



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2018 – 04:08 PM EST

PDB ID : 5IUX  
Title : GLIC-V135C bimane labelled X-ray structure  
Authors : Fourati, Z.; Menny, A.; Delarue, M.  
Deposited on : 2016-03-18  
Resolution : 2.60 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 : rb-20030736  
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) : rb-20030736

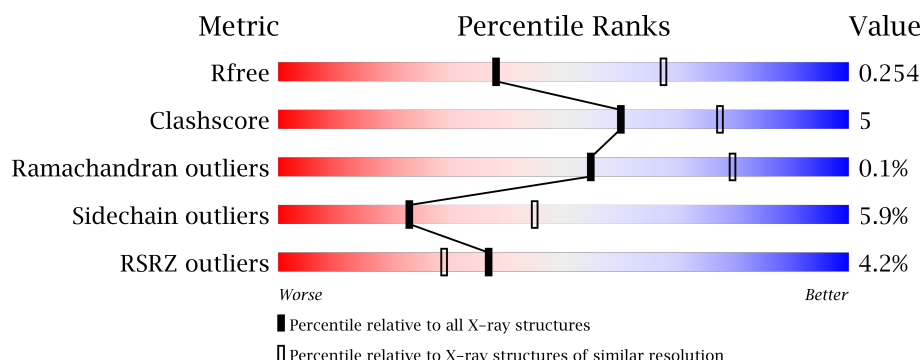
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	317	 4% 85% 12% ..
1	B	317	 3% 85% 12% ..
1	C	317	 5% 78% 20% ..
1	D	317	 5% 84% 14% ..
1	E	317	 4% 82% 15% ..

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
2	LMT	A	501	-	-	-	X
2	LMT	A	506	-	-	-	X
2	LMT	B	602	-	-	-	X
2	LMT	C	602	-	-	-	X
2	LMT	E	402	-	-	-	X
2	LMT	E	403	-	-	-	X
3	PC1	A	502	-	-	-	X
3	PC1	A	503	-	-	-	X
3	PC1	B	601	-	-	-	X
3	PC1	B	603	-	-	-	X
3	PC1	B	604	-	-	-	X
3	PC1	C	601	-	-	-	X
3	PC1	C	603	-	-	-	X
3	PC1	C	604	-	-	-	X
3	PC1	D	602	-	-	-	X
3	PC1	D	603	-	-	-	X
3	PC1	E	404	-	-	-	X
3	PC1	E	405	-	-	-	X
3	PC1	E	406	-	-	-	X
4	ACT	A	505	-	-	X	X
4	ACT	A	509	-	-	X	X
4	ACT	A	510	-	-	X	X
4	ACT	B	607	-	-	X	-
4	ACT	C	608	-	-	X	X
4	ACT	D	607	-	-	-	X
4	ACT	D	608	-	-	X	X
4	ACT	E	401	-	-	X	-
5	6E3	A	507	-	-	-	X
5	6E3	D	604	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13699 atoms, of which 52 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.

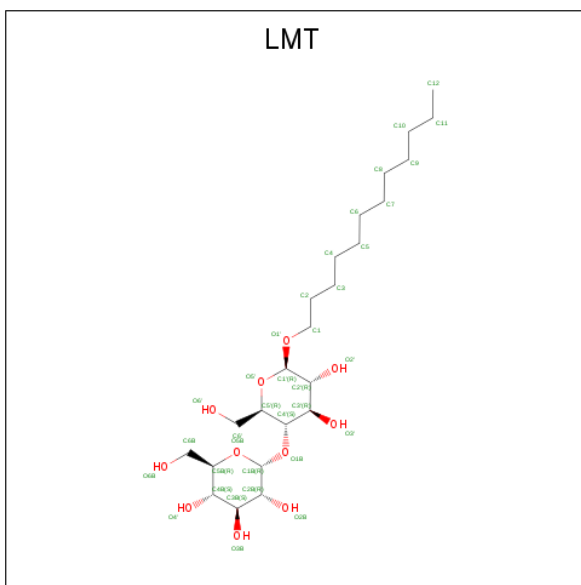
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2524	1662	404	454	4			
1	B	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			
1	C	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			
1	D	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			
1	E	311	Total	C	N	O	S	0	1	0
			2533	1668	406	455	4			

There are 10 discrepancies between the modelled and reference sequences:

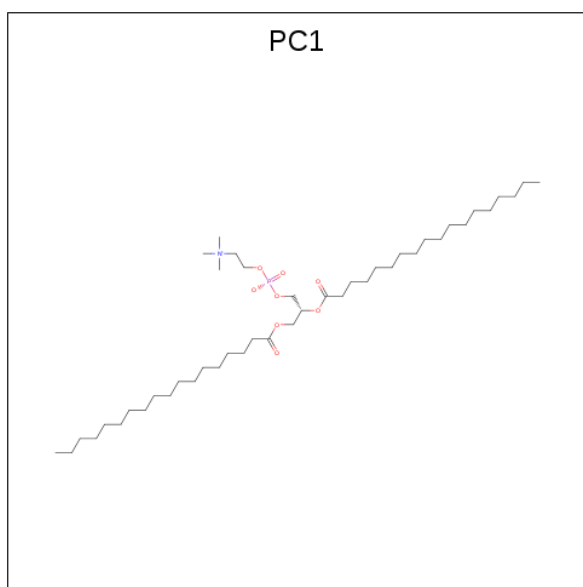
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	CYS	conflict	UNP Q7NDN8
A	135	CYS	VAL	engineered mutation	UNP Q7NDN8
B	27	SER	CYS	conflict	UNP Q7NDN8
B	135	CYS	VAL	engineered mutation	UNP Q7NDN8
C	27	SER	CYS	conflict	UNP Q7NDN8
C	135	CYS	VAL	engineered mutation	UNP Q7NDN8
D	27	SER	CYS	conflict	UNP Q7NDN8
D	135	CYS	VAL	engineered mutation	UNP Q7NDN8
E	27	SER	CYS	conflict	UNP Q7NDN8
E	135	CYS	VAL	engineered mutation	UNP Q7NDN8

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



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

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	A	1	Total	C	O			0	0
			27	23	4				
3	A	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	B	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	B	1	Total	C	O			0	0
			26	22	4				
3	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	C	1	Total	C	O			0	0
			27	23	4				
3	D	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	D	1	Total	C	N	O	P	0	0
			39	29	1	8	1		
3	D	1	Total	C	O			0	0
			22	18	4				
3	E	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
3	E	1	Total	C	N	O	P	0	0
			39	29	1	8	1		

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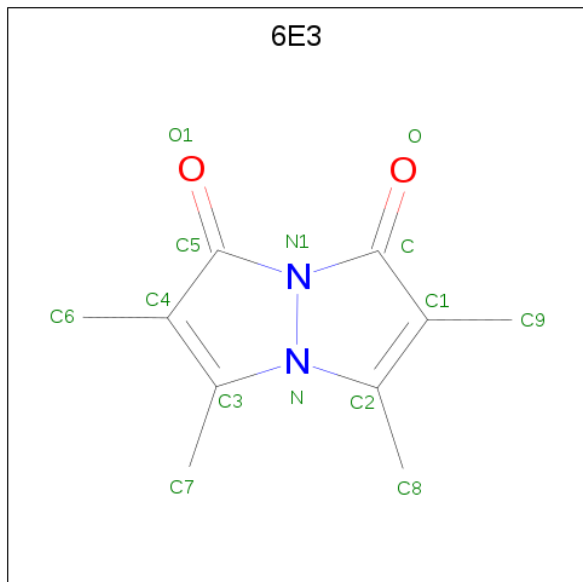
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			27	23	4		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	C	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is 2,3,5,6-tetramethyl-1H,7H-pyrazolo[1,2-a]pyrazole-1,7-dione (three-letter code: 6E3) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			25	10	11	2	2		
5	D	1	Total	C	H	N	O	0	0
			25	10	11	2	2		

- Molecule 6 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Br	0	0
			1	1		
6	A	1	Total	Br	0	0
			1	1		
6	D	1	Total	Br	0	0
			1	1		
6	C	1	Total	Br	0	0
			1	1		
6	E	1	Total	Br	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	Na 1	0	0
7	C	1	Total 1	Na 1	0	0
7	E	1	Total 1	Na 1	0	0

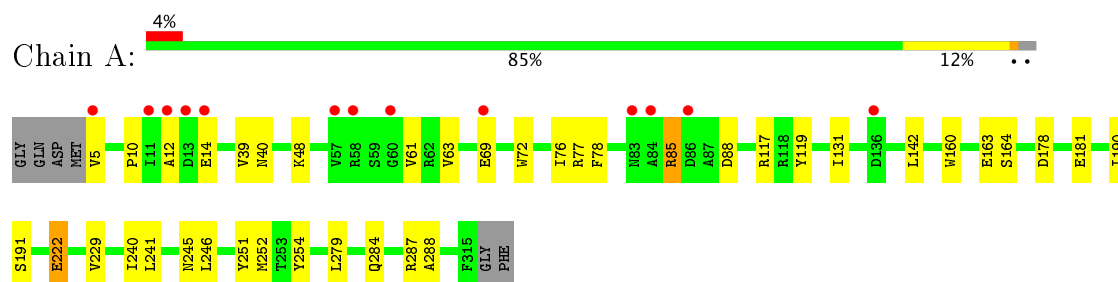
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	26	Total 26	O 26	0	0
8	B	33	Total 33	O 33	0	0
8	C	28	Total 28	O 28	0	0
8	D	29	Total 29	O 29	0	0
8	E	29	Total 29	O 29	0	0

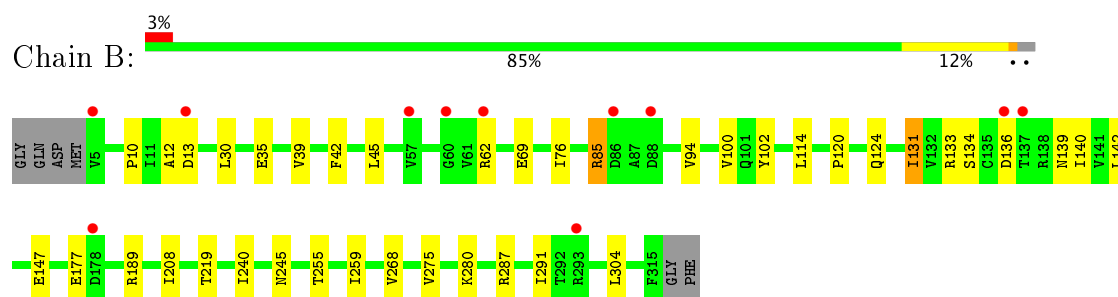
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

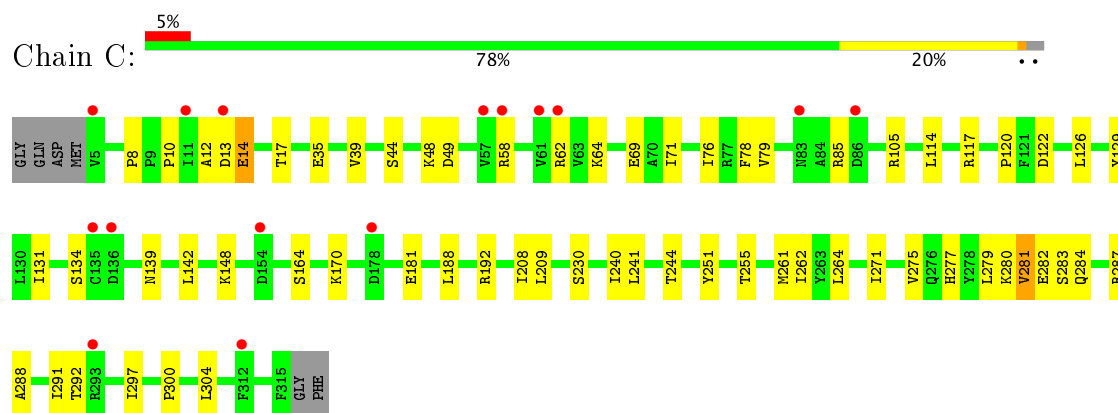
- Molecule 1: Proton-gated ion channel



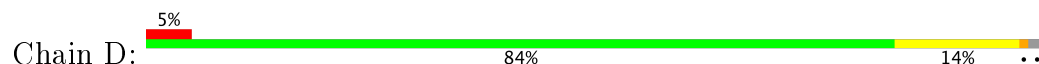
- Molecule 1: Proton-gated ion channel

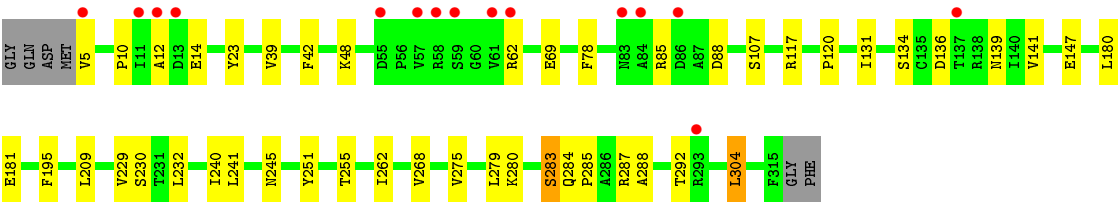


- Molecule 1: Proton-gated ion channel

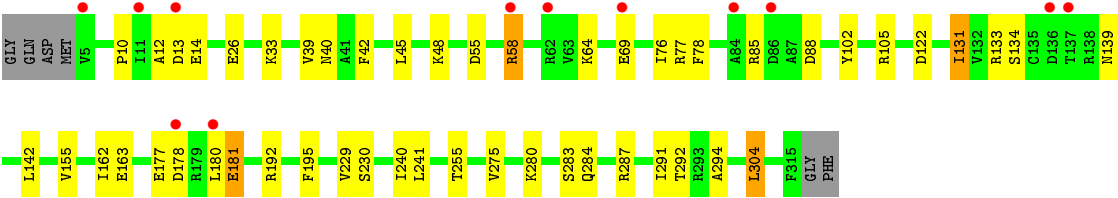
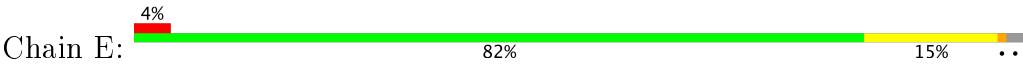


- Molecule 1: Proton-gated ion channel





● Molecule 1: Proton-gated ion channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.03Å 134.07Å 159.94Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 12.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (12.00-2.60) 99.8 (12.00-2.60)	Depositor EDS
$R_{merge}$	3.60	Depositor
$R_{sym}$	5.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.203 , 0.237 0.217 , 0.254	Depositor DCC
$R_{free}$ test set	5709 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 77.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: 6E3, NA, PC1, LMT, BR, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/2592	0.70	0/3543
1	B	0.48	0/2601	0.68	0/3554
1	C	0.49	0/2601	0.71	0/3554
1	D	0.48	0/2601	0.70	0/3554
1	E	0.45	0/2601	0.68	0/3554
All	All	0.48	0/12996	0.70	0/17759

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2524	0	2540	24	0
1	B	2533	0	2553	33	0
1	C	2533	0	2553	32	0
1	D	2533	0	2552	24	0
1	E	2533	0	2553	28	0
2	A	70	0	92	6	0
2	B	35	0	46	3	0
2	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	70	0	92	3	0
3	A	113	0	158	3	0
3	B	112	0	157	6	0
3	C	113	0	158	4	0
3	D	108	0	149	5	0
3	E	113	0	158	5	0
4	A	12	9	9	14	0
4	B	4	3	3	3	0
4	C	8	6	6	3	0
4	D	8	6	6	2	0
4	E	8	6	6	2	0
5	A	14	11	0	1	0
5	D	14	11	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	A	26	0	0	2	0
8	B	33	0	0	3	0
8	C	28	0	0	0	0
8	D	29	0	0	1	0
8	E	29	0	0	0	0
All	All	13647	52	13837	146	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 5.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG21	4:A:505:ACT:H1	1.27	1.14
1:D:131:ILE:HG21	4:D:608:ACT:H2	1.35	1.07
1:A:85:ARG:NH2	4:A:509:ACT:H3	1.88	0.88
3:A:504:PC1:H32	8:A:602:HOH:O	1.82	0.80
1:B:133:ARG:HH12	1:B:177:GLU:HB2	1.53	0.73
1:B:10:PRO:HB2	1:B:12:ALA:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:510:ACT:CH3	1:B:131:ILE:HG21	2.20	0.70
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.54	0.69
1:C:280[A]:LYS:O	1:C:281:VAL:HB	1.93	0.69
1:B:219:THR:HA	1:B:280[A]:LYS:NZ	2.08	0.69
4:A:510:ACT:H3	1:B:131:ILE:HG12	1.76	0.67
3:D:602:PC1:H232	3:D:602:PC1:H31	1.76	0.66
1:A:85:ARG:HH22	4:A:509:ACT:H3	1.58	0.66
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.62	0.65
1:C:280[B]:LYS:O	1:C:281:VAL:HB	1.97	0.64
1:B:42:PHE:HZ	4:C:608:ACT:O	1.81	0.64
1:B:76:ILE:HD12	1:B:142:LEU:HD21	1.78	0.64
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.62	0.64
1:C:78:PHE:CE2	1:C:85:ARG:HD3	2.33	0.64
1:B:219:THR:HA	1:B:280[A]:LYS:HZ1	1.65	0.62
1:D:10:PRO:HB2	1:D:12:ALA:O	2.00	0.61
1:A:131:ILE:CG2	4:A:505:ACT:H1	2.18	0.61
1:A:10:PRO:HB2	1:A:12:ALA:O	2.02	0.60
4:A:505:ACT:O	1:E:42:PHE:CZ	2.56	0.58
4:A:505:ACT:H3	1:E:105:ARG:NH1	2.18	0.58
1:A:85:ARG:HH22	4:A:509:ACT:CH3	2.16	0.58
1:B:85:ARG:HH22	4:B:607:ACT:H1	1.67	0.58
1:E:122:ASP:OD1	1:E:192:ARG:HD2	2.04	0.57
1:E:131:ILE:HG21	4:E:401:ACT:H2	1.85	0.56
1:E:76:ILE:HD12	1:E:142:LEU:HD21	1.87	0.56
1:C:10:PRO:HB2	1:C:12:ALA:O	2.05	0.56
1:D:120:PRO:HD3	1:D:255:THR:OG1	2.06	0.56
1:A:77:ARG:HH21	4:A:505:ACT:C	2.20	0.55
1:B:245:ASN:HB3	8:B:703:HOH:O	2.06	0.55
1:A:279:LEU:HB2	1:A:288:ALA:HB2	1.90	0.54
1:A:85:ARG:HH21	4:A:509:ACT:H3	1.70	0.54
1:E:275:VAL:HG22	3:E:404:PC1:H221	1.89	0.54
1:C:277:HIS:O	1:C:280[B]:LYS:O	2.25	0.53
3:B:601:PC1:H31	8:B:708:HOH:O	2.09	0.53
1:D:245:ASN:HB3	8:D:711:HOH:O	2.09	0.53
1:A:160:TRP:CE3	1:A:190:ILE:HD12	2.44	0.53
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.39	0.53
1:D:268:VAL:HG11	3:D:603:PC1:H281	1.91	0.52
1:E:26:GLU:HB2	1:E:40:ASN:HB3	1.92	0.52
1:B:42:PHE:CZ	4:C:608:ACT:O	2.60	0.51
1:C:134:SER:HB3	1:C:139:ASN:HA	1.92	0.51
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:SER:HB3	1:E:139:ASN:HA	1.91	0.51
1:B:76:ILE:H	4:B:607:ACT:H2	1.76	0.51
1:C:277:HIS:O	1:C:280[A]:LYS:O	2.28	0.51
1:B:268:VAL:HG11	3:B:604:PC1:H281	1.93	0.50
2:A:501:LMT:H6E	2:B:602:LMT:H6'2	1.94	0.50
1:A:117:ARG:HG3	1:A:251:TYR:CD2	2.46	0.50
1:C:297:ILE:O	1:C:300:PRO:HD2	2.12	0.50
1:E:155:VAL:HG12	1:E:162:ILE:HD13	1.94	0.49
1:D:23:TYR:HB3	1:D:42:PHE:HB2	1.95	0.49
2:A:506:LMT:H51	2:B:602:LMT:H82	1.93	0.49
1:C:35:GLU:HG2	1:C:114:LEU:HG	1.93	0.49
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.44	0.49
1:A:119:TYR:CE2	1:A:246:LEU:HD21	2.48	0.49
1:B:94:VAL:HG22	1:B:100:VAL:HG22	1.94	0.49
1:E:291:ILE:HG23	3:E:406:PC1:H232	1.94	0.49
1:A:241:LEU:HD22	1:B:240:ILE:HG12	1.96	0.48
1:A:229:VAL:HG11	1:E:230:SER:HB2	1.95	0.48
1:A:245:ASN:HB3	8:A:605:HOH:O	2.12	0.48
1:D:241:LEU:HD22	1:E:240:ILE:HG12	1.95	0.48
1:D:209:LEU:HD13	1:D:262:ILE:HG23	1.95	0.48
1:E:133:ARG:HH12	1:E:177:GLU:HB2	1.78	0.47
1:B:275:VAL:HG22	3:B:601:PC1:H221	1.97	0.47
1:E:55:ASP:HB3	1:E:58:ARG:HG3	1.94	0.47
1:E:77:ARG:HH21	4:E:401:ACT:C	2.28	0.47
1:C:261:MET:HA	1:C:264:LEU:HD12	1.96	0.47
1:D:275:VAL:HG22	3:D:601:PC1:H221	1.96	0.47
1:C:275:VAL:HG22	3:C:601:PC1:H221	1.95	0.47
1:D:39:VAL:O	1:D:107:SER:HA	2.15	0.47
1:D:304:LEU:HD23	3:E:404:PC1:H211	1.96	0.47
1:B:35:GLU:HA	1:B:114:LEU:CD1	2.45	0.47
1:B:35:GLU:HA	1:B:114:LEU:HD12	1.96	0.47
1:D:139:ASN:HD22	1:D:180:LEU:HD13	1.80	0.46
3:D:602:PC1:H152	3:D:602:PC1:H11	1.97	0.46
1:B:85:ARG:NH2	4:B:607:ACT:H1	2.30	0.46
1:C:280[A]:LYS:O	1:C:281:VAL:CB	2.63	0.45
1:D:117:ARG:HG3	1:D:251:TYR:CD2	2.51	0.45
1:B:255:THR:HG22	1:B:259:ILE:CD1	2.46	0.45
4:A:510:ACT:H2	1:B:131:ILE:HG21	1.97	0.45
1:C:241:LEU:HD22	1:D:240:ILE:HG12	1.98	0.45
1:A:63:VAL:HG21	1:B:136:ASP:HB3	1.99	0.45
1:C:8:PRO:HB3	1:C:49:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:SER:HB2	1:E:229:VAL:HG11	1.99	0.45
1:C:279:LEU:HB2	1:C:288:ALA:HB2	1.97	0.45
1:A:254:TYR:HE1	3:A:502:PC1:H332	1.82	0.45
1:C:120:PRO:HD3	1:C:255:THR:OG1	2.17	0.44
1:C:76:ILE:HD12	1:C:142:LEU:HD21	1.98	0.44
3:C:603:PC1:H322	3:C:603:PC1:H32	1.75	0.44
1:C:131:ILE:HG21	4:C:608:ACT:H1	1.98	0.44
1:A:222:GLU:H	1:A:222:GLU:CD	2.20	0.44
1:B:85:ARG:HG2	6:B:605:BR:BR	2.73	0.44
4:A:510:ACT:H2	1:B:131:ILE:CG2	2.48	0.44
1:B:120:PRO:HD3	1:B:255:THR:OG1	2.18	0.44
1:C:12:ALA:HB3	1:C:14:GLU:HG3	1.98	0.44
1:E:12:ALA:HB3	1:E:14:GLU:HG3	1.99	0.44
1:E:10:PRO:HB2	1:E:12:ALA:O	2.18	0.44
1:A:240:ILE:HG12	1:E:241:LEU:HD22	2.00	0.44
4:A:510:ACT:CH3	1:B:131:ILE:CG2	2.93	0.44
1:B:134:SER:HB3	1:B:139:ASN:HA	2.00	0.44
3:B:603:PC1:H321	3:B:603:PC1:H241	1.99	0.44
1:D:195:PHE:C	1:D:195:PHE:CD1	2.91	0.44
1:B:291:ILE:HG12	3:B:604:PC1:H31	2.00	0.43
2:A:501:LMT:H82	2:A:506:LMT:H52	1.99	0.43
1:B:219:THR:HA	1:B:280[A]:LYS:HZ3	1.83	0.43
1:C:280[B]:LYS:O	1:C:281:VAL:CB	2.66	0.43
1:B:45:LEU:HB2	1:B:102:TYR:HB3	2.01	0.43
1:B:134:SER:HA	1:B:140:ILE:HD12	2.01	0.43
1:E:275:VAL:HG13	3:E:404:PC1:H32	2.01	0.43
1:A:76:ILE:HD12	1:A:142:LEU:HD21	2.00	0.43
1:C:208:ILE:HG22	1:D:232:LEU:HD21	2.01	0.42
1:C:291:ILE:HG23	3:C:604:PC1:H251	2.00	0.42
1:C:117:ARG:HG3	1:C:251:TYR:CD2	2.55	0.42
1:E:131:ILE:HD11	1:E:181:GLU:HG2	2.00	0.42
3:D:602:PC1:H322	3:D:602:PC1:H31	1.88	0.42
1:E:294:ALA:HB3	3:E:406:PC1:H231	2.01	0.42
1:E:33:LYS:HD3	2:E:403:LMT:H6'2	2.02	0.42
2:A:506:LMT:H122	2:B:602:LMT:H12	2.01	0.42
1:C:240:ILE:O	1:C:244:THR:HG23	2.19	0.42
3:A:504:PC1:H2I1	1:E:304:LEU:HD23	2.02	0.42
1:C:105:ARG:HD2	4:D:608:ACT:OXT	2.20	0.42
1:D:279:LEU:HB2	1:D:288:ALA:HB2	2.00	0.42
2:A:506:LMT:H41	2:E:403:LMT:H102	2.01	0.42
1:B:255:THR:HG22	1:B:259:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HB2	1:C:188:LEU:HB3	2.02	0.41
1:C:209:LEU:HD13	1:C:262:ILE:HG23	2.02	0.41
1:C:271:ILE:O	1:C:275:VAL:HG23	2.20	0.41
1:D:134:SER:HB3	1:D:139:ASN:HA	2.02	0.41
1:A:72:TRP:HE1	5:A:507:6E3:C8	2.33	0.41
3:B:601:PC1:C3	8:B:708:HOH:O	2.67	0.41
1:C:79:VAL:HB	1:C:129:TYR:HB2	2.02	0.41
1:D:69:GLU:CD	1:D:69:GLU:H	2.23	0.41
1:D:283:SER:C	1:D:285:PRO:HD3	2.42	0.41
1:A:163:GLU:OE2	1:A:191:SER:HB3	2.21	0.41
1:B:114:LEU:HA	1:B:124:GLN:OE1	2.21	0.40
3:C:603:PC1:H281	3:C:603:PC1:H361	2.03	0.40
1:A:252:MET:HE2	1:E:195:PHE:CZ	2.57	0.40
1:E:45:LEU:HB2	1:E:102:TYR:HB3	2.03	0.40
2:A:506:LMT:H61	2:E:403:LMT:H82	2.04	0.40
1:C:122:ASP:OD1	1:C:192:ARG:HD2	2.22	0.40
1:C:230:SER:HB2	1:D:229:VAL:HG11	2.02	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	309/317 (98%)	297 (96%)	12 (4%)	0	100	100
1	B	310/317 (98%)	297 (96%)	13 (4%)	0	100	100
1	C	310/317 (98%)	292 (94%)	17 (6%)	1 (0%)	44	70
1	D	310/317 (98%)	303 (98%)	7 (2%)	0	100	100
1	E	310/317 (98%)	298 (96%)	12 (4%)	0	100	100
All	All	1549/1585 (98%)	1487 (96%)	61 (4%)	1 (0%)	55	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	281	VAL

### 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	280/284 (99%)	265 (95%)	15 (5%)	26	49
1	B	281/284 (99%)	269 (96%)	12 (4%)	33	61
1	C	281/284 (99%)	260 (92%)	21 (8%)	16	31
1	D	281/284 (99%)	265 (94%)	16 (6%)	24	47
1	E	281/284 (99%)	261 (93%)	20 (7%)	17	34
All	All	1404/1420 (99%)	1320 (94%)	84 (6%)	23	44

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	14	GLU
1	A	39	VAL
1	A	40	ASN
1	A	48	LYS
1	A	61	VAL
1	A	69	GLU
1	A	85	ARG
1	A	88	ASP
1	A	164	SER
1	A	178	ASP
1	A	181	GLU
1	A	222	GLU
1	A	284	GLN
1	A	287	ARG
1	B	13	ASP
1	B	30	LEU

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Mol	Chain	Res	Type
1	B	39	VAL
1	B	62	ARG
1	B	69	GLU
1	B	85	ARG
1	B	131	ILE
1	B	147	GLU
1	B	189	ARG
1	B	208	ILE
1	B	287	ARG
1	B	304	LEU
1	C	13	ASP
1	C	14	GLU
1	C	17	THR
1	C	39	VAL
1	C	44	SER
1	C	48	LYS
1	C	58	ARG
1	C	62	ARG
1	C	64	LYS
1	C	69	GLU
1	C	71	ILE
1	C	148	LYS
1	C	164	SER
1	C	170	LYS
1	C	181	GLU
1	C	282	GLU
1	C	283	SER
1	C	284	GLN
1	C	287	ARG
1	C	292	THR
1	C	304	LEU
1	D	5	VAL
1	D	14	GLU
1	D	48	LYS
1	D	62	ARG
1	D	88	ASP
1	D	136	ASP
1	D	141	VAL
1	D	147	GLU
1	D	181	GLU
1	D	280[A]	LYS
1	D	280[B]	LYS

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Mol	Chain	Res	Type
1	D	283	SER
1	D	284	GLN
1	D	287	ARG
1	D	292	THR
1	D	304	LEU
1	E	13	ASP
1	E	39	VAL
1	E	48	LYS
1	E	58	ARG
1	E	64	LYS
1	E	69	GLU
1	E	88	ASP
1	E	131	ILE
1	E	163	GLU
1	E	178	ASP
1	E	180	LEU
1	E	181	GLU
1	E	255	THR
1	E	280[A]	LYS
1	E	280[B]	LYS
1	E	283	SER
1	E	284	GLN
1	E	287	ARG
1	E	292	THR
1	E	304	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 42 ligands modelled in this entry, 9 are monoatomic - leaving 33 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
2	LMT	A	501	-	36,36,36	1.18	6 (16%)	47,47,47	1.58	10 (21%)
3	PC1	A	502	-	38,38,53	1.37	7 (18%)	43,46,61	1.15	2 (4%)
3	PC1	A	503	-	26,26,53	1.09	3 (11%)	28,28,61	0.91	2 (7%)
3	PC1	A	504	-	46,46,53	1.24	6 (13%)	51,54,61	1.11	3 (5%)
4	ACT	A	505	-	1,3,3	2.16	1 (100%)	0,3,3	0.00	-
2	LMT	A	506	-	36,36,36	1.45	8 (22%)	47,47,47	1.36	4 (8%)
5	6E3	A	507	1	10,15,15	1.82	3 (30%)	6,24,24	3.10	2 (33%)
4	ACT	A	509	-	1,3,3	0.26	0	0,3,3	0.00	-
4	ACT	A	510	-	1,3,3	1.75	0	0,3,3	0.00	-
3	PC1	B	601	-	46,46,53	1.18	4 (8%)	51,54,61	1.01	2 (3%)
2	LMT	B	602	-	36,36,36	1.39	6 (16%)	47,47,47	1.53	8 (17%)
3	PC1	B	603	-	38,38,53	1.29	6 (15%)	43,46,61	1.16	2 (4%)
3	PC1	B	604	-	25,25,53	0.86	1 (4%)	26,26,61	1.08	2 (7%)
4	ACT	B	607	-	1,3,3	1.60	0	0,3,3	0.00	-
3	PC1	C	601	-	46,46,53	1.32	7 (15%)	51,54,61	1.14	2 (3%)
2	LMT	C	602	-	36,36,36	1.42	7 (19%)	47,47,47	1.57	9 (19%)
3	PC1	C	603	-	38,38,53	1.31	6 (15%)	43,46,61	1.11	3 (6%)
3	PC1	C	604	-	26,26,53	1.08	2 (7%)	28,28,61	0.84	1 (3%)
4	ACT	C	607	-	1,3,3	4.49	1 (100%)	0,3,3	0.00	-
4	ACT	C	608	-	1,3,3	3.25	1 (100%)	0,3,3	0.00	-
3	PC1	D	601	-	46,46,53	1.33	7 (15%)	51,54,61	1.31	5 (9%)
3	PC1	D	602	-	38,38,53	1.31	5 (13%)	43,46,61	1.33	4 (9%)
3	PC1	D	603	-	17,20,53	0.69	0	16,20,61	0.80	0
5	6E3	D	604	1	10,15,15	1.83	3 (30%)	6,24,24	3.41	4 (66%)
4	ACT	D	607	-	1,3,3	5.22	1 (100%)	0,3,3	0.00	-
4	ACT	D	608	-	1,3,3	1.92	0	0,3,3	0.00	-
4	ACT	E	401	-	1,3,3	4.68	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LMT	E	402	-	36,36,36	1.52	7 (19%)	47,47,47	1.45	10 (21%)
2	LMT	E	403	-	36,36,36	1.43	8 (22%)	47,47,47	1.19	5 (10%)
3	PC1	E	404	-	46,46,53	1.26	6 (13%)	51,54,61	1.00	3 (5%)
3	PC1	E	405	-	38,38,53	1.29	5 (13%)	43,46,61	1.08	1 (2%)
3	PC1	E	406	-	26,26,53	0.97	1 (3%)	28,28,61	0.78	0
4	ACT	E	409	-	1,3,3	4.70	1 (100%)	0,3,3	0.00	-

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
2	LMT	A	501	-	-	0/21/61/61	0/2/2/2
3	PC1	A	502	-	-	0/42/42/57	0/0/0/0
3	PC1	A	503	-	-	0/27/27/57	0/0/0/0
3	PC1	A	504	-	-	0/50/50/57	0/0/0/0
4	ACT	A	505	-	-	0/0/0/0	0/0/0/0
2	LMT	A	506	-	-	0/21/61/61	0/2/2/2
5	6E3	A	507	1	-	0/0/0/0	0/2/2/2
4	ACT	A	509	-	-	0/0/0/0	0/0/0/0
4	ACT	A	510	-	-	0/0/0/0	0/0/0/0
3	PC1	B	601	-	-	0/50/50/57	0/0/0/0
2	LMT	B	602	-	-	0/21/61/61	0/2/2/2
3	PC1	B	603	-	-	0/42/42/57	0/0/0/0
3	PC1	B	604	-	-	0/25/25/57	0/0/0/0
4	ACT	B	607	-	-	0/0/0/0	0/0/0/0
3	PC1	C	601	-	-	0/50/50/57	0/0/0/0
2	LMT	C	602	-	-	0/21/61/61	0/2/2/2
3	PC1	C	603	-	-	0/42/42/57	0/0/0/0
3	PC1	C	604	-	-	0/27/27/57	0/0/0/0
4	ACT	C	607	-	-	0/0/0/0	0/0/0/0
4	ACT	C	608	-	-	0/0/0/0	0/0/0/0
3	PC1	D	601	-	-	0/50/50/57	0/0/0/0
3	PC1	D	602	-	-	0/42/42/57	0/0/0/0
3	PC1	D	603	-	-	0/15/17/57	0/0/0/0
5	6E3	D	604	1	-	0/0/0/0	0/2/2/2
4	ACT	D	607	-	-	0/0/0/0	0/0/0/0
4	ACT	D	608	-	-	0/0/0/0	0/0/0/0
4	ACT	E	401	-	-	0/0/0/0	0/0/0/0
2	LMT	E	402	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	E	403	-	-	0/21/61/61	0/2/2/2
3	PC1	E	404	-	-	0/50/50/57	0/0/0/0
3	PC1	E	405	-	-	0/42/42/57	0/0/0/0
3	PC1	E	406	-	-	0/27/27/57	0/0/0/0
4	ACT	E	409	-	-	0/0/0/0	0/0/0/0

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	507	6E3	C3-C4	-2.15	1.35	1.39
5	D	604	6E3	C3-C4	-2.06	1.35	1.39
2	C	602	LMT	C3'-C2'	2.00	1.57	1.52
3	C	603	PC1	C12-N	2.01	1.58	1.51
2	E	403	LMT	C1'-C2'	2.03	1.58	1.52
3	B	601	PC1	P-O11	2.04	1.67	1.59
2	A	501	LMT	C3B-C2B	2.05	1.57	1.52
2	B	602	LMT	C3B-C2B	2.05	1.57	1.52
3	A	503	PC1	O21-C21	2.05	1.40	1.34
3	E	404	PC1	P-O11	2.07	1.68	1.59
3	A	504	PC1	C3-C2	2.09	1.56	1.50
3	D	602	PC1	C1-C2	2.10	1.56	1.50
2	A	501	LMT	C3'-C4'	2.10	1.58	1.52
3	C	601	PC1	O21-C21	2.11	1.40	1.34
2	E	403	LMT	C3'-C2'	2.11	1.57	1.52
3	A	503	PC1	O31-C31	2.11	1.39	1.33
3	C	601	PC1	O31-C31	2.12	1.39	1.33
2	A	506	LMT	C4'-C5'	2.14	1.58	1.52
3	C	603	PC1	P-O11	2.14	1.68	1.59
3	A	502	PC1	O21-C21	2.14	1.40	1.34
3	A	504	PC1	C1-C2	2.15	1.56	1.50
4	A	505	ACT	CH3-C	2.16	1.51	1.48
3	B	603	PC1	C3-C2	2.17	1.56	1.50
3	A	502	PC1	C12-N	2.17	1.58	1.51
3	C	603	PC1	C3-C2	2.17	1.56	1.50
2	C	602	LMT	C1B-C2B	2.17	1.58	1.52
2	E	402	LMT	C3'-C2'	2.18	1.57	1.52
3	E	405	PC1	O21-C21	2.19	1.40	1.34
2	A	501	LMT	C4B-C5B	2.19	1.57	1.53
3	E	405	PC1	C12-N	2.20	1.58	1.51
3	B	603	PC1	P-O11	2.21	1.68	1.59
3	D	602	PC1	P-O11	2.22	1.68	1.59
3	E	405	PC1	C1-C2	2.22	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	PC1	O21-C21	2.23	1.40	1.34
3	D	601	PC1	O31-C31	2.23	1.39	1.33
2	C	602	LMT	O5'-C1'	2.24	1.47	1.41
3	D	602	PC1	C12-C11	2.27	1.58	1.51
2	A	506	LMT	C1B-C2B	2.29	1.59	1.52
2	A	501	LMT	C1'-C2'	2.29	1.59	1.52
3	C	603	PC1	C1-C2	2.31	1.57	1.50
3	A	502	PC1	P-O11	2.31	1.69	1.59
3	A	504	PC1	P-O11	2.31	1.69	1.59
3	D	601	PC1	C12-N	2.32	1.59	1.51
2	A	501	LMT	C4B-C3B	2.33	1.58	1.52
3	B	601	PC1	C12-N	2.34	1.59	1.51
3	C	601	PC1	P-O11	2.34	1.69	1.59
3	D	601	PC1	P-O11	2.35	1.69	1.59
3	E	404	PC1	C1-C2	2.35	1.57	1.50
3	C	601	PC1	C12-C11	2.36	1.59	1.51
2	A	506	LMT	C3B-C2B	2.36	1.58	1.52
3	E	404	PC1	C12-N	2.37	1.59	1.51
3	C	604	PC1	O31-C31	2.37	1.40	1.33
3	A	502	PC1	C3-C2	2.40	1.57	1.50
2	E	403	LMT	C4B-C3B	2.42	1.58	1.52
3	B	604	PC1	O31-C31	2.43	1.40	1.33
3	E	405	PC1	C12-C11	2.43	1.59	1.51
3	A	502	PC1	C12-C11	2.43	1.59	1.51
3	A	504	PC1	C12-N	2.44	1.59	1.51
3	C	603	PC1	C12-C11	2.45	1.59	1.51
2	A	501	LMT	C3'-C2'	2.45	1.58	1.52
2	B	602	LMT	C3'-C4'	2.46	1.59	1.52
3	D	602	PC1	O21-C21	2.47	1.41	1.34
3	B	603	PC1	C12-C11	2.47	1.59	1.51
2	E	403	LMT	C1B-C2B	2.47	1.59	1.52
2	E	403	LMT	C3B-C2B	2.49	1.58	1.52
3	B	601	PC1	C12-C11	2.49	1.59	1.51
2	A	506	LMT	C1'-C2'	2.50	1.59	1.52
3	E	404	PC1	C3-C2	2.50	1.57	1.50
2	E	402	LMT	C3B-C2B	2.50	1.58	1.52
2	C	602	LMT	C3B-C2B	2.51	1.58	1.52
3	A	504	PC1	C12-C11	2.56	1.59	1.51
2	E	403	LMT	C4'-C5'	2.62	1.60	1.52
3	B	603	PC1	C1-C2	2.64	1.58	1.50
2	B	602	LMT	C1'-C2'	2.64	1.60	1.52
3	E	404	PC1	C12-C11	2.66	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	PC1	C12-C11	2.68	1.60	1.51
2	E	402	LMT	C4B-C3B	2.73	1.59	1.52
3	A	502	PC1	C1-C2	2.77	1.58	1.50
2	C	602	LMT	C4B-C3B	2.79	1.59	1.52
2	E	402	LMT	C4B-C5B	2.89	1.59	1.53
2	E	402	LMT	C1B-C2B	2.92	1.60	1.52
3	D	601	PC1	C1-C2	2.98	1.59	1.50
2	C	602	LMT	C4B-C5B	2.98	1.59	1.53
2	E	402	LMT	C4'-C5'	3.00	1.61	1.52
2	A	506	LMT	C4B-C3B	3.01	1.60	1.52
2	A	506	LMT	C3'-C2'	3.02	1.60	1.52
3	C	601	PC1	C3-C2	3.02	1.59	1.50
2	B	602	LMT	C4B-C3B	3.02	1.60	1.52
2	B	602	LMT	C4B-C5B	3.06	1.59	1.53
3	E	406	PC1	C3-C2	3.07	1.58	1.50
3	C	601	PC1	C1-C2	3.08	1.59	1.50
2	C	602	LMT	C1'-C2'	3.09	1.61	1.52
3	C	604	PC1	C3-C2	3.14	1.58	1.50
4	C	608	ACT	CH3-C	3.25	1.52	1.48
3	A	503	PC1	C3-C2	3.28	1.58	1.50
2	B	602	LMT	C3'-C2'	3.29	1.60	1.52
2	A	506	LMT	C3'-C4'	3.29	1.61	1.52
2	A	506	LMT	C4B-C5B	3.33	1.60	1.53
3	D	601	PC1	C3-C2	3.40	1.60	1.50
2	E	403	LMT	C3'-C4'	3.40	1.61	1.52
5	A	507	6E3	C-C1	3.45	1.47	1.38
5	D	604	6E3	C-C1	3.54	1.47	1.38
2	E	403	LMT	C4B-C5B	3.56	1.60	1.53
2	E	402	LMT	C3'-C4'	3.86	1.62	1.52
5	D	604	6E3	C5-C4	3.89	1.48	1.38
5	A	507	6E3	C5-C4	3.90	1.48	1.38
3	B	603	PC1	P-O13	4.07	1.76	1.59
3	C	601	PC1	P-O13	4.27	1.77	1.59
3	A	502	PC1	P-O13	4.33	1.77	1.59
3	B	601	PC1	P-O13	4.35	1.77	1.59
3	C	603	PC1	P-O13	4.41	1.77	1.59
3	D	601	PC1	P-O13	4.45	1.78	1.59
4	C	607	ACT	CH3-C	4.49	1.54	1.48
3	E	405	PC1	P-O13	4.49	1.78	1.59
3	D	602	PC1	P-O13	4.52	1.78	1.59
4	E	401	ACT	CH3-C	4.68	1.54	1.48
4	E	409	ACT	CH3-C	4.70	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	404	PC1	P-O13	4.71	1.79	1.59
3	A	504	PC1	P-O13	4.73	1.79	1.59
4	D	607	ACT	CH3-C	5.22	1.55	1.48

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	6E3	C9-C1-C	-6.18	118.68	128.40
5	A	507	6E3	C9-C1-C	-5.66	119.51	128.40
5	D	604	6E3	C6-C4-C5	-4.58	121.20	128.40
5	A	507	6E3	C6-C4-C5	-4.57	121.22	128.40
2	C	602	LMT	C2'-C3'-C4'	-3.88	101.56	109.61
2	A	501	LMT	C3B-C4B-C5B	-3.11	104.75	110.22
2	A	501	LMT	O2'-C2'-C3'	-3.09	103.63	110.36
3	D	601	PC1	O31-C31-O32	-3.05	115.99	123.55
2	A	501	LMT	O5'-C5'-C4'	-3.00	103.61	109.75
2	B	602	LMT	O3'-C3'-C4'	-2.90	103.27	109.87
2	A	501	LMT	C1B-O1B-C4'	-2.89	110.95	118.00
2	A	506	LMT	O2'-C2'-C3'	-2.76	104.35	110.36
2	B	602	LMT	O2B-C2B-C3B	-2.75	104.36	110.36
2	E	403	LMT	O1'-C1'-C2'	-2.75	103.74	108.23
3	D	602	PC1	O31-C31-O32	-2.75	116.73	123.55
2	C	602	LMT	C1B-O1B-C4'	-2.58	111.72	118.00
2	A	501	LMT	O3'-C3'-C4'	-2.47	104.24	109.87
2	C	602	LMT	O3B-C3B-C4B	-2.46	105.01	110.36
2	E	403	LMT	O2B-C2B-C3B	-2.35	105.25	110.36
2	E	402	LMT	O2'-C2'-C3'	-2.29	105.37	110.36
5	D	604	6E3	C9-C1-C2	-2.28	123.86	127.10
2	B	602	LMT	O2'-C2'-C3'	-2.27	105.42	110.36
2	E	403	LMT	C3'-C4'-C5'	-2.27	106.07	110.88
3	B	604	PC1	O31-C31-O32	-2.26	117.94	123.55
2	E	402	LMT	O2B-C2B-C3B	-2.25	105.46	110.36
2	A	501	LMT	O1'-C1'-C2'	-2.22	104.61	108.23
2	A	501	LMT	C4B-C3B-C2B	-2.22	106.92	110.84
2	E	403	LMT	O2'-C2'-C3'	-2.20	105.57	110.36
2	B	602	LMT	O3B-C3B-C4B	-2.15	105.69	110.36
3	C	603	PC1	O31-C31-O32	-2.12	118.29	123.55
2	E	402	LMT	O3B-C3B-C4B	-2.10	105.78	110.36
2	B	602	LMT	O1'-C1'-C2'	-2.10	104.81	108.23
2	C	602	LMT	O5B-C1B-C2B	2.01	114.17	110.30
2	C	602	LMT	O1B-C4'-C5'	2.02	114.32	109.34
3	A	503	PC1	C3-O31-C31	2.02	123.21	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	PC1	C2-O21-C21	2.07	120.52	117.90
2	E	402	LMT	O5B-C5B-C4B	2.07	113.48	109.66
2	E	403	LMT	O1B-C4'-C3'	2.08	112.19	107.19
2	E	402	LMT	C2'-C3'-C4'	2.08	113.92	109.61
5	D	604	6E3	C6-C4-C3	2.14	130.12	127.10
2	C	602	LMT	O5'-C1'-C2'	2.19	114.53	110.30
2	E	402	LMT	O1B-C4'-C3'	2.20	112.50	107.19
3	B	601	PC1	C3-O31-C31	2.24	123.86	117.13
3	D	601	PC1	O31-C31-C32	2.26	118.48	111.90
3	E	404	PC1	C3-O31-C31	2.30	124.04	117.13
3	A	504	PC1	O21-C2-C1	2.30	116.79	108.44
3	E	404	PC1	C2-O21-C21	2.35	123.43	117.88
2	E	402	LMT	O5B-C1B-C2B	2.39	114.91	110.30
2	C	602	LMT	C1B-O5B-C5B	2.43	118.29	113.72
3	C	603	PC1	C3-O31-C31	2.43	124.45	117.13
3	A	503	PC1	C2-O21-C21	2.47	121.03	117.90
2	E	402	LMT	O2B-C2B-C1B	2.50	115.25	110.03
2	A	501	LMT	C1B-O5B-C5B	2.52	118.45	113.72
3	D	602	PC1	C3-O31-C31	2.68	125.18	117.13
2	A	501	LMT	C1'-C2'-C3'	3.10	115.75	109.98
2	B	602	LMT	C1B-O5B-C5B	3.14	119.62	113.72
3	B	604	PC1	C3-O31-C31	3.14	126.23	116.96
2	B	602	LMT	C2'-C3'-C4'	3.17	116.18	109.61
3	A	504	PC1	C2-O21-C21	3.20	125.44	117.88
2	A	501	LMT	O5B-C1B-C2B	3.22	116.50	110.30
3	D	602	PC1	C2-O21-C21	3.24	125.53	117.88
2	A	506	LMT	C1B-O5B-C5B	3.27	119.87	113.72
3	D	601	PC1	C3-O31-C31	3.28	126.99	117.13
3	A	502	PC1	C2-O21-C21	3.37	125.85	117.88
3	B	603	PC1	C2-O21-C21	3.42	125.95	117.88
2	A	506	LMT	C1'-C2'-C3'	3.48	116.44	109.98
2	A	506	LMT	C2'-C3'-C4'	3.67	117.22	109.61
3	D	601	PC1	C2-O21-C21	3.69	126.61	117.88
3	A	504	PC1	O12-P-O14	3.90	132.45	112.28
2	B	602	LMT	C1'-C2'-C3'	3.95	117.32	109.98
2	E	402	LMT	C1-O1'-C1'	3.98	120.70	113.87
3	E	404	PC1	O12-P-O14	3.98	132.88	112.28
3	B	601	PC1	O12-P-O14	3.98	132.89	112.28
3	D	601	PC1	O12-P-O14	4.06	133.29	112.28
3	C	601	PC1	C2-O21-C21	4.11	127.59	117.88
2	C	602	LMT	O1B-C4'-C3'	4.19	117.27	107.19
2	C	602	LMT	C1'-O5'-C5'	4.20	121.62	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	PC1	O12-P-O14	4.23	134.18	112.28
3	E	405	PC1	O12-P-O14	4.24	134.21	112.28
3	D	602	PC1	O12-P-O14	4.31	134.58	112.28
2	E	402	LMT	C1B-O5B-C5B	4.33	121.88	113.72
3	A	502	PC1	O12-P-O14	4.33	134.71	112.28
3	B	603	PC1	O12-P-O14	4.34	134.72	112.28
3	C	601	PC1	O12-P-O14	4.34	134.76	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LMT	2	0
3	A	502	PC1	1	0
3	A	504	PC1	2	0
4	A	505	ACT	5	0
2	A	506	LMT	5	0
5	A	507	6E3	1	0
4	A	509	ACT	4	0
4	A	510	ACT	5	0
3	B	601	PC1	3	0
2	B	602	LMT	3	0
3	B	603	PC1	1	0
3	B	604	PC1	2	0
4	B	607	ACT	3	0
3	C	601	PC1	1	0
3	C	603	PC1	2	0
3	C	604	PC1	1	0
4	C	608	ACT	3	0
3	D	601	PC1	1	0
3	D	602	PC1	3	0
3	D	603	PC1	1	0
4	D	608	ACT	2	0
4	E	401	ACT	2	0
2	E	403	LMT	3	0
3	E	404	PC1	3	0
3	E	406	PC1	2	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<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	311/317 (98%)	-0.27	13 (4%)	37 29	57, 79, 126, 155	0
1	B	311/317 (98%)	-0.31	11 (3%)	44 36	54, 79, 112, 132	0
1	C	311/317 (98%)	-0.20	15 (4%)	31 24	58, 79, 124, 164	0
1	D	311/317 (98%)	-0.21	15 (4%)	31 24	54, 81, 122, 155	0
1	E	311/317 (98%)	-0.21	12 (3%)	40 32	65, 81, 126, 149	0
All	All	1555/1585 (98%)	-0.24	66 (4%)	37 29	54, 80, 123, 164	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	6.2
1	E	5	VAL	5.5
1	C	5	VAL	5.2
1	D	5	VAL	5.1
1	C	58	ARG	5.0
1	D	57	VAL	4.7
1	C	11	ILE	4.6
1	E	11	ILE	4.4
1	D	12	ALA	4.4
1	E	13	ASP	4.3
1	D	58	ARG	4.3
1	A	5	VAL	4.2
1	B	13	ASP	4.2
1	C	13	ASP	4.2
1	D	11	ILE	4.0
1	B	136	ASP	4.0
1	A	11	ILE	4.0
1	D	62	ARG	3.9
1	C	178	ASP	3.9
1	E	58	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	57	VAL	3.8
1	A	84	ALA	3.5
1	A	58	ARG	3.4
1	A	86	ASP	3.3
1	B	178	ASP	3.3
1	D	55	ASP	3.2
1	E	136	ASP	3.1
1	E	62	ARG	3.1
1	E	86	ASP	3.1
1	E	178	ASP	3.1
1	E	137	THR	3.1
1	D	59	SER	3.0
1	D	137	THR	2.9
1	A	14	GLU	2.7
1	D	83	ASN	2.7
1	D	84	ALA	2.6
1	E	180	LEU	2.6
1	B	60	GLY	2.6
1	A	136	ASP	2.6
1	D	13	ASP	2.6
1	B	62	ARG	2.6
1	C	57	VAL	2.4
1	D	86	ASP	2.4
1	C	62	ARG	2.4
1	C	293	ARG	2.4
1	C	136	ASP	2.4
1	A	12	ALA	2.3
1	A	13	ASP	2.3
1	E	84	ALA	2.3
1	C	86	ASP	2.3
1	A	60	GLY	2.3
1	C	312	PHE	2.3
1	C	135	CYS	2.3
1	B	137	THR	2.3
1	C	83	ASN	2.3
1	D	293	ARG	2.3
1	E	69	GLU	2.2
1	B	86	ASP	2.2
1	D	61	VAL	2.1
1	C	61	VAL	2.1
1	A	69	GLU	2.1
1	C	154	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	57	VAL	2.0
1	B	293	ARG	2.0
1	A	83	ASN	2.0
1	B	88	ASP	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<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
4	ACT	D	608	4/4	0.63	0.35	8.03	118,118,122,123	0
4	ACT	A	510	4/4	0.83	0.38	7.92	125,125,128,130	0
2	LMT	A	501	35/35	0.72	0.35	7.73	57,145,160,161	0
2	LMT	B	602	35/35	0.71	0.38	6.76	64,149,169,171	0
2	LMT	E	403	35/35	0.71	0.37	6.73	70,156,174,175	0
2	LMT	A	506	35/35	0.87	0.23	6.31	75,146,162,162	0
2	LMT	C	602	35/35	0.69	0.36	5.99	50,146,167,169	0
2	LMT	E	402	35/35	0.79	0.30	5.37	52,141,164,164	0
3	PC1	B	604	26/54	0.70	0.34	5.24	90,108,125,125	0
5	6E3	D	604	14/14	0.72	0.56	5.11	137,153,156,156	0
3	PC1	E	406	27/54	0.65	0.34	5.10	95,112,134,135	0
3	PC1	A	503	27/54	0.66	0.36	4.82	96,123,134,134	0
5	6E3	A	507	14/14	0.78	0.62	4.32	136,151,152,152	0
3	PC1	D	603	22/54	0.71	0.31	3.93	100,114,133,135	0
3	PC1	B	603	39/54	0.79	0.26	3.61	82,121,151,152	0
3	PC1	C	604	27/54	0.64	0.33	3.50	94,113,132,133	0
4	ACT	A	509	4/4	0.88	0.34	3.31	96,96,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PC1	C	601	47/54	0.75	0.33	3.29	99,118,147,148	0
4	ACT	A	505	4/4	0.94	0.20	3.14	107,107,110,111	0
4	ACT	C	608	4/4	0.82	0.27	2.81	119,119,121,123	0
4	ACT	D	607	4/4	0.91	0.37	2.74	93,93,99,100	0
3	PC1	D	602	39/54	0.74	0.27	2.48	89,118,154,155	0
3	PC1	E	405	39/54	0.75	0.26	2.44	96,129,157,157	0
3	PC1	C	603	39/54	0.71	0.28	2.40	102,126,166,167	0
3	PC1	A	502	39/54	0.78	0.27	2.34	82,111,149,150	0
3	PC1	E	404	47/54	0.78	0.30	2.26	96,112,141,142	0
3	PC1	B	601	47/54	0.76	0.28	2.00	109,117,143,144	0
3	PC1	D	601	47/54	0.77	0.28	1.83	103,116,144,146	0
3	PC1	A	504	47/54	0.76	0.28	1.53	98,113,135,137	0
4	ACT	E	401	4/4	0.79	0.20	1.45	112,112,114,115	0
4	ACT	C	607	4/4	0.88	0.23	1.15	103,104,104,104	0
4	ACT	E	409	4/4	0.89	0.19	0.33	94,96,99,99	0
4	ACT	B	607	4/4	0.96	0.14	-0.36	93,94,95,95	0
7	NA	B	606	1/1	0.78	0.18	-0.38	101,101,101,101	0
7	NA	D	606	1/1	0.91	0.15	-0.44	117,117,117,117	0
7	NA	C	606	1/1	0.95	0.10	-0.80	90,90,90,90	0
7	NA	E	408	1/1	0.91	0.11	-0.89	112,112,112,112	0
6	BR	A	508	1/1	0.83	0.15	-	195,195,195,195	0
6	BR	C	605	1/1	0.85	0.26	-	238,238,238,238	0
6	BR	D	605	1/1	0.92	0.14	-	201,201,201,201	0
6	BR	B	605	1/1	0.73	0.28	-	245,245,245,245	0
6	BR	E	407	1/1	0.94	0.30	-	235,235,235,235	0

## 6.5 Other polymers

There are no such residues in this entry.