



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:05 pm GMT

PDB ID : 3HB3  
Title : High resolution crystal structure of Paracoccus denitrificans cytochrome c oxidase  
Authors : Koepke, J.; Angerer, H.; Peng, G.  
Deposited on : 2009-05-04  
Resolution : 2.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

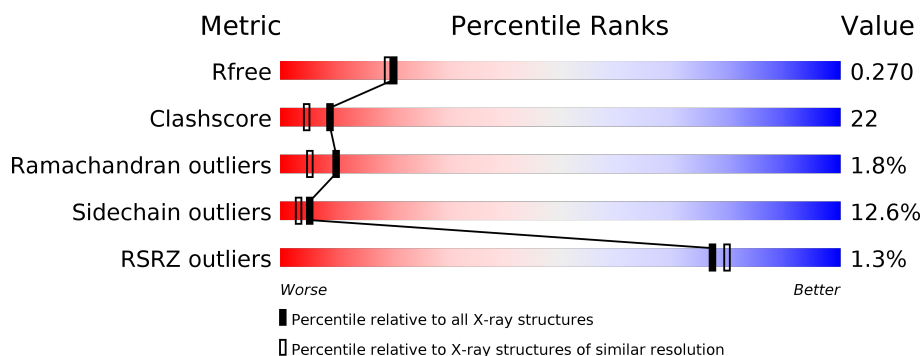
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
2	B	298	
3	C	127	
4	D	120	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	LMT	A	568	-	-	-	X
10	LMT	A	569	-	-	-	X
10	LMT	A	571[A]	-	-	-	X
10	LMT	A	571[B]	-	-	-	X
10	LMT	A	573[A]	-	-	-	X
10	LMT	A	573[B]	-	-	-	X
10	LMT	A	575[A]	-	-	-	X
10	LMT	A	575[B]	-	-	-	X
10	LMT	B	279	-	-	-	X
10	LMT	B	280	-	-	-	X
10	LMT	B	281	-	-	-	X
10	LMT	B	282[A]	-	-	-	X
10	LMT	B	282[B]	-	-	-	X
10	LMT	B	283[A]	-	-	-	X
10	LMT	B	283[B]	-	-	-	X
5	HEA	A	559	X	-	-	-
5	HEA	A	560	X	-	-	-
9	LDA	A	564	-	-	-	X
9	LDA	A	567	-	-	-	X
9	LDA	B	272	-	-	-	X
9	LDA	B	273	-	-	-	X
9	LDA	B	274	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9393 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	529	Total	C	N	O	S	0	3	0
			4200	2819	659	689	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	2	0
			1985	1300	320	357	8			

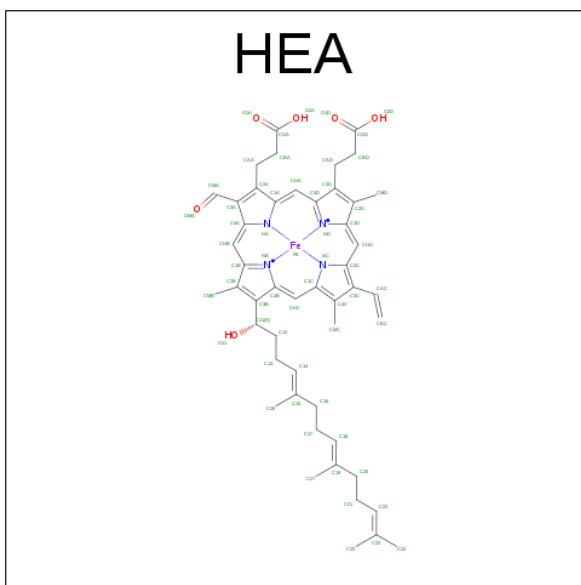
- Molecule 3 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	2	0
			940	591	158	185	6			

- Molecule 4 is a protein called ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	108	Total	C	N	O	S	0	0	0
			831	530	135	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	
			60	49	1	4	6	0
5	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

- Molecule 6 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

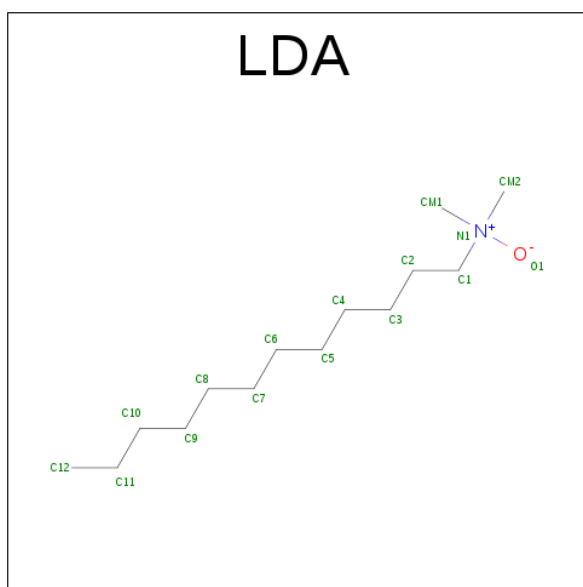
- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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

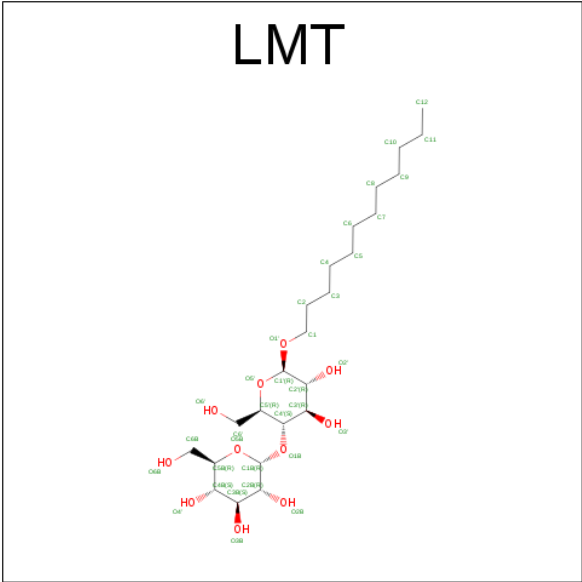
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca		
			1	1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



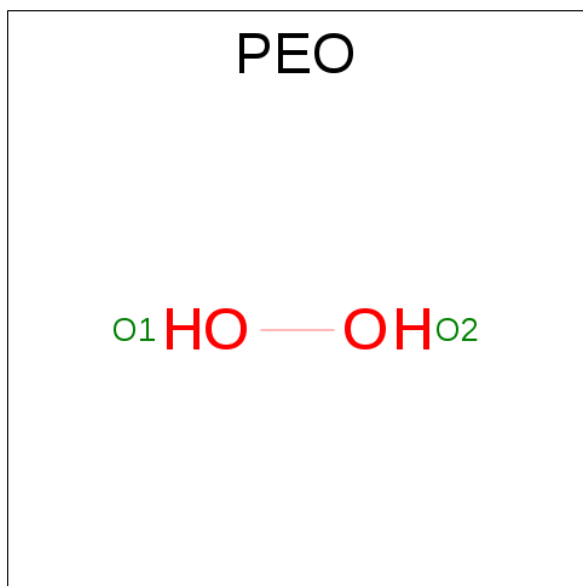
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	A	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1		
9	B	1	Total	C	N	O	0	0
			16	14	1	1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

- 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	0	0
			35	24	11		
10	A	1	Total	C	O	0	0
			35	24	11		
10	A	1	Total	C	O	0	0
			35	24	11		
10	A	1	Total	C	O	0	1
			47	30	17		
10	A	1	Total	C	O	0	1
			58	36	22		
10	A	1	Total	C	O	0	1
			47	30	17		
10	A	1	Total	C	O	0	1
			47	30	17		
10	B	1	Total	C	O	0	0
			35	24	11		
10	B	1	Total	C	O	0	0
			35	24	11		
10	B	1	Total	C	O	0	0
			35	24	11		
10	B	1	Total	C	O	0	1
			47	30	17		
10	B	1	Total	C	O	0	1
			58	36	22		

- Molecule 11 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula:  $\text{H}_2\text{O}_2$ ).



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

- Molecule 12 is water.

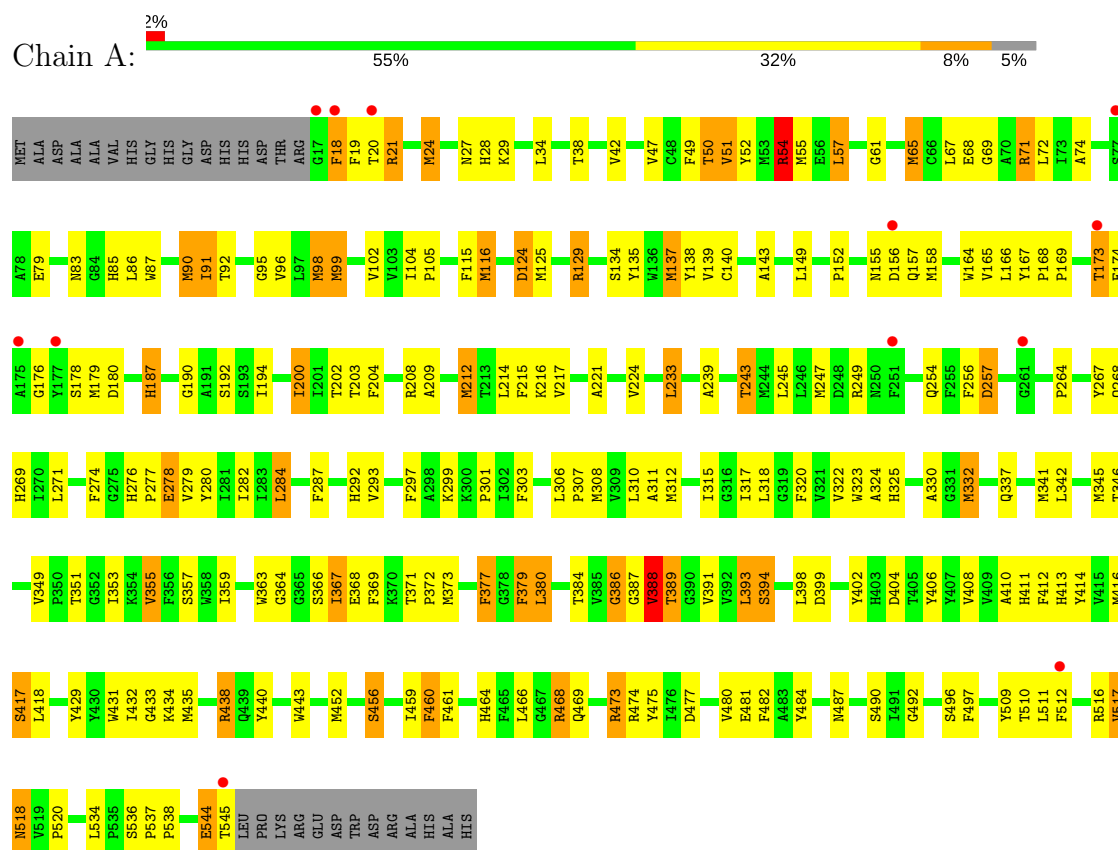
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	158	Total	O	0	0
			158	158		
12	B	228	Total	O	0	0
			228	228		
12	C	87	Total	O	0	0
			87	87		
12	D	81	Total	O	0	0
			81	81		



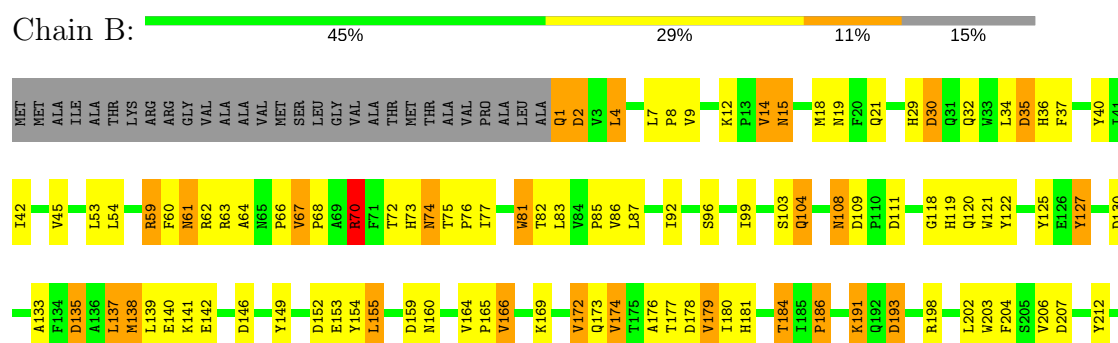
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Cytochrome c oxidase subunit 1-beta



#### • Molecule 2: Cytochrome c oxidase subunit 2

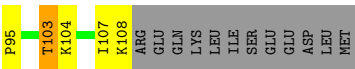
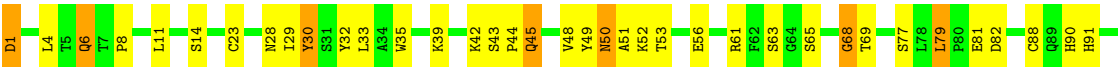




● Molecule 3: ANTIBODY FV FRAGMENT



● Molecule 4: ANTIBODY FV FRAGMENT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.40Å 150.47Å 157.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.25 19.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.98-2.25) 99.2 (19.98-2.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.218 , 0.280 0.211 , 0.270	Depositor DCC
$R_{free}$ test set	2819 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, CU1, CA, MN, LMT, PEO, HEA

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	1.40	19/4368 (0.4%)	1.23	29/5959 (0.5%)
2	B	1.65	18/2050 (0.9%)	1.48	34/2810 (1.2%)
3	C	1.27	0/972	1.20	3/1314 (0.2%)
4	D	1.35	4/852 (0.5%)	1.19	2/1156 (0.2%)
All	All	1.45	41/8242 (0.5%)	1.29	68/11239 (0.6%)

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
1	A	1	0
3	C	0	1
All	All	1	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	GLU	C-O	9.95	1.42	1.23
2	B	122	TYR	CD1-CE1	7.83	1.51	1.39
2	B	9	VAL	CB-CG2	-7.66	1.36	1.52
2	B	203	TRP	CB-CG	6.61	1.62	1.50
1	A	481	GLU	CD-OE2	-6.59	1.18	1.25
4	D	32	TYR	CG-CD1	6.51	1.47	1.39
2	B	212	TYR	CG-CD1	6.45	1.47	1.39
2	B	239	TYR	CD1-CE1	6.40	1.49	1.39
2	B	127	TYR	CE1-CZ	-6.30	1.30	1.38
1	A	367	ILE	CB-CG2	6.23	1.72	1.52
1	A	402	TYR	CD1-CE1	6.21	1.48	1.39
2	B	204	PHE	CD2-CE2	6.20	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	VAL	CB-CG2	6.20	1.65	1.52
4	D	32	TYR	CD1-CE1	6.17	1.48	1.39
2	B	226	TYR	CD1-CE1	6.11	1.48	1.39
2	B	149	TYR	CE2-CZ	6.05	1.46	1.38
1	A	280	TYR	CD2-CE2	5.86	1.48	1.39
1	A	379	PHE	CD1-CE1	5.74	1.50	1.39
1	A	215[A]	PHE	CD2-CE2	5.73	1.50	1.39
1	A	481	GLU	CD-OE1	5.72	1.31	1.25
2	B	172	VAL	CB-CG2	5.63	1.64	1.52
2	B	9	VAL	CB-CG1	5.57	1.64	1.52
1	A	394	SER	CA-CB	5.43	1.61	1.52
2	B	212	TYR	CE2-CZ	5.41	1.45	1.38
1	A	394	SER	CB-OG	5.37	1.49	1.42
1	A	278	GLU	CD-OE1	5.37	1.31	1.25
1	A	406	TYR	CE2-CZ	5.36	1.45	1.38
2	B	239	TYR	CD2-CE2	5.36	1.47	1.39
4	D	56	GLU	CD-OE2	5.33	1.31	1.25
1	A	460	PHE	CE2-CZ	5.29	1.47	1.37
1	A	386	GLY	C-O	5.17	1.31	1.23
4	D	6	GLN	CG-CD	5.17	1.62	1.51
1	A	349	VAL	CA-CB	5.16	1.65	1.54
1	A	353	ILE	C-O	5.13	1.33	1.23
2	B	155	LEU	N-CA	5.12	1.56	1.46
1	A	402	TYR	CB-CG	5.11	1.59	1.51
2	B	206	VAL	CA-CB	5.09	1.65	1.54
2	B	169	LYS	CE-NZ	5.09	1.61	1.49
1	A	355	VAL	CB-CG1	5.04	1.63	1.52
2	B	246	ALA	CA-CB	5.03	1.63	1.52
1	A	388	VAL	CB-CG1	-5.03	1.42	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH2	-14.55	113.02	120.30
1	A	477	ASP	CB-CG-OD2	9.46	126.81	118.30
1	A	473	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	71	ARG	NE-CZ-NH1	9.33	124.97	120.30
2	B	154	TYR	C-N-CA	-9.11	98.93	121.70
1	A	310	LEU	CB-CG-CD1	-8.98	95.74	111.00
2	B	166	VAL	CB-CA-C	-8.77	94.74	111.40
2	B	135	ASP	CB-CG-OD1	8.54	125.99	118.30
1	A	257	ASP	CB-CG-OD2	8.26	125.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ARG	NE-CZ-NH2	-8.13	116.23	120.30
2	B	111	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	71	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	99	MET	CG-SD-CE	-7.56	88.10	100.20
2	B	2	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	468	ARG	CG-CD-NE	-7.39	96.28	111.80
1	A	380	LEU	CB-CG-CD2	-7.29	98.60	111.00
1	A	399	ASP	CB-CG-OD2	7.10	124.69	118.30
2	B	130	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	55	MET	CG-SD-CE	-6.94	89.10	100.20
2	B	179	VAL	CG1-CB-CG2	6.79	121.77	110.90
2	B	35	ASP	CB-CG-OD2	6.75	124.37	118.30
2	B	154	TYR	O-C-N	-6.66	112.05	122.70
2	B	227	MET	CG-SD-CE	-6.61	89.62	100.20
1	A	473	ARG	NE-CZ-NH1	6.57	123.58	120.30
2	B	184	THR	OG1-CB-CG2	-6.54	94.96	110.00
2	B	70	ARG	NE-CZ-NH2	-6.52	117.04	120.30
3	C	90	ASP	CB-CG-OD2	6.46	124.12	118.30
2	B	59	ARG	NE-CZ-NH1	-6.41	117.10	120.30
2	B	152	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	54	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	B	66	PRO	N-CA-C	-6.20	95.99	112.10
2	B	137	LEU	CB-CG-CD2	6.18	121.51	111.00
1	A	124	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	380	LEU	CB-CG-CD1	6.16	121.47	111.00
4	D	1	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	90	MET	CG-SD-CE	-6.08	90.47	100.20
1	A	389	THR	CA-CB-CG2	6.07	120.90	112.40
2	B	146	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	215[A]	PHE	CB-CA-C	6.04	122.48	110.40
3	C	33	THR	N-CA-C	-6.04	94.70	111.00
2	B	30	ASP	CB-CG-OD1	5.99	123.69	118.30
2	B	207	ASP	CB-CG-OD1	5.97	123.67	118.30
2	B	178	ASP	CB-CG-OD1	5.96	123.66	118.30
2	B	109	ASP	CB-CG-OD2	5.90	123.61	118.30
2	B	174	VAL	CB-CA-C	5.72	122.26	111.40
1	A	388	VAL	CA-CB-CG1	5.68	119.42	110.90
1	A	280	TYR	CB-CA-C	5.67	121.74	110.40
1	A	310	LEU	CB-CG-CD2	5.62	120.56	111.00
2	B	179	VAL	CA-CB-CG1	5.54	119.21	110.90
1	A	212	MET	CG-SD-CE	5.46	108.93	100.20
1	A	61	GLY	N-CA-C	-5.42	99.55	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	155	LEU	CB-CG-CD1	-5.38	101.85	111.00
2	B	232	LYS	CD-CE-NZ	-5.26	99.61	111.70
2	B	193	ASP	CB-CG-OD1	5.20	122.98	118.30
2	B	15[A]	ASN	N-CA-CB	5.20	119.95	110.60
2	B	15[B]	ASN	N-CA-CB	5.20	119.95	110.60
3	C	9	GLY	N-CA-C	-5.17	100.17	113.10
2	B	228	PRO	N-CD-CG	5.17	110.96	103.20
1	A	318	LEU	CA-CB-CG	5.15	127.14	115.30
2	B	178	ASP	OD1-CG-OD2	-5.13	113.56	123.30
1	A	284	LEU	CB-CG-CD2	5.11	119.69	111.00
2	B	231	VAL	N-CA-C	-5.10	97.24	111.00
2	B	82	THR	OG1-CB-CG2	-5.09	98.29	110.00
1	A	408	VAL	CA-CB-CG2	5.04	118.46	110.90
2	B	154	TYR	CA-C-N	5.04	128.28	117.20
4	D	90	HIS	N-CA-C	-5.03	97.41	111.00
1	A	408	VAL	CG1-CB-CG2	5.03	118.94	110.90
2	B	191	LYS	N-CA-C	-5.01	97.47	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	389	THR	CB

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	4200	0	4124	231	0
2	B	1985	0	1967	99	0
3	C	940	0	898	47	0
4	D	831	0	807	24	0
5	A	120	0	104	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	96	0	186	8	0
10	A	351	0	234	19	0
10	B	245	0	221	9	0
11	A	2	0	0	0	0
12	A	158	0	0	11	0
12	B	228	0	0	13	0
12	C	87	0	0	10	0
12	D	81	0	0	2	0
All	All	9393	0	8665	398	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 22.

All (398) 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	1.80	1.53
1:A:312:MET:SD	1:A:312:MET:CE	2.01	1.47
1:A:65:MET:SD	1:A:65:MET:CE	2.04	1.46
1:A:373:MET:SD	1:A:373:MET:CE	2.03	1.45
1:A:254:GLN:HB3	1:A:257:ASP:HB3	1.27	1.12
1:A:545:THR:HB	12:A:637:HOH:O	1.49	1.09
1:A:518:ASN:N	1:A:518:ASN:HD22	1.53	1.06
1:A:389:THR:HG21	12:A:852:HOH:O	1.55	1.04
4:D:45:GLN:HG3	12:D:1196:HOH:O	1.62	0.99
4:D:28:ASN:OD1	4:D:68:GLY:HA2	1.62	0.97
1:A:83:ASN:HD21	1:A:157:GLN:HE22	1.02	0.95
2:B:1:GLN:N	12:B:1235:HOH:O	1.95	0.95
1:A:72:LEU:HD23	9:A:567:LDA:H52	1.50	0.92
3:C:93:MET:HE3	3:C:93:MET:HA	1.51	0.91
2:B:227:MET:N	2:B:228:PRO:HD3	1.84	0.91
1:A:518:ASN:ND2	1:A:518:ASN:H	1.68	0.90
1:A:98:MET:HG3	5:A:559:HEA:C3C	2.03	0.89
1:A:239:ALA:O	1:A:243:THR:HG23	1.74	0.88
1:A:369:PHE:H	10:A:573[B]:LMT:H4B	1.39	0.88
1:A:518:ASN:HD22	1:A:518:ASN:H	0.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:HD21	1:A:157:GLN:NE2	1.74	0.85
1:A:102:VAL:O	1:A:105:PRO:HD2	1.76	0.85
2:B:227:MET:HG2	2:B:227:MET:O	1.77	0.83
3:C:31:SER:OG	12:C:1225:HOH:O	1.97	0.82
2:B:40:TYR:HE1	9:B:274:LDA:H31	1.43	0.80
2:B:227:MET:N	2:B:228:PRO:CD	2.44	0.79
1:A:487:ASN:ND2	10:A:572[B]:LMT:O6'	2.12	0.79
1:A:243:THR:O	1:A:247:MET:HG3	1.83	0.78
1:A:187:HIS:CE1	1:A:243:THR:HG22	2.19	0.78
1:A:83:ASN:ND2	1:A:157:GLN:HE22	1.81	0.77
1:A:342:LEU:HA	1:A:345:MET:HE2	1.66	0.75
1:A:54:ARG:HD3	1:A:490:SER:OG	1.86	0.74
3:C:93:MET:CE	3:C:93:MET:HA	2.16	0.74
1:A:468:ARG:NH2	2:B:35:ASP:OD2	2.20	0.74
4:D:6:GLN:HG2	4:D:103:THR:HG22	1.69	0.73
5:A:560:HEA:HHC	5:A:560:HEA:O11	1.88	0.73
1:A:57:LEU:CD2	1:A:87:TRP:HH2	2.01	0.73
4:D:50:ASN:O	4:D:52:LYS:N	2.20	0.73
2:B:227:MET:H	2:B:228:PRO:HD3	1.54	0.73
1:A:337:GLN:HE22	2:B:104:GLN:HE21	1.37	0.73
1:A:342:LEU:HA	1:A:345:MET:CE	2.19	0.73
1:A:27:ASN:HD21	1:A:29[B]:LYS:HB2	1.55	0.71
1:A:190:GLY:O	1:A:194:ILE:HG13	1.90	0.71
1:A:518:ASN:ND2	1:A:518:ASN:N	2.30	0.71
3:C:62:ASP:HB2	12:C:1238:HOH:O	1.90	0.71
1:A:308:MET:HE1	1:A:357:SER:HB2	1.73	0.70
2:B:138:MET:HE1	2:B:226:TYR:HB3	1.73	0.70
1:A:245:LEU:O	1:A:249:ARG:HG3	1.92	0.69
2:B:135:ASP:OD2	12:B:1284:HOH:O	2.10	0.69
4:D:6:GLN:HE21	4:D:103:THR:HG23	1.57	0.69
1:A:57:LEU:HD21	1:A:87:TRP:CH2	2.28	0.69
1:A:57:LEU:CD2	1:A:87:TRP:CH2	2.77	0.68
1:A:98:MET:HB3	5:A:559:HEA:CAC	2.23	0.68
1:A:452:MET:O	1:A:456:SER:HB2	1.94	0.68
1:A:254:GLN:CB	1:A:257:ASP:HB3	2.17	0.67
1:A:91:ILE:HD12	1:A:92:THR:N	2.09	0.67
1:A:452:MET:HE1	5:A:559:HEA:H161	1.77	0.66
2:B:32:GLN:OE1	12:B:610:HOH:O	2.13	0.66
1:A:269:HIS:HD2	1:A:323:TRP:HE1	1.41	0.66
1:A:57:LEU:HD22	1:A:87:TRP:HH2	1.60	0.66
1:A:152:PRO:O	1:A:176:GLY:HA3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:THR:HG23	12:C:925:HOH:O	1.94	0.66
3:C:91:THR:CG2	3:C:116:VAL:H	2.08	0.65
1:A:20:THR:HA	1:A:24:MET:HB2	1.78	0.65
1:A:469:GLN:HE22	2:B:14:VAL:H	1.44	0.65
2:B:74:ASN:HB2	10:B:281:LMT:H12	1.78	0.65
1:A:418:LEU:N	1:A:418:LEU:HD12	2.12	0.65
3:C:9:GLY:HA3	12:C:935:HOH:O	1.96	0.65
4:D:8:PRO:O	4:D:103:THR:HB	1.96	0.65
3:C:91:THR:HB	3:C:115:THR:HA	1.79	0.64
1:A:342:LEU:HD23	1:A:345:MET:CE	2.27	0.64
1:A:187:HIS:HE1	1:A:243:THR:HG22	1.62	0.63
5:A:559:HEA:HMB1	5:A:559:HEA:O11	1.96	0.63
3:C:93:MET:HE1	3:C:112:THR:N	2.13	0.63
4:D:29:ILE:O	4:D:30:TYR:HB2	1.98	0.63
3:C:70:ILE:O	12:C:918:HOH:O	2.16	0.63
1:A:413:HIS:CG	1:A:460:PHE:CE1	2.86	0.63
1:A:284:LEU:O	1:A:287:PHE:HB2	1.99	0.62
1:A:307:PRO:HB2	12:A:1014:HOH:O	1.99	0.62
1:A:366:SER:OG	2:B:62:ARG:HG3	2.00	0.62
3:C:32:TYR:CD2	3:C:98:ARG:HD2	2.34	0.62
5:A:559:HEA:HBC1	5:A:559:HEA:HMC1	1.81	0.62
3:C:40:THR:HB	3:C:41:PRO:CD	2.30	0.61
4:D:33:LEU:HD21	4:D:88:CYS:HB2	1.82	0.61
2:B:180:ILE:HG22	2:B:218:GLU:HG2	1.82	0.61
1:A:484:TYR:H	2:B:15[A]:ASN:HD21	1.49	0.61
1:A:155:ASN:HD21	2:B:222:ILE:HB	1.65	0.61
12:B:307:HOH:O	4:D:30:TYR:HA	1.99	0.61
4:D:50:ASN:H	4:D:91:HIS:CE1	2.20	0.60
1:A:379:PHE:C	1:A:379:PHE:CD1	2.74	0.60
1:A:54:ARG:HD2	1:A:490:SER:HA	1.84	0.60
1:A:308:MET:HE2	1:A:357:SER:HB3	1.84	0.60
2:B:164:VAL:O	2:B:233:ALA:HA	2.02	0.60
1:A:301:PRO:HG2	2:B:72:THR:HG22	1.84	0.60
2:B:70:ARG:HB3	12:B:659:HOH:O	2.01	0.60
3:C:35:SER:OG	3:C:50:SER:OG	2.17	0.59
4:D:4:LEU:HD22	4:D:23:CYS:SG	2.43	0.59
1:A:27:ASN:HD21	1:A:29[C]:LYS:HB2	1.67	0.59
3:C:47:TRP:CZ2	4:D:95:PRO:HB3	2.38	0.59
3:C:93:MET:HE1	3:C:112:THR:CA	2.33	0.59
9:A:564:LDA:H12	10:A:572[A]:LMT:H5'	1.83	0.59
1:A:440:TYR:HA	1:A:510:THR:OG1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HD22	2:B:222:ILE:HD12	1.67	0.58
1:A:342:LEU:HD23	1:A:345:MET:HE3	1.84	0.58
4:D:35:TRP:HB2	4:D:48:VAL:HG13	1.85	0.58
2:B:181:HIS:HB3	2:B:216:CYS:SG	2.43	0.58
4:D:6:GLN:HG2	4:D:103:THR:CG2	2.32	0.58
1:A:413:HIS:CD2	1:A:460:PHE:CZ	2.91	0.58
3:C:91:THR:HG22	3:C:116:VAL:H	1.67	0.58
1:A:412:PHE:CD2	5:A:560:HEA:HAD1	2.38	0.58
1:A:129:ARG:HB3	10:A:574[A]:LMT:H6'1	1.86	0.58
1:A:21:ARG:NH1	10:A:570:LMT:H4B	2.19	0.58
1:A:268:GLN:NE2	12:A:1110:HOH:O	2.36	0.57
4:D:50:ASN:H	4:D:91:HIS:HE1	1.50	0.57
1:A:269:HIS:CD2	1:A:323:TRP:HE1	2.23	0.57
5:A:559:HEA:H122	5:A:559:HEA:HHC	1.85	0.57
2:B:36:HIS:CD2	9:B:273:LDA:HM23	2.39	0.57
1:A:27:ASN:ND2	1:A:29[B]:LYS:HB2	2.20	0.57
1:A:371:THR:HG21	1:A:429:TYR:CD1	2.40	0.57
2:B:36:HIS:HD2	9:B:273:LDA:HM23	1.68	0.57
1:A:158:MET:HG2	12:A:1038:HOH:O	2.05	0.57
3:C:93:MET:HE1	3:C:112:THR:C	2.25	0.57
1:A:18:PHE:O	1:A:20:THR:N	2.38	0.56
3:C:99:HIS:HD2	3:C:104:ALA:O	1.88	0.56
1:A:511:LEU:HD21	10:A:570:LMT:H22	1.88	0.56
1:A:393:LEU:C	5:A:560:HEA:HMA	2.26	0.56
3:C:93:MET:CE	3:C:112:THR:C	2.73	0.56
1:A:355:VAL:O	1:A:359:ILE:HG13	2.06	0.56
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.88	0.55
2:B:141:LYS:HE2	12:B:1156:HOH:O	2.05	0.55
1:A:85:HIS:CD2	1:A:157:GLN:HB3	2.42	0.55
1:A:52:TYR:HD2	1:A:90:MET:HE2	1.71	0.55
9:B:273:LDA:HM21	9:B:276:LDA:HM21	1.88	0.55
1:A:105:PRO:HD3	12:A:969:HOH:O	2.06	0.55
1:A:116:MET:HE3	1:A:200:ILE:HG23	1.88	0.55
1:A:297:PHE:O	1:A:367:ILE:HA	2.05	0.55
1:A:337:GLN:HE22	2:B:104:GLN:NE2	2.03	0.55
1:A:398:LEU:CD1	2:B:34:LEU:HD23	2.36	0.55
5:A:560:HEA:H22	2:B:45:VAL:HG11	1.89	0.55
2:B:138:MET:HB2	2:B:228:PRO:HD2	1.89	0.55
3:C:44:ARG:HG2	12:C:1236:HOH:O	2.07	0.55
1:A:473:ARG:O	1:A:474:ARG:HB2	2.07	0.55
3:C:76:LYS:HD3	12:C:813:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:HB3	10:A:571[A]:LMT:H4B	1.88	0.54
1:A:57:LEU:HD22	1:A:87:TRP:CH2	2.41	0.54
12:A:1324:HOH:O	2:B:198:ARG:HD3	2.08	0.54
2:B:227:MET:CG	2:B:227:MET:O	2.50	0.54
3:C:19[A]:LYS:HE2	12:C:907:HOH:O	2.08	0.54
1:A:50:THR:HG23	5:A:559:HEA:HMB3	1.90	0.54
1:A:475:TYR:HE1	2:B:224:HIS:NE2	2.06	0.54
2:B:81:TRP:CE3	10:B:281:LMT:C12	2.90	0.54
2:B:73:HIS:HB2	12:B:1057:HOH:O	2.08	0.54
1:A:308:MET:CE	1:A:357:SER:HB2	2.36	0.54
1:A:413:HIS:CD2	1:A:460:PHE:CE1	2.96	0.54
3:C:27:PHE:CE2	3:C:29:PHE:HA	2.43	0.54
2:B:29:HIS:HD2	12:B:863:HOH:O	1.90	0.54
3:C:93:MET:HE1	3:C:111:GLY:C	2.29	0.53
1:A:99:MET:HE3	1:A:282:ILE:HD11	1.91	0.53
1:A:91:ILE:HD12	1:A:91:ILE:C	2.28	0.53
2:B:138:MET:CE	2:B:226:TYR:HB3	2.39	0.53
1:A:135:TYR:O	1:A:139:VAL:HG23	2.09	0.53
1:A:308:MET:CE	1:A:357:SER:CB	2.86	0.53
2:B:81:TRP:CE3	10:B:281:LMT:H121	2.43	0.53
1:A:393:LEU:CB	5:A:560:HEA:HMA	2.39	0.52
1:A:387:GLY:HA3	5:A:560:HEA:C15	2.40	0.52
1:A:116:MET:HE1	1:A:204:PHE:HB2	1.91	0.52
1:A:239:ALA:O	1:A:243:THR:CG2	2.50	0.52
3:C:35:SER:OG	3:C:99:HIS:HE1	1.92	0.52
1:A:116:MET:CE	1:A:200:ILE:HG23	2.39	0.52
2:B:118:GLY:H	2:B:176:ALA:HA	1.74	0.52
2:B:108:ASN:H	2:B:108:ASN:ND2	2.07	0.52
2:B:61:ASN:HD22	2:B:61:ASN:C	2.13	0.52
1:A:464:HIS:O	1:A:468:ARG:HG3	2.10	0.52
1:A:475:TYR:CE1	2:B:224:HIS:CD2	2.98	0.51
5:A:559:HEA:C12	5:A:559:HEA:HHC	2.41	0.51
2:B:172:VAL:HG12	2:B:174:VAL:HG12	1.93	0.51
1:A:208:ARG:HG2	1:A:212:MET:HG2	1.90	0.51
5:A:560:HEA:HMC1	5:A:560:HEA:HBC1	1.91	0.51
1:A:417:SER:HB2	5:A:559:HEA:HMC2	1.91	0.51
2:B:81:TRP:HE3	10:B:281:LMT:C12	2.23	0.51
1:A:278:GLU:O	1:A:282:ILE:HG13	2.10	0.51
1:A:276:HIS:O	1:A:279:VAL:HG22	2.11	0.51
2:B:21:GLN:NE2	12:B:295:HOH:O	2.41	0.51
1:A:369:PHE:HB2	10:A:573[B]:LMT:H6'2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:ASP:OD1	2:B:160:ASN:N	2.43	0.51
3:C:22:CYS:HB3	3:C:79:LEU:HB3	1.92	0.51
2:B:1:GLN:HA	2:B:1:GLN:OE1	2.11	0.51
1:A:364:GLY:HA2	2:B:60:PHE:CE1	2.47	0.51
1:A:165:VAL:HB	1:A:271:LEU:HD21	1.92	0.50
1:A:330:ALA:HA	2:B:193:ASP:OD2	2.11	0.50
1:A:52:TYR:HD2	1:A:90:MET:CE	2.24	0.50
1:A:473:ARG:HG3	1:A:474:ARG:HD2	1.92	0.50
1:A:47:VAL:O	1:A:51:VAL:HG23	2.12	0.50
2:B:19:ASN:HD21	9:B:272:LDA:H21	1.76	0.50
3:C:88:SER:O	3:C:91:THR:HG23	2.12	0.50
3:C:93:MET:CE	3:C:112:THR:N	2.74	0.50
1:A:38:THR:CG2	1:A:138:TYR:CE2	2.94	0.50
1:A:65:MET:CE	1:A:65:MET:CG	2.88	0.50
1:A:125:MET:HA	1:A:125:MET:HE3	1.93	0.49
3:C:101:TYR:HB3	4:D:49:TYR:CD2	2.46	0.49
2:B:138:MET:SD	2:B:155:LEU:HD23	2.52	0.49
2:B:155:LEU:HD21	2:B:226:TYR:CE1	2.47	0.49
1:A:418:LEU:N	1:A:418:LEU:CD1	2.74	0.49
4:D:61:ARG:CZ	4:D:79:LEU:HD23	2.42	0.49
1:A:18:PHE:O	1:A:21:ARG:N	2.33	0.49
1:A:209:ALA:O	1:A:212:MET:HB3	2.11	0.49
1:A:27:ASN:HD21	1:A:29[A]:LYS:CG	2.25	0.49
2:B:119:HIS:HE1	2:B:177:THR:HG21	1.77	0.49
2:B:19:ASN:HB3	12:B:314:HOH:O	2.12	0.49
10:A:575[B]:LMT:H5B	10:A:575[B]:LMT:O2B	2.13	0.49
1:A:202:THR:O	1:A:203:THR:C	2.51	0.49
1:A:168:PRO:HD2	1:A:267:TYR:CD2	2.48	0.48
1:A:391:VAL:O	1:A:394:SER:OG	2.28	0.48
3:C:108:TRP:CE3	4:D:44:PRO:HD2	2.48	0.48
1:A:137:MET:O	1:A:138:TYR:C	2.48	0.48
1:A:92:THR:O	1:A:96:VAL:HG23	2.14	0.48
3:C:38:ARG:HD3	3:C:48:VAL:HG21	1.94	0.48
1:A:27:ASN:HD21	1:A:29[A]:LYS:HG3	1.78	0.48
1:A:412:PHE:CB	5:A:560:HEA:C2D	2.91	0.48
1:A:452:MET:HG3	1:A:452:MET:O	2.12	0.48
2:B:138:MET:HE1	2:B:226:TYR:CB	2.41	0.48
2:B:61:ASN:ND2	2:B:64:ALA:H	2.11	0.48
3:C:8:GLY:O	3:C:18:LEU:HD11	2.13	0.48
3:C:39:GLN:O	3:C:92:ALA:HB1	2.13	0.48
4:D:81:GLU:OE1	4:D:81:GLU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:TRP:CD1	10:B:281:LMT:H61	2.48	0.48
10:A:570:LMT:H2B	10:A:570:LMT:H6E	1.95	0.48
1:A:384:THR:O	1:A:388:VAL:HB	2.14	0.48
2:B:133:ALA:O	2:B:250:PHE:HB3	2.13	0.48
1:A:373:MET:O	1:A:377:PHE:HB2	2.14	0.48
1:A:38:THR:HG21	1:A:138:TYR:CE2	2.49	0.48
1:A:520:PRO:HA	1:A:534:LEU:O	2.14	0.48
2:B:81:TRP:CZ3	10:B:281:LMT:H121	2.49	0.48
3:C:51:ILE:HD11	3:C:55:GLY:HA2	1.96	0.48
1:A:102:VAL:C	1:A:105:PRO:HD2	2.33	0.48
1:A:386:GLY:HA2	1:A:389:THR:HG22	1.96	0.48
1:A:410:ALA:O	1:A:411:HIS:C	2.53	0.48
2:B:19:ASN:HD21	9:B:272:LDA:H41	1.78	0.48
3:C:109:GLY:O	4:D:43:SER:OG	2.14	0.47
1:A:379:PHE:O	1:A:379:PHE:CD1	2.67	0.47
1:A:115:PHE:CZ	1:A:431:TRP:CG	3.02	0.47
2:B:1:GLN:N	2:B:4:LEU:HB2	2.28	0.47
1:A:98:MET:HG3	5:A:559:HEA:CAC	2.45	0.47
1:A:169:PRO:O	1:A:173:THR:HB	2.13	0.47
2:B:140[B]:GLU:OE2	12:B:1161:HOH:O	2.20	0.47
1:A:292:HIS:H	1:A:292:HIS:CD2	2.32	0.47
2:B:120:GLN:HB3	2:B:121:TRP:CE2	2.50	0.47
1:A:393:LEU:HB3	5:A:560:HEA:HMA	1.97	0.47
2:B:127:TYR:N	2:B:127:TYR:CD1	2.81	0.47
10:B:280:LMT:O3'	10:B:280:LMT:H1B	2.14	0.47
1:A:67:LEU:C	1:A:69:GLY:H	2.17	0.46
1:A:125:MET:HE3	1:A:203:THR:OG1	2.15	0.46
1:A:217:VAL:CG1	1:A:221:ALA:HB3	2.45	0.46
3:C:44:ARG:CG	12:C:1236:HOH:O	2.63	0.46
1:A:341:MET:O	1:A:345:MET:HE2	2.15	0.46
1:A:416:MET:HG2	5:A:560:HEA:CBC	2.46	0.46
1:A:398:LEU:HD13	2:B:34:LEU:HD23	1.98	0.46
2:B:72:THR:O	2:B:73:HIS:HB3	2.16	0.46
4:D:61:ARG:NE	4:D:82:ASP:OD2	2.42	0.46
1:A:388:VAL:HG13	2:B:42:ILE:HD12	1.96	0.46
1:A:292:HIS:N	1:A:292:HIS:CD2	2.84	0.46
1:A:389:THR:CG2	1:A:411:HIS:HA	2.45	0.46
1:A:68:GLU:N	1:A:68:GLU:OE1	2.37	0.46
1:A:18:PHE:HD2	1:A:18:PHE:H	1.62	0.46
1:A:364:GLY:HA2	2:B:60:PHE:CD1	2.51	0.46
1:A:233:LEU:HB3	1:A:320:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:TYR:CD1	1:A:509:TYR:C	2.89	0.45
2:B:40:TYR:CE1	9:B:274:LDA:H31	2.36	0.45
1:A:167:TYR:HB2	12:A:1274:HOH:O	2.16	0.45
1:A:311:ALA:O	1:A:315:ILE:HD12	2.16	0.45
2:B:61:ASN:ND2	2:B:61:ASN:C	2.70	0.45
1:A:277:PRO:O	1:A:278:GLU:C	2.55	0.45
1:A:322:VAL:O	1:A:325:HIS:ND1	2.49	0.45
1:A:54:ARG:CD	1:A:490:SER:HA	2.46	0.45
1:A:484:TYR:OH	10:B:279:LMT:H5'	2.16	0.45
3:C:42:GLU:H	3:C:42:GLU:CD	2.19	0.45
1:A:137:MET:HB2	1:A:192:SER:HB2	1.98	0.45
1:A:432:ILE:HD13	1:A:510:THR:HG21	1.97	0.45
1:A:545:THR:CB	12:A:637:HOH:O	2.32	0.45
2:B:67:VAL:HA	2:B:68:PRO:HD2	1.82	0.45
3:C:87:LYS:HG2	3:C:87:LYS:H	1.62	0.45
1:A:140:CYS:O	1:A:143:ALA:N	2.45	0.45
1:A:200:ILE:HA	1:A:200:ILE:HD12	1.87	0.45
1:A:306:LEU:N	1:A:307:PRO:HD2	2.32	0.45
1:A:71:ARG:NH2	1:A:79:GLU:O	2.50	0.45
1:A:267:TYR:OH	1:A:271:LEU:HD13	2.16	0.45
1:A:460:PHE:O	1:A:461:PHE:C	2.52	0.45
2:B:165:PRO:HA	2:B:234:VAL:O	2.16	0.45
1:A:98:MET:HG3	5:A:559:HEA:C2C	2.47	0.44
1:A:115:PHE:O	1:A:116:MET:C	2.53	0.44
1:A:475:TYR:HE1	2:B:224:HIS:CD2	2.36	0.44
3:C:68:PHE:N	3:C:68:PHE:CD1	2.85	0.44
1:A:324:ALA:HB1	1:A:332:MET:HE1	2.00	0.44
1:A:475:TYR:CE1	2:B:224:HIS:NE2	2.84	0.44
1:A:34:LEU:HB3	1:A:135:TYR:CE1	2.53	0.44
4:D:6:GLN:NE2	4:D:103:THR:HG23	2.28	0.44
1:A:325:HIS:HB2	5:A:560:HEA:OMA	2.17	0.44
2:B:138:MET:HE1	2:B:226:TYR:CD1	2.53	0.44
1:A:312:MET:CE	1:A:312:MET:CG	2.93	0.44
1:A:29[C]:LYS:HE3	1:A:538:PRO:HB2	2.00	0.44
2:B:125:TYR:O	2:B:133:ALA:HA	2.18	0.44
9:A:564:LDA:H21	10:A:572[A]:LMT:H6'2	2.00	0.44
1:A:468:ARG:HD3	2:B:18:MET:O	2.18	0.44
1:A:104:ILE:HB	12:A:969:HOH:O	2.17	0.43
1:A:52:TYR:CD2	1:A:90:MET:HE2	2.51	0.43
2:B:81:TRP:CE3	10:B:281:LMT:H123	2.53	0.43
1:A:342:LEU:HD23	1:A:345:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:572[B]:LMT:O2B	10:A:572[B]:LMT:H5'	2.18	0.43
1:A:28:HIS:HE1	12:A:857:HOH:O	2.01	0.43
1:A:155:ASN:ND2	2:B:222:ILE:HD12	2.33	0.43
1:A:306:LEU:N	1:A:307:PRO:CD	2.81	0.43
5:A:560:HEA:O11	5:A:560:HEA:CHC	2.61	0.43
1:A:443:TRP:HZ2	10:A:569:LMT:H1'	1.84	0.43
1:A:116:MET:CE	1:A:204:PHE:HB2	2.48	0.43
9:A:565:LDA:HM23	9:A:565:LDA:H21	1.59	0.43
2:B:155:LEU:HD21	2:B:226:TYR:HE1	1.84	0.43
2:B:34:LEU:O	2:B:37:PHE:HB3	2.19	0.43
9:B:273:LDA:H21	9:B:273:LDA:HM12	1.51	0.43
1:A:431:TRP:O	1:A:435:MET:HG3	2.19	0.43
1:A:165:VAL:HB	1:A:271:LEU:CD2	2.49	0.43
1:A:412:PHE:HB2	5:A:560:HEA:HMD3	2.01	0.43
2:B:180:ILE:CG2	2:B:218:GLU:HG2	2.48	0.42
3:C:6:GLU:HA	3:C:21:SER:O	2.19	0.42
4:D:6:GLN:N	12:D:643:HOH:O	2.50	0.42
1:A:433:GLY:HA2	1:A:438:ARG:O	2.18	0.42
2:B:127:TYR:N	2:B:127:TYR:HD1	2.17	0.42
3:C:6:GLU:OE2	3:C:109:GLY:HA3	2.19	0.42
1:A:149:LEU:O	1:A:149:LEU:HG	2.18	0.42
1:A:276:HIS:HB3	1:A:277:PRO:HD3	2.01	0.42
2:B:12:LYS:HE3	2:B:153:GLU:CG	2.49	0.42
2:B:30:ASP:HB3	2:B:99:ILE:HG23	2.01	0.42
1:A:416:MET:HG2	5:A:560:HEA:HBC2	2.02	0.42
1:A:417:SER:C	1:A:418:LEU:HD12	2.39	0.42
5:A:559:HEA:H253	5:A:559:HEA:H211	1.67	0.42
5:A:560:HEA:H252	2:B:45:VAL:HG21	2.01	0.42
1:A:416:MET:CG	5:A:560:HEA:HAC	2.50	0.42
2:B:1:GLN:H1	2:B:4:LEU:HB2	1.83	0.42
2:B:7:LEU:HA	2:B:8:PRO:HD2	1.89	0.42
3:C:48:VAL:O	3:C:61:PRO:HD2	2.20	0.42
1:A:303:PHE:CD1	1:A:303:PHE:C	2.93	0.42
1:A:351:THR:HG21	5:A:560:HEA:H14	2.01	0.42
2:B:103:SER:OG	2:B:104:GLN:N	2.52	0.42
1:A:155:ASN:HD22	2:B:222:ILE:CD1	2.33	0.41
3:C:6:GLU:OE1	3:C:96:CYS:N	2.49	0.41
5:A:559:HEA:HAA2	5:A:559:HEA:HHA	1.90	0.41
1:A:389:THR:HG23	1:A:411:HIS:HA	2.02	0.41
1:A:341:MET:HG3	1:A:394:SER:O	2.20	0.41
1:A:459:ILE:HG21	1:A:459:ILE:HD13	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLU:CD	1:A:68:GLU:H	2.22	0.41
2:B:119:HIS:CE1	2:B:177:THR:CG2	3.03	0.41
1:A:155:ASN:ND2	2:B:222:ILE:CD1	2.84	0.41
1:A:249:ARG:HD3	1:A:249:ARG:HH11	1.74	0.41
1:A:293:VAL:O	1:A:297:PHE:HD1	2.03	0.41
1:A:371:THR:N	1:A:372:PRO:CD	2.83	0.41
1:A:72:LEU:HB2	9:A:567:LDA:H32	2.02	0.41
1:A:21:ARG:HH12	10:A:570:LMT:H4B	1.84	0.41
3:C:12:VAL:HB	3:C:13:GLN:H	1.67	0.41
1:A:256:PHE:HB3	1:A:264:PRO:HA	2.02	0.41
1:A:95:GLY:O	1:A:99:MET:HG2	2.21	0.41
2:B:141:LYS:CE	12:B:1156:HOH:O	2.66	0.41
1:A:414:TYR:CE1	1:A:418:LEU:HD22	2.56	0.41
1:A:137:MET:HG2	1:A:137:MET:H	1.54	0.41
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.90	0.41
1:A:480:VAL:HG11	12:B:1312:HOH:O	2.20	0.41
1:A:65:MET:O	1:A:83:ASN:HB3	2.20	0.41
4:D:49:TYR:CE1	4:D:53:THR:CG2	3.04	0.41
1:A:180:ASP:OD2	1:A:249:ARG:NH1	2.53	0.41
1:A:536:SER:HA	1:A:537:PRO:HA	1.80	0.41
1:A:42:VAL:HG23	1:A:42:VAL:H	1.66	0.41
2:B:119:HIS:HE1	2:B:177:THR:CG2	2.34	0.41
2:B:222:ILE:CD1	2:B:222:ILE:CB	2.87	0.41
1:A:164:TRP:CE2	1:A:165:VAL:HG13	2.56	0.40
2:B:202:LEU:HD12	2:B:202:LEU:C	2.41	0.40
1:A:416:MET:HG2	5:A:560:HEA:CAC	2.52	0.40
1:A:271:LEU:O	1:A:271:LEU:HG	2.20	0.40
2:B:75:THR:N	2:B:76:PRO:HD2	2.36	0.40
1:A:49:PHE:N	1:A:49:PHE:CD1	2.87	0.40
5:A:559:HEA:H132	5:A:559:HEA:H263	1.62	0.40
2:B:139:LEU:HA	2:B:139:LEU:HD23	1.89	0.40
3:C:62:ASP:N	12:C:1238:HOH:O	2.53	0.40
1:A:27:ASN:ND2	1:A:29[A]:LYS:HG3	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	530/558 (95%)	462 (87%)	61 (12%)	7 (1%)	14	9
2	B	252/298 (85%)	216 (86%)	31 (12%)	5 (2%)	9	4
3	C	118/127 (93%)	105 (89%)	11 (9%)	2 (2%)	11	6
4	D	106/120 (88%)	99 (93%)	3 (3%)	4 (4%)	4	1
All	All	1006/1103 (91%)	882 (88%)	106 (10%)	18 (2%)	10	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PHE
1	A	544	GLU
2	B	74	ASN
3	C	12	VAL
2	B	235	SER
3	C	109	GLY
4	D	68	GLY
4	D	77	SER
1	A	299	LYS
1	A	482	PHE
1	A	492	GLY
4	D	30	TYR
4	D	51	ALA
1	A	393	LEU
2	B	92	ILE
2	B	67	VAL
1	A	517	VAL
2	B	186	PRO

### 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%)	390 (90%)	45 (10%)	8	6
2	B	213/243 (88%)	184 (86%)	29 (14%)	4	2
3	C	103/107 (96%)	85 (82%)	18 (18%)	2	1
4	D	92/104 (88%)	77 (84%)	15 (16%)	3	1
All	All	843/908 (93%)	736 (87%)	107 (13%)	5	3

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	21	ARG
1	A	24	MET
1	A	50	THR
1	A	54	ARG
1	A	57	LEU
1	A	65	MET
1	A	86	LEU
1	A	91	ILE
1	A	98	MET
1	A	116	MET
1	A	124	ASP
1	A	129	ARG
1	A	134	SER
1	A	137	MET
1	A	156	ASP
1	A	166	LEU
1	A	173	THR
1	A	174	GLU
1	A	178	SER
1	A	179	MET
1	A	187	HIS
1	A	200	ILE
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	216	LYS
1	A	224	VAL
1	A	233	LEU
1	A	243	THR
1	A	274	PHE
1	A	317	ILE
1	A	332	MET
1	A	368	GLU
1	A	377	PHE
1	A	380	LEU
1	A	388	VAL
1	A	404	ASP
1	A	417	SER
1	A	434	LYS
1	A	438	ARG
1	A	456	SER
1	A	496	SER
1	A	516[A]	ARG
1	A	516[B]	ARG
1	A	518	ASN
1	A	544	GLU
2	B	1	GLN
2	B	2	ASP
2	B	4	LEU
2	B	14	VAL
2	B	53	LEU
2	B	54	LEU
2	B	59	ARG
2	B	61	ASN
2	B	63	ARG
2	B	70	ARG
2	B	77	ILE
2	B	81	TRP
2	B	83	LEU
2	B	85	PRO
2	B	87	LEU
2	B	96	SER
2	B	104	GLN
2	B	108	ASN
2	B	137	LEU
2	B	138	MET
2	B	142	GLU

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Mol	Chain	Res	Type
2	B	166	VAL
2	B	173	GLN
2	B	179	VAL
2	B	184	THR
2	B	186	PRO
2	B	191	LYS
2	B	232	LYS
2	B	247	LYS
3	C	3	LYS
3	C	5	GLN
3	C	6	GLU
3	C	11	LEU
3	C	13	GLN
3	C	17	SER
3	C	19[A]	LYS
3	C	19[B]	LYS
3	C	21	SER
3	C	33	THR
3	C	42	GLU
3	C	44	ARG
3	C	48	VAL
3	C	50	SER
3	C	83	MET
3	C	87	LYS
3	C	88	SER
3	C	91	THR
4	D	1	ASP
4	D	11	LEU
4	D	14	SER
4	D	39	LYS
4	D	42	LYS
4	D	45	GLN
4	D	50	ASN
4	D	63	SER
4	D	65	SER
4	D	69	THR
4	D	79	LEU
4	D	103	THR
4	D	104	LYS
4	D	107	ILE
4	D	108	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	28	HIS
1	A	85	HIS
1	A	155	ASN
1	A	157	GLN
1	A	187	HIS
1	A	268	GLN
1	A	269	HIS
1	A	469	GLN
1	A	486	ASN
1	A	487	ASN
1	A	518	ASN
2	B	21	GLN
2	B	29	HIS
2	B	61	ASN
2	B	104	GLN
2	B	108	ASN
2	B	192	GLN
2	B	208	GLN
3	C	13	GLN
3	C	99	HIS
4	D	45	GLN
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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 5 are monoatomic - leaving 34 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	44,67,67	3.04	12 (27%)	37,103,103	4.16	24 (64%)
5	HEA	A	560	1,11	44,67,67	3.63	16 (36%)	37,103,103	4.70	22 (59%)
9	LDA	A	564	-	13,15,15	2.38	2 (15%)	14,17,17	0.58	0
9	LDA	A	565	-	13,15,15	2.43	2 (15%)	14,17,17	0.54	0
9	LDA	A	566	-	13,15,15	2.45	2 (15%)	14,17,17	0.46	0
9	LDA	A	567	-	13,15,15	2.39	2 (15%)	14,17,17	0.65	0
10	LMT	A	568	-	36,36,36	4.54	13 (36%)	47,47,47	1.00	3 (6%)
10	LMT	A	569	-	36,36,36	4.57	14 (38%)	47,47,47	1.37	5 (10%)
10	LMT	A	570	-	36,36,36	4.55	13 (36%)	47,47,47	1.29	5 (10%)
10	LMT	A	571[A]	-	36,36,36	4.50	13 (36%)	47,47,47	1.74	6 (12%)
10	LMT	A	571[B]	-	36,36,36	4.50	13 (36%)	47,47,47	1.76	7 (14%)
10	LMT	A	572[A]	-	36,36,36	4.62	13 (36%)	47,47,47	1.24	2 (4%)
10	LMT	A	572[B]	-	36,36,36	4.58	13 (36%)	47,47,47	1.31	7 (14%)
10	LMT	A	573[A]	-	36,36,36	4.53	13 (36%)	47,47,47	1.50	7 (14%)
10	LMT	A	573[B]	-	36,36,36	4.56	14 (38%)	47,47,47	1.41	7 (14%)
10	LMT	A	574[A]	-	36,36,36	4.57	13 (36%)	47,47,47	1.37	5 (10%)
10	LMT	A	574[B]	-	36,36,36	4.59	13 (36%)	47,47,47	1.08	2 (4%)
10	LMT	A	575[A]	-	36,36,36	4.54	13 (36%)	47,47,47	1.51	8 (17%)
10	LMT	A	575[B]	-	36,36,36	4.53	13 (36%)	47,47,47	1.58	8 (17%)
11	PEO	A	576	5,6	1,1,1	0.73	0	0,0,0	0.00	-
9	LDA	B	272	-	13,15,15	2.33	2 (15%)	14,17,17	0.82	1 (7%)
9	LDA	B	273	-	13,15,15	2.42	2 (15%)	14,17,17	0.52	0
9	LDA	B	274	-	13,15,15	2.39	2 (15%)	14,17,17	0.51	0
9	LDA	B	275	-	13,15,15	2.44	2 (15%)	14,17,17	0.55	0
9	LDA	B	276	-	13,15,15	2.41	2 (15%)	14,17,17	0.59	0
9	LDA	B	277	-	13,15,15	2.44	2 (15%)	14,17,17	0.52	0
10	LMT	B	278	-	36,36,36	4.49	13 (36%)	47,47,47	1.34	6 (12%)
10	LMT	B	279	-	36,36,36	4.53	13 (36%)	47,47,47	1.48	5 (10%)
10	LMT	B	280	-	36,36,36	4.57	13 (36%)	47,47,47	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	LMT	B	281	-	36,36,36	4.52	13 (36%)	47,47,47	1.20	5 (10%)
10	LMT	B	282[A]	-	36,36,36	4.55	13 (36%)	47,47,47	1.33	7 (14%)
10	LMT	B	282[B]	-	36,36,36	4.55	13 (36%)	47,47,47	1.30	6 (12%)
10	LMT	B	283[A]	-	36,36,36	4.64	13 (36%)	47,47,47	1.21	2 (4%)
10	LMT	B	283[B]	-	36,36,36	4.65	13 (36%)	47,47,47	1.12	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
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[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	571[B]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	572[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	572[B]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	573[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	573[B]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	574[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	574[B]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	575[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	A	575[B]	-	-	0/21/61/61	0/2/2/2
11	PEO	A	576	5,6	-	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
9	LDA	B	277	-	-	0/13/13/13	0/0/0/0
10	LMT	B	278	-	-	1/21/61/61	0/2/2/2
10	LMT	B	279	-	-	0/21/61/61	0/2/2/2
10	LMT	B	280	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LMT	B	281	-	-	0/21/61/61	0/2/2/2
10	LMT	B	282[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	B	282[B]	-	-	0/21/61/61	0/2/2/2
10	LMT	B	283[A]	-	-	0/21/61/61	0/2/2/2
10	LMT	B	283[B]	-	-	0/21/61/61	0/2/2/2

All (323) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	560	HEA	O11-C11	-11.38	1.16	1.42
10	A	573[B]	LMT	C4B-C5B	-9.38	1.33	1.53
10	B	283[A]	LMT	C4B-C5B	-9.25	1.33	1.53
10	A	572[B]	LMT	C4B-C5B	-9.16	1.33	1.53
10	A	571[A]	LMT	C4B-C5B	-9.16	1.33	1.53
10	A	575[B]	LMT	C4B-C5B	-9.16	1.33	1.53
10	A	573[A]	LMT	C4B-C5B	-9.16	1.33	1.53
10	B	282[A]	LMT	C4B-C5B	-9.15	1.33	1.53
10	A	572[A]	LMT	C4B-C5B	-9.14	1.33	1.53
10	A	574[B]	LMT	C4B-C5B	-9.11	1.33	1.53
10	A	574[A]	LMT	C4B-C5B	-9.10	1.33	1.53
10	A	571[B]	LMT	C4B-C5B	-9.09	1.33	1.53
10	B	282[B]	LMT	C4B-C5B	-9.08	1.33	1.53
10	B	283[B]	LMT	C4B-C5B	-9.08	1.33	1.53
10	A	575[A]	LMT	C4B-C5B	-9.03	1.33	1.53
10	B	283[B]	LMT	O3'-C3'	-9.00	1.22	1.43
10	B	279	LMT	O2B-C2B	-8.96	1.22	1.43
10	A	568	LMT	C4B-C5B	-8.93	1.34	1.53
10	B	283[A]	LMT	O3'-C3'	-8.92	1.22	1.43
10	B	280	LMT	O3B-C3B	-8.92	1.22	1.43
10	B	280	LMT	C4B-C5B	-8.91	1.34	1.53
10	B	282[B]	LMT	O3B-C3B	-8.91	1.22	1.43
10	A	572[A]	LMT	O2B-C2B	-8.91	1.22	1.43
10	B	283[B]	LMT	O4'-C4B	-8.91	1.22	1.43
10	B	278	LMT	C4B-C5B	-8.91	1.34	1.53
10	B	282[B]	LMT	O4'-C4B	-8.90	1.22	1.43
10	B	283[A]	LMT	O2B-C2B	-8.90	1.22	1.43
10	B	283[B]	LMT	O3B-C3B	-8.89	1.22	1.43
10	A	575[B]	LMT	O4'-C4B	-8.89	1.22	1.43
10	B	283[A]	LMT	O3B-C3B	-8.89	1.22	1.43
10	A	573[B]	LMT	O2B-C2B	-8.89	1.22	1.43
10	A	573[B]	LMT	O3B-C3B	-8.89	1.22	1.43
10	A	572[B]	LMT	O4'-C4B	-8.89	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	574[B]	LMT	O3B-C3B	-8.88	1.22	1.43
10	B	283[B]	LMT	O2B-C2B	-8.88	1.22	1.43
10	A	575[A]	LMT	O2B-C2B	-8.88	1.22	1.43
10	B	282[A]	LMT	O2B-C2B	-8.87	1.22	1.43
10	A	575[B]	LMT	O3B-C3B	-8.87	1.22	1.43
10	A	572[A]	LMT	O3'-C3'	-8.87	1.22	1.43
10	A	575[A]	LMT	O3B-C3B	-8.87	1.22	1.43
10	A	573[B]	LMT	O4'-C4B	-8.86	1.22	1.43
10	A	574[A]	LMT	O2B-C2B	-8.86	1.22	1.43
10	A	572[B]	LMT	O2B-C2B	-8.86	1.22	1.43
10	A	571[B]	LMT	O4'-C4B	-8.86	1.22	1.43
10	A	574[B]	LMT	O2B-C2B	-8.86	1.22	1.43
10	A	574[A]	LMT	O3B-C3B	-8.86	1.22	1.43
10	B	282[B]	LMT	O2B-C2B	-8.86	1.22	1.43
10	A	574[A]	LMT	O4'-C4B	-8.86	1.22	1.43
10	A	571[A]	LMT	O3B-C3B	-8.86	1.22	1.43
10	A	573[A]	LMT	O4'-C4B	-8.85	1.22	1.43
10	A	571[B]	LMT	O3B-C3B	-8.85	1.22	1.43
10	A	571[A]	LMT	O2B-C2B	-8.85	1.22	1.43
10	A	573[A]	LMT	O2B-C2B	-8.85	1.22	1.43
10	A	574[B]	LMT	O4'-C4B	-8.85	1.22	1.43
10	A	575[A]	LMT	O4'-C4B	-8.85	1.22	1.43
10	B	283[A]	LMT	O4'-C4B	-8.85	1.22	1.43
10	B	282[A]	LMT	O4'-C4B	-8.84	1.22	1.43
10	B	281	LMT	C4B-C5B	-8.84	1.34	1.53
10	A	572[B]	LMT	O3B-C3B	-8.84	1.22	1.43
10	B	280	LMT	O3'-C3'	-8.84	1.22	1.43
10	A	572[A]	LMT	O4'-C4B	-8.83	1.22	1.43
10	A	572[A]	LMT	O3B-C3B	-8.82	1.22	1.43
10	B	279	LMT	O3'-C3'	-8.82	1.22	1.43
10	A	570	LMT	O3B-C3B	-8.82	1.22	1.43
10	A	572[B]	LMT	O3'-C3'	-8.81	1.22	1.43
10	B	280	LMT	O2B-C2B	-8.81	1.22	1.43
10	A	570	LMT	O2B-C2B	-8.81	1.22	1.43
10	B	282[A]	LMT	O3B-C3B	-8.80	1.22	1.43
10	A	574[B]	LMT	O3'-C3'	-8.80	1.22	1.43
10	A	574[A]	LMT	O3'-C3'	-8.80	1.22	1.43
10	A	571[B]	LMT	O2B-C2B	-8.80	1.22	1.43
10	A	569	LMT	O4'-C4B	-8.79	1.22	1.43
10	A	575[B]	LMT	O2B-C2B	-8.79	1.22	1.43
10	A	571[A]	LMT	O4'-C4B	-8.78	1.22	1.43
10	A	569	LMT	O2B-C2B	-8.78	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	573[A]	LMT	O3B-C3B	-8.78	1.22	1.43
10	B	278	LMT	O3'-C3'	-8.77	1.22	1.43
10	A	568	LMT	O4'-C4B	-8.77	1.22	1.43
10	A	570	LMT	C4B-C5B	-8.76	1.34	1.53
10	B	280	LMT	O4'-C4B	-8.76	1.22	1.43
10	A	570	LMT	O4'-C4B	-8.75	1.22	1.43
10	A	569	LMT	C4B-C5B	-8.75	1.34	1.53
10	A	568	LMT	O3'-C3'	-8.74	1.22	1.43
10	B	281	LMT	O2B-C2B	-8.73	1.22	1.43
10	A	570	LMT	O3'-C3'	-8.72	1.22	1.43
10	B	281	LMT	O4'-C4B	-8.71	1.22	1.43
10	A	569	LMT	O3B-C3B	-8.71	1.22	1.43
10	A	569	LMT	O3'-C3'	-8.71	1.22	1.43
10	B	279	LMT	O3B-C3B	-8.71	1.22	1.43
10	A	568	LMT	O3B-C3B	-8.70	1.22	1.43
10	A	575[B]	LMT	O3'-C3'	-8.68	1.23	1.43
10	A	575[A]	LMT	O3'-C3'	-8.68	1.23	1.43
10	A	568	LMT	O2B-C2B	-8.68	1.23	1.43
10	B	281	LMT	O3B-C3B	-8.68	1.23	1.43
10	B	281	LMT	O3'-C3'	-8.67	1.23	1.43
10	B	279	LMT	O4'-C4B	-8.65	1.23	1.43
10	B	282[A]	LMT	O3'-C3'	-8.63	1.23	1.43
10	B	282[B]	LMT	O3'-C3'	-8.63	1.23	1.43
10	A	571[B]	LMT	O3'-C3'	-8.61	1.23	1.43
10	A	571[A]	LMT	O3'-C3'	-8.61	1.23	1.43
10	A	573[A]	LMT	O3'-C3'	-8.61	1.23	1.43
10	A	573[B]	LMT	O3'-C3'	-8.61	1.23	1.43
10	B	278	LMT	O2B-C2B	-8.60	1.23	1.43
10	B	278	LMT	O3B-C3B	-8.59	1.23	1.43
10	B	278	LMT	O4'-C4B	-8.53	1.23	1.43
10	B	279	LMT	C4B-C5B	-8.50	1.35	1.53
9	A	566	LDA	O1-N1	-8.48	1.25	1.42
9	B	277	LDA	O1-N1	-8.43	1.25	1.42
9	B	275	LDA	O1-N1	-8.41	1.25	1.42
9	A	565	LDA	O1-N1	-8.40	1.25	1.42
9	B	273	LDA	O1-N1	-8.38	1.25	1.42
9	B	276	LDA	O1-N1	-8.32	1.25	1.42
9	A	564	LDA	O1-N1	-8.26	1.25	1.42
9	B	274	LDA	O1-N1	-8.26	1.25	1.42
9	A	567	LDA	O1-N1	-8.25	1.25	1.42
9	B	272	LDA	O1-N1	-8.10	1.26	1.42
5	A	559	HEA	O11-C11	-7.95	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	283[B]	LMT	C3B-C2B	-7.50	1.33	1.52
10	A	569	LMT	C3'-C2'	-7.45	1.33	1.52
10	B	283[A]	LMT	C3'-C2'	-7.42	1.33	1.52
10	B	279	LMT	C3B-C2B	-7.41	1.33	1.52
10	A	574[B]	LMT	C4B-C3B	-7.39	1.33	1.52
10	A	569	LMT	C3B-C2B	-7.38	1.33	1.52
10	B	283[B]	LMT	C3'-C2'	-7.38	1.33	1.52
10	A	573[B]	LMT	C4B-C3B	-7.37	1.33	1.52
10	B	283[B]	LMT	C4B-C3B	-7.37	1.33	1.52
10	B	283[A]	LMT	C4B-C3B	-7.33	1.33	1.52
10	B	281	LMT	C3'-C2'	-7.31	1.33	1.52
10	A	574[B]	LMT	C3B-C2B	-7.31	1.33	1.52
10	A	575[A]	LMT	C3B-C2B	-7.30	1.33	1.52
10	B	283[A]	LMT	C3B-C2B	-7.29	1.33	1.52
10	A	572[B]	LMT	C4B-C3B	-7.29	1.33	1.52
10	B	282[A]	LMT	C4B-C3B	-7.28	1.33	1.52
10	A	570	LMT	C3'-C2'	-7.28	1.33	1.52
10	A	572[A]	LMT	C3'-C2'	-7.28	1.33	1.52
10	A	575[A]	LMT	C4B-C3B	-7.28	1.33	1.52
10	B	282[B]	LMT	C4B-C3B	-7.27	1.33	1.52
10	B	282[A]	LMT	C3B-C2B	-7.27	1.33	1.52
10	A	574[B]	LMT	C3'-C2'	-7.27	1.33	1.52
10	A	574[A]	LMT	C3'-C2'	-7.27	1.33	1.52
10	A	575[B]	LMT	C4B-C3B	-7.25	1.33	1.52
10	B	280	LMT	C3'-C2'	-7.24	1.33	1.52
10	B	280	LMT	C3B-C2B	-7.24	1.33	1.52
10	A	572[A]	LMT	C4B-C3B	-7.23	1.33	1.52
10	A	568	LMT	C3'-C2'	-7.23	1.34	1.52
10	A	572[A]	LMT	C3B-C2B	-7.23	1.34	1.52
10	A	571[B]	LMT	C4B-C3B	-7.22	1.34	1.52
10	A	572[B]	LMT	C3B-C2B	-7.22	1.34	1.52
10	A	571[B]	LMT	C3B-C2B	-7.21	1.34	1.52
10	A	573[A]	LMT	C3B-C2B	-7.20	1.34	1.52
10	B	282[B]	LMT	C3B-C2B	-7.20	1.34	1.52
10	A	574[A]	LMT	C4B-C3B	-7.20	1.34	1.52
10	B	278	LMT	C3'-C2'	-7.19	1.34	1.52
10	A	573[A]	LMT	C4B-C3B	-7.19	1.34	1.52
10	A	571[A]	LMT	C4B-C3B	-7.19	1.34	1.52
10	A	570	LMT	C4B-C3B	-7.19	1.34	1.52
10	A	568	LMT	C3B-C2B	-7.17	1.34	1.52
10	B	279	LMT	C3'-C2'	-7.16	1.34	1.52
10	A	568	LMT	C4B-C3B	-7.16	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	281	LMT	C3B-C2B	-7.16	1.34	1.52
10	B	280	LMT	C4B-C3B	-7.15	1.34	1.52
10	A	572[A]	LMT	C4'-C5'	-7.15	1.33	1.52
10	A	573[B]	LMT	C3B-C2B	-7.14	1.34	1.52
10	A	569	LMT	C4B-C3B	-7.14	1.34	1.52
10	A	572[B]	LMT	C3'-C2'	-7.14	1.34	1.52
10	A	570	LMT	C3B-C2B	-7.13	1.34	1.52
10	A	574[A]	LMT	C3B-C2B	-7.13	1.34	1.52
10	B	282[A]	LMT	C3'-C2'	-7.13	1.34	1.52
10	B	282[B]	LMT	C3'-C2'	-7.13	1.34	1.52
10	A	575[B]	LMT	C3B-C2B	-7.12	1.34	1.52
10	A	571[A]	LMT	C3B-C2B	-7.12	1.34	1.52
10	B	278	LMT	C3B-C2B	-7.10	1.34	1.52
10	B	283[B]	LMT	C4'-C5'	-7.10	1.33	1.52
10	B	281	LMT	C4B-C3B	-7.09	1.34	1.52
10	A	572[B]	LMT	C4'-C5'	-7.07	1.33	1.52
10	B	278	LMT	C4B-C3B	-7.05	1.34	1.52
10	B	279	LMT	C4B-C3B	-7.04	1.34	1.52
10	B	283[B]	LMT	C3'-C4'	-7.04	1.33	1.52
10	A	570	LMT	C4'-C5'	-7.03	1.34	1.52
10	B	283[A]	LMT	C4'-C5'	-7.00	1.34	1.52
10	B	283[A]	LMT	C3'-C4'	-6.94	1.33	1.52
10	A	575[B]	LMT	C4'-C5'	-6.94	1.34	1.52
10	A	575[A]	LMT	C4'-C5'	-6.94	1.34	1.52
10	B	279	LMT	C4'-C5'	-6.94	1.34	1.52
10	A	572[A]	LMT	C3'-C4'	-6.93	1.33	1.52
10	A	568	LMT	C4'-C5'	-6.92	1.34	1.52
10	A	571[B]	LMT	C4'-C5'	-6.85	1.34	1.52
10	A	571[A]	LMT	C4'-C5'	-6.85	1.34	1.52
10	A	573[A]	LMT	C3'-C2'	-6.85	1.34	1.52
10	A	573[B]	LMT	C3'-C2'	-6.85	1.34	1.52
10	B	280	LMT	C4'-C5'	-6.82	1.34	1.52
10	A	569	LMT	C4'-C5'	-6.80	1.34	1.52
10	A	570	LMT	C3'-C4'	-6.80	1.34	1.52
10	A	575[B]	LMT	C3'-C2'	-6.78	1.35	1.52
10	A	575[A]	LMT	C3'-C2'	-6.78	1.35	1.52
10	A	574[B]	LMT	C4'-C5'	-6.75	1.34	1.52
10	A	574[A]	LMT	C4'-C5'	-6.75	1.34	1.52
10	B	281	LMT	C4'-C5'	-6.73	1.34	1.52
10	A	568	LMT	C3'-C4'	-6.73	1.34	1.52
10	B	281	LMT	C3'-C4'	-6.72	1.34	1.52
10	B	278	LMT	C3'-C4'	-6.67	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	283[B]	LMT	C1B-C2B	-6.67	1.33	1.52
10	B	280	LMT	C3'-C4'	-6.67	1.34	1.52
10	A	569	LMT	C3'-C4'	-6.67	1.34	1.52
10	A	572[B]	LMT	C1'-C2'	-6.67	1.33	1.52
10	A	570	LMT	C1'-C2'	-6.64	1.33	1.52
10	B	280	LMT	C1'-C2'	-6.63	1.33	1.52
10	A	572[B]	LMT	C3'-C4'	-6.62	1.34	1.52
10	B	279	LMT	C1B-C2B	-6.62	1.33	1.52
10	A	573[A]	LMT	C4'-C5'	-6.61	1.35	1.52
10	A	573[B]	LMT	C4'-C5'	-6.61	1.35	1.52
10	B	282[A]	LMT	C4'-C5'	-6.59	1.35	1.52
10	B	282[B]	LMT	C4'-C5'	-6.59	1.35	1.52
10	A	574[B]	LMT	C3'-C4'	-6.58	1.34	1.52
10	A	574[A]	LMT	C3'-C4'	-6.58	1.34	1.52
10	B	283[A]	LMT	C1'-C2'	-6.58	1.33	1.52
10	A	569	LMT	C1'-C2'	-6.57	1.33	1.52
10	A	574[B]	LMT	C1'-C2'	-6.56	1.33	1.52
10	A	574[A]	LMT	C1'-C2'	-6.56	1.33	1.52
10	A	571[B]	LMT	C3'-C2'	-6.55	1.35	1.52
10	A	571[A]	LMT	C3'-C2'	-6.55	1.35	1.52
10	B	282[A]	LMT	C1'-C2'	-6.55	1.33	1.52
10	B	282[B]	LMT	C1'-C2'	-6.55	1.33	1.52
10	B	278	LMT	C4'-C5'	-6.55	1.35	1.52
10	B	281	LMT	C1'-C2'	-6.52	1.33	1.52
10	A	572[A]	LMT	C1B-C2B	-6.50	1.33	1.52
10	A	575[B]	LMT	C3'-C4'	-6.49	1.34	1.52
10	A	575[A]	LMT	C3'-C4'	-6.49	1.34	1.52
10	B	279	LMT	C3'-C4'	-6.49	1.34	1.52
10	A	574[A]	LMT	C1B-C2B	-6.47	1.34	1.52
10	B	282[A]	LMT	C1B-C2B	-6.47	1.34	1.52
10	A	572[A]	LMT	C1'-C2'	-6.46	1.34	1.52
10	A	573[A]	LMT	C1B-C2B	-6.45	1.34	1.52
10	B	283[B]	LMT	C1'-C2'	-6.45	1.34	1.52
10	B	282[B]	LMT	C1B-C2B	-6.44	1.34	1.52
10	B	281	LMT	C1B-C2B	-6.43	1.34	1.52
10	A	568	LMT	C1'-C2'	-6.43	1.34	1.52
10	A	575[A]	LMT	C1B-C2B	-6.43	1.34	1.52
10	A	569	LMT	C1B-C2B	-6.42	1.34	1.52
10	B	282[A]	LMT	C3'-C4'	-6.42	1.35	1.52
10	B	282[B]	LMT	C3'-C4'	-6.42	1.35	1.52
10	B	279	LMT	C1'-C2'	-6.41	1.34	1.52
10	A	573[A]	LMT	C3'-C4'	-6.39	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	573[B]	LMT	C3'-C4'	-6.39	1.35	1.52
10	A	570	LMT	C1B-C2B	-6.38	1.34	1.52
10	B	280	LMT	C1B-C2B	-6.38	1.34	1.52
10	A	568	LMT	C1B-C2B	-6.38	1.34	1.52
10	B	283[A]	LMT	C1B-C2B	-6.38	1.34	1.52
10	A	572[B]	LMT	C1B-C2B	-6.37	1.34	1.52
10	A	575[B]	LMT	C1B-C2B	-6.37	1.34	1.52
10	B	278	LMT	C1'-C2'	-6.36	1.34	1.52
10	A	574[B]	LMT	C1B-C2B	-6.35	1.34	1.52
10	A	571[A]	LMT	C1B-C2B	-6.34	1.34	1.52
10	A	571[B]	LMT	C3'-C4'	-6.34	1.35	1.52
10	A	571[A]	LMT	C3'-C4'	-6.34	1.35	1.52
10	A	573[B]	LMT	C1B-C2B	-6.28	1.34	1.52
10	A	571[B]	LMT	C1B-C2B	-6.28	1.34	1.52
10	A	573[A]	LMT	C1'-C2'	-6.25	1.34	1.52
10	A	573[B]	LMT	C1'-C2'	-6.25	1.34	1.52
10	A	571[B]	LMT	C1'-C2'	-6.21	1.34	1.52
10	A	571[A]	LMT	C1'-C2'	-6.21	1.34	1.52
10	B	278	LMT	C1B-C2B	-6.19	1.34	1.52
10	A	575[B]	LMT	C1'-C2'	-6.12	1.35	1.52
10	A	575[A]	LMT	C1'-C2'	-6.12	1.35	1.52
5	A	560	HEA	C4A-NA	-5.80	1.29	1.36
5	A	559	HEA	C4A-NA	-5.07	1.30	1.36
5	A	559	HEA	C1A-NA	-4.72	1.31	1.36
5	A	559	HEA	C1D-ND	-3.78	1.32	1.36
5	A	560	HEA	C1A-NA	-3.58	1.32	1.36
5	A	560	HEA	C4B-NB	-2.62	1.33	1.36
9	B	275	LDA	C1-N1	-2.37	1.46	1.51
9	B	277	LDA	C1-N1	-2.34	1.46	1.51
9	A	566	LDA	C1-N1	-2.30	1.46	1.51
9	B	273	LDA	C1-N1	-2.30	1.46	1.51
9	A	565	LDA	C1-N1	-2.26	1.46	1.51
9	B	276	LDA	C1-N1	-2.23	1.46	1.51
9	A	567	LDA	C1-N1	-2.21	1.46	1.51
9	B	274	LDA	C1-N1	-2.21	1.46	1.51
9	A	564	LDA	C1-N1	-2.14	1.46	1.51
9	B	272	LDA	C1-N1	-2.14	1.46	1.51
5	A	559	HEA	C4C-NC	-2.11	1.31	1.36
10	A	569	LMT	O1B-C1B	2.03	1.47	1.41
5	A	560	HEA	C24-C23	2.03	1.56	1.50
5	A	560	HEA	C17-C18	2.05	1.57	1.50
10	A	573[B]	LMT	O1B-C1B	2.15	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	560	HEA	C3B-C2B	2.25	1.48	1.41
5	A	560	HEA	C4D-CHA	2.57	1.47	1.40
5	A	560	HEA	C4C-CHD	3.04	1.48	1.40
5	A	559	HEA	C1B-CHB	3.06	1.48	1.40
10	A	570	LMT	O1'-C1'	3.17	1.45	1.40
10	A	572[B]	LMT	O1'-C1'	3.25	1.45	1.40
10	B	281	LMT	O1'-C1'	3.27	1.45	1.40
10	A	571[B]	LMT	O1'-C1'	3.45	1.46	1.40
10	A	571[A]	LMT	O1'-C1'	3.45	1.46	1.40
10	A	568	LMT	O1'-C1'	3.52	1.46	1.40
10	B	279	LMT	O1'-C1'	3.53	1.46	1.40
10	B	282[A]	LMT	O1'-C1'	3.54	1.46	1.40
10	B	282[B]	LMT	O1'-C1'	3.54	1.46	1.40
10	B	283[B]	LMT	O1'-C1'	3.54	1.46	1.40
10	A	572[A]	LMT	O1'-C1'	3.59	1.46	1.40
10	A	574[B]	LMT	O1'-C1'	3.63	1.46	1.40
10	A	574[A]	LMT	O1'-C1'	3.63	1.46	1.40
10	B	283[A]	LMT	O1'-C1'	3.65	1.46	1.40
10	B	280	LMT	O1'-C1'	3.67	1.46	1.40
10	A	575[B]	LMT	O1'-C1'	3.68	1.46	1.40
10	A	575[A]	LMT	O1'-C1'	3.68	1.46	1.40
10	A	569	LMT	O1'-C1'	3.69	1.46	1.40
5	A	559	HEA	C3D-C2D	3.76	1.48	1.37
5	A	560	HEA	C3D-C2D	3.78	1.48	1.37
10	A	573[A]	LMT	O1'-C1'	3.78	1.46	1.40
10	A	573[B]	LMT	O1'-C1'	3.78	1.46	1.40
5	A	559	HEA	C3C-C2C	3.84	1.45	1.40
10	B	278	LMT	O1'-C1'	3.89	1.47	1.40
5	A	559	HEA	OMA-CMA	4.97	1.38	1.21
5	A	560	HEA	C3A-C2A	5.43	1.47	1.40
5	A	560	HEA	OMA-CMA	5.60	1.40	1.21
5	A	559	HEA	C18-C19	7.09	1.50	1.33
5	A	559	HEA	C14-C15	7.38	1.51	1.33
5	A	560	HEA	C22-C23	7.41	1.54	1.32
5	A	560	HEA	C3C-C2C	7.51	1.50	1.40
5	A	560	HEA	C18-C19	7.96	1.52	1.33
5	A	559	HEA	C22-C23	8.72	1.57	1.32
5	A	560	HEA	C14-C15	9.50	1.56	1.33

All (156) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	560	HEA	C13-C12-C11	-14.69	92.22	114.46
5	A	560	HEA	OMA-CMA-C3A	-9.61	102.99	125.08
5	A	559	HEA	C16-C15-C14	-8.94	102.81	121.10
5	A	560	HEA	CAA-CBA-CGA	-8.77	97.67	112.66
5	A	560	HEA	C1B-C2B-C3B	-8.34	101.19	107.00
5	A	559	HEA	C12-C13-C14	-8.07	91.13	112.33
5	A	559	HEA	C17-C18-C19	-8.01	107.57	127.68
5	A	559	HEA	C13-C14-C15	-7.66	108.45	127.68
5	A	560	HEA	C17-C18-C19	-7.08	109.89	127.68
5	A	559	HEA	C21-C22-C23	-6.67	103.99	127.80
5	A	559	HEA	C20-C19-C18	-6.58	107.63	121.10
5	A	559	HEA	CAA-CBA-CGA	-6.32	101.86	112.66
5	A	560	HEA	C13-C14-C15	-6.22	112.07	127.68
5	A	560	HEA	CAD-CBD-CGD	-6.06	102.31	112.66
5	A	560	HEA	C21-C22-C23	-5.64	107.68	127.80
5	A	559	HEA	C1B-C2B-C3B	-4.72	103.71	107.00
5	A	559	HEA	C13-C12-C11	-4.69	107.36	114.46
5	A	559	HEA	C26-C15-C14	-4.57	111.48	123.69
5	A	560	HEA	C20-C19-C18	-4.20	112.50	121.10
5	A	560	HEA	C25-C23-C22	-4.17	110.07	122.65
5	A	559	HEA	OMA-CMA-C3A	-4.16	115.53	125.08
5	A	559	HEA	C24-C23-C22	-3.88	110.94	122.65
10	A	571[B]	LMT	C1'-O5'-C5'	-3.72	106.71	113.72
10	A	571[A]	LMT	C1'-O5'-C5'	-3.72	106.71	113.72
10	A	572[B]	LMT	C1'-O5'-C5'	-3.63	106.89	113.72
5	A	559	HEA	C27-C19-C20	-3.62	109.00	115.29
5	A	560	HEA	C26-C15-C16	-3.53	109.15	115.29
5	A	559	HEA	CBD-CAD-C3D	-3.46	105.87	112.48
10	A	570	LMT	C1B-O5B-C5B	-3.42	107.28	113.72
5	A	560	HEA	C26-C15-C14	-3.38	114.67	123.69
10	A	575[B]	LMT	C1'-O5'-C5'	-3.25	107.59	113.72
10	A	575[A]	LMT	C1'-O5'-C5'	-3.25	107.59	113.72
10	A	575[B]	LMT	C1B-O5B-C5B	-2.98	108.11	113.72
5	A	560	HEA	CBD-CAD-C3D	-2.88	106.98	112.48
10	A	573[A]	LMT	C1B-O5B-C5B	-2.88	108.30	113.72
10	B	278	LMT	C1B-O5B-C5B	-2.86	108.32	113.72
5	A	559	HEA	C27-C19-C18	-2.77	116.29	123.69
10	A	574[A]	LMT	C1B-O5B-C5B	-2.74	108.55	113.72
5	A	559	HEA	C25-C23-C22	-2.70	114.51	122.65
10	A	572[B]	LMT	O5'-C1'-C2'	-2.59	105.31	110.30
10	B	282[B]	LMT	C1B-O5B-C5B	-2.51	108.98	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	572[B]	LMT	C1B-O5B-C5B	-2.46	109.08	113.72
5	A	559	HEA	C3A-C4A-NA	-2.44	106.33	110.94
10	A	571[B]	LMT	C1B-O5B-C5B	-2.44	109.12	113.72
10	B	279	LMT	C1'-O5'-C5'	-2.38	109.23	113.72
10	B	282[A]	LMT	C1B-O1B-C4'	-2.32	112.34	118.00
10	A	574[A]	LMT	C1B-O1B-C4'	-2.32	112.35	118.00
5	A	560	HEA	C27-C19-C18	-2.26	117.65	123.69
10	A	568	LMT	C1B-O1B-C4'	-2.21	112.60	118.00
5	A	559	HEA	CMC-C2C-C1C	-2.16	125.14	128.46
10	A	570	LMT	C2'-C3'-C4'	-2.14	105.16	109.61
10	A	574[B]	LMT	O1B-C4'-C5'	-2.11	104.17	109.34
9	B	272	LDA	CM2-N1-CM1	-2.06	107.04	110.99
10	A	575[A]	LMT	C1B-O1B-C4'	-2.04	113.03	118.00
5	A	560	HEA	C24-C23-C22	-2.01	116.57	122.65
10	A	573[A]	LMT	O5'-C5'-C6'	2.01	111.23	106.41
10	A	573[B]	LMT	O5'-C5'-C6'	2.01	111.23	106.41
10	A	575[B]	LMT	O5B-C5B-C6B	2.09	111.41	106.41
10	B	283[B]	LMT	O5B-C5B-C4B	2.09	113.51	109.66
10	A	572[B]	LMT	O1B-C1B-C2B	2.09	112.83	108.11
10	B	283[B]	LMT	O1'-C1'-C2'	2.11	111.68	108.23
10	B	279	LMT	O1'-C1'-C2'	2.13	111.70	108.23
10	B	281	LMT	O1B-C1B-C2B	2.13	112.91	108.11
10	A	569	LMT	O1'-C1'-C2'	2.15	111.74	108.23
10	B	283[A]	LMT	O1'-C1'-C2'	2.17	111.77	108.23
10	B	280	LMT	O1'-C1'-C2'	2.18	111.80	108.23
10	A	573[B]	LMT	C1B-C2B-C3B	2.18	114.04	109.98
10	A	575[B]	LMT	O5'-C1'-C2'	2.26	114.65	110.30
10	A	575[A]	LMT	O5'-C1'-C2'	2.26	114.65	110.30
10	A	575[B]	LMT	O1'-C1'-C2'	2.26	111.92	108.23
10	A	575[A]	LMT	O1'-C1'-C2'	2.26	111.92	108.23
10	B	280	LMT	O1B-C1B-C2B	2.27	113.22	108.11
10	A	575[A]	LMT	O1B-C4'-C3'	2.28	112.68	107.19
10	B	282[A]	LMT	O1B-C4'-C3'	2.29	112.70	107.19
5	A	560	HEA	C12-C13-C14	2.29	118.36	112.33
10	A	571[B]	LMT	O1B-C4'-C3'	2.31	112.76	107.19
10	B	278	LMT	O1B-C1B-C2B	2.34	113.37	108.11
5	A	560	HEA	CMD-C2D-C3D	2.35	129.38	124.94
5	A	560	HEA	O11-C11-C3B	2.36	118.61	111.83
10	B	278	LMT	O5B-C5B-C6B	2.41	112.17	106.41
10	A	572[B]	LMT	O1B-C4'-C3'	2.42	113.02	107.19
10	B	278	LMT	C2'-C3'-C4'	2.44	114.66	109.61
10	A	568	LMT	O1'-C1'-C2'	2.46	112.24	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	559	HEA	CMB-C2B-C1B	2.47	132.26	128.46
10	B	282[A]	LMT	O1'-C1'-C2'	2.49	112.29	108.23
10	B	282[B]	LMT	O1'-C1'-C2'	2.49	112.29	108.23
10	B	281	LMT	O1'-C1'-C2'	2.53	112.37	108.23
10	B	281	LMT	C3'-C4'-C5'	2.55	116.28	110.88
10	A	573[B]	LMT	O1B-C1B-C2B	2.60	113.98	108.11
10	A	574[A]	LMT	O1B-C4'-C5'	2.67	115.91	109.34
10	A	571[A]	LMT	C1B-C2B-C3B	2.76	115.11	109.98
10	A	573[A]	LMT	C3'-C4'-C5'	2.77	116.75	110.88
10	A	573[B]	LMT	C3'-C4'-C5'	2.77	116.75	110.88
10	A	571[A]	LMT	C4B-C3B-C2B	2.80	115.78	110.84
10	B	278	LMT	C1'-C2'-C3'	2.80	115.19	109.98
5	A	560	HEA	C17-C16-C15	2.83	122.50	112.93
10	A	569	LMT	O1B-C1B-C2B	2.86	114.55	108.11
10	A	572[B]	LMT	O1'-C1'-C2'	2.89	112.95	108.23
10	A	572[A]	LMT	O1B-C4'-C3'	2.89	114.16	107.19
10	A	571[B]	LMT	O1B-C1B-C2B	2.96	114.78	108.11
5	A	559	HEA	CMC-C2C-C3C	3.00	130.47	124.89
10	B	282[A]	LMT	C1-O1'-C1'	3.09	119.16	113.87
10	B	282[B]	LMT	C1-O1'-C1'	3.09	119.16	113.87
5	A	560	HEA	CMC-C2C-C3C	3.09	130.63	124.89
5	A	559	HEA	C26-C15-C16	3.13	120.73	115.29
10	B	282[A]	LMT	C2'-C3'-C4'	3.14	116.11	109.61
10	B	282[B]	LMT	C2'-C3'-C4'	3.14	116.11	109.61
10	A	573[A]	LMT	C1'-C2'-C3'	3.18	115.88	109.98
10	A	573[B]	LMT	C1'-C2'-C3'	3.18	115.88	109.98
10	A	570	LMT	O1B-C4'-C3'	3.22	114.94	107.19
10	A	569	LMT	O5B-C5B-C4B	3.27	115.69	109.66
5	A	560	HEA	C16-C17-C18	3.40	123.62	111.97
10	A	572[B]	LMT	C1-O1'-C1'	3.45	119.80	113.87
10	B	281	LMT	C1-O1'-C1'	3.49	119.86	113.87
10	A	575[B]	LMT	C1-O1'-C1'	3.52	119.91	113.87
10	A	575[A]	LMT	C1-O1'-C1'	3.52	119.91	113.87
10	A	570	LMT	O1B-C4'-C5'	3.52	118.01	109.34
10	B	281	LMT	O5'-C5'-C4'	3.58	117.07	109.75
10	A	568	LMT	C1-O1'-C1'	3.58	120.02	113.87
10	A	569	LMT	C1-O1'-C1'	3.62	120.08	113.87
10	A	570	LMT	C1-O1'-C1'	3.67	120.16	113.87
10	A	569	LMT	O5'-C5'-C4'	3.69	117.31	109.75
10	B	282[A]	LMT	O5'-C5'-C4'	3.73	117.39	109.75
10	B	282[B]	LMT	O5'-C5'-C4'	3.73	117.39	109.75
10	B	282[A]	LMT	C3'-C4'-C5'	3.75	118.83	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	282[B]	LMT	C3'-C4'-C5'	3.75	118.83	110.88
10	A	573[A]	LMT	O1B-C4'-C3'	3.86	116.48	107.19
10	B	279	LMT	C3B-C4B-C5B	3.99	117.24	110.22
10	A	575[B]	LMT	C2'-C3'-C4'	4.00	117.89	109.61
10	A	575[A]	LMT	C2'-C3'-C4'	4.00	117.89	109.61
5	A	559	HEA	C12-C11-C3B	4.11	122.68	112.65
10	A	573[A]	LMT	C2'-C3'-C4'	4.13	118.18	109.61
10	A	573[B]	LMT	C2'-C3'-C4'	4.13	118.18	109.61
5	A	559	HEA	CBA-CAA-C2A	4.18	120.45	112.47
10	A	574[A]	LMT	O1B-C4'-C3'	4.29	117.53	107.19
10	A	573[A]	LMT	C1-O1'-C1'	4.33	121.29	113.87
10	A	573[B]	LMT	C1-O1'-C1'	4.33	121.29	113.87
10	B	279	LMT	O5B-C5B-C4B	4.61	118.15	109.66
10	B	278	LMT	C1-O1'-C1'	4.78	122.08	113.87
10	A	571[B]	LMT	C1-O1'-C1'	4.83	122.16	113.87
10	A	571[A]	LMT	C1-O1'-C1'	4.83	122.16	113.87
10	B	279	LMT	C1-O1'-C1'	4.90	122.27	113.87
10	B	280	LMT	C1-O1'-C1'	4.96	122.38	113.87
10	B	283[B]	LMT	C1-O1'-C1'	4.97	122.39	113.87
10	A	574[B]	LMT	C1-O1'-C1'	5.03	122.50	113.87
10	A	574[A]	LMT	C1-O1'-C1'	5.03	122.50	113.87
5	A	559	HEA	O11-C11-C3B	5.10	126.50	111.83
10	A	575[B]	LMT	C1'-C2'-C3'	5.24	119.72	109.98
10	A	575[A]	LMT	C1'-C2'-C3'	5.24	119.72	109.98
10	A	572[A]	LMT	C1-O1'-C1'	5.42	123.17	113.87
10	A	571[B]	LMT	C2'-C3'-C4'	5.68	121.39	109.61
10	A	571[A]	LMT	C2'-C3'-C4'	5.68	121.39	109.61
10	B	283[A]	LMT	C1-O1'-C1'	5.95	124.08	113.87
10	A	571[B]	LMT	C1'-C2'-C3'	6.13	121.37	109.98
10	A	571[A]	LMT	C1'-C2'-C3'	6.13	121.37	109.98
5	A	560	HEA	C12-C11-C3B	8.29	132.91	112.65

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

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Mol	Chain	Res	Type	Atom
5	A	559	HEA	NB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	278	LMT	C1-O1'-C1'-O5'

There are no ring outliers.

22 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	559	HEA	14	0
5	A	560	HEA	18	0
9	A	564	LDA	2	0
9	A	565	LDA	1	0
9	A	567	LDA	2	0
10	A	569	LMT	1	0
10	A	570	LMT	4	0
10	A	571[A]	LMT	1	0
10	A	571[B]	LMT	1	0
10	A	572[A]	LMT	2	0
10	A	572[B]	LMT	2	0
10	A	573[B]	LMT	3	0
10	A	574[A]	LMT	1	0
10	A	574[B]	LMT	2	0
10	A	575[B]	LMT	2	0
9	B	272	LDA	2	0
9	B	273	LDA	4	0
9	B	274	LDA	2	0
9	B	276	LDA	1	0
10	B	279	LMT	1	0
10	B	280	LMT	1	0
10	B	281	LMT	7	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	529/558 (94%)	-0.54	12 (2%) 61 64	18, 39, 62, 101	0
2	B	252/298 (84%)	-0.74	0 100 100	15, 32, 50, 63	0
3	C	118/127 (92%)	-0.33	1 (0%) 86 87	20, 45, 65, 74	0
4	D	108/120 (90%)	-0.54	0 100 100	21, 41, 61, 69	0
All	All	1007/1103 (91%)	-0.57	13 (1%) 77 80	15, 38, 61, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLY	6.9
1	A	545	THR	5.8
3	C	118	SER	4.0
1	A	251	PHE	3.8
1	A	175	ALA	3.1
1	A	20	THR	3.0
1	A	18	PHE	2.9
1	A	177	TYR	2.8
1	A	156	ASP	2.5
1	A	261	GLY	2.3
1	A	173	THR	2.1
1	A	512	PHE	2.1
1	A	77	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	LMT	B	282[A]	35/35	0.52	0.42	22.64	57,120,122,122	12
10	LMT	B	282[B]	35/35	0.52	0.42	22.64	57,118,122,122	12
9	LDA	B	272	16/16	0.70	0.25	10.82	26,37,86,87	0
10	LMT	A	573[B]	35/35	0.59	0.35	10.67	50,102,107,108	12
10	LMT	A	573[A]	35/35	0.59	0.35	10.67	50,102,107,108	12
9	LDA	A	564	16/16	0.64	0.24	9.23	44,80,111,113	0
9	LDA	A	567	16/16	0.53	0.34	8.44	81,99,113,114	0
10	LMT	B	279	35/35	0.79	0.23	8.05	70,89,106,107	0
10	LMT	B	283[B]	35/35	0.63	0.32	7.35	71,76,84,85	23
10	LMT	B	283[A]	35/35	0.63	0.32	7.35	71,86,88,88	23
10	LMT	A	569	35/35	0.69	0.28	6.64	70,97,101,102	0
10	LMT	A	571[B]	35/35	0.63	0.35	6.02	79,104,112,112	12
10	LMT	A	571[A]	35/35	0.63	0.35	6.02	79,110,112,112	12
10	LMT	A	568	35/35	0.78	0.22	5.29	88,110,114,114	0
9	LDA	B	274	16/16	0.64	0.26	5.03	60,82,106,107	0
10	LMT	B	280	35/35	0.65	0.25	4.80	88,130,134,134	0
10	LMT	B	281	35/35	0.72	0.35	4.41	68,110,125,126	0
9	LDA	B	273	16/16	0.71	0.20	3.24	99,105,113,113	0
10	LMT	A	575[A]	35/35	0.68	0.28	2.93	91,121,127,127	12
10	LMT	A	575[B]	35/35	0.68	0.28	2.93	91,117,127,127	12
5	HEA	A	560	60/60	0.97	0.11	0.98	20,36,45,53	0
10	LMT	A	570	35/35	0.82	0.16	0.82	54,87,103,107	0
5	HEA	A	559	60/60	0.97	0.11	0.75	11,23,36,51	0
6	CU1	B	270	1/1	0.99	0.06	-1.94	35,35,35,35	0
6	CU1	B	271	1/1	0.99	0.06	-2.28	32,32,32,32	0
8	CA	A	563	1/1	0.97	0.04	-2.49	35,35,35,35	0
7	MN	A	562	1/1	0.99	0.05	-3.68	34,34,34,34	0
6	CU1	A	561	1/1	0.99	0.01	-	43,43,43,43	0
10	LMT	A	574[A]	35/35	0.45	0.49	-	140,155,159,159	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	LMT	B	278	35/35	0.86	0.20	-	52,73,107,107	0
11	PEO	A	576	2/2	0.98	0.07	-	17,17,17,32	0
9	LDA	B	276	16/16	0.31	0.43	-	96,115,127,127	0
9	LDA	A	566	16/16	0.47	0.47	-	120,125,127,127	0
10	LMT	A	572[B]	35/35	0.55	0.35	-	100,106,108,108	23
10	LMT	A	574[B]	35/35	0.45	0.49	-	140,157,159,159	12
9	LDA	A	565	16/16	0.39	0.30	-	91,107,124,124	0
9	LDA	B	277	16/16	0.35	0.39	-	141,150,156,156	0
9	LDA	B	275	16/16	0.34	0.32	-	138,141,144,144	0
10	LMT	A	572[A]	35/35	0.55	0.35	-	100,105,108,108	23

## 6.5 Other polymers [i](#)

There are no such residues in this entry.