Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:24 AM GMT

PDB ID	:	3EHB
Title	:	A D-Pathway Mutation Decouples the Paracoccus Denitrificans Cytochrome c Oxidase by Altering the side chain orientation of a distant, conserved Glutamate
Authors	:	Koepke, J.; Mueller, H.; Peng, G.
Deposited on	:	2008-09-12
Resolution	:	2.32 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:

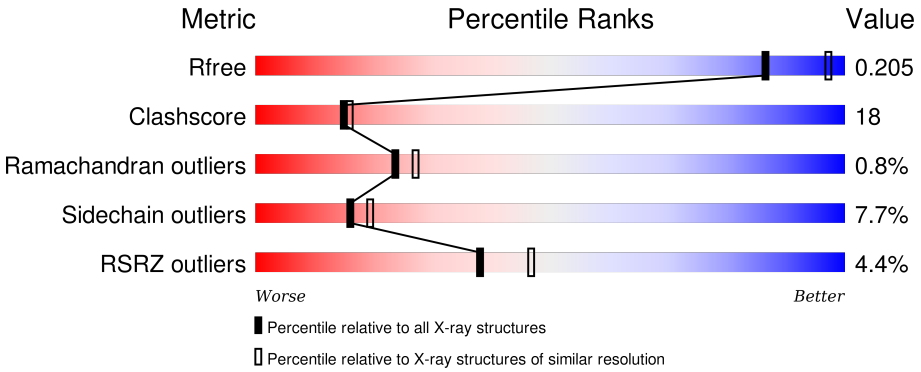
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	558	5% 62% 28% 5% 5%
2	B	298	% 59% 22% • 15%
3	C	127	9% 64% 25% 5% 6%
4	D	120	% 64% 23% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	LMT	A	568	-	-	-	X
10	LMT	A	569	-	-	-	X
10	LMT	A	571	-	-	-	X
10	LMT	A	572	-	-	-	X
10	LMT	A	573	-	-	-	X
10	LMT	A	574	-	-	-	X
10	LMT	A	575	-	-	-	X
10	LMT	B	278	-	-	-	X
10	LMT	B	279	-	-	-	X
10	LMT	D	121	-	-	-	X
5	HEA	A	559	X	-	-	-
5	HEA	A	560	X	-	-	-
7	MG	A	562	-	-	-	X
9	LDA	A	564	-	-	-	X
9	LDA	A	565	-	-	-	X
9	LDA	A	566	-	-	-	X
9	LDA	A	567	-	-	-	X
9	LDA	B	272	-	-	-	X
9	LDA	B	273	-	-	-	X
9	LDA	B	274	-	-	-	X
9	LDA	B	275	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9036 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 Cytochrome c oxidase subunit 1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	3	1
			4199	2818	656	692	33			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	ASP	ASN	ENGINEERED	UNP P98002

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	1	1
			1982	1298	320	356	8			

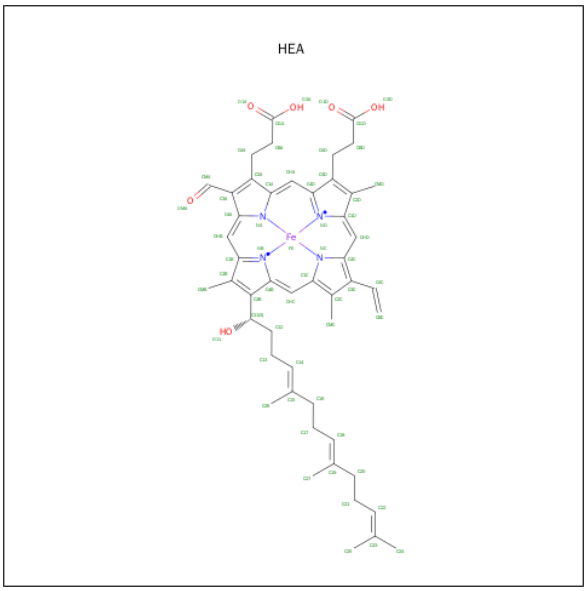
- Molecule 3 is a protein called FV fragment Chain H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	119	Total	C	N	O	S	0	2	1
			941	591	159	185	6			

- Molecule 4 is a protein called FV fragment Chain L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	109	Total	C	N	O	S	0	0	1
			832	530	136	164	2			

- Molecule 5 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cu	0	0
			2	2		
6	A	1	Total	Cu	0	0
			1	1		

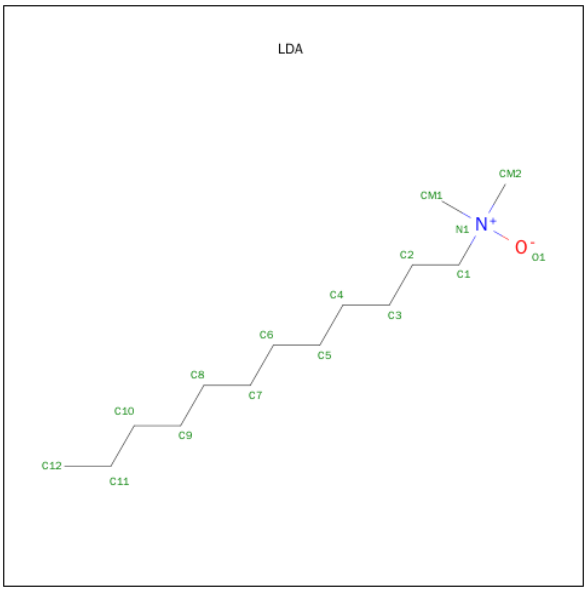
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

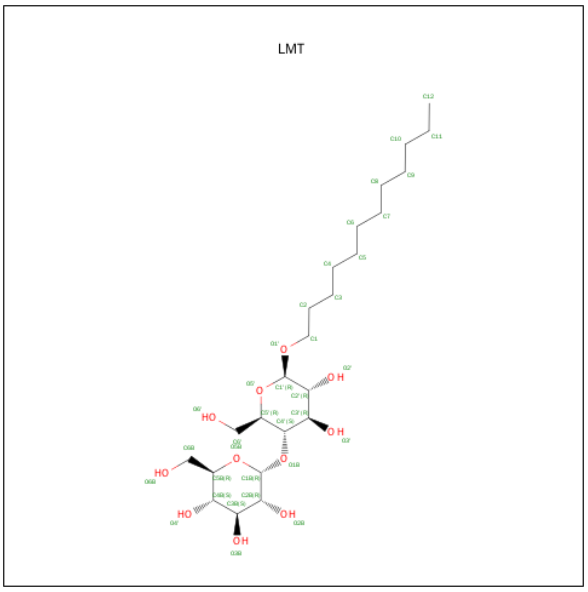
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



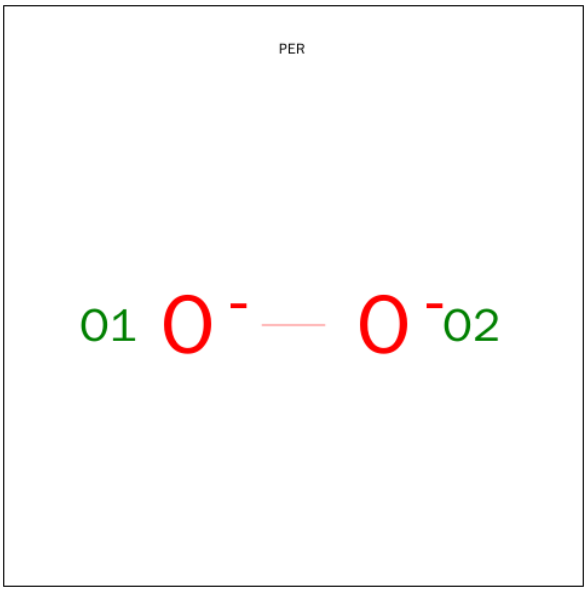
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	A	1	Total C O 35 24 11	0	0
10	B	1	Total C O 47 36 11	0	1
10	B	1	Total C O 35 24 11	0	0
10	B	1	Total C O 35 24 11	0	0
10	D	1	Total C O 35 24 11	0	0

- Molecule 11 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O 2 2	0	0

- Molecule 12 is water.

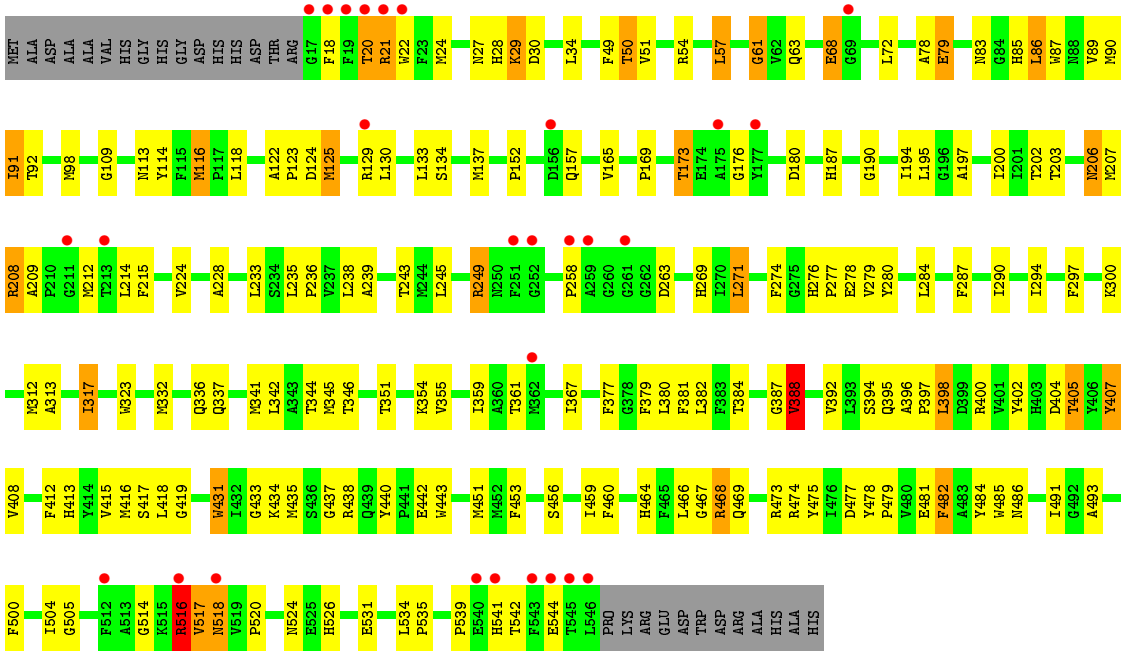
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	117	Total O 117 117	0	0
12	B	138	Total O 138 138	0	0
12	C	70	Total O 70 70	0	0
12	D	54	Total O 54 54	0	0

3 Residue-property plots (i)

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

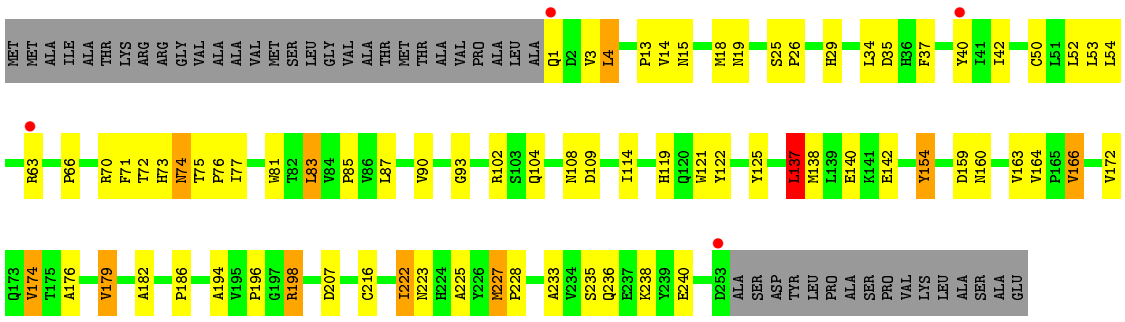
- Molecule 1: Cytochrome c oxidase subunit 1-beta

Chain A:



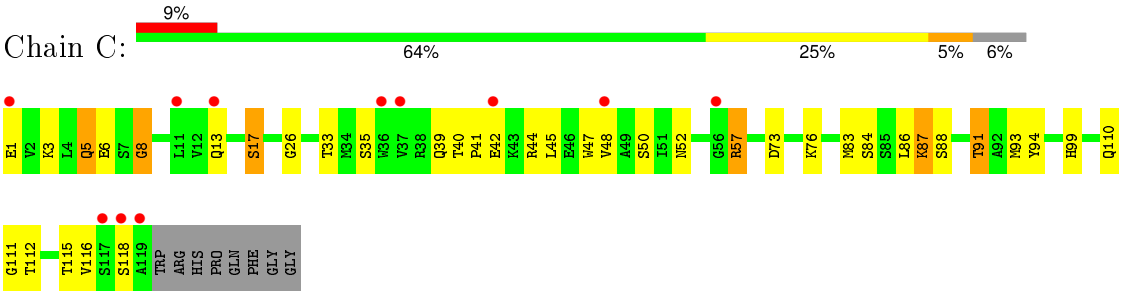
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



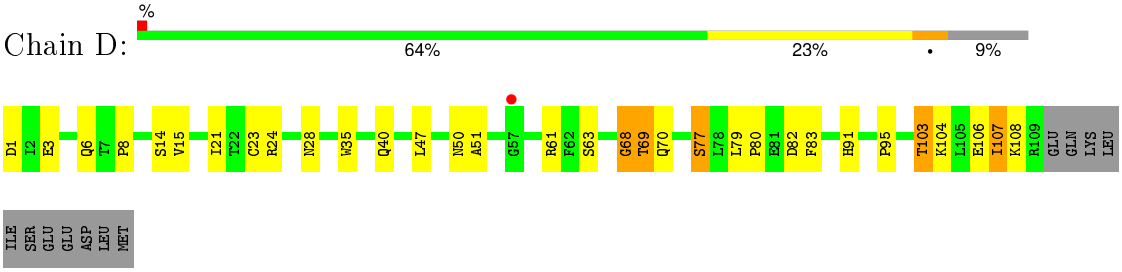
- Molecule 3: FV fragment Chain H

Chain C:



• Molecule 4: FV fragment Chain L

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.46Å 151.33Å 157.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.69 – 2.32 19.69 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.69-2.32) 98.9 (19.69-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.242 0.204 , 0.205	Depositor DCC
R_{free} test set	2622 reflections (3.11%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.2	EDS
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 87148 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9036	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MG, CA, LMT, LDA, PER, HEA, CU

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	1.20	6/4367 (0.1%)	1.08	18/5959 (0.3%)
2	B	1.38	7/2043 (0.3%)	1.18	10/2801 (0.4%)
3	C	1.14	0/973	1.05	1/1316 (0.1%)
4	D	1.28	2/853 (0.2%)	1.10	0/1158
All	All	1.25	15/8236 (0.2%)	1.11	29/11234 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	23	CYS	CB-SG	-8.64	1.67	1.82
2	B	125	TYR	CE2-CZ	7.65	1.48	1.38
1	A	407	TYR	CD2-CE2	7.47	1.50	1.39
2	B	182	ALA	CA-CB	6.48	1.66	1.52
1	A	460	PHE	CE2-CZ	6.47	1.49	1.37
4	D	51	ALA	CA-CB	6.19	1.65	1.52
2	B	125	TYR	CD2-CE2	5.60	1.47	1.39
1	A	482	PHE	CE1-CZ	5.40	1.47	1.37
1	A	468	ARG	CG-CD	5.38	1.65	1.51
2	B	154	TYR	CG-CD2	5.35	1.46	1.39
2	B	163	VAL	CB-CG1	5.35	1.64	1.52
1	A	431	TRP	CE3-CZ3	5.13	1.47	1.38
1	A	392	VAL	CB-CG1	5.02	1.63	1.52
2	B	222	ILE	CG1-CD1	5.01	1.85	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	176	ALA	CA-CB	5.00	1.62	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	A	468	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	A	54	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	A	263	ASP	CB-CG-OD1	8.92	126.33	118.30
1	A	249	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	B	137	LEU	CB-CG-CD2	7.86	124.35	111.00
2	B	137	LEU	CB-CG-CD1	-7.30	98.59	111.00
2	B	154	TYR	C-N-CA	-7.29	103.46	121.70
1	A	263	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	A	468	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	388	VAL	CG1-CB-CG2	6.89	121.92	110.90
1	A	271	LEU	CA-CB-CG	-6.74	99.80	115.30
2	B	163	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	A	124	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	61	GLY	N-CA-C	-6.55	96.72	113.10
2	B	66	PRO	N-CA-C	-6.55	95.07	112.10
2	B	238	LYS	CD-CE-NZ	-6.51	96.72	111.70
2	B	166	VAL	CB-CA-C	-6.44	99.16	111.40
1	A	408	VAL	CG1-CB-CG2	6.30	120.98	110.90
1	A	400	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	468	ARG	CG-CD-NE	-6.26	98.65	111.80
1	A	215[A]	PHE	CB-CA-C	5.69	121.79	110.40
2	B	227	MET	CG-SD-CE	5.55	109.08	100.20
2	B	179	VAL	CG1-CB-CG2	5.50	119.70	110.90
1	A	86	LEU	CB-CG-CD2	5.36	120.11	111.00
1	A	208	ARG	NE-CZ-NH1	-5.23	117.69	120.30
3	C	8	GLY	N-CA-C	5.12	125.90	113.10
2	B	207	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	516	ARG	NE-CZ-NH2	5.09	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	8	GLY	Peptide

5.2 Too-close contacts (i)

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	4199	0	4116	177	0
2	B	1982	0	1965	63	0
3	C	941	0	898	26	0
4	D	832	0	807	23	0
5	A	120	0	104	24	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	64	0	124	5	0
9	B	80	0	155	15	0
10	A	280	0	335	27	0
10	B	117	0	133	8	0
10	D	35	0	39	3	0
11	A	2	0	0	0	0
12	A	117	0	0	4	0
12	B	138	0	0	5	0
12	C	70	0	0	4	0
12	D	54	0	0	2	0
All	All	9036	0	8676	305	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 (305) 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)
2:B:222:ILE:CG1	2:B:222:ILE:CD1	1.85	1.55
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.07	1.44
1:A:276:HIS:NE2	1:A:280:TYR:CE2	1.96	1.31
10:A:575:LMT:O6B	10:A:575:LMT:C6B	1.81	1.28
1:A:342:LEU:HA	1:A:345:MET:CE	1.78	1.13
1:A:342:LEU:HA	1:A:345:MET:HE2	1.29	1.08
1:A:276:HIS:CE1	1:A:280:TYR:HE2	1.71	1.06
1:A:208:ARG:NH1	1:A:212:MET:O	1.93	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLN:HB2	2:B:4:LEU:HB2	1.42	1.00
1:A:342:LEU:HD23	1:A:345:MET:HE1	1.47	0.94
2:B:29:HIS:HD2	12:B:386:HOH:O	1.51	0.93
10:A:570:LMT:H2B	10:A:570:LMT:H6E	1.47	0.93
1:A:169:PRO:O	1:A:173:THR:HB	1.67	0.93
10:A:575:LMT:H4'	10:A:575:LMT:H3B	1.51	0.93
1:A:342:LEU:HD23	1:A:345:MET:CE	2.04	0.87
1:A:402:TYR:O	1:A:405:THR:HB	1.75	0.86
2:B:74:ASN:OD1	2:B:76:PRO:HD2	1.75	0.86
4:D:8:PRO:O	4:D:103:THR:HB	1.74	0.86
1:A:418:LEU:N	1:A:418:LEU:HD12	1.93	0.83
1:A:276:HIS:CE1	1:A:280:TYR:CE2	2.55	0.82
3:C:5:GLN:HG3	12:C:171:HOH:O	1.81	0.80
1:A:98:MET:HB3	5:A:559:HEA:CAC	2.13	0.79
10:A:571:LMT:O3'	10:A:571:LMT:H1B	1.80	0.78
1:A:29[A]:LYS:HG2	1:A:114:TYR:CZ	2.19	0.78
1:A:469:GLN:HE22	2:B:14:VAL:H	1.33	0.76
1:A:468:ARG:NH2	2:B:35:ASP:OD2	2.19	0.76
3:C:35:SER:OG	3:C:99:HIS:HE1	1.69	0.75
1:A:317:ILE:C	1:A:317:ILE:HD12	2.07	0.75
1:A:83:ASN:HD21	1:A:157:GLN:HE22	1.32	0.75
1:A:83:ASN:HD21	1:A:157:GLN:NE2	1.85	0.74
4:D:50:ASN:H	4:D:91:HIS:HE1	1.35	0.74
1:A:116:MET:CE	1:A:200:ILE:HG23	2.19	0.73
4:D:50:ASN:H	4:D:91:HIS:CE1	2.06	0.73
1:A:405:THR:CG2	1:A:407:TYR:H	2.02	0.73
3:C:91:THR:HG22	3:C:116:VAL:H	1.54	0.72
1:A:91:ILE:HD12	1:A:92:THR:N	2.04	0.72
1:A:417:SER:C	1:A:418:LEU:HD12	2.10	0.72
1:A:116:MET:HE3	1:A:200:ILE:HG23	1.74	0.69
1:A:412:PHE:HB2	5:A:560:HEA:HMD3	1.75	0.68
1:A:342:LEU:CA	1:A:345:MET:HE2	2.18	0.67
1:A:98:MET:HG3	5:A:559:HEA:C3C	2.25	0.67
3:C:1:GLU:OE2	3:C:26:GLY:O	2.13	0.67
1:A:415:VAL:O	1:A:419:GLY:HA3	1.95	0.67
1:A:418:LEU:CD1	1:A:418:LEU:N	2.57	0.66
2:B:154:TYR:O	2:B:154:TYR:CD1	2.49	0.65
1:A:206:ASN:HD22	1:A:206:ASN:N	1.95	0.65
1:A:206:ASN:ND2	1:A:206:ASN:N	2.45	0.65
4:D:6:GLN:NE2	4:D:103:THR:HG23	2.11	0.65
1:A:152:PRO:O	1:A:176:GLY:HA3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLN:HB2	2:B:4:LEU:HD22	1.78	0.64
1:A:287:PHE:HB3	1:A:312:MET:HE2	1.79	0.64
9:B:272:LDA:H11	9:B:275:LDA:HM22	1.78	0.64
1:A:21:ARG:HD3	1:A:22:TRP:CD1	2.33	0.64
1:A:130:LEU:HD22	1:A:195:LEU:HD22	1.80	0.64
4:D:6:GLN:HE21	4:D:103:THR:HG23	1.63	0.64
1:A:190:GLY:O	1:A:194:ILE:HG13	1.97	0.64
1:A:337:GLN:HE22	2:B:104:GLN:NE2	1.96	0.63
4:D:104:LYS:HE2	4:D:106:GLU:OE2	1.97	0.63
1:A:405:THR:HG22	1:A:407:TYR:H	1.63	0.63
1:A:202:THR:O	1:A:206:ASN:ND2	2.31	0.63
5:A:560:HEA:HHC	5:A:560:HEA:O11	1.98	0.63
1:A:245:LEU:O	1:A:249:ARG:HG3	1.98	0.63
9:A:565:LDA:HM23	10:A:571:LMT:H5'	1.81	0.63
2:B:37:PHE:HD1	9:B:273:LDA:H11	1.64	0.63
1:A:337:GLN:HE22	2:B:104:GLN:HE21	1.44	0.63
1:A:269:HIS:HD2	1:A:323:TRP:HE1	1.46	0.62
2:B:1:GLN:CB	2:B:4:LEU:HB2	2.23	0.62
1:A:342:LEU:HD22	10:A:574:LMT:H81	1.81	0.62
1:A:336:GLN:HE22	9:A:566:LDA:H22	1.65	0.61
1:A:433:GLY:HA2	1:A:438:ARG:O	1.99	0.61
1:A:473:ARG:O	1:A:474:ARG:HB2	2.00	0.61
1:A:381:PHE:CD2	1:A:382:LEU:CD2	2.84	0.61
1:A:381:PHE:CD2	1:A:382:LEU:HD23	2.35	0.61
4:D:24:ARG:HD2	4:D:70:GLN:HE22	1.64	0.61
1:A:485:TRP:HH2	10:B:278:LMT:H11	1.63	0.61
2:B:227:MET:N	2:B:228:PRO:CD	2.64	0.60
1:A:187:HIS:CE1	1:A:243:THR:HG22	2.36	0.60
1:A:284:LEU:O	1:A:287:PHE:HB2	2.02	0.60
1:A:412:PHE:CD2	5:A:560:HEA:HAD1	2.36	0.60
1:A:239:ALA:O	1:A:243:THR:HG23	2.01	0.60
3:C:57:ARG:HH11	3:C:57:ARG:HG3	1.67	0.60
5:A:560:HEA:HMB1	5:A:560:HEA:H122	1.85	0.59
1:A:129:ARG:HG3	10:A:575:LMT:H31	1.84	0.59
1:A:351:THR:HG21	5:A:560:HEA:H14	1.84	0.59
1:A:297:PHE:O	1:A:367:ILE:HA	2.01	0.59
1:A:312:MET:HE3	12:A:579:HOH:O	2.02	0.59
1:A:484:TYR:H	2:B:15:ASN:HD21	1.51	0.59
4:D:69:THR:HG22	4:D:70:GLN:HG2	1.84	0.59
1:A:287:PHE:HB3	1:A:312:MET:CE	2.34	0.58
1:A:464:HIS:O	1:A:468:ARG:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:ND2	1:A:157:GLN:HE22	2.01	0.58
3:C:47:TRP:HE1	3:C:50:SER:HB2	1.69	0.58
1:A:451:MET:HG2	10:A:572:LMT:H92	1.86	0.58
10:A:574:LMT:H91	2:B:90:VAL:HA	1.86	0.57
1:A:341:MET:HG3	1:A:394:SER:O	2.04	0.57
1:A:468:ARG:HD3	2:B:18:MET:O	2.04	0.57
1:A:85:HIS:O	1:A:89:VAL:HG23	2.03	0.57
3:C:93:MET:CE	3:C:112:THR:C	2.73	0.57
9:B:274:LDA:H12	10:B:279:LMT:H121	1.85	0.57
1:A:412:PHE:CB	5:A:560:HEA:C2D	2.83	0.57
1:A:116:MET:HE1	1:A:200:ILE:HG23	1.87	0.56
1:A:443:TRP:HZ2	10:A:569:LMT:H11	1.69	0.56
3:C:88:SER:O	3:C:91:THR:HG23	2.05	0.56
3:C:91:THR:HB	3:C:115:THR:HA	1.88	0.56
1:A:27:ASN:HB3	1:A:30:ASP:OD2	2.06	0.55
4:D:6:GLN:HG2	4:D:103:THR:HG22	1.88	0.55
2:B:19:ASN:ND2	9:B:272:LDA:H32	2.20	0.55
3:C:47:TRP:CZ2	4:D:95:PRO:HB3	2.41	0.55
1:A:125:MET:HA	1:A:125:MET:HE3	1.88	0.55
1:A:129:ARG:CG	10:A:575:LMT:H31	2.36	0.55
2:B:3:VAL:HG13	2:B:4:LEU:HD13	1.89	0.55
2:B:19:ASN:HD21	9:B:272:LDA:H51	1.70	0.55
1:A:412:PHE:HB3	5:A:560:HEA:C2D	2.36	0.55
10:A:570:LMT:H6E	10:A:570:LMT:C2B	2.30	0.55
1:A:468:ARG:NH1	2:B:19:ASN:OD1	2.40	0.55
1:A:485:TRP:CH2	10:B:278:LMT:H11	2.42	0.55
3:C:87:LYS:HE2	12:C:135:HOH:O	2.07	0.55
1:A:109:GLY:O	1:A:113:ASN:HB2	2.07	0.54
1:A:276:HIS:O	1:A:279:VAL:HG22	2.07	0.54
4:D:40:GLN:HB2	12:D:132:HOH:O	2.07	0.54
2:B:109:ASP:HB3	12:B:372:HOH:O	2.07	0.54
1:A:405:THR:HG23	1:A:407:TYR:H	1.71	0.54
2:B:75:THR:O	2:B:76:PRO:C	2.46	0.54
1:A:78:ALA:O	1:A:79:GLU:C	2.46	0.54
1:A:412:PHE:CE1	1:A:413:HIS:CE1	2.96	0.54
1:A:344:THR:HG22	5:A:560:HEA:HMB2	1.91	0.53
2:B:19:ASN:HD21	9:B:272:LDA:H32	1.73	0.53
3:C:86:LEU:HB3	3:C:116:VAL:HG21	1.90	0.53
1:A:57:LEU:HD22	1:A:87:TRP:HH2	1.74	0.53
1:A:18:PHE:HB3	1:A:21:ARG:HB2	1.91	0.53
4:D:79:LEU:HB3	4:D:80:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG22	10:A:574:LMT:H41	1.91	0.53
1:A:481:GLU:HG2	2:B:13:PRO:O	2.09	0.53
1:A:274:PHE:CZ	1:A:278[A]:GLU:HG3	2.44	0.53
2:B:73:HIS:O	2:B:74:ASN:HB2	2.09	0.53
2:B:83:LEU:O	2:B:87:LEU:HD23	2.08	0.52
1:A:346:THR:HG22	10:A:574:LMT:H22	1.91	0.52
3:C:39:GLN:HB2	3:C:45:LEU:HD23	1.91	0.52
10:A:571:LMT:O3'	10:A:571:LMT:C1B	2.56	0.52
2:B:40:TYR:HE1	9:B:275:LDA:H31	1.74	0.52
1:A:313:ALA:O	1:A:317:ILE:HG23	2.09	0.52
10:D:121:LMT:H1B	10:D:121:LMT:O3'	2.09	0.52
1:A:524:ASN:OD1	1:A:526:HIS:HB2	2.09	0.52
4:D:61:ARG:HG3	4:D:61:ARG:HH11	1.75	0.52
2:B:138:MET:HG3	2:B:228:PRO:HG3	1.92	0.52
1:A:300:LYS:HD3	1:A:361:THR:O	2.10	0.51
1:A:416:MET:HG2	5:A:560:HEA:HBC2	1.91	0.51
1:A:290:ILE:O	1:A:294:ILE:HG13	2.10	0.51
1:A:68:GLU:CD	1:A:68:GLU:H	2.13	0.51
1:A:206:ASN:HD22	1:A:206:ASN:H	1.59	0.51
1:A:21:ARG:HD3	1:A:22:TRP:NE1	2.25	0.51
1:A:438:ARG:NH2	1:A:514:GLY:O	2.41	0.51
1:A:516:ARG:NH2	1:A:518:ASN:HB3	2.25	0.51
4:D:21:ILE:HG23	4:D:103:THR:HG21	1.92	0.51
1:A:412:PHE:CB	5:A:560:HEA:HMD3	2.39	0.51
1:A:187:HIS:HE1	1:A:243:THR:HG22	1.76	0.51
1:A:394:SER:HA	5:A:560:HEA:OMA	2.10	0.51
2:B:52:LEU:HD13	10:B:279:LMT:H102	1.92	0.50
1:A:416:MET:HG2	5:A:560:HEA:CBC	2.41	0.50
5:A:559:HEA:HHC	5:A:559:HEA:C12	2.42	0.50
3:C:17:SER:HB2	3:C:84:SER:HA	1.93	0.50
1:A:27:ASN:ND2	1:A:29[B]:LYS:HB2	2.27	0.50
1:A:504:ILE:CD1	10:A:570:LMT:H122	2.42	0.50
3:C:83:MET:HB3	3:C:86:LEU:HD21	1.94	0.50
1:A:440:TYR:OH	1:A:442:GLU:OE1	2.19	0.49
4:D:6:GLN:HG2	4:D:103:THR:CG2	2.42	0.49
2:B:1:GLN:HB2	2:B:4:LEU:CD2	2.42	0.49
1:A:125:MET:HE3	1:A:203:THR:HG21	1.94	0.49
1:A:122:ALA:HB2	1:A:207:MET:O	2.12	0.49
10:A:568:LMT:O2B	10:A:568:LMT:O3'	2.30	0.48
1:A:355:VAL:HG21	5:A:560:HEA:H18	1.94	0.48
1:A:27:ASN:HD21	1:A:29[C]:LYS:HE2	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:MET:HE3	10:A:574:LMT:H81	1.96	0.48
1:A:405:THR:HG23	1:A:467:GLY:HA2	1.94	0.48
1:A:456:SER:HA	1:A:459:ILE:HD12	1.96	0.48
2:B:216:CYS:HB2	2:B:227:MET:HG3	1.96	0.48
1:A:379:PHE:CD1	1:A:379:PHE:C	2.86	0.48
1:A:396:ALA:HB3	1:A:397:PRO:HD3	1.95	0.48
2:B:121:TRP:CD2	2:B:223:ASN:HB2	2.49	0.48
2:B:174:VAL:HG23	2:B:194:ALA:HB2	1.95	0.48
2:B:40:TYR:CE1	9:B:275:LDA:H31	2.49	0.47
2:B:164:VAL:O	2:B:233:ALA:HA	2.13	0.47
1:A:395:GLN:C	1:A:397:PRO:HD2	2.35	0.47
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.49	0.47
3:C:94:TYR:O	3:C:111:GLY:HA2	2.14	0.47
10:A:574:LMT:H11	10:A:574:LMT:O2'	2.14	0.47
5:A:559:HEA:HBC1	5:A:559:HEA:HMC1	1.95	0.47
1:A:484:TYR:N	2:B:15:ASN:HD21	2.11	0.47
1:A:133:LEU:O	1:A:137:MET:HG2	2.14	0.47
9:A:566:LDA:HM12	9:A:566:LDA:H22	1.80	0.47
2:B:25:SER:HB2	2:B:26:PRO:HD2	1.95	0.47
1:A:125:MET:CE	1:A:203:THR:CB	2.93	0.47
4:D:28:ASN:OD1	4:D:68:GLY:HA2	2.15	0.47
1:A:478:TYR:O	1:A:479:PRO:C	2.53	0.47
1:A:459:ILE:HD11	1:A:493:ALA:HA	1.97	0.47
1:A:518:ASN:HD22	1:A:518:ASN:H	1.63	0.46
1:A:412:PHE:CG	5:A:560:HEA:HMD3	2.50	0.46
9:A:564:LDA:H21	9:A:564:LDA:HM23	1.67	0.46
1:A:520:PRO:HA	1:A:534:LEU:O	2.16	0.46
1:A:342:LEU:CD2	1:A:345:MET:HE3	2.46	0.46
1:A:491:ILE:HD13	10:A:572:LMT:H6'1	1.98	0.46
12:A:606:HOH:O	2:B:198:ARG:HD2	2.15	0.46
9:B:276:LDA:H21	9:B:276:LDA:HM21	1.70	0.46
3:C:40:THR:HB	3:C:41:PRO:HD2	1.98	0.46
3:C:5:GLN:OE1	3:C:110[B]:GLN:NE2	2.49	0.46
1:A:271:LEU:O	1:A:271:LEU:HG	2.04	0.46
1:A:29[B]:LYS:HD2	1:A:114:TYR:OH	2.15	0.46
1:A:417:SER:HB2	5:A:559:HEA:HMC2	1.98	0.46
2:B:19:ASN:HB3	12:B:309:HOH:O	2.16	0.45
1:A:398:LEU:HD13	2:B:34:LEU:HD23	1.97	0.45
1:A:342:LEU:CD2	1:A:345:MET:CE	2.85	0.45
2:B:70:ARG:HG3	12:B:391:HOH:O	2.16	0.45
1:A:541:HIS:NE2	12:A:609:HOH:O	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:HIS:C	2:B:73:HIS:CD2	2.90	0.45
5:A:559:HEA:H122	5:A:559:HEA:HHC	1.97	0.45
1:A:187:HIS:CE1	1:A:243:THR:CG2	2.99	0.45
1:A:332:MET:HG3	1:A:337:GLN:HG3	1.98	0.45
1:A:516:ARG:O	1:A:517:VAL:HG23	2.16	0.45
1:A:317:ILE:CD1	1:A:317:ILE:C	2.83	0.45
1:A:125:MET:CE	1:A:203:THR:OG1	2.65	0.45
1:A:516:ARG:CZ	1:A:518:ASN:HB3	2.46	0.44
1:A:118:LEU:HD23	12:A:674:HOH:O	2.17	0.44
1:A:388:VAL:HG13	2:B:42:ILE:HD12	2.00	0.44
1:A:387:GLY:HA3	5:A:560:HEA:C15	2.47	0.44
1:A:209:ALA:O	1:A:212:MET:HB3	2.18	0.44
1:A:381:PHE:HD2	1:A:382:LEU:CD2	2.30	0.44
2:B:109:ASP:N	2:B:109:ASP:OD1	2.49	0.44
1:A:431:TRP:O	1:A:435:MET:HG3	2.18	0.44
4:D:61:ARG:NE	4:D:82:ASP:OD2	2.35	0.44
2:B:114:ILE:O	2:B:172:VAL:HA	2.17	0.44
10:D:121:LMT:H12	10:D:121:LMT:O2'	2.17	0.44
1:A:384:THR:O	1:A:388:VAL:HB	2.18	0.44
1:A:276:HIS:CD2	1:A:280:TYR:CE2	2.95	0.44
1:A:355:VAL:O	1:A:359:ILE:HG13	2.17	0.43
2:B:71:PHE:CZ	10:B:279:LMT:H32	2.54	0.43
2:B:74:ASN:HD22	10:B:279:LMT:H12	1.84	0.43
1:A:336:GLN:HE22	9:A:566:LDA:HM12	1.83	0.43
1:A:354:LYS:HE3	1:A:354:LYS:HB3	1.88	0.43
4:D:83:PHE:CZ	4:D:107:ILE:HG23	2.53	0.43
4:D:24:ARG:HD2	4:D:70:GLN:NE2	2.33	0.43
1:A:235:LEU:N	1:A:236:PRO:CD	2.81	0.43
1:A:505:GLY:HA3	10:A:569:LMT:H62	2.01	0.43
1:A:165:VAL:HB	1:A:271:LEU:CD2	2.48	0.43
1:A:342:LEU:HD23	1:A:345:MET:HE3	1.93	0.43
10:D:121:LMT:C1B	10:D:121:LMT:O3'	2.66	0.43
1:A:453:PHE:C	1:A:453:PHE:CD2	2.92	0.43
3:C:52:ASN:HB2	12:C:178:HOH:O	2.18	0.43
1:A:180:ASP:OD1	1:A:249:ARG:HD3	2.19	0.42
1:A:28:HIS:HD2	1:A:113:ASN:O	2.00	0.42
3:C:44:ARG:HB2	3:C:44:ARG:HE	1.54	0.42
2:B:154:TYR:O	2:B:154:TYR:CG	2.72	0.42
9:B:274:LDA:H12	10:B:279:LMT:C12	2.50	0.42
2:B:227:MET:HA	2:B:228:PRO:HD2	1.80	0.42
3:C:39:GLN:HA	3:C:44:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PHE:HB2	5:A:559:HEA:H261	2.01	0.42
1:A:98:MET:HB3	5:A:559:HEA:CBC	2.50	0.42
1:A:381:PHE:CD2	1:A:382:LEU:HD21	2.54	0.42
1:A:412:PHE:HB2	5:A:560:HEA:CMD	2.47	0.42
1:A:437:GLY:O	1:A:516:ARG:NH1	2.43	0.42
9:B:274:LDA:H72	9:B:274:LDA:H41	1.77	0.42
9:B:274:LDA:HM21	10:B:279:LMT:H121	2.00	0.42
9:B:275:LDA:H21	9:B:275:LDA:HM23	1.80	0.42
2:B:37:PHE:CD1	9:B:273:LDA:H11	2.48	0.42
1:A:258:PRO:HG3	2:B:196:PRO:HB2	2.02	0.42
1:A:50:THR:HG22	1:A:51:VAL:N	2.34	0.42
1:A:61:GLY:N	1:A:477:ASP:OD1	2.51	0.42
1:A:30:ASP:O	1:A:34:LEU:HG	2.19	0.42
10:A:575:LMT:C4'	10:A:575:LMT:H3B	2.37	0.41
10:A:574:LMT:H3B	10:A:574:LMT:H4'	2.01	0.41
4:D:8:PRO:O	4:D:103:THR:CB	2.58	0.41
3:C:3:LYS:HD3	12:C:171:HOH:O	2.19	0.41
4:D:24:ARG:CD	4:D:70:GLN:NE2	2.82	0.41
1:A:197:ALA:HB1	1:A:228:ALA:HB1	2.02	0.41
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.93	0.41
2:B:160:ASN:ND2	12:B:394:HOH:O	2.46	0.41
2:B:102:ARG:HD3	12:D:159:HOH:O	2.20	0.41
4:D:35:TRP:O	4:D:47:LEU:HB2	2.21	0.41
2:B:159:ASP:OD1	2:B:160:ASN:N	2.51	0.41
9:B:273:LDA:HM23	9:B:273:LDA:H22	1.76	0.41
10:A:568:LMT:H61	10:A:568:LMT:H31	1.71	0.41
2:B:122:TYR:CB	2:B:137:LEU:HD22	2.50	0.41
2:B:236:GLN:O	2:B:240:GLU:HG3	2.20	0.41
1:A:535:PRO:HD2	1:A:539:PRO:HD3	2.03	0.41
1:A:208:ARG:HB3	1:A:212:MET:HG2	2.03	0.41
1:A:405:THR:HG23	1:A:467:GLY:CA	2.50	0.41
1:A:381:PHE:CD1	2:B:50:CYS:SG	3.14	0.41
1:A:434:LYS:HE3	1:A:531:GLU:O	2.21	0.41
3:C:57:ARG:NH1	3:C:57:ARG:HG3	2.34	0.41
1:A:49:PHE:HA	1:A:90:MET:CE	2.51	0.41
3:C:73:ASP:OD2	3:C:76:LYS:HG3	2.21	0.41
4:D:24:ARG:CD	4:D:70:GLN:HE22	2.33	0.41
2:B:227:MET:N	2:B:228:PRO:HD3	2.35	0.41
1:A:491:ILE:HG23	10:A:572:LMT:H2'	2.03	0.41
1:A:482:PHE:O	1:A:486:ASN:OD1	2.39	0.41
1:A:123:PRO:HB3	1:A:542:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:574:LMT:H92	2:B:93:GLY:HA3	2.03	0.40
2:B:72:THR:O	2:B:73:HIS:HB3	2.21	0.40
2:B:119:HIS:O	2:B:121:TRP:HA	2.20	0.40
1:A:20:THR:O	1:A:24:MET:HB2	2.22	0.40
1:A:280:TYR:O	1:A:284:LEU:HD23	2.22	0.40
10:A:574:LMT:H5B	10:A:574:LMT:H4'	2.03	0.40
1:A:238:LEU:HD22	1:A:274:PHE:CE1	2.56	0.40
1:A:475:TYR:CZ	2:B:225:ALA:HA	2.57	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	531/558 (95%)	494 (93%)	34 (6%)	3 (1%)	30	35
2	B	252/298 (85%)	240 (95%)	10 (4%)	2 (1%)	24	27
3	C	119/127 (94%)	110 (92%)	8 (7%)	1 (1%)	24	27
4	D	107/120 (89%)	101 (94%)	4 (4%)	2 (2%)	10	8
All	All	1009/1103 (92%)	945 (94%)	56 (6%)	8 (1%)	24	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	74	ASN
3	C	118	SER
1	A	79	GLU
4	D	77	SER
2	B	235	SER
1	A	544	GLU
1	A	517	VAL

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Mol	Chain	Res	Type
4	D	68	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	435/454 (96%)	405 (93%)	30 (7%)	19 24
2	B	212/243 (87%)	194 (92%)	18 (8%)	13 15
3	C	103/107 (96%)	94 (91%)	9 (9%)	13 14
4	D	92/104 (88%)	82 (89%)	10 (11%)	8 8
All	All	842/908 (93%)	775 (92%)	67 (8%)	16 18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ARG
1	A	29[A]	LYS
1	A	29[B]	LYS
1	A	29[C]	LYS
1	A	50	THR
1	A	57	LEU
1	A	63	GLN
1	A	68	GLU
1	A	72	LEU
1	A	86	LEU
1	A	91	ILE
1	A	116	MET
1	A	125	MET
1	A	134	SER
1	A	173	THR
1	A	206	ASN
1	A	214	LEU
1	A	224	VAL
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	277	PRO
1	A	317	ILE
1	A	377	PHE
1	A	380	LEU
1	A	388	VAL
1	A	398	LEU
1	A	404	ASP
1	A	405	THR
1	A	516	ARG
1	A	518	ASN
2	B	4	LEU
2	B	53	LEU
2	B	54	LEU
2	B	63	ARG
2	B	77	ILE
2	B	81	TRP
2	B	83	LEU
2	B	85	PRO
2	B	108	ASN
2	B	137	LEU
2	B	140[A]	GLU
2	B	140[B]	GLU
2	B	142	GLU
2	B	166	VAL
2	B	174	VAL
2	B	179	VAL
2	B	186	PRO
2	B	198	ARG
3	C	5	GLN
3	C	13	GLN
3	C	17	SER
3	C	33	THR
3	C	42	GLU
3	C	48	VAL
3	C	57	ARG
3	C	87	LYS
3	C	91	THR
4	D	1	ASP
4	D	3	GLU
4	D	14	SER
4	D	15	VAL
4	D	63	SER

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Mol	Chain	Res	Type
4	D	69	THR
4	D	77	SER
4	D	103	THR
4	D	107	ILE
4	D	108	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	28	HIS
1	A	59	HIS
1	A	155	ASN
1	A	157	GLN
1	A	206	ASN
1	A	250	ASN
1	A	268	GLN
1	A	269	HIS
1	A	469	GLN
1	A	486	ASN
1	A	518	ASN
2	B	15	ASN
2	B	21	GLN
2	B	29	HIS
2	B	73	HIS
2	B	104	GLN
2	B	108	ASN
2	B	173	GLN
2	B	208	GLN
3	C	99	HIS
4	D	6	GLN
4	D	37	GLN
4	D	90	HIS
4	D	91	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 for Mogul analysis.

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	$\#\|Z\| > 2$
5	HEA	A	559	1	40,67,67	3.38	14 (35%)	41,103,103	4.49	24 (58%)
5	HEA	A	560	1,11	40,67,67	4.15	18 (45%)	41,103,103	4.87	26 (63%)
9	LDA	A	564	-	15,15,15	3.76	2 (13%)	16,17,17	0.66	0
9	LDA	A	565	-	15,15,15	3.45	1 (6%)	16,17,17	0.82	1 (6%)
9	LDA	A	566	-	15,15,15	3.43	1 (6%)	16,17,17	0.88	1 (6%)
9	LDA	A	567	-	15,15,15	3.61	2 (13%)	16,17,17	0.74	0
10	LMT	A	568	-	36,36,36	4.31	15 (41%)	47,47,47	1.24	4 (8%)
10	LMT	A	569	-	36,36,36	4.32	16 (44%)	47,47,47	2.11	13 (27%)
10	LMT	A	570	-	36,36,36	4.22	16 (44%)	47,47,47	1.44	5 (10%)
10	LMT	A	571	-	36,36,36	4.27	16 (44%)	47,47,47	1.50	6 (12%)
10	LMT	A	572	-	36,36,36	4.01	17 (47%)	47,47,47	1.60	5 (10%)
10	LMT	A	573	-	36,36,36	4.01	16 (44%)	47,47,47	1.68	6 (12%)
10	LMT	A	574	-	36,36,36	4.23	15 (41%)	47,47,47	1.70	6 (12%)
10	LMT	A	575	-	36,36,36	4.41	16 (44%)	47,47,47	1.57	8 (17%)
11	PER	A	576	5	0,1,1	0.00	-	0,0,0	0.00	-
9	LDA	B	272	-	15,15,15	3.57	2 (13%)	16,17,17	0.72	0
9	LDA	B	273	-	15,15,15	3.65	1 (6%)	16,17,17	0.73	0
9	LDA	B	274	-	15,15,15	3.59	1 (6%)	16,17,17	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	LDA	B	275	-	15,15,15	3.50	2 (13%)	16,17,17	0.57	0
9	LDA	B	276	-	15,15,15	3.73	1 (6%)	16,17,17	0.67	0
10	LMT	B	277[A]	-	36,36,36	4.22	16 (44%)	47,47,47	2.02	9 (19%)
10	LMT	B	277[B]	-	36,36,36	4.22	16 (44%)	47,47,47	1.94	8 (17%)
10	LMT	B	278	-	36,36,36	4.19	13 (36%)	47,47,47	1.75	10 (21%)
10	LMT	B	279	-	36,36,36	4.22	14 (38%)	47,47,47	1.26	5 (10%)
10	LMT	D	121	-	36,36,36	4.05	15 (41%)	47,47,47	2.16	12 (25%)

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
5	HEA	A	559	1	4/4/7/16	0/24/76/76	0/0/8/8
5	HEA	A	560	1,11	4/4/7/16	0/24/76/76	0/0/8/8
9	LDA	A	564	-	-	0/13/13/13	0/0/0/0
9	LDA	A	565	-	-	0/13/13/13	0/0/0/0
9	LDA	A	566	-	-	0/13/13/13	0/0/0/0
9	LDA	A	567	-	-	0/13/13/13	0/0/0/0
10	LMT	A	568	-	-	0/21/61/61	0/2/2/2
10	LMT	A	569	-	-	0/21/61/61	0/2/2/2
10	LMT	A	570	-	-	0/21/61/61	0/2/2/2
10	LMT	A	571	-	-	0/21/61/61	0/2/2/2
10	LMT	A	572	-	-	0/21/61/61	0/2/2/2
10	LMT	A	573	-	-	0/21/61/61	0/2/2/2
10	LMT	A	574	-	-	1/21/61/61	0/2/2/2
10	LMT	A	575	-	-	0/21/61/61	0/2/2/2
11	PER	A	576	5	-	0/0/0/0	0/0/0/0
9	LDA	B	272	-	-	0/13/13/13	0/0/0/0
9	LDA	B	273	-	-	0/13/13/13	0/0/0/0
9	LDA	B	274	-	-	0/13/13/13	0/0/0/0
9	LDA	B	275	-	-	0/13/13/13	0/0/0/0
9	LDA	B	276	-	-	0/13/13/13	0/0/0/0
10	LMT	B	277[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	B	277[B]	-	-	0/21/61/61	0/2/2/2
10	LMT	B	278	-	-	0/21/61/61	0/2/2/2
10	LMT	B	279	-	-	0/21/61/61	0/2/2/2
10	LMT	D	121	-	-	0/21/61/61	0/2/2/2

All (246) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	564	LDA	O1-N1	-14.20	1.26	1.39
9	B	276	LDA	O1-N1	-14.19	1.26	1.39
9	B	273	LDA	O1-N1	-13.98	1.26	1.39
9	A	567	LDA	O1-N1	-13.69	1.26	1.39
9	B	274	LDA	O1-N1	-13.62	1.26	1.39
9	B	272	LDA	O1-N1	-13.60	1.26	1.39
9	B	275	LDA	O1-N1	-13.23	1.27	1.39
9	A	566	LDA	O1-N1	-13.12	1.27	1.39
9	A	565	LDA	O1-N1	-13.12	1.27	1.39
5	A	560	HEA	O11-C11	-11.25	1.16	1.42
10	A	569	LMT	O2B-C2B	-8.76	1.22	1.43
10	A	571	LMT	C4B-C5B	-8.75	1.34	1.53
10	B	277[B]	LMT	O4'-C4B	-8.74	1.22	1.43
10	B	277[A]	LMT	O4'-C4B	-8.74	1.22	1.43
10	A	569	LMT	O3B-C3B	-8.64	1.22	1.43
10	B	278	LMT	O4'-C4B	-8.62	1.22	1.43
5	A	559	HEA	O11-C11	-8.58	1.22	1.42
10	A	569	LMT	C4B-C5B	-8.46	1.35	1.53
10	A	568	LMT	O3'-C3'	-8.43	1.22	1.43
10	B	279	LMT	O3'-C3'	-8.43	1.22	1.43
10	A	570	LMT	O3B-C3B	-8.34	1.23	1.43
10	A	574	LMT	C4B-C5B	-8.33	1.35	1.53
10	B	277[B]	LMT	O2B-C2B	-8.31	1.23	1.43
10	B	277[A]	LMT	O2B-C2B	-8.31	1.23	1.43
10	A	572	LMT	O3'-C3'	-8.29	1.23	1.43
10	A	568	LMT	O3B-C3B	-8.28	1.23	1.43
10	A	574	LMT	O3'-C3'	-8.28	1.23	1.43
10	A	568	LMT	O2B-C2B	-8.26	1.23	1.43
10	A	571	LMT	O4'-C4B	-8.25	1.23	1.43
10	A	574	LMT	O2B-C2B	-8.24	1.23	1.43
10	A	574	LMT	O3B-C3B	-8.22	1.23	1.43
10	B	279	LMT	O3B-C3B	-8.22	1.23	1.43
10	A	570	LMT	O2B-C2B	-8.21	1.23	1.43
10	B	278	LMT	O2B-C2B	-8.18	1.23	1.43
10	A	570	LMT	C4B-C5B	-8.16	1.35	1.53
10	A	575	LMT	O2B-C2B	-8.16	1.23	1.43
10	B	278	LMT	O3'-C3'	-8.15	1.23	1.43
10	A	575	LMT	O3'-C3'	-8.15	1.23	1.43
10	B	278	LMT	O3B-C3B	-8.14	1.23	1.43
10	A	571	LMT	O3B-C3B	-8.13	1.23	1.43
10	A	575	LMT	O4'-C4B	-8.11	1.23	1.43
10	A	570	LMT	O4'-C4B	-8.10	1.23	1.43
10	A	573	LMT	O2B-C2B	-8.10	1.23	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	279	LMT	O4'-C4B	-8.09	1.23	1.43
10	B	279	LMT	O2B-C2B	-8.07	1.23	1.43
10	B	277[B]	LMT	O3'-C3'	-8.06	1.23	1.43
10	B	277[A]	LMT	O3'-C3'	-8.06	1.23	1.43
10	B	278	LMT	C4B-C5B	-8.06	1.36	1.53
10	B	279	LMT	C4B-C5B	-8.05	1.36	1.53
10	A	574	LMT	O4'-C4B	-8.05	1.23	1.43
10	A	568	LMT	C4B-C5B	-8.02	1.36	1.53
10	A	571	LMT	O3'-C3'	-8.01	1.23	1.43
10	A	573	LMT	O3B-C3B	-7.99	1.23	1.43
10	A	573	LMT	C4B-C5B	-7.99	1.36	1.53
10	A	570	LMT	O3'-C3'	-7.98	1.23	1.43
10	D	121	LMT	O2B-C2B	-7.97	1.23	1.43
10	A	569	LMT	O3'-C3'	-7.97	1.23	1.43
10	A	572	LMT	O3B-C3B	-7.97	1.23	1.43
10	B	277[B]	LMT	C4B-C5B	-7.97	1.36	1.53
10	B	277[A]	LMT	C4B-C5B	-7.97	1.36	1.53
10	D	121	LMT	O3B-C3B	-7.94	1.24	1.43
10	A	568	LMT	O4'-C4B	-7.90	1.24	1.43
10	A	571	LMT	O2B-C2B	-7.87	1.24	1.43
10	D	121	LMT	O3'-C3'	-7.85	1.24	1.43
10	A	575	LMT	C4B-C5B	-7.84	1.36	1.53
10	A	569	LMT	O4'-C4B	-7.78	1.24	1.43
10	A	573	LMT	O3'-C3'	-7.77	1.24	1.43
10	B	277[B]	LMT	O3B-C3B	-7.75	1.24	1.43
10	B	277[A]	LMT	O3B-C3B	-7.75	1.24	1.43
10	A	575	LMT	O3B-C3B	-7.74	1.24	1.43
10	A	572	LMT	O4'-C4B	-7.74	1.24	1.43
10	A	572	LMT	O2B-C2B	-7.68	1.24	1.43
10	A	572	LMT	C4B-C5B	-7.61	1.37	1.53
10	A	573	LMT	O4'-C4B	-7.60	1.24	1.43
10	A	568	LMT	C3'-C2'	-7.47	1.32	1.52
10	A	569	LMT	C3'-C2'	-7.38	1.33	1.52
10	D	121	LMT	O4'-C4B	-7.37	1.25	1.43
10	A	569	LMT	C3B-C2B	-7.12	1.33	1.52
10	B	278	LMT	C3'-C2'	-6.94	1.34	1.52
10	A	574	LMT	C3'-C2'	-6.84	1.34	1.52
10	A	568	LMT	C3B-C2B	-6.81	1.34	1.52
10	A	568	LMT	C4B-C3B	-6.68	1.34	1.52
10	A	569	LMT	C4B-C3B	-6.67	1.34	1.52
10	A	571	LMT	C4B-C3B	-6.63	1.35	1.52
10	A	573	LMT	C3B-C2B	-6.61	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	279	LMT	C3'-C2'	-6.61	1.35	1.52
10	A	571	LMT	C1'-C2'	-6.59	1.32	1.52
10	B	279	LMT	C4'-C5'	-6.58	1.34	1.52
10	A	570	LMT	C4'-C5'	-6.56	1.34	1.52
10	B	279	LMT	C4B-C3B	-6.55	1.35	1.52
10	D	121	LMT	C4B-C5B	-6.54	1.39	1.53
10	A	575	LMT	C3'-C2'	-6.54	1.35	1.52
10	A	568	LMT	C3'-C4'	-6.50	1.34	1.52
10	D	121	LMT	C3'-C2'	-6.48	1.35	1.52
10	D	121	LMT	C4'-C5'	-6.48	1.35	1.52
10	B	277[B]	LMT	C1B-C2B	-6.45	1.33	1.52
10	B	277[A]	LMT	C1B-C2B	-6.45	1.33	1.52
10	A	570	LMT	C3B-C2B	-6.45	1.35	1.52
10	A	571	LMT	C3'-C2'	-6.42	1.35	1.52
10	B	278	LMT	C3B-C2B	-6.40	1.35	1.52
10	A	570	LMT	C3'-C2'	-6.40	1.35	1.52
10	A	574	LMT	C3B-C2B	-6.39	1.35	1.52
10	B	279	LMT	C3B-C2B	-6.38	1.35	1.52
10	B	277[B]	LMT	C4B-C3B	-6.37	1.35	1.52
10	B	277[A]	LMT	C4B-C3B	-6.37	1.35	1.52
10	B	277[B]	LMT	C3'-C4'	-6.36	1.34	1.52
10	B	277[A]	LMT	C3'-C4'	-6.36	1.34	1.52
10	A	570	LMT	C4B-C3B	-6.36	1.35	1.52
10	A	571	LMT	C3B-C2B	-6.36	1.35	1.52
10	A	575	LMT	C4B-C3B	-6.29	1.35	1.52
10	A	570	LMT	C3'-C4'	-6.22	1.34	1.52
10	A	574	LMT	C4B-C3B	-6.21	1.36	1.52
10	B	278	LMT	C1B-C2B	-6.21	1.34	1.52
10	A	575	LMT	C3B-C2B	-6.20	1.36	1.52
10	B	279	LMT	C3'-C4'	-6.20	1.34	1.52
10	A	568	LMT	C1'-C2'	-6.19	1.34	1.52
10	A	572	LMT	C4B-C3B	-6.18	1.36	1.52
10	A	572	LMT	C3'-C2'	-6.17	1.36	1.52
10	B	278	LMT	C4B-C3B	-6.17	1.36	1.52
10	B	279	LMT	C1B-C2B	-6.16	1.34	1.52
10	D	121	LMT	C3B-C2B	-6.13	1.36	1.52
10	B	277[B]	LMT	C3B-C2B	-6.12	1.36	1.52
10	B	277[A]	LMT	C3B-C2B	-6.12	1.36	1.52
10	A	568	LMT	C4'-C5'	-6.12	1.36	1.52
10	D	121	LMT	C3'-C4'	-6.09	1.35	1.52
10	A	575	LMT	C4'-C5'	-6.07	1.36	1.52
10	A	571	LMT	C4'-C5'	-6.05	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	121	LMT	C1'-C2'	-6.05	1.34	1.52
10	A	573	LMT	C4B-C3B	-6.04	1.36	1.52
10	D	121	LMT	C4B-C3B	-5.98	1.36	1.52
10	A	569	LMT	C3'-C4'	-5.90	1.35	1.52
10	A	574	LMT	C1B-C2B	-5.86	1.35	1.52
10	B	278	LMT	C1'-C2'	-5.85	1.35	1.52
10	B	277[B]	LMT	C4'-C5'	-5.85	1.36	1.52
10	B	277[A]	LMT	C4'-C5'	-5.85	1.36	1.52
10	A	574	LMT	C4'-C5'	-5.84	1.36	1.52
10	A	574	LMT	C1'-C2'	-5.82	1.35	1.52
10	A	574	LMT	C3'-C4'	-5.82	1.36	1.52
10	B	278	LMT	C4'-C5'	-5.81	1.36	1.52
10	A	575	LMT	C1'-C2'	-5.81	1.35	1.52
10	A	570	LMT	C1'-C2'	-5.79	1.35	1.52
10	A	569	LMT	C1'-C2'	-5.79	1.35	1.52
10	A	572	LMT	C3B-C2B	-5.74	1.37	1.52
10	B	277[B]	LMT	C3'-C2'	-5.74	1.37	1.52
10	B	277[A]	LMT	C3'-C2'	-5.74	1.37	1.52
10	A	573	LMT	C1B-C2B	-5.72	1.35	1.52
10	A	569	LMT	C1B-C2B	-5.70	1.35	1.52
10	A	575	LMT	C3'-C4'	-5.67	1.36	1.52
10	A	570	LMT	C1B-C2B	-5.64	1.35	1.52
10	A	571	LMT	C3'-C4'	-5.61	1.36	1.52
10	A	575	LMT	C1B-C2B	-5.57	1.35	1.52
10	A	572	LMT	C4'-C5'	-5.56	1.37	1.52
10	A	569	LMT	C4'-C5'	-5.53	1.37	1.52
10	A	573	LMT	C4'-C5'	-5.49	1.37	1.52
10	A	573	LMT	C3'-C2'	-5.48	1.38	1.52
10	A	568	LMT	C1B-C2B	-5.46	1.36	1.52
10	B	278	LMT	C3'-C4'	-5.41	1.37	1.52
10	B	279	LMT	C1'-C2'	-5.41	1.36	1.52
10	A	572	LMT	C1'-C2'	-5.40	1.36	1.52
10	A	571	LMT	C1B-C2B	-5.40	1.36	1.52
10	A	572	LMT	C3'-C4'	-5.39	1.37	1.52
10	D	121	LMT	C1B-C2B	-5.18	1.37	1.52
10	A	573	LMT	C1'-C2'	-5.17	1.37	1.52
10	A	573	LMT	C3'-C4'	-5.05	1.38	1.52
10	B	277[B]	LMT	C1'-C2'	-4.63	1.38	1.52
10	B	277[A]	LMT	C1'-C2'	-4.63	1.38	1.52
10	A	572	LMT	C1B-C2B	-4.59	1.38	1.52
5	A	560	HEA	C4A-NA	-4.49	1.30	1.36
5	A	559	HEA	C1A-NA	-3.42	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	559	HEA	C4A-NA	-2.89	1.32	1.36
5	A	560	HEA	C1A-NA	-2.79	1.32	1.36
9	A	564	LDA	C1-N1	-2.60	1.46	1.51
5	A	559	HEA	C1D-ND	-2.53	1.33	1.36
9	B	275	LDA	C1-N1	-2.50	1.46	1.51
5	A	560	HEA	C4B-NB	-2.37	1.33	1.36
9	A	567	LDA	C1-N1	-2.12	1.47	1.51
5	A	560	HEA	C1D-ND	-2.10	1.33	1.36
9	B	272	LDA	C1-N1	-2.08	1.47	1.51
5	A	560	HEA	C1B-CHB	2.01	1.45	1.39
10	B	279	LMT	O2'-C2'	2.03	1.47	1.43
10	A	568	LMT	O1B-C1B	2.03	1.47	1.41
5	A	559	HEA	C3B-C2B	2.04	1.48	1.41
10	A	571	LMT	O5'-C1'	2.05	1.47	1.41
10	A	573	LMT	O5B-C1B	2.08	1.47	1.41
10	B	277[B]	LMT	O1B-C1B	2.08	1.47	1.41
10	B	277[A]	LMT	O1B-C1B	2.08	1.47	1.41
10	A	570	LMT	O5B-C1B	2.10	1.47	1.41
10	A	570	LMT	O1B-C1B	2.10	1.47	1.41
10	A	572	LMT	O2'-C2'	2.11	1.48	1.43
10	D	121	LMT	O2'-C2'	2.12	1.48	1.43
10	B	277[B]	LMT	O5'-C1'	2.14	1.47	1.41
10	B	277[A]	LMT	O5'-C1'	2.14	1.47	1.41
5	A	559	HEA	C1B-CHB	2.18	1.45	1.39
5	A	560	HEA	C24-C23	2.21	1.56	1.50
5	A	559	HEA	C4D-CHA	2.21	1.45	1.39
10	A	568	LMT	O5'-C1'	2.23	1.47	1.41
10	A	574	LMT	O5B-C1B	2.23	1.47	1.41
10	A	574	LMT	O1B-C1B	2.25	1.47	1.41
10	A	575	LMT	O5'-C1'	2.25	1.47	1.41
10	A	573	LMT	O1B-C4'	2.29	1.49	1.43
5	A	560	HEA	C1C-CHC	2.29	1.46	1.39
10	A	569	LMT	O1B-C1B	2.30	1.47	1.41
10	A	570	LMT	O1B-C4'	2.31	1.49	1.43
5	A	560	HEA	C4D-CHA	2.39	1.46	1.39
10	A	572	LMT	O5B-C1B	2.46	1.48	1.41
10	A	572	LMT	O5'-C1'	2.49	1.48	1.41
10	A	572	LMT	O1B-C1B	2.50	1.48	1.41
5	A	560	HEA	C4C-CHD	2.50	1.46	1.39
10	A	571	LMT	O1B-C1B	2.50	1.48	1.41
10	A	575	LMT	O1B-C1B	2.56	1.48	1.41
10	A	569	LMT	O5'-C1'	2.60	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	573	LMT	O1B-C1B	2.62	1.48	1.41
10	D	121	LMT	O1B-C1B	2.62	1.48	1.41
5	A	560	HEA	C13-C14	2.67	1.58	1.50
10	A	571	LMT	O5B-C1B	2.75	1.48	1.41
10	A	569	LMT	O5B-C1B	2.83	1.49	1.41
10	B	277[B]	LMT	O5B-C1B	2.85	1.49	1.41
10	B	277[A]	LMT	O5B-C1B	2.85	1.49	1.41
5	A	560	HEA	C3D-C2D	3.07	1.46	1.37
5	A	559	HEA	C3D-C2D	3.31	1.47	1.37
10	B	279	LMT	O1'-C1'	3.48	1.46	1.40
10	A	570	LMT	O1'-C1'	3.59	1.46	1.40
10	A	569	LMT	O1'-C1'	3.63	1.46	1.40
10	B	278	LMT	O1'-C1'	3.64	1.46	1.40
10	A	573	LMT	O1'-C1'	4.01	1.47	1.40
10	A	572	LMT	O1'-C1'	4.02	1.47	1.40
5	A	559	HEA	C3A-C2A	4.08	1.45	1.40
10	A	571	LMT	O1'-C1'	4.27	1.47	1.40
10	A	568	LMT	O1'-C1'	4.36	1.48	1.40
10	A	575	LMT	O1'-C1'	4.38	1.48	1.40
5	A	559	HEA	C3C-C2C	4.43	1.46	1.40
10	A	574	LMT	O1'-C1'	4.55	1.48	1.40
10	D	121	LMT	O1'-C1'	4.65	1.48	1.40
5	A	560	HEA	C3A-C2A	5.31	1.47	1.40
10	B	277[B]	LMT	O1'-C1'	5.47	1.50	1.40
10	B	277[A]	LMT	O1'-C1'	5.47	1.50	1.40
5	A	560	HEA	OMA-CMA	6.37	1.41	1.21
5	A	559	HEA	OMA-CMA	6.48	1.42	1.21
5	A	560	HEA	C22-C23	7.12	1.54	1.32
5	A	559	HEA	C22-C23	8.00	1.56	1.32
5	A	560	HEA	C3C-C2C	8.39	1.51	1.40
5	A	559	HEA	C14-C15	8.89	1.50	1.33
10	A	575	LMT	O6B-C6B	8.98	1.81	1.42
5	A	559	HEA	C18-C19	9.50	1.51	1.33
5	A	560	HEA	C18-C19	9.86	1.52	1.33
5	A	560	HEA	C14-C15	13.05	1.58	1.33

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	560	HEA	C13-C12-C11	-18.42	90.03	114.51
5	A	559	HEA	C17-C18-C19	-10.86	104.14	127.76
5	A	560	HEA	C27-C19-C18	-9.79	104.27	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	559	HEA	C16-C15-C14	-9.70	102.64	121.05
5	A	560	HEA	C13-C14-C15	-8.76	108.71	127.76
5	A	559	HEA	C12-C13-C14	-8.33	89.08	112.40
5	A	559	HEA	C13-C14-C15	-7.24	112.01	127.76
5	A	560	HEA	C26-C15-C14	-6.58	110.58	123.50
5	A	559	HEA	CAA-CBA-CGA	-6.57	100.70	112.75
5	A	559	HEA	C27-C19-C18	-6.18	111.36	123.50
5	A	559	HEA	C13-C12-C11	-6.09	106.42	114.51
5	A	560	HEA	CAD-CBD-CGD	-6.08	101.61	112.75
5	A	560	HEA	CAA-CBA-CGA	-5.68	102.33	112.75
5	A	559	HEA	C20-C19-C18	-5.25	111.09	121.05
5	A	560	HEA	OMA-CMA-C3A	-5.07	114.86	125.11
5	A	559	HEA	C27-C19-C20	-5.00	107.77	115.41
5	A	559	HEA	C26-C15-C14	-4.82	114.03	123.50
5	A	560	HEA	C26-C15-C16	-4.62	108.34	115.41
5	A	559	HEA	C26-C15-C16	-4.43	108.64	115.41
5	A	559	HEA	CMC-C2C-C1C	-4.35	121.17	128.36
10	D	121	LMT	C1B-O5B-C5B	-4.30	105.40	113.75
5	A	560	HEA	C17-C18-C19	-4.13	118.78	127.76
5	A	560	HEA	C1A-C2A-C3A	-4.13	102.94	107.07
10	A	569	LMT	C1'-C2'-C3'	-4.03	102.03	109.97
10	B	277[B]	LMT	C1'-O5'-C5'	-4.03	105.92	113.75
10	B	277[A]	LMT	C1'-O5'-C5'	-4.03	105.92	113.75
9	B	274	LDA	CM2-N1-CM1	-3.90	104.43	108.83
5	A	559	HEA	CBD-CAD-C3D	-3.80	105.72	112.53
5	A	560	HEA	C17-C16-C15	-3.58	101.05	112.71
5	A	559	HEA	C24-C23-C22	-3.58	111.10	122.61
10	A	570	LMT	C1B-O5B-C5B	-3.50	106.94	113.75
10	B	279	LMT	C1'-O5'-C5'	-3.47	107.01	113.75
5	A	560	HEA	C4B-C3B-C11	-3.11	123.63	127.01
10	A	575	LMT	O6B-C6B-C5B	-3.07	101.20	111.33
10	B	278	LMT	C1B-O5B-C5B	-3.07	107.79	113.75
10	B	278	LMT	C1'-C2'-C3'	-2.99	104.08	109.97
10	A	569	LMT	C2'-C3'-C4'	-2.97	103.08	109.60
10	B	278	LMT	O5B-C1B-C2B	-2.88	104.37	110.28
5	A	560	HEA	C21-C22-C23	-2.83	116.84	127.73
5	A	560	HEA	C25-C23-C22	-2.74	113.78	122.61
5	A	560	HEA	C24-C23-C22	-2.73	113.81	122.61
5	A	559	HEA	O11-C11-C12	-2.67	103.22	109.73
10	A	573	LMT	C1'-O5'-C5'	-2.63	108.64	113.75
10	B	277[B]	LMT	C6B-C5B-C4B	-2.59	106.62	113.02
10	B	277[A]	LMT	C6B-C5B-C4B	-2.59	106.62	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	559	HEA	C21-C20-C19	-2.55	104.41	112.71
10	B	279	LMT	C1B-O5B-C5B	-2.55	108.80	113.75
9	A	565	LDA	CM2-N1-CM1	-2.49	106.02	108.83
9	A	566	LDA	O1-N1-CM2	-2.49	105.73	109.05
10	A	569	LMT	C3-C2-C1	-2.40	102.76	113.47
5	A	560	HEA	C20-C19-C18	-2.36	116.57	121.05
10	B	278	LMT	O1B-C1B-O5B	-2.35	104.73	110.68
5	A	559	HEA	OMA-CMA-C3A	-2.34	120.39	125.11
5	A	559	HEA	C21-C22-C23	-2.33	118.75	127.73
5	A	560	HEA	CMC-C2C-C1C	-2.12	124.86	128.36
10	A	571	LMT	C3B-C4B-C5B	-2.10	106.54	110.20
10	A	570	LMT	O5'-C5'-C6'	-2.08	101.11	106.36
10	A	575	LMT	C1B-C2B-C3B	2.02	113.95	109.97
10	D	121	LMT	C1'-O5'-C5'	2.06	117.75	113.75
10	D	121	LMT	C3'-C4'-C5'	2.07	115.51	110.84
10	A	571	LMT	C4-C3-C2	2.09	125.33	114.53
10	D	121	LMT	O5B-C5B-C4B	2.10	113.62	109.68
10	B	278	LMT	O3'-C3'-C4'	2.13	114.90	109.87
5	A	560	HEA	CBA-CAA-C2A	2.14	116.36	112.53
5	A	560	HEA	C20-C21-C22	2.15	117.31	111.69
10	B	278	LMT	O2B-C2B-C3B	2.15	115.17	110.34
10	A	568	LMT	O5'-C5'-C4'	2.19	114.37	109.75
10	D	121	LMT	O1B-C1B-C2B	2.20	113.45	108.10
10	B	278	LMT	O5B-C5B-C6B	2.20	111.93	106.36
10	A	569	LMT	O4'-C4B-C5B	2.23	115.16	109.24
10	A	569	LMT	C4-C3-C2	2.26	126.19	114.53
10	B	279	LMT	O5'-C5'-C6'	2.31	112.20	106.36
10	A	569	LMT	C1B-C2B-C3B	2.32	114.55	109.97
10	A	574	LMT	O1B-C1B-C2B	2.33	113.77	108.10
5	A	560	HEA	CMB-C2B-C1B	2.33	132.22	128.36
10	A	569	LMT	O5B-C1B-C2B	2.34	115.07	110.28
10	A	571	LMT	O5B-C1B-C2B	2.37	115.13	110.28
10	D	121	LMT	O5'-C5'-C4'	2.41	114.84	109.75
10	A	570	LMT	O1B-C1B-C2B	2.42	113.99	108.10
5	A	559	HEA	CMB-C2B-C3B	2.45	130.14	125.14
10	A	569	LMT	O1'-C1-C2	2.47	119.71	109.88
10	D	121	LMT	O1'-C1'-C2'	2.48	111.18	108.04
10	B	277[B]	LMT	O1B-C1B-O5B	2.50	117.01	110.68
10	B	277[A]	LMT	O1B-C1B-O5B	2.50	117.01	110.68
10	A	569	LMT	O1B-C1B-C2B	2.51	114.21	108.10
10	B	278	LMT	C2'-C3'-C4'	2.59	115.29	109.60
10	A	569	LMT	O5'-C5'-C4'	2.60	115.23	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	573	LMT	O1B-C1B-C2B	2.61	114.46	108.10
10	B	278	LMT	O2'-C2'-C1'	2.62	115.76	110.02
10	A	575	LMT	O1B-C4'-C3'	2.63	113.94	107.17
10	A	568	LMT	O1'-C1'-C2'	2.64	111.37	108.04
10	B	277[B]	LMT	O5B-C5B-C6B	2.67	113.11	106.36
10	B	277[A]	LMT	O5B-C5B-C6B	2.67	113.11	106.36
10	B	277[B]	LMT	C1'-C2'-C3'	2.70	115.30	109.97
10	B	277[A]	LMT	C1'-C2'-C3'	2.70	115.30	109.97
10	A	575	LMT	O1'-C1'-C2'	2.72	111.48	108.04
10	A	571	LMT	C3'-C4'-C5'	2.75	117.05	110.84
10	D	121	LMT	C2'-C3'-C4'	2.79	115.73	109.60
10	A	572	LMT	O5'-C5'-C4'	2.89	115.85	109.75
10	A	572	LMT	O2B-C2B-C1B	2.92	116.42	110.02
5	A	559	HEA	C4B-C3B-C11	2.93	130.19	127.01
10	A	575	LMT	O1B-C1B-C2B	3.00	115.40	108.10
10	A	568	LMT	O1B-C1B-C2B	3.09	115.61	108.10
10	A	574	LMT	C3'-C4'-C5'	3.09	117.82	110.84
5	A	560	HEA	CAD-C3D-C4D	3.10	130.37	127.01
5	A	560	HEA	C16-C15-C14	3.13	126.98	121.05
10	B	279	LMT	O1'-C1'-C2'	3.17	112.05	108.04
10	A	575	LMT	C3B-C4B-C5B	3.24	115.85	110.20
5	A	560	HEA	CAA-C2A-C1A	3.33	130.63	127.01
10	A	573	LMT	C1'-C2'-C3'	3.39	116.64	109.97
10	A	571	LMT	C2'-C3'-C4'	3.46	117.20	109.60
10	A	574	LMT	C2'-C3'-C4'	3.59	117.49	109.60
10	A	569	LMT	O3'-C3'-C4'	3.64	118.48	109.87
10	B	277[B]	LMT	O5B-C5B-C4B	3.71	116.65	109.68
10	B	277[A]	LMT	O5B-C5B-C4B	3.71	116.65	109.68
10	A	572	LMT	O1B-C1B-C2B	3.76	117.26	108.10
10	B	279	LMT	C1-O1'-C1'	3.84	120.66	113.94
10	A	570	LMT	O1B-C4'-C5'	3.93	119.66	109.32
10	A	574	LMT	O5'-C5'-C4'	3.94	118.07	109.75
10	A	575	LMT	O5B-C5B-C4B	3.99	117.17	109.68
10	A	573	LMT	O1'-C1'-C2'	4.01	113.10	108.04
5	A	560	HEA	CMC-C2C-C3C	4.18	133.26	125.09
10	A	568	LMT	C1-O1'-C1'	4.31	121.48	113.94
10	A	573	LMT	C2'-C3'-C4'	4.58	119.65	109.60
10	D	121	LMT	C3B-C4B-C5B	4.65	118.30	110.20
10	B	277[A]	LMT	C1-O1'-C1'	4.78	122.29	113.94
10	D	121	LMT	C1B-C2B-C3B	4.78	119.40	109.97
10	B	277[B]	LMT	C3B-C4B-C5B	4.82	118.60	110.20
10	B	277[A]	LMT	C3B-C4B-C5B	4.82	118.60	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	572	LMT	C1-O1'-C1'	4.87	122.45	113.94
5	A	559	HEA	O11-C11-C3B	5.13	126.96	111.82
10	D	121	LMT	C4B-C3B-C2B	5.26	120.60	110.79
10	A	574	LMT	C1-O1'-C1'	5.32	123.25	113.94
10	A	569	LMT	O2'-C2'-C1'	5.40	121.87	110.02
10	A	575	LMT	C1-O1'-C1'	5.43	123.44	113.94
10	A	571	LMT	C1-O1'-C1'	5.47	123.51	113.94
10	A	572	LMT	O1'-C1'-C2'	5.49	114.98	108.04
5	A	560	HEA	C12-C13-C14	5.54	127.91	112.40
10	A	570	LMT	C1-O1'-C1'	5.82	124.11	113.94
10	A	574	LMT	O1'-C1'-C2'	5.87	115.45	108.04
10	A	573	LMT	C1-O1'-C1'	6.04	124.50	113.94
5	A	559	HEA	CMC-C2C-C3C	6.05	136.93	125.09
5	A	559	HEA	CBA-CAA-C2A	6.55	124.27	112.53
10	B	278	LMT	O1'-C1'-C2'	6.89	116.75	108.04
10	D	121	LMT	C1-O1'-C1'	7.48	127.02	113.94
10	B	277[B]	LMT	O1'-C1'-C2'	7.65	117.70	108.04
10	B	277[A]	LMT	O1'-C1'-C2'	7.65	117.70	108.04
10	A	569	LMT	O1'-C1'-C2'	8.07	118.23	108.04
5	A	559	HEA	C12-C11-C3B	8.29	129.75	112.59
5	A	560	HEA	C12-C11-C3B	9.78	132.82	112.59

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	560	HEA	C11
5	A	560	HEA	ND
5	A	560	HEA	NA
5	A	560	HEA	NB
5	A	559	HEA	C11
5	A	559	HEA	ND
5	A	559	HEA	NA
5	A	559	HEA	NB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	574	LMT	C1-O1'-C1'-O5'

There are no ring outliers.

20 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	559	HEA	8	0
5	A	560	HEA	16	0
9	A	564	LDA	1	0
9	A	565	LDA	1	0
9	A	566	LDA	3	0
10	A	568	LMT	2	0
10	A	569	LMT	2	0
10	A	570	LMT	3	0
10	A	571	LMT	3	0
10	A	572	LMT	3	0
10	A	574	LMT	9	0
10	A	575	LMT	5	0
9	B	272	LDA	4	0
9	B	273	LDA	3	0
9	B	274	LDA	4	0
9	B	275	LDA	4	0
9	B	276	LDA	1	0
10	B	278	LMT	2	0
10	B	279	LMT	6	0
10	D	121	LMT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	530/558 (94%)	-0.11	28 (5%) 30 39	41, 55, 79, 125	0
2	B	253/298 (84%)	-0.41	4 (1%) 74 80	36, 50, 70, 86	0
3	C	119/127 (93%)	0.22	11 (9%) 11 16	39, 60, 82, 112	0
4	D	109/120 (90%)	-0.10	1 (0%) 85 89	42, 57, 71, 82	0
All	All	1011/1103 (91%)	-0.15	44 (4%) 38 47	36, 55, 77, 125	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	119	ALA	8.7
1	A	545	THR	8.2
1	A	17	GLY	7.3
1	A	18	PHE	6.7
1	A	546	LEU	6.6
3	C	118	SER	6.6
1	A	20	THR	6.1
1	A	19	PHE	5.1
1	A	177	TYR	4.1
1	A	544	GLU	4.0
1	A	251	PHE	3.8
1	A	541	HIS	3.5
2	B	1	GLN	3.3
1	A	259	ALA	3.3
3	C	117	SER	3.2
1	A	543	PHE	3.1
1	A	518	ASN	2.9
1	A	156	ASP	2.9
1	A	211	GLY	2.8
1	A	175	ALA	2.8
3	C	13	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLY	2.7
3	C	37	VAL	2.7
1	A	252	GLY	2.6
4	D	57	GLY	2.5
1	A	213	THR	2.5
1	A	69	GLY	2.5
1	A	129	ARG	2.5
3	C	36	TRP	2.4
1	A	21	ARG	2.4
3	C	48	VAL	2.3
1	A	362	MET	2.3
3	C	56	GLY	2.3
1	A	258	PRO	2.2
1	A	22	TRP	2.2
2	B	63	ARG	2.1
1	A	540	GLU	2.1
1	A	512	PHE	2.1
3	C	1	GLU	2.1
1	A	516	ARG	2.1
2	B	253	ASP	2.1
2	B	40	TYR	2.1
3	C	11	LEU	2.0
3	C	42	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	LMT	A	572	35/35	0.36	0.42	35.16	84,112,123,123	0
10	LMT	A	574	35/35	0.43	0.45	23.86	64,134,147,148	0
9	LDA	A	564	16/16	0.44	0.43	16.85	68,75,106,109	0
10	LMT	A	571	35/35	0.39	0.44	15.96	81,116,145,146	0
9	LDA	B	272	16/16	0.44	0.38	15.61	46,67,114,117	0
9	LDA	B	274	16/16	0.65	0.28	11.19	83,98,111,111	0
10	LMT	B	278	35/35	0.85	0.29	10.69	68,86,99,100	0
10	LMT	A	568	35/35	0.78	0.34	8.51	83,103,108,109	0
10	LMT	D	121	35/35	0.54	0.41	7.61	93,103,108,110	0
9	LDA	A	565	16/16	0.65	0.31	6.78	72,85,94,95	0
9	LDA	A	566	16/16	0.68	0.32	6.42	92,97,113,113	0
10	LMT	A	569	35/35	0.63	0.36	5.66	84,98,111,111	0
10	LMT	A	573	35/35	0.36	0.42	5.34	65,102,131,132	0
10	LMT	B	279	35/35	0.76	0.40	4.67	68,120,136,137	0
10	LMT	A	575	35/35	0.30	0.46	4.25	97,142,149,150	0
9	LDA	B	273	16/16	0.76	0.28	3.24	81,85,98,100	0
9	LDA	B	275	16/16	0.74	0.27	3.23	55,81,113,115	0
9	LDA	A	567	16/16	0.66	0.27	2.13	96,103,104,105	0
7	MG	A	562	1/1	0.98	0.15	2.05	28,28,28,28	0
10	LMT	A	570	35/35	0.70	0.27	1.65	69,104,122,125	0
5	HEA	A	559	60/60	0.95	0.16	1.58	37,47,51,56	0
5	HEA	A	560	60/60	0.96	0.13	0.60	34,52,54,62	0
6	CU	B	270	1/1	0.99	0.07	-0.92	48,48,48,48	0
6	CU	B	271	1/1	0.99	0.06	-1.75	50,50,50,50	0
8	CA	A	563	1/1	0.97	0.06	-2.88	53,53,53,53	0
9	LDA	B	276	16/16	0.48	0.41	-	121,128,130,130	0
6	CU	A	561	1/1	1.00	0.03	-	54,54,54,54	0
10	LMT	B	277[A]	35/35	0.85	0.28	-	67,81,87,88	12
10	LMT	B	277[B]	35/35	0.85	0.28	-	65,78,87,88	12
11	PER	A	576	2/2	0.99	0.10	-	49,49,49,56	0

6.5 Other polymers (i)

There are no such residues in this entry.