Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 02:14 PM JST

PDB ID	:	8ZXS / pdb_00008zxs
Title	:	Crystal structure of multidrug efflux transporter OqxB from Klebsiella pneumoniae
Authors	:	Murakami, S.; Yamashita, E.; Okada, U.
Deposited on	:	2024-06-15
Resolution	:	2.75 Å(reported)

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

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

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

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

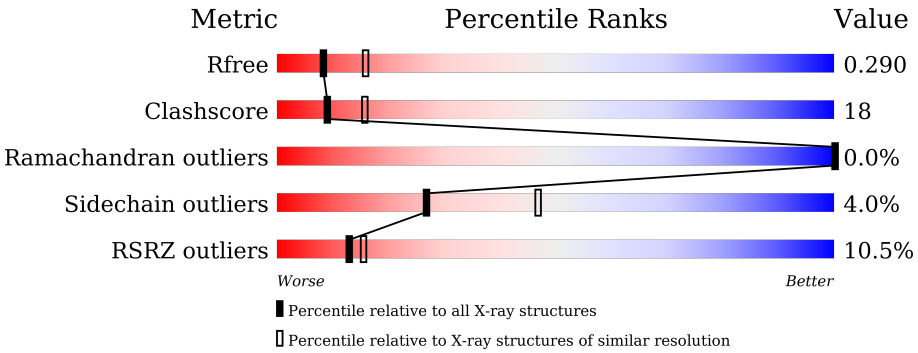
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1056	11% 61% 36%
1	B	1056	13% 61% 37%
1	C	1056	8% 64% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23984 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.

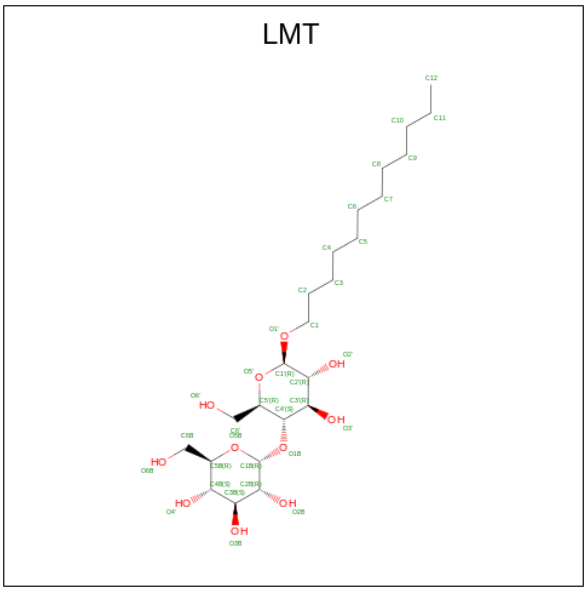
- Molecule 1 is a protein called Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1040	Total	C	N	O	S	0	0	0
			7912	5098	1334	1446	34			
1	B	1042	Total	C	N	O	S	0	0	0
			7932	5110	1340	1448	34			
1	C	1041	Total	C	N	O	S	0	0	0
			7923	5104	1338	1447	34			

There are 18 discrepancies between the modelled and reference sequences:

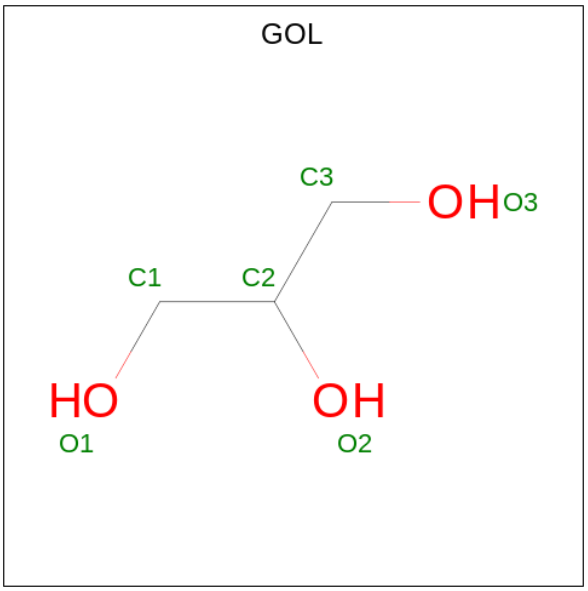
Chain	Residue	Modelled	Actual	Comment	Reference
A	1051	HIS	-	expression tag	UNP U5U6L7
A	1052	HIS	-	expression tag	UNP U5U6L7
A	1053	HIS	-	expression tag	UNP U5U6L7
A	1054	HIS	-	expression tag	UNP U5U6L7
A	1055	HIS	-	expression tag	UNP U5U6L7
A	1056	HIS	-	expression tag	UNP U5U6L7
B	1051	HIS	-	expression tag	UNP U5U6L7
B	1052	HIS	-	expression tag	UNP U5U6L7
B	1053	HIS	-	expression tag	UNP U5U6L7
B	1054	HIS	-	expression tag	UNP U5U6L7
B	1055	HIS	-	expression tag	UNP U5U6L7
B	1056	HIS	-	expression tag	UNP U5U6L7
C	1051	HIS	-	expression tag	UNP U5U6L7
C	1052	HIS	-	expression tag	UNP U5U6L7
C	1053	HIS	-	expression tag	UNP U5U6L7
C	1054	HIS	-	expression tag	UNP U5U6L7
C	1055	HIS	-	expression tag	UNP U5U6L7
C	1056	HIS	-	expression tag	UNP U5U6L7

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

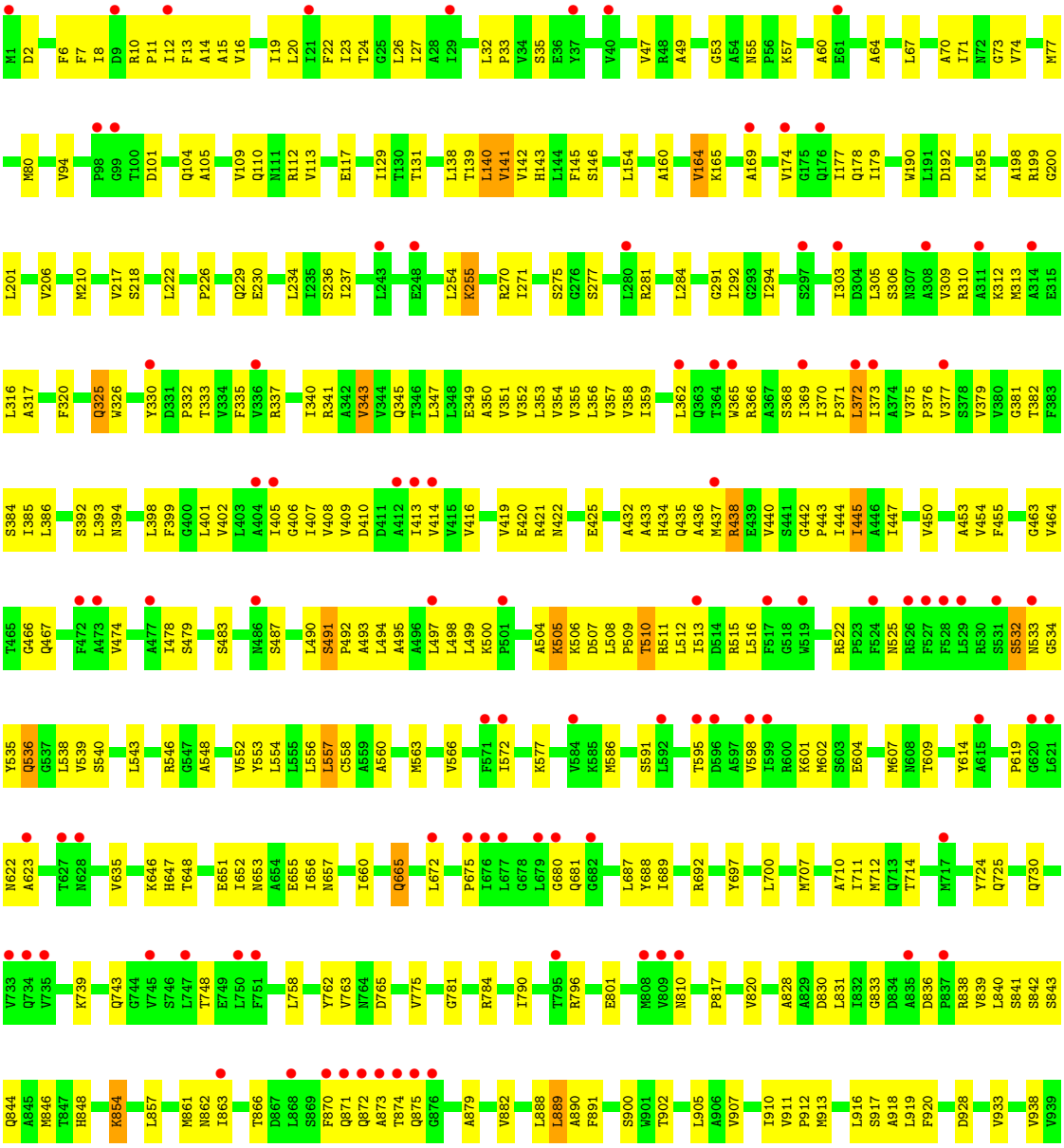
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O 1 1	0	0

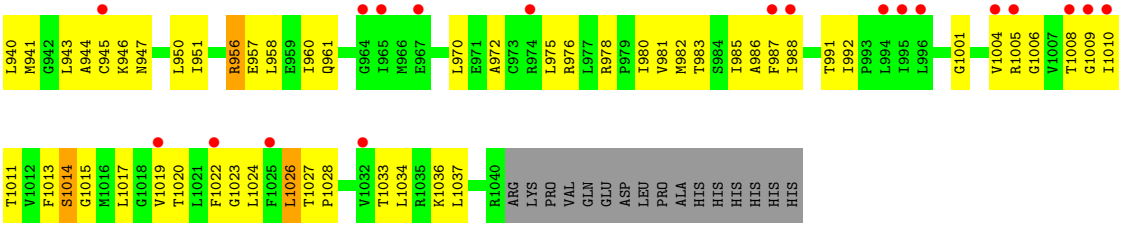
3 Residue-property plots (i)

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

- Molecule 1: Efflux pump membrane transporter

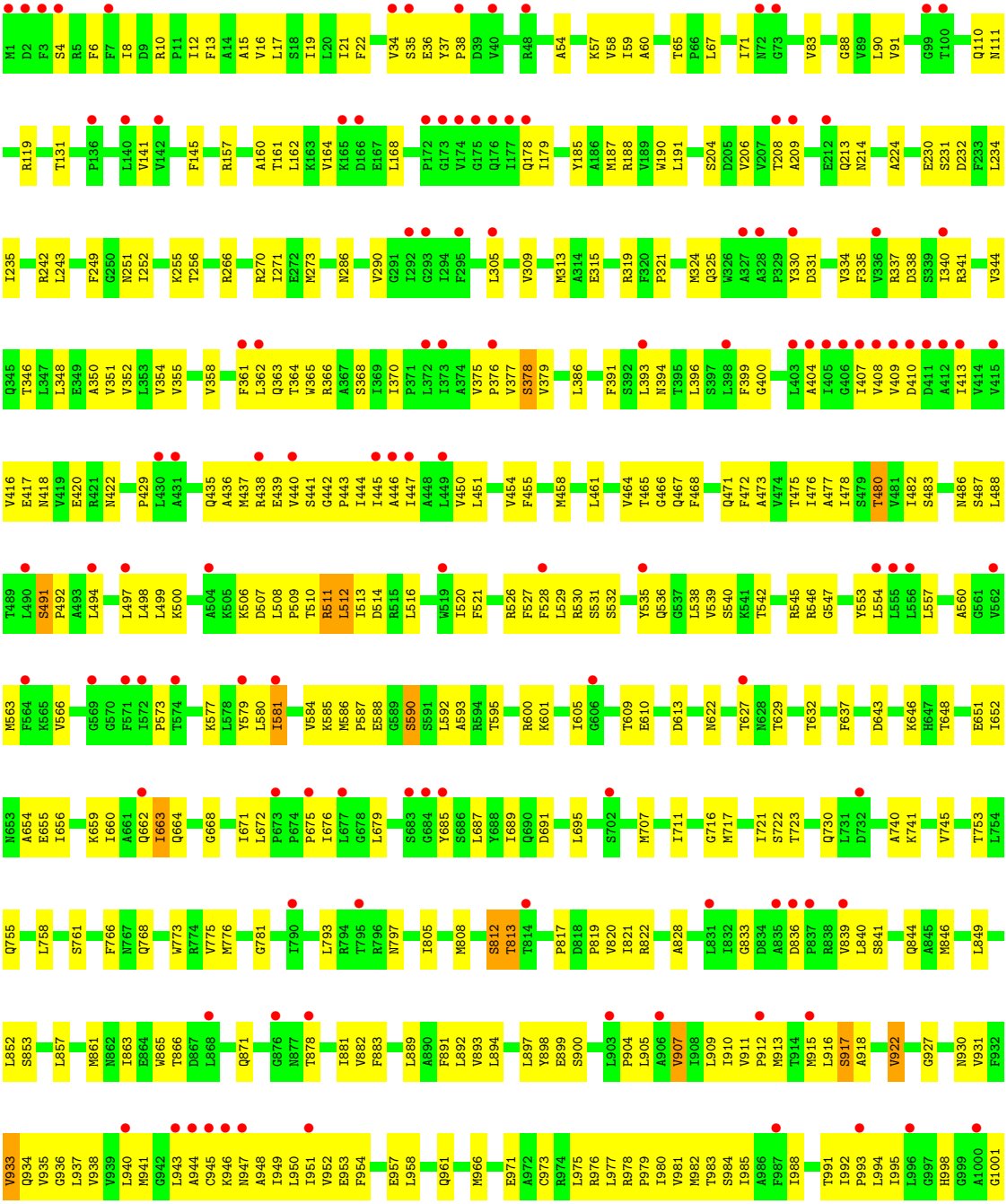
Chain A:

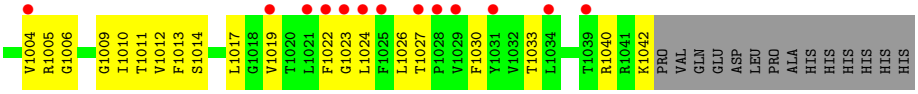




• Molecule 1: Efflux pump membrane transporter

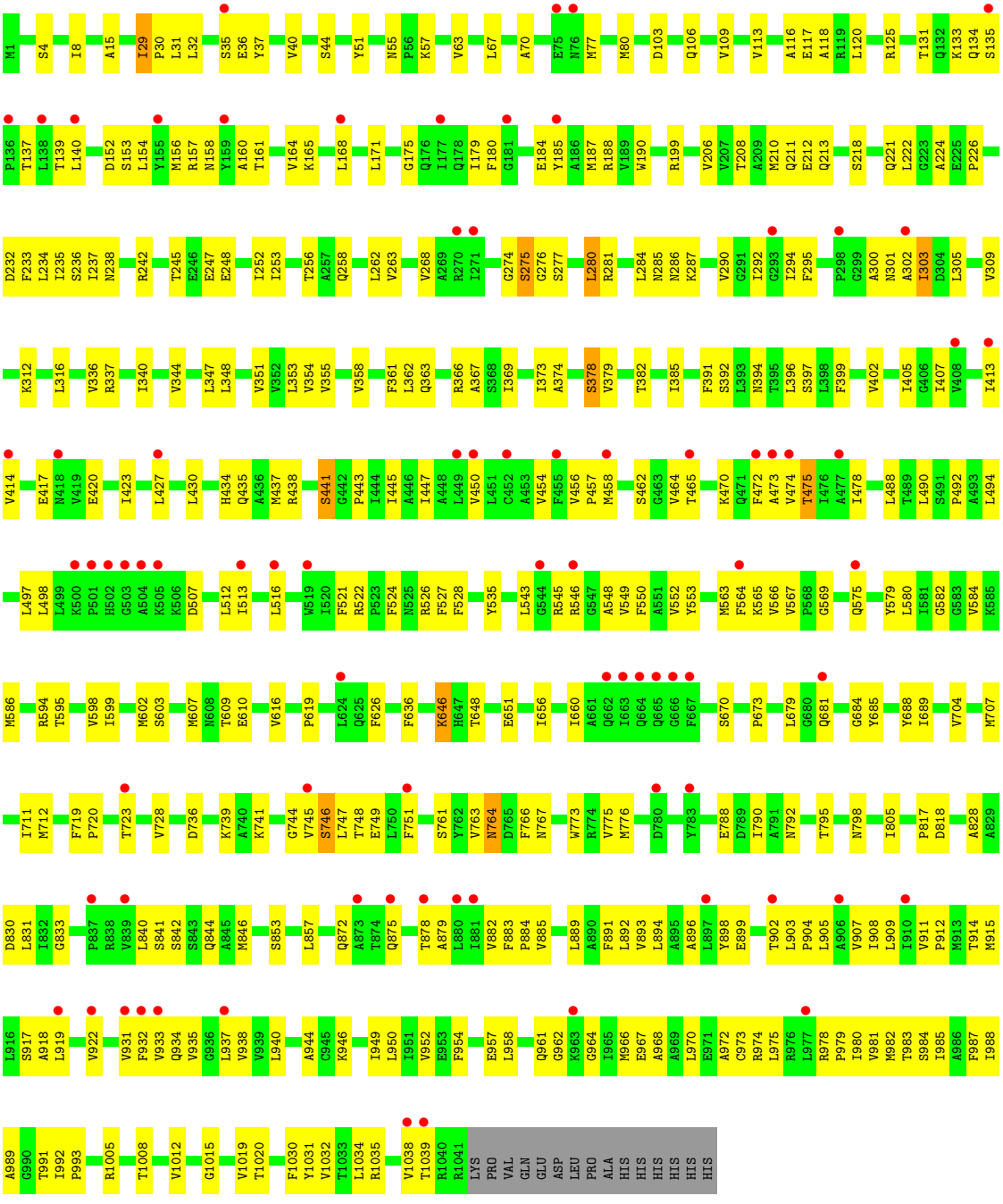
Chain B:





• Molecule 1: Efflux pump membrane transporter

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.39Å 165.94Å 249.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.04 – 2.75 43.04 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.04-2.75) 99.7 (43.04-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.236 , 0.288 0.240 , 0.290	Depositor DCC
R_{free} test set	6847 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	93.2	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23984	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.22	0/8069	0.49	1/10988 (0.0%)
1	B	0.23	0/8089	0.50	3/11013 (0.0%)
1	C	0.22	0/8080	0.45	0/11002
All	All	0.22	0/24238	0.48	4/33003 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	536	GLN	N-CA-CB	5.59	118.94	110.28
1	B	512	LEU	CA-CB-CG	5.53	135.65	116.30
1	B	520	ILE	CA-C-N	-5.20	113.56	120.63
1	B	520	ILE	C-N-CA	-5.20	113.56	120.63

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	7912	0	8114	324	0
1	B	7932	0	8140	325	0
1	C	7923	0	8127	264	0
2	A	105	0	137	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	70	0	91	0	0
2	C	35	0	45	3	0
3	A	6	0	8	0	0
4	C	1	0	0	0	0
All	All	23984	0	24662	881	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 18.

All (881) 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:422:ASN:ND2	1:A:432:ALA:O	1.98	0.97
1:B:745:VAL:HB	1:B:808:MET:HE1	1.51	0.91
1:C:154:LEU:O	1:C:158:ASN:ND2	2.04	0.91
1:A:23:ILE:HA	1:A:26:LEU:HD12	1.53	0.89
1:A:370:ILE:HD11	1:A:416:VAL:HG11	1.54	0.89
1:A:464:VAL:HA	1:A:467:GLN:HG2	1.55	0.88
1:A:55:ASN:HD22	1:C:238:ASN:HB2	1.41	0.84
1:A:586:MET:HG3	1:A:595:THR:HG22	1.57	0.84
1:B:512:LEU:HD13	1:B:516:LEU:HD21	1.60	0.84
1:A:1014:SER:HA	1:A:1017:LEU:HD12	1.60	0.83
1:A:179:ILE:HD12	1:A:292:ILE:HD12	1.60	0.83
1:B:16:VAL:HG11	1:C:896:ALA:HB2	1.62	0.82
1:A:421:ARG:NH1	1:A:422:ASN:OD1	2.09	0.82
1:B:337:ARG:HA	1:B:340:ILE:HG22	1.61	0.82
1:C:399:PHE:CE2	1:C:1005:ARG:HG3	2.16	0.81
1:B:22:PHE:HB2	1:B:377:VAL:HG23	1.62	0.81
1:B:444:ILE:HD11	1:B:488:LEU:HG	1.64	0.79
1:A:370:ILE:CD1	1:A:416:VAL:HG11	2.13	0.79
1:A:413:ILE:HD13	1:A:983:THR:HG22	1.64	0.79
1:C:285:ASN:O	1:C:287:LYS:NZ	2.13	0.78
1:A:687:LEU:HD13	1:A:863:ILE:HG13	1.65	0.78
1:A:604:GLU:HA	1:A:607:MET:HG3	1.64	0.77
1:A:370:ILE:HD12	1:A:371:PRO:HD3	1.67	0.77
1:A:680:GLY:HA2	2:A:1102:LMT:H2'	1.67	0.76
1:A:463:GLY:O	1:A:466:GLY:N	2.18	0.75
1:A:408:VAL:HG22	1:A:483:SER:HB2	1.68	0.75
1:C:300:ALA:O	1:C:301:ASN:ND2	2.20	0.75
1:B:676:ILE:HD11	1:B:679:LEU:HB2	1.69	0.74
1:A:913:MET:HB3	1:A:1022:PHE:HD1	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:964:GLY:O	1:C:968:ALA:N	2.20	0.73
1:C:399:PHE:HE2	1:C:1005:ARG:HG3	1.51	0.73
1:A:165:LYS:HG3	1:A:177:ILE:HD11	1.71	0.73
1:A:142:VAL:HG22	1:A:292:ILE:HB	1.69	0.73
1:A:370:ILE:HD12	1:A:371:PRO:CD	2.18	0.73
1:B:945:CYS:O	1:B:949:ILE:HG13	1.89	0.73
1:C:63:VAL:O	1:C:67:LEU:HD12	1.89	0.73
1:C:139:THR:HG22	1:C:140:LEU:HD23	1.71	0.72
1:B:168:LEU:HD11	1:B:313:MET:HE1	1.72	0.72
1:B:413:ILE:HD11	1:B:983:THR:HG22	1.70	0.72
1:A:382:THR:HG23	1:A:478:ILE:HD11	1.72	0.72
1:A:563:MET:HA	1:A:566:VAL:HG22	1.72	0.72
1:A:707:MET:HE3	1:A:711:ILE:HD11	1.70	0.72
2:A:1101:LMT:H3'	1:C:31:LEU:HD21	1.72	0.71
1:A:765:ASP:OD1	1:B:119:ARG:NH1	2.23	0.71
1:A:563:MET:HE2	1:A:919:LEU:HB3	1.71	0.71
1:C:788:GLU:O	1:C:792:ASN:ND2	2.19	0.71
1:A:1023:GLY:O	1:A:1027:THR:OG1	2.08	0.71
1:B:251:ASN:OD1	1:B:266:ARG:NH1	2.23	0.71
1:B:497:LEU:HG	1:B:498:LEU:HD22	1.73	0.70
1:C:103:ASP:OD1	1:C:133:LYS:NZ	2.25	0.70
1:A:73:GLY:H	1:A:77:MET:HE1	1.55	0.70
1:B:513:ILE:O	1:B:521:PHE:HZ	1.75	0.70
1:A:2:ASP:HB2	1:A:438:ARG:HG3	1.73	0.69
1:B:214:ASN:HB2	1:B:243:LEU:HD12	1.74	0.69
1:B:447:ILE:O	1:B:451:LEU:HG	1.92	0.69
1:B:560:ALA:HB2	1:B:916:LEU:HD22	1.73	0.69
1:A:317:ALA:HA	1:A:320:PHE:CE2	2.28	0.69
1:B:83:VAL:HG22	1:B:821:ILE:HD12	1.73	0.69
1:B:687:LEU:HD21	1:B:863:ILE:HB	1.75	0.69
1:C:77:MET:HE1	1:C:80:MET:HB2	1.74	0.69
1:B:446:ALA:O	1:B:450:VAL:HG23	1.93	0.68
1:B:441:SER:HB2	1:B:488:LEU:HD21	1.74	0.68
1:A:15:ALA:O	1:A:19:ILE:HG12	1.94	0.68
1:B:506:LYS:O	1:B:510:THR:OG1	2.09	0.68
1:B:375:VAL:HG21	1:B:409:VAL:HG12	1.75	0.68
1:B:510:THR:HA	1:B:513:ILE:HG13	1.76	0.68
1:C:967:GLU:HA	1:C:970:LEU:HD12	1.75	0.68
1:B:514:ASP:HA	1:B:521:PHE:CE1	2.29	0.68
1:B:513:ILE:HD12	1:B:514:ASP:N	2.09	0.68
1:C:57:LYS:HE2	1:C:817:PRO:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:HH21	1:C:184:GLU:HG3	1.58	0.67
1:C:221:GLN:HG3	1:C:234:LEU:HD11	1.77	0.67
1:A:357:VAL:HG21	1:A:986:ALA:HB2	1.75	0.67
1:B:984:SER:O	1:B:988:ILE:HG13	1.95	0.67
1:A:406:GLY:HA3	1:A:987:PHE:HZ	1.59	0.66
1:B:506:LYS:HD2	1:B:511:ARG:HG2	1.75	0.66
1:A:435:GLN:HG2	1:A:438:ARG:HH12	1.61	0.66
1:C:567:VAL:HG11	1:C:919:LEU:HD23	1.78	0.66
1:A:437:MET:HA	1:A:437:MET:HE3	1.76	0.66
1:C:361:PHE:HD1	1:C:982:MET:HE2	1.59	0.66
1:A:312:LYS:O	1:A:316:LEU:HD12	1.94	0.66
1:A:464:VAL:HG13	1:A:871:GLN:HE22	1.59	0.66
1:A:7:PHE:HB3	1:A:14:ALA:HB2	1.76	0.65
1:B:512:LEU:HD13	1:B:516:LEU:CD2	2.26	0.65
1:A:416:VAL:HA	1:A:419:VAL:HG12	1.76	0.65
1:B:894:LEU:HB3	1:B:904:PRO:HB3	1.79	0.65
1:A:543:LEU:HD21	1:A:1028:PRO:HB2	1.78	0.65
1:B:417:GLU:OE2	1:B:978:ARG:NH1	2.29	0.65
1:B:507:ASP:OD1	1:B:508:LEU:N	2.30	0.65
1:B:988:ILE:HA	1:B:991:THR:HG22	1.77	0.65
1:A:602:MET:HB3	1:A:660:ILE:HG21	1.79	0.65
1:C:707:MET:HE1	1:C:853:SER:HA	1.79	0.65
1:A:357:VAL:HG13	1:A:985:ILE:HD11	1.79	0.64
1:B:57:LYS:NZ	1:B:817:PRO:O	2.30	0.64
1:C:966:MET:SD	1:C:966:MET:N	2.63	0.64
1:A:572:ILE:H	1:A:572:ILE:HD12	1.62	0.64
1:A:535:TYR:HA	1:A:538:LEU:HD12	1.79	0.64
1:B:446:ALA:HB2	1:B:897:LEU:HD13	1.79	0.64
1:B:905:LEU:HD12	1:B:905:LEU:H	1.64	0.63
1:C:188:ARG:HD3	1:C:190:TRP:CZ2	2.32	0.63
1:A:192:ASP:OD2	1:A:195:LYS:NZ	2.29	0.63
1:A:656:ILE:O	1:A:660:ILE:HG13	1.98	0.63
1:B:507:ASP:OD1	1:B:509:PRO:HD2	1.98	0.63
1:A:509:PRO:O	1:A:513:ILE:HD12	1.98	0.63
1:C:933:VAL:O	1:C:937:LEU:HD23	1.98	0.63
1:A:762:TYR:OH	1:B:119:ARG:NH1	2.32	0.63
1:B:386:LEU:HD21	1:B:475:THR:HG22	1.78	0.63
1:C:535:TYR:HE2	1:C:973:CYS:HB3	1.63	0.63
1:A:303:ILE:HD11	1:A:337:ARG:HB2	1.80	0.63
1:A:358:VAL:HG23	1:A:362:LEU:HD12	1.80	0.63
1:B:853:SER:O	1:B:857:LEU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PHE:HE2	1:B:577:LYS:HD2	1.65	0.62
1:B:536:GLN:O	1:B:540:SER:OG	2.16	0.62
1:C:946:LYS:HA	1:C:949:ILE:HD12	1.80	0.62
1:A:1004:VAL:O	1:A:1008:THR:HG23	1.98	0.62
1:C:443:PRO:O	1:C:447:ILE:HG13	1.98	0.62
1:B:573:PRO:HD3	1:B:930:ASN:HB2	1.81	0.62
1:C:1031:TYR:O	1:C:1035:ARG:HB2	1.98	0.62
1:B:37:TYR:HD2	1:B:396:LEU:HD21	1.64	0.62
1:A:976:ARG:HH11	1:A:976:ARG:HG3	1.64	0.62
1:B:545:ARG:HH21	1:B:547:GLY:H	1.47	0.62
1:B:949:ILE:HD12	1:B:950:LEU:N	2.15	0.62
1:C:984:SER:O	1:C:988:ILE:HG12	2.00	0.62
1:A:178:GLN:OE1	2:A:1103:LMT:O2'	2.15	0.61
1:A:349:GLU:HG3	1:A:353:LEU:HD13	1.80	0.61
1:A:700:LEU:HD23	1:A:724:TYR:CZ	2.35	0.61
1:B:934:GLN:HA	1:B:937:LEU:HG	1.81	0.61
1:B:476:ILE:HD12	1:B:477:ALA:N	2.15	0.61
1:B:444:ILE:HA	1:B:447:ILE:HG12	1.81	0.61
1:C:399:PHE:HZ	1:C:1005:ARG:HA	1.65	0.61
1:C:905:LEU:O	1:C:909:LEU:HD12	1.99	0.61
1:A:71:ILE:HA	1:A:112:ARG:HD3	1.82	0.61
1:A:142:VAL:HG21	1:A:313:MET:HE2	1.82	0.61
1:A:546:ARG:NH2	1:A:1036:LYS:HD3	2.15	0.61
1:C:954:PHE:HE2	1:C:975:LEU:HB2	1.65	0.61
1:A:495:ALA:O	1:A:499:LEU:HG	2.01	0.61
1:A:536:GLN:HB2	1:A:970:LEU:HD21	1.82	0.60
1:B:443:PRO:HG3	1:B:953:GLU:HG2	1.83	0.60
1:B:1030:PHE:HA	1:B:1033:THR:HG22	1.82	0.60
1:C:932:PHE:HB3	1:C:1008:THR:HG23	1.82	0.60
1:C:918:ALA:O	1:C:922:VAL:HG23	2.00	0.60
1:A:379:VAL:O	1:A:382:THR:HB	2.01	0.60
1:A:730:GLN:HG2	1:C:236:SER:HB2	1.83	0.60
1:B:758:LEU:HD11	1:B:793:LEU:HD11	1.83	0.60
1:C:206:VAL:O	1:C:210:MET:HG3	2.01	0.60
1:B:305:LEU:O	1:B:309:VAL:HG12	2.00	0.60
1:C:586:MET:HG3	1:C:595:THR:HG22	1.83	0.60
1:A:381:GLY:O	1:A:384:SER:OG	2.20	0.60
1:C:685:TYR:CZ	1:C:833:GLY:HA3	2.36	0.60
1:A:652:ILE:O	1:A:656:ILE:HG13	2.01	0.60
1:A:907:VAL:O	1:A:910:ILE:HG13	2.02	0.60
1:B:947:ASN:O	1:B:951:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:MET:HE2	1:C:595:THR:HA	1.84	0.60
1:A:646:LYS:O	1:A:647:HIS:ND1	2.28	0.60
1:A:546:ARG:HH22	1:A:1036:LYS:HD3	1.65	0.60
1:A:563:MET:HE1	1:A:920:PHE:HA	1.84	0.60
1:B:418:ASN:ND2	1:B:436:ALA:O	2.34	0.60
1:C:549:VAL:HA	1:C:552:VAL:HG12	1.83	0.60
1:C:979:PRO:O	1:C:983:THR:HG23	2.02	0.60
1:A:978:ARG:O	1:A:982:MET:HG2	2.00	0.60
1:B:981:VAL:O	1:B:985:ILE:HG22	2.02	0.59
1:B:1023:GLY:O	1:B:1027:THR:OG1	2.18	0.59
1:A:494:LEU:O	1:A:498:LEU:HB2	2.01	0.59
1:A:532:SER:O	1:A:535:TYR:N	2.35	0.59
1:C:362:LEU:HD12	1:C:367:ALA:HB1	1.84	0.59
1:C:447:ILE:HD13	1:C:946:LYS:HG3	1.84	0.59
1:B:465:THR:HA	1:B:468:PHE:CD1	2.38	0.59
1:C:358:VAL:HG12	1:C:413:ILE:HD11	1.84	0.59
1:A:23:ILE:HD12	1:A:24:THR:N	2.18	0.59
1:B:695:LEU:HD12	1:B:861:MET:HE3	1.85	0.59
1:B:740:ALA:HA	1:B:808:MET:HE2	1.84	0.59
1:B:535:TYR:HA	1:B:538:LEU:HD12	1.84	0.59
1:B:545:ARG:NH2	1:B:547:GLY:H	2.01	0.59
1:B:994:LEU:HD22	1:B:1009:GLY:C	2.28	0.59
1:C:967:GLU:HA	1:C:970:LEU:CD1	2.33	0.59
1:A:375:VAL:HG11	1:A:409:VAL:HG12	1.85	0.59
1:B:587:PRO:O	1:B:590:SER:OG	2.21	0.58
1:C:940:LEU:HD11	1:C:1012:VAL:HA	1.86	0.58
1:A:577:LYS:NZ	1:A:675:PRO:O	2.30	0.58
1:A:972:ALA:HA	1:A:975:LEU:HD12	1.83	0.58
1:C:187:MET:HB3	1:C:775:VAL:HG12	1.85	0.58
1:B:378:SER:HB3	1:B:486:ASN:HD21	1.68	0.58
1:C:399:PHE:HD1	1:C:472:PHE:CE1	2.21	0.58
1:B:917:SER:OG	1:B:1014:SER:O	2.21	0.58
1:C:63:VAL:HG12	1:C:67:LEU:HD11	1.85	0.58
1:A:353:LEU:O	1:A:357:VAL:HG23	2.02	0.58
1:A:928:ASP:OD2	1:A:928:ASP:N	2.37	0.58
1:C:535:TYR:CE2	1:C:973:CYS:HB3	2.38	0.58
1:C:543:LEU:O	1:C:546:ARG:NH1	2.37	0.58
1:B:581:ILE:HD12	1:B:581:ILE:O	2.04	0.58
1:B:351:VAL:O	1:B:354:VAL:HG12	2.04	0.58
1:B:546:ARG:H	1:B:546:ARG:CD	2.16	0.58
1:B:652:ILE:HA	1:B:655:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:O	1:B:65:THR:HG23	2.04	0.57
1:B:979:PRO:O	1:B:983:THR:HG23	2.04	0.57
1:A:1020:THR:O	1:A:1024:LEU:HD12	2.04	0.57
1:B:352:VAL:O	1:B:355:VAL:HG22	2.04	0.57
1:B:839:VAL:HG12	1:B:840:LEU:HD23	1.86	0.57
1:A:440:VAL:O	1:A:444:ILE:HG13	2.03	0.57
1:A:940:LEU:HD22	1:A:1015:GLY:HA3	1.84	0.57
1:C:185:TYR:HB2	1:C:773:TRP:CE3	2.38	0.57
1:C:545:ARG:HH21	1:C:548:ALA:HB2	1.68	0.57
1:A:200:GLY:O	1:A:796:ARG:NH2	2.36	0.57
1:B:648:THR:O	1:B:651:GLU:HG2	2.05	0.57
1:B:685:TYR:CZ	1:B:833:GLY:HA3	2.40	0.57
1:A:11:PRO:HG3	1:A:497:LEU:HD21	1.85	0.57
1:B:526:ARG:O	1:B:530:ARG:HG3	2.04	0.57
1:B:651:GLU:O	1:B:654:ALA:N	2.38	0.57
1:A:1006:GLY:O	1:A:1010:ILE:HD12	2.05	0.57
1:C:846:MET:HE2	1:C:872:GLN:HG2	1.85	0.57
1:A:71:ILE:HB	1:A:80:MET:HE1	1.87	0.57
1:A:405:ILE:O	1:A:409:VAL:HG13	2.04	0.57
1:A:872:GLN:HA	1:A:875:GLN:HG2	1.87	0.57
1:B:957:GLU:O	1:B:961:GLN:NE2	2.37	0.57
1:C:184:GLU:O	1:C:276:GLY:N	2.37	0.57
1:C:905:LEU:C	1:C:909:LEU:HD12	2.29	0.57
1:A:230:GLU:HG2	1:B:593:ALA:HB1	1.87	0.57
1:B:410:ASP:HB3	1:B:946:LYS:HZ1	1.69	0.57
1:A:493:ALA:O	1:A:497:LEU:HD22	2.05	0.57
1:C:4:SER:O	1:C:8:ILE:HG12	2.05	0.56
1:B:707:MET:O	1:B:711:ILE:HD12	2.04	0.56
1:B:944:ALA:HB2	1:B:1019:VAL:HG22	1.86	0.56
1:A:758:LEU:HD11	1:A:790:ILE:HG23	1.88	0.56
1:A:947:ASN:O	1:A:951:ILE:HG23	2.06	0.56
1:B:841:SER:OG	1:B:844:GLN:OE1	2.19	0.56
1:B:934:GLN:O	1:B:938:VAL:HG22	2.06	0.56
1:C:312:LYS:O	1:C:316:LEU:HG	2.05	0.56
1:C:603:SER:O	1:C:607:MET:HG3	2.06	0.56
1:A:370:ILE:HD12	1:A:371:PRO:N	2.20	0.56
1:A:842:SER:O	1:A:846:MET:HG3	2.05	0.56
1:C:40:VAL:HB	1:C:464:VAL:HG12	1.88	0.56
1:B:334:VAL:O	1:B:338:ASP:N	2.35	0.56
1:C:109:VAL:O	1:C:113:VAL:HG13	2.05	0.56
1:C:281:ARG:HB2	1:C:619:PRO:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:VAL:O	1:A:556:LEU:HB2	2.06	0.56
1:A:697:TYR:CD2	1:A:817:PRO:HG3	2.40	0.56
1:B:375:VAL:HG22	1:B:408:VAL:HG12	1.87	0.56
1:C:989:ALA:HA	1:C:992:ILE:HG12	1.86	0.56
1:B:512:LEU:O	1:B:516:LEU:HD22	2.06	0.56
1:A:406:GLY:O	1:A:409:VAL:HG22	2.06	0.56
1:A:707:MET:O	1:A:711:ILE:HD12	2.05	0.56
1:B:443:PRO:O	1:B:447:ILE:HG23	2.05	0.56
1:B:910:ILE:HG21	1:B:1027:THR:HG22	1.87	0.56
1:A:944:ALA:HB2	1:A:1019:VAL:HG22	1.86	0.55
1:B:465:THR:HA	1:B:468:PHE:HD1	1.71	0.55
1:A:22:PHE:CE1	1:A:26:LEU:HD11	2.41	0.55
1:A:340:ILE:HG12	1:A:398:LEU:HD21	1.87	0.55
1:B:37:TYR:CD2	1:B:396:LEU:HD21	2.40	0.55
1:C:720:PRO:HB2	1:C:831:LEU:HG	1.87	0.55
1:B:17:LEU:O	1:B:21:ILE:HG12	2.06	0.55
1:B:937:LEU:O	1:B:941:MET:HG3	2.07	0.55
1:C:748:THR:HA	1:C:751:PHE:HD2	1.71	0.55
1:A:110:GLN:OE1	1:B:111:ASN:HB3	2.06	0.55
1:A:347:LEU:HD13	1:A:379:VAL:HG11	1.89	0.55
1:C:29:ILE:HG23	1:C:30:PRO:HD3	1.87	0.55
1:C:160:ALA:HA	1:C:164:VAL:HB	1.87	0.55
1:A:422:ASN:HD21	1:A:436:ALA:N	2.04	0.55
1:B:971:GLU:O	1:B:975:LEU:HG	2.07	0.55
1:A:421:ARG:NH2	1:A:425:GLU:HG3	2.22	0.55
1:A:447:ILE:HA	1:A:450:VAL:HG22	1.89	0.55
1:A:455:PHE:HE1	1:A:938:VAL:HG12	1.70	0.55
1:B:671:ILE:HD12	1:B:672:LEU:H	1.72	0.55
1:C:303:ILE:HG23	1:C:337:ARG:HH11	1.72	0.55
1:A:10:ARG:HD3	1:B:899:GLU:OE2	2.07	0.54
1:A:16:VAL:CG2	1:B:892:LEU:HB3	2.37	0.54
1:C:4:SER:HB3	1:C:437:MET:HG3	1.89	0.54
1:C:437:MET:HE3	1:C:492:PRO:HB3	1.87	0.54
1:C:465:THR:HG22	1:C:931:VAL:HG11	1.89	0.54
1:A:23:ILE:O	1:A:27:ILE:HD12	2.06	0.54
1:A:913:MET:HB3	1:A:1022:PHE:CD1	2.38	0.54
1:B:581:ILE:CD1	1:B:671:ILE:HG23	2.37	0.54
1:C:903:LEU:HD11	1:C:952:VAL:HG13	1.88	0.54
1:B:422:ASN:ND2	1:B:435:GLN:HB3	2.22	0.54
1:B:553:TYR:CD2	1:B:913:MET:HE2	2.43	0.54
1:C:158:ASN:HA	1:C:161:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:984:SER:HB3	1:C:1020:THR:HG21	1.90	0.54
1:A:13:PHE:O	1:A:16:VAL:HG12	2.08	0.54
1:A:226:PRO:O	1:B:781:GLY:HA3	2.08	0.54
1:B:985:ILE:HA	1:B:988:ILE:HD11	1.88	0.54
1:A:714:THR:HG21	1:A:848:HIS:CE1	2.43	0.54
1:B:933:VAL:O	1:B:937:LEU:HG	2.08	0.54
1:B:1013:PHE:O	1:B:1017:LEU:HG	2.08	0.54
1:C:458:MET:HG3	1:C:473:ALA:HB2	1.90	0.54
1:B:580:LEU:HD12	1:B:656:ILE:HD11	1.90	0.54
1:B:949:ILE:HD12	1:B:950:LEU:H	1.73	0.54
1:C:458:MET:HE1	1:C:882:VAL:HG22	1.89	0.54
1:C:911:VAL:HG22	1:C:912:PRO:HD3	1.90	0.54
1:B:355:VAL:HB	1:B:368:SER:HB3	1.90	0.53
1:C:221:GLN:HA	1:C:237:ILE:HG13	1.90	0.53
1:A:950:LEU:HB3	1:A:976:ARG:NH1	2.23	0.53
1:B:437:MET:HA	1:B:440:VAL:HG22	1.88	0.53
1:C:351:VAL:O	1:C:355:VAL:HG13	2.07	0.53
1:A:539:VAL:O	1:A:543:LEU:HG	2.08	0.53
1:B:255:LYS:HD2	1:B:256:THR:H	1.73	0.53
1:C:891:PHE:CD2	1:C:904:PRO:HB2	2.44	0.53
1:C:1008:THR:O	1:C:1012:VAL:HG22	2.09	0.53
1:C:284:LEU:HD12	1:C:616:VAL:HG12	1.90	0.53
1:A:60:ALA:HA	1:A:64:ALA:HB3	1.91	0.53
1:A:217:VAL:HG22	1:B:755:GLN:OE1	2.08	0.53
1:B:937:LEU:C	1:B:941:MET:HE3	2.34	0.53
1:C:981:VAL:O	1:C:985:ILE:HG12	2.07	0.53
1:A:8:ILE:HD13	1:A:493:ALA:HA	1.91	0.53
1:B:994:LEU:HD21	1:B:1013:PHE:CD1	2.43	0.53
1:C:747:LEU:H	1:C:747:LEU:HD12	1.73	0.53
1:A:352:VAL:O	1:A:355:VAL:HG22	2.09	0.53
1:A:598:VAL:O	1:A:602:MET:HG2	2.08	0.53
1:C:385:ILE:HG21	1:C:478:ILE:HG13	1.91	0.53
1:C:564:PHE:HB3	1:C:565:LYS:HD2	1.91	0.53
1:C:958:LEU:O	1:C:962:GLY:N	2.29	0.53
1:A:49:ALA:HA	1:A:129:ILE:HG22	1.90	0.53
1:A:160:ALA:HA	1:A:164:VAL:CG1	2.38	0.53
1:A:536:GLN:O	1:A:540:SER:OG	2.21	0.53
1:B:365:TRP:HB3	1:B:510:THR:HG22	1.90	0.53
1:B:410:ASP:HB3	1:B:946:LYS:NZ	2.24	0.53
1:C:242:ARG:NH1	1:C:767:ASN:OD1	2.41	0.53
1:C:253:ILE:HG12	1:C:262:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:HA	1:C:402:VAL:HG12	1.91	0.53
1:C:399:PHE:HD1	1:C:472:PHE:HE1	1.56	0.53
1:A:714:THR:HG21	1:A:848:HIS:HE1	1.73	0.53
1:B:560:ALA:HA	1:B:916:LEU:HD13	1.90	0.53
1:A:450:VAL:HG12	1:A:890:ALA:HA	1.91	0.53
1:B:766:PHE:CE2	1:B:773:TRP:HB2	2.44	0.52
1:A:399:PHE:CE1	1:A:1008:THR:HG21	2.43	0.52
1:B:487:SER:HA	1:B:491:SER:OG	2.09	0.52
1:B:978:ARG:O	1:B:982:MET:HG3	2.09	0.52
1:C:584:VAL:HG21	1:C:598:VAL:HG11	1.91	0.52
1:A:305:LEU:O	1:A:309:VAL:HG13	2.09	0.52
1:A:689:ILE:O	1:A:828:ALA:HA	2.09	0.52
1:B:319:ARG:HG3	1:B:319:ARG:HH11	1.73	0.52
1:B:514:ASP:O	1:B:521:PHE:HE1	1.92	0.52
1:B:740:ALA:HA	1:B:808:MET:CE	2.39	0.52
1:B:913:MET:SD	1:B:913:MET:N	2.82	0.52
1:B:988:ILE:HA	1:B:991:THR:CG2	2.39	0.52
1:C:29:ILE:HA	1:C:32:LEU:HD12	1.91	0.52
1:A:11:PRO:CG	1:A:497:LEU:HD21	2.40	0.52
1:B:716:GLY:HA3	1:B:836:ASP:OD1	2.09	0.52
1:B:878:THR:O	1:B:881:ILE:HG13	2.09	0.52
1:B:13:PHE:O	1:B:16:VAL:HG12	2.09	0.52
1:B:57:LYS:HE2	1:B:730:GLN:HE22	1.75	0.52
1:B:936:GLY:O	1:B:940:LEU:HG	2.09	0.52
1:B:191:LEU:HD21	1:B:206:VAL:HG11	1.91	0.52
1:C:379:VAL:HG21	1:C:405:ILE:HG22	1.91	0.52
1:A:366:ARG:HD3	1:A:499:LEU:HA	1.91	0.52
1:A:410:ASP:O	1:A:414:VAL:HG13	2.10	0.52
1:C:211:GLN:HG2	1:C:763:VAL:HG13	1.91	0.52
1:C:465:THR:HG21	1:C:875:GLN:HG3	1.92	0.52
1:A:47:VAL:HG22	1:A:131:THR:HG23	1.92	0.52
1:A:508:LEU:HB3	1:A:509:PRO:HD3	1.92	0.52
1:B:745:VAL:HG23	1:B:797:ASN:HB3	1.92	0.52
1:B:889:LEU:O	1:B:893:VAL:HG12	2.10	0.52
1:B:979:PRO:HA	1:B:982:MET:HG3	1.90	0.52
1:A:366:ARG:HH21	1:A:500:LYS:HB2	1.73	0.52
1:A:379:VAL:HG23	1:A:401:LEU:HD22	1.91	0.52
1:A:508:LEU:O	1:A:512:LEU:HG	2.09	0.52
1:B:204:SER:O	1:B:208:THR:HG23	2.10	0.52
1:B:508:LEU:HD12	1:B:508:LEU:H	1.75	0.52
1:B:508:LEU:HB2	1:B:509:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:MET:HE2	1:B:595:THR:HA	1.92	0.52
1:B:613:ASP:OD2	1:B:613:ASP:N	2.41	0.52
1:C:361:PHE:CD1	1:C:982:MET:HE2	2.42	0.52
1:A:1033:THR:O	1:A:1036:LYS:HG2	2.10	0.51
1:B:209:ALA:O	1:B:213:GLN:HG3	2.10	0.51
1:C:441:SER:O	1:C:445:ILE:HG13	2.10	0.51
1:B:187:MET:HB3	1:B:775:VAL:HG13	1.92	0.51
1:B:334:VAL:HG13	1:B:335:PHE:HD1	1.76	0.51
1:A:657:ASN:HA	1:A:660:ILE:HD11	1.93	0.51
1:A:846:MET:HE1	1:A:873:ALA:HB2	1.91	0.51
1:B:420:GLU:HG2	1:B:499:LEU:HD21	1.92	0.51
1:A:687:LEU:HG	1:A:831:LEU:HB2	1.93	0.51
1:B:65:THR:HG22	1:B:822:ARG:CZ	2.41	0.51
1:B:992:ILE:N	1:B:993:PRO:HD2	2.25	0.51
1:B:511:ARG:NH2	1:B:514:ASP:OD1	2.44	0.51
1:A:739:LYS:O	1:A:743:GLN:HG3	2.11	0.51
1:B:954:PHE:HE1	1:B:976:ARG:HH11	1.58	0.51
1:A:358:VAL:HG11	1:A:368:SER:HA	1.93	0.51
1:A:692:ARG:NE	1:A:862:ASN:OD1	2.43	0.51
1:A:443:PRO:O	1:A:447:ILE:HD12	2.10	0.51
1:A:609:THR:HG23	1:A:655:GLU:OE1	2.10	0.51
1:C:894:LEU:HD11	1:C:907:VAL:HG11	1.93	0.51
1:A:281:ARG:HB2	1:A:619:PRO:HG2	1.92	0.51
1:A:918:ALA:HB2	1:A:940:LEU:HD21	1.92	0.51
1:A:1006:GLY:O	1:A:1009:GLY:N	2.44	0.51
1:B:922:VAL:HG12	1:B:927:GLY:HA3	1.91	0.51
1:C:373:ILE:HD11	1:C:490:LEU:HD21	1.93	0.51
1:C:569:GLY:O	1:C:841:SER:OG	2.26	0.51
1:C:648:THR:HG23	1:C:651:GLU:H	1.76	0.51
1:A:67:LEU:O	1:A:71:ILE:HD12	2.11	0.50
1:A:1033:THR:O	1:A:1037:LEU:HD23	2.11	0.50
1:B:15:ALA:O	1:B:19:ILE:HG13	2.12	0.50
1:B:473:ALA:HA	1:B:476:ILE:HG13	1.93	0.50
1:B:573:PRO:HG3	1:B:930:ASN:HB2	1.93	0.50
1:A:553:TYR:HD1	1:A:1026:LEU:HD21	1.74	0.50
1:A:933:VAL:HG23	1:A:1011:THR:HG21	1.93	0.50
1:C:889:LEU:O	1:C:893:VAL:HG22	2.11	0.50
1:A:985:ILE:HA	1:A:988:ILE:HG13	1.93	0.50
1:B:878:THR:O	1:B:882:VAL:HG13	2.12	0.50
1:C:369:ILE:O	1:C:373:ILE:HG23	2.11	0.50
1:C:494:LEU:O	1:C:498:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:776:MET:HE3	1:C:776:MET:HA	1.94	0.50
1:A:681:GLN:NE2	1:A:833:GLY:O	2.44	0.50
1:B:361:PHE:HD1	1:B:978:ARG:HG3	1.76	0.50
1:B:440:VAL:O	1:B:444:ILE:HG23	2.11	0.50
1:B:442:GLY:O	1:B:445:ILE:HG13	2.11	0.50
1:C:528:PHE:HE2	1:C:978:ARG:HB2	1.76	0.50
1:C:934:GLN:O	1:C:938:VAL:HG13	2.11	0.50
1:A:206:VAL:O	1:A:210:MET:HG3	2.11	0.50
1:A:356:LEU:O	1:A:359:ILE:HG13	2.11	0.50
1:B:12:ILE:HB	1:C:899:GLU:CD	2.36	0.50
1:B:386:LEU:HD22	1:B:391:PHE:HB2	1.92	0.50
1:C:208:THR:HA	1:C:211:GLN:HG3	1.94	0.50
1:C:354:VAL:O	1:C:358:VAL:HG13	2.12	0.50
1:C:456:VAL:HG13	1:C:457:PRO:HD3	1.94	0.50
1:B:36:GLU:OE2	1:B:577:LYS:NZ	2.44	0.50
1:B:513:ILE:O	1:B:521:PHE:CZ	2.60	0.50
1:B:545:ARG:HH21	1:B:546:ARG:HD3	1.77	0.50
1:C:688:TYR:CE1	1:C:830:ASP:HB3	2.47	0.50
1:B:249:PHE:O	1:B:252:ILE:HG13	2.12	0.49
1:B:663:ILE:HD12	1:B:663:ILE:O	2.12	0.49
1:C:764:ASN:O	1:C:775:VAL:HG22	2.11	0.49
1:A:20:LEU:HD21	1:B:889:LEU:CD2	2.42	0.49
1:B:605:ILE:HD13	1:B:659:LYS:HG3	1.94	0.49
1:C:213:GLN:CD	1:C:252:ILE:HG23	2.37	0.49
1:B:34:VAL:HG22	1:B:393:LEU:HB2	1.93	0.49
1:C:188:ARG:HH21	1:C:276:GLY:C	2.21	0.49
1:C:188:ARG:NE	1:C:275:SER:O	2.27	0.49
1:C:347:LEU:O	1:C:351:VAL:HG13	2.12	0.49
1:C:361:PHE:CD1	1:C:982:MET:HB3	2.47	0.49
1:A:447:ILE:HG21	1:A:946:LYS:HB2	1.94	0.49
1:A:958:LEU:HA	1:A:961:GLN:OE1	2.13	0.49
1:B:918:ALA:O	1:B:1011:THR:OG1	2.29	0.49
1:C:363:GLN:HG2	1:C:521:PHE:CD1	2.48	0.49
1:C:435:GLN:OE1	1:C:438:ARG:NH1	2.46	0.49
1:C:689:ILE:HD12	1:C:704:VAL:HG22	1.93	0.49
1:B:454:VAL:HG12	1:B:455:PHE:CD1	2.47	0.49
1:B:506:LYS:O	1:B:507:ASP:HB3	2.12	0.49
1:C:885:VAL:O	1:C:889:LEU:HD23	2.12	0.49
1:C:914:THR:HB	1:C:1019:VAL:HB	1.93	0.49
1:A:369:ILE:O	1:A:372:LEU:HB3	2.13	0.49
1:A:917:SER:O	1:A:1014:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HD21	1:B:309:VAL:HG23	1.94	0.49
1:B:418:ASN:HD21	1:B:439:GLU:HG3	1.77	0.49
1:C:358:VAL:O	1:C:362:LEU:HB2	2.12	0.49
1:A:672:LEU:HD12	1:A:672:LEU:H	1.77	0.49
1:A:987:PHE:O	1:A:991:THR:HG23	2.12	0.49
1:C:351:VAL:HG12	1:C:405:ILE:HD13	1.95	0.49
1:C:512:LEU:O	1:C:516:LEU:HD12	2.12	0.49
1:C:987:PHE:O	1:C:991:THR:HG23	2.13	0.49
1:B:286:ASN:HD21	1:B:600:ARG:HA	1.78	0.49
1:B:1001:GLY:O	1:B:1005:ARG:HG2	2.13	0.49
1:C:171:LEU:HD21	1:C:312:LYS:HB2	1.93	0.49
1:C:707:MET:HE2	1:C:857:LEU:HG	1.95	0.49
1:A:104:GLN:HE22	1:C:103:ASP:HB3	1.77	0.49
1:A:154:LEU:HD13	1:A:275:SER:HB2	1.93	0.49
1:A:992:ILE:HD12	1:A:992:ILE:H	1.77	0.49
1:B:185:TYR:HB2	1:B:773:TRP:CE3	2.48	0.49
1:A:817:PRO:HG2	1:A:820:VAL:HG22	1.95	0.49
1:B:472:PHE:CD2	1:B:935:VAL:HG21	2.48	0.49
1:B:478:ILE:HG23	1:B:482:ILE:HD11	1.95	0.49
1:B:622:ASN:C	1:B:622:ASN:HD22	2.21	0.49
1:B:966:MET:H	1:B:966:MET:CE	2.25	0.48
1:C:553:TYR:CD1	1:C:1030:PHE:HZ	2.31	0.48
1:B:83:VAL:HG11	1:B:627:THR:HG21	1.95	0.48
1:C:749:GLU:OE1	1:C:795:THR:OG1	2.31	0.48
1:A:406:GLY:HA3	1:A:987:PHE:CZ	2.45	0.48
1:A:687:LEU:HD22	1:A:863:ILE:HD11	1.96	0.48
1:C:399:PHE:CZ	1:C:1005:ARG:HA	2.46	0.48
1:C:563:MET:O	1:C:567:VAL:HG12	2.13	0.48
1:C:1038:VAL:HG12	1:C:1039:THR:HG23	1.95	0.48
1:B:820:VAL:C	1:B:821:ILE:HD13	2.37	0.48
1:C:392:SER:OG	1:C:394:ASN:ND2	2.38	0.48
1:C:723:THR:HG22	1:C:830:ASP:OD2	2.13	0.48
1:A:725:GLN:O	1:A:817:PRO:HA	2.13	0.48
1:A:957:GLU:O	1:A:961:GLN:HG3	2.13	0.48
1:B:256:THR:HG23	1:C:741:LYS:HE3	1.95	0.48
1:B:819:PRO:HG2	1:B:821:ILE:HD11	1.94	0.48
1:C:598:VAL:O	1:C:602:MET:HG3	2.14	0.48
1:C:915:MET:SD	1:C:937:LEU:HD12	2.54	0.48
1:A:351:VAL:O	1:A:354:VAL:HG12	2.14	0.48
1:B:461:LEU:HD11	1:B:882:VAL:HG21	1.95	0.48
1:B:954:PHE:HE1	1:B:976:ARG:NH1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:CA	1:C:402:VAL:HG12	2.44	0.48
1:A:8:ILE:HG21	1:A:434:HIS:CD2	2.49	0.48
1:A:375:VAL:O	1:A:379:VAL:HG12	2.14	0.48
1:B:67:LEU:O	1:B:71:ILE:HG13	2.14	0.48
1:B:476:ILE:O	1:B:480:THR:HG22	2.13	0.48
1:B:966:MET:H	1:B:966:MET:HE3	1.78	0.48
1:C:340:ILE:O	1:C:344:VAL:HG13	2.14	0.48
1:C:470:LYS:O	1:C:474:VAL:HG22	2.14	0.48
1:A:1010:ILE:HD12	1:A:1010:ILE:H	1.79	0.48
1:B:849:LEU:HA	1:B:852:LEU:HD13	1.96	0.48
1:C:563:MET:HA	1:C:566:VAL:HG12	1.95	0.48
1:C:748:THR:HA	1:C:751:PHE:CD2	2.49	0.48
1:A:255:LYS:HB2	1:A:255:LYS:HE3	1.55	0.47
1:A:350:ALA:HB2	1:A:405:ILE:HD13	1.96	0.47
1:A:933:VAL:CG2	1:A:1011:THR:HG21	2.44	0.47
1:B:230:GLU:OE2	1:C:594:ARG:NH1	2.46	0.47
1:B:478:ILE:O	1:B:482:ILE:HD12	2.13	0.47
1:B:629:THR:HB	1:B:632:THR:OG1	2.13	0.47
1:A:421:ARG:NH1	1:A:422:ASN:HA	2.29	0.47
1:A:956:ARG:O	1:A:960:ILE:HG12	2.14	0.47
1:B:676:ILE:CD1	1:B:679:LEU:HB2	2.42	0.47
1:C:420:GLU:HA	1:C:423:ILE:HG12	1.95	0.47
1:C:954:PHE:CD2	1:C:972:ALA:HA	2.49	0.47
1:B:464:VAL:HG12	1:B:468:PHE:CE1	2.49	0.47
1:B:721:ILE:HD12	1:B:722:SER:H	1.79	0.47
1:B:931:VAL:HA	1:B:934:GLN:OE1	2.14	0.47
1:C:374:ALA:O	1:C:378:SER:OG	2.31	0.47
1:C:841:SER:H	1:C:844:GLN:HE21	1.60	0.47
1:C:348:LEU:O	1:C:351:VAL:HG22	2.14	0.47
1:A:373:ILE:O	1:A:376:PRO:HD2	2.14	0.47
1:A:522:ARG:HA	1:A:525:ASN:OD1	2.15	0.47
1:A:861:MET:HE3	1:A:861:MET:HB2	1.78	0.47
1:A:55:ASN:ND2	1:C:238:ASN:HB2	2.19	0.47
1:A:210:MET:HE2	1:A:210:MET:HB3	1.82	0.47
1:A:505:LYS:HD2	1:A:507:ASP:HA	1.97	0.47
1:A:601:LYS:NZ	1:A:665:GLN:HE22	2.11	0.47
1:B:450:VAL:HG22	1:B:893:VAL:HG13	1.96	0.47
1:B:553:TYR:OH	1:B:909:LEU:O	2.24	0.47
1:B:1040:ARG:HE	1:B:1040:ARG:HB3	1.53	0.47
1:C:286:ASN:OD1	1:C:603:SER:OG	2.29	0.47
1:A:646:LYS:HA	1:A:646:LYS:HD3	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:MET:HE3	1:C:77:MET:HB2	1.81	0.47
1:C:117:GLU:HA	1:C:120:LEU:HD12	1.97	0.47
1:C:179:ILE:HD13	1:C:292:ILE:HG23	1.96	0.47
1:C:763:VAL:HB	1:C:775:VAL:HG23	1.96	0.47
1:A:340:ILE:O	1:A:343:VAL:HG12	2.15	0.47
1:A:534:GLY:O	1:A:538:LEU:HG	2.13	0.47
1:B:601:LYS:HD2	1:B:601:LYS:HA	1.55	0.47
1:A:160:ALA:HA	1:A:164:VAL:HG13	1.97	0.47
1:A:399:PHE:CZ	1:A:1008:THR:HG21	2.50	0.47
1:B:346:THR:O	1:B:350:ALA:N	2.44	0.47
1:C:35:SER:O	1:C:394:ASN:HA	2.14	0.47
1:C:106:GLN:NE2	1:C:131:THR:O	2.47	0.47
1:C:305:LEU:O	1:C:309:VAL:HG23	2.15	0.47
1:B:363:GLN:HE21	1:B:521:PHE:HB3	1.79	0.46
1:B:911:VAL:N	1:B:912:PRO:HD2	2.30	0.46
1:B:1006:GLY:O	1:B:1010:ILE:HB	2.15	0.46
1:C:883:PHE:HB2	1:C:884:PRO:HD3	1.97	0.46
1:A:511:ARG:HG3	1:A:512:LEU:N	2.29	0.46
1:B:224:ALA:HA	1:B:234:LEU:HD11	1.96	0.46
1:B:375:VAL:O	1:B:379:VAL:HG13	2.16	0.46
1:B:563:MET:HA	1:B:566:VAL:HG12	1.96	0.46
1:B:973:CYS:O	1:B:977:LEU:HB2	2.16	0.46
1:A:940:LEU:HD12	1:A:941:MET:N	2.31	0.46
1:B:6:PHE:HE1	1:B:10:ARG:NE	2.13	0.46
1:B:399:PHE:HB3	1:B:472:PHE:HE1	1.81	0.46
1:B:943:LEU:HD12	1:B:946:LYS:HD3	1.98	0.46
1:A:554:LEU:HA	1:A:557:LEU:HD22	1.97	0.46
1:B:178:GLN:C	1:B:179:ILE:HD13	2.41	0.46
1:B:422:ASN:HD21	1:B:435:GLN:HB3	1.79	0.46
1:C:70:ALA:HB2	1:C:116:ALA:HB2	1.97	0.46
1:C:161:THR:HG21	1:C:184:GLU:HG2	1.98	0.46
1:A:332:PRO:HA	1:A:335:PHE:HE2	1.80	0.46
1:B:907:VAL:HG21	1:B:949:ILE:HG23	1.96	0.46
1:A:109:VAL:O	1:A:113:VAL:HG13	2.15	0.46
1:B:59:ILE:HD11	1:B:88:GLY:HA2	1.97	0.46
1:B:1022:PHE:O	1:B:1026:LEU:HB3	2.16	0.46
1:C:285:ASN:O	1:C:286:ASN:HB2	2.16	0.46
1:C:656:ILE:O	1:C:660:ILE:HG23	2.16	0.46
1:C:917:SER:HB2	1:C:1015:GLY:HA2	1.96	0.46
1:C:681:GLN:HA	1:C:681:GLN:OE1	2.16	0.46
1:B:57:LYS:HE2	1:B:730:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:H	1:B:57:LYS:HD2	1.81	0.46
1:B:812:SER:OG	1:B:813:THR:N	2.48	0.46
1:C:437:MET:O	1:C:441:SER:HB3	2.16	0.46
1:C:978:ARG:HG3	1:C:982:MET:HE3	1.97	0.46
1:A:870:PHE:O	1:A:874:THR:HG23	2.16	0.46
1:A:905:LEU:HB2	1:A:1034:LEU:HD11	1.98	0.46
1:C:44:SER:OG	1:C:134:GLN:O	2.30	0.46
1:C:180:PHE:O	1:C:280:LEU:HB3	2.16	0.46
1:C:427:LEU:HD12	1:C:427:LEU:HA	1.79	0.46
1:A:306:SER:OG	1:A:333:THR:HG21	2.16	0.45
1:A:420:GLU:OE1	1:A:499:LEU:HD13	2.16	0.45
1:B:711:ILE:HG23	1:B:717:MET:HE3	1.98	0.45
1:A:101:ASP:HB3	1:A:104:GLN:HB3	1.98	0.45
1:A:707:MET:O	1:A:710:ALA:N	2.49	0.45
1:A:763:VAL:HG22	1:A:775:VAL:O	2.16	0.45
1:A:854:LYS:HA	1:A:854:LYS:HD2	1.56	0.45
1:B:354:VAL:O	1:B:358:VAL:HG23	2.16	0.45
1:B:400:GLY:O	1:B:476:ILE:HG22	2.15	0.45
1:C:37:TYR:OH	1:C:575:GLN:OE1	2.35	0.45
1:C:391:PHE:CZ	1:C:474:VAL:HG21	2.51	0.45
1:C:567:VAL:CG1	1:C:919:LEU:HD23	2.45	0.45
1:A:375:VAL:HA	1:A:408:VAL:HG11	1.99	0.45
1:A:918:ALA:CB	1:A:940:LEU:HD21	2.46	0.45
1:B:337:ARG:HA	1:B:340:ILE:CG2	2.41	0.45
1:A:8:ILE:HD11	1:A:492:PRO:HB2	1.98	0.45
1:A:844:GLN:H	1:A:844:GLN:CD	2.23	0.45
1:B:440:VAL:HA	1:B:443:PRO:HG2	1.98	0.45
1:B:528:PHE:O	1:B:532:SER:OG	2.17	0.45
1:C:450:VAL:O	1:C:454:VAL:HG23	2.17	0.45
1:C:497:LEU:CD2	2:C:1101:LMT:H3B	2.46	0.45
1:C:978:ARG:O	1:C:982:MET:HG2	2.17	0.45
1:B:160:ALA:HA	1:B:164:VAL:HB	1.97	0.45
1:B:188:ARG:HD3	1:B:776:MET:HB2	1.98	0.45
1:B:331:ASP:O	1:B:334:VAL:HG12	2.17	0.45
1:B:335:PHE:O	1:B:338:ASP:HB3	2.16	0.45
1:B:370:ILE:HD12	1:B:416:VAL:HG22	1.97	0.45
1:B:461:LEU:HB2	1:B:466:GLY:CA	2.47	0.45
1:B:527:PHE:HD2	1:B:527:PHE:O	2.00	0.45
1:B:947:ASN:OD1	1:B:948:ALA:N	2.49	0.45
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.55	0.45
1:A:291:GLY:C	1:A:292:ILE:HD13	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:O	1:A:425:GLU:HG2	2.17	0.45
1:C:36:GLU:HB2	1:C:336:VAL:HG13	1.97	0.45
1:C:841:SER:H	1:C:844:GLN:NE2	2.14	0.45
1:A:6:PHE:CD1	1:A:6:PHE:C	2.95	0.45
1:A:317:ALA:HA	1:A:320:PHE:CD2	2.52	0.45
1:B:37:TYR:OH	1:B:675:PRO:O	2.24	0.45
1:B:573:PRO:CD	1:B:930:ASN:HB2	2.45	0.45
1:C:135:SER:C	1:C:137:THR:H	2.25	0.45
1:C:891:PHE:HE2	1:C:905:LEU:HD12	1.82	0.45
1:C:954:PHE:CE2	1:C:975:LEU:HB2	2.49	0.45
1:B:930:ASN:O	1:B:933:VAL:N	2.50	0.45
1:A:73:GLY:N	1:A:77:MET:HE1	2.27	0.45
1:A:556:LEU:HD22	1:A:913:MET:SD	2.56	0.45
1:B:429:PRO:HB3	1:B:499:LEU:O	2.16	0.45
1:B:691:ASP:HB2	1:B:861:MET:HE2	1.97	0.45
1:B:741:LYS:O	1:B:741:LYS:NZ	2.43	0.45
1:B:976:ARG:O	1:B:980:ILE:HG13	2.17	0.45
1:C:245:THR:HG23	1:C:248:GLU:H	1.82	0.45
1:C:366:ARG:NH1	1:C:507:ASP:OD2	2.50	0.45
1:C:790:ILE:O	1:C:805:ILE:HD11	2.17	0.45
1:A:440:VAL:HA	1:A:443:PRO:HG2	1.98	0.45
1:A:652:ILE:HD12	1:A:652:ILE:H	1.82	0.45
1:B:157:ARG:N	1:B:290:VAL:HG11	2.32	0.45
1:B:539:VAL:HA	1:B:542:THR:OG1	2.16	0.45
1:C:407:ILE:HD11	1:C:987:PHE:HE1	1.82	0.45
1:C:414:VAL:O	1:C:417:GLU:HG3	2.17	0.45
1:C:935:VAL:O	1:C:938:VAL:HG22	2.16	0.45
1:A:6:PHE:C	1:A:6:PHE:HD1	2.25	0.44
1:A:688:TYR:CE2	1:A:830:ASP:HB3	2.53	0.44
1:A:1001:GLY:O	1:A:1005:ARG:HG2	2.17	0.44
1:B:1024:LEU:HD23	1:B:1024:LEU:HA	1.81	0.44
1:C:458:MET:HE2	1:C:458:MET:N	2.32	0.44
1:A:332:PRO:O	1:A:335:PHE:HD2	2.00	0.44
1:A:515:ARG:HH21	1:A:516:LEU:HD21	1.82	0.44
1:B:242:ARG:NH1	1:C:51:TYR:OH	2.49	0.44
1:B:334:VAL:HA	1:B:337:ARG:HG2	1.98	0.44
1:C:185:TYR:HA	1:C:274:GLY:O	2.17	0.44
1:A:165:LYS:HG3	1:A:177:ILE:CD1	2.46	0.44
1:A:478:ILE:HG13	1:A:479:SER:N	2.31	0.44
1:A:490:LEU:HG	1:A:494:LEU:HD13	1.98	0.44
1:A:533:ASN:HA	1:A:536:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ASP:OD1	1:A:838:ARG:NH1	2.51	0.44
1:B:141:VAL:CG1	1:B:330:TYR:HB3	2.48	0.44
1:B:545:ARG:HE	1:B:545:ARG:C	2.26	0.44
1:A:138:LEU:HD12	1:A:294:ILE:O	2.17	0.44
1:A:140:LEU:HD13	1:A:141:VAL:N	2.32	0.44
1:A:536:GLN:HA	1:A:539:VAL:HG22	1.99	0.44
1:A:947:ASN:ND2	1:A:980:ILE:HG23	2.31	0.44
1:A:1013:PHE:CE2	1:A:1017:LEU:HD11	2.52	0.44
1:A:74:VAL:HG23	1:A:112:ARG:HD2	2.00	0.44
1:A:105:ALA:O	1:A:109:VAL:HG23	2.17	0.44
1:A:648:THR:O	1:A:651:GLU:N	2.51	0.44
1:A:985:ILE:HA	1:A:988:ILE:CG1	2.47	0.44
1:B:270:ARG:C	1:B:271:ILE:HD13	2.42	0.44
1:C:157:ARG:HD2	1:C:179:ILE:HG21	1.99	0.44
1:C:300:ALA:C	1:C:302:ALA:H	2.25	0.44
1:A:370:ILE:CG2	1:A:494:LEU:HB3	2.46	0.44
1:A:487:SER:HA	1:A:491:SER:OG	2.17	0.44
1:A:557:LEU:HD23	1:A:558:CYS:H	1.83	0.44
1:B:435:GLN:HA	1:B:438:ARG:HD2	2.00	0.44
1:A:310:ARG:HG3	1:A:326:TRP:HH2	1.83	0.44
1:A:450:VAL:O	1:A:454:VAL:HG13	2.18	0.44
1:B:335:PHE:CE2	1:B:577:LYS:HD2	2.50	0.44
1:C:185:TYR:HB2	1:C:773:TRP:CZ3	2.53	0.44
1:C:684:GLY:HA3	1:C:833:GLY:O	2.17	0.44
1:A:341:ARG:NH1	1:A:345:GLN:OE1	2.50	0.44
1:A:407:ILE:HG13	1:A:408:VAL:N	2.33	0.44
1:A:910:ILE:HG21	1:A:1027:THR:HG23	1.99	0.44
1:B:110:GLN:OE1	1:B:131:THR:OG1	2.19	0.44
1:B:527:PHE:HD2	1:B:531:SER:HG	1.65	0.44
1:B:585:LYS:NZ	1:B:588:GLU:OE1	2.51	0.44
1:B:588:GLU:N	1:B:588:GLU:OE1	2.50	0.44
1:C:36:GLU:HG2	1:C:37:TYR:CD2	2.53	0.44
1:A:622:ASN:HD22	1:A:623:ALA:N	2.16	0.43
1:A:841:SER:H	1:A:844:GLN:NE2	2.16	0.43
1:A:844:GLN:OE1	1:A:844:GLN:N	2.44	0.43
1:B:4:SER:OG	1:B:437:MET:SD	2.73	0.43
1:C:156:MET:HB2	1:C:290:VAL:HG21	2.00	0.43
1:C:472:PHE:O	1:C:475:THR:HG22	2.17	0.43
1:A:32:LEU:HB3	1:A:393:LEU:HD11	2.00	0.43
1:A:201:LEU:HD13	1:A:254:LEU:HD23	2.00	0.43
1:A:366:ARG:NH2	1:A:500:LYS:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD12	1:B:91:VAL:N	2.33	0.43
1:B:508:LEU:HB2	1:B:509:PRO:CD	2.48	0.43
1:A:165:LYS:HE3	1:A:177:ILE:HD11	2.01	0.43
1:A:351:VAL:O	1:A:355:VAL:HG13	2.17	0.43
1:B:38:PRO:HD3	1:B:394:ASN:CG	2.44	0.43
1:B:586:MET:HB3	1:B:587:PRO:HD2	2.01	0.43
1:B:913:MET:HB3	1:B:1022:PHE:CD2	2.54	0.43
1:B:954:PHE:HA	1:B:957:GLU:HG3	2.00	0.43
1:C:175:GLY:N	1:C:295:PHE:O	2.49	0.43
1:C:1035:ARG:HA	1:C:1035:ARG:HD2	1.78	0.43
1:A:16:VAL:HG23	1:B:892:LEU:HB3	1.99	0.43
1:C:616:VAL:CG2	1:C:636:PHE:HB2	2.48	0.43
1:A:169:ALA:HA	1:A:174:VAL:HG21	2.00	0.43
1:B:8:ILE:H	1:B:8:ILE:HD12	1.82	0.43
1:B:407:ILE:O	1:B:946:LYS:NZ	2.52	0.43
1:B:437:MET:HE1	1:B:492:PRO:HG3	2.00	0.43
1:B:482:ILE:O	1:B:486:ASN:ND2	2.51	0.43
1:B:513:ILE:HD12	1:B:514:ASP:H	1.79	0.43
1:C:579:TYR:CZ	1:C:673:PRO:HB3	2.53	0.43
1:A:226:PRO:HD3	1:B:190:TRP:CH2	2.53	0.43
1:A:419:VAL:HG11	1:A:495:ALA:HB1	2.01	0.43
1:B:145:PHE:CE2	1:B:325:GLN:HB2	2.54	0.43
1:B:464:VAL:O	1:B:467:GLN:N	2.52	0.43
1:B:584:VAL:HG22	1:B:586:MET:HG2	2.01	0.43
1:C:171:LEU:HD12	1:C:171:LEU:H	1.83	0.43
1:C:512:LEU:C	1:C:516:LEU:HD12	2.44	0.43
1:A:284:LEU:HD11	1:A:614:TYR:CD1	2.54	0.43
1:A:375:VAL:HG22	1:A:376:PRO:HD3	2.00	0.43
1:A:474:VAL:O	1:A:478:ILE:HG23	2.19	0.43
1:B:321:PRO:HD2	1:B:324:MET:CE	2.49	0.43
1:C:55:ASN:OD1	1:C:57:LYS:HG3	2.18	0.43
1:C:210:MET:HB2	1:C:763:VAL:HG11	2.01	0.43
1:C:902:THR:HG23	1:C:1034:LEU:HB3	1.99	0.43
1:A:382:THR:HG21	1:A:401:LEU:HD21	2.01	0.43
1:A:557:LEU:HD23	1:A:558:CYS:N	2.34	0.43
1:B:391:PHE:HE2	1:B:471:GLN:HA	1.84	0.43
1:C:134:GLN:NE2	1:C:135:SER:O	2.52	0.43
1:C:766:PHE:CE1	1:C:773:TRP:HB2	2.54	0.43
1:A:35:SER:O	1:A:394:ASN:HA	2.18	0.43
1:A:57:LYS:HE2	1:C:238:ASN:ND2	2.34	0.43
1:C:117:GLU:HA	1:C:120:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:THR:HG21	1:C:875:GLN:CG	2.48	0.43
1:C:974:ARG:NH2	1:C:975:LEU:HD21	2.34	0.43
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.79	0.42
1:A:879:ALA:HA	1:A:882:VAL:HB	2.01	0.42
1:B:950:LEU:HD23	1:B:950:LEU:HA	1.84	0.42
1:B:1009:GLY:HA2	1:B:1012:VAL:HB	2.00	0.42
1:A:143:HIS:O	1:A:326:TRP:HA	2.19	0.42
1:A:421:ARG:HH22	1:A:425:GLU:HG3	1.84	0.42
1:A:442:GLY:O	1:A:445:ILE:HG13	2.18	0.42
1:A:712:MET:HE2	1:A:712:MET:HB3	1.85	0.42
1:B:334:VAL:O	1:B:337:ARG:HG2	2.19	0.42
1:B:461:LEU:HB2	1:B:466:GLY:HA2	2.01	0.42
1:B:662:GLN:C	1:B:664:GLN:HE22	2.28	0.42
1:B:898:TYR:OH	1:B:949:ILE:O	2.38	0.42
1:C:303:ILE:HG23	1:C:337:ARG:NH1	2.32	0.42
1:C:361:PHE:CE1	1:C:524:PHE:HZ	2.37	0.42
1:C:904:PRO:O	1:C:908:ILE:HG12	2.19	0.42
1:A:67:LEU:O	1:A:70:ALA:N	2.48	0.42
1:C:234:LEU:C	1:C:235:ILE:HD13	2.44	0.42
1:A:943:LEU:HA	1:A:946:LYS:HD2	2.00	0.42
1:C:160:ALA:O	1:C:165:LYS:N	2.39	0.42
1:C:950:LEU:HD12	1:C:980:ILE:HG12	2.01	0.42
1:B:351:VAL:O	1:B:355:VAL:HG13	2.20	0.42
1:B:386:LEU:HD22	1:B:391:PHE:CB	2.49	0.42
1:B:689:ILE:O	1:B:828:ALA:HA	2.19	0.42
1:C:736:ASP:CG	1:C:739:LYS:HB2	2.44	0.42
1:A:218:SER:HB2	1:B:54:ALA:HA	2.01	0.42
1:A:505:LYS:HE3	1:A:505:LYS:HB3	1.68	0.42
1:A:653:ASN:O	1:A:657:ASN:HB2	2.19	0.42
1:B:464:VAL:H	1:B:871:GLN:HE22	1.66	0.42
1:C:430:LEU:O	1:C:434:HIS:HD2	2.03	0.42
1:A:532:SER:O	1:A:535:TYR:HB3	2.20	0.42
1:A:577:LYS:HA	1:A:577:LYS:HD3	1.71	0.42
1:A:602:MET:HB3	1:A:660:ILE:CG2	2.47	0.42
1:B:16:VAL:CG2	1:C:892:LEU:HB3	2.49	0.42
1:B:497:LEU:HG	1:B:498:LEU:CD2	2.46	0.42
1:B:609:THR:HG22	1:B:610:GLU:H	1.84	0.42
1:B:836:ASP:N	1:B:836:ASP:OD2	2.51	0.42
1:B:966:MET:SD	1:B:966:MET:N	2.89	0.42
1:C:744:GLY:O	1:C:798:ASN:N	2.52	0.42
1:A:19:ILE:O	1:A:23:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ARG:HA	1:B:344:VAL:HG12	2.01	0.42
1:A:386:LEU:HD12	1:A:386:LEU:HA	1.90	0.42
1:A:548:ALA:O	1:A:552:VAL:HG12	2.20	0.42
1:B:891:PHE:HD1	1:B:904:PRO:HB2	1.85	0.42
1:C:582:GLY:HA2	1:C:670:SER:HA	2.01	0.42
1:C:707:MET:CE	1:C:853:SER:HA	2.49	0.42
1:C:932:PHE:O	1:C:935:VAL:HG22	2.20	0.42
1:A:80:MET:HE2	1:A:94:VAL:HG22	2.02	0.42
1:A:117:GLU:CG	1:A:129:ILE:HD11	2.50	0.42
1:A:270:ARG:C	1:A:271:ILE:HD13	2.44	0.42
1:A:330:TYR:HE2	1:A:332:PRO:HB3	1.85	0.42
1:A:373:ILE:O	1:A:377:VAL:HG22	2.18	0.42
1:A:781:GLY:HA3	1:C:226:PRO:O	2.20	0.42
1:B:871:GLN:HE21	1:B:871:GLN:HB3	1.64	0.42
1:C:152:ASP:O	1:C:156:MET:HG3	2.20	0.42
1:A:33:PRO:HB2	1:A:392:SER:HB2	2.02	0.41
1:A:375:VAL:HA	1:A:408:VAL:CG1	2.50	0.41
1:A:839:VAL:O	1:A:840:LEU:HD23	2.20	0.41
1:A:902:THR:HA	1:A:905:LEU:HD12	2.01	0.41
1:B:234:LEU:C	1:B:235:ILE:HD13	2.45	0.41
1:C:187:MET:O	1:C:775:VAL:HA	2.20	0.41
1:C:363:GLN:HG2	1:C:521:PHE:CG	2.55	0.41
1:C:712:MET:HE3	1:C:719:PHE:HB2	2.01	0.41
1:A:370:ILE:HD12	1:A:370:ILE:C	2.45	0.41
1:B:376:PRO:O	1:B:379:VAL:HG22	2.20	0.41
1:B:660:ILE:HD13	1:B:668:GLY:C	2.45	0.41
1:C:168:LEU:HA	1:C:171:LEU:CD1	2.51	0.41
1:A:222:LEU:HG	1:A:237:ILE:HD11	2.01	0.41
1:A:560:ALA:HA	1:A:916:LEU:HD12	2.01	0.41
1:B:846:MET:HG3	1:B:865:TRP:CH2	2.55	0.41
1:C:199:ARG:HD2	1:C:263:VAL:HG11	2.02	0.41
1:C:312:LYS:HA	1:C:312:LYS:HD3	1.84	0.41
1:C:355:VAL:HA	1:C:358:VAL:HG22	2.02	0.41
1:A:275:SER:OG	1:A:277:SER:O	2.38	0.41
1:A:447:ILE:HA	1:A:450:VAL:CG2	2.49	0.41
1:A:511:ARG:HG3	1:A:512:LEU:HD23	2.01	0.41
1:A:748:THR:HG21	1:C:212:GLU:HG2	2.00	0.41
1:A:981:VAL:O	1:A:985:ILE:HG23	2.19	0.41
1:B:334:VAL:HG13	1:B:335:PHE:CD1	2.53	0.41
1:B:554:LEU:O	1:B:557:LEU:HG	2.21	0.41
1:C:728:VAL:HG21	1:C:818:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:944:ALA:HB2	1:C:1019:VAL:HG21	2.03	0.41
1:A:237:ILE:CD1	1:B:758:LEU:HD23	2.50	0.41
1:A:409:VAL:O	1:A:413:ILE:HD12	2.21	0.41
1:A:790:ILE:HD11	1:C:222:LEU:HD21	2.02	0.41
1:B:161:THR:HG22	1:B:162:LEU:HD23	2.01	0.41
1:B:410:ASP:OD1	1:B:983:THR:HG21	2.21	0.41
1:C:396:LEU:HA	1:C:399:PHE:HB2	2.02	0.41
1:A:888:LEU:HA	1:A:891:PHE:HB3	2.03	0.41
1:A:911:VAL:HG22	1:A:912:PRO:HD3	2.01	0.41
1:B:527:PHE:O	1:B:531:SER:OG	2.36	0.41
1:B:912:PRO:O	1:B:915:MET:HB3	2.20	0.41
1:B:994:LEU:HD21	1:B:1013:PHE:HD1	1.84	0.41
1:C:399:PHE:HA	1:C:402:VAL:HG22	2.02	0.41
1:B:660:ILE:HD12	1:B:660:ILE:C	2.46	0.41
1:C:522:ARG:O	1:C:526:ARG:HG3	2.20	0.41
1:A:145:PHE:CZ	1:A:325:GLN:HG3	2.56	0.41
1:A:164:VAL:HB	1:A:316:LEU:HD22	2.03	0.41
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.69	0.41
1:B:273:MET:HE2	1:B:273:MET:HB2	1.82	0.41
1:B:458:MET:HE1	1:B:883:PHE:HE2	1.86	0.41
1:B:643:ASP:OD1	1:B:643:ASP:N	2.54	0.41
1:B:745:VAL:CB	1:B:808:MET:HE1	2.37	0.41
1:C:15:ALA:HB1	2:C:1101:LMT:H32	2.02	0.41
1:A:343:VAL:HG23	1:A:402:VAL:HG23	2.01	0.41
1:A:375:VAL:HG12	1:A:408:VAL:HG12	2.03	0.41
1:A:453:ALA:HB1	1:A:889:LEU:HB3	2.03	0.41
1:A:1005:ARG:HG2	1:A:1005:ARG:H	1.65	0.41
1:B:54:ALA:HB1	1:B:58:VAL:HG13	2.03	0.41
1:B:344:VAL:O	1:B:348:LEU:HD13	2.21	0.41
1:B:513:ILE:O	1:B:514:ASP:C	2.63	0.41
1:B:991:THR:HG23	1:B:1013:PHE:CZ	2.55	0.41
1:C:118:ALA:HA	1:C:125:ARG:HH11	1.85	0.41
1:C:382:THR:HG23	1:C:478:ILE:HG22	2.03	0.41
1:C:711:ILE:HD12	1:C:720:PRO:HG3	2.03	0.41
1:A:190:TRP:CH2	1:C:226:PRO:HD3	2.56	0.41
1:A:385:ILE:HD13	1:A:385:ILE:HA	1.83	0.41
1:A:409:VAL:C	1:A:413:ILE:HD12	2.46	0.41
1:B:498:LEU:O	1:B:500:LYS:HE3	2.20	0.41
1:B:717:MET:H	1:B:717:MET:HG3	1.73	0.41
1:B:1004:VAL:HG13	1:B:1005:ARG:HD3	2.02	0.41
1:A:198:ALA:HB3	1:A:199:ARG:HH11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:OG	1:B:755:GLN:NE2	2.54	0.40
1:A:714:THR:CG2	1:A:848:HIS:HE1	2.35	0.40
1:B:450:VAL:HG22	1:B:893:VAL:CG1	2.52	0.40
1:B:458:MET:HB2	1:B:473:ALA:CB	2.51	0.40
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.92	0.40
1:C:353:LEU:HD12	1:C:993:PRO:HD3	2.02	0.40
1:C:527:PHE:CD1	1:C:527:PHE:C	2.99	0.40
1:A:53:GLY:C	1:C:218:SER:HB2	2.46	0.40
1:A:419:VAL:HG23	1:A:433:ALA:HA	2.03	0.40
1:A:506:LYS:HD2	1:A:510:THR:HB	2.03	0.40
1:B:315:GLU:CD	1:B:319:ARG:HH22	2.29	0.40
1:B:335:PHE:HZ	1:B:577:LYS:HA	1.86	0.40
1:B:579:TYR:HA	1:B:637:PHE:O	2.21	0.40
1:B:994:LEU:HB2	1:B:1010:ILE:HG13	2.04	0.40
1:C:745:VAL:HG12	1:C:746:SER:O	2.22	0.40
1:C:957:GLU:O	1:C:961:GLN:HB3	2.21	0.40
1:A:748:THR:CG2	1:C:212:GLU:HG2	2.51	0.40
1:A:831:LEU:HD23	1:A:831:LEU:HA	1.92	0.40
1:A:910:ILE:O	1:A:913:MET:HB2	2.21	0.40
1:B:891:PHE:CD1	1:B:904:PRO:HB2	2.57	0.40
1:C:232:ASP:C	1:C:233:PHE:HD1	2.29	0.40
1:C:689:ILE:O	1:C:828:ALA:HA	2.21	0.40
1:C:831:LEU:HD12	1:C:831:LEU:HA	1.96	0.40
1:C:878:THR:OG1	1:C:879:ALA:N	2.54	0.40
1:C:898:TYR:HD1	1:C:903:LEU:CD2	2.35	0.40
1:A:444:ILE:HA	1:A:447:ILE:HD12	2.03	0.40
1:A:784:ARG:NH1	1:C:224:ALA:HB3	2.37	0.40
1:B:404:ALA:O	1:B:408:VAL:HG23	2.22	0.40
1:B:464:VAL:O	1:B:468:PHE:CD1	2.74	0.40
1:C:497:LEU:HD21	2:C:1101:LMT:H3B	2.04	0.40
1:C:610:GLU:OE1	1:C:646:LYS:NZ	2.38	0.40
1:C:988:ILE:HG12	1:C:988:ILE:H	1.72	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	1038/1056 (98%)	1002 (96%)	35 (3%)	1 (0%)	48 70
1	B	1040/1056 (98%)	989 (95%)	51 (5%)	0	100 100
1	C	1039/1056 (98%)	1006 (97%)	33 (3%)	0	100 100
All	All	3117/3168 (98%)	2997 (96%)	119 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ALA

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	849/864 (98%)	814 (96%)	35 (4%)	26 46
1	B	851/864 (98%)	816 (96%)	35 (4%)	26 46
1	C	850/864 (98%)	819 (96%)	31 (4%)	30 51
All	All	2550/2592 (98%)	2449 (96%)	101 (4%)	27 47

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	139	THR
1	A	140	LEU
1	A	141	VAL
1	A	146	SER
1	A	164	VAL
1	A	229	GLN
1	A	236	SER

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Mol	Chain	Res	Type
1	A	255	LYS
1	A	325	GLN
1	A	343	VAL
1	A	365	TRP
1	A	372	LEU
1	A	438	ARG
1	A	445	ILE
1	A	491	SER
1	A	505	LYS
1	A	510	THR
1	A	532	SER
1	A	557	LEU
1	A	591	SER
1	A	635	VAL
1	A	665	GLN
1	A	801	GLU
1	A	810	ASN
1	A	843	SER
1	A	854	LYS
1	A	857	LEU
1	A	866	THR
1	A	889	LEU
1	A	900	SER
1	A	945	CYS
1	A	956	ARG
1	A	1014	SER
1	A	1026	LEU
1	B	35	SER
1	B	231	SER
1	B	232	ASP
1	B	362	LEU
1	B	364	THR
1	B	366	ARG
1	B	378	SER
1	B	480	THR
1	B	483	SER
1	B	491	SER
1	B	494	LEU
1	B	511	ARG
1	B	529	LEU
1	B	581	ILE
1	B	590	SER

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Mol	Chain	Res	Type
1	B	646	LYS
1	B	663	ILE
1	B	723	THR
1	B	753	THR
1	B	761	SER
1	B	768	GLN
1	B	805	ILE
1	B	812	SER
1	B	813	THR
1	B	866	THR
1	B	900	SER
1	B	907	VAL
1	B	917	SER
1	B	922	VAL
1	B	933	VAL
1	B	952	VAL
1	B	958	LEU
1	B	995	ILE
1	B	998	HIS
1	B	1042	LYS
1	C	29	ILE
1	C	153	SER
1	C	247	GLU
1	C	256	THR
1	C	258	GLN
1	C	268	VAL
1	C	275	SER
1	C	277	SER
1	C	280	LEU
1	C	294	ILE
1	C	303	ILE
1	C	378	SER
1	C	397	SER
1	C	441	SER
1	C	462	SER
1	C	475	THR
1	C	488	LEU
1	C	513	ILE
1	C	550	PHE
1	C	580	LEU
1	C	599	ILE
1	C	609	THR

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Mol	Chain	Res	Type
1	C	626	PHE
1	C	646	LYS
1	C	679	LEU
1	C	746	SER
1	C	761	SER
1	C	764	ASN
1	C	840	LEU
1	C	842	SER
1	C	1032	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	132	GLN
1	A	533	ASN
1	A	622	ASN
1	A	628	ASN
1	A	657	ASN
1	A	665	GLN
1	A	727	ASN
1	A	848	HIS
1	A	855	GLN
1	B	143	HIS
1	B	176	GLN
1	B	221	GLN
1	B	286	ASN
1	B	345	GLN
1	B	418	ASN
1	B	536	GLN
1	B	608	ASN
1	B	664	GLN
1	B	730	GLN
1	B	871	GLN
1	C	158	ASN
1	C	238	ASN
1	C	434	HIS
1	C	644	GLN
1	C	844	GLN
1	C	871	GLN
1	C	961	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides 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	GOL	A	1104	-	5,5,5	0.91	0	5,5,5	0.98	0
2	LMT	B	1102	-	36,36,36	1.13	4 (11%)	47,47,47	1.03	2 (4%)
2	LMT	A	1101	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	2 (4%)
2	LMT	B	1101	-	36,36,36	1.14	4 (11%)	47,47,47	0.96	1 (2%)
2	LMT	A	1103	-	36,36,36	1.10	4 (11%)	47,47,47	1.09	4 (8%)
2	LMT	C	1101	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
2	LMT	A	1102	-	36,36,36	1.14	4 (11%)	47,47,47	0.95	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1104	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	B	1102	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	9/21/61/61	0/2/2/2
2	LMT	B	1101	-	-	7/21/61/61	0/2/2/2
2	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	6/21/61/61	0/2/2/2
2	LMT	A	1102	-	-	9/21/61/61	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	LMT	O3'-C3'	-2.73	1.36	1.43
2	C	1101	LMT	O3'-C3'	-2.72	1.36	1.43
2	A	1102	LMT	O3'-C3'	-2.69	1.36	1.43
2	A	1101	LMT	O3'-C3'	-2.54	1.37	1.43
2	B	1102	LMT	O3'-C3'	-2.53	1.37	1.43
2	A	1103	LMT	O3'-C3'	-2.43	1.37	1.43
2	C	1101	LMT	O2'-C2'	-2.33	1.37	1.43
2	A	1103	LMT	O2'-C2'	-2.32	1.37	1.43
2	B	1102	LMT	O2'-C2'	-2.27	1.37	1.43
2	B	1101	LMT	O2B-C2B	-2.26	1.37	1.43
2	A	1102	LMT	O3B-C3B	-2.25	1.37	1.43
2	B	1102	LMT	O2B-C2B	-2.24	1.37	1.43
2	C	1101	LMT	O4'-C4B	-2.23	1.37	1.43
2	B	1101	LMT	O2'-C2'	-2.22	1.37	1.43
2	A	1102	LMT	O2B-C2B	-2.19	1.37	1.43
2	A	1101	LMT	O3B-C3B	-2.19	1.37	1.43
2	A	1101	LMT	O2'-C2'	-2.19	1.37	1.43
2	C	1101	LMT	O3B-C3B	-2.16	1.37	1.43
2	B	1101	LMT	O3B-C3B	-2.16	1.37	1.43
2	C	1101	LMT	O2B-C2B	-2.15	1.37	1.43
2	B	1102	LMT	O3B-C3B	-2.15	1.37	1.43
2	A	1103	LMT	O3B-C3B	-2.14	1.37	1.43
2	A	1103	LMT	O2B-C2B	-2.09	1.38	1.43
2	A	1101	LMT	O2B-C2B	-2.06	1.38	1.43
2	A	1102	LMT	O2'-C2'	-2.03	1.38	1.43
2	A	1101	LMT	O4'-C4B	-2.02	1.38	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	LMT	C3'-C4'-C5'	-3.26	103.45	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1102	LMT	C1'-O5'-C5'	-3.20	107.41	113.69
2	B	1101	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
2	A	1103	LMT	C1'-O5'-C5'	-2.71	108.37	113.69
2	B	1102	LMT	C3'-C4'-C5'	-2.56	105.07	110.93
2	A	1102	LMT	C3'-C4'-C5'	-2.53	105.13	110.93
2	A	1101	LMT	C1'-O5'-C5'	-2.52	108.75	113.69
2	A	1103	LMT	O5B-C5B-C4B	2.50	114.24	109.69
2	A	1101	LMT	C3'-C4'-C5'	-2.47	105.25	110.93
2	A	1103	LMT	O1'-C1'-C2'	2.35	111.97	108.30
2	A	1103	LMT	O5'-C1'-C2'	-2.29	105.51	110.35
2	A	1102	LMT	O5B-C5B-C4B	2.28	113.83	109.69
2	A	1102	LMT	C1'-O5'-C5'	-2.09	109.58	113.69
2	C	1101	LMT	C1'-O5'-C5'	-2.04	109.68	113.69

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	O5'-C1'-O1'-C1
2	A	1103	LMT	C2'-C1'-O1'-C1
2	A	1103	LMT	O5'-C1'-O1'-C1
2	B	1101	LMT	C2-C1-O1'-C1'
2	B	1102	LMT	C2'-C1'-O1'-C1
2	B	1102	LMT	O5'-C1'-O1'-C1
2	C	1101	LMT	C2-C1-O1'-C1'
3	A	1104	GOL	O1-C1-C2-O2
3	A	1104	GOL	O1-C1-C2-C3
2	B	1101	LMT	C4B-C5B-C6B-O6B
2	A	1103	LMT	O5'-C5'-C6'-O6'
2	B	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	B	1102	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C1-C2-C3-C4
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	A	1102	LMT	O1'-C1-C2-C3
2	A	1102	LMT	O5'-C1'-O1'-C1
2	A	1101	LMT	O1'-C1-C2-C3
2	A	1102	LMT	C4B-C5B-C6B-O6B
2	A	1102	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
2	A	1103	LMT	C7-C8-C9-C10
2	A	1102	LMT	C2'-C1'-O1'-C1
2	B	1102	LMT	O5'-C5'-C6'-O6'
2	B	1102	LMT	C6-C7-C8-C9
2	A	1103	LMT	C4-C5-C6-C7
2	C	1101	LMT	C2-C3-C4-C5
2	A	1103	LMT	C2B-C1B-O1B-C4'
2	A	1101	LMT	C7-C8-C9-C10
2	B	1102	LMT	C7-C8-C9-C10
2	A	1101	LMT	C3-C4-C5-C6
2	A	1103	LMT	C5-C6-C7-C8
2	A	1103	LMT	C1-C2-C3-C4
2	B	1102	LMT	C1-C2-C3-C4
2	B	1102	LMT	C4-C5-C6-C7
2	A	1103	LMT	C6-C7-C8-C9
2	A	1102	LMT	C7-C8-C9-C10
2	B	1102	LMT	C5-C6-C7-C8
2	B	1101	LMT	O1'-C1-C2-C3
2	A	1103	LMT	O5B-C1B-O1B-C4'
2	B	1102	LMT	O1'-C1-C2-C3
2	B	1101	LMT	C2-C3-C4-C5
2	A	1101	LMT	C9-C10-C11-C12
2	A	1102	LMT	C1-C2-C3-C4
2	A	1103	LMT	C4'-C5'-C6'-O6'
2	A	1103	LMT	C2-C3-C4-C5
2	C	1101	LMT	C5-C6-C7-C8
2	A	1102	LMT	C2-C1-O1'-C1'
2	C	1101	LMT	C3-C4-C5-C6
2	A	1101	LMT	C11-C10-C9-C8
2	B	1101	LMT	C4-C5-C6-C7
2	A	1102	LMT	O5B-C1B-O1B-C4'

There are no ring outliers.

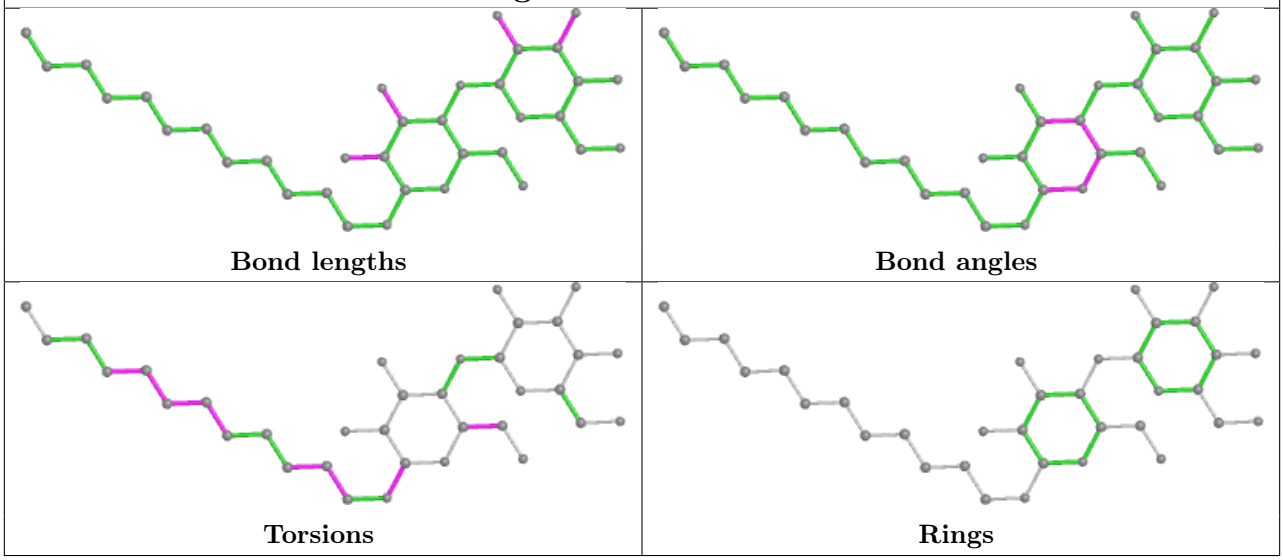
4 monomers are involved in 6 short contacts:

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

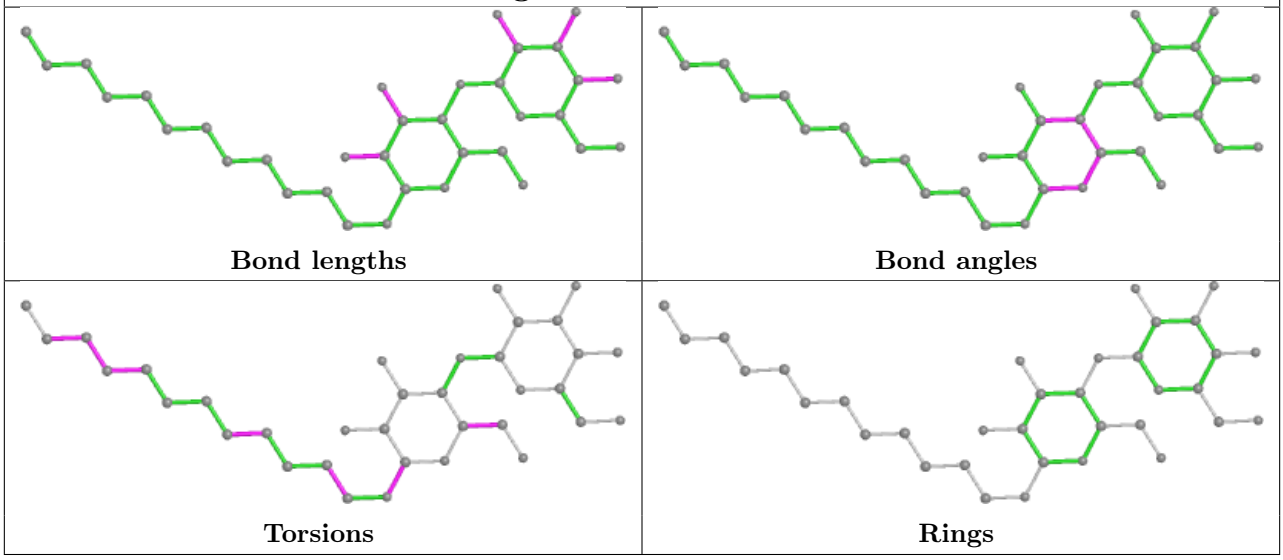
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

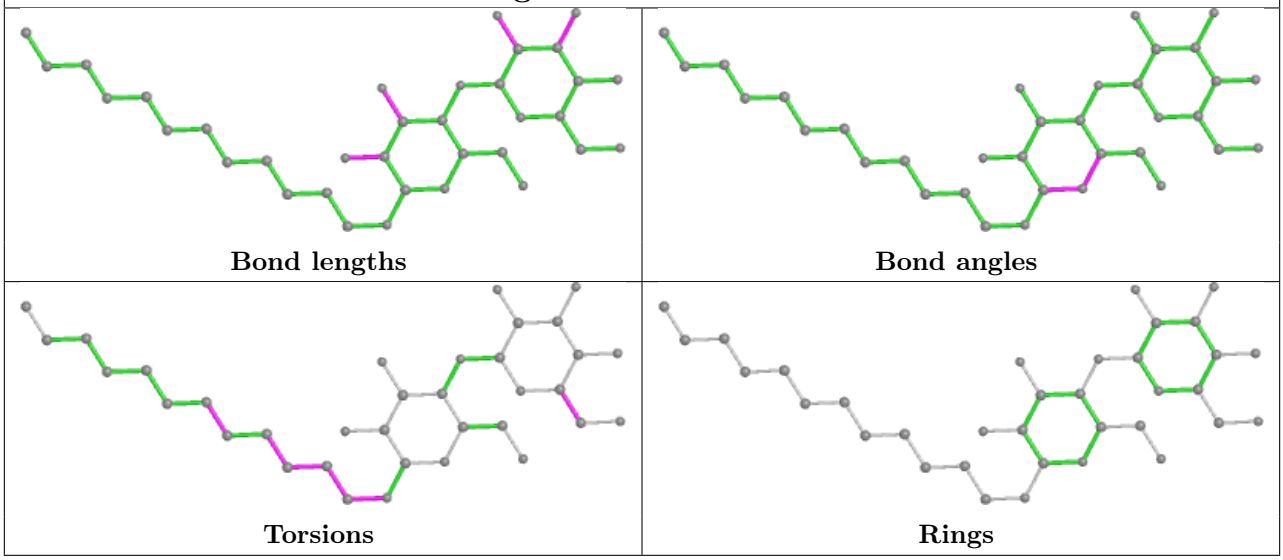
Ligand LMT B 1102



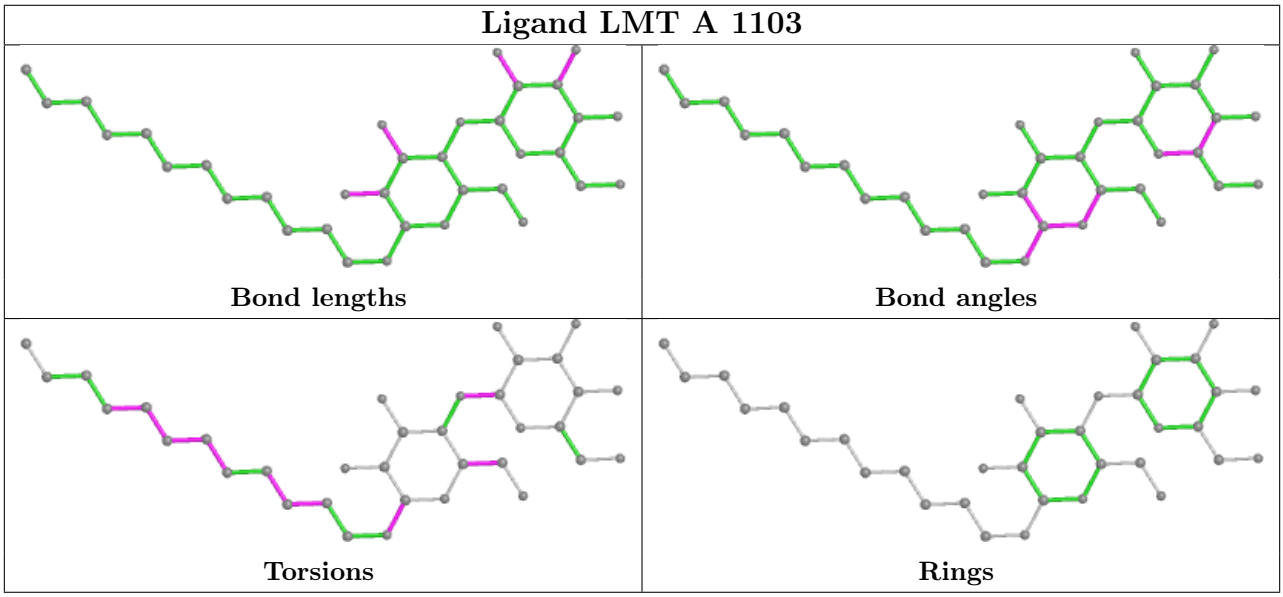
Ligand LMT A 1101



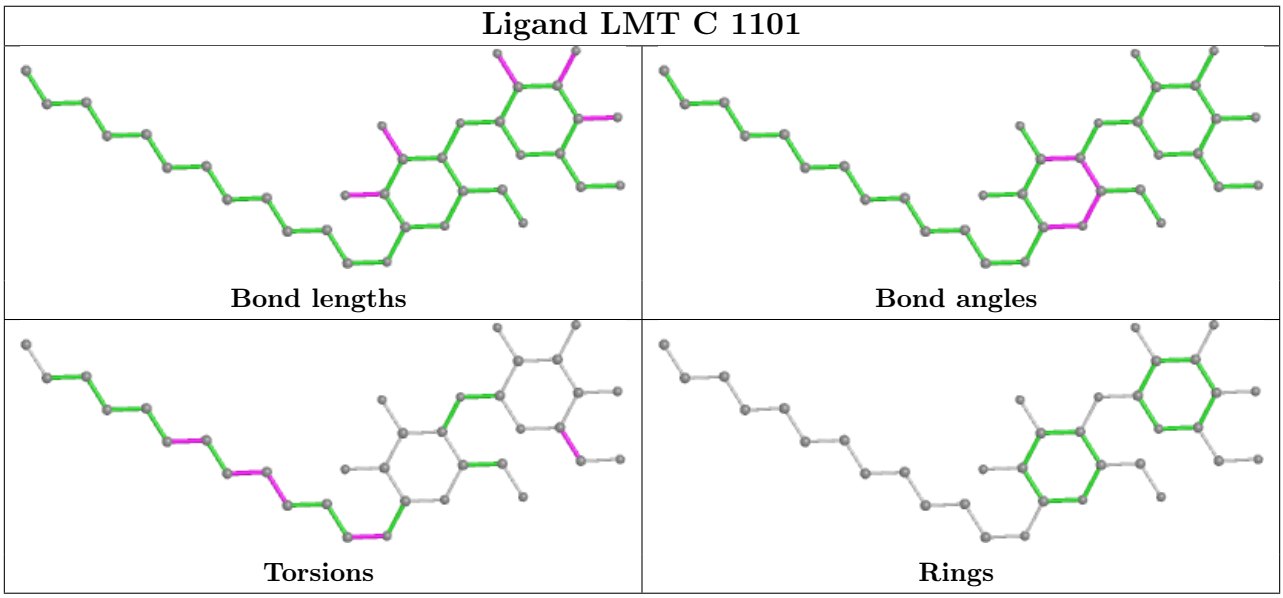
Ligand LMT B 1101



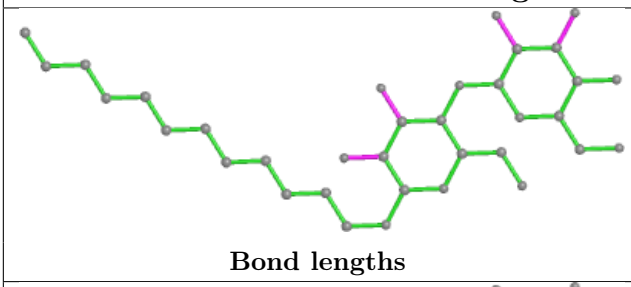
Ligand LMT A 1103



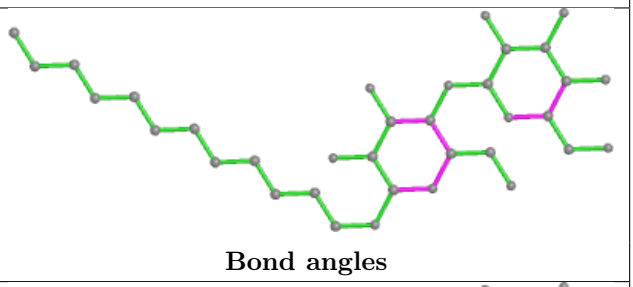
Ligand LMT C 1101



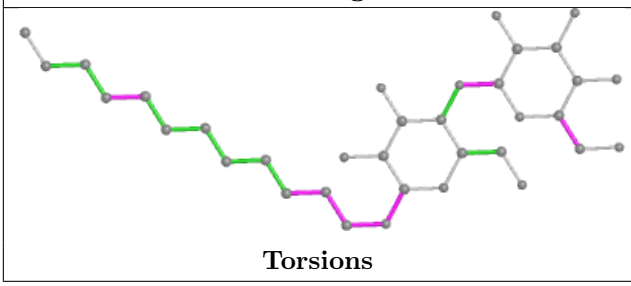
Ligand LMT A 1102



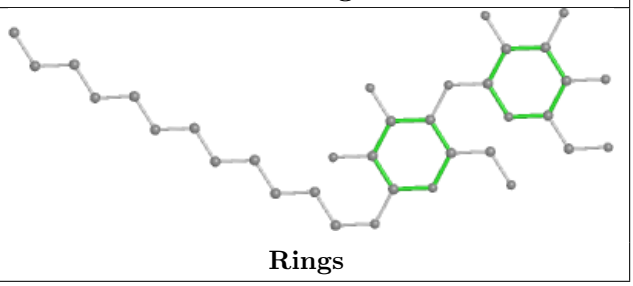
Bond lengths



Bond angles



Torsions



Rings

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	1040/1056 (98%)	0.59	115 (11%) 12 14	70, 117, 183, 244	0
1	B	1042/1056 (98%)	0.72	133 (12%) 9 11	73, 138, 205, 230	0
1	C	1041/1056 (98%)	0.45	80 (7%) 21 24	67, 103, 150, 237	0
All	All	3123/3168 (98%)	0.59	328 (10%) 13 15	67, 115, 197, 244	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ILE	7.7
1	C	76	ASN	7.7
1	A	169	ALA	7.5
1	A	871	GLN	7.2
1	B	943	LEU	6.7
1	B	409	VAL	6.6
1	B	412	ALA	6.5
1	B	906	ALA	6.0
1	B	3	PHE	5.8
1	A	174	VAL	5.6
1	B	944	ALA	5.6
1	B	406	GLY	5.5
1	A	873	ALA	5.5
1	B	177	ILE	5.3
1	A	528	PHE	5.3
1	B	140	LEU	5.0
1	B	178	GLN	5.0
1	B	174	VAL	4.9
1	A	994	LEU	4.8
1	C	880	LEU	4.8
1	B	142	VAL	4.7
1	A	734	GLN	4.7
1	B	176	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	305	LEU	4.6
1	A	872	GLN	4.6
1	B	1019	VAL	4.5
1	A	620	GLY	4.5
1	B	99	GLY	4.5
1	C	455	PHE	4.5
1	B	7	PHE	4.5
1	C	449	LEU	4.4
1	C	501	PRO	4.4
1	A	751	PHE	4.4
1	B	1025	PHE	4.4
1	A	592	LEU	4.3
1	A	750	LEU	4.3
1	A	524	PHE	4.3
1	B	411	ASP	4.3
1	C	783	TYR	4.3
1	A	874	THR	4.2
1	B	684	GLY	4.2
1	A	628	ASN	4.2
1	C	666	GLY	4.1
1	A	571	PHE	4.1
1	B	677	LEU	4.1
1	A	747	LEU	4.0
1	B	292	ILE	4.0
1	C	839	VAL	4.0
1	A	875	GLN	4.0
1	C	681	GLN	4.0
1	A	987	PHE	4.0
1	B	413	ILE	4.0
1	A	377	VAL	3.9
1	C	963	LYS	3.9
1	B	362	LEU	3.9
1	B	1	MET	3.8
1	C	500	LYS	3.8
1	A	682	GLY	3.8
1	A	533	ASN	3.8
1	B	410	ASP	3.7
1	B	293	GLY	3.6
1	B	569	GLY	3.6
1	A	311	ALA	3.5
1	A	412	ALA	3.5
1	B	404	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	40	VAL	3.5
1	A	1009	GLY	3.5
1	B	1027	THR	3.5
1	C	780	ASP	3.4
1	C	1038	VAL	3.4
1	A	995	ILE	3.4
1	B	1034	LEU	3.4
1	A	365	TRP	3.3
1	B	1028	PRO	3.3
1	A	1	MET	3.3
1	C	298	PRO	3.3
1	B	673	PRO	3.2
1	A	404	ALA	3.2
1	A	280	LEU	3.2
1	B	2	ASP	3.2
1	B	73	GLY	3.2
1	B	1039	THR	3.2
1	C	473	ALA	3.2
1	A	745	VAL	3.2
1	C	624	LEU	3.2
1	C	474	VAL	3.2
1	A	519	TRP	3.2
1	A	99	GLY	3.2
1	C	544	GLY	3.2
1	B	340	ILE	3.2
1	B	1031	TYR	3.2
1	C	270	ARG	3.2
1	B	393	LEU	3.1
1	A	595	THR	3.1
1	B	564	PHE	3.1
1	A	531	SER	3.1
1	B	912	PRO	3.1
1	A	373	ILE	3.0
1	C	937	LEU	3.0
1	A	314	ALA	3.0
1	C	450	VAL	3.0
1	B	490	LEU	3.0
1	B	675	PRO	3.0
1	B	212	GLU	3.0
1	A	37	TYR	3.0
1	A	529	LEU	3.0
1	B	581	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	40	VAL	3.0
1	C	662	GLN	3.0
1	B	449	LEU	2.9
1	C	919	LEU	2.9
1	A	627	THR	2.9
1	C	875	GLN	2.9
1	B	72	ASN	2.9
1	B	528	PHE	2.9
1	B	571	PHE	2.9
1	C	564	PHE	2.9
1	A	676	ILE	2.8
1	B	100	THR	2.8
1	C	665	GLN	2.8
1	B	1022	PHE	2.8
1	C	516	LEU	2.8
1	B	405	ILE	2.8
1	C	933	VAL	2.8
1	B	915	MET	2.8
1	B	165	LYS	2.8
1	B	35	SER	2.8
1	C	135	SER	2.8
1	B	662	GLN	2.8
1	B	166	ASP	2.8
1	C	138	LEU	2.8
1	C	181	GLY	2.8
1	B	373	ILE	2.8
1	C	881	ILE	2.8
1	A	835	ALA	2.8
1	C	1039	THR	2.8
1	B	1021	LEU	2.8
1	A	572	ILE	2.7
1	A	996	LEU	2.7
1	B	579	TYR	2.7
1	A	596	ASP	2.7
1	A	176	GLN	2.7
1	B	814	THR	2.7
1	C	503	GLY	2.7
1	C	177	ILE	2.7
1	C	75	GLU	2.7
1	A	1019	VAL	2.7
1	A	1022	PHE	2.7
1	C	271	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	810	ASN	2.7
1	C	408	VAL	2.7
1	A	497	LEU	2.7
1	B	136	PRO	2.7
1	B	878	THR	2.7
1	A	21	ILE	2.7
1	A	599	ILE	2.7
1	A	717	MET	2.6
1	A	615	ALA	2.6
1	B	361	PHE	2.6
1	A	1004	VAL	2.6
1	A	680	GLY	2.6
1	C	910	ILE	2.6
1	B	330	TYR	2.6
1	A	733	VAL	2.6
1	B	172	PRO	2.6
1	C	136	PRO	2.6
1	C	575	GLN	2.6
1	A	527	PHE	2.6
1	B	504	ALA	2.6
1	B	987	PHE	2.6
1	C	878	THR	2.6
1	B	790	ILE	2.6
1	C	293	GLY	2.6
1	C	505	LYS	2.5
1	B	430	LEU	2.5
1	C	977	LEU	2.5
1	B	415	VAL	2.5
1	A	808	MET	2.5
1	A	967	GLU	2.5
1	C	452	CYS	2.5
1	C	185	TYR	2.5
1	C	897	LEU	2.5
1	B	993	PRO	2.5
1	C	664	GLN	2.5
1	A	584	VAL	2.5
1	B	1029	VAL	2.5
1	C	751	PHE	2.5
1	A	623	ALA	2.5
1	B	327	ALA	2.5
1	A	965	ILE	2.5
1	B	175	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	795	THR	2.5
1	B	519	TRP	2.5
1	A	837	PRO	2.5
1	A	1032	VAL	2.5
1	A	486	ASN	2.5
1	B	835	ALA	2.5
1	C	418	ASN	2.5
1	C	504	ALA	2.5
1	A	868	LEU	2.4
1	B	398	LEU	2.4
1	B	295	PHE	2.4
1	B	535	TYR	2.4
1	A	12	ILE	2.4
1	B	1023	GLY	2.4
1	A	372	LEU	2.4
1	A	672	LEU	2.4
1	C	837	PRO	2.4
1	A	297	SER	2.4
1	B	4	SER	2.4
1	A	809	VAL	2.4
1	B	34	VAL	2.4
1	A	29	ILE	2.4
1	A	9	ASP	2.4
1	C	465	THR	2.4
1	B	554	LEU	2.4
1	B	555	LEU	2.4
1	B	868	LEU	2.4
1	C	168	LEU	2.4
1	A	1005	ARG	2.4
1	B	376	PRO	2.4
1	A	413	ILE	2.4
1	C	302	ALA	2.4
1	B	208	THR	2.4
1	C	427	LEU	2.4
1	A	526	ARG	2.4
1	C	458	MET	2.4
1	A	988	ILE	2.4
1	B	447	ILE	2.4
1	C	546	ARG	2.3
1	A	1025	PHE	2.3
1	A	513	ILE	2.3
1	A	1010	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	945	CYS	2.3
1	B	947	ASN	2.3
1	B	497	LEU	2.3
1	A	517	PHE	2.3
1	B	372	LEU	2.3
1	A	437	MET	2.3
1	A	1008	THR	2.3
1	A	675	PRO	2.3
1	A	735	VAL	2.3
1	B	572	ILE	2.3
1	A	477	ALA	2.3
1	B	209	ALA	2.3
1	B	1000	ALA	2.3
1	A	362	LEU	2.3
1	A	679	LEU	2.3
1	B	940	LEU	2.3
1	B	627	THR	2.3
1	C	932	PHE	2.3
1	B	446	ALA	2.3
1	C	723	THR	2.2
1	B	38	PRO	2.2
1	A	303	ILE	2.2
1	C	472	PHE	2.2
1	A	308	ALA	2.2
1	A	621	LEU	2.2
1	B	996	LEU	2.2
1	B	562	VAL	2.2
1	A	369	ILE	2.2
1	C	513	ILE	2.2
1	C	667	PHE	2.2
1	B	431	ALA	2.2
1	C	873	ALA	2.2
1	A	364	THR	2.2
1	A	501	PRO	2.2
1	A	405	ILE	2.2
1	A	945	CYS	2.2
1	B	328	ALA	2.2
1	C	477	ALA	2.2
1	B	903	LEU	2.2
1	B	876	GLY	2.2
1	B	574	THR	2.2
1	A	330	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1004	VAL	2.2
1	B	946	LYS	2.2
1	B	831	LEU	2.2
1	B	173	GLY	2.2
1	B	336	VAL	2.1
1	B	408	VAL	2.1
1	C	413	ILE	2.1
1	C	922	VAL	2.1
1	A	964	GLY	2.1
1	B	837	PRO	2.1
1	A	472	PHE	2.1
1	B	445	ILE	2.1
1	C	931	VAL	2.1
1	A	677	LEU	2.1
1	B	403	LEU	2.1
1	A	473	ALA	2.1
1	B	438	ARG	2.1
1	C	519	TRP	2.1
1	C	502	HIS	2.1
1	A	795	THR	2.1
1	C	35	SER	2.1
1	A	336	VAL	2.1
1	C	414	VAL	2.1
1	C	663	ILE	2.1
1	B	685	TYR	2.1
1	C	155	TYR	2.1
1	C	159	TYR	2.1
1	B	1024	LEU	2.1
1	C	140	LEU	2.1
1	A	974	ARG	2.1
1	A	876	GLY	2.1
1	B	606	GLY	2.1
1	A	863	ILE	2.1
1	A	243	LEU	2.1
1	B	556	LEU	2.1
1	A	61	GLU	2.0
1	A	248	GLU	2.0
1	B	951	ILE	2.0
1	A	414	VAL	2.0
1	A	870	PHE	2.0
1	C	745	VAL	2.0
1	B	494	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	732	ASP	2.0
1	B	836	ASP	2.0
1	C	906	ALA	2.0
1	A	98	PRO	2.0
1	C	902	THR	2.0
1	A	598	VAL	2.0
1	B	440	VAL	2.0
1	B	839	VAL	2.0
1	B	48	ARG	2.0
1	B	683	SER	2.0
1	B	702	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

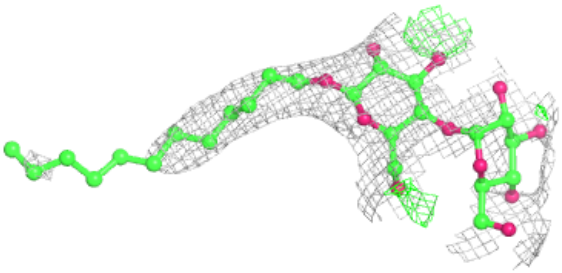
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

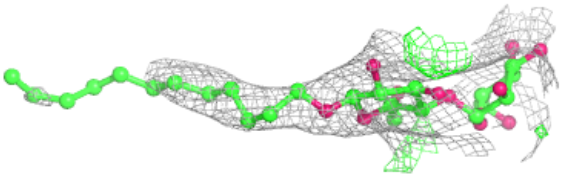
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1104	6/6	0.61	0.13	140,147,159,162	0
2	LMT	A	1101	35/35	0.82	0.17	98,126,165,169	0
2	LMT	B	1102	35/35	0.84	0.24	106,138,147,150	0
2	LMT	A	1102	35/35	0.87	0.20	100,147,172,174	0
2	LMT	A	1103	35/35	0.88	0.20	102,133,150,152	0
2	LMT	B	1101	35/35	0.88	0.18	108,160,182,189	0
2	LMT	C	1101	35/35	0.89	0.12	81,105,125,127	0

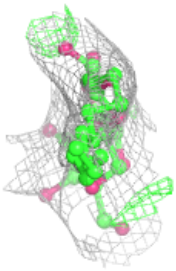
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

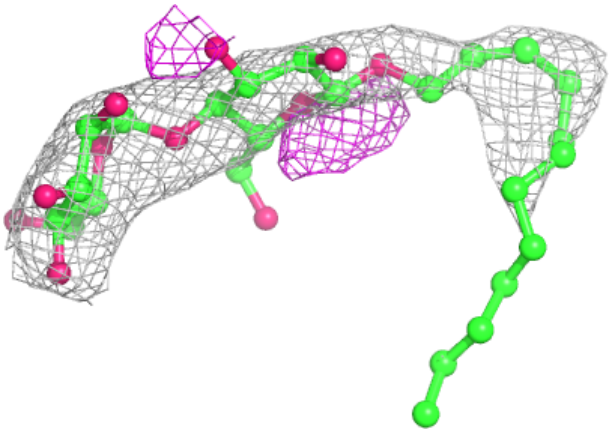


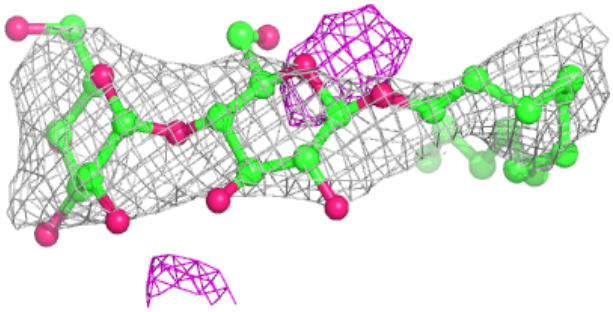


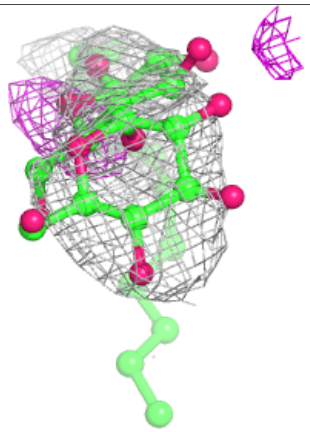


Electron density around LMT B 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

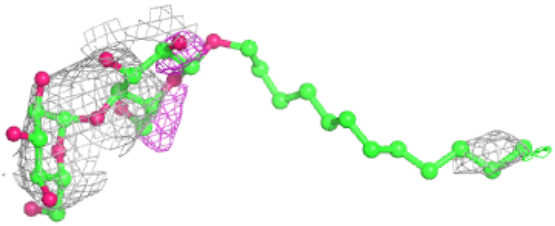


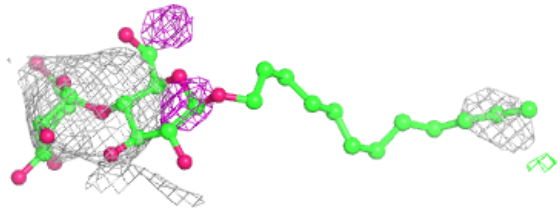


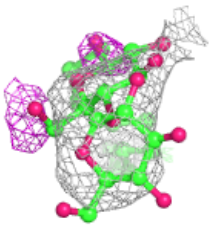


Electron density around LMT A 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

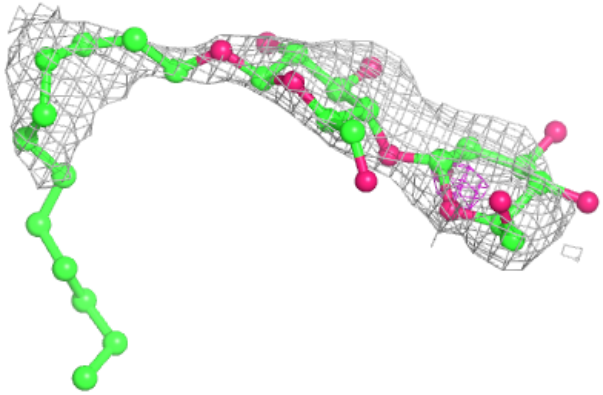


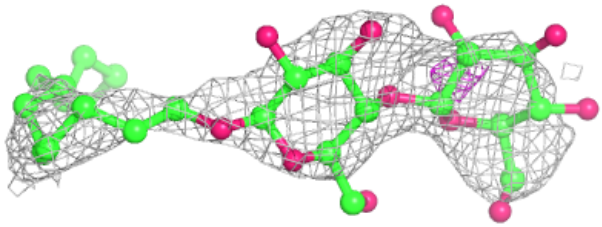


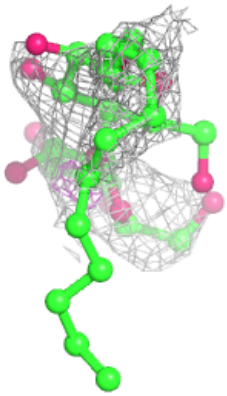


Electron density around LMT A 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

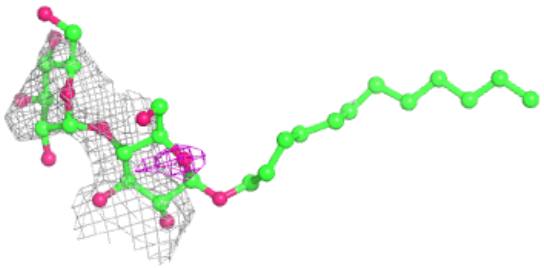


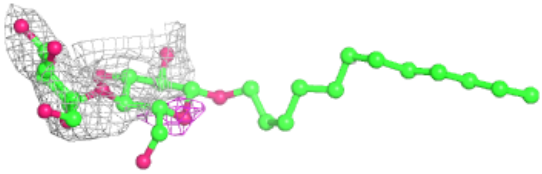


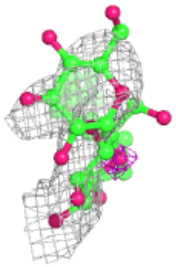


Electron density around LMT B 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

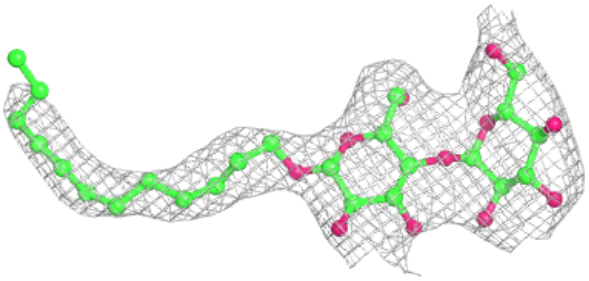


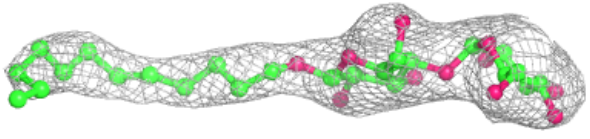


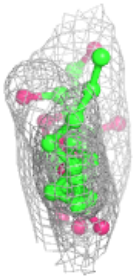


Electron density around LMT C 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.