:GLU:HG3	1.83	0.61
1:A:717:ARG:NH1	4:A:1105:DM2:O19	2.33	0.61
1:A:445:ILE:O	1:A:448:VAL:HG22	2.01	0.61
1:C:509:LYS:HB3	1:C:510:LYS:CB	2.30	0.61
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.30	0.60
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.82	0.60
1:B:447:MET:HA	1:B:447:MET:CE	2.31	0.60
2:E:30:VAL:O	2:E:34:MET:HB2	2.01	0.60
1:A:586:ARG:NH2	1:A:660:ASP:CB	2.64	0.60
4:B:1104:DM2:O5'	4:B:1104:DM2:H112	2.01	0.60
2:D:12:SER:O	2:D:16:LYS:HG2	2.01	0.60
1:A:85:THR:O	1:A:85:THR:HG22	2.00	0.60
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.83	0.60
1:A:360:GLN:HG2	1:A:513:PHE:CG	2.37	0.60
1:A:717:ARG:CZ	4:A:1105:DM2:H1	2.32	0.60
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.84	0.60
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.31	0.60
1:A:843:LEU:O	1:A:847:LEU:HG	2.01	0.60
1:C:314:GLU:HG2	1:C:317:PHE:CE1	2.36	0.60
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.84	0.60
1:A:1036:LYS:HA	1:A:1037:ASN:HB3	1.83	0.60
1:A:971:ARG:HH11	1:A:971:ARG:HG3	1.66	0.60
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.31	0.60
1:B:519:MET:HE3	1:B:520:PHE:N	2.16	0.60
1:A:714:THR:HG22	1:A:715:SER:OG	2.01	0.60
1:A:1001:ASN:O	1:A:1005:THR:CG2	2.50	0.60
1:B:138:MET:HE3	1:B:325:TYR:HD2	1.66	0.60
4:A:1105:DM2:C6'	4:A:1105:DM2:H2'2	2.20	0.60
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.84	0.60
1:C:366:LEU:HD23	1:C:496:MET:CE	2.32	0.60
1:A:672:VAL:HG23	1:A:673:GLU:N	2.17	0.59
1:B:919:ARG:CD	1:B:1005:THR:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:LEU:HD12	3:A:1102:LMT:C12	2.32	0.59
1:B:960:LEU:HD21	1:B:1027:VAL:HG22	1.84	0.59
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.66	0.59
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.84	0.59
1:A:56:THR:O	1:A:60:THR:HB	2.01	0.59
1:A:971:ARG:HG3	1:A:971:ARG:NH1	2.17	0.59
1:B:352:PHE:CE1	1:B:365:THR:HG23	2.38	0.59
1:B:468:ARG:O	1:B:472:ILE:HD12	2.02	0.59
1:C:255:GLN:NE2	1:C:256:ASP:N	2.46	0.59
1:A:716:VAL:O	10:A:1641:HOH:O	2.16	0.59
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.67	0.59
1:A:1030:ARG:NE	1:A:1030:ARG:HA	2.17	0.59
1:B:919:ARG:CG	1:B:919:ARG:NH1	2.60	0.59
1:B:809:TRP:NE1	2:D:79:LEU:HD22	2.18	0.59
1:C:669:PRO:HG3	1:C:675:GLY:O	2.03	0.59
1:A:356:TYR:CA	1:A:365:THR:HG21	2.30	0.59
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.85	0.59
1:A:958:LYS:HA	1:A:958:LYS:HE2	1.85	0.58
1:A:987:MET:HE1	1:A:1008:MET:HE2	1.85	0.58
1:A:674:LEU:HB3	1:A:675:GLY:C	2.23	0.58
1:A:38:ILE:HD12	1:A:39:ALA:N	2.18	0.58
1:A:866:GLU:CD	1:A:866:GLU:H	1.95	0.58
1:A:1023:PRO:O	1:A:1027:VAL:HG13	2.02	0.58
2:E:74:ASN:HD21	2:E:105:ASP:HB2	1.67	0.58
1:A:586:ARG:HD3	10:A:1596:HOH:O	2.02	0.58
1:C:895:TRP:CD1	5:C:1102:D12:H82	2.38	0.58
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.84	0.58
1:C:1035:ARG:HA	1:C:1036:LYS:CG	2.34	0.58
3:A:1102:LMT:H5B	3:A:1102:LMT:C6'	2.33	0.58
1:B:522:LYS:NZ	1:B:522:LYS:CB	2.67	0.58
1:B:447:MET:HA	1:B:447:MET:HE2	1.84	0.57
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.34	0.57
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.86	0.57
1:A:865:GLN:HA	1:A:866:GLU:O	2.04	0.57
1:A:866:GLU:CB	1:A:867:ARG:HA	2.34	0.57
1:C:671:ILE:CG1	1:C:674:LEU:HG	2.34	0.57
1:C:694:LYS:HG2	10:C:1307:HOH:O	2.05	0.57
1:C:867:ARG:NH1	10:C:1225:HOH:O	2.36	0.57
1:A:614:GLY:HA2	1:A:621:GLY:O	2.04	0.57
1:C:673:GLU:HG3	10:C:1483:HOH:O	2.03	0.57
1:A:987:MET:HE1	1:A:990:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:PRO:O	1:B:6:ILE:HG13	2.03	0.57
1:A:717:ARG:HH12	4:A:1105:DM2:C20	2.16	0.57
2:E:74:ASN:ND2	2:E:105:ASP:HB2	2.19	0.57
1:A:408:ASP:OD1	1:A:940:LYS:NZ	2.26	0.57
1:A:717:ARG:HH22	4:A:1105:DM2:C1	2.18	0.56
1:A:38:ILE:C	1:A:38:ILE:CD1	2.73	0.56
1:B:405:LEU:HD22	1:B:481:SER:HB2	1.88	0.56
1:A:412:VAL:HG11	1:A:489:THR:CG2	2.35	0.56
4:A:1105:DM2:H10	4:A:1106:DM2:C1	2.36	0.56
1:B:399:VAL:HA	1:B:402:ILE:HD12	1.87	0.56
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.88	0.56
2:E:92:HIS:O	2:E:96:VAL:HG23	2.04	0.56
1:A:958:LYS:HE2	1:A:958:LYS:CA	2.35	0.56
2:D:25:GLY:HA2	2:D:62:ILE:HD12	1.87	0.56
1:A:543:VAL:O	1:A:547:ILE:HG12	2.06	0.56
1:A:472:ILE:N	1:A:472:ILE:HD13	2.20	0.56
2:D:48:TRP:HE3	2:D:53:LEU:HD13	1.71	0.56
1:A:540:ARG:CD	1:A:540:ARG:H	2.05	0.56
1:B:716:VAL:HG13	10:B:1490:HOH:O	2.05	0.56
2:E:42:ALA:O	2:E:50:PRO:HD3	2.06	0.56
1:A:438:ILE:HD12	1:A:439:GLN:N	2.20	0.56
1:A:985:GLY:O	1:A:988:PRO:HD2	2.06	0.56
3:A:1104:LMT:H4B	10:A:1275:HOH:O	2.05	0.56
1:B:865:GLN:O	1:B:868:LEU:N	2.35	0.56
4:A:1106:DM2:O14	10:A:1692:HOH:O	2.18	0.55
1:C:1011:MET:HE2	1:C:1011:MET:HA	1.86	0.55
1:A:376:LEU:HD13	1:A:405:LEU:HD12	1.88	0.55
1:B:708:LYS:C	1:B:710:PRO:HD3	2.26	0.55
1:A:836:SER:O	1:A:839:GLU:HG3	2.06	0.55
1:C:659:LYS:HE2	1:C:660:ASP:OD2	2.06	0.55
1:B:867:ARG:O	1:B:868:LEU:HD12	2.07	0.55
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.88	0.55
1:A:867:ARG:N	1:A:868:LEU:HD23	2.22	0.55
1:A:677:ALA:O	1:A:678:THR:HG23	2.07	0.55
1:A:987:MET:CE	1:A:990:VAL:HG21	2.36	0.55
1:C:368:PRO:HD3	1:C:413:VAL:HG21	1.86	0.55
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.87	0.55
1:C:33:ALA:O	1:C:337:ILE:HD11	2.06	0.55
1:B:461:GLY:HA3	1:B:865:GLN:OE1	2.07	0.55
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.89	0.55
1:C:1030:ARG:O	1:C:1034:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:THR:OG1	1:B:309:GLU:HG3	2.06	0.55
1:A:836:SER:OG	1:A:839:GLU:HG2	2.06	0.55
1:A:1040:ILE:O	1:A:1041:GLU:HB2	2.07	0.55
1:A:8:ARG:NH1	5:A:1107:D12:H111	2.21	0.55
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.89	0.55
1:A:276:ASP:O	1:A:614:GLY:HA3	2.07	0.55
1:C:853:THR:HG21	10:C:1723:HOH:O	2.07	0.55
1:A:152:GLU:N	1:A:152:GLU:OE1	2.31	0.54
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.71	0.54
1:A:444:GLY:HA2	3:A:1103:LMT:H12	1.88	0.54
1:C:808:ARG:HD2	10:C:1749:HOH:O	2.06	0.54
1:A:522:LYS:HG3	1:A:526:HIS:CE1	2.43	0.54
1:A:649:MET:CE	1:A:653:ARG:NH1	2.70	0.54
1:A:255:GLN:CD	1:A:255:GLN:N	2.59	0.54
1:A:361:ASN:O	1:A:365:THR:HG23	2.08	0.54
1:C:139:VAL:O	1:C:326:PRO:HD2	2.07	0.54
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.88	0.54
1:C:21:LEU:O	1:C:25:LEU:HG	2.07	0.54
1:B:961:ILE:HG22	1:B:965:LEU:HD23	1.89	0.54
1:B:875:SER:CB	3:B:1101:LMT:H6'2	2.33	0.54
2:E:31:ARG:NH1	2:E:31:ARG:HG2	2.18	0.54
3:B:1101:LMT:C2	3:B:1101:LMT:O2'	2.52	0.54
1:C:898:PRO:O	1:C:902:MET:HG2	2.07	0.54
1:C:509:LYS:O	1:C:514:GLY:HA3	2.07	0.54
1:B:255:GLN:C	1:B:257:GLY:H	2.10	0.54
1:C:111:LEU:HD21	1:C:127:VAL:HG22	1.88	0.54
1:A:537:SER:HB2	1:A:540:ARG:NH1	2.22	0.54
1:C:895:TRP:C	1:C:898:PRO:HD2	2.28	0.54
1:C:491:ALA:O	1:C:495:THR:HG23	2.08	0.54
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.89	0.53
1:B:178:PHE:C	4:B:1104:DM2:H213	2.28	0.53
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.90	0.53
1:A:896:SER:O	1:A:899:PHE:HD2	1.91	0.53
1:B:357:LEU:HD11	1:B:516:PHE:CE2	2.43	0.53
1:C:489:THR:HB	1:C:490:PRO:HD3	1.89	0.53
1:A:1035:ARG:HG3	1:A:1036:LYS:HZ2	1.71	0.53
1:A:449:LEU:HB3	1:A:478:MET:SD	2.48	0.53
1:B:115:MET:N	1:B:116:PRO:CD	2.71	0.53
1:B:760:ASN:HB2	8:B:1106:GOL:H31	1.90	0.53
1:A:510:LYS:HD2	1:A:511:GLY:N	2.23	0.53
1:B:396:PHE:HA	1:B:399:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.90	0.53
1:B:530:SER:O	1:B:534:ILE:HG13	2.08	0.53
1:B:960:LEU:C	1:B:960:LEU:HD23	2.28	0.53
1:A:717:ARG:NH2	4:A:1105:DM2:C1	2.71	0.53
1:A:537:SER:O	1:A:538:THR:CB	2.56	0.53
1:B:605:ASN:OD1	1:B:637:ARG:HG2	2.08	0.53
1:A:418:ARG:HE	1:A:970:MET:HE3	1.72	0.53
1:A:881:LEU:CD1	3:A:1102:LMT:H112	2.39	0.53
1:C:973:ARG:O	1:C:977:MET:HG3	2.09	0.53
1:C:120:GLN:HB2	10:C:1522:HOH:O	2.08	0.53
1:B:211:ASN:HB2	1:B:240:LEU:HD22	1.90	0.53
2:E:59:HIS:O	2:E:63:VAL:HG23	2.08	0.53
1:A:777:ALA:O	1:A:781:MET:HG2	2.09	0.53
1:A:866:GLU:O	1:A:868:LEU:HB2	2.06	0.53
1:A:671:ILE:N	1:A:674:LEU:HD12	2.11	0.53
1:C:95:GLU:HG3	10:C:1718:HOH:O	2.09	0.53
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.89	0.53
1:C:563:PHE:CE2	1:C:564:LEU:HD22	2.44	0.53
1:C:70:ASN:HB2	10:C:1427:HOH:O	2.08	0.53
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.24	0.53
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.11	0.53
1:A:148:THR:HG23	10:A:1514:HOH:O	2.10	0.52
1:A:919:ARG:O	1:A:919:ARG:HD3	2.10	0.52
1:A:342:LYS:HG3	3:A:1104:LMT:H92	1.92	0.52
1:A:339:GLU:O	1:A:343:THR:HG23	2.08	0.52
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.91	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.90	0.52
1:A:554:TYR:CE1	1:A:558:ARG:CZ	2.92	0.52
1:B:885:PHE:HD1	1:B:902:MET:CE	2.22	0.52
1:C:111:LEU:HD21	1:C:127:VAL:CG2	2.40	0.52
1:A:989:LEU:HD23	1:A:1000:GLN:OE1	2.10	0.52
2:D:165:LEU:O	2:D:166:GLN:C	2.48	0.52
1:A:676:THR:HG21	4:A:1106:DM2:H1'	1.90	0.52
1:C:671:ILE:HG13	1:C:674:LEU:HG	1.91	0.52
1:C:799:VAL:HG23	1:C:804:PHE:HE1	1.74	0.52
1:C:943:ILE:O	1:C:947:GLU:HB3	2.08	0.52
4:B:1104:DM2:O5'	4:B:1104:DM2:C11	2.57	0.52
1:A:1035:ARG:HG3	1:A:1036:LYS:CD	2.40	0.52
1:B:678:THR:HA	1:B:837:THR:HG22	1.91	0.52
1:B:138:MET:HE3	1:B:325:TYR:CD2	2.44	0.52
2:E:29:GLU:O	2:E:33:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ARG:HH22	1:A:660:ASP:CB	2.23	0.52
1:B:678:THR:HA	1:B:837:THR:CG2	2.39	0.52
1:B:695:LEU:HD13	1:B:825:MET:HG3	1.92	0.52
1:A:676:THR:CB	4:A:1105:DM2:H213	2.37	0.52
1:A:617:PHE:CD2	4:A:1106:DM2:H2	2.45	0.52
1:A:418:ARG:NH2	1:A:970:MET:CE	2.72	0.52
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.88	0.52
1:A:360:GLN:HG2	1:A:513:PHE:CE2	2.44	0.52
1:B:837:THR:O	1:B:841:MET:HG3	2.09	0.52
1:A:416:VAL:HG22	1:A:431:THR:HA	1.92	0.52
1:A:542:LEU:HD12	1:A:542:LEU:N	2.25	0.52
1:C:40:PRO:HB2	1:C:94:PHE:O	2.09	0.52
1:B:6:ILE:HD11	1:B:431:THR:HG22	1.92	0.52
1:A:1036:LYS:HA	1:A:1037:ASN:CB	2.39	0.52
1:B:960:LEU:HD23	1:B:960:LEU:O	2.10	0.52
1:C:404:LEU:HD11	1:C:937:LEU:CD2	2.40	0.52
2:E:26:ARG:HB3	2:E:29:GLU:HB2	1.93	0.52
1:A:401:ALA:O	1:A:405:LEU:HG	2.10	0.52
1:C:33:ALA:O	1:C:391:ASN:HA	2.10	0.52
1:B:328:ASP:O	1:B:331:PRO:HD2	2.10	0.52
1:A:489:THR:HB	1:A:490:PRO:HD3	1.92	0.51
1:A:1041:GLU:CD	1:A:1042:HIS:H	2.13	0.51
1:C:735:LYS:NZ	10:C:1641:HOH:O	2.40	0.51
1:B:255:GLN:C	1:B:257:GLY:N	2.64	0.51
1:A:38:ILE:HG22	1:A:465:ALA:HB3	1.93	0.51
1:B:138:MET:CE	1:B:140:VAL:HG22	2.40	0.51
1:A:427:PRO:O	1:A:431:THR:HG23	2.11	0.51
1:B:873:ALA:N	1:B:874:PRO:CD	2.73	0.51
1:C:193:LEU:CD1	1:C:265:VAL:HB	2.40	0.51
1:A:712:MET:HG3	1:A:713:LEU:HD13	1.92	0.51
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.39	0.51
1:B:897:ILE:N	1:B:898:PRO:CD	2.74	0.51
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.45	0.51
1:A:910:ILE:HG23	1:A:911:GLY:N	2.26	0.51
2:E:134:LYS:O	2:E:134:LYS:HG2	2.11	0.51
1:B:527:TYR:CZ	1:B:968:VAL:CG1	2.93	0.51
1:A:1035:ARG:HG3	1:A:1036:LYS:HD3	1.93	0.51
1:A:504:ASP:C	1:A:505:HIS:ND1	2.64	0.51
1:B:255:GLN:OE1	1:B:255:GLN:CA	2.58	0.51
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.93	0.51
1:C:177:LEU:HD13	1:C:179:GLY:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TYR:CE2	1:B:968:VAL:CG1	2.92	0.51
1:B:955:LYS:HA	1:B:955:LYS:HE2	1.92	0.51
1:C:32:VAL:CG1	1:C:337:ILE:HD13	2.40	0.51
1:B:240:LEU:HG	1:B:245:GLU:HB3	1.91	0.51
1:A:538:THR:H	1:A:540:ARG:HD3	1.76	0.51
2:E:40:VAL:HG13	10:E:250:HOH:O	2.11	0.51
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.92	0.51
1:A:343:THR:HG21	1:A:1000:GLN:OE1	2.11	0.51
1:B:386:PHE:HB3	1:B:388:PHE:CE2	2.45	0.50
1:B:866:GLU:C	1:B:868:LEU:H	2.14	0.50
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.92	0.50
1:A:344:LEU:HD21	1:A:376:LEU:CD2	2.42	0.50
4:A:1105:DM2:C6'	4:A:1105:DM2:C2'	2.82	0.50
1:A:418:ARG:NE	1:A:970:MET:CE	2.75	0.50
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.93	0.50
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.93	0.50
1:A:263:ARG:NH2	2:D:155:ASN:O	2.44	0.50
2:E:31:ARG:CG	2:E:31:ARG:HH11	2.16	0.50
1:C:980:LEU:HD12	1:C:984:LEU:CD2	2.42	0.50
1:C:653:ARG:NH1	10:C:1450:HOH:O	2.44	0.50
1:A:420:MET:HE3	1:A:500:ILE:HG13	1.93	0.50
1:A:617:PHE:CD2	4:A:1106:DM2:C2	2.94	0.50
2:D:93:LEU:HB3	2:D:94:GLU:OE1	2.12	0.50
1:B:960:LEU:CD2	1:B:960:LEU:C	2.80	0.50
1:C:641:GLU:OE1	1:C:641:GLU:N	2.30	0.50
1:C:364:ALA:O	1:C:368:PRO:HD2	2.12	0.50
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.77	0.50
1:C:226:LYS:NZ	10:C:1497:HOH:O	2.45	0.50
1:B:454:VAL:HB	1:B:455:PRO:HD3	1.94	0.50
1:B:555:LEU:HD21	1:B:914:LEU:HD12	1.94	0.50
1:B:522:LYS:HZ2	1:B:522:LYS:HB2	1.77	0.50
1:B:862:MET:HE2	10:B:1463:HOH:O	2.11	0.50
1:B:873:ALA:O	1:B:877:TYR:CD2	2.65	0.49
1:B:672:VAL:HG23	1:B:673:GLU:CD	2.32	0.49
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.45	0.49
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.93	0.49
1:A:717:ARG:NH2	4:A:1105:DM2:C2	2.73	0.49
1:A:554:TYR:HE1	1:A:558:ARG:NH2	2.11	0.49
1:A:895:TRP:CG	6:A:1108:D10:H71	2.47	0.49
1:B:527:TYR:OH	1:B:968:VAL:HG13	2.09	0.49
1:A:662:MET:HB3	1:A:664:PHE:CE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ILE:HB	1:C:368:PRO:CD	2.42	0.49
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.94	0.49
1:A:676:THR:O	1:A:678:THR:N	2.45	0.49
1:A:729:ILE:CD1	1:C:234:ILE:HG23	2.43	0.49
1:A:57:VAL:HG11	1:A:88:VAL:HG22	1.91	0.49
1:B:255:GLN:O	1:B:257:GLY:N	2.45	0.49
1:B:169:THR:O	1:B:172:VAL:HG13	2.12	0.49
2:D:82:THR:HB	2:D:83:PRO:HD2	1.94	0.49
2:E:41:ASN:HD21	2:E:72:ASP:HB2	1.77	0.49
1:B:408:ASP:OD2	1:B:940:LYS:NZ	2.36	0.49
1:C:666:PHE:CD2	1:C:677:ALA:HB2	2.48	0.49
1:C:867:ARG:HG2	10:C:1225:HOH:O	2.13	0.49
3:B:1102:LMT:H5B	3:B:1102:LMT:H6D	1.92	0.49
1:B:867:ARG:HG2	1:B:867:ARG:O	2.13	0.49
1:A:903:LEU:O	1:A:906:PRO:HD2	2.12	0.49
1:C:951:ASP:O	1:C:955:LYS:HG2	2.12	0.49
1:A:538:THR:H	1:A:540:ARG:CD	2.25	0.49
1:B:874:PRO:HD2	1:B:875:SER:H	1.77	0.49
1:A:836:SER:O	1:A:837:THR:C	2.51	0.49
2:D:98:VAL:HA	2:D:101:LYS:HE2	1.94	0.49
1:C:702:LEU:HD11	1:C:844:MET:CE	2.43	0.49
1:B:872:GLN:C	1:B:874:PRO:CD	2.82	0.49
1:C:1034:SER:O	1:C:1035:ARG:C	2.51	0.49
1:A:60:THR:CG2	1:A:119:PRO:HG2	2.43	0.48
1:A:649:MET:HE3	1:A:653:ARG:NH1	2.28	0.48
1:A:254:ASN:HB2	1:A:258:SER:OG	2.13	0.48
1:B:121:GLU:H	1:B:121:GLU:CD	2.15	0.48
1:B:973:ARG:O	1:B:977:MET:HG3	2.13	0.48
1:C:57:VAL:HG11	1:C:88:VAL:HG23	1.94	0.48
1:A:695:LEU:HD13	1:A:825:MET:HG3	1.94	0.48
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.49	0.48
1:A:617:PHE:CB	4:A:1105:DM2:C14	2.83	0.48
1:B:987:MET:CG	1:B:1008:MET:CE	2.90	0.48
1:B:1008:MET:O	1:B:1012:VAL:HG23	2.12	0.48
1:A:418:ARG:HH21	1:A:970:MET:HE1	1.79	0.48
1:C:370:ILE:O	1:C:373:PRO:HD2	2.14	0.48
1:C:151:GLN:OE1	1:C:278:ILE:HG23	2.12	0.48
1:B:555:LEU:CD2	1:B:914:LEU:HD13	2.43	0.48
1:A:545:TYR:OH	1:A:906:PRO:HG2	2.13	0.48
1:A:910:ILE:CG2	1:A:911:GLY:N	2.76	0.48
1:A:866:GLU:CG	1:A:867:ARG:CB	2.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:LEU:N	1:A:868:LEU:HD22	2.29	0.48
2:E:163:GLU:CG	2:E:164:ILE:N	2.77	0.48
1:A:633:ASP:OD1	3:A:1104:LMT:O4'	2.24	0.48
1:B:303:ALA:O	1:B:307:ARG:HG3	2.13	0.48
1:A:867:ARG:HA	1:A:869:SER:H	1.77	0.48
1:A:987:MET:CE	1:A:987:MET:CA	2.69	0.48
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.12	0.48
1:A:259:ARG:NH2	10:A:1533:HOH:O	2.46	0.48
1:A:729:ILE:HD11	1:C:234:ILE:HG23	1.95	0.48
1:A:483:LEU:HD12	1:A:483:LEU:HA	1.72	0.48
2:E:31:ARG:O	2:E:35:ALA:N	2.42	0.48
1:C:423:GLU:HB3	1:C:425:LEU:HD13	1.94	0.48
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.44	0.48
1:A:153:ASP:OD1	1:A:182:TYR:OH	2.26	0.48
1:A:418:ARG:NH2	1:A:970:MET:HE1	2.29	0.48
1:A:57:VAL:HG11	1:A:88:VAL:CG2	2.44	0.48
1:A:708:LYS:C	1:A:710:PRO:HD3	2.34	0.48
2:D:115:THR:HB	2:D:116:PRO:HD2	1.95	0.48
1:B:139:VAL:HG13	1:B:178:PHE:HE2	1.78	0.48
1:A:845:GLU:HG2	1:A:857:TYR:CZ	2.49	0.48
1:B:649:MET:HB3	1:B:653:ARG:NH2	2.28	0.48
1:A:711:ASP:N	1:A:711:ASP:OD1	2.41	0.48
3:A:1104:LMT:H2B	3:A:1104:LMT:H5'	1.96	0.47
1:A:836:SER:O	1:A:839:GLU:N	2.46	0.47
1:C:750:LEU:HD23	1:C:750:LEU:O	2.14	0.47
1:A:867:ARG:O	1:A:867:ARG:CG	2.58	0.47
1:A:676:THR:CB	4:A:1105:DM2:C21	2.79	0.47
2:E:31:ARG:NH1	2:E:31:ARG:CG	2.73	0.47
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.49	0.47
1:A:717:ARG:CZ	4:A:1105:DM2:C1	2.92	0.47
1:A:456:MET:C	1:A:458:PHE:H	2.17	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.96	0.47
1:A:553:ALA:O	1:A:557:VAL:HG13	2.14	0.47
1:B:39:ALA:HB2	1:B:673:GLU:HG2	1.96	0.47
1:C:895:TRP:CD1	5:C:1102:D12:H101	2.49	0.47
1:A:971:ARG:HH11	1:A:971:ARG:CG	2.27	0.47
1:B:578:LEU:HD22	1:B:661:ALA:HB2	1.95	0.47
1:C:743:ILE:O	1:C:743:ILE:HD12	2.13	0.47
1:B:247:GLY:HA2	1:B:268:ILE:HD12	1.97	0.47
1:A:966:ASP:HA	1:A:969:ARG:HG2	1.96	0.47
1:C:2:PRO:O	1:C:6:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:N	10:A:1602:HOH:O	2.48	0.47
1:B:842:GLU:O	1:B:846:GLN:HG3	2.15	0.47
5:A:1107:D12:H91	10:B:1683:HOH:O	2.14	0.47
1:A:454:VAL:N	1:A:455:PRO:CD	2.78	0.47
1:B:986:VAL:HG23	1:B:989:LEU:HD12	1.97	0.47
1:B:11:PHE:O	1:B:11:PHE:HD2	1.97	0.47
1:A:532:GLY:O	1:A:536:ARG:HD3	2.13	0.47
1:A:11:PHE:HD2	1:A:11:PHE:O	1.98	0.47
1:A:537:SER:OG	1:A:540:ARG:HD3	2.14	0.47
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.38	0.47
1:B:555:LEU:HA	1:B:555:LEU:HD12	1.76	0.47
1:A:526:HIS:O	1:A:530:SER:OG	2.30	0.47
1:B:713:LEU:HD22	1:B:843:LEU:HD23	1.96	0.47
1:A:505:HIS:HD2	1:A:521:GLU:OE1	1.98	0.47
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.15	0.47
1:C:363:ARG:O	1:C:367:ILE:HG13	2.15	0.47
2:D:154:ILE:HG13	2:D:155:ASN:N	2.28	0.47
1:C:680:PHE:CZ	1:C:829:GLY:HA3	2.50	0.47
1:C:732:ASP:OD2	1:C:735:LYS:HE3	2.15	0.47
1:C:358:PHE:CG	1:C:977:MET:HG2	2.50	0.47
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.50	0.47
1:B:972:LEU:HD22	1:B:976:LEU:HD13	1.96	0.47
1:C:340:VAL:HG11	1:C:395:MET:CB	2.44	0.47
1:B:104:GLN:OE1	1:B:131:LYS:HG3	2.15	0.47
1:C:493:CYS:O	1:C:497:LEU:HB2	2.15	0.47
1:A:534:ILE:HG23	1:A:541:TYR:CE2	2.48	0.46
1:A:414:GLU:OE2	1:A:974:PRO:HG3	2.14	0.46
1:A:1036:LYS:CA	1:A:1037:ASN:HB3	2.44	0.46
1:B:468:ARG:HG2	1:B:472:ILE:CD1	2.44	0.46
1:A:376:LEU:HD13	1:A:405:LEU:CD1	2.45	0.46
1:A:462:SER:OG	1:A:463:THR:N	2.49	0.46
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.97	0.46
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.96	0.46
1:A:866:GLU:CG	1:A:867:ARG:CA	2.72	0.46
4:A:1105:DM2:C1	4:A:1106:DM2:H112	2.45	0.46
1:A:351:VAL:O	1:A:355:MET:HG2	2.16	0.46
1:A:892:TYR:OH	1:A:946:VAL:HG22	2.15	0.46
1:B:616:GLY:HA3	1:B:619:GLY:O	2.15	0.46
1:C:359:LEU:O	1:C:361:ASN:N	2.36	0.46
1:A:717:ARG:HH12	4:A:1105:DM2:C19	2.29	0.46
1:C:255:GLN:HE21	1:C:256:ASP:CB	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:THR:HB	2:E:50:PRO:HD2	1.98	0.46
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.15	0.46
1:B:120:GLN:HB3	10:B:1620:HOH:O	2.15	0.46
2:E:28:ASP:O	2:E:29:GLU:C	2.53	0.46
1:B:138:MET:CE	1:B:140:VAL:CG2	2.93	0.46
1:A:420:MET:HG2	1:A:430:ALA:CB	2.45	0.46
1:A:729:ILE:CD1	1:C:234:ILE:CG2	2.93	0.46
3:A:1101:LMT:H4O1	3:B:1101:LMT:H2B	1.78	0.46
1:B:873:ALA:N	1:B:874:PRO:HD3	2.31	0.46
1:A:842:GLU:O	1:A:846:GLN:HG3	2.16	0.46
1:A:668:LEU:HA	1:A:668:LEU:HD23	1.82	0.46
1:A:456:MET:HG3	1:A:471:SER:HG	1.80	0.46
1:A:151:GLN:NE2	10:A:1203:HOH:O	2.18	0.46
1:A:1036:LYS:N	1:A:1036:LYS:HD3	2.31	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.46	0.46
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.97	0.46
1:B:178:PHE:CA	4:B:1104:DM2:H213	2.46	0.46
1:B:709:HIS:N	1:B:710:PRO:HD3	2.30	0.46
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.48	0.46
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.97	0.46
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.68	0.46
1:B:714:THR:CG2	1:B:832:ALA:HA	2.46	0.46
1:C:11:PHE:HD1	1:C:11:PHE:O	1.98	0.46
1:A:226:LYS:HD3	1:A:227:GLY:N	2.31	0.46
1:C:868:LEU:C	1:C:868:LEU:HD23	2.36	0.46
1:B:868:LEU:C	1:B:870:GLY:H	2.19	0.46
1:B:342:LYS:HD3	1:B:346:GLU:OE2	2.16	0.46
1:C:893:GLU:HG3	1:C:893:GLU:O	2.16	0.46
1:A:355:MET:CA	1:A:355:MET:CE	2.93	0.45
1:A:709:HIS:N	1:A:710:PRO:CD	2.76	0.45
1:B:426:PRO:HD2	1:B:429:GLU:CG	2.46	0.45
3:A:1104:LMT:H12	3:A:1104:LMT:H41	1.58	0.45
1:C:395:MET:HA	1:C:395:MET:CE	2.46	0.45
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.46	0.45
1:A:908:GLY:CA	1:A:1014:ALA:HB2	2.47	0.45
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.98	0.45
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.51	0.45
1:A:921:LEU:HA	1:A:921:LEU:HD12	1.76	0.45
1:A:919:ARG:NH1	1:A:919:ARG:CG	2.46	0.45
1:A:708:LYS:O	1:A:708:LYS:CG	2.64	0.45
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LEU:HA	1:A:669:PRO:HD3	1.82	0.45
1:C:575:MET:SD	1:C:664:PHE:HD2	2.39	0.45
1:B:872:GLN:C	1:B:874:PRO:HD2	2.37	0.45
1:A:522:LYS:HA	1:A:522:LYS:HE3	1.99	0.45
1:A:554:TYR:O	1:A:558:ARG:HG2	2.17	0.45
1:A:729:ILE:HD12	1:C:234:ILE:CG2	2.46	0.45
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.46	0.45
1:A:868:LEU:N	1:A:868:LEU:CD2	2.79	0.45
1:A:60:THR:HG23	1:A:119:PRO:CG	2.46	0.45
1:A:445:ILE:HD13	1:A:940:LYS:HG3	1.99	0.45
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.99	0.45
1:A:925:VAL:O	1:A:929:VAL:HG22	2.17	0.45
1:A:373:PRO:HB3	3:A:1101:LMT:H121	1.98	0.45
1:A:764:ASP:OD1	1:A:765:ARG:HD3	2.17	0.45
1:A:1035:ARG:CG	1:A:1036:LYS:NZ	2.78	0.45
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.47	0.45
1:B:418:ARG:HD3	10:B:1229:HOH:O	2.16	0.45
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.98	0.45
1:B:744:ASN:N	10:B:1544:HOH:O	2.19	0.45
3:A:1104:LMT:H1B	3:A:1104:LMT:H5'	1.61	0.45
1:A:866:GLU:HG2	1:A:867:ARG:CG	2.46	0.45
1:C:672:VAL:N	1:C:673:GLU:OE2	2.49	0.45
1:B:968:VAL:HG13	10:B:1377:HOH:O	2.16	0.45
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.75	0.45
1:A:987:MET:HE1	1:A:1008:MET:HE1	1.90	0.45
1:C:867:ARG:CG	1:C:867:ARG:HH11	2.18	0.45
1:B:386:PHE:HB3	1:B:388:PHE:HD2	1.80	0.45
1:C:177:LEU:HD13	1:C:179:GLY:O	2.16	0.45
1:A:505:HIS:C	1:A:507:GLU:N	2.71	0.45
1:A:897:ILE:N	1:A:898:PRO:CD	2.80	0.45
1:A:987:MET:HE3	1:A:1008:MET:SD	2.55	0.44
1:A:968:VAL:CG2	1:A:1023:PRO:HG3	2.47	0.44
1:C:971:ARG:C	1:C:974:PRO:HD2	2.37	0.44
1:A:421:ALA:HB2	1:A:500:ILE:HG21	1.99	0.44
1:B:489:THR:N	1:B:490:PRO:CD	2.80	0.44
3:B:1102:LMT:H6D	3:B:1102:LMT:C5B	2.47	0.44
1:A:554:TYR:CE1	1:A:558:ARG:NH2	2.85	0.44
2:D:82:THR:HB	2:D:83:PRO:CD	2.47	0.44
1:C:664:PHE:CD2	1:C:717:ARG:HD3	2.52	0.44
1:A:418:ARG:CZ	1:A:970:MET:CE	2.95	0.44
1:C:620:ARG:NH1	10:C:1579:HOH:O	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ALA:HB2	10:A:1623:HOH:O	2.17	0.44
1:C:242:SER:HB2	1:C:244:GLU:OE1	2.18	0.44
3:A:1103:LMT:H6'1	1:C:8:ARG:NH2	2.21	0.44
1:A:537:SER:HB2	1:A:540:ARG:CZ	2.46	0.44
1:A:879:ILE:HD12	1:A:879:ILE:C	2.37	0.44
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.99	0.44
2:E:100:LEU:HD13	2:E:135:TYR:CD1	2.52	0.44
1:A:682:PHE:HB2	1:A:859:TRP:CZ3	2.51	0.44
1:A:148:THR:CG2	10:A:1514:HOH:O	2.64	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	2.00	0.44
1:C:314:GLU:CG	1:C:317:PHE:CE1	3.01	0.44
1:B:189:ASN:CG	1:B:192:GLU:HG2	2.38	0.44
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.41	0.44
1:A:953:MET:HA	1:A:958:LYS:O	2.17	0.44
1:A:679:GLY:HA3	4:A:1105:DM2:H212	2.00	0.44
4:B:1104:DM2:O6	4:B:1104:DM2:C21	2.55	0.44
1:A:879:ILE:HG13	1:A:880:SER:N	2.33	0.44
1:A:277:ILE:HA	1:A:613:ASN:O	2.18	0.44
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.79	0.44
1:C:199:THR:HB	1:C:200:PRO:HD2	2.00	0.44
1:A:886:LEU:HB3	1:C:14:VAL:HG13	1.99	0.44
1:A:1035:ARG:HD2	1:A:1035:ARG:HA	1.60	0.44
1:B:351:VAL:HG21	1:B:406:VAL:HG22	2.00	0.44
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.78	0.43
2:E:150:PHE:CE2	2:E:154:ILE:HD11	2.52	0.43
1:A:360:GLN:HG2	1:A:513:PHE:CD1	2.53	0.43
1:B:351:VAL:O	1:B:355:MET:HG2	2.18	0.43
1:A:307:ARG:HD3	10:A:1357:HOH:O	2.18	0.43
1:A:617:PHE:CD2	4:A:1106:DM2:C1	3.01	0.43
1:B:414:GLU:HG2	1:B:977:MET:HE1	1.97	0.43
1:C:367:ILE:HB	1:C:368:PRO:HD3	2.00	0.43
1:A:449:LEU:HD23	1:A:478:MET:SD	2.58	0.43
1:B:104:GLN:OE1	1:B:131:LYS:HE2	2.18	0.43
1:A:350:LEU:HD13	1:A:984:LEU:O	2.18	0.43
1:B:575:MET:CE	10:B:1517:HOH:O	2.66	0.43
1:A:672:VAL:C	1:A:674:LEU:H	2.20	0.43
1:A:537:SER:O	1:A:538:THR:OG1	2.34	0.43
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.00	0.43
1:A:618:ALA:HA	1:A:619:GLY:HA2	1.40	0.43
1:A:57:VAL:CG1	1:A:88:VAL:HG23	2.48	0.43
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD23	1:B:578:LEU:N	2.34	0.43
1:B:832:ALA:O	1:B:835:LYS:HB2	2.18	0.43
1:C:666:PHE:CE2	1:C:677:ALA:HB2	2.53	0.43
1:A:240:LEU:HG	1:A:245:GLU:HB3	2.00	0.43
1:C:79:SER:HB2	10:C:1265:HOH:O	2.17	0.43
1:B:615:PHE:CD2	1:B:626:ILE:HD12	2.53	0.43
2:E:32:ILE:HD13	2:E:32:ILE:N	2.32	0.43
1:A:968:VAL:HG21	1:A:1023:PRO:CG	2.48	0.43
1:A:616:GLY:C	1:A:618:ALA:N	2.70	0.43
3:B:1101:LMT:C2'	3:B:1101:LMT:H22	2.49	0.43
1:A:1030:ARG:HE	1:A:1030:ARG:HA	1.81	0.43
1:C:695:LEU:HA	1:C:695:LEU:HD23	1.88	0.43
2:E:41:ASN:ND2	2:E:72:ASP:HB2	2.34	0.43
4:A:1106:DM2:H1'	4:A:1106:DM2:O8	2.19	0.43
1:A:575:MET:HB2	1:A:617:PHE:HE1	1.83	0.43
3:A:1103:LMT:C2	3:A:1103:LMT:O5'	2.67	0.43
1:A:1027:VAL:CG2	1:A:1028:VAL:N	2.81	0.43
1:B:659:LYS:HB3	1:B:660:ASP:H	1.59	0.43
1:A:344:LEU:HD21	1:A:376:LEU:HD21	1.99	0.43
1:B:328:ASP:OD1	1:B:330:THR:HB	2.19	0.43
1:A:1038:GLU:HG3	1:A:1038:GLU:O	2.18	0.43
1:B:456:MET:CG	1:B:467:TYR:HB3	2.44	0.43
1:C:702:LEU:HD11	1:C:844:MET:HE1	2.00	0.43
1:B:563:PHE:O	1:B:924:ASP:HB2	2.19	0.43
2:D:28:ASP:HB3	2:D:31:ARG:NH2	2.34	0.43
1:A:961:ILE:HG22	1:A:962:GLU:N	2.33	0.43
3:B:1101:LMT:O2'	3:B:1101:LMT:C1	2.67	0.43
1:C:428:LYS:HG3	1:C:494:ALA:HB1	2.00	0.43
1:A:717:ARG:NH1	4:A:1105:DM2:C19	2.82	0.43
1:A:961:ILE:HD11	1:A:1031:ARG:NH2	2.34	0.43
1:B:875:SER:O	1:B:879:ILE:HG13	2.19	0.43
1:A:524:THR:O	1:A:527:TYR:HB3	2.19	0.43
1:A:1036:LYS:HA	1:A:1037:ASN:HA	1.83	0.43
1:A:695:LEU:HA	1:A:695:LEU:HD23	1.85	0.43
1:C:721:LEU:HB2	1:C:814:PRO:HG2	2.00	0.43
1:B:493:CYS:O	1:B:497:LEU:HB2	2.19	0.43
1:A:617:PHE:O	4:A:1105:DM2:H141	2.19	0.42
1:B:677:ALA:O	1:B:678:THR:CB	2.67	0.42
1:B:441:ALA:O	1:B:445:ILE:HG13	2.19	0.42
1:A:450:SER:O	1:A:454:VAL:HG23	2.18	0.42
1:A:958:LYS:N	1:A:958:LYS:HE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:VAL:HA	1:A:478:MET:HE2	2.01	0.42
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.51	0.42
1:A:456:MET:HB3	10:A:1602:HOH:O	2.19	0.42
1:A:1012:VAL:HG12	1:A:1013:THR:N	2.34	0.42
1:B:678:THR:CA	1:B:837:THR:HG22	2.49	0.42
1:B:758:TYR:CE2	1:B:770:LYS:HE2	2.54	0.42
1:B:618:ALA:HB1	1:B:719:ASN:O	2.19	0.42
1:C:382:VAL:HG11	1:C:476:SER:OG	2.19	0.42
1:A:862:MET:CE	4:A:1105:DM2:H211	2.50	0.42
1:A:676:THR:HG21	4:A:1106:DM2:C1'	2.49	0.42
1:C:309:GLU:HG3	1:C:313:MET:HE3	1.97	0.42
1:B:126:GLY:CA	1:C:116:PRO:HB3	2.46	0.42
1:C:897:ILE:N	1:C:898:PRO:CD	2.82	0.42
1:A:945:ILE:HG12	1:A:971:ARG:HG2	2.00	0.42
1:C:901:VAL:O	1:C:904:VAL:HG12	2.19	0.42
2:E:113:GLY:O	2:E:143:ASP:HA	2.19	0.42
2:D:94:GLU:CD	2:D:94:GLU:N	2.56	0.42
1:B:672:VAL:HG12	7:B:1103:LMU:H61	1.97	0.42
1:A:881:LEU:HD12	3:A:1102:LMT:C11	2.50	0.42
1:B:678:THR:CA	1:B:837:THR:CG2	2.98	0.42
2:D:82:THR:O	2:D:85:HIS:HB2	2.19	0.42
1:A:898:PRO:O	1:A:902:MET:HG3	2.20	0.42
1:A:176:GLN:HG2	1:A:615:PHE:CE1	2.55	0.42
1:B:17:ILE:HD11	6:B:1105:D10:H42	2.01	0.42
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.55	0.42
2:D:142:GLN:HA	2:D:147:LYS:O	2.18	0.42
1:C:544:LEU:HD12	1:C:544:LEU:HA	1.77	0.42
1:B:874:PRO:CD	1:B:875:SER:H	2.33	0.42
1:A:987:MET:HB3	1:A:988:PRO:HD3	2.02	0.42
1:B:744:ASN:O	1:B:748:THR:CG2	2.64	0.42
2:E:73:VAL:HG13	2:E:74:ASN:OD1	2.19	0.42
1:C:281:PHE:CE2	1:C:324:VAL:HG21	2.54	0.42
1:A:575:MET:HG3	1:A:617:PHE:HD1	1.85	0.42
1:A:418:ARG:HH21	1:A:970:MET:CE	2.33	0.42
1:C:1011:MET:CE	1:C:1011:MET:CA	2.91	0.42
1:C:1013:THR:HB	1:C:1017:LEU:HD22	2.01	0.42
1:A:281:PHE:O	1:A:284:GLN:HG2	2.20	0.42
2:E:94:GLU:HG3	10:E:225:HOH:O	2.19	0.42
1:A:987:MET:HE2	1:A:990:VAL:CG2	2.49	0.42
1:C:894:SER:O	1:C:898:PRO:HG2	2.19	0.42
1:B:522:LYS:NZ	1:B:522:LYS:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.50	0.42
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.90	0.42
1:A:895:TRP:CD1	6:A:1108:D10:H71	2.54	0.42
1:C:743:ILE:CD1	1:C:747:ASN:OD1	2.68	0.42
1:B:185:ARG:HD2	10:B:1528:HOH:O	2.20	0.42
1:C:950:LYS:HE2	1:C:954:ASP:OD1	2.20	0.42
1:A:866:GLU:CD	1:A:867:ARG:HG3	2.40	0.42
1:A:676:THR:O	1:A:677:ALA:C	2.59	0.42
1:C:674:LEU:N	1:C:674:LEU:HD23	2.35	0.42
1:A:1035:ARG:HG3	1:A:1036:LYS:CE	2.50	0.42
1:B:454:VAL:N	1:B:455:PRO:CD	2.83	0.42
1:C:951:ASP:OD1	1:C:955:LYS:HE3	2.20	0.42
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.19	0.42
1:B:726:GLN:OE1	1:B:812:GLY:HA3	2.20	0.42
1:C:21:LEU:C	1:C:21:LEU:HD12	2.40	0.41
1:A:418:ARG:CZ	1:A:970:MET:HE2	2.49	0.41
1:A:412:VAL:CG1	1:A:489:THR:HG22	2.47	0.41
1:A:85:THR:CG2	1:A:85:THR:O	2.66	0.41
1:A:284:GLN:HB2	1:A:285:PRO:HD2	2.02	0.41
1:A:360:GLN:NE2	1:A:517:ASN:OD1	2.38	0.41
1:C:366:LEU:O	1:C:369:THR:HB	2.21	0.41
1:B:522:LYS:HZ3	1:B:522:LYS:HB3	1.86	0.41
2:D:126:LEU:HD22	2:D:164:ILE:HD12	2.02	0.41
1:C:83:ASP:C	1:C:83:ASP:OD1	2.59	0.41
1:A:867:ARG:N	1:A:868:LEU:CG	2.63	0.41
1:C:527:TYR:CE2	1:C:968:VAL:CG1	2.86	0.41
1:A:1041:GLU:CG	1:A:1042:HIS:N	2.48	0.41
1:A:1:MET:N	1:A:2:PRO:CD	2.84	0.41
1:B:960:LEU:HD22	1:B:1027:VAL:HG22	2.01	0.41
1:A:448:VAL:O	1:A:451:ALA:HB3	2.21	0.41
1:A:845:GLU:HG2	1:A:857:TYR:OH	2.20	0.41
1:C:750:LEU:CD2	1:C:750:LEU:C	2.88	0.41
1:A:307:ARG:NH1	10:A:1357:HOH:O	2.07	0.41
1:C:251:LEU:O	1:C:252:LYS:HB3	2.21	0.41
2:D:92:HIS:O	2:D:96:VAL:HG23	2.21	0.41
1:B:568:ASP:CG	1:B:644:VAL:HG23	2.40	0.41
1:A:673:GLU:O	1:A:674:LEU:C	2.59	0.41
1:A:418:ARG:HE	1:A:970:MET:CE	2.34	0.41
1:A:372:VAL:HB	1:A:373:PRO:CD	2.50	0.41
1:A:60:THR:CG2	1:A:119:PRO:CG	2.98	0.41
2:D:23:ARG:HB2	2:D:53:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:GLN:O	1:B:866:GLU:C	2.59	0.41
1:A:558:ARG:HD3	1:A:558:ARG:HA	1.82	0.41
1:A:891:LEU:HD12	3:A:1103:LMT:H11	2.00	0.41
2:E:160:ASP:O	2:E:164:ILE:HG13	2.21	0.41
1:A:952:LEU:O	1:A:956:GLU:HB2	2.21	0.41
1:B:307:ARG:NH1	1:B:328:ASP:OD2	2.51	0.41
1:B:542:LEU:O	1:B:546:LEU:HD13	2.20	0.41
1:A:867:ARG:N	1:A:868:LEU:CA	2.82	0.41
1:C:670:ALA:HB3	1:C:862:MET:CE	2.51	0.41
1:C:360:GLN:HG2	1:C:513:PHE:CD1	2.55	0.41
1:A:881:LEU:HD12	3:A:1102:LMT:H112	2.02	0.41
1:C:463:THR:CG2	1:C:467:TYR:CZ	3.04	0.41
1:A:554:TYR:CZ	1:A:558:ARG:NH1	2.89	0.41
1:B:485:ALA:HA	1:B:489:THR:OG1	2.21	0.41
1:A:307:ARG:NE	10:A:1366:HOH:O	2.42	0.41
1:B:162:MET:O	1:B:166:ILE:HG12	2.20	0.41
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.91	0.41
1:B:851:LEU:HB3	1:B:852:PRO:HD2	2.01	0.41
4:A:1105:DM2:O8	4:A:1105:DM2:C2'	2.56	0.41
1:B:458:PHE:CD2	3:B:1101:LMT:H41	2.56	0.41
1:B:940:LYS:HG2	10:B:1356:HOH:O	2.21	0.41
1:B:578:LEU:HD22	1:B:661:ALA:CB	2.51	0.41
1:A:670:ALA:CB	10:A:1623:HOH:O	2.69	0.41
2:E:89:HIS:CG	2:E:119:LEU:HG	2.56	0.41
1:A:919:ARG:HG2	1:A:919:ARG:HH11	1.73	0.40
1:B:575:MET:HE3	10:B:1517:HOH:O	2.21	0.40
1:C:637:ARG:N	1:C:638:PRO:CD	2.84	0.40
1:B:366:LEU:HD22	1:B:366:LEU:HA	1.89	0.40
2:E:34:MET:SD	2:E:40:VAL:HG12	2.62	0.40
1:C:1:MET:N	1:C:2:PRO:CD	2.83	0.40
1:C:815:ARG:CZ	10:C:1596:HOH:O	2.49	0.40
1:A:1036:LYS:CA	1:A:1037:ASN:CB	2.99	0.40
1:B:138:MET:HE2	1:B:140:VAL:HG23	2.04	0.40
1:B:866:GLU:O	1:B:868:LEU:N	2.54	0.40
1:C:799:VAL:CG2	1:C:804:PHE:HE1	2.33	0.40
1:A:727:PHE:CE2	1:A:729:ILE:HG12	2.56	0.40
1:A:1007:VAL:O	1:A:1011:MET:HG2	2.21	0.40
1:A:188:MET:CE	1:A:773:VAL:HG12	2.52	0.40
1:C:483:LEU:HA	1:C:483:LEU:HD12	1.90	0.40
1:B:657:GLN:HA	1:B:657:GLN:OE1	2.21	0.40
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:MET:HG3	1:A:617:PHE:CD1	2.56	0.40
1:A:672:VAL:HG22	1:A:673:GLU:N	2.02	0.40
1:A:990:VAL:HG12	1:A:1004:GLY:C	2.41	0.40
1:C:739:LEU:N	1:C:739:LEU:HD12	2.35	0.40
2:E:150:PHE:HA	2:E:165:LEU:HD12	2.03	0.40
1:A:957:GLY:O	1:A:958:LYS:C	2.59	0.40
1:A:13:TRP:HH2	1:A:370:ILE:HD13	1.86	0.40
2:D:42:ALA:O	2:D:50:PRO:HD3	2.21	0.40
1:A:326:PRO:O	1:A:630:SER:HB2	2.21	0.40
1:A:540:ARG:HG2	1:A:541:TYR:CE1	2.57	0.40
1:B:987:MET:N	1:B:988:PRO:CD	2.83	0.40
1:C:21:LEU:HD12	1:C:22:ALA:H	1.85	0.40
1:A:510:LYS:HD2	1:A:511:GLY:H	1.84	0.40
1:C:947:GLU:HG3	1:C:948:PHE:N	2.36	0.40
1:A:956:GLU:CA	1:A:956:GLU:OE2	2.69	0.40
1:C:284:GLN:HG3	1:C:285:PRO:HD2	2.03	0.40
1:B:672:VAL:HG23	1:B:673:GLU:OE2	2.20	0.40
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.51	0.40
1:B:866:GLU:C	1:B:868:LEU:N	2.75	0.40
1:A:462:SER:O	1:A:463:THR:C	2.58	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	1040/1057 (98%)	979 (94%)	47 (4%)	14 (1%)	15 10
1	B	1031/1057 (98%)	997 (97%)	29 (3%)	5 (0%)	34 34
1	C	1034/1057 (98%)	997 (96%)	35 (3%)	2 (0%)	52 61
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	150/169 (89%)	141 (94%)	7 (5%)	2 (1%)	15 10
All	All	3409/3509 (97%)	3265 (96%)	121 (4%)	23 (1%)	26 26

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	617	PHE
1	A	672	VAL
1	A	677	ALA
1	B	659	LYS
1	C	510	LYS
1	A	960	LEU
1	A	1037	ASN
1	B	256	ASP
1	B	867	ARG
1	A	837	THR
1	A	955	LYS
1	A	1040	ILE
1	A	1041	GLU
1	B	869	SER
1	C	1035	ARG
2	E	29	GLU
1	A	958	LYS
1	A	674	LEU
1	A	1025	PHE
2	E	28	ASP
1	B	874	PRO
1	A	419	VAL

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	848/863 (98%)	786 (93%)	62 (7%)	17 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	839/863 (97%)	788 (94%)	51 (6%)	23	23
1	C	842/863 (98%)	795 (94%)	47 (6%)	26	27
2	D	120/132 (91%)	114 (95%)	6 (5%)	30	33
2	E	117/132 (89%)	111 (95%)	6 (5%)	29	32
All	All	2766/2853 (97%)	2594 (94%)	172 (6%)	23	22

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	25	LEU
1	A	30	LEU
1	A	37	THR
1	A	49	TYR
1	A	60	THR
1	A	113	LEU
1	A	214	VAL
1	A	240	LEU
1	A	262	LEU
1	A	263	ARG
1	A	270	LEU
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	343	THR
1	A	366	LEU
1	A	429	GLU
1	A	431	THR
1	A	449	LEU
1	A	472	ILE
1	A	483	LEU
1	A	492	LEU
1	A	505	HIS
1	A	518	ARG
1	A	530	SER
1	A	540	ARG
1	A	577	GLN
1	A	630	SER
1	A	649	MET
1	A	659	LYS
1	A	673	GLU

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Mol	Chain	Res	Type
1	A	678	THR
1	A	695	LEU
1	A	708	LYS
1	A	711	ASP
1	A	713	LEU
1	A	715	SER
1	A	717	ARG
1	A	742	SER
1	A	801	PHE
1	A	828	LEU
1	A	836	SER
1	A	839	GLU
1	A	866	GLU
1	A	868	LEU
1	A	879	ILE
1	A	881	LEU
1	A	902	MET
1	A	919	ARG
1	A	921	LEU
1	A	931	LEU
1	A	946	VAL
1	A	968	VAL
1	A	971	ARG
1	A	984	LEU
1	A	987	MET
1	A	991	ILE
1	A	1005	THR
1	A	1030	ARG
1	A	1040	ILE
1	A	1042	HIS
1	B	11	PHE
1	B	21	LEU
1	B	30	LEU
1	B	49	TYR
1	B	75	LEU
1	B	108	GLN
1	B	111	LEU
1	B	240	LEU
1	B	255	GLN
1	B	261	LEU
1	B	270	LEU
1	B	274	ASN

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	353	LEU
1	B	365	THR
1	B	366	LEU
1	B	377	LEU
1	B	386	PHE
1	B	468	ARG
1	B	480	LEU
1	B	497	LEU
1	B	510	LYS
1	B	555	LEU
1	B	574	THR
1	B	578	LEU
1	B	600	THR
1	B	610	PHE
1	B	633	ASP
1	B	641	GLU
1	B	660	ASP
1	B	672	VAL
1	B	695	LEU
1	B	713	LEU
1	B	714	THR
1	B	748	THR
1	B	758	TYR
1	B	801	PHE
1	B	869	SER
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	907	LEU
1	B	914	LEU
1	B	919	ARG
1	B	921	LEU
1	B	937	LEU
1	B	965	LEU
1	B	972	LEU
1	B	980	LEU
1	B	992	SER
1	B	1030	ARG
1	C	11	PHE
1	C	21	LEU
1	C	49	TYR

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Mol	Chain	Res	Type
1	C	75	LEU
1	C	95	GLU
1	C	96	SER
1	C	121	GLU
1	C	135	SER
1	C	152	GLU
1	C	177	LEU
1	C	193	LEU
1	C	255	GLN
1	C	289	LEU
1	C	310	LEU
1	C	324	VAL
1	C	344	LEU
1	C	383	LEU
1	C	404	LEU
1	C	483	LEU
1	C	544	LEU
1	C	558	ARG
1	C	564	LEU
1	C	671	ILE
1	C	673	GLU
1	C	676	THR
1	C	690	LEU
1	C	695	LEU
1	C	717	ARG
1	C	743	ILE
1	C	750	LEU
1	C	784	ASP
1	C	799	VAL
1	C	801	PHE
1	C	811	TYR
1	C	822	LEU
1	C	828	LEU
1	C	853	THR
1	C	867	ARG
1	C	876	LEU
1	C	891	LEU
1	C	948	PHE
1	C	960	LEU
1	C	968	VAL
1	C	976	LEU
1	C	1011	MET

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Mol	Chain	Res	Type
1	C	1017	LEU
1	C	1032	ARG
2	D	45	VAL
2	D	53	LEU
2	D	61	GLU
2	D	79	LEU
2	D	94	GLU
2	D	154	ILE
2	E	34	MET
2	E	79	LEU
2	E	119	LEU
2	E	123	ARG
2	E	134	LYS
2	E	159	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	255	GLN
2	E	69	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
3	LMT	A	1101	-	36,36,36	1.21	4 (11%)	47,47,47	1.25	5 (10%)
3	LMT	A	1102	-	36,36,36	1.20	3 (8%)	47,47,47	1.16	5 (10%)
3	LMT	A	1103	-	36,36,36	1.16	4 (11%)	47,47,47	1.23	4 (8%)
3	LMT	A	1104	-	36,36,36	1.23	4 (11%)	47,47,47	0.98	5 (10%)
4	DM2	A	1105	-	41,43,43	2.48	11 (26%)	55,67,67	1.32	6 (10%)
4	DM2	A	1106	-	41,43,43	2.51	13 (31%)	55,67,67	1.64	10 (18%)
5	D12	A	1107	-	11,11,11	0.28	0	10,10,10	0.84	0
6	D10	A	1108	-	9,9,9	0.26	0	8,8,8	0.75	0
6	D10	A	1109	-	9,9,9	0.24	0	8,8,8	0.69	0
3	LMT	B	1101	-	36,36,36	1.24	4 (11%)	47,47,47	1.30	4 (8%)
3	LMT	B	1102	-	36,36,36	1.19	4 (11%)	47,47,47	1.13	4 (8%)
7	LMU	B	1103	-	36,36,36	1.24	4 (11%)	47,47,47	1.21	7 (14%)
4	DM2	B	1104	-	41,43,43	2.52	10 (24%)	55,67,67	1.41	8 (14%)
6	D10	B	1105	-	9,9,9	0.31	0	8,8,8	0.83	0
8	GOL	B	1106	-	5,5,5	0.33	0	5,5,5	0.49	0
8	GOL	B	1107	-	5,5,5	0.34	0	5,5,5	0.16	0
9	HEX	B	1108	-	5,5,5	0.20	0	4,4,4	0.52	0
5	D12	B	1109	-	11,11,11	0.22	0	10,10,10	0.72	0
3	LMT	C	1101	-	36,36,36	1.17	4 (11%)	47,47,47	1.06	3 (6%)
5	D12	C	1102	-	11,11,11	0.16	0	10,10,10	0.56	0
8	GOL	C	1103	-	5,5,5	0.41	0	5,5,5	0.50	0
6	D10	C	1104	-	9,9,9	0.23	0	8,8,8	0.72	0
9	HEX	C	1105	-	5,5,5	0.21	0	4,4,4	0.55	0
5	D12	C	1106	-	11,11,11	0.30	0	10,10,10	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1104	-	-	0/21/61/61	0/2/2/2
4	DM2	A	1105	-	-	0/13/60/60	0/5/5/5
4	DM2	A	1106	-	-	0/13/60/60	0/5/5/5
5	D12	A	1107	-	-	0/9/9/9	0/0/0/0
6	D10	A	1108	-	-	0/7/7/7	0/0/0/0
6	D10	A	1109	-	-	0/7/7/7	0/0/0/0
3	LMT	B	1101	-	-	1/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	0/21/61/61	0/2/2/2
7	LMU	B	1103	-	-	1/21/61/61	0/2/2/2
4	DM2	B	1104	-	-	0/13/60/60	0/5/5/5
6	D10	B	1105	-	-	0/7/7/7	0/0/0/0
8	GOL	B	1106	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1107	-	-	0/4/4/4	0/0/0/0
9	HEX	B	1108	-	-	0/3/3/3	0/0/0/0
5	D12	B	1109	-	-	0/9/9/9	0/0/0/0
3	LMT	C	1101	-	-	0/21/61/61	0/2/2/2
5	D12	C	1102	-	-	0/9/9/9	0/0/0/0
8	GOL	C	1103	-	-	0/4/4/4	0/0/0/0
6	D10	C	1104	-	-	0/7/7/7	0/0/0/0
9	HEX	C	1105	-	-	0/3/3/3	0/0/0/0
5	D12	C	1106	-	-	0/9/9/9	0/0/0/0

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	DM2	C4'-C5'	-3.63	1.45	1.52
7	B	1103	LMU	C3'-C4'	-3.50	1.42	1.52
4	B	1104	DM2	C4'-C5'	-3.38	1.45	1.52
3	B	1102	LMT	C3'-C4'	-3.07	1.43	1.52
3	B	1101	LMT	C3'-C4'	-3.05	1.43	1.52
3	C	1101	LMT	C3'-C4'	-3.01	1.43	1.52
3	A	1104	LMT	C3'-C4'	-2.94	1.44	1.52
3	A	1102	LMT	C3'-C4'	-2.94	1.44	1.52
4	A	1105	DM2	C4'-C5'	-2.84	1.47	1.52
3	A	1101	LMT	C3'-C4'	-2.81	1.44	1.52
3	A	1103	LMT	C3'-C4'	-2.74	1.44	1.52
4	A	1106	DM2	C9-C16	-2.58	1.34	1.39
3	B	1101	LMT	C3B-C2B	-2.45	1.45	1.52
3	A	1101	LMT	C3B-C2B	-2.45	1.46	1.52
3	A	1102	LMT	C3B-C2B	-2.43	1.46	1.52
4	A	1105	DM2	C9-C16	-2.36	1.35	1.39
4	A	1106	DM2	O10-C10	-2.35	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1104	LMT	C3B-C2B	-2.34	1.46	1.52
4	B	1104	DM2	C9-C16	-2.34	1.35	1.39
3	A	1103	LMT	C3B-C2B	-2.32	1.46	1.52
7	B	1103	LMU	C3'-C2'	-2.17	1.46	1.52
3	B	1102	LMT	C3B-C2B	-2.14	1.46	1.52
3	C	1101	LMT	C3B-C2B	-2.14	1.46	1.52
3	A	1103	LMT	O1B-C1B	-2.01	1.36	1.41
4	A	1105	DM2	C7-C6	2.01	1.52	1.47
4	A	1106	DM2	O8-C8	2.11	1.42	1.37
3	C	1101	LMT	O5'-C5'	2.15	1.49	1.44
4	A	1106	DM2	C7-C6	2.16	1.53	1.47
3	B	1101	LMT	O5'-C5'	2.16	1.49	1.44
3	A	1101	LMT	O5'-C5'	2.18	1.49	1.44
3	A	1104	LMT	O5'-C5'	2.20	1.49	1.44
4	A	1106	DM2	O4-C4	2.22	1.40	1.37
4	A	1105	DM2	C2'-C1'	2.22	1.56	1.51
3	B	1102	LMT	O5'-C5'	2.23	1.49	1.44
4	A	1105	DM2	O4-C4	2.24	1.40	1.37
7	B	1103	LMU	O3'-C3'	2.34	1.48	1.43
4	B	1104	DM2	O4-C4	2.49	1.41	1.37
4	A	1106	DM2	C17-C16	2.60	1.44	1.40
4	A	1105	DM2	C15-C16	2.60	1.54	1.51
4	A	1106	DM2	C2'-C1'	2.66	1.56	1.51
4	B	1104	DM2	C2'-C1'	2.88	1.57	1.51
4	B	1104	DM2	C15-C16	2.92	1.55	1.51
4	A	1106	DM2	C15-C16	2.92	1.55	1.51
4	A	1106	DM2	C5-C6	3.04	1.55	1.47
4	B	1104	DM2	C5-C6	3.05	1.55	1.47
4	A	1105	DM2	C5-C6	3.06	1.55	1.47
4	B	1104	DM2	C17-C16	3.36	1.45	1.40
4	A	1105	DM2	C17-C16	3.38	1.45	1.40
3	A	1103	LMT	O5B-C1B	3.68	1.51	1.41
3	C	1101	LMT	O5B-C1B	3.70	1.51	1.41
7	B	1103	LMU	O5B-C1B	3.71	1.51	1.41
3	B	1102	LMT	O5B-C1B	3.73	1.51	1.41
3	A	1104	LMT	O5B-C1B	3.85	1.51	1.41
3	B	1101	LMT	O5B-C1B	3.92	1.51	1.41
3	A	1102	LMT	O5B-C1B	3.93	1.51	1.41
3	A	1101	LMT	O5B-C1B	3.97	1.52	1.41
4	B	1104	DM2	C8-C9	6.00	1.51	1.40
4	A	1106	DM2	C8-C9	6.17	1.51	1.40
4	A	1105	DM2	C8-C9	6.17	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	DM2	O19-C19	7.56	1.36	1.22
4	A	1105	DM2	O19-C19	7.58	1.36	1.22
4	B	1104	DM2	O19-C19	7.64	1.36	1.22
4	A	1106	DM2	O6-C6	8.42	1.38	1.22
4	A	1105	DM2	O6-C6	8.47	1.38	1.22
4	B	1104	DM2	O6-C6	8.55	1.38	1.22

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1106	DM2	O4-C4-C3	-4.17	117.33	124.35
3	B	1101	LMT	C1B-O1B-C4'	-3.66	108.43	118.01
4	A	1106	DM2	C1-C20-C19	-3.66	113.18	119.28
4	A	1105	DM2	O4-C4-C3	-3.47	118.51	124.35
4	B	1104	DM2	O4-C4-C3	-3.31	118.78	124.35
3	A	1103	LMT	C1B-O1B-C4'	-2.98	110.21	118.01
4	B	1104	DM2	C1-C20-C19	-2.52	115.09	119.28
4	A	1106	DM2	C20-C5-C6	-2.39	115.87	119.72
4	A	1105	DM2	C20-C5-C6	-2.35	115.92	119.72
3	C	1101	LMT	C1B-O1B-C4'	-2.30	111.98	118.01
3	B	1102	LMT	C1B-O1B-C4'	-2.18	112.30	118.01
7	B	1103	LMU	C1B-O5B-C5B	-2.14	109.60	113.75
4	B	1104	DM2	O13-C13-C12	-2.11	119.61	122.22
4	A	1105	DM2	C1-C20-C19	-2.06	115.85	119.28
3	A	1102	LMT	C1B-C2B-C3B	-2.05	105.93	109.97
4	B	1104	DM2	C20-C5-C6	-2.04	116.42	119.72
7	B	1103	LMU	O5'-C5'-C6'	2.00	111.41	106.36
3	B	1101	LMT	O5B-C5B-C4B	2.01	113.45	109.68
3	A	1104	LMT	O1'-C1-C2	2.01	117.88	109.88
7	B	1103	LMU	C4B-C3B-C2B	2.03	114.58	110.79
4	A	1106	DM2	C14-C13-C12	2.07	119.95	117.66
7	B	1103	LMU	O6'-C6'-C5'	2.08	118.20	111.33
7	B	1103	LMU	C1-O1'-C1'	2.09	117.60	113.94
3	A	1101	LMT	O6B-C6B-C5B	2.11	118.29	111.33
4	A	1105	DM2	O5'-C5'-C4'	2.11	113.18	109.53
4	A	1106	DM2	O12-C12-C13	2.11	113.09	108.44
3	B	1102	LMT	O1'-C1-C2	2.12	118.31	109.88
3	A	1104	LMT	O1'-C1'-C2'	2.13	110.73	108.04
4	B	1104	DM2	C14-C13-C12	2.14	120.03	117.66
3	C	1101	LMT	O1'-C1-C2	2.15	118.41	109.88
3	A	1104	LMT	O1B-C4'-C5'	2.18	115.04	109.32
3	A	1104	LMT	O6'-C6'-C5'	2.20	118.60	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	LMT	O6B-C6B-C5B	2.27	118.84	111.33
4	A	1106	DM2	C5-C20-C19	2.27	124.09	120.75
4	A	1106	DM2	C7-C18-C17	2.39	123.45	119.73
3	A	1101	LMT	C1B-O5B-C5B	2.41	118.42	113.75
3	A	1103	LMT	O5'-C1'-C2'	2.48	115.37	110.28
7	B	1103	LMU	C3B-C4B-C5B	2.50	114.55	110.20
3	B	1102	LMT	O6B-C6B-C5B	2.51	119.63	111.33
3	A	1102	LMT	O1'-C1'-C2'	2.56	111.27	108.04
4	A	1106	DM2	O10-C1'-C2'	2.56	113.05	108.38
7	B	1103	LMU	O5'-C1'-C2'	2.67	115.75	110.28
3	A	1102	LMT	C3B-C4B-C5B	2.74	114.97	110.20
4	B	1104	DM2	C4-C5-C6	2.93	126.32	122.34
3	B	1101	LMT	O1'-C1'-C2'	2.94	111.76	108.04
3	C	1101	LMT	C1-O1'-C1'	3.03	119.25	113.94
3	A	1104	LMT	C1-O1'-C1'	3.06	119.29	113.94
3	A	1101	LMT	C3B-C4B-C5B	3.16	115.71	110.20
4	A	1105	DM2	C4-C5-C6	3.19	126.67	122.34
3	A	1101	LMT	C1-O1'-C1'	3.22	119.57	113.94
3	A	1102	LMT	O5B-C5B-C4B	3.32	115.91	109.68
3	A	1103	LMT	C1'-C2'-C3'	3.40	116.67	109.97
3	B	1102	LMT	C1-O1'-C1'	3.46	119.98	113.94
4	B	1104	DM2	C21-O4-C4	3.54	122.91	117.54
4	A	1105	DM2	O4-C4-C5	3.56	121.31	115.78
3	A	1101	LMT	O5B-C5B-C4B	3.62	116.48	109.68
4	B	1104	DM2	O4-C4-C5	3.64	121.44	115.78
3	A	1103	LMT	C2'-C3'-C4'	4.00	118.39	109.60
4	A	1106	DM2	C4-C5-C6	4.05	127.83	122.34
3	B	1101	LMT	C1-O1'-C1'	4.24	121.36	113.94
4	A	1106	DM2	O4-C4-C5	4.43	122.67	115.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1101	LMT	C1-O1'-C1'-O5'
7	B	1103	LMU	C1'-O1'-C1-C2

There are no ring outliers.

17 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	LMT	3	0
3	A	1102	LMT	8	0
3	A	1103	LMT	11	0
3	A	1104	LMT	6	0
4	A	1105	DM2	33	0
4	A	1106	DM2	12	0
5	A	1107	D12	3	0
6	A	1108	D10	2	0
3	B	1101	LMT	10	0
3	B	1102	LMT	4	0
7	B	1103	LMU	4	0
4	B	1104	DM2	9	0
6	B	1105	D10	1	0
8	B	1106	GOL	1	0
3	C	1101	LMT	1	0
5	C	1102	D12	2	0
8	C	1103	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1042/1057 (98%)	0.08	57 (5%) 29 32	23, 48, 95, 151	0
1	B	1033/1057 (97%)	-0.12	32 (3%) 52 57	23, 46, 75, 131	0
1	C	1036/1057 (98%)	-0.08	31 (2%) 54 58	25, 43, 74, 151	0
2	D	156/169 (92%)	-0.10	4 (2%) 59 63	33, 45, 74, 110	0
2	E	152/169 (89%)	1.00	32 (21%) 1 1	38, 56, 87, 104	0
All	All	3419/3509 (97%)	0.00	156 (4%) 36 40	23, 46, 83, 151	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	11	GLY	9.2
1	C	1036	LYS	8.6
1	B	678	THR	7.2
2	E	34	MET	7.0
1	A	868	LEU	5.6
1	A	515	TRP	5.4
1	A	674	LEU	5.3
1	A	869	SER	5.2
2	E	68	LYS	5.1
1	A	512	PHE	5.0
2	E	66	LEU	5.0
1	A	677	ALA	4.8
1	C	362	PHE	4.8
1	B	677	ALA	4.7
1	A	918	PHE	4.6
2	E	30	VAL	4.6
1	A	518	ARG	4.6
1	A	866	GLU	4.6
1	C	1035	ARG	4.6
1	B	510	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
2	E	33	LEU	4.6
2	E	35	ALA	4.5
1	A	865	GLN	4.5
1	A	498	LYS	4.5
1	A	500	ILE	4.4
1	C	513	PHE	4.4
1	A	541	TYR	4.4
2	E	31	ARG	4.3
1	A	836	SER	4.3
2	E	67	LEU	4.1
1	C	497	LEU	4.1
1	C	739	LEU	4.1
1	A	618	ALA	4.0
1	C	1034	SER	4.0
1	B	871	ASN	3.9
1	C	1033	PHE	3.9
1	A	1040	ILE	3.9
1	A	506	GLY	3.9
2	E	61	GLU	3.8
2	E	40	VAL	3.8
2	E	32	ILE	3.8
1	C	510	LYS	3.7
2	E	62	ILE	3.6
1	B	255	GLN	3.6
1	B	868	LEU	3.6
1	A	514	GLY	3.6
1	A	1042	HIS	3.6
1	A	362	PHE	3.5
2	E	69	ASN	3.4
2	E	64	GLU	3.4
2	E	37	GLY	3.3
1	A	874	PRO	3.3
1	B	712	MET	3.3
2	E	73	VAL	3.3
1	C	512	PHE	3.2
1	C	500	ILE	3.2
1	C	811	TYR	3.2
2	E	70	GLY	3.2
2	E	65	VAL	3.1
1	B	674	LEU	3.1
1	A	536	ARG	3.1
1	B	869	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	38	ALA	3.1
1	A	867	ARG	3.0
1	A	835	LYS	3.0
2	E	60	LEU	3.0
1	A	427	PRO	3.0
2	E	106	VAL	3.0
1	B	511	GLY	2.9
1	C	793	ALA	2.9
1	B	837	THR	2.9
1	B	508	GLY	2.9
1	A	873	ALA	2.9
1	A	522	LYS	2.9
2	E	27	ASP	2.9
2	E	139	VAL	2.9
1	B	501	ALA	2.8
1	A	672	VAL	2.8
1	C	363	ARG	2.8
1	B	603	LYS	2.8
1	A	543	VAL	2.8
1	B	834	GLY	2.8
1	A	554	TYR	2.7
1	B	657	GLN	2.7
1	A	540	ARG	2.7
1	B	600	THR	2.7
1	A	510	LYS	2.7
1	A	534	ILE	2.7
1	C	255	GLN	2.7
2	E	63	VAL	2.7
1	A	513	PHE	2.6
1	A	619	GLY	2.6
1	B	596	HIS	2.6
1	A	676	THR	2.6
2	E	101	LYS	2.6
1	C	736	ALA	2.6
1	B	638	PRO	2.6
1	A	537	SER	2.6
2	E	71	ALA	2.6
1	A	956	GLU	2.6
1	A	511	GLY	2.5
1	C	498	LYS	2.5
1	A	832	ALA	2.5
1	C	28	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	429	GLU	2.5
1	B	874	PRO	2.5
1	B	256	ASP	2.5
1	A	993	THR	2.5
1	A	531	VAL	2.5
1	B	641	GLU	2.5
1	A	673	GLU	2.5
1	A	497	LEU	2.5
1	A	557	VAL	2.5
1	B	257	GLY	2.4
1	A	462	SER	2.4
1	B	604	ASN	2.4
2	D	150	PHE	2.4
1	B	558	ARG	2.4
1	A	509	LYS	2.4
1	B	509	LYS	2.4
1	C	554	TYR	2.4
1	A	870	GLY	2.4
1	C	29	LYS	2.4
1	C	501	ALA	2.4
1	B	877	TYR	2.4
1	A	501	ALA	2.4
1	A	425	LEU	2.3
1	A	871	ASN	2.3
1	C	508	GLY	2.3
2	E	29	GLU	2.3
1	C	737	GLN	2.3
1	B	597	TYR	2.3
1	A	712	MET	2.3
1	C	425	LEU	2.3
1	A	496	MET	2.2
1	A	657	GLN	2.2
1	C	495	THR	2.2
1	B	3	ASN	2.2
1	B	500	ILE	2.2
1	C	955	LYS	2.2
2	E	36	ASN	2.2
2	E	165	LEU	2.2
1	A	529	ASP	2.1
1	B	653	ARG	2.1
2	D	12	SER	2.1
1	C	734	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	133	LEU	2.1
2	E	137	ALA	2.1
1	B	601	LYS	2.1
1	C	361	ASN	2.1
1	A	461	GLY	2.0
1	C	803	ALA	2.0
1	A	363	ARG	2.0
2	E	54	ALA	2.0
2	E	97	GLU	2.0
1	C	738	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	GOL	B	1107	6/6	0.74	0.39	14.59	95,119,134,143	0
3	LMT	A	1104	35/35	0.90	0.31	6.58	74,94,100,104	0
4	DM2	B	1104	39/39	0.75	0.26	5.45	93,121,139,142	0
3	LMT	B	1102	35/35	0.90	0.21	4.04	63,77,111,112	0
9	HEX	C	1105	6/6	0.71	0.20	3.85	84,101,105,105	0
7	LMU	B	1103	35/35	0.74	0.22	3.84	65,84,96,105	0
8	GOL	B	1106	6/6	0.89	0.27	3.20	73,88,107,114	0
9	HEX	B	1108	6/6	0.69	0.15	2.88	84,101,109,109	0
5	D12	B	1109	12/12	0.71	0.19	2.71	52,73,88,91	0
3	LMT	A	1103	35/35	0.86	0.16	2.70	59,95,115,119	0
8	GOL	C	1103	6/6	0.93	0.15	2.53	37,48,59,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	D12	A	1107	12/12	0.72	0.20	2.28	58,82,125,125	0
3	LMT	A	1102	35/35	0.80	0.27	1.86	73,105,119,120	0
3	LMT	C	1101	35/35	0.93	0.14	1.85	62,74,93,97	0
3	LMT	B	1101	35/35	0.79	0.27	1.52	73,114,134,136	0
4	DM2	A	1106	39/39	0.70	0.24	0.95	81,141,174,176	0
3	LMT	A	1101	35/35	0.94	0.13	0.95	49,74,107,108	0
4	DM2	A	1105	39/39	0.83	0.18	0.29	75,91,110,115	0
5	D12	C	1102	12/12	0.56	0.16	-0.01	58,91,99,100	0
6	D10	A	1108	10/10	0.73	0.18	-	85,103,113,113	0
6	D10	C	1104	10/10	0.76	0.18	-	80,97,104,107	0
6	D10	A	1109	10/10	0.55	0.29	-	83,107,121,121	0
6	D10	B	1105	10/10	0.76	0.18	-	75,97,109,110	0
5	D12	C	1106	12/12	0.75	0.13	-	81,98,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.