Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:58 PM GMT

PDB ID	:	4DX5
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	:	1.90 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:

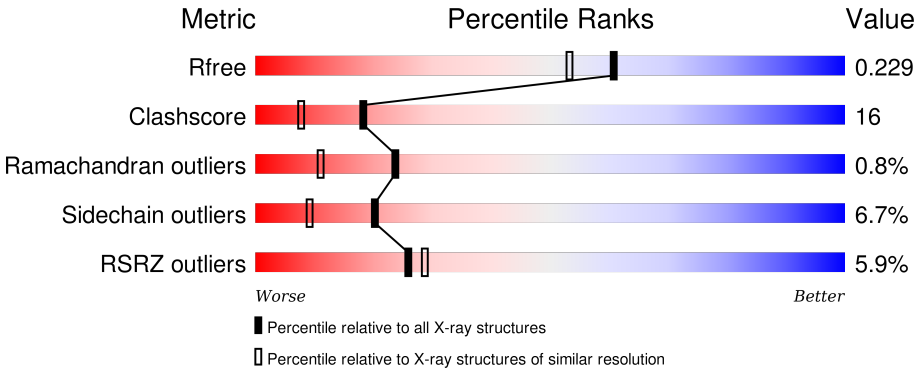
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	8% 70% 23% 5% •
1	B	1057	5% 78% 17% • •
1	C	1057	4% 79% 16% • •
2	D	169	3% 77% 13% • 8%
2	E	169	14% 63% 23% • • 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
10	C14	B	1109	-	-	-	X
11	LMU	B	1114	-	-	-	X
12	DD9	C	1111	-	-	-	X
14	UND	C	1119	-	-	-	X
3	GOL	A	1101	-	-	-	X
3	GOL	A	1110	-	-	-	X
3	GOL	B	1101	-	-	-	X
3	GOL	B	1102	-	-	-	X
3	GOL	B	1113	-	-	-	X
3	GOL	B	1115	-	-	-	X
3	GOL	B	1116	-	-	X	X
3	GOL	B	1117	-	-	-	X
3	GOL	C	1101	-	-	-	X
3	GOL	C	1114	-	-	-	X
3	GOL	C	1115	-	-	-	X
3	GOL	C	1117	-	-	-	X
3	GOL	D	201	-	-	-	X
3	GOL	D	202	-	-	-	X
4	LMT	A	1102	-	-	-	X
4	LMT	A	1109	-	-	-	X
4	LMT	B	1104	-	-	-	X
4	LMT	B	1110	-	-	-	X
4	LMT	B	1111	-	-	-	X
5	OCT	A	1105	-	-	-	X
5	OCT	C	1106	-	-	-	X
5	OCT	C	1112	-	-	-	X
6	D10	A	1107	-	-	-	X
6	D10	B	1107	-	-	-	X
6	D10	C	1107	-	-	-	X
6	D10	C	1120	-	-	-	X
7	HEX	B	1108	-	-	-	X
7	HEX	B	1112	-	-	-	X
7	HEX	C	1113	-	-	-	X
8	D12	A	1111	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29010 atoms, of which 587 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	1044	Total	C	N	O	S	0	0	0
			7943	5106	1315	1478	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	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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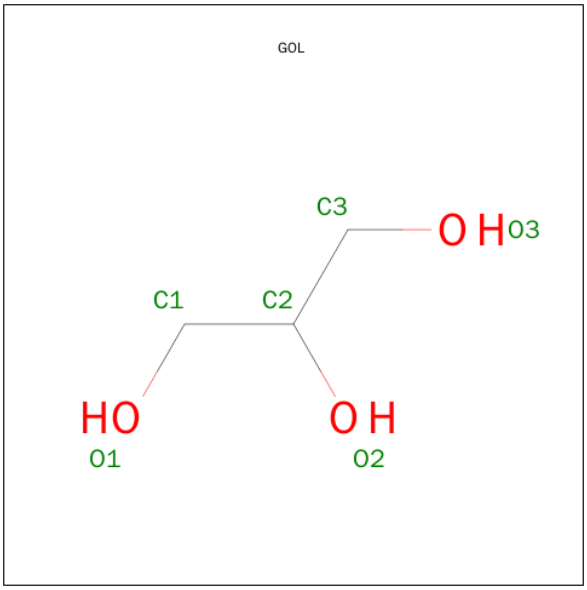
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	EXPRESSION TAG	UNP P31224

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			

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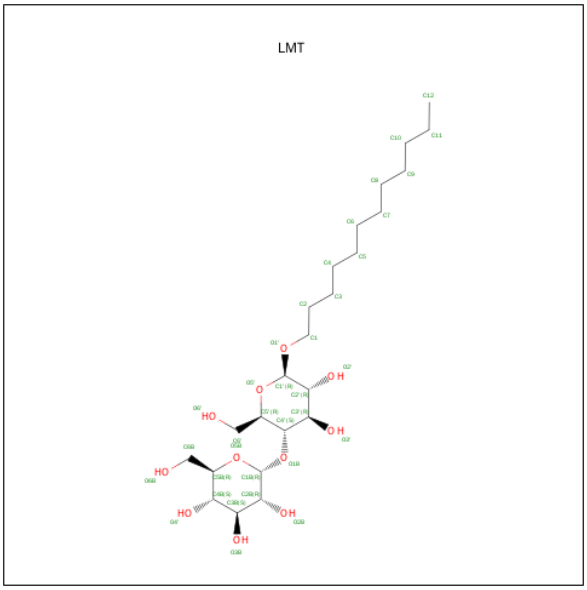
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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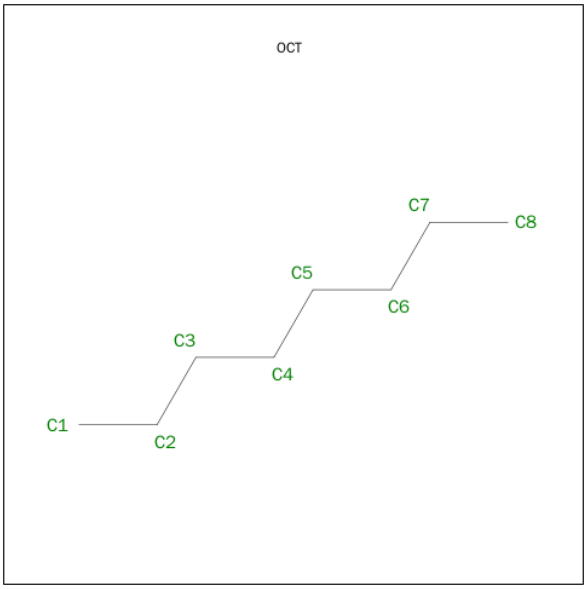
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0
4	C	1	Total C O 35 24 11	0	0

- Molecule 5 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H 26 8 18	0	0
5	A	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0

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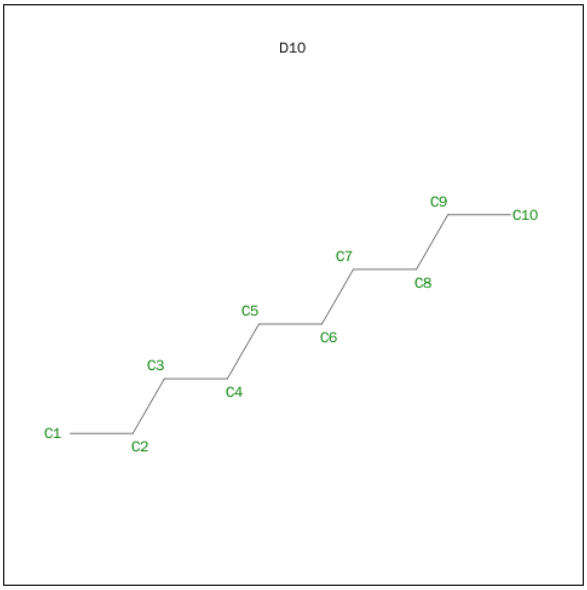
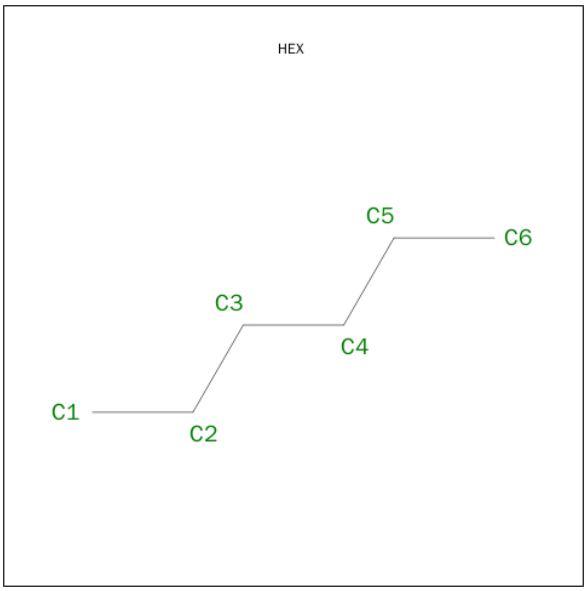
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C H 26 8 18	0	0

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



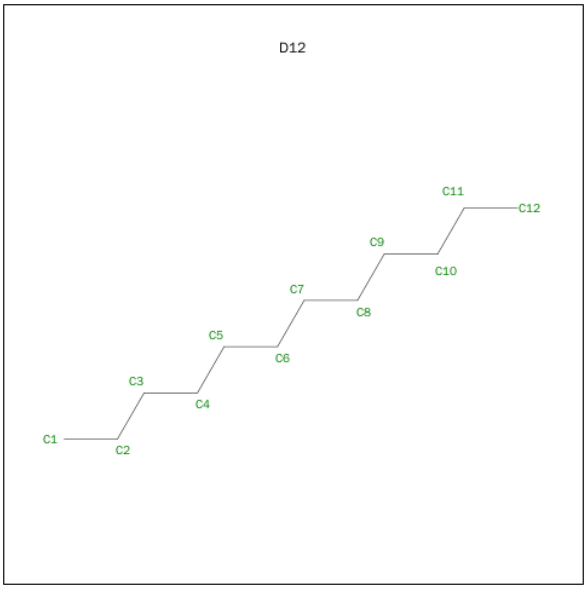
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0

- Molecule 7 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



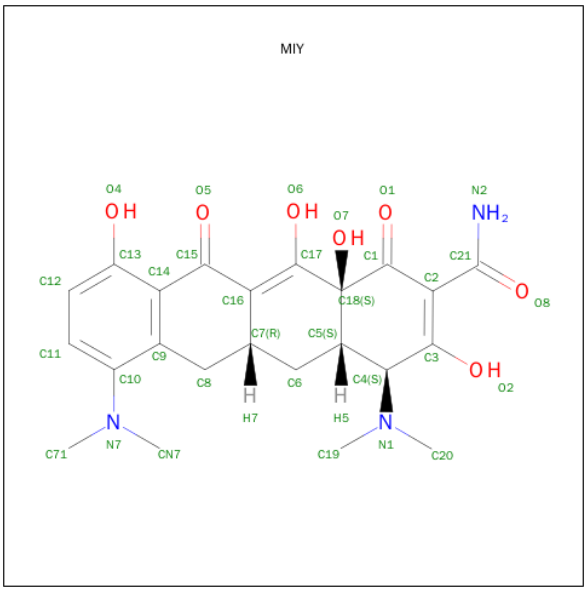
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H 20 6 14	0	0
7	B	1	Total C H 20 6 14	0	0
7	B	1	Total C H 20 6 14	0	0
7	C	1	Total C H 20 6 14	0	0
7	C	1	Total C H 20 6 14	0	0

- Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



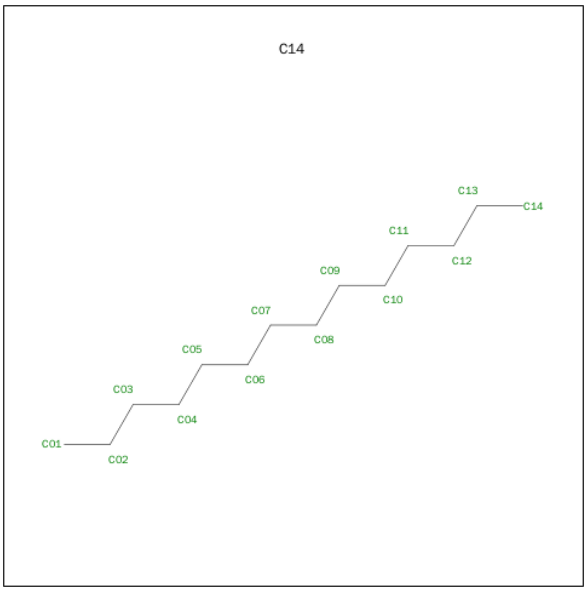
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H 38 12 26	0	0
8	B	1	Total C H 38 12 26	0	0
8	C	1	Total C H 38 12 26	0	0
8	C	1	Total C H 38 12 26	0	0

- Molecule 9 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: $C_{23}H_{27}N_3O_7$).



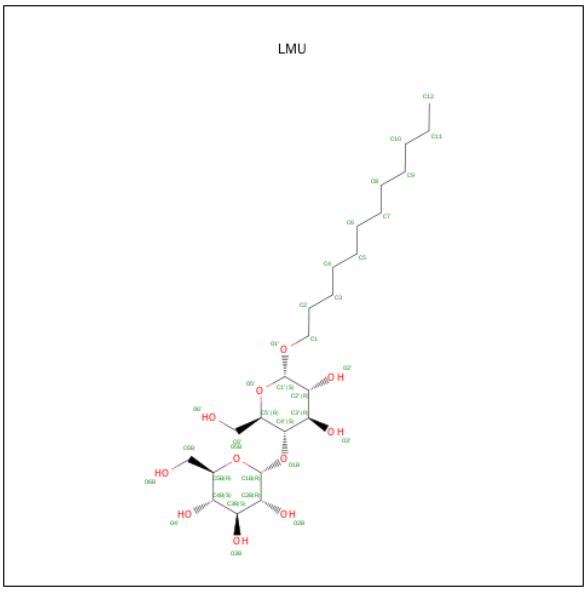
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C H N O 60 23 27 3 7	0	0

- Molecule 10 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



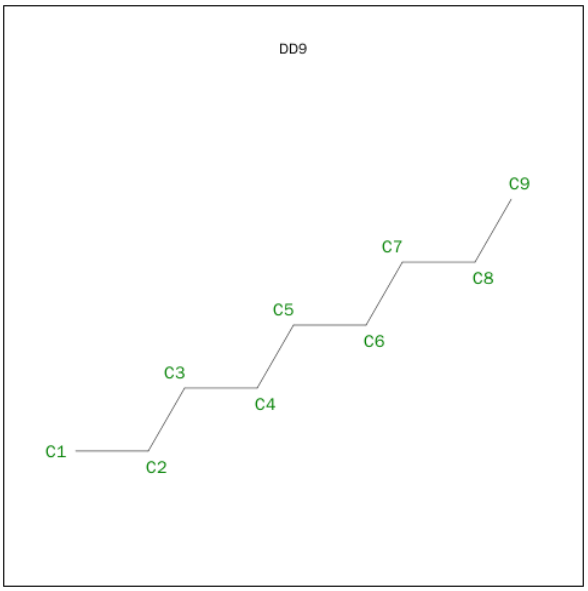
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H		0	0
			44	14	30			

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



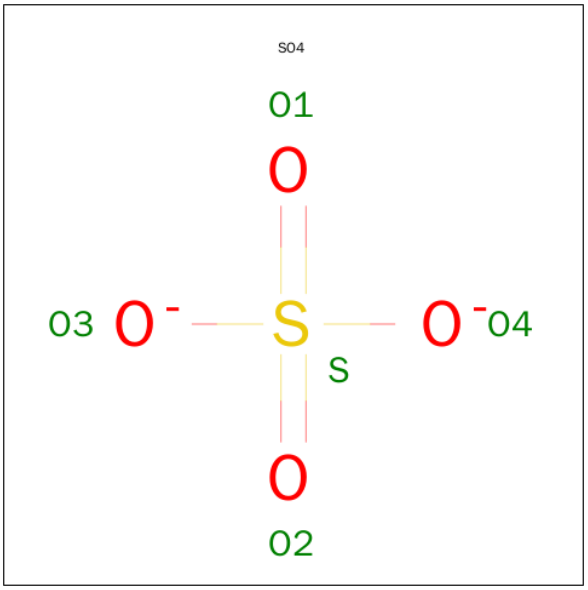
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 12 is NONANE (three-letter code: DD9) (formula: C_9H_{20}).



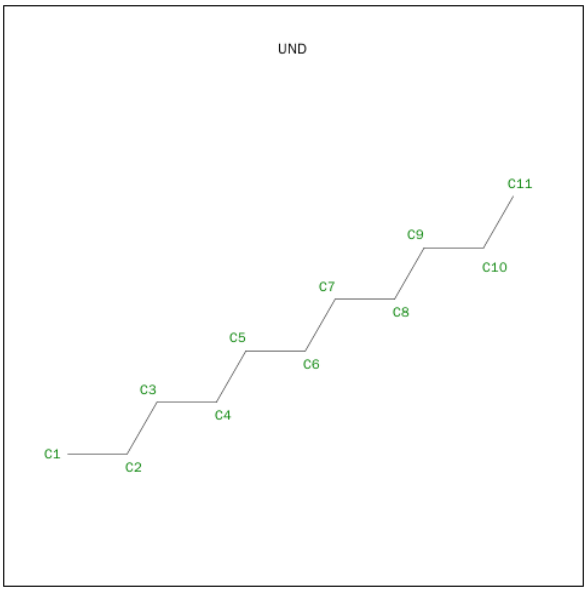
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C H 29 9 20	0	0

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total O S 5 4 1	0	0

- Molecule 14 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C H 35 11 24	0	0

- Molecule 15 is water.

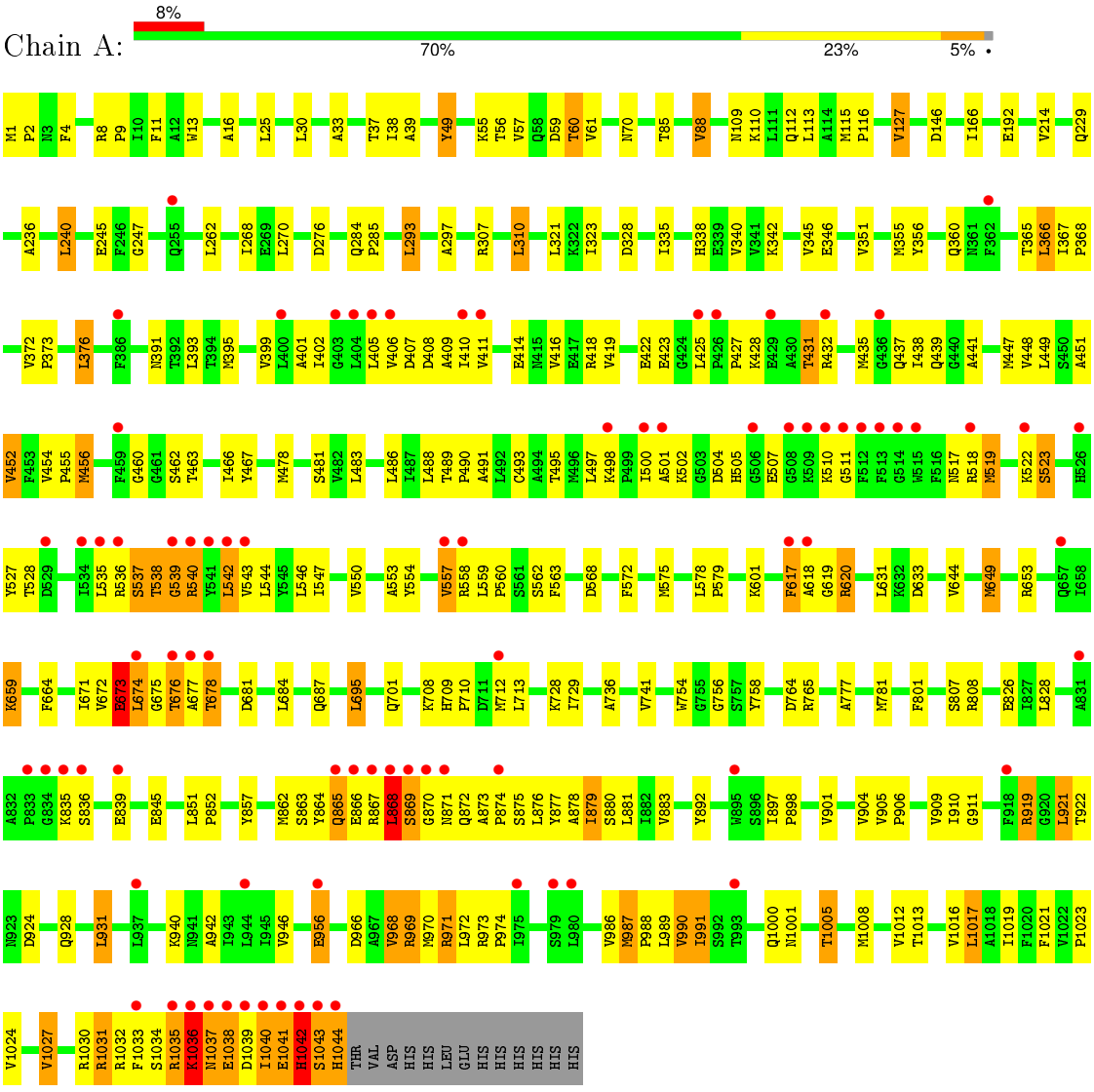
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	540	Total O 540 540	0	0
15	B	531	Total O 531 531	0	0
15	D	87	Total O 87 87	0	0
15	E	42	Total O 42 42	0	0
15	C	583	Total O 583 583	0	0

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 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.

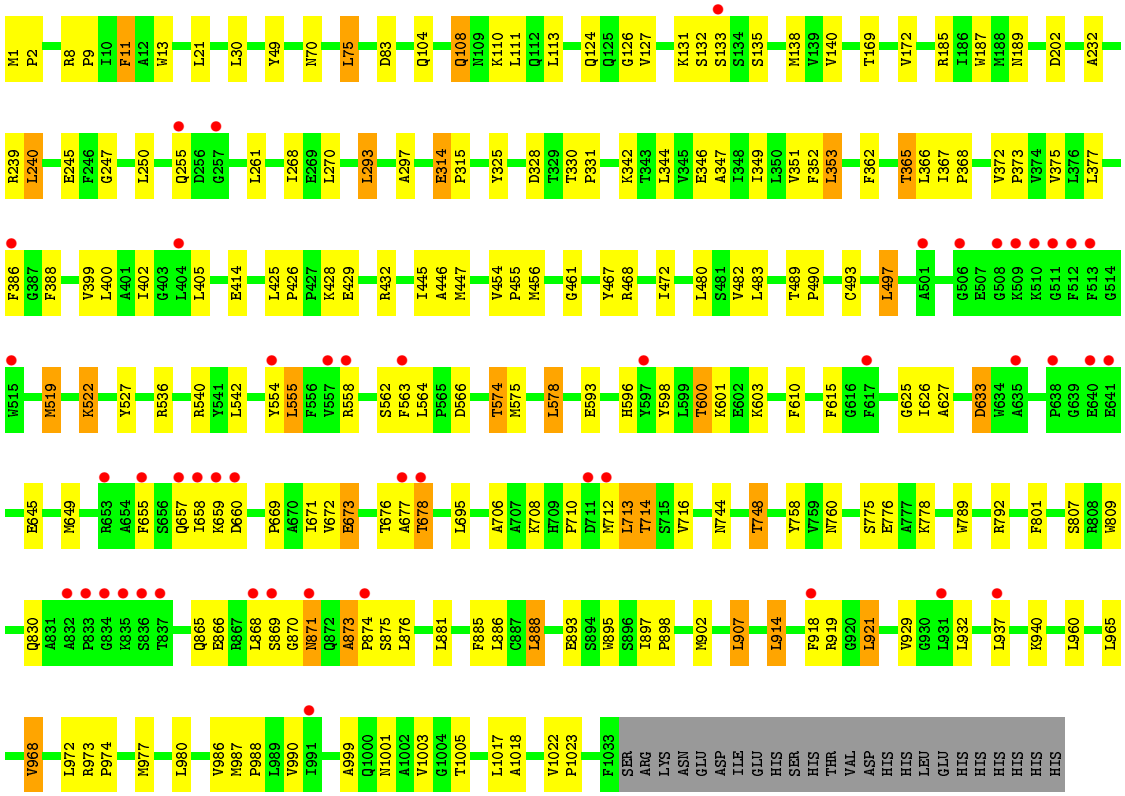
- Molecule 1: Acriflavine resistance protein B

Chain A:



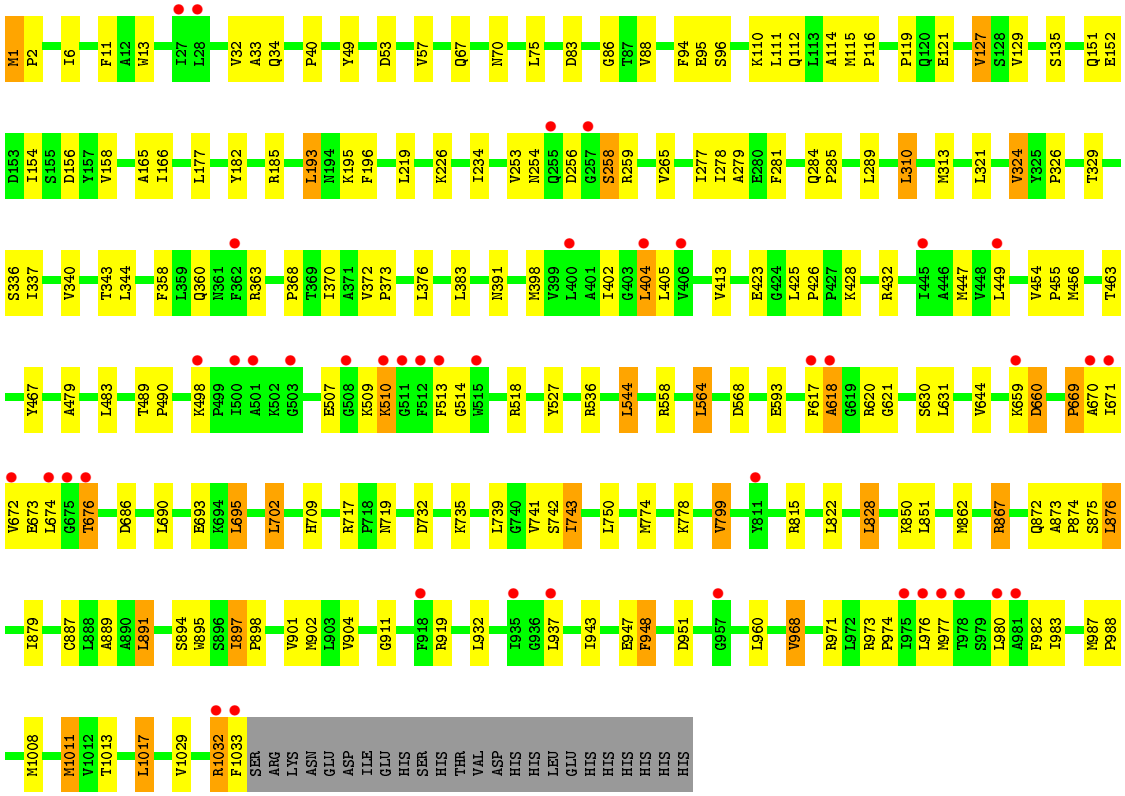
- Molecule 1: Acriflavine resistance protein B

Chain B:



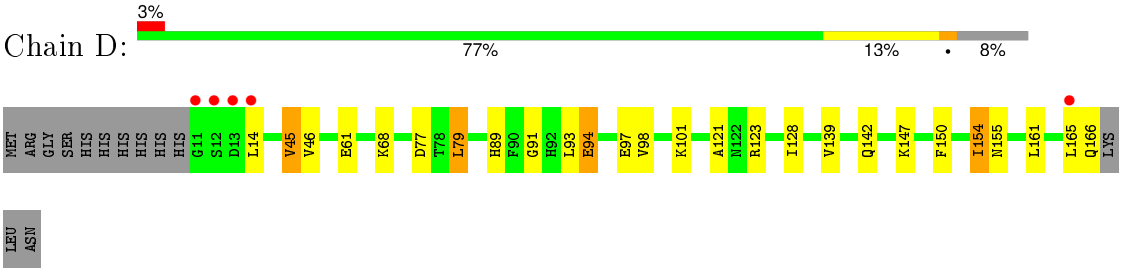
• Molecule 1: Acriflavine resistance protein B

Chain C:



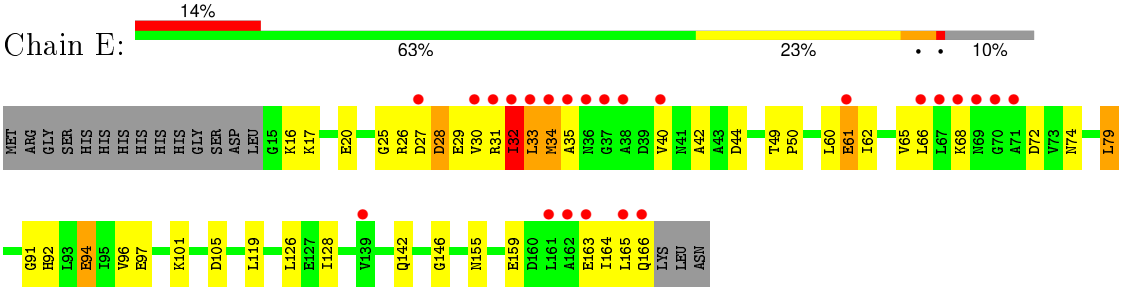
• Molecule 2: DARPIN

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	145.99Å 161.72Å 245.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.47 – 1.90 39.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.47-1.90) 99.4 (39.47-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.200 , 0.231 0.201 , 0.229	Depositor DCC
R_{free} test set	22550 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.6	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 451016 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29010	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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, DD9, D10, D12, LMT, HEX, LMU, MIY, UND, SO4, OCT, C14

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	0/8095	0.54	1/10991 (0.0%)
1	B	0.37	0/7999	0.53	0/10863
1	C	0.39	0/7999	0.55	0/10863
2	D	0.34	0/1196	0.48	0/1626
2	E	0.31	0/1170	0.46	0/1591
All	All	0.37	0/26459	0.53	1/35934 (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	-5.61	100.75	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	7943	0	8084	363	0
1	B	7849	0	8001	201	0
1	C	7849	0	8001	195	0
2	D	1177	0	1159	23	0
2	E	1151	0	1136	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	2	0
3	B	36	0	48	11	0
3	C	24	0	32	5	0
3	D	12	8	16	0	0
3	E	6	0	8	1	0
4	A	140	0	184	33	0
4	B	105	0	138	17	0
4	C	35	0	46	1	0
5	A	16	36	36	0	0
5	C	40	90	90	1	0
6	A	10	22	22	1	0
6	B	20	44	44	1	0
6	C	30	66	66	0	0
7	A	6	14	14	0	0
7	B	12	28	28	0	0
7	C	12	28	28	0	0
8	A	12	26	26	8	0
8	B	12	26	26	1	0
8	C	24	52	52	1	0
9	B	33	27	26	2	0
10	B	14	30	30	2	0
11	B	35	46	45	3	0
12	C	9	20	20	0	0
13	C	5	0	0	0	0
14	C	11	24	24	0	0
15	A	540	0	0	15	0
15	B	531	0	0	16	0
15	C	583	0	0	18	0
15	D	87	0	0	4	0
15	E	42	0	0	1	0
All	All	28423	587	27446	841	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 16.

All (841) 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:1040:ILE:CA	1:A:1041:GLU:HB2	1.68	1.18
1:B:414:GLU:HG3	1:B:977:MET:CE	1.76	1.16
1:A:1038:GLU:CB	1:A:1039:ASP:HA	1.74	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:GLU:N	2:D:94:GLU:OE2	1.82	1.12
1:A:971:ARG:HG3	1:A:971:ARG:HH11	0.99	1.11
1:A:1038:GLU:HB2	1:A:1039:ASP:HA	1.14	1.10
1:C:509:LYS:CA	1:C:510:LYS:HB2	1.80	1.09
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.29	1.09
1:A:1040:ILE:HG22	1:A:1041:GLU:CB	1.81	1.09
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.29	1.08
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.26	1.08
1:A:676:THR:H	1:A:862:MET:HE1	1.14	1.07
1:A:865:GLN:N	1:A:866:GLU:HB2	1.68	1.07
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.13	1.07
1:A:987:MET:HE1	1:A:1008:MET:SD	1.95	1.06
1:A:542:LEU:HD12	1:A:542:LEU:H	1.18	1.06
1:C:509:LYS:HA	1:C:510:LYS:HB2	1.06	1.05
1:A:1040:ILE:HA	1:A:1041:GLU:HB2	1.27	1.05
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.38	1.04
1:A:866:GLU:C	1:A:868:LEU:HB2	1.79	1.04
1:C:527:TYR:CE2	1:C:968:VAL:HG13	1.92	1.03
1:A:538:THR:HG22	1:A:539:GLY:H	1.19	1.03
1:C:70:ASN:O	1:C:110:LYS:NZ	1.90	1.03
1:A:618:ALA:H	1:A:619:GLY:HA2	1.23	1.03
1:B:414:GLU:CG	1:B:977:MET:HE1	1.88	1.03
1:A:672:VAL:HG23	1:A:673:GLU:H	1.20	1.03
1:A:538:THR:O	1:A:540:ARG:N	1.92	1.02
1:C:671:ILE:HD11	1:C:674:LEU:CD1	1.90	1.02
1:A:617:PHE:HD1	1:A:617:PHE:N	1.53	1.02
1:A:865:GLN:HA	1:A:868:LEU:HG	1.41	1.01
1:A:865:GLN:CA	1:A:868:LEU:HG	1.90	1.01
1:C:185:ARG:HH12	3:C:1115:GOL:H31	1.24	1.01
1:A:1040:ILE:CB	1:A:1041:GLU:HB2	1.90	1.01
4:B:1104:LMT:H5B	4:B:1104:LMT:H6E	1.44	1.00
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.39	0.99
1:B:885:PHE:HB2	1:B:902:MET:HE1	1.42	0.96
1:A:1035:ARG:HD2	1:A:1035:ARG:N	1.80	0.95
1:A:659:LYS:HD3	1:A:659:LYS:H	1.33	0.94
1:A:971:ARG:HG3	1:A:971:ARG:NH1	1.72	0.94
1:A:618:ALA:HB3	1:A:619:GLY:O	1.67	0.93
1:A:865:GLN:N	1:A:865:GLN:OE1	2.01	0.93
1:A:538:THR:HG22	1:A:539:GLY:N	1.80	0.93
1:C:423:GLU:HB2	1:C:425:LEU:HD13	1.50	0.92
1:A:1027:VAL:O	1:A:1031:ARG:HG2	1.66	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.34	0.92
1:A:867:ARG:N	1:A:868:LEU:HB2	1.84	0.91
1:A:1035:ARG:HD2	1:A:1035:ARG:H	1.32	0.91
1:A:1038:GLU:HB2	1:A:1039:ASP:CA	2.00	0.91
1:A:1040:ILE:CG2	1:A:1041:GLU:HB2	2.00	0.90
1:C:509:LYS:HA	1:C:510:LYS:CB	1.97	0.90
2:E:32:ILE:O	2:E:34:MET:N	2.05	0.89
2:E:32:ILE:O	2:E:35:ALA:N	2.04	0.89
1:B:919:ARG:NE	15:B:1353:HOH:O	2.04	0.89
1:A:1031:ARG:NH1	1:A:1039:ASP:OD2	2.06	0.89
1:A:868:LEU:O	1:A:869:SER:HB2	1.73	0.89
1:A:659:LYS:CD	1:A:659:LYS:H	1.82	0.88
1:A:1040:ILE:HG22	1:A:1041:GLU:HB2	1.55	0.87
2:D:123:ARG:NH1	15:D:338:HOH:O	2.06	0.87
1:A:971:ARG:CG	1:A:971:ARG:HH11	1.86	0.87
1:A:617:PHE:CD1	1:A:617:PHE:N	2.29	0.86
1:A:672:VAL:O	1:A:675:GLY:N	2.09	0.86
1:B:677:ALA:O	1:B:678:THR:HB	1.75	0.85
1:A:617:PHE:HD1	1:A:617:PHE:H	0.85	0.85
1:C:259:ARG:NH1	2:E:155:ASN:OD1	2.10	0.85
1:A:919:ARG:NH2	1:A:990:VAL:O	2.10	0.85
2:E:60:LEU:HD22	2:E:94:GLU:HG2	1.58	0.85
1:B:131:LYS:NZ	15:B:1633:HOH:O	2.09	0.84
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.35	0.84
1:B:885:PHE:CB	1:B:902:MET:HE1	2.06	0.84
1:B:1:MET:N	15:B:1286:HOH:O	2.10	0.84
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.06	0.84
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.07	0.84
1:A:1040:ILE:CG2	1:A:1041:GLU:CB	2.54	0.83
1:A:672:VAL:HG23	1:A:673:GLU:N	1.92	0.83
1:B:75:LEU:HD13	3:B:1101:GOL:H32	1.57	0.83
1:A:342:LYS:HD2	4:A:1109:LMT:H1'	1.59	0.83
1:A:881:LEU:HD22	4:A:1103:LMT:H122	1.61	0.83
1:A:1042:HIS:CD2	1:A:1043:SER:N	2.47	0.83
1:A:542:LEU:CD1	1:A:542:LEU:H	1.91	0.83
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.60	0.83
1:B:625:GLY:C	1:B:626:ILE:HD12	1.98	0.82
1:A:542:LEU:N	1:A:542:LEU:HD12	1.95	0.82
1:B:352:PHE:CE2	1:B:365:THR:HG21	2.13	0.82
1:B:748:THR:HG21	15:B:1499:HOH:O	1.79	0.82
1:A:987:MET:HA	1:A:987:MET:CE	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.60	0.81
1:A:1:MET:N	15:A:1630:HOH:O	2.13	0.81
1:C:509:LYS:CA	1:C:510:LYS:CB	2.56	0.81
2:E:34:MET:CE	2:E:40:VAL:HG12	2.10	0.81
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.62	0.80
1:A:1042:HIS:HD2	1:A:1043:SER:N	1.79	0.80
1:A:836:SER:OG	1:A:839:GLU:HG3	1.80	0.80
1:A:672:VAL:CG2	1:A:673:GLU:H	1.94	0.80
1:A:1012:VAL:O	1:A:1016:VAL:HG22	1.80	0.80
1:C:370:ILE:O	1:C:373:PRO:HD2	1.81	0.80
1:A:38:ILE:HD11	1:A:674:LEU:HD21	1.64	0.80
2:E:30:VAL:O	2:E:34:MET:HB2	1.82	0.79
1:A:1040:ILE:HG22	1:A:1041:GLU:CG	2.12	0.79
4:B:1110:LMT:H21	4:B:1110:LMT:O2'	1.83	0.79
1:A:729:ILE:HD11	1:C:234:ILE:CG2	2.13	0.79
1:B:873:ALA:CB	1:B:874:PRO:HD3	2.13	0.79
1:B:868:LEU:O	1:B:870:GLY:N	2.16	0.78
1:A:618:ALA:N	1:A:619:GLY:HA2	1.94	0.78
1:C:363:ARG:HH11	1:C:498:LYS:HE3	1.49	0.78
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.84	0.78
1:A:1038:GLU:CG	1:A:1039:ASP:HA	2.13	0.77
1:A:146:ASP:OD1	15:A:1501:HOH:O	2.01	0.77
1:A:538:THR:CG2	1:A:542:LEU:HD11	2.14	0.77
1:B:876:LEU:HD21	4:B:1110:LMT:H11	1.65	0.77
1:A:676:THR:O	1:A:678:THR:N	2.17	0.77
1:C:593:GLU:OE1	15:C:1684:HOH:O	2.02	0.76
1:A:659:LYS:HD3	1:A:659:LYS:N	1.99	0.76
2:D:94:GLU:CD	2:D:94:GLU:H	1.85	0.76
2:E:34:MET:CE	2:E:34:MET:HA	2.16	0.75
1:B:600:THR:HG22	1:B:601:LYS:N	2.00	0.75
1:B:990:VAL:O	15:B:1353:HOH:O	2.04	0.75
1:C:659:LYS:NZ	1:C:660:ASP:OD2	2.19	0.75
1:A:4:PHE:O	1:A:8:ARG:HD2	1.85	0.75
1:A:1040:ILE:CB	1:A:1041:GLU:CB	2.64	0.75
4:A:1102:LMT:H6'1	4:B:1110:LMT:O3B	1.85	0.75
2:D:45:VAL:HG22	15:D:351:HOH:O	1.86	0.74
1:A:535:LEU:HD22	1:A:1027:VAL:HG11	1.69	0.74
1:A:38:ILE:CD1	1:A:674:LEU:HD21	2.18	0.74
1:A:360:GLN:NE2	1:A:517:ASN:OD1	2.20	0.74
1:A:672:VAL:O	1:A:674:LEU:N	2.20	0.74
1:B:625:GLY:O	1:B:626:ILE:HD12	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LYS:CE	1:B:432:ARG:HH22	2.00	0.74
9:B:1103:MIY:HN72	9:B:1103:MIY:H81	1.69	0.74
1:A:538:THR:O	1:A:540:ARG:HG2	1.88	0.74
2:E:34:MET:HA	2:E:34:MET:HE3	1.69	0.74
1:B:633:ASP:OD1	1:B:633:ASP:N	2.20	0.73
1:A:537:SER:O	1:A:538:THR:HB	1.86	0.73
1:B:744:ASN:O	1:B:748:THR:HG23	1.86	0.73
1:B:873:ALA:HB3	1:B:874:PRO:CD	2.14	0.73
1:B:555:LEU:HD21	1:B:914:LEU:CD1	2.19	0.73
1:A:708:LYS:C	1:A:710:PRO:HD3	2.08	0.73
1:B:974:PRO:HA	1:B:977:MET:HE2	1.70	0.73
1:A:866:GLU:OE1	1:A:866:GLU:HA	1.88	0.73
1:A:865:GLN:HA	1:A:868:LEU:CG	2.19	0.72
1:A:504:ASP:O	1:A:505:HIS:ND1	2.14	0.72
1:A:507:GLU:HG2	1:A:518:ARG:HD3	1.70	0.72
1:C:321:LEU:O	15:C:1513:HOH:O	2.07	0.72
2:E:28:ASP:O	2:E:31:ARG:HB3	1.89	0.72
8:A:1111:D12:H111	1:B:447:MET:HG3	1.69	0.72
2:E:164:ILE:O	2:E:166:GLN:N	2.19	0.72
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.90	0.72
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.71	0.72
1:B:352:PHE:CE2	1:B:365:THR:CG2	2.72	0.72
1:A:527:TYR:CE2	1:A:968:VAL:HG13	2.25	0.72
1:A:546:LEU:O	1:A:550:VAL:HG23	1.88	0.72
1:A:1040:ILE:CA	1:A:1041:GLU:CB	2.58	0.72
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.72	0.72
1:A:1035:ARG:HA	1:A:1036:LYS:HE2	1.70	0.71
1:A:676:THR:N	1:A:862:MET:HE1	1.99	0.71
1:A:539:GLY:CA	1:A:542:LEU:HD13	2.20	0.71
1:C:867:ARG:NH1	1:C:867:ARG:HG2	2.05	0.71
1:C:115:MET:N	1:C:116:PRO:HD2	2.05	0.71
1:C:259:ARG:NH1	15:C:1437:HOH:O	2.19	0.71
1:A:342:LYS:CD	4:A:1109:LMT:H1'	2.20	0.71
1:C:135:SER:HB3	1:C:672:VAL:O	1.89	0.71
1:A:881:LEU:HD21	4:A:1103:LMT:H92	1.73	0.71
1:A:867:ARG:H	1:A:869:SER:H	1.39	0.71
1:A:987:MET:CE	1:A:1008:MET:SD	2.76	0.70
1:A:729:ILE:HD11	1:C:234:ILE:HG21	1.72	0.70
1:A:866:GLU:C	1:A:867:ARG:HG3	2.12	0.70
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.71	0.70
1:B:386:PHE:HB3	1:B:388:PHE:CE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:HIS:HB3	4:A:1109:LMT:H11	1.74	0.70
1:B:386:PHE:HB3	1:B:388:PHE:CD1	2.26	0.70
1:C:673:GLU:OE2	1:C:673:GLU:N	2.25	0.70
1:C:32:VAL:CG1	1:C:337:ILE:HD13	2.22	0.69
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.22	0.69
1:B:1018:ALA:O	1:B:1022:VAL:HG13	1.93	0.69
1:A:866:GLU:O	1:A:867:ARG:HG3	1.93	0.69
1:C:617:PHE:O	1:C:618:ALA:CB	2.40	0.69
1:A:881:LEU:CD2	4:A:1103:LMT:H122	2.21	0.69
1:A:942:ALA:O	1:A:946:VAL:HG13	1.92	0.69
1:B:522:LYS:HE3	1:B:522:LYS:HA	1.73	0.69
1:A:671:ILE:HG22	1:A:674:LEU:HD23	1.74	0.69
4:B:1111:LMT:H6'1	4:B:1111:LMT:O6'	1.92	0.69
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.71	0.68
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.29	0.68
1:A:968:VAL:CG2	1:A:1023:PRO:HG3	2.23	0.68
1:C:151:GLN:HG2	3:C:1117:GOL:O3	1.94	0.68
1:B:706:ALA:HB3	1:B:716:VAL:HG11	1.76	0.68
1:B:232:ALA:HA	3:B:1115:GOL:H31	1.75	0.68
1:A:519:MET:O	1:A:523:SER:OG	2.11	0.68
1:A:987:MET:HA	1:A:987:MET:HE2	1.76	0.67
1:C:151:GLN:NE2	1:C:279:ALA:O	2.27	0.67
1:A:866:GLU:O	1:A:868:LEU:HD23	1.93	0.67
1:C:671:ILE:H	1:C:862:MET:HE1	1.58	0.67
2:E:164:ILE:C	2:E:166:GLN:H	1.97	0.67
1:A:537:SER:HB3	1:A:540:ARG:HH11	1.60	0.67
4:B:1104:LMT:C5B	4:B:1104:LMT:H6E	2.21	0.67
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.24	0.67
2:E:60:LEU:CD2	2:E:94:GLU:HG2	2.25	0.67
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.78	0.66
1:A:504:ASP:C	1:A:505:HIS:HD1	1.98	0.66
1:A:553:ALA:O	1:A:557:VAL:HG12	1.95	0.66
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.77	0.66
1:A:866:GLU:C	1:A:867:ARG:CG	2.63	0.66
1:C:185:ARG:NH1	3:C:1115:GOL:H31	2.06	0.66
4:B:1111:LMT:O5B	4:B:1111:LMT:H5'	1.95	0.66
1:C:872:GLN:OE1	15:C:1449:HOH:O	2.12	0.66
1:A:676:THR:H	1:A:862:MET:CE	2.00	0.66
1:A:538:THR:HG23	1:A:542:LEU:HD11	1.77	0.66
2:E:25:GLY:HA2	2:E:62:ILE:CD1	2.25	0.66
2:E:44:ASP:OD2	3:E:201:GOL:O3	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ALA:O	1:A:495:THR:HG23	1.95	0.66
1:B:776:GLU:OE1	15:B:1321:HOH:O	2.13	0.66
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.78	0.66
1:A:192:GLU:OE1	15:A:1390:HOH:O	2.13	0.66
1:A:538:THR:HG22	1:A:542:LEU:HD11	1.78	0.66
1:C:671:ILE:CD1	1:C:674:LEU:CD1	2.73	0.65
1:A:276:ASP:OD2	1:A:620:ARG:NH1	2.29	0.65
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.77	0.65
1:C:57:VAL:HG11	1:C:88:VAL:HG23	1.78	0.65
1:C:95:GLU:OE2	15:C:1567:HOH:O	2.15	0.65
1:A:966:ASP:O	1:A:970:MET:HG3	1.96	0.65
1:C:671:ILE:HG13	1:C:674:LEU:HG	1.78	0.65
1:A:865:GLN:H	1:A:866:GLU:HB2	1.61	0.65
1:A:676:THR:HG23	1:A:862:MET:HE3	1.79	0.65
1:A:1040:ILE:HG22	1:A:1041:GLU:HG3	1.80	0.64
1:A:671:ILE:CG2	1:A:674:LEU:HD23	2.27	0.64
1:B:104:GLN:OE1	1:B:131:LYS:HD2	1.97	0.64
1:A:709:HIS:N	1:A:710:PRO:HD3	2.13	0.64
1:A:1040:ILE:HG22	1:A:1041:GLU:HB3	1.73	0.64
1:A:346:GLU:HG3	4:A:1109:LMT:H102	1.79	0.64
1:A:8:ARG:HH12	8:A:1111:D12:H13	1.62	0.63
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.80	0.63
1:C:669:PRO:HD2	15:C:1773:HOH:O	1.99	0.63
1:A:601:LYS:NZ	15:A:1324:HOH:O	2.31	0.63
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.79	0.63
1:B:596:HIS:O	1:B:600:THR:HB	1.98	0.63
15:B:1438:HOH:O	1:C:743:ILE:HD11	1.99	0.63
1:A:307:ARG:NE	15:A:1662:HOH:O	2.30	0.62
1:B:456:MET:CG	1:B:467:TYR:HB3	2.29	0.62
1:A:527:TYR:OH	1:A:1019:ILE:O	2.09	0.62
2:D:154:ILE:HG13	2:D:155:ASN:N	2.12	0.62
1:A:865:GLN:HA	1:A:866:GLU:O	1.99	0.62
1:C:447:MET:CE	1:C:891:LEU:HG	2.29	0.62
1:A:346:GLU:CG	4:A:1109:LMT:H102	2.30	0.62
1:A:365:THR:O	1:A:368:PRO:HD2	1.99	0.62
1:A:510:LYS:HD2	1:A:511:GLY:H	1.65	0.62
1:B:468:ARG:O	1:B:472:ILE:HD13	2.00	0.62
1:C:509:LYS:HB3	1:C:510:LYS:HB3	1.82	0.62
11:B:1114:LMU:O5'	11:B:1114:LMU:H21	1.98	0.62
1:A:423:GLU:OE2	1:A:425:LEU:HD11	2.00	0.62
1:C:509:LYS:CB	1:C:510:LYS:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:O	1:A:431:THR:HG23	2.00	0.61
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.82	0.61
1:A:507:GLU:HG2	1:A:518:ARG:CD	2.30	0.61
1:A:865:GLN:CB	1:A:868:LEU:HG	2.30	0.61
1:A:881:LEU:HD13	4:A:1103:LMT:H122	1.82	0.61
1:A:8:ARG:NH1	8:A:1111:D12:H13	2.15	0.61
1:A:70:ASN:O	1:A:110:LYS:HE3	2.00	0.61
1:A:1040:ILE:HA	1:A:1041:GLU:CB	2.17	0.61
1:B:108:GLN:CG	1:C:112:GLN:HG3	2.19	0.61
1:C:671:ILE:HG13	1:C:671:ILE:O	2.01	0.61
4:A:1102:LMT:O6'	4:A:1102:LMT:O5B	2.18	0.61
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.81	0.61
1:A:563:PHE:O	1:A:924:ASP:HB2	2.00	0.61
1:B:974:PRO:HA	1:B:977:MET:CE	2.30	0.61
1:A:987:MET:HA	1:A:987:MET:HE3	1.82	0.61
1:B:885:PHE:CD1	1:B:902:MET:HE1	2.36	0.61
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.33	0.61
1:A:867:ARG:N	1:A:869:SER:H	1.97	0.61
1:B:540:ARG:NH2	4:B:1104:LMT:H6'1	2.16	0.61
1:A:342:LYS:HE3	4:A:1109:LMT:H92	1.83	0.61
1:A:1042:HIS:CD2	1:A:1042:HIS:C	2.73	0.61
1:A:537:SER:HB3	1:A:540:ARG:HD2	1.83	0.60
1:A:649:MET:HE3	1:A:653:ARG:NH1	2.16	0.60
1:B:973:ARG:O	1:B:977:MET:HG3	2.01	0.60
1:B:600:THR:CG2	1:B:601:LYS:N	2.64	0.60
1:A:701:GLN:OE1	15:A:1598:HOH:O	2.16	0.60
1:A:956:GLU:OE2	1:A:956:GLU:CA	2.48	0.60
2:D:89:HIS:CD2	2:D:123:ARG:HD3	2.36	0.60
1:B:247:GLY:HA2	1:B:268:ILE:HD12	1.83	0.60
1:C:815:ARG:NH2	15:C:1329:HOH:O	2.34	0.60
1:A:868:LEU:HD22	1:A:868:LEU:N	2.17	0.60
1:B:428:LYS:CE	1:B:432:ARG:NH2	2.65	0.60
1:B:809:TRP:NE1	2:D:79:LEU:HD22	2.16	0.60
1:B:428:LYS:HE3	1:B:432:ARG:HH22	1.65	0.60
1:C:617:PHE:O	1:C:618:ALA:HB2	2.01	0.60
1:A:1037:ASN:O	1:A:1038:GLU:HB3	2.02	0.59
1:A:463:THR:HG23	1:A:467:TYR:HE2	1.67	0.59
2:E:163:GLU:O	2:E:166:GLN:HB2	2.02	0.59
2:E:68:LYS:O	2:E:68:LYS:HG2	2.00	0.59
1:B:135:SER:OG	15:B:1652:HOH:O	2.16	0.59
1:A:971:ARG:NH1	15:A:1735:HOH:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.32	0.59
1:A:49:TYR:HE2	1:A:60:THR:HG21	1.67	0.59
1:A:987:MET:HE3	1:A:987:MET:CA	2.32	0.59
1:B:677:ALA:O	1:B:678:THR:CB	2.49	0.59
1:A:342:LYS:HD2	4:A:1109:LMT:C1'	2.32	0.59
1:C:336:SER:O	1:C:340:VAL:HG23	2.03	0.59
1:A:575:MET:SD	1:A:664:PHE:CE1	2.96	0.59
1:A:676:THR:HG23	1:A:862:MET:CE	2.33	0.59
1:A:538:THR:CG2	1:A:539:GLY:N	2.54	0.58
2:E:34:MET:HE1	2:E:40:VAL:CG1	2.26	0.58
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.23	0.58
4:B:1110:LMT:O2'	4:B:1110:LMT:C2	2.51	0.58
1:A:863:SER:HA	1:A:866:GLU:HG3	1.84	0.58
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.85	0.58
1:C:671:ILE:HG12	1:C:862:MET:SD	2.44	0.58
1:C:815:ARG:NE	15:C:1329:HOH:O	2.04	0.58
1:C:509:LYS:O	1:C:514:GLY:HA3	2.03	0.58
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.86	0.58
1:C:111:LEU:HD21	1:C:127:VAL:HG22	1.84	0.58
1:A:500:ILE:O	15:A:1731:HOH:O	2.17	0.58
1:B:429:GLU:OE1	15:B:1581:HOH:O	2.16	0.58
1:B:352:PHE:HE2	1:B:365:THR:HG21	1.67	0.58
1:A:989:LEU:HD23	1:A:1000:GLN:OE1	2.03	0.58
1:A:868:LEU:N	1:A:868:LEU:CD2	2.66	0.58
1:A:987:MET:CA	1:A:987:MET:CE	2.82	0.58
1:A:971:ARG:HG3	15:A:1735:HOH:O	2.03	0.57
1:B:555:LEU:HD21	1:B:914:LEU:HD13	1.85	0.57
1:A:562:SER:OG	1:A:922:THR:HG21	2.04	0.57
1:A:8:ARG:HH12	8:A:1111:D12:C1	2.18	0.57
1:A:510:LYS:HD2	1:A:511:GLY:N	2.19	0.57
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.24	0.57
1:B:428:LYS:HE2	1:B:432:ARG:NH1	2.19	0.57
1:B:873:ALA:O	1:B:876:LEU:N	2.37	0.57
1:A:360:GLN:HE22	1:A:517:ASN:CG	2.06	0.57
4:A:1102:LMT:H6'1	4:B:1110:LMT:C3B	2.35	0.57
1:B:536:ARG:NH2	15:B:1522:HOH:O	2.37	0.57
1:B:676:THR:HB	1:B:678:THR:HG22	1.86	0.57
1:A:877:TYR:O	1:A:881:LEU:HD23	2.05	0.57
1:C:670:ALA:HB3	1:C:862:MET:HE1	1.85	0.57
1:C:111:LEU:HD21	1:C:127:VAL:CG2	2.35	0.57
1:C:875:SER:O	1:C:879:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:ARG:O	1:C:974:PRO:HD2	2.05	0.57
1:B:645:GLU:OE1	1:B:649:MET:HE1	2.05	0.57
1:A:672:VAL:HG23	1:A:673:GLU:CD	2.26	0.56
1:A:539:GLY:HA2	1:A:542:LEU:HD13	1.88	0.56
2:E:32:ILE:O	2:E:33:LEU:C	2.43	0.56
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.88	0.56
1:A:435:MET:O	1:A:439:GLN:HB3	2.06	0.56
1:A:862:MET:HG2	15:A:1417:HOH:O	2.04	0.56
1:C:527:TYR:CE2	1:C:968:VAL:CG1	2.79	0.56
1:A:870:GLY:HA3	4:A:1103:LMT:O3B	2.06	0.56
1:A:901:VAL:O	1:A:904:VAL:HG22	2.05	0.56
1:C:358:PHE:CG	1:C:977:MET:HG2	2.41	0.56
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.87	0.56
1:C:111:LEU:CD2	1:C:129:VAL:CG2	2.84	0.56
1:C:509:LYS:CB	1:C:510:LYS:CB	2.85	0.55
1:B:885:PHE:HA	1:B:902:MET:HE2	1.86	0.55
1:A:868:LEU:O	1:A:869:SER:CB	2.51	0.55
1:B:461:GLY:HA3	1:B:865:GLN:OE1	2.06	0.55
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.88	0.55
2:E:27:ASP:OD2	2:E:61:GLU:HB3	2.06	0.55
1:A:1035:ARG:N	1:A:1035:ARG:CD	2.53	0.55
1:C:671:ILE:CD1	1:C:674:LEU:HG	2.36	0.55
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.88	0.55
1:A:956:GLU:N	1:A:956:GLU:OE2	2.40	0.55
1:A:402:ILE:O	1:A:406:VAL:HG12	2.05	0.55
4:A:1102:LMT:O4'	4:B:1110:LMT:H3B	2.05	0.55
1:A:527:TYR:HE2	1:A:968:VAL:HG13	1.68	0.55
1:B:428:LYS:HE2	1:B:432:ARG:HH12	1.69	0.55
1:C:620:ARG:NH1	15:C:1722:HOH:O	2.25	0.55
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.86	0.55
1:C:67:GLN:OE1	15:C:1673:HOH:O	2.18	0.55
1:C:670:ALA:HB3	1:C:862:MET:CE	2.37	0.55
1:A:928:GLN:HG2	4:A:1103:LMT:H22	1.88	0.55
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.06	0.55
1:B:885:PHE:HD1	1:B:902:MET:CE	2.20	0.55
4:A:1103:LMT:O3'	4:A:1103:LMT:H1B	2.06	0.54
1:A:401:ALA:O	1:A:405:LEU:HG	2.06	0.54
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.87	0.54
2:E:72:ASP:OD2	15:E:339:HOH:O	2.18	0.54
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.89	0.54
1:B:428:LYS:HE2	1:B:432:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1111:LMT:H3'	4:B:1111:LMT:O2B	2.06	0.54
1:A:729:ILE:CD1	1:C:234:ILE:CG2	2.84	0.54
1:B:240:LEU:HG	1:B:245:GLU:HB3	1.90	0.54
2:D:98:VAL:HA	2:D:101:LYS:HE2	1.90	0.54
1:A:675:GLY:HA3	1:A:862:MET:HE2	1.89	0.54
3:B:1116:GOL:H2	1:C:119:PRO:HA	1.89	0.54
1:C:33:ALA:O	1:C:391:ASN:HA	2.08	0.54
1:C:702:LEU:HG	1:C:851:LEU:HD11	1.89	0.54
1:C:898:PRO:O	1:C:902:MET:HG2	2.07	0.54
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.10	0.54
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.88	0.54
2:D:165:LEU:C	2:D:166:GLN:HG2	2.27	0.54
1:B:671:ILE:HG22	1:B:673:GLU:HG2	1.88	0.54
1:B:973:ARG:HG2	1:B:977:MET:CE	2.37	0.54
1:A:538:THR:O	1:A:539:GLY:C	2.46	0.54
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.38	0.54
1:A:971:ARG:NH2	15:A:1736:HOH:O	2.36	0.54
1:A:881:LEU:CD1	4:A:1103:LMT:H122	2.37	0.54
1:B:428:LYS:HE2	1:B:432:ARG:HH22	1.73	0.54
1:B:472:ILE:N	1:B:472:ILE:HD12	2.23	0.54
1:C:971:ARG:C	1:C:974:PRO:HD2	2.27	0.54
1:C:226:LYS:NZ	15:C:1560:HOH:O	2.41	0.54
1:C:360:GLN:HG2	1:C:513:PHE:CD1	2.43	0.54
2:E:49:THR:HB	2:E:50:PRO:HD2	1.90	0.54
1:A:881:LEU:HD13	4:A:1103:LMT:C12	2.38	0.53
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.74	0.53
1:B:239:ARG:HH21	3:B:1116:GOL:H11	1.73	0.53
1:A:1038:GLU:OE1	1:A:1039:ASP:HA	2.08	0.53
1:C:423:GLU:HB3	1:C:425:LEU:HD13	1.87	0.53
1:A:968:VAL:HG21	1:A:1023:PRO:CG	2.34	0.53
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.90	0.53
2:E:16:LYS:O	2:E:20:GLU:HG3	2.08	0.53
1:A:1035:ARG:O	1:A:1036:LYS:C	2.47	0.53
1:B:615:PHE:O	1:B:626:ILE:HD13	2.08	0.53
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.91	0.53
1:B:645:GLU:O	1:B:649:MET:HG3	2.09	0.53
1:A:240:LEU:HG	1:A:245:GLU:HB3	1.91	0.53
1:B:562:SER:HA	1:B:677:ALA:HB3	1.91	0.53
1:C:151:GLN:OE1	1:C:278:ILE:HG23	2.09	0.53
2:E:42:ALA:O	2:E:50:PRO:HD3	2.09	0.53
2:D:165:LEU:O	2:D:166:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1110:LMT:H21	4:B:1110:LMT:H2O2	1.74	0.52
1:A:729:ILE:HD11	1:C:234:ILE:HG23	1.87	0.52
1:B:974:PRO:CA	1:B:977:MET:HE2	2.36	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.91	0.52
1:A:345:VAL:HG21	4:A:1109:LMT:H61	1.89	0.52
3:B:1116:GOL:O1	3:B:1116:GOL:O3	2.27	0.52
1:B:807:SER:OG	3:B:1113:GOL:H31	2.09	0.52
1:A:57:VAL:CG1	1:A:88:VAL:CG2	2.83	0.52
1:A:633:ASP:OD2	4:A:1109:LMT:O4'	2.26	0.52
1:B:352:PHE:CD2	1:B:365:THR:HG23	2.44	0.52
1:A:85:THR:O	1:A:85:THR:HG22	2.08	0.52
1:A:865:GLN:CA	1:A:866:GLU:HB2	2.38	0.52
4:B:1111:LMT:C5'	4:B:1111:LMT:O5B	2.57	0.52
2:D:150:PHE:O	2:D:154:ILE:HG23	2.08	0.52
1:A:423:GLU:HB2	1:A:425:LEU:HG	1.92	0.52
1:A:1037:ASN:O	1:A:1038:GLU:CB	2.58	0.52
1:A:674:LEU:CD2	1:A:674:LEU:N	2.72	0.52
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.39	0.52
1:C:447:MET:HE3	1:C:891:LEU:HG	1.92	0.52
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.90	0.52
1:C:428:LYS:NZ	1:C:432:ARG:HH21	2.08	0.52
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.09	0.52
1:A:543:VAL:O	1:A:547:ILE:HG12	2.10	0.52
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.36	0.52
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.93	0.52
1:B:428:LYS:HE3	1:B:432:ARG:NH2	2.23	0.51
1:C:617:PHE:CD2	1:C:676:THR:HG21	2.46	0.51
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.92	0.51
1:B:645:GLU:HG2	1:B:649:MET:CE	2.40	0.51
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.39	0.51
1:C:40:PRO:HB2	1:C:94:PHE:O	2.11	0.51
1:A:672:VAL:C	1:A:674:LEU:N	2.64	0.51
9:B:1103:MIY:HN72	9:B:1103:MIY:C8	2.40	0.51
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.92	0.51
1:C:193:LEU:HD13	1:C:265:VAL:HB	1.92	0.51
2:E:92:HIS:O	2:E:96:VAL:HG23	2.10	0.51
1:B:885:PHE:HA	1:B:902:MET:CE	2.40	0.51
1:A:1042:HIS:O	1:A:1043:SER:CB	2.58	0.51
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.41	0.51
1:C:115:MET:N	1:C:116:PRO:CD	2.74	0.51
1:C:324:VAL:HG12	1:C:326:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:NE2	15:C:1648:HOH:O	2.44	0.51
1:C:671:ILE:CG1	1:C:671:ILE:O	2.58	0.51
1:A:672:VAL:CG2	1:A:673:GLU:N	2.61	0.51
1:C:447:MET:HE1	1:C:891:LEU:HG	1.93	0.51
2:D:46:VAL:O	2:D:77:ASP:HB2	2.10	0.51
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.10	0.51
1:C:1011:MET:HA	1:C:1011:MET:CE	2.41	0.51
1:B:13:TRP:CD1	10:B:1109:C14:H051	2.46	0.51
1:A:537:SER:O	1:A:538:THR:CB	2.54	0.51
2:E:26:ARG:O	2:E:30:VAL:HG23	2.11	0.51
1:C:423:GLU:HB3	1:C:425:LEU:CD1	2.41	0.51
1:B:328:ASP:O	1:B:331:PRO:HD2	2.10	0.51
1:B:400:LEU:HD13	1:B:929:VAL:HG12	1.93	0.51
1:B:542:LEU:N	1:B:542:LEU:HD23	2.26	0.51
1:B:493:CYS:HA	1:B:497:LEU:HD22	1.92	0.51
1:C:509:LYS:HB3	1:C:510:LYS:CB	2.40	0.51
1:C:943:ILE:O	1:C:947:GLU:HB3	2.11	0.51
1:B:555:LEU:CD2	1:B:914:LEU:HD13	2.41	0.51
1:C:741:VAL:CG1	1:C:799:VAL:HG11	2.41	0.51
1:B:672:VAL:HG22	1:B:673:GLU:OE2	2.11	0.50
1:C:671:ILE:N	1:C:862:MET:HE1	2.26	0.50
2:D:94:GLU:HG2	15:D:347:HOH:O	2.11	0.50
1:A:881:LEU:CD2	4:A:1103:LMT:H92	2.41	0.50
1:A:422:GLU:C	1:A:423:GLU:HG3	2.32	0.50
1:A:376:LEU:HD13	1:A:405:LEU:CD1	2.41	0.50
1:A:862:MET:O	1:A:866:GLU:HG2	2.10	0.50
2:E:31:ARG:HH12	2:E:65:VAL:HG22	1.76	0.50
2:E:164:ILE:C	2:E:166:GLN:N	2.62	0.50
1:C:671:ILE:CG1	1:C:674:LEU:HG	2.41	0.50
2:E:28:ASP:O	2:E:31:ARG:CB	2.57	0.50
2:D:121:ALA:HB1	2:D:161:LEU:HD21	1.94	0.50
1:A:13:TRP:NE1	6:A:1107:D10:H32	2.27	0.50
1:B:362:PHE:O	1:B:365:THR:HG22	2.12	0.50
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.42	0.50
1:C:709:HIS:HE1	15:C:1731:HOH:O	1.94	0.50
1:A:8:ARG:HH22	8:A:1111:D12:C1	2.24	0.50
1:C:428:LYS:NZ	1:C:432:ARG:NH2	2.59	0.50
1:B:871:ASN:ND2	1:B:871:ASN:O	2.41	0.50
15:A:1655:HOH:O	2:D:154:ILE:HD11	2.11	0.50
2:E:74:ASN:HD21	2:E:105:ASP:HB2	1.77	0.49
1:C:1032:ARG:HG3	1:C:1032:ARG:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ILE:HD11	1:C:674:LEU:CG	2.41	0.49
1:A:39:ALA:HB2	1:A:673:GLU:HG3	1.93	0.49
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.74	0.49
1:A:49:TYR:CE2	1:A:60:THR:HG21	2.46	0.49
1:A:865:GLN:C	1:A:868:LEU:HG	2.32	0.49
1:A:284:GLN:HB2	1:A:285:PRO:HD2	1.94	0.49
1:C:536:ARG:HH21	4:C:1102:LMT:C3B	2.25	0.49
1:A:431:THR:O	1:A:435:MET:HG2	2.13	0.49
1:B:897:ILE:N	1:B:898:PRO:CD	2.75	0.49
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.47	0.49
1:A:897:ILE:N	1:A:898:PRO:CD	2.76	0.49
1:A:376:LEU:HD13	1:A:405:LEU:HD12	1.94	0.49
1:C:152:GLU:CD	1:C:152:GLU:H	2.15	0.49
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.94	0.49
2:E:163:GLU:HG3	2:E:164:ILE:N	2.28	0.49
1:A:712:MET:SD	1:A:835:LYS:HD2	2.53	0.49
3:C:1101:GOL:O1	3:C:1101:GOL:O3	2.14	0.49
1:B:138:MET:CE	1:B:140:VAL:HG22	2.43	0.49
1:A:428:LYS:O	1:A:432:ARG:HG3	2.13	0.49
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.95	0.49
2:E:97:GLU:O	2:E:101:LYS:HG3	2.13	0.49
1:A:676:THR:C	1:A:678:THR:H	2.15	0.49
1:A:1001:ASN:O	1:A:1005:THR:CG2	2.59	0.49
1:A:454:VAL:N	1:A:455:PRO:CD	2.76	0.49
1:C:281:PHE:CE1	1:C:324:VAL:HG11	2.47	0.48
1:A:865:GLN:CD	1:A:865:GLN:N	2.67	0.48
1:A:539:GLY:C	1:A:542:LEU:HD13	2.34	0.48
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.95	0.48
15:B:1683:HOH:O	1:C:70:ASN:HB2	2.12	0.48
1:B:352:PHE:CE2	1:B:365:THR:HG23	2.48	0.48
1:B:400:LEU:HD13	1:B:929:VAL:CG1	2.43	0.48
1:B:133:SER:HA	15:B:1724:HOH:O	2.13	0.48
1:A:1:MET:CA	15:A:1630:HOH:O	2.60	0.48
10:B:1109:C14:H052	1:C:895:TRP:HE1	1.79	0.48
1:C:617:PHE:CE2	1:C:676:THR:HG21	2.48	0.48
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.43	0.48
1:C:621:GLY:N	15:C:1227:HOH:O	2.28	0.48
1:B:600:THR:HG22	1:B:601:LYS:H	1.77	0.48
1:A:355:MET:CE	1:A:410:ILE:HD11	2.44	0.48
1:A:33:ALA:O	1:A:391:ASN:HA	2.14	0.48
1:C:732:ASP:OD2	1:C:735:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:MET:HE2	1:B:447:MET:HA	1.95	0.47
1:B:716:VAL:HG13	1:B:716:VAL:O	2.14	0.47
1:C:983:ILE:HG13	1:C:1011:MET:HG2	1.96	0.47
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.49	0.47
1:A:493:CYS:O	1:A:497:LEU:HB2	2.13	0.47
4:A:1104:LMT:O3'	4:A:1104:LMT:H1B	2.13	0.47
1:B:375:VAL:CG1	1:B:405:LEU:HD13	2.44	0.47
4:A:1102:LMT:C4B	4:B:1110:LMT:H3B	2.45	0.47
1:A:866:GLU:OE1	1:A:866:GLU:CA	2.58	0.47
1:A:546:LEU:HD23	1:A:546:LEU:N	2.29	0.47
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.96	0.47
1:C:489:THR:HB	1:C:490:PRO:HD3	1.95	0.47
1:A:418:ARG:CZ	1:A:970:MET:CE	2.92	0.47
1:A:1043:SER:HA	1:A:1044:HIS:HA	1.49	0.47
1:A:405:LEU:N	1:A:405:LEU:HD23	2.28	0.47
1:A:544:LEU:HD12	1:A:544:LEU:O	2.14	0.47
1:A:1044:HIS:C	1:A:1044:HIS:ND1	2.67	0.47
1:A:418:ARG:CZ	1:A:970:MET:HE2	2.45	0.47
1:A:214:VAL:HG22	1:A:236:ALA:HB3	1.96	0.47
1:C:405:LEU:HD12	1:C:405:LEU:C	2.34	0.47
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.97	0.47
1:A:987:MET:N	1:A:988:PRO:CD	2.78	0.47
1:A:507:GLU:OE1	1:A:518:ARG:NH1	2.44	0.47
1:A:865:GLN:HB2	1:A:868:LEU:HG	1.96	0.47
4:A:1109:LMT:O2B	4:A:1109:LMT:H4'	2.13	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.47
2:D:68:LYS:NZ	15:D:350:HOH:O	2.11	0.47
1:C:404:LEU:HD11	1:C:937:LEU:CD2	2.44	0.47
1:C:329:THR:HB	15:C:1558:HOH:O	2.15	0.47
1:A:1038:GLU:CD	1:A:1039:ASP:HA	2.33	0.46
1:C:659:LYS:NZ	1:C:660:ASP:HB2	2.30	0.46
1:A:649:MET:HE1	1:A:653:ARG:CZ	2.45	0.46
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.97	0.46
1:C:987:MET:CG	1:C:1008:MET:HE1	2.46	0.46
1:A:1035:ARG:CA	1:A:1036:LYS:HE2	2.40	0.46
1:C:564:LEU:HD23	1:C:670:ALA:HB1	1.97	0.46
1:C:156:ASP:OD1	1:C:182:TYR:HB2	2.15	0.46
1:B:919:ARG:HB3	1:B:921:LEU:HD22	1.96	0.46
1:B:669:PRO:HD3	11:B:1114:LMU:O6'	2.15	0.46
1:C:428:LYS:HZ1	1:C:432:ARG:NH2	2.13	0.46
1:B:127:VAL:N	3:B:1102:GOL:O1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:LYS:O	1:A:1037:ASN:OD1	2.33	0.46
1:A:1042:HIS:HD2	1:A:1043:SER:CA	2.27	0.46
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.74	0.46
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.96	0.46
2:E:49:THR:HB	2:E:50:PRO:CD	2.45	0.46
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.96	0.46
1:B:563:PHE:CE2	1:B:677:ALA:HB2	2.51	0.46
1:A:649:MET:CE	1:A:653:ARG:NH1	2.79	0.46
1:C:1011:MET:HE3	1:C:1011:MET:HA	1.97	0.46
1:B:138:MET:HE3	1:B:325:TYR:HD2	1.80	0.46
1:C:778:LYS:NZ	15:C:1454:HOH:O	2.49	0.46
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.46
1:B:563:PHE:CE2	1:B:677:ALA:N	2.84	0.46
1:C:895:TRP:C	1:C:898:PRO:HD2	2.36	0.46
1:B:247:GLY:CA	1:B:268:ILE:HD12	2.45	0.46
1:B:673:GLU:CD	1:B:673:GLU:H	2.17	0.46
1:C:947:GLU:HG3	1:C:948:PHE:N	2.31	0.46
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.97	0.46
1:B:999:ALA:O	1:B:1003:VAL:HG13	2.15	0.46
1:C:901:VAL:O	1:C:904:VAL:HG12	2.16	0.46
1:A:764:ASP:OD1	1:A:765:ARG:HD3	2.16	0.46
1:A:864:TYR:C	1:A:866:GLU:HB2	2.33	0.46
1:C:895:TRP:CD2	5:C:1103:OCT:H13	2.51	0.46
1:C:360:GLN:HG2	1:C:513:PHE:CE1	2.51	0.46
1:C:281:PHE:CZ	1:C:324:VAL:HG11	2.51	0.46
1:B:375:VAL:HG11	1:B:405:LEU:HD13	1.97	0.46
1:B:554:TYR:O	1:B:558:ARG:HG3	2.15	0.46
2:E:34:MET:CE	2:E:40:VAL:CG1	2.88	0.46
1:A:356:TYR:HA	1:A:365:THR:HG21	1.98	0.46
1:A:463:THR:HG23	1:A:467:TYR:CE2	2.50	0.46
1:C:111:LEU:HD23	1:C:129:VAL:CG2	2.46	0.46
1:C:195:LYS:HE3	1:C:196:PHE:CZ	2.51	0.46
1:A:393:LEU:HD11	1:A:466:ILE:HG13	1.98	0.46
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.97	0.46
1:A:554:TYR:CZ	1:A:558:ARG:HD2	2.51	0.45
1:A:1031:ARG:O	1:A:1033:PHE:N	2.49	0.45
1:A:55:LYS:NZ	1:A:59:ASP:OD2	2.47	0.45
1:B:11:PHE:O	1:B:11:PHE:HD1	1.98	0.45
1:B:386:PHE:HB3	1:B:388:PHE:HE1	1.78	0.45
1:B:428:LYS:HE2	1:B:432:ARG:CZ	2.47	0.45
1:C:32:VAL:HG12	1:C:337:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:SER:O	1:A:879:ILE:HG23	2.15	0.45
1:A:987:MET:N	1:A:988:PRO:HD2	2.31	0.45
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.45
1:A:910:ILE:HG23	1:A:911:GLY:N	2.31	0.45
2:D:93:LEU:HB3	2:D:94:GLU:OE2	2.17	0.45
1:A:408:ASP:OD1	1:A:940:LYS:NZ	2.39	0.45
1:A:1040:ILE:CG2	1:A:1041:GLU:HB3	2.40	0.45
1:A:672:VAL:CG2	1:A:673:GLU:CD	2.84	0.45
1:C:659:LYS:NZ	1:C:660:ASP:CG	2.69	0.45
1:A:956:GLU:HA	1:A:956:GLU:OE2	2.14	0.45
1:A:1030:ARG:O	1:A:1034:SER:HB3	2.16	0.45
1:B:655:PHE:C	1:B:657:GLN:H	2.20	0.45
1:B:426:PRO:HD2	1:B:429:GLU:CG	2.46	0.45
1:B:138:MET:HE3	1:B:325:TYR:CD2	2.52	0.45
1:A:537:SER:HB2	1:A:538:THR:H	1.47	0.45
1:B:447:MET:CE	1:B:447:MET:HA	2.46	0.45
1:C:114:ALA:C	1:C:116:PRO:HD2	2.38	0.45
1:A:449:LEU:O	1:A:452:VAL:HG13	2.16	0.45
1:C:774:MET:SD	3:C:1115:GOL:O3	2.75	0.44
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.99	0.44
1:B:564:LEU:CD1	1:B:671:ILE:HD12	2.47	0.44
1:A:346:GLU:HG2	4:A:1109:LMT:H122	1.99	0.44
1:A:892:TYR:CZ	1:A:946:VAL:HG22	2.53	0.44
1:A:416:VAL:O	1:A:419:VAL:HB	2.17	0.44
1:A:372:VAL:HB	1:A:373:PRO:CD	2.47	0.44
1:C:479:ALA:O	1:C:483:LEU:HD23	2.17	0.44
2:E:32:ILE:C	2:E:34:MET:N	2.69	0.44
1:C:977:MET:HE2	1:C:977:MET:HB3	1.89	0.44
4:A:1104:LMT:H5B	4:A:1104:LMT:O6'	2.18	0.44
1:B:426:PRO:HB2	1:B:429:GLU:OE1	2.17	0.44
1:B:645:GLU:OE1	1:B:649:MET:CE	2.65	0.44
2:E:17:LYS:HA	2:E:17:LYS:HD2	1.59	0.44
1:B:75:LEU:HD13	3:B:1101:GOL:C3	2.39	0.44
1:A:712:MET:HA	1:A:835:LYS:HG3	1.98	0.44
1:C:195:LYS:HE3	1:C:196:PHE:CE2	2.52	0.44
1:A:16:ALA:HB2	1:A:488:LEU:HD22	2.00	0.44
1:C:671:ILE:CD1	1:C:674:LEU:CG	2.96	0.44
1:A:881:LEU:CD1	4:A:1103:LMT:C12	2.96	0.44
1:C:889:ALA:HA	1:C:894:SER:O	2.18	0.44
1:B:127:VAL:H	3:B:1102:GOL:C1	2.29	0.44
1:C:376:LEU:HD11	1:C:402:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ARG:HA	2:E:79:LEU:HD23	2.00	0.44
1:C:894:SER:O	1:C:898:PRO:HG2	2.17	0.44
1:B:187:TRP:HB3	1:B:776:GLU:HG3	1.98	0.44
1:B:349:ILE:O	1:B:353:LEU:HD22	2.17	0.44
1:C:897:ILE:CD1	1:C:897:ILE:N	2.81	0.44
1:B:708:LYS:C	1:B:710:PRO:HD3	2.38	0.44
1:A:127:VAL:HG22	1:B:113:LEU:HD22	1.99	0.44
1:C:876:LEU:CD1	1:C:932:LEU:HD11	2.48	0.44
1:A:1030:ARG:NE	1:A:1030:ARG:HA	2.33	0.44
4:B:1110:LMT:O5B	4:B:1110:LMT:H6D	2.17	0.43
1:A:38:ILE:HD12	1:A:674:LEU:HD21	1.97	0.43
2:E:32:ILE:HD13	2:E:32:ILE:N	2.33	0.43
1:C:32:VAL:HG12	1:C:337:ILE:HD13	1.97	0.43
1:A:728:LYS:O	1:A:807:SER:HA	2.18	0.43
1:C:254:ASN:N	1:C:258:SER:O	2.39	0.43
1:B:519:MET:SD	1:B:519:MET:C	2.97	0.43
1:B:873:ALA:CB	1:B:874:PRO:CD	2.81	0.43
1:A:57:VAL:HG11	1:A:88:VAL:HG22	1.94	0.43
1:C:719:ASN:HB2	1:C:828:LEU:HD22	1.99	0.43
1:A:489:THR:N	1:A:490:PRO:CD	2.81	0.43
1:B:885:PHE:CG	1:B:902:MET:HE1	2.54	0.43
4:A:1109:LMT:H4B	4:A:1109:LMT:H1B	1.57	0.43
1:A:56:THR:O	1:A:60:THR:HB	2.18	0.43
1:B:593:GLU:OE2	1:B:658:ILE:HD13	2.17	0.43
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.70	0.43
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.98	0.43
1:A:537:SER:CB	1:A:540:ARG:HH11	2.26	0.43
1:A:8:ARG:NH2	8:A:1111:D12:H13	2.33	0.43
3:B:1116:GOL:H12	15:B:1469:HOH:O	2.17	0.43
1:B:8:ARG:HH11	1:B:8:ARG:HG3	1.84	0.43
1:A:909:VAL:HA	1:A:931:LEU:HD21	2.00	0.43
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.18	0.43
1:A:368:PRO:HA	1:A:409:ALA:HB1	2.00	0.43
1:B:987:MET:N	1:B:988:PRO:CD	2.81	0.43
1:A:687:GLN:NE2	15:A:1616:HOH:O	2.51	0.43
1:B:536:ARG:NH1	4:B:1104:LMT:O2B	2.51	0.43
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.19	0.43
1:A:879:ILE:HD12	1:A:883:VAL:HG23	1.99	0.43
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.71	0.43
1:A:528:THR:CG2	1:A:969:ARG:HB3	2.49	0.43
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:O	1:A:112:GLN:HG3	2.18	0.43
1:B:885:PHE:CZ	8:B:1106:D12:H112	2.54	0.43
1:A:681:ASP:OD1	1:A:826:GLU:OE1	2.36	0.43
1:A:991:ILE:HG23	1:A:991:ILE:O	2.17	0.43
1:B:489:THR:HG21	15:B:1728:HOH:O	2.19	0.43
1:A:1038:GLU:CB	1:A:1039:ASP:CA	2.62	0.43
4:A:1102:LMT:C5B	4:A:1102:LMT:H6'	2.30	0.43
1:A:671:ILE:O	1:A:674:LEU:HB2	2.19	0.43
1:B:973:ARG:HG2	1:B:977:MET:HE2	2.00	0.42
1:A:672:VAL:C	1:A:674:LEU:H	2.21	0.42
1:A:1:MET:N	1:A:2:PRO:CD	2.82	0.42
1:A:554:TYR:OH	1:A:558:ARG:NE	2.51	0.42
1:C:398:MET:O	1:C:402:ILE:HG12	2.18	0.42
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.84	0.42
1:B:885:PHE:HB2	1:B:902:MET:CE	2.31	0.42
1:C:1013:THR:HB	1:C:1017:LEU:HD22	2.00	0.42
1:A:372:VAL:HB	1:A:373:PRO:HD3	2.00	0.42
1:C:57:VAL:HG11	1:C:88:VAL:CG2	2.44	0.42
1:C:463:THR:CG2	1:C:467:TYR:CZ	3.02	0.42
1:A:1038:GLU:HB2	1:A:1040:ILE:O	2.20	0.42
1:A:672:VAL:HG23	1:A:673:GLU:OE2	2.19	0.42
1:B:809:TRP:CD1	2:D:79:LEU:HD22	2.54	0.42
1:A:684:LEU:HD23	1:A:695:LEU:HD22	2.01	0.42
1:C:509:LYS:HG2	1:C:510:LYS:HE3	2.00	0.42
1:B:600:THR:HG22	1:B:601:LYS:HD3	2.01	0.42
1:B:776:GLU:HB3	15:B:1321:HOH:O	2.19	0.42
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.39	0.42
1:A:9:PRO:HD2	1:B:893:GLU:OE1	2.19	0.42
1:B:895:TRP:CD1	6:B:1105:D10:H32	2.55	0.42
1:C:121:GLU:HB2	15:C:1336:HOH:O	2.19	0.42
1:A:879:ILE:HG13	1:A:880:SER:N	2.34	0.42
1:B:655:PHE:C	1:B:657:GLN:N	2.72	0.42
1:B:314:GLU:N	1:B:315:PRO:CD	2.83	0.42
2:E:32:ILE:HB	2:E:33:LEU:H	1.49	0.42
1:A:500:ILE:N	15:A:1731:HOH:O	2.53	0.42
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.49	0.42
2:E:142:GLN:HB3	2:E:146:GLY:HA2	2.00	0.42
1:B:578:LEU:HD23	1:B:578:LEU:N	2.35	0.42
1:C:1029:VAL:O	1:C:1033:PHE:HD2	2.02	0.42
1:A:892:TYR:OH	1:A:946:VAL:HG22	2.19	0.42
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:SER:N	15:B:1652:HOH:O	2.50	0.42
1:C:193:LEU:CD1	1:C:265:VAL:HB	2.49	0.42
1:A:736:ALA:HA	1:A:741:VAL:HG22	2.01	0.42
1:B:564:LEU:HD12	1:B:671:ILE:HD12	2.01	0.42
2:D:91:GLY:HA2	2:D:128:ILE:HD12	2.02	0.42
1:C:165:ALA:HB3	1:C:313:MET:CE	2.50	0.42
1:A:758:TYR:OH	3:A:1101:GOL:O3	2.33	0.42
4:A:1109:LMT:H2B	4:A:1109:LMT:C6'	2.50	0.42
1:B:575:MET:HE1	1:B:626:ILE:HD11	2.01	0.42
1:B:866:GLU:C	1:B:868:LEU:N	2.72	0.42
1:B:645:GLU:CD	1:B:649:MET:HE1	2.39	0.42
1:A:351:VAL:O	1:A:355:MET:HG2	2.20	0.42
1:B:124:GLN:HG2	1:B:758:TYR:CE2	2.55	0.42
1:A:777:ALA:O	1:A:781:MET:HG2	2.20	0.42
1:A:867:ARG:HA	1:A:869:SER:N	2.34	0.41
2:E:31:ARG:HH12	2:E:65:VAL:CG2	2.32	0.41
1:B:330:THR:N	1:B:331:PRO:CD	2.83	0.41
1:A:489:THR:HB	1:A:490:PRO:HD3	2.01	0.41
2:D:14:LEU:HD23	2:D:14:LEU:HA	1.79	0.41
1:C:447:MET:SD	1:C:887:CYS:HB3	2.61	0.41
1:A:416:VAL:HG22	1:A:431:THR:HA	2.01	0.41
1:C:456:MET:HG3	1:C:467:TYR:HB3	2.02	0.41
1:B:446:ALA:HB2	1:B:482:VAL:HG21	2.02	0.41
1:A:673:GLU:H	1:A:673:GLU:CD	2.23	0.41
1:A:539:GLY:N	1:A:542:LEU:CD1	2.84	0.41
1:C:425:LEU:HA	1:C:426:PRO:HD3	1.91	0.41
1:A:986:VAL:O	1:A:989:LEU:HB2	2.20	0.41
2:E:74:ASN:ND2	2:E:105:ASP:HB2	2.35	0.41
1:A:8:ARG:HH22	8:A:1111:D12:H13	1.85	0.41
1:C:873:ALA:N	1:C:874:PRO:CD	2.83	0.41
1:B:347:ALA:O	1:B:351:VAL:HG23	2.19	0.41
1:B:907:LEU:HG	1:B:1017:LEU:HB3	2.02	0.41
1:B:932:LEU:HA	1:B:932:LEU:HD23	1.89	0.41
1:C:544:LEU:HA	1:C:544:LEU:HD12	1.70	0.41
1:A:865:GLN:O	1:A:865:GLN:CG	2.69	0.41
2:E:31:ARG:O	2:E:32:ILE:O	2.38	0.41
1:B:744:ASN:O	1:B:748:THR:CG2	2.63	0.41
1:B:566:ASP:OD1	11:B:1114:LMU:O6B	2.38	0.41
1:C:404:LEU:HD13	1:C:982:PHE:CD1	2.55	0.41
1:A:875:SER:O	1:A:878:ALA:HB3	2.20	0.41
1:A:8:ARG:CZ	8:A:1111:D12:H13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:GLN:HA	2:D:147:LYS:O	2.20	0.41
1:A:845:GLU:HG2	1:A:857:TYR:CZ	2.55	0.41
1:A:578:LEU:HB3	1:A:579:PRO:HD2	2.03	0.41
1:B:575:MET:CE	1:B:626:ILE:HD11	2.51	0.41
1:C:277:ILE:C	1:C:278:ILE:HG13	2.40	0.41
1:B:760:ASN:HB2	3:B:1116:GOL:O1	2.21	0.41
1:A:449:LEU:HD23	1:A:478:MET:SD	2.60	0.41
1:A:448:VAL:O	1:A:451:ALA:HB3	2.21	0.41
1:C:154:ILE:O	1:C:158:VAL:HG23	2.20	0.41
1:A:38:ILE:HD11	1:A:674:LEU:CD2	2.42	0.41
1:B:885:PHE:CD1	1:B:902:MET:CE	3.00	0.41
1:A:709:HIS:N	1:A:710:PRO:CD	2.80	0.41
1:B:888:LEU:HB3	1:B:898:PRO:HB3	2.03	0.41
1:A:372:VAL:N	1:A:373:PRO:HD2	2.35	0.41
1:C:376:LEU:HD11	1:C:402:ILE:HD11	2.02	0.41
1:B:8:ARG:N	1:B:9:PRO:CD	2.84	0.41
1:B:342:LYS:HD3	1:B:346:GLU:OE2	2.20	0.41
1:A:407:ASP:O	1:A:411:VAL:HG23	2.20	0.41
1:A:1040:ILE:H	1:A:1040:ILE:HG12	1.51	0.41
1:A:674:LEU:HD23	1:A:674:LEU:N	2.36	0.41
1:B:426:PRO:HD2	1:B:429:GLU:HG3	2.03	0.41
1:C:2:PRO:O	1:C:6:ILE:HG13	2.21	0.41
1:B:189:ASN:OD1	1:B:189:ASN:C	2.58	0.41
1:B:70:ASN:O	1:B:110:LYS:HE3	2.21	0.41
1:A:438:ILE:O	1:A:441:ALA:N	2.53	0.41
1:C:368:PRO:HD3	1:C:413:VAL:HG21	2.02	0.41
1:B:83:ASP:C	1:B:83:ASP:OD1	2.59	0.41
1:C:83:ASP:OD1	1:C:83:ASP:C	2.58	0.41
2:D:93:LEU:O	2:D:97:GLU:HG3	2.21	0.41
1:A:335:ILE:HG23	4:A:1109:LMT:H6D	2.03	0.41
1:A:575:MET:SD	1:A:664:PHE:CZ	3.14	0.41
1:B:169:THR:O	1:B:172:VAL:HG13	2.21	0.41
1:A:921:LEU:HA	1:A:921:LEU:HD12	1.83	0.41
1:A:501:ALA:O	1:A:502:LYS:C	2.58	0.41
1:B:489:THR:N	1:B:490:PRO:CD	2.84	0.40
1:C:507:GLU:HG2	1:C:518:ARG:HG2	2.02	0.40
1:C:919:ARG:NH2	15:C:1637:HOH:O	2.55	0.40
1:A:1038:GLU:CG	1:A:1039:ASP:CA	2.94	0.40
1:C:53:ASP:O	1:C:57:VAL:HG23	2.22	0.40
1:C:111:LEU:HD23	1:C:129:VAL:HG21	2.04	0.40
1:A:897:ILE:N	1:A:898:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLY:HA3	3:A:1110:GOL:H32	2.03	0.40
1:A:115:MET:HB2	1:A:116:PRO:HD3	2.03	0.40
2:E:62:ILE:O	2:E:66:LEU:HG	2.20	0.40
1:B:386:PHE:HB3	1:B:388:PHE:HD1	1.77	0.40
1:A:456:MET:HE2	1:A:467:TYR:CD1	2.56	0.40
1:C:326:PRO:O	1:C:630:SER:HB2	2.21	0.40
1:C:404:LEU:HG	1:C:449:LEU:HD13	2.04	0.40
1:B:454:VAL:N	1:B:455:PRO:CD	2.84	0.40
1:C:13:TRP:NE1	8:C:1104:D12:H92	2.37	0.40
1:B:352:PHE:HE2	1:B:365:THR:CG2	2.25	0.40
1:B:712:MET:HG3	1:B:713:LEU:HD13	2.03	0.40
1:A:460:GLY:N	1:A:872:GLN:HE22	2.18	0.40
1:B:918:PHE:CD1	1:B:918:PHE:C	2.94	0.40
1:A:538:THR:CG2	1:A:539:GLY:H	2.00	0.40
1:B:126:GLY:CA	1:C:116:PRO:HB3	2.51	0.40
1:C:111:LEU:HD22	1:C:129:VAL:HG22	2.03	0.40
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.95	0.40
1:A:876:LEU:HA	1:A:876:LEU:HD23	1.90	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	1042/1057 (99%)	986 (95%)	40 (4%)	16 (2%)	13 3
1	B	1031/1057 (98%)	1004 (97%)	22 (2%)	5 (0%)	34 21
1	C	1031/1057 (98%)	1002 (97%)	26 (2%)	3 (0%)	46 35
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100 100
2	E	150/169 (89%)	145 (97%)	2 (1%)	3 (2%)	9 2
All	All	3408/3509 (97%)	3289 (96%)	92 (3%)	27 (1%)	24 11

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	539	GLY
1	A	673	GLU
1	A	677	ALA
1	A	1036	LYS
1	A	1038	GLU
1	A	1043	SER
1	B	659	LYS
1	B	869	SER
1	C	510	LYS
1	C	618	ALA
2	E	32	ILE
2	E	33	LEU
2	E	165	LEU
1	A	620	ARG
1	A	869	SER
1	A	1032	ARG
1	A	1041	GLU
1	A	1042	HIS
1	B	678	THR
1	B	873	ALA
1	A	871	ASN
1	A	1031	ARG
1	A	1037	ASN
1	B	603	LYS
1	A	868	LEU
1	C	669	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	850/863 (98%)	783 (92%)	67 (8%)	15 6
1	B	839/863 (97%)	785 (94%)	54 (6%)	22 10
1	C	839/863 (97%)	791 (94%)	48 (6%)	25 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	120/132 (91%)	114 (95%)	6 (5%)	30 18
2	E	117/132 (89%)	107 (92%)	10 (8%)	13 5
All	All	2765/2853 (97%)	2580 (93%)	185 (7%)	20 9

All (185) 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	127	VAL
1	A	229	GLN
1	A	240	LEU
1	A	262	LEU
1	A	270	LEU
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	366	LEU
1	A	376	LEU
1	A	431	THR
1	A	437	GLN
1	A	447	MET
1	A	452	VAL
1	A	456	MET
1	A	462	SER
1	A	483	LEU
1	A	486	LEU
1	A	498	LYS
1	A	519	MET
1	A	522	LYS
1	A	523	SER
1	A	536	ARG
1	A	537	SER
1	A	540	ARG
1	A	542	LEU
1	A	557	VAL

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Mol	Chain	Res	Type
1	A	617	PHE
1	A	649	MET
1	A	659	LYS
1	A	673	GLU
1	A	674	LEU
1	A	676	THR
1	A	678	THR
1	A	695	LEU
1	A	713	LEU
1	A	801	PHE
1	A	828	LEU
1	A	865	GLN
1	A	868	LEU
1	A	879	ILE
1	A	919	ARG
1	A	921	LEU
1	A	931	LEU
1	A	956	GLU
1	A	968	VAL
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	987	MET
1	A	990	VAL
1	A	991	ILE
1	A	1005	THR
1	A	1017	LEU
1	A	1027	VAL
1	A	1035	ARG
1	A	1036	LYS
1	A	1040	ILE
1	A	1042	HIS
1	A	1044	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	132	SER
1	B	240	LEU

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Mol	Chain	Res	Type
1	B	250	LEU
1	B	255	GLN
1	B	261	LEU
1	B	270	LEU
1	B	293	LEU
1	B	314	GLU
1	B	353	LEU
1	B	365	THR
1	B	366	LEU
1	B	377	LEU
1	B	399	VAL
1	B	480	LEU
1	B	483	LEU
1	B	497	LEU
1	B	519	MET
1	B	522	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	660	ASP
1	B	673	GLU
1	B	695	LEU
1	B	713	LEU
1	B	714	THR
1	B	748	THR
1	B	778	LYS
1	B	801	PHE
1	B	871	ASN
1	B	875	SER
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	907	LEU
1	B	914	LEU
1	B	921	LEU
1	B	937	LEU
1	B	960	LEU
1	B	965	LEU
1	B	968	VAL

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Mol	Chain	Res	Type
1	B	972	LEU
1	B	980	LEU
1	B	986	VAL
1	C	1	MET
1	C	11	PHE
1	C	49	TYR
1	C	75	LEU
1	C	96	SER
1	C	127	VAL
1	C	177	LEU
1	C	193	LEU
1	C	253	VAL
1	C	256	ASP
1	C	258	SER
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	544	LEU
1	C	558	ARG
1	C	564	LEU
1	C	660	ASP
1	C	676	THR
1	C	690	LEU
1	C	693	GLU
1	C	695	LEU
1	C	702	LEU
1	C	717	ARG
1	C	739	LEU
1	C	742	SER
1	C	743	ILE
1	C	750	LEU
1	C	799	VAL
1	C	822	LEU
1	C	828	LEU
1	C	850	LYS
1	C	867	ARG
1	C	876	LEU
1	C	891	LEU
1	C	897	ILE

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Mol	Chain	Res	Type
1	C	948	PHE
1	C	951	ASP
1	C	960	LEU
1	C	968	VAL
1	C	976	LEU
1	C	980	LEU
1	C	1011	MET
1	C	1017	LEU
1	C	1032	ARG
2	D	45	VAL
2	D	61	GLU
2	D	79	LEU
2	D	94	GLU
2	D	139	VAL
2	D	154	ILE
2	E	28	ASP
2	E	29	GLU
2	E	32	ILE
2	E	34	MET
2	E	61	GLU
2	E	79	LEU
2	E	94	GLU
2	E	119	LEU
2	E	126	LEU
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	A	1042	HIS
1	B	274	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)

51 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	GOL	A	1101	-	5,5,5	0.26	0	5,5,5	0.57	0
4	LMT	A	1102	-	36,36,36	1.15	3 (8%)	47,47,47	1.48	9 (19%)
4	LMT	A	1103	-	36,36,36	1.16	3 (8%)	47,47,47	1.14	2 (4%)
4	LMT	A	1104	-	36,36,36	1.20	3 (8%)	47,47,47	1.12	4 (8%)
5	OCT	A	1105	-	7,7,7	0.34	0	6,6,6	0.80	0
5	OCT	A	1106	-	7,7,7	0.22	0	6,6,6	0.61	0
6	D10	A	1107	-	9,9,9	0.25	0	8,8,8	0.70	0
7	HEX	A	1108	-	5,5,5	0.23	0	4,4,4	0.68	0
4	LMT	A	1109	-	36,36,36	1.11	3 (8%)	47,47,47	1.54	11 (23%)
3	GOL	A	1110	-	5,5,5	0.35	0	5,5,5	0.67	0
8	D12	A	1111	-	11,11,11	0.42	0	10,10,10	1.10	0
3	GOL	B	1101	-	5,5,5	0.29	0	5,5,5	0.32	0
3	GOL	B	1102	-	5,5,5	0.37	0	5,5,5	0.30	0
9	MIY	B	1103	-	35,36,36	3.28	17 (48%)	40,58,58	2.28	14 (35%)
4	LMT	B	1104	-	36,36,36	1.13	3 (8%)	47,47,47	1.26	4 (8%)
6	D10	B	1105	-	9,9,9	0.35	0	8,8,8	0.90	0
8	D12	B	1106	-	11,11,11	0.22	0	10,10,10	0.73	0
6	D10	B	1107	-	9,9,9	0.31	0	8,8,8	0.95	0
7	HEX	B	1108	-	5,5,5	0.25	0	4,4,4	0.60	0
10	C14	B	1109	-	13,13,13	0.27	0	12,12,12	0.93	0
4	LMT	B	1110	-	36,36,36	1.20	3 (8%)	47,47,47	1.38	7 (14%)
4	LMT	B	1111	-	36,36,36	1.17	3 (8%)	47,47,47	1.05	3 (6%)
7	HEX	B	1112	-	5,5,5	0.20	0	4,4,4	0.52	0
3	GOL	B	1113	-	5,5,5	0.33	0	5,5,5	0.53	0
11	LMU	B	1114	-	36,36,36	1.13	4 (11%)	47,47,47	2.37	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	1115	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	B	1116	-	5,5,5	0.36	0	5,5,5	0.12	0
3	GOL	B	1117	-	5,5,5	0.45	0	5,5,5	0.38	0
3	GOL	C	1101	-	5,5,5	0.24	0	5,5,5	0.50	0
4	LMT	C	1102	-	36,36,36	1.15	3 (8%)	47,47,47	1.07	1 (2%)
5	OCT	C	1103	-	7,7,7	0.29	0	6,6,6	0.76	0
8	D12	C	1104	-	11,11,11	0.27	0	10,10,10	0.79	0
5	OCT	C	1105	-	7,7,7	0.30	0	6,6,6	1.15	1 (16%)
5	OCT	C	1106	-	7,7,7	0.24	0	6,6,6	0.64	0
6	D10	C	1107	-	9,9,9	0.37	0	8,8,8	1.00	0
8	D12	C	1108	-	11,11,11	0.39	0	10,10,10	1.10	1 (10%)
6	D10	C	1109	-	9,9,9	0.26	0	8,8,8	0.80	0
7	HEX	C	1110	-	5,5,5	0.24	0	4,4,4	0.70	0
12	DD9	C	1111	-	8,8,8	0.23	0	7,7,7	0.75	0
5	OCT	C	1112	-	7,7,7	0.24	0	6,6,6	0.74	0
7	HEX	C	1113	-	5,5,5	0.20	0	4,4,4	0.49	0
3	GOL	C	1114	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	C	1115	-	5,5,5	0.46	0	5,5,5	0.69	0
5	OCT	C	1116	-	7,7,7	0.30	0	6,6,6	0.86	0
3	GOL	C	1117	-	5,5,5	0.48	0	5,5,5	0.44	0
13	SO4	C	1118	-	4,4,4	0.28	0	6,6,6	0.13	0
14	UND	C	1119	-	10,10,10	0.24	0	9,9,9	0.73	0
6	D10	C	1120	-	9,9,9	0.24	0	8,8,8	0.71	0
3	GOL	D	201	-	5,5,5	0.30	0	5,5,5	0.33	0
3	GOL	D	202	-	5,5,5	0.31	0	5,5,5	0.42	0
3	GOL	E	201	-	5,5,5	0.29	0	5,5,5	0.28	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	GOL	A	1101	-	-	0/4/4/4	0/0/0/0
4	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
4	LMT	A	1103	-	-	0/21/61/61	0/2/2/2
4	LMT	A	1104	-	-	0/21/61/61	0/2/2/2
5	OCT	A	1105	-	-	0/5/5/5	0/0/0/0
5	OCT	A	1106	-	-	0/5/5/5	0/0/0/0
6	D10	A	1107	-	-	0/7/7/7	0/0/0/0
7	HEX	A	1108	-	-	0/3/3/3	0/0/0/0
4	LMT	A	1109	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1110	-	-	0/4/4/4	0/0/0/0
8	D12	A	1111	-	-	0/9/9/9	0/0/0/0
3	GOL	B	1101	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1102	-	-	0/4/4/4	0/0/0/0
9	MIY	B	1103	-	-	0/12/70/70	0/4/4/4
4	LMT	B	1104	-	-	0/21/61/61	0/2/2/2
6	D10	B	1105	-	-	0/7/7/7	0/0/0/0
8	D12	B	1106	-	-	0/9/9/9	0/0/0/0
6	D10	B	1107	-	-	0/7/7/7	0/0/0/0
7	HEX	B	1108	-	-	0/3/3/3	0/0/0/0
10	C14	B	1109	-	-	0/11/11/11	0/0/0/0
4	LMT	B	1110	-	-	0/21/61/61	0/2/2/2
4	LMT	B	1111	-	-	0/21/61/61	0/2/2/2
7	HEX	B	1112	-	-	0/3/3/3	0/0/0/0
3	GOL	B	1113	-	-	0/4/4/4	0/0/0/0
11	LMU	B	1114	-	-	0/21/61/61	0/2/2/2
3	GOL	B	1115	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1116	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1117	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1101	-	-	0/4/4/4	0/0/0/0
4	LMT	C	1102	-	-	0/21/61/61	0/2/2/2
5	OCT	C	1103	-	-	0/5/5/5	0/0/0/0
8	D12	C	1104	-	-	0/9/9/9	0/0/0/0
5	OCT	C	1105	-	-	0/5/5/5	0/0/0/0
5	OCT	C	1106	-	-	0/5/5/5	0/0/0/0
6	D10	C	1107	-	-	0/7/7/7	0/0/0/0
8	D12	C	1108	-	-	0/9/9/9	0/0/0/0
6	D10	C	1109	-	-	0/7/7/7	0/0/0/0
7	HEX	C	1110	-	-	0/3/3/3	0/0/0/0
12	DD9	C	1111	-	-	0/6/6/6	0/0/0/0
5	OCT	C	1112	-	-	0/5/5/5	0/0/0/0
7	HEX	C	1113	-	-	0/3/3/3	0/0/0/0
3	GOL	C	1114	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1115	-	-	0/4/4/4	0/0/0/0
5	OCT	C	1116	-	-	0/5/5/5	0/0/0/0
3	GOL	C	1117	-	-	0/4/4/4	0/0/0/0
13	SO4	C	1118	-	-	0/0/0/0	0/0/0/0
14	UND	C	1119	-	-	0/8/8/8	0/0/0/0
6	D10	C	1120	-	-	0/7/7/7	0/0/0/0
3	GOL	D	201	-	-	0/4/4/4	0/0/0/0
3	GOL	D	202	-	-	0/4/4/4	0/0/0/0
3	GOL	E	201	-	-	0/4/4/4	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1103	MIY	C18-C1	-4.21	1.48	1.55
9	B	1103	MIY	C14-C9	-4.07	1.34	1.40
9	B	1103	MIY	O7-C18	-3.61	1.36	1.42
4	B	1110	LMT	C3'-C4'	-3.23	1.43	1.52
4	A	1104	LMT	C3'-C4'	-3.16	1.43	1.52
4	B	1111	LMT	C3'-C4'	-3.14	1.43	1.52
4	A	1103	LMT	C3'-C4'	-3.05	1.43	1.52
9	B	1103	MIY	C7-C16	-3.05	1.48	1.51
4	C	1102	LMT	C3'-C4'	-3.00	1.43	1.52
4	A	1102	LMT	C3'-C4'	-2.89	1.44	1.52
4	A	1109	LMT	C3'-C4'	-2.85	1.44	1.52
4	B	1104	LMT	C3'-C4'	-2.85	1.44	1.52
11	B	1114	LMU	O2B-C2B	-2.14	1.37	1.43
9	B	1103	MIY	C5-C4	2.18	1.56	1.54
9	B	1103	MIY	C10-N7	2.19	1.48	1.42
11	B	1114	LMU	C4B-C3B	2.53	1.59	1.52
9	B	1103	MIY	C11-C10	2.56	1.44	1.39
9	B	1103	MIY	C2-C21	2.57	1.52	1.47
4	A	1103	LMT	O5'-C5'	2.59	1.50	1.44
4	C	1102	LMT	O5'-C5'	2.62	1.50	1.44
4	B	1111	LMT	O5'-C5'	2.66	1.51	1.44
4	B	1110	LMT	O5'-C5'	2.70	1.51	1.44
4	A	1109	LMT	O5'-C5'	2.76	1.51	1.44
9	B	1103	MIY	O6-C17	2.76	1.42	1.33
4	A	1104	LMT	O5'-C5'	2.77	1.51	1.44
4	B	1104	LMT	O5'-C5'	2.93	1.51	1.44
4	A	1102	LMT	O5'-C5'	2.94	1.51	1.44
11	B	1114	LMU	O4'-C4B	3.07	1.50	1.43
9	B	1103	MIY	C8-C9	3.20	1.57	1.51
11	B	1114	LMU	C4B-C5B	3.30	1.60	1.53
4	A	1109	LMT	O5B-C1B	3.38	1.50	1.41
4	B	1104	LMT	O5B-C1B	3.38	1.50	1.41
9	B	1103	MIY	C21-N2	3.55	1.43	1.33
4	A	1102	LMT	O5B-C1B	3.57	1.51	1.41
4	C	1102	LMT	O5B-C1B	3.62	1.51	1.41
4	A	1103	LMT	O5B-C1B	3.68	1.51	1.41
4	A	1104	LMT	O5B-C1B	3.69	1.51	1.41
4	B	1111	LMT	O5B-C1B	3.81	1.51	1.41
9	B	1103	MIY	C16-C17	3.88	1.40	1.36
4	B	1110	LMT	O5B-C1B	3.90	1.51	1.41
9	B	1103	MIY	C11-C12	4.11	1.46	1.38
9	B	1103	MIY	C14-C13	4.15	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1103	MIY	O5-C15	7.23	1.38	1.23
9	B	1103	MIY	O1-C1	7.65	1.36	1.22
9	B	1103	MIY	C10-C9	9.23	1.53	1.40

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1103	MIY	C11-C12-C13	-6.31	114.02	120.49
4	A	1109	LMT	C1B-O5B-C5B	-4.24	105.51	113.75
11	B	1114	LMU	C1'-O5'-C5'	-3.93	106.12	113.75
9	B	1103	MIY	C18-C17-C16	-3.72	118.49	122.95
4	A	1104	LMT	C1B-O1B-C4'	-3.14	109.80	118.01
11	B	1114	LMU	C1B-O1B-C4'	-2.88	110.48	118.01
9	B	1103	MIY	O6-C17-C16	-2.82	121.14	123.84
4	B	1110	LMT	C1B-O1B-C4'	-2.77	110.76	118.01
4	A	1102	LMT	C1B-O1B-C4'	-2.53	111.41	118.01
5	C	1105	OCT	C6-C5-C4	-2.45	101.88	114.53
9	B	1103	MIY	O7-C18-C17	-2.43	105.48	109.85
9	B	1103	MIY	C20-N1-C4	-2.35	108.33	114.07
9	B	1103	MIY	C11-C10-N7	-2.31	118.36	121.59
9	B	1103	MIY	C11-C10-C9	-2.30	117.50	120.47
8	C	1108	D12	C9-C8-C7	-2.27	102.83	114.53
9	B	1103	MIY	O5-C15-C16	-2.20	117.45	120.73
4	A	1109	LMT	C1B-C2B-C3B	-2.20	105.64	109.97
9	B	1103	MIY	C5-C18-C1	-2.12	108.75	111.17
4	A	1109	LMT	O1B-C4'-C3'	-2.09	101.77	107.17
4	B	1110	LMT	O6'-C6'-C5'	2.01	117.96	111.33
4	B	1110	LMT	O5'-C1'-C2'	2.02	114.42	110.28
4	A	1109	LMT	O1'-C1'-C2'	2.03	110.60	108.04
4	B	1111	LMT	O5'-C5'-C6'	2.03	111.48	106.36
4	A	1102	LMT	O6B-C6B-C5B	2.04	118.08	111.33
4	A	1102	LMT	O1'-C1'-C2'	2.09	110.67	108.04
4	A	1102	LMT	C1B-O5B-C5B	2.10	117.81	113.75
4	A	1102	LMT	O1'-C1-C2	2.11	118.27	109.88
11	B	1114	LMU	O5'-C5'-C4'	2.12	114.23	109.75
4	B	1104	LMT	O1B-C1B-C2B	2.14	113.31	108.10
4	B	1104	LMT	O6B-C6B-C5B	2.16	118.46	111.33
4	A	1102	LMT	C1-O1'-C1'	2.17	117.73	113.94
9	B	1103	MIY	C12-C11-C10	2.18	124.06	119.29
4	A	1104	LMT	O6B-C6B-C5B	2.20	118.61	111.33
4	A	1109	LMT	C1-O1'-C1'	2.24	117.86	113.94
4	A	1104	LMT	O6'-C6'-C5'	2.27	118.83	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	LMT	O6'-C6'-C5'	2.39	119.24	111.33
11	B	1114	LMU	O1B-C4'-C3'	2.43	113.44	107.17
4	B	1111	LMT	O6B-C6B-C5B	2.44	119.38	111.33
4	A	1109	LMT	C3B-C4B-C5B	2.44	114.45	110.20
4	B	1110	LMT	C1B-O5B-C5B	2.44	118.49	113.75
4	B	1104	LMT	C2'-C3'-C4'	2.55	115.19	109.60
4	B	1110	LMT	O5B-C5B-C4B	2.56	114.48	109.68
11	B	1114	LMU	C6B-C5B-C4B	2.69	119.65	113.02
4	A	1109	LMT	O6'-C6'-C5'	2.77	120.49	111.33
4	A	1109	LMT	O5'-C5'-C4'	2.79	115.64	109.75
4	B	1110	LMT	O1'-C1'-C2'	2.87	111.66	108.04
4	A	1103	LMT	C2'-C3'-C4'	2.88	115.91	109.60
9	B	1103	MIY	C18-C5-C4	3.02	115.78	111.73
11	B	1114	LMU	O5B-C1B-C2B	3.06	116.56	110.28
4	B	1111	LMT	C1-O1'-C1'	3.12	119.40	113.94
11	B	1114	LMU	C6'-C5'-C4'	3.25	122.69	113.25
4	A	1109	LMT	O1B-C1B-C2B	3.30	116.13	108.10
4	A	1104	LMT	C1-O1'-C1'	3.47	120.01	113.94
9	B	1103	MIY	C12-C13-C14	3.47	124.78	120.21
4	A	1109	LMT	C3'-C4'-C5'	3.48	118.71	110.84
4	A	1109	LMT	C2'-C3'-C4'	3.48	117.25	109.60
4	C	1102	LMT	C1-O1'-C1'	3.59	120.22	113.94
4	A	1103	LMT	C1-O1'-C1'	3.70	120.41	113.94
11	B	1114	LMU	O4'-C4B-C5B	3.94	119.68	109.24
11	B	1114	LMU	C3B-C4B-C5B	4.10	117.35	110.20
4	A	1102	LMT	O5B-C5B-C4B	4.25	117.65	109.68
9	B	1103	MIY	O6-C17-C18	4.29	120.35	113.50
4	B	1104	LMT	C1-O1'-C1'	4.59	121.96	113.94
4	A	1102	LMT	C3B-C4B-C5B	4.61	118.23	110.20
4	B	1110	LMT	C1-O1'-C1'	4.65	122.07	113.94
11	B	1114	LMU	O4'-C4B-C3B	4.79	121.11	110.34
11	B	1114	LMU	O5B-C5B-C4B	4.85	118.78	109.68
11	B	1114	LMU	O5B-C5B-C6B	5.19	119.46	106.36
11	B	1114	LMU	O5'-C5'-C6'	5.43	120.07	106.36
9	B	1103	MIY	C9-C10-N7	6.10	124.13	118.94
11	B	1114	LMU	O1'-C1'-C2'	6.49	116.24	108.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	GOL	1	0
4	A	1102	LMT	6	0
4	A	1103	LMT	11	0
4	A	1104	LMT	2	0
6	A	1107	D10	1	0
4	A	1109	LMT	14	0
3	A	1110	GOL	1	0
8	A	1111	D12	8	0
3	B	1101	GOL	2	0
3	B	1102	GOL	2	0
9	B	1103	MIY	2	0
4	B	1104	LMT	4	0
6	B	1105	D10	1	0
8	B	1106	D12	1	0
10	B	1109	C14	2	0
4	B	1110	LMT	9	0
4	B	1111	LMT	4	0
3	B	1113	GOL	1	0
11	B	1114	LMU	3	0
3	B	1115	GOL	1	0
3	B	1116	GOL	5	0
3	C	1101	GOL	1	0
4	C	1102	LMT	1	0
5	C	1103	OCT	1	0
8	C	1104	D12	1	0
3	C	1115	GOL	3	0
3	C	1117	GOL	1	0
3	E	201	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	1044/1057 (98%)	0.26	84 (8%) 15 17	17, 43, 87, 136	0
1	B	1033/1057 (97%)	0.10	48 (4%) 36 39	19, 41, 69, 133	0
1	C	1033/1057 (97%)	0.05	42 (4%) 41 45	20, 36, 61, 104	0
2	D	156/169 (92%)	-0.07	5 (3%) 51 54	30, 39, 66, 110	0
2	E	152/169 (89%)	0.76	24 (15%) 3 3	34, 50, 83, 106	0
All	All	3418/3509 (97%)	0.16	203 (5%) 26 29	17, 40, 75, 136	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	11	GLY	12.5
1	A	1043	SER	7.3
1	B	677	ALA	7.3
1	A	868	LEU	6.9
1	A	869	SER	6.2
2	E	165	LEU	6.1
2	E	33	LEU	6.0
1	A	918	PHE	5.9
1	B	678	THR	5.3
1	C	28	LEU	5.2
1	B	512	PHE	5.1
1	A	518	ARG	5.1
2	D	12	SER	5.0
2	E	31	ARG	4.9
2	E	34	MET	4.9
1	B	515	TRP	4.8
2	E	35	ALA	4.8
1	A	515	TRP	4.8
1	A	1042	HIS	4.7
1	A	1044	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	1033	PHE	4.6
1	A	937	LEU	4.6
2	E	66	LEU	4.5
1	A	1035	ARG	4.4
2	E	37	GLY	4.4
1	C	811	TYR	4.4
1	A	512	PHE	4.3
1	B	511	GLY	4.2
1	A	1040	ILE	4.2
2	E	68	LYS	4.2
1	B	871	ASN	4.1
1	A	506	GLY	4.1
1	C	617	PHE	4.1
1	A	459	PHE	4.0
1	B	658	ILE	4.0
1	A	1036	LYS	4.0
1	C	672	VAL	4.0
1	B	657	GLN	4.0
1	A	678	THR	3.9
1	C	1032	ARG	3.9
1	C	508	GLY	3.8
1	B	659	LYS	3.8
1	A	712	MET	3.7
1	A	425	LEU	3.7
1	A	513	PHE	3.7
2	E	38	ALA	3.7
1	A	866	GLU	3.7
1	A	386	PHE	3.7
1	A	871	ASN	3.6
1	A	529	ASP	3.6
1	B	255	GLN	3.6
1	C	513	PHE	3.6
1	A	835	LYS	3.6
1	C	362	PHE	3.6
1	A	870	GLY	3.6
1	A	539	GLY	3.6
1	B	638	PRO	3.5
1	A	498	LYS	3.5
1	A	542	LEU	3.5
1	A	956	GLU	3.5
1	B	635	ALA	3.5
1	A	362	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	540	ARG	3.4
1	C	510	LYS	3.4
1	A	411	VAL	3.4
1	B	513	PHE	3.4
1	A	1033	PHE	3.4
1	B	508	GLY	3.4
1	A	508	GLY	3.3
1	C	255	GLN	3.3
1	B	868	LEU	3.3
2	E	162	ALA	3.2
1	B	510	LYS	3.2
2	E	70	GLY	3.2
1	A	677	ALA	3.2
1	A	541	TYR	3.2
1	B	558	ARG	3.2
1	A	836	SER	3.2
1	C	676	THR	3.2
1	A	255	GLN	3.2
1	A	404	LEU	3.2
1	B	653	ARG	3.1
2	E	166	GLN	3.1
2	E	163	GLU	3.1
2	E	30	VAL	3.1
1	A	617	PHE	3.1
1	B	597	TYR	3.1
1	B	640	GLU	3.1
1	B	834	GLY	3.1
1	C	671	ILE	3.0
1	C	935	ILE	3.0
1	C	975	ILE	3.0
1	A	543	VAL	3.0
1	C	406	VAL	3.0
1	A	501	ALA	3.0
1	A	867	ARG	3.0
1	B	937	LEU	3.0
2	E	61	GLU	3.0
1	C	957	GLY	3.0
1	A	500	ILE	3.0
1	A	557	VAL	2.9
1	C	918	PHE	2.9
1	A	526	HIS	2.9
2	D	14	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	386	PHE	2.9
2	D	165	LEU	2.9
2	E	27	ASP	2.8
1	A	975	ILE	2.8
1	B	918	PHE	2.8
2	E	32	ILE	2.8
1	A	833	PRO	2.8
1	A	944	LEU	2.8
1	C	512	PHE	2.8
1	A	839	GLU	2.8
1	C	670	ALA	2.7
2	E	36	ASN	2.7
2	E	69	ASN	2.7
2	D	13	ASP	2.7
1	A	514	GLY	2.7
1	A	1037	ASN	2.7
1	A	674	LEU	2.7
1	A	1039	ASP	2.7
1	C	937	LEU	2.7
1	B	554	TYR	2.6
1	B	836	SER	2.6
1	C	618	ALA	2.6
1	A	536	ARG	2.6
1	A	534	ILE	2.6
1	B	833	PRO	2.6
1	A	979	SER	2.6
1	B	557	VAL	2.6
1	C	978	THR	2.6
1	A	657	GLN	2.6
1	C	400	LEU	2.5
1	B	641	GLU	2.5
1	A	895	TRP	2.5
1	B	655	PHE	2.5
1	A	1041	GLU	2.5
1	C	976	LEU	2.5
1	A	993	THR	2.5
1	C	675	GLY	2.5
1	B	506	GLY	2.5
1	C	503	GLY	2.5
1	B	832	ALA	2.5
1	A	522	LYS	2.4
1	C	498	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	445	ILE	2.4
1	C	257	GLY	2.4
1	A	510	LYS	2.4
2	E	161	LEU	2.4
1	A	676	THR	2.4
1	A	865	GLN	2.4
1	B	712	MET	2.4
1	B	837	THR	2.4
1	B	563	PHE	2.4
1	C	981	ALA	2.4
1	A	1038	GLU	2.4
1	A	834	GLY	2.4
1	C	404	LEU	2.4
1	C	674	LEU	2.4
1	B	509	LYS	2.4
1	B	991	ILE	2.3
1	C	515	TRP	2.3
1	C	659	LYS	2.3
1	C	501	ALA	2.3
1	A	511	GLY	2.3
2	E	40	VAL	2.3
1	B	617	PHE	2.3
1	A	400	LEU	2.3
1	C	449	LEU	2.3
1	C	27	ILE	2.3
1	A	403	GLY	2.3
1	B	257	GLY	2.3
1	A	980	LEU	2.2
1	B	711	ASP	2.2
2	E	67	LEU	2.2
1	A	436	GLY	2.2
1	B	874	PRO	2.2
1	C	977	MET	2.2
1	B	133	SER	2.2
1	A	410	ILE	2.2
1	C	980	LEU	2.2
2	E	139	VAL	2.2
1	B	501	ALA	2.2
1	C	511	GLY	2.2
1	B	404	LEU	2.2
1	A	406	VAL	2.2
1	B	660	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	558	ARG	2.1
1	A	429	GLU	2.1
1	B	869	SER	2.1
1	A	509	LYS	2.1
1	A	432	ARG	2.1
1	C	500	ILE	2.1
1	A	426	PRO	2.1
1	A	874	PRO	2.1
1	A	618	ALA	2.1
1	B	931	LEU	2.1
1	B	835	LYS	2.1
1	A	831	ALA	2.0
1	A	405	LEU	2.0
2	E	71	ALA	2.0
1	A	535	LEU	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
5	OCT	C	1112	8/8	0.38	0.32	14.01	79,97,102,103	0
3	GOL	C	1115	6/6	0.92	0.20	10.04	30,39,51,52	0
6	D10	C	1107	10/10	0.74	0.28	9.47	72,92,96,99	0
4	LMT	A	1109	35/35	0.74	0.34	8.41	70,95,104,105	0
7	HEX	B	1108	6/6	0.79	0.22	7.84	66,79,87,87	0
3	GOL	B	1117	6/6	0.86	0.27	6.47	55,55,64,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	D	202	6/6	0.77	0.17	6.41	53,69,83,88	0
7	HEX	B	1112	6/6	0.51	0.24	5.86	79,96,103,103	0
3	GOL	B	1101	6/6	0.90	0.14	5.24	34,41,52,58	0
3	GOL	C	1117	6/6	0.75	0.29	5.14	41,53,58,61	0
3	GOL	D	201	6/6	0.92	0.10	5.06	55,60,64,71	0
3	GOL	B	1113	6/6	0.90	0.18	4.98	56,64,67,68	0
6	D10	A	1107	10/10	0.42	0.25	4.63	75,92,106,108	0
4	LMT	B	1111	35/35	0.65	0.34	4.39	78,120,130,131	0
4	LMT	A	1102	35/35	0.84	0.17	4.36	50,71,95,101	0
5	OCT	C	1106	8/8	0.58	0.19	4.22	73,88,101,101	0
3	GOL	C	1114	6/6	0.82	0.18	4.03	59,67,69,70	0
7	HEX	C	1113	6/6	0.73	0.27	3.82	71,89,105,105	0
10	C14	B	1109	14/14	0.77	0.18	3.70	70,87,106,109	0
3	GOL	B	1116	6/6	0.91	0.19	3.51	67,75,82,87	0
6	D10	C	1120	10/10	0.62	0.21	3.22	72,94,116,116	0
3	GOL	A	1101	6/6	0.91	0.13	3.16	38,47,54,58	0
11	LMU	B	1114	35/35	0.71	0.24	2.99	76,100,115,118	0
14	UND	C	1119	11/11	0.64	0.31	2.88	64,98,118,118	0
12	DD9	C	1111	9/9	0.76	0.20	2.87	56,80,98,101	0
4	LMT	B	1104	35/35	0.89	0.20	2.81	53,68,98,99	0
6	D10	B	1107	10/10	0.69	0.19	2.75	64,94,113,113	0
3	GOL	B	1102	6/6	0.91	0.12	2.67	40,58,64,69	0
5	OCT	A	1105	8/8	0.69	0.30	2.43	73,89,93,94	0
4	LMT	B	1110	35/35	0.67	0.31	2.36	65,121,126,129	0
3	GOL	B	1115	6/6	0.74	0.19	2.23	56,68,71,72	0
3	GOL	C	1101	6/6	0.89	0.17	2.04	50,57,69,74	0
3	GOL	A	1110	6/6	0.94	0.13	2.01	28,40,54,56	0
7	HEX	C	1110	6/6	0.73	0.17	1.99	77,93,98,98	0
8	D12	C	1108	12/12	0.82	0.22	1.88	40,63,90,90	0
7	HEX	A	1108	6/6	0.76	0.18	1.87	89,110,112,112	0
4	LMT	A	1104	35/35	0.90	0.13	1.62	51,74,104,108	0
9	MIY	B	1103	33/33	0.86	0.16	1.15	52,74,112,116	0
3	GOL	E	201	6/6	0.89	0.14	0.97	56,59,64,68	0
8	D12	A	1111	12/12	0.88	0.13	0.93	53,73,98,98	0
4	LMT	A	1103	35/35	0.71	0.24	0.81	68,88,105,106	0
5	OCT	C	1116	8/8	0.80	0.15	0.65	61,75,84,85	0
8	D12	C	1104	12/12	0.67	0.14	0.58	68,85,98,99	0
5	OCT	C	1103	8/8	0.90	0.10	0.55	65,80,84,86	0
4	LMT	C	1102	35/35	0.94	0.12	0.15	50,64,79,80	0
5	OCT	C	1105	8/8	0.81	0.14	-0.21	67,83,101,105	0
6	D10	B	1105	10/10	0.82	0.19	-	69,85,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	OCT	A	1106	8/8	0.80	0.18	-	66,82,86,86	0
13	SO4	C	1118	5/5	0.99	0.11	-	62,67,76,78	0
6	D10	C	1109	10/10	0.64	0.34	-	73,90,102,102	0
8	D12	B	1106	12/12	0.66	0.25	-	74,92,108,109	0

6.5 Other polymers

There are no such residues in this entry.