Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:57 PM GMT

PDB ID	:	4DX6
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	:	2.90 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:

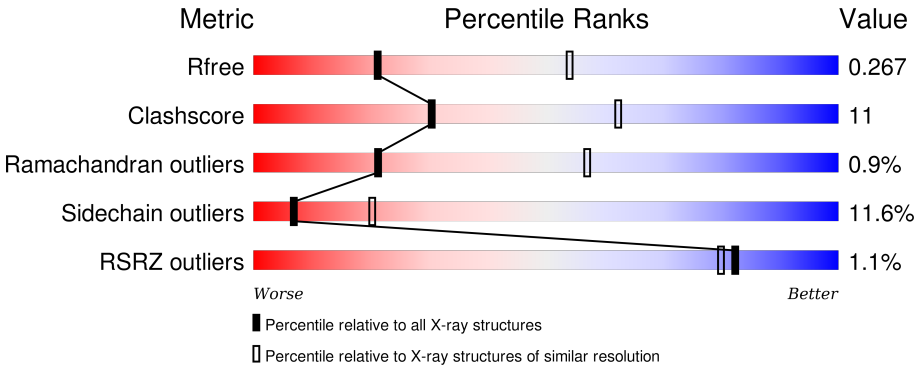
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	65% 29%
1	B	1057	70% 24%
1	C	1057	67% 27%
2	D	169	72% 18% 8%
2	E	169	2% 54% 29% 7% 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	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	B	1101	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7947	5108	1316	1479	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7853	5054	1296	1459	44			
1	C	1034	Total	C	N	O	S	0	0	0
			7859	5057	1297	1461	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	ASN	GLY	CONFLICT	UNP P31224
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	616	ASN	GLY	CONFLICT	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	616	ASN	GLY	CONFLICT	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

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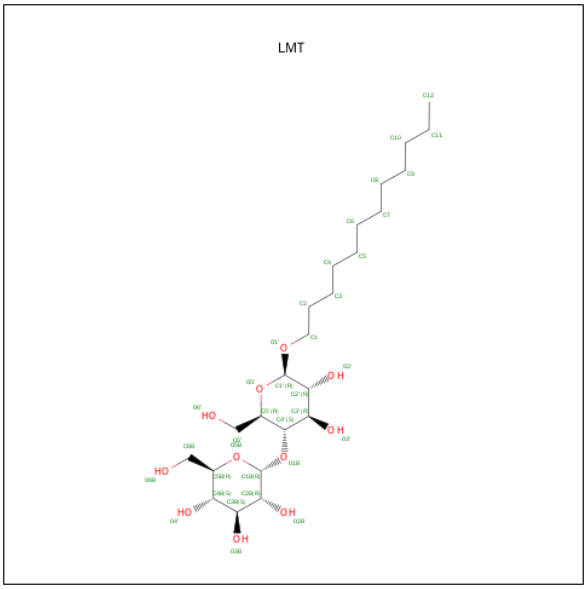
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	EXPRESSION TAG	UNP P31224
C	1055	HIS	-	EXPRESSION TAG	UNP P31224
C	1056	HIS	-	EXPRESSION TAG	UNP P31224
C	1057	HIS	-	EXPRESSION TAG	UNP P31224

- 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	B	1	Total	C	O		0	0
			35	24	11			
3	B	1	Total	C	O		0	0
			35	24	11			
3	C	1	Total	C	O		0	0
			35	24	11			

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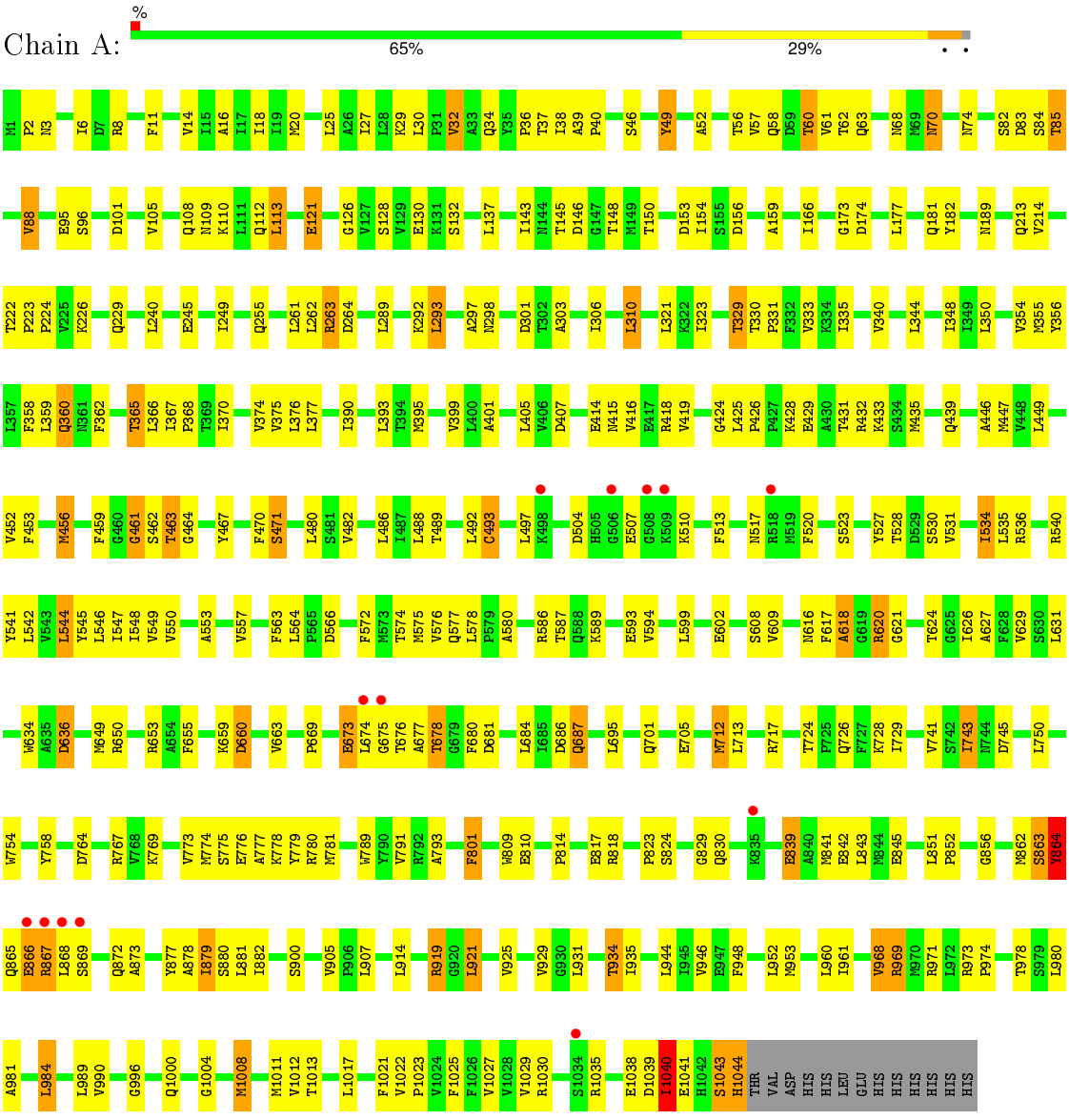
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

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.

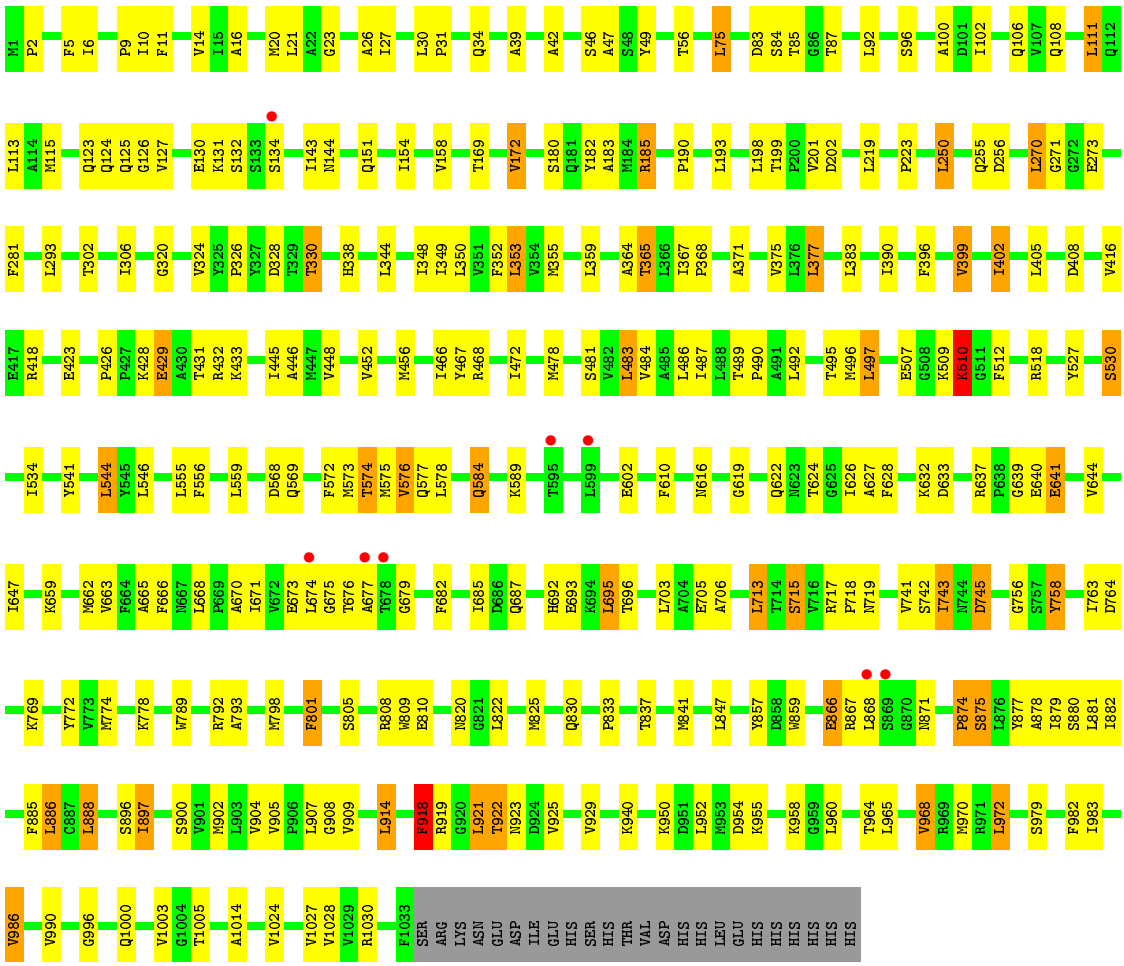
- Molecule 1: Acriflavine resistance protein B

Chain A:



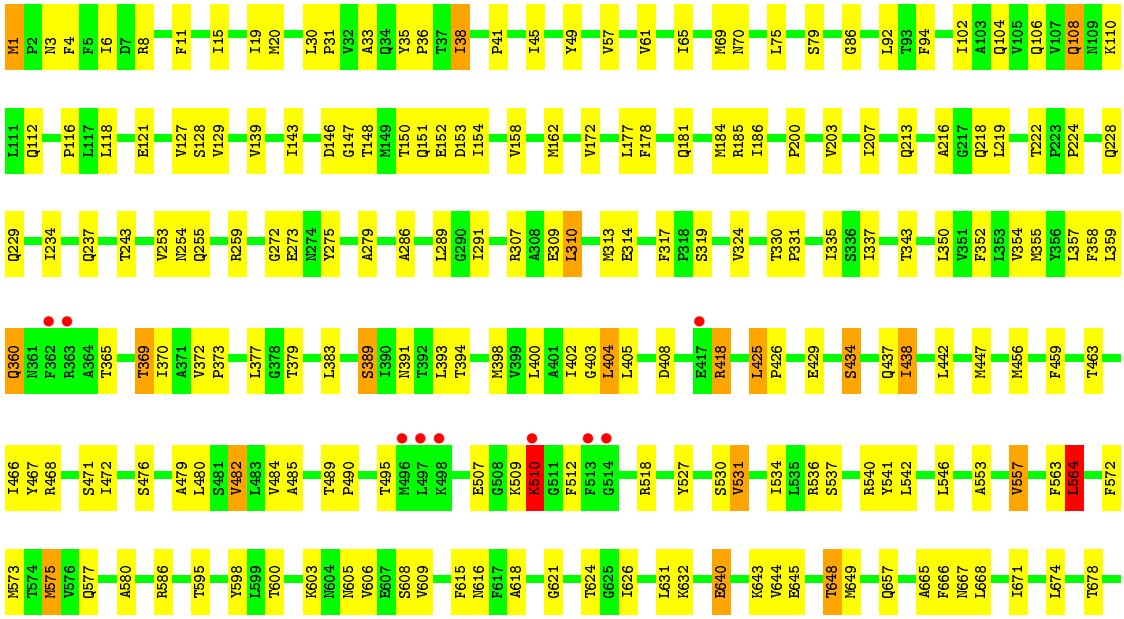
- Molecule 1: Acriflavine resistance protein B

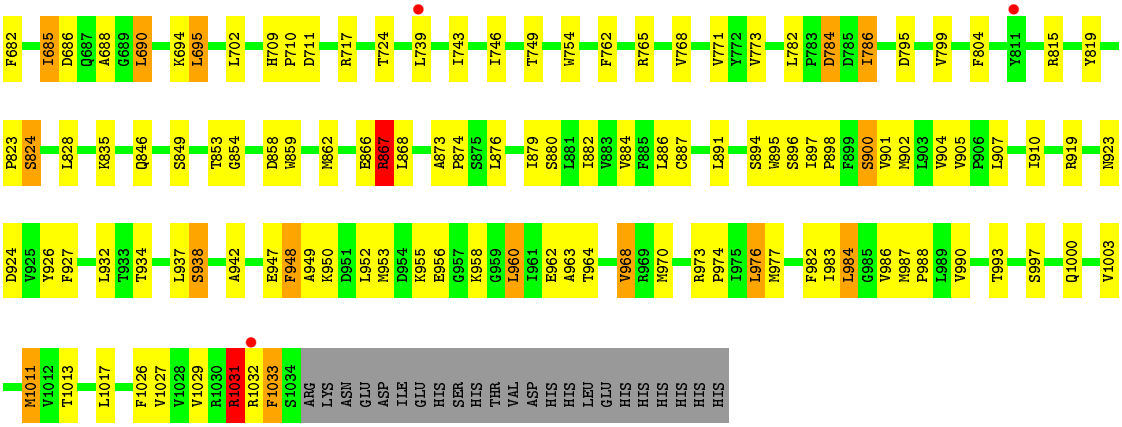
Chain B:



• Molecule 1: Acriflavine resistance protein B

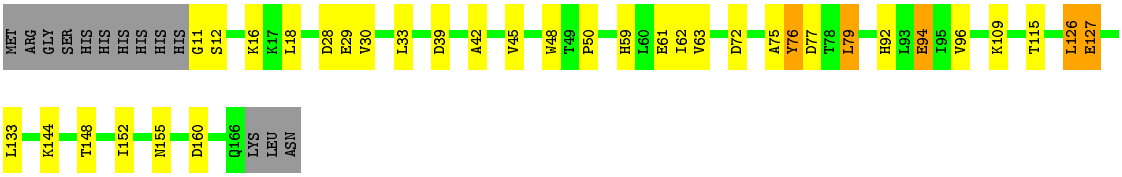
Chain C:





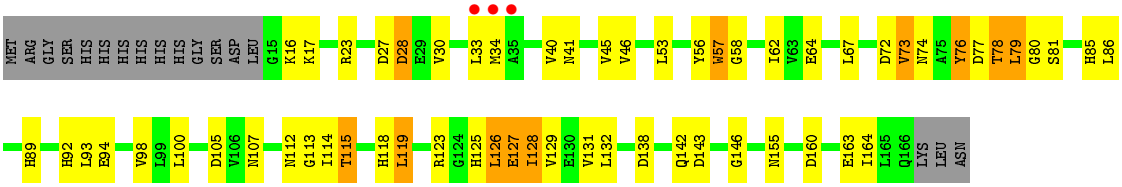
- Molecule 2: DARPIN

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	145.69Å 165.45Å 245.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.90 49.28 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.28-2.90) 95.0 (49.28-2.29)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.209 , 0.270 0.202 , 0.267	Depositor DCC
R_{free} test set	6582 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 252313 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	26232	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: LMT

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	0.44	0/8099	0.64	0/10997
1	B	0.41	0/8003	0.60	1/10869 (0.0%)
1	C	0.44	0/8009	0.63	2/10877 (0.0%)
2	D	0.38	0/1196	0.58	0/1626
2	E	0.42	0/1170	0.63	0/1591
All	All	0.43	0/26477	0.62	3/35960 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	867	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	564	LEU	CA-CB-CG	5.20	127.27	115.30
1	B	250	LEU	CA-CB-CG	5.18	127.20	115.30

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	7947	0	8087	211	0
1	B	7853	0	8004	154	0
1	C	7859	0	8009	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1177	0	1159	24	0
2	E	1151	0	1136	39	0
3	A	70	0	92	4	0
3	B	105	0	138	4	0
3	C	70	0	92	3	0
All	All	26232	0	26717	583	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 11.

All (583) 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:621:GLY:H	1:A:624:THR:HG21	1.31	0.95
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.57	0.86
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.59	0.84
1:C:616:ASN:HB3	1:C:618:ALA:H	1.41	0.84
1:A:764:ASP:OD2	1:A:769:LYS:NZ	2.16	0.79
1:A:350:LEU:HD23	1:A:984:LEU:HD13	1.65	0.79
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.64	0.78
1:A:674:LEU:HB3	1:A:675:GLY:HA2	1.65	0.78
1:A:867:ARG:HB3	1:A:868:LEU:HB2	1.64	0.78
1:C:876:LEU:HD11	1:C:932:LEU:HD11	1.65	0.78
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.65	0.76
1:A:356:TYR:HA	1:A:365:THR:HG21	1.67	0.76
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.66	0.76
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.66	0.75
1:A:866:GLU:HB2	1:A:867:ARG:HA	1.69	0.75
1:C:563:PHE:HB2	1:C:866:GLU:HG3	1.67	0.74
1:B:866:GLU:OE2	3:B:1103:LMT:O4'	2.07	0.72
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.53	0.72
1:B:979:SER:O	1:B:983:ILE:HG12	1.90	0.72
1:A:14:VAL:HG22	1:B:886:LEU:HD12	1.73	0.71
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.72	0.70
1:A:809:TRP:HE1	2:E:78:THR:HG23	1.57	0.70
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.73	0.70
2:E:46:VAL:O	2:E:78:THR:HG22	1.92	0.70
1:B:919:ARG:NH2	1:B:990:VAL:O	2.26	0.69
1:B:897:ILE:O	1:B:900:SER:OG	2.11	0.68
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.76	0.68
1:A:56:THR:O	1:A:60:THR:HB	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:LEU:HD22	1:C:1027:VAL:HG22	1.76	0.67
2:E:115:THR:OG1	2:E:118:HIS:ND1	2.27	0.67
1:A:74:ASN:HB3	1:A:95:GLU:HB2	1.76	0.67
1:C:357:LEU:O	1:C:360:GLN:NE2	2.28	0.67
1:B:445:ILE:HG21	1:B:940:LYS:HE2	1.75	0.67
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.60	0.66
1:A:459:PHE:HB2	1:A:464:GLY:HA2	1.78	0.66
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.78	0.65
1:A:775:SER:HG	1:A:789:TRP:HZ2	1.44	0.65
1:C:536:ARG:NH2	3:C:1102:LMT:O3B	2.28	0.65
1:C:907:LEU:HD22	1:C:1017:LEU:HD23	1.79	0.65
1:A:934:THR:HG22	1:A:1011:MET:HE2	1.77	0.65
1:A:602:GLU:OE1	1:A:650:ARG:NH1	2.30	0.65
1:B:950:LYS:NZ	1:B:954:ASP:OD1	2.25	0.64
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.80	0.64
1:B:742:SER:HB3	1:B:745:ASP:HB2	1.79	0.64
2:E:28:ASP:OD1	2:E:28:ASP:N	2.31	0.64
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.79	0.63
1:A:70:ASN:O	1:A:110:LYS:HE3	1.98	0.63
1:A:616:ASN:O	1:A:618:ALA:N	2.31	0.63
1:C:104:GLN:HE22	1:C:108:GLN:HG3	1.63	0.63
1:A:534:ILE:HB	1:A:541:TYR:CZ	2.34	0.63
1:B:584:GLN:HB3	1:B:622:GLN:HG2	1.81	0.63
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.81	0.62
1:C:104:GLN:NE2	1:C:108:GLN:HG3	2.13	0.62
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.34	0.62
2:E:56:TYR:HB2	2:E:86:LEU:HD13	1.81	0.62
1:C:49:TYR:HB3	1:C:57:VAL:HG22	1.80	0.62
1:B:574:THR:HA	1:B:665:ALA:HA	1.82	0.62
1:A:137:LEU:O	1:A:329:THR:OG1	2.17	0.62
1:B:507:GLU:O	1:B:518:ARG:NH1	2.32	0.61
1:C:150:THR:O	1:C:154:ILE:HG13	2.00	0.61
1:B:26:ALA:O	1:B:30:LEU:HB2	2.01	0.61
1:A:674:LEU:HB3	1:A:675:GLY:CA	2.31	0.61
1:A:109:ASN:O	1:A:112:GLN:HG2	2.01	0.61
1:A:669:PRO:HG2	1:A:674:LEU:HD21	1.83	0.61
1:A:355:MET:HB3	1:A:365:THR:HB	1.83	0.61
1:C:8:ARG:NH2	3:C:1101:LMT:O4'	2.33	0.61
1:B:405:LEU:HD22	1:B:481:SER:HB2	1.82	0.60
1:C:575:MET:HG3	1:C:666:PHE:HE1	1.65	0.60
1:A:416:VAL:HG22	1:A:431:THR:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLN:NE2	1:B:758:TYR:O	2.34	0.60
2:E:123:ARG:HG2	2:E:125:HIS:CE1	2.37	0.60
1:B:75:LEU:HD21	1:B:92:LEU:HB3	1.84	0.59
1:B:801:PHE:O	1:B:805:SER:OG	2.19	0.59
2:E:126:LEU:H	2:E:126:LEU:HD12	1.66	0.59
1:C:150:THR:HG23	1:C:153:ASP:H	1.67	0.59
1:C:151:GLN:HE21	1:C:286:ALA:H	1.49	0.59
1:A:16:ALA:HB2	1:A:488:LEU:HD22	1.83	0.59
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.85	0.59
1:B:576:VAL:HB	1:B:663:VAL:HG22	1.85	0.59
2:E:74:ASN:HD21	2:E:105:ASP:H	1.49	0.59
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.84	0.58
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	1.84	0.58
1:B:134:SER:OG	1:B:673:GLU:OE2	2.21	0.58
1:A:774:MET:HG2	1:A:775:SER:H	1.68	0.58
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.37	0.58
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.68	0.58
1:A:29:LYS:HE3	3:B:1102:LMT:H1'	1.86	0.58
1:C:370:ILE:O	1:C:373:PRO:HD2	2.04	0.58
1:C:690:LEU:HD21	1:C:854:GLY:HA3	1.85	0.58
1:A:907:LEU:HD22	1:A:1017:LEU:HB3	1.85	0.58
1:A:101:ASP:O	1:A:105:VAL:HG23	2.04	0.58
1:A:980:LEU:O	1:A:984:LEU:HB2	2.03	0.57
1:A:461:GLY:O	1:A:463:THR:N	2.37	0.57
1:C:70:ASN:O	1:C:110:LYS:NZ	2.38	0.57
1:A:839:GLU:HA	1:A:842:GLU:HB3	1.86	0.57
1:B:952:LEU:HD22	1:B:958:LYS:HD2	1.87	0.57
1:C:540:ARG:NH2	3:C:1102:LMT:O6'	2.38	0.57
1:B:871:ASN:HD22	3:B:1102:LMT:H6'1	1.69	0.57
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.87	0.57
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.87	0.57
1:A:878:ALA:O	1:A:882:ILE:HG12	2.05	0.57
1:B:897:ILE:HD12	1:B:950:LYS:HD2	1.87	0.56
1:A:166:ILE:HD12	1:A:306:ILE:HG23	1.87	0.56
2:E:67:LEU:HD21	2:E:73:VAL:HG23	1.86	0.56
1:C:904:VAL:HG13	1:C:938:SER:HB2	1.86	0.56
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	1.88	0.56
1:C:186:ILE:HB	1:C:773:VAL:HG12	1.87	0.56
1:A:401:ALA:O	1:A:405:LEU:HG	2.05	0.56
1:A:726:GLN:N	1:A:810:GLU:O	2.33	0.56
1:A:636:ASP:N	1:A:636:ASP:OD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:94:GLU:O	2:E:98:VAL:HG23	2.05	0.56
1:A:867:ARG:H	1:A:868:LEU:HB2	1.71	0.56
1:B:396:PHE:HA	1:B:399:VAL:HG13	1.88	0.56
1:C:150:THR:HG22	1:C:153:ASP:OD1	2.06	0.56
1:A:609:VAL:HG22	1:A:629:VAL:HG22	1.88	0.56
1:A:27:ILE:HD13	3:A:1101:LMT:H61	1.88	0.56
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.87	0.56
1:B:673:GLU:O	1:B:675:GLY:N	2.38	0.56
2:E:58:GLY:HA3	2:E:92:HIS:CE1	2.42	0.55
1:C:563:PHE:O	1:C:924:ASP:HB2	2.07	0.55
1:C:531:VAL:HA	1:C:534:ILE:HB	1.88	0.55
1:C:365:THR:O	1:C:369:THR:OG1	2.24	0.55
1:B:1024:VAL:O	1:B:1028:VAL:HG12	2.06	0.55
1:A:996:GLY:O	1:A:1000:GLN:HG3	2.06	0.55
1:A:415:ASN:OD1	1:A:418:ARG:NH1	2.39	0.55
1:B:715:SER:O	1:B:717:ARG:NH1	2.38	0.55
1:C:682:PHE:HB2	1:C:859:TRP:CZ3	2.41	0.55
1:B:352:PHE:HD2	1:B:353:LEU:HD13	1.72	0.55
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.88	0.55
2:D:126:LEU:H	2:D:126:LEU:HD12	1.71	0.55
2:E:30:VAL:O	2:E:34:MET:HB2	2.07	0.55
1:B:692:HIS:O	1:B:696:THR:HG23	2.07	0.55
1:A:49:TYR:CE2	1:A:121:GLU:HG3	2.41	0.55
2:D:48:TRP:CD1	2:D:77:ASP:HB3	2.40	0.54
1:C:507:GLU:HG2	1:C:518:ARG:HG2	1.89	0.54
2:D:29:GLU:O	2:D:33:LEU:HD12	2.08	0.54
1:C:379:THR:HG23	1:C:476:SER:HB2	1.89	0.54
1:C:151:GLN:NE2	1:C:286:ALA:H	2.05	0.54
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.88	0.54
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.88	0.54
1:A:453:PHE:O	1:A:471:SER:OG	2.24	0.54
1:A:20:MET:HG3	1:A:377:LEU:HD13	1.88	0.54
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.07	0.54
1:B:877:TYR:HE2	3:B:1103:LMT:H11	1.72	0.54
1:B:144:ASN:HB2	1:B:154:ILE:HD11	1.89	0.54
1:A:393:LEU:HD22	1:A:470:PHE:HE1	1.72	0.54
2:E:113:GLY:O	2:E:143:ASP:HA	2.08	0.54
1:C:485:ALA:HA	1:C:489:THR:OG1	2.08	0.54
1:A:574:THR:HB	1:A:627:ALA:HB3	1.89	0.53
1:C:203:VAL:O	1:C:207:ILE:HG13	2.08	0.53
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:ALA:O	1:A:781:MET:HG2	2.09	0.53
1:A:576:VAL:HG22	1:A:663:VAL:HG22	1.90	0.53
1:C:181:GLN:O	1:C:272:GLY:HA2	2.08	0.53
1:C:36:PRO:O	1:C:38:ILE:HG23	2.08	0.53
1:C:882:ILE:O	1:C:886:LEU:HG	2.08	0.53
1:B:10:ILE:HD12	1:C:895:TRP:NE1	2.23	0.53
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.89	0.53
1:C:418:ARG:HH12	1:C:970:MET:HG2	1.74	0.53
1:B:328:ASP:OD1	1:B:330:THR:HB	2.08	0.53
1:A:1022:VAL:HA	1:A:1025:PHE:HD1	1.74	0.53
1:C:648:THR:HG22	1:C:665:ALA:HB1	1.90	0.53
1:B:416:VAL:HG21	1:B:431:THR:HG22	1.91	0.53
1:A:366:LEU:O	1:A:370:ILE:HG12	2.08	0.53
1:B:42:ALA:HB3	1:B:132:SER:HB2	1.91	0.53
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.43	0.53
1:C:438:ILE:HG12	1:C:442:LEU:HG	1.91	0.53
1:C:150:THR:OG1	1:C:151:GLN:N	2.41	0.52
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.90	0.52
1:C:600:THR:O	1:C:603:LYS:HE3	2.09	0.52
2:E:41:ASN:HD21	2:E:72:ASP:HB2	1.75	0.52
1:C:3:ASN:HA	1:C:6:ILE:HD12	1.91	0.52
1:A:393:LEU:HD22	1:A:470:PHE:CE1	2.44	0.52
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.90	0.52
1:B:83:ASP:OD2	1:B:85:THR:OG1	2.27	0.52
2:E:93:LEU:HD13	2:E:128:ILE:HG12	1.90	0.52
1:B:925:VAL:O	1:B:929:VAL:HG23	2.09	0.52
1:A:545:TYR:O	1:A:549:VAL:HG23	2.10	0.52
1:A:960:LEU:HG	1:A:1027:VAL:HG12	1.92	0.52
2:E:89:HIS:CD2	2:E:119:LEU:HG	2.45	0.52
1:A:435:MET:O	1:A:439:GLN:HB2	2.10	0.52
2:E:85:HIS:NE2	2:E:114:ILE:O	2.30	0.52
1:C:667:ASN:OD1	1:C:668:LEU:N	2.42	0.52
1:A:544:LEU:O	1:A:548:ILE:HG12	2.10	0.51
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.45	0.51
1:A:867:ARG:HG3	1:A:868:LEU:HD13	1.92	0.51
1:C:949:ALA:O	1:C:953:MET:HG3	2.10	0.51
1:B:573:MET:HE3	1:B:666:PHE:CE2	2.45	0.51
1:A:817:GLU:HB2	1:A:824:SER:O	2.11	0.51
1:B:676:THR:OG1	1:B:679:GLY:HA3	2.09	0.51
1:A:879:ILE:HG12	1:A:880:SER:N	2.21	0.51
1:C:480:LEU:O	1:C:484:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ARG:HB3	1:A:868:LEU:CB	2.39	0.51
1:A:355:MET:HA	1:A:355:MET:HE2	1.92	0.51
1:B:584:GLN:HB3	1:B:622:GLN:CG	2.41	0.51
1:C:218:GLN:HA	1:C:234:ILE:HG13	1.92	0.51
1:B:423:GLU:OE1	1:B:433:LYS:NZ	2.41	0.51
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.93	0.51
1:B:632:LYS:O	1:B:637:ARG:NE	2.31	0.51
1:C:102:ILE:O	1:C:106:GLN:HG3	2.10	0.51
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.92	0.51
1:C:595:THR:HG23	1:C:609:VAL:HG11	1.93	0.51
1:B:16:ALA:O	1:B:20:MET:HG3	2.10	0.51
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.91	0.51
1:A:750:LEU:HB2	1:A:801:PHE:CZ	2.46	0.51
1:A:255:GLN:CD	1:A:255:GLN:H	2.14	0.51
1:B:616:ASN:HB3	1:B:619:GLY:O	2.11	0.51
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.45	0.51
1:A:865:GLN:HA	1:A:867:ARG:N	2.26	0.50
2:D:30:VAL:HG21	2:D:62:ILE:HG12	1.92	0.50
1:A:676:THR:O	1:A:678:THR:N	2.38	0.50
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.94	0.50
1:A:110:LYS:O	1:A:113:LEU:HB2	2.12	0.50
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.46	0.50
1:C:873:ALA:N	1:C:874:PRO:HD2	2.27	0.50
1:A:146:ASP:CB	1:A:148:THR:HG23	2.41	0.50
1:B:355:MET:O	1:B:359:LEU:HB2	2.12	0.50
1:A:594:VAL:HA	1:A:655:PHE:CE1	2.47	0.50
1:C:564:LEU:HD12	1:C:926:TYR:CE1	2.47	0.50
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.93	0.50
1:C:575:MET:HG3	1:C:666:PHE:CE1	2.46	0.50
1:B:960:LEU:HD21	1:B:1027:VAL:HA	1.93	0.50
1:A:14:VAL:O	1:A:18:ILE:HG12	2.12	0.50
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.93	0.50
1:C:45:ILE:HG12	1:C:129:VAL:HG22	1.93	0.50
1:C:645:GLU:O	1:C:649:MET:HB2	2.12	0.50
1:C:644:VAL:O	1:C:648:THR:OG1	2.29	0.49
1:A:263:ARG:NH2	2:D:155:ASN:O	2.43	0.49
2:E:160:ASP:O	2:E:163:GLU:HG2	2.12	0.49
1:B:39:ALA:HB2	1:B:673:GLU:HG2	1.94	0.49
1:C:784:ASP:N	1:C:784:ASP:OD2	2.43	0.49
1:A:775:SER:OG	1:A:789:TRP:HZ2	1.95	0.49
2:E:89:HIS:O	2:E:123:ARG:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.12	0.49
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.12	0.49
1:B:30:LEU:HB3	1:B:390:ILE:HD12	1.95	0.49
1:B:875:SER:O	1:B:879:ILE:HG12	2.11	0.49
1:A:303:ALA:HB2	1:A:330:THR:HG21	1.94	0.49
1:A:865:GLN:HA	1:A:866:GLU:C	2.33	0.49
2:E:56:TYR:HD1	2:E:57:TRP:CE3	2.30	0.49
2:D:48:TRP:HD1	2:D:77:ASP:HB3	1.77	0.49
1:A:864:TYR:C	1:A:867:ARG:HB2	2.33	0.49
1:C:573:MET:HB2	1:C:666:PHE:CE2	2.48	0.49
1:C:997:SER:HA	1:C:1000:GLN:HG3	1.95	0.49
1:A:85:THR:HG21	1:A:620:ARG:HG2	1.95	0.49
1:C:331:PRO:O	1:C:335:ILE:HG22	2.13	0.49
1:B:866:GLU:O	1:B:868:LEU:N	2.46	0.48
1:B:809:TRP:NE1	2:D:79:LEU:HD22	2.28	0.48
1:B:885:PHE:HA	1:B:902:MET:HE1	1.96	0.48
1:B:426:PRO:HD2	1:B:429:GLU:HG3	1.95	0.48
1:C:352:PHE:HD1	1:C:369:THR:HG21	1.78	0.48
1:A:63:GLN:CD	1:C:768:VAL:HG23	2.33	0.48
1:C:640:GLU:HA	1:C:643:LYS:HG2	1.95	0.48
1:A:575:MET:HE3	1:A:575:MET:HB3	1.56	0.48
2:E:23:ARG:HB2	2:E:53:LEU:HD13	1.94	0.48
2:E:76:TYR:HD2	2:E:76:TYR:H	1.61	0.48
1:C:880:SER:O	1:C:884:VAL:HG23	2.12	0.48
1:C:983:ILE:HG13	1:C:1011:MET:HG2	1.95	0.48
1:A:544:LEU:HA	1:A:547:ILE:HD12	1.95	0.48
1:A:594:VAL:HG13	1:A:655:PHE:CZ	2.49	0.48
2:E:160:ASP:O	2:E:164:ILE:HG13	2.14	0.48
1:C:228:GLN:HG3	1:C:229:GLN:N	2.27	0.48
2:D:148:THR:O	2:D:152:ILE:HG12	2.13	0.48
1:A:578:LEU:HD13	1:A:587:THR:HG23	1.96	0.48
1:A:527:TYR:CE1	1:A:968:VAL:HG13	2.48	0.48
2:D:72:ASP:HB3	2:D:75:ALA:HB2	1.96	0.48
1:B:446:ALA:HA	1:B:478:MET:HE1	1.94	0.48
1:A:68:ASN:O	1:A:110:LYS:HB3	2.13	0.48
1:A:530:SER:O	1:A:534:ILE:HG23	2.14	0.48
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.44	0.48
1:C:309:GLU:O	1:C:313:MET:HG3	2.12	0.47
1:B:964:THR:O	1:B:968:VAL:HB	2.14	0.47
2:E:125:HIS:O	2:E:129:VAL:HG23	2.13	0.47
2:E:127:GLU:O	2:E:131:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:SER:HB2	1:B:273:GLU:HG3	1.95	0.47
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.34	0.47
1:B:371:ALA:O	1:B:375:VAL:HG23	2.13	0.47
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.97	0.47
1:A:528:THR:HG21	1:A:969:ARG:HB3	1.97	0.47
1:B:982:PHE:O	1:B:986:VAL:HG13	2.15	0.47
2:E:27:ASP:HA	2:E:62:ILE:HD11	1.96	0.47
1:A:360:GLN:HG3	1:A:513:PHE:CD1	2.49	0.47
1:C:459:PHE:CE1	1:C:876:LEU:HD23	2.50	0.47
1:C:948:PHE:CE1	1:C:970:MET:HE2	2.49	0.47
1:B:5:PHE:CD1	1:B:487:ILE:HG23	2.50	0.47
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.97	0.47
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.97	0.47
1:B:448:VAL:O	1:B:452:VAL:HG23	2.15	0.47
2:D:12:SER:O	2:D:16:LYS:HG2	2.15	0.47
1:A:358:PHE:HE2	1:A:520:PHE:HE1	1.62	0.47
1:C:621:GLY:O	1:C:624:THR:HB	2.14	0.47
1:C:20:MET:HG2	1:C:377:LEU:HD12	1.96	0.47
1:A:527:TYR:HE1	1:A:968:VAL:HG13	1.80	0.47
1:A:2:PRO:O	1:A:6:ILE:HG13	2.15	0.47
1:B:616:ASN:HB2	1:B:624:THR:HB	1.96	0.47
1:A:1043:SER:HA	1:A:1044:HIS:HA	1.57	0.47
1:C:61:VAL:O	1:C:65:ILE:HG13	2.14	0.47
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.96	0.47
1:A:572:PHE:HE1	1:A:631:LEU:HD21	1.80	0.47
1:A:919:ARG:NH2	1:A:990:VAL:O	2.48	0.47
1:C:151:GLN:NE2	1:C:279:ALA:O	2.47	0.46
1:A:919:ARG:HB3	1:A:921:LEU:HD22	1.97	0.46
1:C:358:PHE:CD1	1:C:977:MET:HG2	2.50	0.46
2:E:77:ASP:O	2:E:80:GLY:N	2.48	0.46
1:B:154:ILE:O	1:B:158:VAL:HG23	2.15	0.46
2:D:92:HIS:O	2:D:96:VAL:HG23	2.14	0.46
3:A:1102:LMT:H6D	3:A:1102:LMT:H5B	1.96	0.46
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.51	0.46
1:C:259:ARG:HH22	2:E:155:ASN:CG	2.17	0.46
2:D:94:GLU:CD	2:D:94:GLU:H	2.18	0.46
1:C:671:ILE:H	1:C:862:MET:HE1	1.80	0.46
1:C:984:LEU:HD12	1:C:987:MET:HG3	1.98	0.46
1:A:132:SER:HB3	1:A:173:GLY:HA3	1.96	0.46
1:A:925:VAL:O	1:A:929:VAL:HG22	2.16	0.46
1:C:509:LYS:HA	1:C:510:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.76	0.46
1:C:958:LYS:HB2	1:C:963:ALA:HB2	1.98	0.46
1:C:33:ALA:O	1:C:337:ILE:HD11	2.16	0.46
1:B:377:LEU:HA	1:B:377:LEU:HD12	1.75	0.46
1:B:986:VAL:O	1:B:990:VAL:HG23	2.15	0.46
1:A:809:TRP:NE1	2:E:78:THR:HG23	2.26	0.46
1:B:905:VAL:O	1:B:909:VAL:HG23	2.15	0.46
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.97	0.46
1:A:108:GLN:HG3	1:A:108:GLN:O	2.16	0.46
1:B:14:VAL:HG13	1:C:886:LEU:HB3	1.97	0.46
1:B:100:ALA:HB1	1:B:131:LYS:HD3	1.98	0.46
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.51	0.46
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.97	0.46
1:A:407:ASP:HB2	1:A:978:THR:HG21	1.98	0.46
1:A:774:MET:HG2	1:A:775:SER:N	2.30	0.46
1:A:459:PHE:CE2	1:A:873:ALA:HB2	2.51	0.45
1:C:383:LEU:HA	1:C:383:LEU:HD12	1.79	0.45
1:C:200:PRO:HD2	1:C:749:THR:HG23	1.98	0.45
2:E:123:ARG:HG2	2:E:125:HIS:HE1	1.79	0.45
3:A:1102:LMT:H41	3:A:1102:LMT:H72	1.56	0.45
1:B:534:ILE:HG23	1:B:541:TYR:CE1	2.51	0.45
1:A:156:ASP:HB2	1:A:182:TYR:CD1	2.51	0.45
1:C:685:ILE:HD11	1:C:858:ASP:HB2	1.97	0.45
1:C:846:GLN:O	1:C:849:SER:OG	2.34	0.45
1:A:416:VAL:HG11	1:A:431:THR:HG22	1.99	0.45
1:A:1013:THR:HB	1:A:1017:LEU:HD23	1.97	0.45
1:A:687:GLN:HG3	1:A:856:GLY:N	2.30	0.45
1:B:428:LYS:HE3	1:B:432:ARG:NH2	2.32	0.45
1:A:674:LEU:HD22	1:A:676:THR:N	2.31	0.45
1:C:686:ASP:HB3	1:C:823:PRO:HB2	1.97	0.45
1:C:139:VAL:HG13	1:C:178:PHE:HE1	1.82	0.45
1:C:425:LEU:HA	1:C:425:LEU:HD12	1.86	0.45
1:B:472:ILE:HD13	1:B:472:ILE:HA	1.89	0.45
1:B:111:LEU:O	1:B:115:MET:HG2	2.16	0.45
1:A:780:ARG:HG3	1:A:780:ARG:HH11	1.82	0.45
1:A:877:TYR:HA	1:A:880:SER:HB3	1.97	0.45
1:B:874:PRO:HG2	1:B:875:SER:H	1.82	0.45
1:A:83:ASP:OD2	1:A:85:THR:HG23	2.16	0.45
1:B:448:VAL:HG21	1:B:888:LEU:HD13	1.98	0.45
1:A:395:MET:O	1:A:399:VAL:HG23	2.17	0.45
1:A:589:LYS:O	1:A:593:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ALA:O	1:C:482:VAL:HG13	2.17	0.45
1:A:867:ARG:CB	1:A:868:LEU:HB2	2.41	0.45
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.98	0.45
1:A:546:LEU:O	1:A:550:VAL:HG23	2.17	0.45
1:A:517:ASN:HD22	1:A:517:ASN:N	2.15	0.45
1:C:400:LEU:O	1:C:404:LEU:HD22	2.17	0.44
2:E:100:LEU:HD23	2:E:100:LEU:HA	1.74	0.44
1:B:185:ARG:HD2	1:B:185:ARG:HA	1.74	0.44
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.50	0.44
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.71	0.44
1:B:878:ALA:O	1:B:882:ILE:HG13	2.17	0.44
1:B:402:ILE:HD12	1:B:402:ILE:HA	1.74	0.44
1:A:673:GLU:OE1	1:A:865:GLN:NE2	2.51	0.44
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.81	0.44
1:B:575:MET:O	1:B:663:VAL:HA	2.17	0.44
1:A:463:THR:O	1:A:467:TYR:HD2	1.99	0.44
1:A:449:LEU:O	1:A:452:VAL:HG13	2.18	0.44
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.18	0.44
1:B:764:ASP:OD2	1:B:769:LYS:NZ	2.50	0.44
1:B:584:GLN:N	1:B:622:GLN:HG2	2.33	0.44
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.33	0.44
1:B:9:PRO:HG3	1:B:495:THR:HG21	1.98	0.44
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.17	0.44
1:C:36:PRO:HD3	1:C:391:ASN:ND2	2.33	0.44
1:A:750:LEU:HB2	1:A:801:PHE:HZ	1.82	0.44
1:C:447:MET:SD	1:C:887:CYS:HB3	2.57	0.44
1:A:599:LEU:HA	1:A:599:LEU:HD23	1.78	0.44
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.53	0.44
1:B:364:ALA:HB2	1:B:497:LEU:HD11	1.99	0.44
1:C:754:TRP:CZ2	1:C:786:ILE:HG13	2.52	0.44
1:A:56:THR:HG23	1:C:213:GLN:HG2	1.99	0.44
1:B:685:ILE:HG22	1:B:687:GLN:HG2	2.00	0.44
2:D:11:GLY:N	2:D:16:LYS:HD3	2.33	0.44
1:B:169:THR:O	1:B:172:VAL:HG13	2.17	0.44
1:C:900:SER:OG	1:C:1026:PHE:HA	2.17	0.44
1:C:674:LEU:HA	1:C:674:LEU:HD23	1.78	0.44
1:B:30:LEU:HA	1:B:31:PRO:HD3	1.88	0.44
1:A:467:TYR:CZ	1:A:925:VAL:HG22	2.53	0.44
1:C:434:SER:O	1:C:438:ILE:HG23	2.17	0.44
1:C:510:LYS:O	1:C:510:LYS:HG2	2.17	0.44
1:A:948:PHE:O	1:A:952:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:LYS:HE3	2:D:144:LYS:HB2	1.82	0.44
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.99	0.44
1:A:27:ILE:HG23	3:A:1101:LMT:H41	2.00	0.44
1:B:144:ASN:HA	1:B:320:GLY:O	2.18	0.44
1:A:681:ASP:H	1:A:863:SER:HB2	1.83	0.44
1:C:688:ALA:HB3	1:C:690:LEU:HD22	1.99	0.43
1:C:984:LEU:HA	1:C:984:LEU:HD12	1.77	0.43
1:B:841:MET:HG2	1:B:859:TRP:CZ2	2.53	0.43
1:C:901:VAL:HG13	1:C:942:ALA:HB3	2.00	0.43
1:B:706:ALA:HB1	1:B:713:LEU:HD23	1.99	0.43
1:C:577:GLN:HB2	1:C:577:GLN:HE21	1.57	0.43
1:B:492:LEU:O	1:B:496:MET:HB2	2.18	0.43
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.79	0.43
1:A:150:THR:O	1:A:154:ILE:HG13	2.18	0.43
1:B:2:PRO:HG3	1:B:486:LEU:HD23	2.01	0.43
2:E:142:GLN:HB3	2:E:146:GLY:HA2	1.99	0.43
1:C:41:PRO:HG2	1:C:94:PHE:HB2	2.00	0.43
2:D:76:TYR:N	2:D:76:TYR:CD2	2.86	0.43
1:C:255:GLN:OE1	1:C:255:GLN:N	2.49	0.43
2:D:127:GLU:H	2:D:127:GLU:HG2	1.27	0.43
1:A:531:VAL:O	1:A:535:LEU:HG	2.17	0.43
1:B:23:GLY:O	1:B:27:ILE:HG13	2.19	0.43
1:C:746:ILE:HG13	1:C:804:PHE:CE2	2.54	0.43
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.35	0.43
1:A:174:ASP:HB3	1:A:292:LYS:HG3	1.99	0.43
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.77	0.43
1:C:216:ALA:HB3	1:C:234:ILE:O	2.19	0.43
1:C:1029:VAL:C	1:C:1031:ARG:H	2.22	0.43
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.99	0.43
1:C:598:TYR:HB3	1:C:606:VAL:HG21	2.01	0.43
1:B:530:SER:O	1:B:534:ILE:HG13	2.19	0.43
1:A:298:ASN:HB3	1:A:301:ASP:HB2	2.01	0.43
1:A:36:PRO:O	1:A:38:ILE:HG23	2.18	0.43
1:A:586:ARG:HH12	1:A:660:ASP:HB3	1.84	0.43
1:B:125:GLN:NE2	1:B:772:TYR:OH	2.52	0.43
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.54	0.43
1:A:415:ASN:O	1:A:419:VAL:HG23	2.19	0.43
2:D:76:TYR:N	2:D:76:TYR:HD2	2.17	0.43
1:C:398:MET:O	1:C:402:ILE:HG12	2.18	0.43
1:B:641:GLU:H	1:B:641:GLU:HG3	1.49	0.43
1:B:918:PHE:C	1:B:918:PHE:CD1	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HG11	1:A:405:LEU:HD22	2.01	0.42
1:B:677:ALA:C	1:B:679:GLY:H	2.22	0.42
1:C:102:ILE:HA	1:C:102:ILE:HD13	1.79	0.42
1:C:350:LEU:O	1:C:354:VAL:HG23	2.19	0.42
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.19	0.42
1:B:302:THR:O	1:B:306:ILE:HG13	2.19	0.42
1:B:352:PHE:HE1	1:B:365:THR:HG21	1.83	0.42
1:B:418:ARG:HD2	1:B:970:MET:HG2	2.00	0.42
1:B:741:VAL:HG22	1:B:793:ALA:HB2	2.02	0.42
1:A:1038:GLU:OE2	1:A:1039:ASP:HA	2.19	0.42
1:A:1030:ARG:HD2	1:A:1030:ARG:HA	1.86	0.42
1:C:553:ALA:O	1:C:557:VAL:HG22	2.18	0.42
1:A:684:LEU:O	1:A:824:SER:HA	2.18	0.42
1:C:259:ARG:NH2	2:E:155:ASN:OD1	2.33	0.42
1:A:428:LYS:O	1:A:432:ARG:HB2	2.19	0.42
2:D:59:HIS:O	2:D:63:VAL:HG23	2.20	0.42
1:A:547:ILE:O	1:A:550:VAL:HB	2.18	0.42
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.19	0.42
1:C:984:LEU:O	1:C:987:MET:HB2	2.19	0.42
1:C:527:TYR:O	1:C:530:SER:HB3	2.19	0.42
1:C:403:GLY:HA3	1:C:982:PHE:HA	2.00	0.42
1:C:31:PRO:HB2	1:C:389:SER:HB3	2.01	0.42
1:A:189:ASN:ND2	1:A:779:TYR:CZ	2.88	0.42
1:A:1004:GLY:O	1:A:1008:MET:HB2	2.19	0.42
1:A:743:ILE:HG12	1:A:743:ILE:H	1.57	0.42
1:B:914:LEU:HA	1:B:914:LEU:HD13	1.92	0.42
1:A:370:ILE:O	1:A:374:VAL:HG23	2.20	0.42
1:A:905:VAL:HG22	1:A:935:ILE:HG23	2.02	0.42
1:B:466:ILE:HD11	1:B:671:ILE:HD12	2.02	0.42
1:A:58:GLN:HA	1:A:62:THR:OG1	2.19	0.42
2:D:18:LEU:HD23	2:D:39:ASP:O	2.19	0.42
1:A:809:TRP:NE1	2:E:79:LEU:HD22	2.35	0.42
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.55	0.42
1:A:712:MET:HB3	1:A:713:LEU:HD13	2.01	0.42
1:B:193:LEU:HB3	1:B:198:LEU:O	2.20	0.42
1:C:456:MET:HE2	1:C:467:TYR:HB3	2.02	0.42
1:C:976:LEU:HA	1:C:976:LEU:HD12	1.83	0.42
1:C:605:ASN:O	1:C:632:LYS:N	2.50	0.42
1:C:426:PRO:HG2	1:C:429:GLU:HB3	2.01	0.42
1:B:602:GLU:OE1	1:B:647:ILE:HG23	2.20	0.42
2:E:119:LEU:HD12	2:E:119:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:HB3	1:A:52:ALA:HB3	2.02	0.42
1:C:185:ARG:HD3	1:C:272:GLY:O	2.20	0.42
1:C:509:LYS:HA	1:C:510:LYS:CB	2.49	0.42
1:B:639:GLY:O	1:B:641:GLU:N	2.52	0.42
1:B:509:LYS:HG2	1:B:510:LYS:H	1.85	0.42
1:C:1:MET:O	1:C:4:PHE:HB3	2.19	0.42
1:B:541:TYR:HA	1:B:544:LEU:HB2	2.02	0.41
1:A:159:ALA:HB2	1:A:177:LEU:HD22	2.02	0.41
1:C:955:LYS:N	1:C:955:LYS:HD2	2.35	0.41
1:C:57:VAL:HG21	1:C:86:GLY:CA	2.41	0.41
1:A:331:PRO:O	1:A:335:ILE:HG13	2.20	0.41
1:A:261:LEU:O	1:A:264:ASP:HB2	2.21	0.41
1:B:904:VAL:O	1:B:907:LEU:HB2	2.19	0.41
1:B:199:THR:OG1	1:B:201:VAL:HB	2.20	0.41
2:D:133:LEU:HA	2:D:133:LEU:HD23	1.80	0.41
1:A:934:THR:HG22	1:A:1011:MET:HG2	2.02	0.41
1:C:38:ILE:HD11	1:C:671:ILE:HG21	2.02	0.41
1:C:61:VAL:HA	1:C:118:LEU:HD22	2.03	0.41
1:B:568:ASP:OD2	1:B:644:VAL:N	2.44	0.41
1:A:701:GLN:O	1:A:705:GLU:HG2	2.21	0.41
1:C:158:VAL:HG22	1:C:162:MET:SD	2.60	0.41
1:B:183:ALA:N	1:B:271:GLY:O	2.53	0.41
2:E:17:LYS:HB2	2:E:33:LEU:HD13	2.03	0.41
1:A:542:LEU:HA	1:A:542:LEU:HD13	1.75	0.41
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.81	0.41
1:B:960:LEU:CD2	1:B:1027:VAL:HG22	2.50	0.41
1:A:344:LEU:O	1:A:348:ILE:HG13	2.20	0.41
1:C:314:GLU:HA	1:C:317:PHE:CE1	2.56	0.41
2:E:107:ASN:HD21	2:E:138:ASP:HB2	1.85	0.41
1:C:819:TYR:N	1:C:824:SER:HB3	2.34	0.41
1:B:921:LEU:HB3	1:B:922:THR:H	1.60	0.41
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.89	0.41
1:B:695:LEU:HD23	1:B:695:LEU:HA	1.61	0.41
1:B:575:MET:HE3	1:B:575:MET:HB2	1.75	0.41
1:C:534:ILE:HG23	1:C:541:TYR:CE2	2.55	0.41
1:C:897:ILE:HD11	1:C:950:LYS:HD3	2.02	0.41
1:C:330:THR:N	1:C:331:PRO:HD2	2.36	0.41
1:C:937:LEU:HB3	1:C:1011:MET:HE3	2.03	0.41
1:C:934:THR:HA	1:C:937:LEU:HD12	2.01	0.41
1:A:159:ALA:HB3	1:A:181:GLN:HG3	2.01	0.41
1:C:709:HIS:N	1:C:710:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:TYR:HB3	1:B:270:LEU:HD12	2.02	0.41
1:C:690:LEU:HB3	1:C:694:LYS:HB2	2.02	0.41
1:C:671:ILE:HG13	1:C:671:ILE:O	2.20	0.41
1:A:1038:GLU:CD	1:A:1039:ASP:HA	2.40	0.41
1:B:344:LEU:O	1:B:348:ILE:HG12	2.20	0.41
1:A:914:LEU:HD23	1:A:914:LEU:HA	1.89	0.41
1:A:480:LEU:HD13	1:A:480:LEU:HA	1.84	0.41
1:C:468:ARG:O	1:C:472:ILE:HG22	2.20	0.41
1:A:669:PRO:CG	1:A:674:LEU:HD21	2.50	0.41
1:C:35:TYR:CD2	1:C:671:ILE:HG22	2.56	0.41
1:A:358:PHE:HE2	1:A:520:PHE:CE1	2.39	0.41
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.84	0.41
1:A:851:LEU:HD23	1:A:851:LEU:HA	1.82	0.41
1:B:756:GLY:HA3	1:B:774:MET:HE2	2.02	0.41
1:A:428:LYS:HG2	1:A:432:ARG:HH21	1.85	0.41
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.41
1:A:367:ILE:HB	1:A:368:PRO:HD3	2.02	0.41
1:A:741:VAL:HG12	1:A:793:ALA:HB2	2.02	0.41
2:D:42:ALA:O	2:D:50:PRO:HD3	2.21	0.41
1:B:527:TYR:CD2	1:B:972:LEU:HG	2.56	0.41
1:C:952:LEU:O	1:C:956:GLU:HB2	2.21	0.41
1:C:1033:PHE:N	1:C:1033:PHE:CD2	2.89	0.41
1:C:310:LEU:HA	1:C:310:LEU:HD12	1.94	0.41
1:B:743:ILE:HG12	1:B:743:ILE:H	1.57	0.41
1:C:146:ASP:O	1:C:148:THR:N	2.54	0.41
1:A:563:PHE:CD1	1:A:564:LEU:HG	2.55	0.41
1:B:483:LEU:HD13	1:B:483:LEU:HA	1.75	0.41
1:A:864:TYR:HB3	1:A:865:GLN:H	1.74	0.41
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.44	0.41
1:B:921:LEU:HA	1:B:921:LEU:HD12	1.82	0.41
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.56	0.41
1:B:102:ILE:O	1:B:106:GLN:HG3	2.20	0.41
1:C:69:MET:HG3	1:C:92:LEU:HD21	2.03	0.41
1:A:355:MET:O	1:A:359:LEU:HB2	2.20	0.40
1:C:907:LEU:O	1:C:910:ILE:HG22	2.21	0.40
2:E:76:TYR:N	2:E:76:TYR:CD2	2.88	0.40
1:B:115:MET:HE1	1:B:123:GLN:HA	2.02	0.40
2:E:128:ILE:O	2:E:132:LEU:HG	2.21	0.40
1:B:190:PRO:HB3	1:B:789:TRP:CZ3	2.56	0.40
1:A:649:MET:HE1	1:A:653:ARG:HH11	1.87	0.40
1:B:349:ILE:O	1:B:353:LEU:HD22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.56	0.40
1:A:159:ALA:CB	1:A:181:GLN:HG3	2.52	0.40
2:D:109:LYS:HG2	2:D:115:THR:HG22	2.04	0.40
1:A:32:VAL:HG12	1:A:390:ILE:HB	2.02	0.40
1:C:15:ILE:O	1:C:19:ILE:HG13	2.21	0.40
1:A:745:ASP:HB3	1:A:791:VAL:HG11	2.04	0.40
1:A:841:MET:O	1:A:845:GLU:HG3	2.22	0.40
1:C:964:THR:O	1:C:968:VAL:HB	2.21	0.40
1:C:30:LEU:HA	1:C:31:PRO:HD3	1.96	0.40
1:C:184:MET:HB3	1:C:771:VAL:HG22	2.03	0.40
1:C:986:VAL:O	1:C:990:VAL:HG23	2.22	0.40
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.03	0.40
1:A:489:THR:O	1:A:493:CYS:HB2	2.21	0.40
1:B:559:LEU:HD23	1:B:923:ASN:HB2	2.04	0.40
1:C:923:ASN:OD1	1:C:927:PHE:HD2	2.05	0.40
2:D:126:LEU:HD12	2:D:126:LEU:N	2.36	0.40
1:C:489:THR:OG1	1:C:490:PRO:HD3	2.21	0.40
1:B:809:TRP:CD1	2:D:79:LEU:HD22	2.56	0.40
1:A:1039:ASP:H	1:A:1040:ILE:HD12	1.86	0.40
1:B:703:LEU:HD11	1:B:718:PRO:HG3	2.03	0.40
1:A:553:ALA:O	1:A:557:VAL:HG22	2.21	0.40
1:A:84:SER:OG	1:A:814:PRO:HA	2.22	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%)	963 (92%)	63 (6%)	16 (2%)	13 42
1	B	1031/1057 (98%)	954 (92%)	66 (6%)	11 (1%)	17 51
1	C	1032/1057 (98%)	963 (93%)	66 (6%)	3 (0%)	46 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	154/169 (91%)	144 (94%)	10 (6%)	0	100	100
2	E	150/169 (89%)	139 (93%)	10 (7%)	1 (1%)	26	63
All	All	3409/3509 (97%)	3163 (93%)	215 (6%)	31 (1%)	21	57

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	SER
1	A	864	TYR
1	A	866	GLU
1	A	1040	ILE
1	B	510	LYS
1	B	674	LEU
1	A	618	ALA
1	B	640	GLU
1	B	659	LYS
1	C	147	GLY
1	C	1031	ARG
1	A	424	GLY
1	A	617	PHE
1	A	634	TRP
1	A	869	SER
1	B	670	ALA
1	B	867	ARG
1	B	874	PRO
1	B	918	PHE
1	C	510	LYS
1	A	504	ASP
1	A	852	PRO
1	B	34	GLN
1	A	126	GLY
1	A	145	THR
1	A	677	ALA
1	A	1043	SER
1	B	820	ASN
1	B	833	PRO
1	A	461	GLY
2	E	45	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	851/864 (98%)	747 (88%)	104 (12%)	6 18
1	B	840/864 (97%)	748 (89%)	92 (11%)	8 23
1	C	841/864 (97%)	742 (88%)	99 (12%)	6 19
2	D	120/132 (91%)	111 (92%)	9 (8%)	17 44
2	E	117/132 (89%)	101 (86%)	16 (14%)	4 13
All	All	2769/2856 (97%)	2449 (88%)	320 (12%)	7 20

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	11	PHE
1	A	25	LEU
1	A	30	LEU
1	A	32	VAL
1	A	37	THR
1	A	46	SER
1	A	49	TYR
1	A	60	THR
1	A	70	ASN
1	A	82	SER
1	A	85	THR
1	A	88	VAL
1	A	96	SER
1	A	113	LEU
1	A	121	GLU
1	A	128	SER
1	A	130	GLU
1	A	143	ILE
1	A	153	ASP
1	A	214	VAL
1	A	222	THR
1	A	226	LYS

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	240	LEU
1	A	245	GLU
1	A	249	ILE
1	A	262	LEU
1	A	263	ARG
1	A	289	LEU
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	329	THR
1	A	360	GLN
1	A	362	PHE
1	A	365	THR
1	A	376	LEU
1	A	425	LEU
1	A	433	LYS
1	A	447	MET
1	A	456	MET
1	A	463	THR
1	A	471	SER
1	A	486	LEU
1	A	492	LEU
1	A	493	CYS
1	A	507	GLU
1	A	510	LYS
1	A	523	SER
1	A	534	ILE
1	A	536	ARG
1	A	540	ARG
1	A	544	LEU
1	A	566	ASP
1	A	577	GLN
1	A	608	SER
1	A	620	ARG
1	A	626	ILE
1	A	636	ASP
1	A	659	LYS
1	A	660	ASP
1	A	673	GLU
1	A	678	THR
1	A	687	GLN

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Mol	Chain	Res	Type
1	A	695	LEU
1	A	712	MET
1	A	717	ARG
1	A	728	LYS
1	A	729	ILE
1	A	743	ILE
1	A	758	TYR
1	A	767	ARG
1	A	773	VAL
1	A	776	GLU
1	A	778	LYS
1	A	801	PHE
1	A	830	GLN
1	A	839	GLU
1	A	862	MET
1	A	863	SER
1	A	864	TYR
1	A	867	ARG
1	A	872	GLN
1	A	879	ILE
1	A	881	LEU
1	A	919	ARG
1	A	921	LEU
1	A	931	LEU
1	A	934	THR
1	A	944	LEU
1	A	946	VAL
1	A	953	MET
1	A	961	ILE
1	A	968	VAL
1	A	969	ARG
1	A	971	ARG
1	A	973	ARG
1	A	984	LEU
1	A	1008	MET
1	A	1035	ARG
1	A	1040	ILE
1	A	1041	GLU
1	A	1044	HIS
1	B	6	ILE
1	B	11	PHE
1	B	21	LEU

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Mol	Chain	Res	Type
1	B	46	SER
1	B	49	TYR
1	B	75	LEU
1	B	84	SER
1	B	87	THR
1	B	96	SER
1	B	111	LEU
1	B	130	GLU
1	B	143	ILE
1	B	151	GLN
1	B	172	VAL
1	B	185	ARG
1	B	250	LEU
1	B	255	GLN
1	B	256	ASP
1	B	270	LEU
1	B	293	LEU
1	B	330	THR
1	B	338	HIS
1	B	353	LEU
1	B	365	THR
1	B	377	LEU
1	B	383	LEU
1	B	399	VAL
1	B	402	ILE
1	B	408	ASP
1	B	429	GLU
1	B	468	ARG
1	B	483	LEU
1	B	497	LEU
1	B	510	LYS
1	B	512	PHE
1	B	530	SER
1	B	544	LEU
1	B	546	LEU
1	B	555	LEU
1	B	556	PHE
1	B	569	GLN
1	B	572	PHE
1	B	574	THR
1	B	576	VAL
1	B	577	GLN

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Mol	Chain	Res	Type
1	B	578	LEU
1	B	584	GLN
1	B	589	LYS
1	B	610	PHE
1	B	626	ILE
1	B	628	PHE
1	B	633	ASP
1	B	641	GLU
1	B	662	MET
1	B	668	LEU
1	B	693	GLU
1	B	695	LEU
1	B	713	LEU
1	B	715	SER
1	B	719	ASN
1	B	743	ILE
1	B	745	ASP
1	B	758	TYR
1	B	763	ILE
1	B	778	LYS
1	B	798	MET
1	B	801	PHE
1	B	808	ARG
1	B	810	GLU
1	B	822	LEU
1	B	825	MET
1	B	830	GLN
1	B	837	THR
1	B	866	GLU
1	B	875	SER
1	B	880	SER
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	896	SER
1	B	897	ILE
1	B	914	LEU
1	B	918	PHE
1	B	921	LEU
1	B	922	THR
1	B	955	LYS
1	B	965	LEU

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Mol	Chain	Res	Type
1	B	968	VAL
1	B	972	LEU
1	B	986	VAL
1	B	1003	VAL
1	B	1030	ARG
1	C	1	MET
1	C	11	PHE
1	C	38	ILE
1	C	75	LEU
1	C	79	SER
1	C	108	GLN
1	C	121	GLU
1	C	127	VAL
1	C	128	SER
1	C	143	ILE
1	C	152	GLU
1	C	177	LEU
1	C	237	GLN
1	C	243	THR
1	C	253	VAL
1	C	254	ASN
1	C	273	GLU
1	C	289	LEU
1	C	307	ARG
1	C	310	LEU
1	C	319	SER
1	C	324	VAL
1	C	355	MET
1	C	359	LEU
1	C	360	GLN
1	C	369	THR
1	C	389	SER
1	C	394	THR
1	C	404	LEU
1	C	408	ASP
1	C	418	ARG
1	C	425	LEU
1	C	434	SER
1	C	437	GLN
1	C	438	ILE
1	C	463	THR
1	C	471	SER

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Mol	Chain	Res	Type
1	C	482	VAL
1	C	495	THR
1	C	510	LYS
1	C	512	PHE
1	C	531	VAL
1	C	537	SER
1	C	542	LEU
1	C	546	LEU
1	C	557	VAL
1	C	564	LEU
1	C	575	MET
1	C	586	ARG
1	C	608	SER
1	C	615	PHE
1	C	626	ILE
1	C	640	GLU
1	C	648	THR
1	C	657	GLN
1	C	678	THR
1	C	685	ILE
1	C	690	LEU
1	C	695	LEU
1	C	702	LEU
1	C	711	ASP
1	C	717	ARG
1	C	739	LEU
1	C	743	ILE
1	C	765	ARG
1	C	782	LEU
1	C	784	ASP
1	C	786	ILE
1	C	795	ASP
1	C	799	VAL
1	C	815	ARG
1	C	824	SER
1	C	828	LEU
1	C	835	LYS
1	C	853	THR
1	C	867	ARG
1	C	868	LEU
1	C	879	ILE
1	C	891	LEU

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Mol	Chain	Res	Type
1	C	894	SER
1	C	896	SER
1	C	900	SER
1	C	902	MET
1	C	905	VAL
1	C	919	ARG
1	C	938	SER
1	C	947	GLU
1	C	948	PHE
1	C	960	LEU
1	C	962	GLU
1	C	968	VAL
1	C	976	LEU
1	C	984	LEU
1	C	993	THR
1	C	1003	VAL
1	C	1011	MET
1	C	1031	ARG
1	C	1032	ARG
1	C	1033	PHE
2	D	28	ASP
2	D	45	VAL
2	D	61	GLU
2	D	76	TYR
2	D	79	LEU
2	D	94	GLU
2	D	126	LEU
2	D	127	GLU
2	D	160	ASP
2	E	16	LYS
2	E	28	ASP
2	E	40	VAL
2	E	57	TRP
2	E	64	GLU
2	E	73	VAL
2	E	76	TYR
2	E	78	THR
2	E	79	LEU
2	E	81	SER
2	E	112	ASN
2	E	115	THR
2	E	119	LEU

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Mol	Chain	Res	Type
2	E	126	LEU
2	E	127	GLU
2	E	128	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	692	HIS
1	A	747	ASN
1	C	104	GLN
1	C	151	GLN
1	C	237	GLN
1	C	439	GLN
1	C	577	GLN
2	E	92	HIS
2	E	125	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 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	1.16	3 (8%)	47,47,47	1.45	7 (14%)
3	LMT	A	1102	-	36,36,36	1.13	3 (8%)	47,47,47	1.47	7 (14%)
3	LMT	B	1101	-	36,36,36	1.15	3 (8%)	47,47,47	1.32	8 (17%)
3	LMT	B	1102	-	36,36,36	1.15	4 (11%)	47,47,47	1.40	7 (14%)
3	LMT	B	1103	-	36,36,36	1.15	4 (11%)	47,47,47	1.65	13 (27%)
3	LMT	C	1101	-	36,36,36	1.11	3 (8%)	47,47,47	1.15	3 (6%)
3	LMT	C	1102	-	36,36,36	1.17	3 (8%)	47,47,47	1.28	5 (10%)

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	B	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	B	1103	-	-	0/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	C	1102	-	-	0/21/61/61	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	LMT	C3'-C4'	-2.97	1.44	1.52
3	B	1102	LMT	C3'-C4'	-2.81	1.44	1.52
3	C	1102	LMT	C3'-C4'	-2.81	1.44	1.52
3	C	1101	LMT	C3'-C4'	-2.78	1.44	1.52
3	B	1101	LMT	C3'-C4'	-2.76	1.44	1.52
3	A	1101	LMT	C3'-C4'	-2.75	1.44	1.52
3	B	1103	LMT	C3'-C4'	-2.51	1.45	1.52
3	B	1102	LMT	O1B-C4'	2.01	1.48	1.43
3	B	1103	LMT	O1B-C4'	2.18	1.49	1.43
3	C	1101	LMT	O5'-C5'	2.51	1.50	1.44
3	A	1101	LMT	O5'-C5'	2.54	1.50	1.44
3	B	1103	LMT	O5'-C5'	2.65	1.51	1.44
3	C	1102	LMT	O5'-C5'	2.69	1.51	1.44
3	B	1102	LMT	O5'-C5'	2.82	1.51	1.44
3	A	1102	LMT	O5'-C5'	2.84	1.51	1.44
3	B	1101	LMT	O5'-C5'	2.87	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	LMT	O5B-C1B	3.50	1.50	1.41
3	A	1102	LMT	O5B-C1B	3.80	1.51	1.41
3	C	1102	LMT	O5B-C1B	3.80	1.51	1.41
3	B	1103	LMT	O5B-C1B	3.96	1.52	1.41
3	B	1102	LMT	O5B-C1B	3.97	1.52	1.41
3	B	1101	LMT	O5B-C1B	4.00	1.52	1.41
3	A	1101	LMT	O5B-C1B	4.11	1.52	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	LMT	O1'-C1-C2	2.02	117.93	109.88
3	C	1102	LMT	O1'-C1-C2	2.04	117.99	109.88
3	A	1102	LMT	O5B-C5B-C6B	2.05	111.53	106.36
3	B	1102	LMT	O6'-C6'-C5'	2.12	118.34	111.33
3	A	1101	LMT	O5B-C5B-C4B	2.14	113.69	109.68
3	B	1102	LMT	O5'-C1'-C2'	2.18	114.74	110.28
3	C	1102	LMT	O1'-C1'-C2'	2.21	110.83	108.04
3	B	1103	LMT	O5'-C1'-C2'	2.21	114.82	110.28
3	A	1102	LMT	O6B-C6B-C5B	2.24	118.74	111.33
3	A	1101	LMT	O6'-C6'-C5'	2.26	118.79	111.33
3	B	1103	LMT	C3'-C4'-C5'	2.27	115.97	110.84
3	B	1102	LMT	O6B-C6B-C5B	2.28	118.86	111.33
3	B	1103	LMT	O6'-C6'-C5'	2.28	118.87	111.33
3	B	1103	LMT	C3B-C4B-C5B	2.28	114.17	110.20
3	B	1101	LMT	C1B-O5B-C5B	2.30	118.22	113.75
3	B	1103	LMT	O1B-C1B-C2B	2.32	113.74	108.10
3	B	1101	LMT	O3B-C3B-C2B	2.33	115.57	110.34
3	B	1101	LMT	O6B-C6B-C5B	2.36	119.11	111.33
3	A	1102	LMT	O6'-C6'-C5'	2.36	119.12	111.33
3	B	1103	LMT	C4B-C3B-C2B	2.37	115.22	110.79
3	C	1101	LMT	O6'-C6'-C5'	2.38	119.19	111.33
3	B	1102	LMT	O1B-C1B-C2B	2.42	113.99	108.10
3	B	1102	LMT	C1'-C2'-C3'	2.42	114.74	109.97
3	B	1103	LMT	C1B-C2B-C3B	2.44	114.78	109.97
3	B	1101	LMT	O5B-C5B-C4B	2.52	114.41	109.68
3	B	1103	LMT	O5B-C5B-C4B	2.54	114.45	109.68
3	B	1101	LMT	O1'-C1'-C2'	2.57	111.28	108.04
3	B	1103	LMT	O1B-C4'-C5'	2.62	116.20	109.32
3	B	1103	LMT	O5B-C1B-C2B	2.64	115.69	110.28
3	C	1102	LMT	C2'-C3'-C4'	2.64	115.40	109.60
3	B	1101	LMT	O6'-C6'-C5'	2.73	120.34	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	LMT	C1-O1'-C1'	2.75	118.75	113.94
3	C	1101	LMT	C1-O1'-C1'	2.75	118.76	113.94
3	A	1101	LMT	C1-O1'-C1'	2.92	119.04	113.94
3	C	1101	LMT	C2'-C3'-C4'	2.98	116.15	109.60
3	B	1103	LMT	C1B-O1B-C4'	3.06	125.99	118.01
3	B	1101	LMT	C2'-C3'-C4'	3.08	116.36	109.60
3	A	1102	LMT	C4B-C3B-C2B	3.27	116.89	110.79
3	B	1103	LMT	C1-O1'-C1'	3.29	119.69	113.94
3	B	1102	LMT	C2'-C3'-C4'	3.30	116.85	109.60
3	C	1102	LMT	C1-O1'-C1'	3.33	119.76	113.94
3	C	1102	LMT	O5B-C5B-C4B	3.39	116.04	109.68
3	A	1101	LMT	C2'-C3'-C4'	3.41	117.09	109.60
3	A	1101	LMT	C1'-C2'-C3'	3.45	116.77	109.97
3	B	1103	LMT	C2'-C3'-C4'	3.46	117.20	109.60
3	A	1102	LMT	O5B-C5B-C4B	3.56	116.36	109.68
3	A	1102	LMT	C1-O1'-C1'	3.70	120.42	113.94
3	A	1101	LMT	O5'-C1'-C2'	3.83	118.14	110.28
3	B	1102	LMT	C1-O1'-C1'	4.76	122.27	113.94
3	A	1102	LMT	C3B-C4B-C5B	4.97	118.86	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	LMT	2	0
3	A	1102	LMT	2	0
3	B	1102	LMT	2	0
3	B	1103	LMT	2	0
3	C	1101	LMT	1	0
3	C	1102	LMT	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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%)	-0.51	13 (1%) 81 78	13, 57, 113, 163	0
1	B	1033/1057 (97%)	-0.54	8 (0%) 87 86	24, 61, 101, 159	0
1	C	1034/1057 (97%)	-0.56	12 (1%) 81 78	17, 53, 92, 164	0
2	D	156/169 (92%)	-0.61	0 100 100	41, 60, 90, 117	0
2	E	152/169 (89%)	-0.19	3 (1%) 68 64	32, 59, 99, 119	0
All	All	3419/3509 (97%)	-0.53	36 (1%) 82 80	13, 58, 102, 164	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	THR	11.6
1	A	868	LEU	8.2
1	A	869	SER	5.2
1	C	497	LEU	4.2
1	B	134	SER	3.9
1	A	675	GLY	3.9
1	B	674	LEU	3.7
1	C	496	MET	3.6
1	C	363	ARG	3.3
1	C	510	LYS	3.2
1	A	1034	SER	3.1
2	E	34	MET	3.0
1	C	1032	ARG	3.0
1	B	677	ALA	3.0
1	A	508	GLY	2.9
1	C	513	PHE	2.9
1	B	868	LEU	2.9
1	C	362	PHE	2.8
2	E	35	ALA	2.7
1	C	417	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	835	LYS	2.7
1	A	518	ARG	2.6
1	A	674	LEU	2.5
1	A	866	GLU	2.5
1	B	595	THR	2.3
1	C	811	TYR	2.2
1	A	509	LYS	2.2
1	A	506	GLY	2.2
1	A	867	ARG	2.2
1	B	599	LEU	2.2
1	C	739	LEU	2.2
1	A	498	LYS	2.1
1	B	869	SER	2.1
2	E	33	LEU	2.1
1	C	498	LYS	2.1
1	C	514	GLY	2.1

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
3	LMT	A	1102	35/35	0.79	0.39	4.22	90,116,154,157	0
3	LMT	B	1101	35/35	0.89	0.19	2.38	66,102,122,125	0
3	LMT	A	1101	35/35	0.89	0.20	2.03	32,107,156,157	0
3	LMT	B	1103	35/35	0.82	0.27	1.74	42,147,193,195	0
3	LMT	B	1102	35/35	0.74	0.24	1.66	52,134,161,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	LMT	C	1101	35/35	0.86	0.18	1.43	55,97,134,136	0
3	LMT	C	1102	35/35	0.93	0.17	1.30	63,87,104,110	0

6.5 Other polymers (i)

There are no such residues in this entry.