



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:23 am GMT

PDB ID : 4O1O  
Title : Crystal Structure of RNase L in complex with 2-5A  
Authors : Huang, H.; Zeqiraj, E.; Ceccarelli, D.F.; Sicheri, F.  
Deposited on : 2013-12-16  
Resolution : 3.27 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

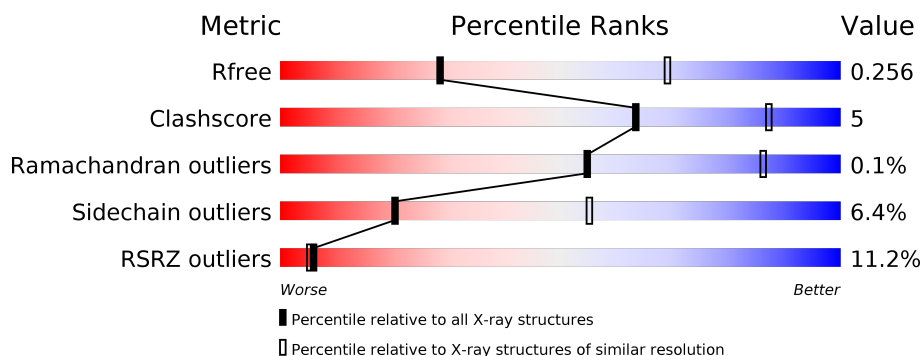
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.27 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	1006 (3.34-3.22)
Clashscore	112137	1070 (3.34-3.22)
Ramachandran outliers	110173	1050 (3.34-3.22)
Sidechain outliers	110143	1049 (3.34-3.22)
RSRZ outliers	101464	1011 (3.34-3.22)

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	717	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	717	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>6%</div> </div> </div>
1	C	717	<div> <div>17%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>6%</div> </div> </div>
1	D	717	<div> <div>20%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21697 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.

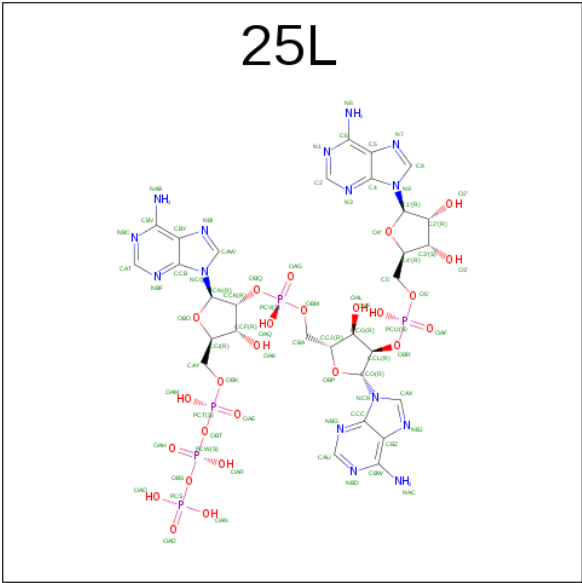
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5352	3358	945	1027	22			
1	B	672	Total	C	N	O	S	0	0	0
			5352	3358	945	1027	22			
1	C	671	Total	C	N	O	S	0	0	0
			5345	3354	944	1025	22			
1	D	672	Total	C	N	O	S	0	0	0
			5348	3355	944	1027	22			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	EXPRESSION TAG	UNP A5H025
A	17	ALA	-	EXPRESSION TAG	UNP A5H025
A	18	MET	-	EXPRESSION TAG	UNP A5H025
A	19	ASP	-	EXPRESSION TAG	UNP A5H025
A	20	PRO	-	EXPRESSION TAG	UNP A5H025
B	16	GLY	-	EXPRESSION TAG	UNP A5H025
B	17	ALA	-	EXPRESSION TAG	UNP A5H025
B	18	MET	-	EXPRESSION TAG	UNP A5H025
B	19	ASP	-	EXPRESSION TAG	UNP A5H025
B	20	PRO	-	EXPRESSION TAG	UNP A5H025
C	16	GLY	-	EXPRESSION TAG	UNP A5H025
C	17	ALA	-	EXPRESSION TAG	UNP A5H025
C	18	MET	-	EXPRESSION TAG	UNP A5H025
C	19	ASP	-	EXPRESSION TAG	UNP A5H025
C	20	PRO	-	EXPRESSION TAG	UNP A5H025
D	16	GLY	-	EXPRESSION TAG	UNP A5H025
D	17	ALA	-	EXPRESSION TAG	UNP A5H025
D	18	MET	-	EXPRESSION TAG	UNP A5H025
D	19	ASP	-	EXPRESSION TAG	UNP A5H025
D	20	PRO	-	EXPRESSION TAG	UNP A5H025

- Molecule 2 is [[[(2R,3R,4R,5R)-5-(6-AMINOPURIN-9-YL)-4-[[[(2R,3R,4R,5R)-5-(6-AMINOPURIN-9-YL)-4-[[[(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL]OXY-3-HYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL]OXY-3-HYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL] PHOSPHONO HYDROGEN PHOSPHATE (three-letter code: 25L) (formula: C<sub>30</sub>H<sub>40</sub>N<sub>15</sub>O<sub>25</sub>P<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			75	30	15	25	5		
2	B	1	Total	C	N	O	P	0	0
			75	30	15	25	5		
2	C	1	Total	C	N	O	P	0	0
			75	30	15	25	5		
2	D	1	Total	C	N	O	P	0	0
			75	30	15	25	5		

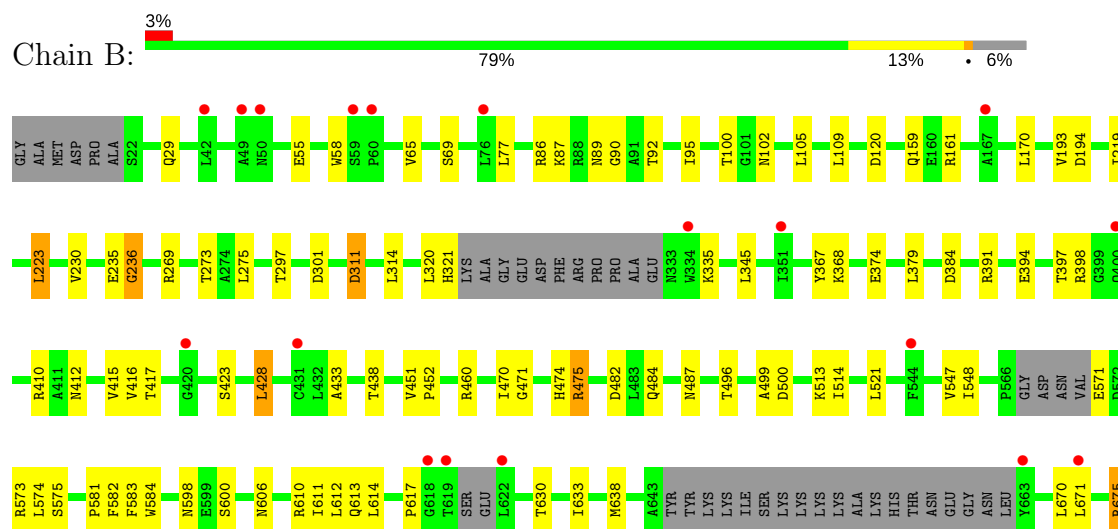
### 3 Residue-property plots

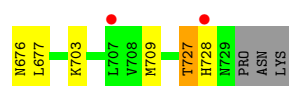
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Ribonuclease L

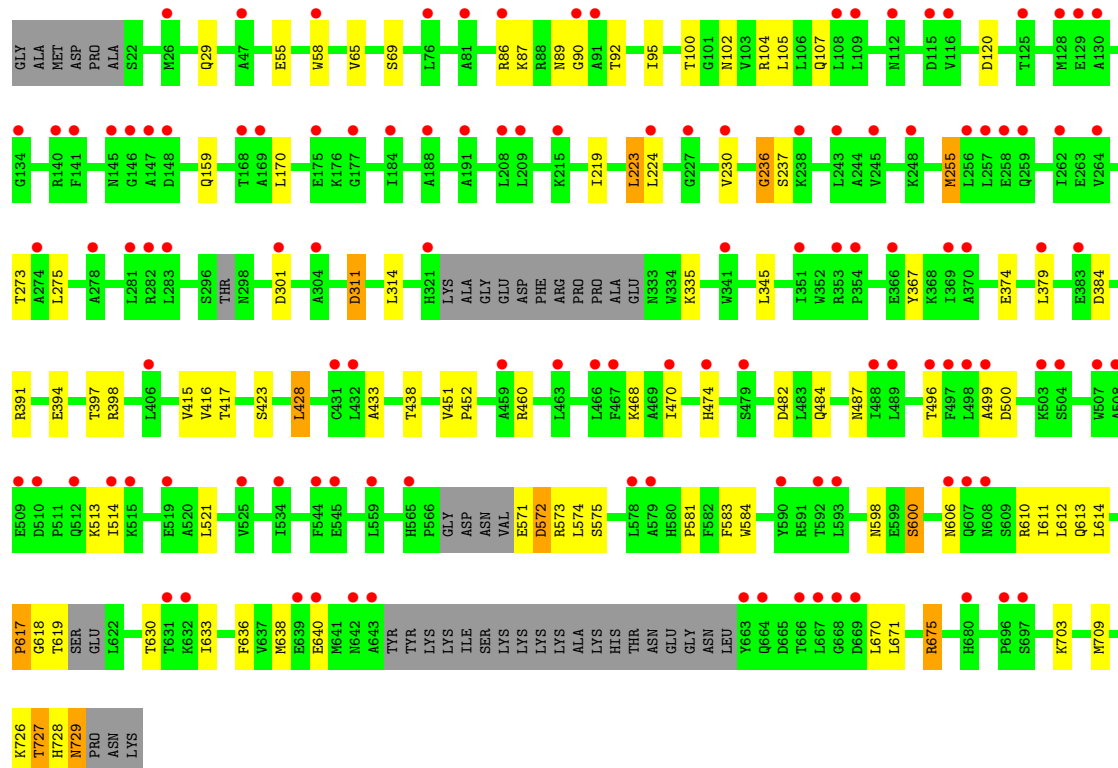
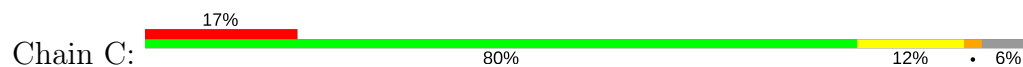


#### • Molecule 1: Ribonuclease L

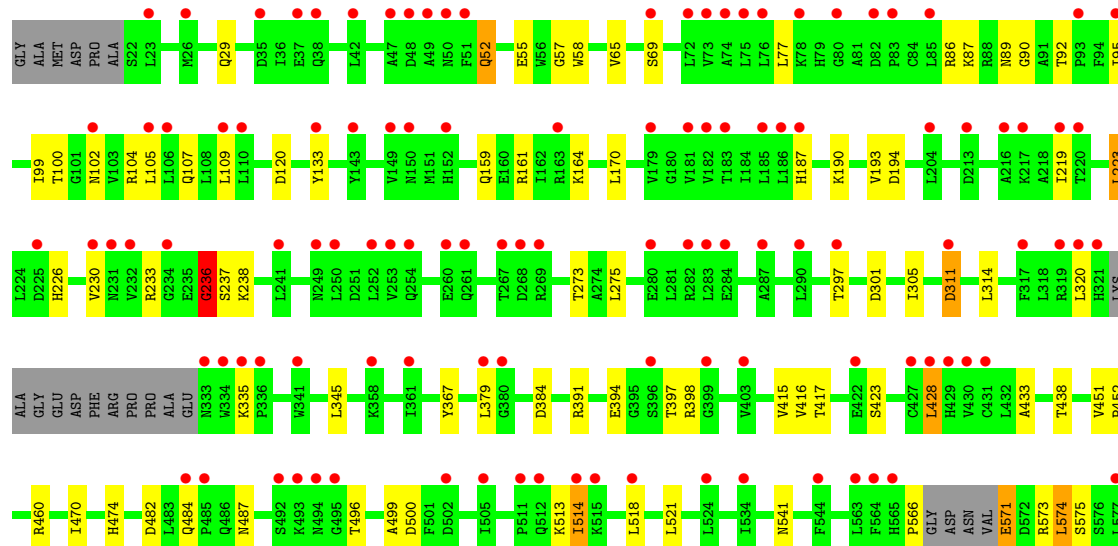
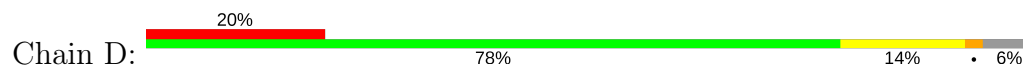


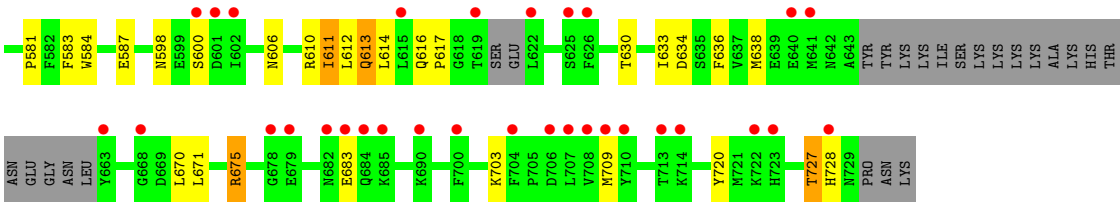


• Molecule 1: Ribonuclease L



• Molecule 1: Ribonuclease L





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.79Å 111.97Å 268.46Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	49.70 – 3.27 49.73 – 3.27	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.70-3.27) 92.8 (49.73-3.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.230 , 0.289 0.229 , 0.256	Depositor DCC
$R_{free}$ test set	1596 reflections (3.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.398 for h,-k,-l	Xtriage
Reported twinning fraction	0.476 for H, K, L 0.524 for -H, -K, L	Depositor
Outliers	0 of 51181 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
25L

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	0.55	0/5445	0.69	4/7349 (0.1%)
1	B	0.53	0/5445	0.68	3/7349 (0.0%)
1	C	0.45	0/5437	0.66	5/7336 (0.1%)
1	D	0.45	0/5441	0.67	5/7345 (0.1%)
All	All	0.50	0/21768	0.68	17/29379 (0.1%)

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	0	1
1	C	0	2
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	GLY	N-CA-C	-9.08	90.39	113.10
1	A	236	GLY	N-CA-C	-6.94	95.75	113.10
1	D	236	GLY	N-CA-C	-6.89	95.87	113.10
1	C	236	GLY	N-CA-C	-6.84	96.01	113.10
1	B	69	SER	N-CA-CB	-6.65	100.53	110.50
1	C	237	SER	N-CA-C	-6.43	93.65	111.00
1	C	499	ALA	N-CA-C	6.24	127.86	111.00
1	D	499	ALA	N-CA-C	6.09	127.44	111.00
1	B	499	ALA	N-CA-C	5.95	127.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ALA	C-N-CA	-5.90	106.96	121.70
1	D	69	SER	N-CA-CB	-5.86	101.71	110.50
1	D	320	LEU	N-CA-C	5.83	126.75	111.00
1	C	69	SER	N-CA-CB	-5.78	101.83	110.50
1	C	617	PRO	O-C-N	-5.28	114.22	123.20
1	A	69	SER	N-CA-CB	-5.16	102.76	110.50
1	A	237	SER	N-CA-C	-5.10	97.24	111.00
1	D	320	LEU	CB-CA-C	-5.05	100.61	110.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	ALA	Peptide
1	C	236	GLY	Peptide
1	C	572	ASP	Peptide
1	D	236	GLY	Peptide
1	D	571	GLU	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5352	0	5268	53	0
1	B	5352	0	5268	44	0
1	C	5345	0	5260	49	0
1	D	5348	0	5257	74	0
2	A	75	0	34	0	0
2	B	75	0	34	4	0
2	C	75	0	34	3	0
2	D	75	0	34	7	0
All	All	21697	0	21189	208	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 (208) 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:512:GLN:O	1:A:515:LYS:HG2	1.47	1.13
1:C:618:GLY:O	1:C:619:THR:OG1	1.85	0.93
1:D:613:GLN:O	1:D:613:GLN:NE2	2.06	0.87
1:C:571:GLU:OE1	1:C:572:ASP:N	2.12	0.82
1:D:613:GLN:HG3	1:D:614:LEU:N	2.00	0.76
1:A:183:THR:HG21	1:D:226:HIS:CE1	2.22	0.75
1:C:468:LYS:NZ	1:C:728:HIS:CE1	2.54	0.75
1:D:514:ILE:HG22	1:D:573:ARG:NH2	2.02	0.75
1:D:518:LEU:CD2	1:D:574:LEU:HD11	2.19	0.72
1:D:613:GLN:O	1:D:617:PRO:HG3	1.91	0.71
1:D:571:GLU:N	1:D:573:ARG:CG	2.55	0.70
1:A:187:HIS:HB2	1:D:187:HIS:CD2	2.27	0.70
1:A:301:ASP:O	1:A:305:ILE:HD12	1.92	0.69
1:D:611:ILE:O	1:D:614:LEU:HB2	1.93	0.67
1:D:571:GLU:N	1:D:573:ARG:HG3	2.09	0.67
1:A:499:ALA:O	1:A:500:ASP:HB3	1.94	0.66
1:A:144:GLU:OE2	1:D:190:LYS:HE3	1.94	0.66
1:D:52:GLN:HG2	1:D:52:GLN:O	1.96	0.65
1:A:515:LYS:HG3	1:A:516:ARG:N	2.11	0.65
1:A:571:GLU:N	1:A:571:GLU:OE2	2.29	0.65
1:A:89:ASN:O	1:A:120:ASP:HB2	1.96	0.65
1:D:611:ILE:HA	1:D:614:LEU:HD12	1.78	0.65
1:C:89:ASN:O	1:C:120:ASP:HB2	1.97	0.65
1:D:301:ASP:O	1:D:305:ILE:HD12	1.98	0.64
1:D:613:GLN:C	1:D:613:GLN:HE21	2.01	0.64
1:D:89:ASN:O	1:D:120:ASP:HB2	1.97	0.64
1:D:518:LEU:HD22	1:D:574:LEU:HD11	1.79	0.63
1:A:613:GLN:O	1:A:617:PRO:HG3	1.98	0.62
1:B:89:ASN:O	1:B:120:ASP:HB2	1.99	0.62
1:C:468:LYS:HZ3	1:C:728:HIS:CE1	2.18	0.62
2:B:1000:25L:HCF	2:B:1000:25L:HAW	1.82	0.62
1:B:613:GLN:O	1:B:617:PRO:HG3	2.01	0.61
1:A:598:ASN:OD1	1:A:675:ARG:NH1	2.33	0.61
1:B:598:ASN:OD1	1:B:675:ARG:NH1	2.34	0.61
1:C:598:ASN:OD1	1:C:675:ARG:NH1	2.33	0.61
1:D:514:ILE:CG2	1:D:573:ARG:NH2	2.64	0.61
1:B:451:VAL:HB	1:B:452:PRO:HD2	1.83	0.60
1:D:598:ASN:OD1	1:D:675:ARG:NH1	2.34	0.60
1:C:89:ASN:HB3	2:C:1000:25L:HCJ	1.84	0.60
1:B:581:PRO:HA	1:B:584:TRP:CG	2.37	0.59
1:D:451:VAL:HB	1:D:452:PRO:HD2	1.84	0.59
1:D:514:ILE:HG22	1:D:573:ARG:HH22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:VAL:HB	1:A:452:PRO:HD2	1.84	0.59
1:D:581:PRO:HA	1:D:584:TRP:CG	2.38	0.59
1:C:451:VAL:HB	1:C:452:PRO:HD2	1.84	0.59
1:A:394:GLU:HA	1:A:428:LEU:HB2	1.84	0.58
1:C:394:GLU:HA	1:C:428:LEU:HB2	1.85	0.58
1:C:581:PRO:HG2	1:C:709:MET:HE1	1.86	0.57
1:A:581:PRO:HG2	1:A:709:MET:HE1	1.87	0.57
1:C:728:HIS:ND1	1:C:728:HIS:O	2.38	0.57
1:A:515:LYS:HG3	1:A:516:ARG:H	1.70	0.56
1:B:87:LYS:HE2	2:B:1000:25L:OAP	2.04	0.56
1:C:311:ASP:HB3	1:C:314:LEU:HB3	1.87	0.56
1:A:470:ILE:HG22	1:A:474:HIS:CE1	2.41	0.56
1:B:311:ASP:HB3	1:B:314:LEU:HB3	1.87	0.56
1:B:581:PRO:HG2	1:B:709:MET:HE1	1.87	0.56
1:D:164:LYS:HE3	2:D:1000:25L:OAD	2.06	0.56
1:D:581:PRO:HG2	1:D:709:MET:HE1	1.87	0.56
1:A:311:ASP:HB3	1:A:314:LEU:HB3	1.87	0.56
1:D:470:ILE:HG22	1:D:474:HIS:CE1	2.41	0.56
1:A:187:HIS:CB	1:D:187:HIS:CD2	2.88	0.56
1:D:311:ASP:HB3	1:D:314:LEU:HB3	1.88	0.56
1:B:394:GLU:HA	1:B:428:LEU:HB2	1.87	0.56
1:D:571:GLU:N	1:D:573:ARG:HG2	2.21	0.56
1:A:581:PRO:HA	1:A:584:TRP:CG	2.41	0.55
1:D:394:GLU:HA	1:D:428:LEU:HB2	1.87	0.55
1:A:633:ILE:HG21	1:A:638:MET:SD	2.47	0.55
1:B:219:ILE:HG22	1:B:223:LEU:HD22	1.89	0.55
1:B:235:GLU:HG2	1:B:236:GLY:N	2.20	0.55
1:A:394:GLU:OE1	1:B:269:ARG:NH2	2.40	0.54
1:C:581:PRO:HA	1:C:584:TRP:CG	2.42	0.54
1:D:219:ILE:HG22	1:D:223:LEU:HD22	1.89	0.54
1:A:219:ILE:HG22	1:A:223:LEU:HD22	1.88	0.54
1:C:219:ILE:HG22	1:C:223:LEU:HD22	1.89	0.54
1:B:415:VAL:HG12	1:B:416:VAL:O	2.08	0.54
1:C:636:PHE:CZ	1:C:640:GLU:OE2	2.62	0.53
1:D:633:ILE:HG21	1:D:638:MET:SD	2.49	0.53
1:A:183:THR:CG2	1:D:226:HIS:CE1	2.90	0.53
1:A:301:ASP:O	1:A:305:ILE:CD1	2.55	0.53
1:B:633:ILE:HG21	1:B:638:MET:SD	2.49	0.53
1:C:633:ILE:HG21	1:C:638:MET:SD	2.49	0.52
1:B:571:GLU:N	1:B:571:GLU:CD	2.62	0.52
1:C:470:ILE:HG22	1:C:474:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:GLN:HG3	1:D:57:GLY:HA2	1.92	0.52
1:B:320:LEU:O	1:B:321:HIS:HB2	2.08	0.52
1:A:58:TRP:CH2	1:A:87:LYS:HE3	2.45	0.52
1:B:581:PRO:HA	1:B:584:TRP:CD1	2.45	0.52
1:A:415:VAL:HG12	1:A:416:VAL:O	2.10	0.51
1:D:415:VAL:HG12	1:D:416:VAL:O	2.10	0.51
1:C:89:ASN:CB	2:C:1000:25L:HCJ	2.40	0.51
1:A:308:ARG:HG3	2:B:1000:25L:O3'	2.10	0.51
1:B:482:ASP:O	1:B:487:ASN:ND2	2.43	0.51
1:A:581:PRO:HA	1:A:584:TRP:CD1	2.47	0.50
1:C:415:VAL:HG12	1:C:416:VAL:O	2.11	0.50
1:D:133:TYR:OH	2:D:1000:25L:NBD	2.36	0.50
1:D:581:PRO:HA	1:D:584:TRP:CD1	2.46	0.50
1:B:471:GLY:O	1:B:475:ARG:HG3	2.12	0.50
1:D:164:LYS:CE	2:D:1000:25L:OAD	2.60	0.50
1:D:587:GLU:O	1:D:587:GLU:HG2	2.11	0.50
1:A:630:THR:O	1:A:633:ILE:HG22	2.12	0.50
1:A:58:TRP:CZ2	1:A:87:LYS:HE3	2.46	0.49
1:C:618:GLY:C	1:C:619:THR:HG1	1.93	0.49
1:D:236:GLY:HA3	1:D:238:LYS:HG3	1.94	0.49
1:D:301:ASP:O	1:D:305:ILE:CD1	2.59	0.49
1:C:224:LEU:HD12	1:C:255:MET:HG2	1.94	0.49
1:D:610:ARG:O	1:D:613:GLN:CG	2.61	0.49
1:D:233:ARG:HD2	1:D:237:SER:O	2.12	0.49
1:B:470:ILE:HG22	1:B:474:HIS:CE1	2.48	0.49
1:C:468:LYS:HZ1	1:C:728:HIS:CE1	2.28	0.49
1:B:630:THR:O	1:B:633:ILE:HG22	2.13	0.48
1:A:159:GLN:HE22	1:B:391:ARG:NH2	2.11	0.48
1:D:87:LYS:HE2	2:D:1000:25L:OAP	2.13	0.48
1:D:482:ASP:O	1:D:487:ASN:ND2	2.46	0.48
1:C:600:SER:HB3	1:D:683:GLU:HA	1.95	0.48
1:C:630:THR:O	1:C:633:ILE:HG22	2.14	0.48
1:B:65:VAL:O	1:B:100:THR:HG21	2.14	0.48
1:B:235:GLU:CG	1:B:236:GLY:N	2.77	0.47
1:C:482:ASP:O	1:C:487:ASN:ND2	2.46	0.47
1:C:58:TRP:CH2	1:C:87:LYS:HE3	2.49	0.47
1:D:630:THR:O	1:D:633:ILE:HG22	2.14	0.47
1:C:460:ARG:HG2	1:C:583:PHE:HA	1.95	0.47
1:D:611:ILE:HG22	1:D:720:TYR:OH	2.15	0.47
1:A:482:ASP:O	1:A:487:ASN:ND2	2.47	0.47
1:A:571:GLU:C	1:A:573:ARG:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HD12	1:C:255:MET:CG	2.45	0.47
1:A:460:ARG:HG2	1:A:583:PHE:HA	1.96	0.47
1:B:58:TRP:CH2	1:B:87:LYS:HE3	2.50	0.47
1:C:159:GLN:HE22	1:D:391:ARG:NH2	2.13	0.47
1:D:460:ARG:HG2	1:D:583:PHE:HA	1.95	0.47
1:C:581:PRO:HA	1:C:584:TRP:CD1	2.50	0.47
1:D:58:TRP:CH2	1:D:87:LYS:HE3	2.50	0.47
1:A:161:ARG:HB2	1:B:374:GLU:O	2.16	0.46
1:C:92:THR:OG1	1:C:95:ILE:HG12	2.16	0.46
1:D:102:ASN:HB3	1:D:105:LEU:HD12	1.98	0.46
1:A:727:THR:HG23	1:A:728:HIS:N	2.29	0.46
1:A:367:TYR:HA	1:A:379:LEU:HD12	1.97	0.46
1:A:547:VAL:O	1:A:548:ILE:C	2.54	0.46
1:C:367:TYR:HA	1:C:379:LEU:HD12	1.97	0.46
1:A:65:VAL:O	1:A:100:THR:HG21	2.16	0.46
1:A:92:THR:OG1	1:A:95:ILE:HG12	2.16	0.46
1:B:102:ASN:HB3	1:B:105:LEU:HD12	1.98	0.46
1:C:224:LEU:CD1	1:C:255:MET:CG	2.93	0.46
1:A:417:THR:HB	1:A:433:ALA:HB2	1.98	0.46
1:C:255:MET:HG3	1:C:255:MET:O	2.15	0.46
1:C:417:THR:HB	1:C:433:ALA:HB2	1.98	0.46
1:C:374:GLU:O	1:D:161:ARG:HB2	2.16	0.46
1:A:374:GLU:O	1:B:161:ARG:HB2	2.15	0.46
1:B:460:ARG:HG2	1:B:583:PHE:HA	1.97	0.45
1:D:65:VAL:O	1:D:100:THR:HG21	2.16	0.45
1:B:58:TRP:CZ2	1:B:87:LYS:HE3	2.51	0.45
1:C:58:TRP:CZ2	1:C:87:LYS:HE3	2.50	0.45
1:D:99:ILE:CD1	2:D:1000:25L:HAU	2.47	0.45
1:C:571:GLU:CG	1:C:572:ASP:H	2.29	0.45
1:D:566:PRO:HB2	1:D:573:ARG:HD2	1.97	0.45
1:D:164:LYS:HE3	2:D:1000:25L:OAR	2.16	0.45
1:C:571:GLU:CD	1:C:572:ASP:H	2.20	0.45
1:B:367:TYR:HA	1:B:379:LEU:HD12	1.98	0.45
1:D:86:ARG:NH1	1:D:90:GLY:O	2.50	0.44
1:B:92:THR:OG1	1:B:95:ILE:HG12	2.16	0.44
1:D:727:THR:HG23	1:D:728:HIS:N	2.33	0.44
1:C:65:VAL:O	1:C:100:THR:HG21	2.17	0.44
1:D:518:LEU:HD21	1:D:574:LEU:CD1	2.47	0.44
1:A:102:ASN:HB3	1:A:105:LEU:HD12	1.99	0.44
1:D:616:GLN:N	1:D:617:PRO:HD3	2.33	0.44
1:D:92:THR:OG1	1:D:95:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLY:HA3	1:A:238:LYS:HG3	1.99	0.44
1:B:193:VAL:HG13	1:B:194:ASP:N	2.32	0.44
1:C:102:ASN:HB3	1:C:105:LEU:HD12	1.99	0.44
1:D:417:THR:HB	1:D:433:ALA:HB2	2.00	0.44
1:B:417:THR:HB	1:B:433:ALA:HB2	2.00	0.43
1:B:727:THR:HG23	1:B:728:HIS:N	2.34	0.43
1:A:86:ARG:NH1	1:A:90:GLY:O	2.51	0.43
1:D:193:VAL:HG13	1:D:194:ASP:N	2.33	0.43
1:D:367:TYR:HA	1:D:379:LEU:HD12	1.99	0.43
1:D:58:TRP:CZ2	1:D:87:LYS:HE3	2.53	0.43
2:D:1000:25L:HCF	2:D:1000:25L:OAN	2.18	0.43
1:A:391:ARG:NH2	1:B:159:GLN:HE22	2.17	0.43
1:B:86:ARG:NH1	1:B:90:GLY:O	2.52	0.43
1:B:547:VAL:O	1:B:548:ILE:C	2.55	0.43
1:C:86:ARG:NH1	1:C:90:GLY:O	2.51	0.43
1:D:634:ASP:OD1	1:D:636:PHE:HD2	2.02	0.42
1:A:530:LYS:HG3	1:A:534:ILE:HD13	2.00	0.42
1:D:470:ILE:CG2	1:D:474:HIS:CE1	3.03	0.42
1:A:572:ASP:OD1	1:A:572:ASP:N	2.52	0.42
1:B:606:ASN:O	1:B:612:LEU:HD12	2.20	0.42
1:D:606:ASN:O	1:D:612:LEU:HD12	2.20	0.42
1:C:613:GLN:O	1:C:617:PRO:HG3	2.20	0.42
1:A:641:MET:HG2	1:A:673:PHE:CE1	2.54	0.42
1:C:727:THR:O	1:C:729:ASN:N	2.52	0.42
1:C:391:ARG:NH2	1:D:159:GLN:HE22	2.18	0.42
1:A:470:ILE:CG2	1:A:474:HIS:CE1	3.03	0.41
1:C:224:LEU:CD1	1:C:255:MET:HG3	2.50	0.41
1:D:514:ILE:CG2	1:D:573:ARG:HH21	2.34	0.41
1:B:77:LEU:HD11	1:B:109:LEU:HD23	2.03	0.41
1:A:158:ASP:OD2	1:B:368:LYS:NZ	2.43	0.41
1:C:606:ASN:O	1:C:612:LEU:HD12	2.20	0.41
2:B:1000:25L:OBS	2:B:1000:25L:HAYA	2.21	0.41
1:B:412:ASN:ND2	1:B:415:VAL:HG23	2.36	0.41
1:D:616:GLN:N	1:D:617:PRO:CD	2.84	0.41
1:B:460:ARG:HD2	1:B:582:PHE:O	2.20	0.41
1:C:104:ARG:HA	1:C:107:GLN:OE1	2.21	0.41
1:D:610:ARG:O	1:D:613:GLN:HG3	2.20	0.41
1:C:58:TRP:HZ2	2:C:1000:25L:OAP	2.04	0.41
1:A:633:ILE:HG12	1:A:634:ASP:N	2.36	0.40
1:B:676:ASN:O	1:B:677:LEU:C	2.59	0.40
1:A:512:GLN:HG3	1:A:515:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:HA	1:D:107:GLN:OE1	2.21	0.40
1:D:77:LEU:HD11	1:D:109:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	662/717 (92%)	634 (96%)	28 (4%)	0	100	100
1	B	662/717 (92%)	632 (96%)	29 (4%)	1 (0%)	51	82
1	C	659/717 (92%)	630 (96%)	28 (4%)	1 (0%)	51	82
1	D	662/717 (92%)	635 (96%)	27 (4%)	0	100	100
All	All	2645/2868 (92%)	2531 (96%)	112 (4%)	2 (0%)	55	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	ASP
1	C	301	ASP

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	578/617 (94%)	540 (93%)	38 (7%)	19	54
1	B	578/617 (94%)	541 (94%)	37 (6%)	20	55
1	C	577/617 (94%)	540 (94%)	37 (6%)	20	55
1	D	577/617 (94%)	542 (94%)	35 (6%)	22	57
All	All	2310/2468 (94%)	2163 (94%)	147 (6%)	20	55

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	55	GLU
1	A	170	LEU
1	A	223	LEU
1	A	230	VAL
1	A	232	VAL
1	A	237	SER
1	A	273	THR
1	A	275	LEU
1	A	297	THR
1	A	311	ASP
1	A	335	LYS
1	A	345	LEU
1	A	384	ASP
1	A	397	THR
1	A	398	ARG
1	A	423	SER
1	A	428	LEU
1	A	438	THR
1	A	484	GLN
1	A	496	THR
1	A	500	ASP
1	A	513	LYS
1	A	514	ILE
1	A	515	LYS
1	A	521	LEU
1	A	573	ARG
1	A	574	LEU
1	A	575	SER
1	A	600	SER
1	A	610	ARG
1	A	611	ILE
1	A	614	LEU

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Mol	Chain	Res	Type
1	A	670	LEU
1	A	671	LEU
1	A	675	ARG
1	A	703	LYS
1	A	727	THR
1	B	29	GLN
1	B	55	GLU
1	B	170	LEU
1	B	223	LEU
1	B	230	VAL
1	B	273	THR
1	B	275	LEU
1	B	297	THR
1	B	311	ASP
1	B	335	LYS
1	B	345	LEU
1	B	384	ASP
1	B	397	THR
1	B	398	ARG
1	B	410	ARG
1	B	423	SER
1	B	428	LEU
1	B	438	THR
1	B	475	ARG
1	B	484	GLN
1	B	496	THR
1	B	500	ASP
1	B	513	LYS
1	B	514	ILE
1	B	521	LEU
1	B	573	ARG
1	B	574	LEU
1	B	575	SER
1	B	600	SER
1	B	610	ARG
1	B	611	ILE
1	B	614	LEU
1	B	670	LEU
1	B	671	LEU
1	B	675	ARG
1	B	703	LYS
1	B	727	THR

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Mol	Chain	Res	Type
1	C	29	GLN
1	C	55	GLU
1	C	170	LEU
1	C	223	LEU
1	C	230	VAL
1	C	255	MET
1	C	273	THR
1	C	275	LEU
1	C	311	ASP
1	C	335	LYS
1	C	345	LEU
1	C	384	ASP
1	C	397	THR
1	C	398	ARG
1	C	423	SER
1	C	428	LEU
1	C	438	THR
1	C	484	GLN
1	C	496	THR
1	C	500	ASP
1	C	513	LYS
1	C	514	ILE
1	C	521	LEU
1	C	573	ARG
1	C	574	LEU
1	C	575	SER
1	C	600	SER
1	C	610	ARG
1	C	611	ILE
1	C	614	LEU
1	C	670	LEU
1	C	671	LEU
1	C	675	ARG
1	C	703	LYS
1	C	726	LYS
1	C	727	THR
1	C	729	ASN
1	D	29	GLN
1	D	52	GLN
1	D	55	GLU
1	D	170	LEU
1	D	223	LEU

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Mol	Chain	Res	Type
1	D	230	VAL
1	D	273	THR
1	D	275	LEU
1	D	297	THR
1	D	311	ASP
1	D	335	LYS
1	D	345	LEU
1	D	384	ASP
1	D	397	THR
1	D	398	ARG
1	D	423	SER
1	D	428	LEU
1	D	438	THR
1	D	484	GLN
1	D	496	THR
1	D	500	ASP
1	D	513	LYS
1	D	514	ILE
1	D	521	LEU
1	D	541	ASN
1	D	574	LEU
1	D	575	SER
1	D	600	SER
1	D	611	ILE
1	D	613	GLN
1	D	670	LEU
1	D	671	LEU
1	D	675	ARG
1	D	703	LYS
1	D	727	THR

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

Mol	Chain	Res	Type
1	A	38	GLN
1	A	159	GLN
1	A	385	GLN
1	A	429	HIS
1	A	512	GLN
1	A	607	GLN
1	A	608	ASN
1	A	613	GLN

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Mol	Chain	Res	Type
1	A	616	GLN
1	B	38	GLN
1	B	159	GLN
1	B	385	GLN
1	B	608	ASN
1	C	38	GLN
1	C	159	GLN
1	C	385	GLN
1	C	607	GLN
1	C	608	ASN
1	C	613	GLN
1	C	616	GLN
1	C	728	HIS
1	D	38	GLN
1	D	159	GLN
1	D	321	HIS
1	D	385	GLN
1	D	541	ASN
1	D	608	ASN
1	D	613	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	25L	A	1000	-	69,83,83	2.37	8 (11%)	73,130,130	3.99	17 (23%)
2	25L	B	1000	-	69,83,83	2.67	13 (18%)	73,130,130	3.48	21 (28%)
2	25L	C	1000	-	69,83,83	2.77	12 (17%)	73,130,130	3.58	13 (17%)
2	25L	D	1000	-	69,83,83	2.72	10 (14%)	73,130,130	3.43	13 (17%)

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	25L	A	1000	-	-	0/40/100/100	0/9/9/9
2	25L	B	1000	-	-	0/40/100/100	0/9/9/9
2	25L	C	1000	-	-	0/40/100/100	0/9/9/9
2	25L	D	1000	-	-	0/40/100/100	0/9/9/9

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	25L	CBZ-NBJ	-2.16	1.32	1.39
2	B	1000	25L	CBY-NBI	-2.10	1.32	1.39
2	B	1000	25L	C5-C4	2.17	1.45	1.40
2	C	1000	25L	O4'-C1'	2.20	1.44	1.41
2	B	1000	25L	CBZ-CCC	2.39	1.45	1.40
2	A	1000	25L	C5-C4	2.47	1.46	1.40
2	B	1000	25L	OBP-CCO	2.51	1.44	1.41
2	B	1000	25L	CBY-CCB	2.53	1.46	1.40
2	D	1000	25L	O4'-C1'	2.66	1.44	1.41
2	A	1000	25L	CBZ-CCC	2.98	1.47	1.40
2	D	1000	25L	CBZ-CCC	3.12	1.47	1.40
2	C	1000	25L	OBP-CCO	3.13	1.45	1.41
2	B	1000	25L	OBO-CCN	3.25	1.45	1.41
2	D	1000	25L	CBY-CCB	3.38	1.48	1.40
2	C	1000	25L	CBZ-CCC	3.38	1.48	1.40
2	C	1000	25L	C5-C4	3.50	1.48	1.40
2	D	1000	25L	C5-C4	3.56	1.48	1.40
2	B	1000	25L	O4'-C1'	3.62	1.46	1.41
2	C	1000	25L	CBY-CCB	3.67	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	25L	CAT-NBC	6.37	1.45	1.33
2	A	1000	25L	C2-N1	6.56	1.46	1.33
2	B	1000	25L	CAU-NBD	6.86	1.46	1.33
2	A	1000	25L	CAT-NBF	7.03	1.43	1.32
2	B	1000	25L	C2-N1	7.05	1.47	1.33
2	B	1000	25L	CAT-NBC	7.15	1.47	1.33
2	C	1000	25L	C2-N1	7.26	1.47	1.33
2	A	1000	25L	CAU-NBD	7.34	1.47	1.33
2	D	1000	25L	CAU-NBD	7.48	1.48	1.33
2	D	1000	25L	C2-N1	7.50	1.48	1.33
2	C	1000	25L	CAT-NBC	7.56	1.48	1.33
2	D	1000	25L	CAT-NBC	7.95	1.48	1.33
2	C	1000	25L	CAU-NBD	7.98	1.48	1.33
2	C	1000	25L	CAT-NBF	8.47	1.46	1.32
2	A	1000	25L	CAU-NBG	8.59	1.46	1.32
2	B	1000	25L	CAU-NBG	8.61	1.46	1.32
2	A	1000	25L	C2-N3	8.67	1.46	1.32
2	D	1000	25L	CAT-NBF	9.03	1.47	1.32
2	D	1000	25L	C2-N3	9.10	1.47	1.32
2	C	1000	25L	C2-N3	9.24	1.47	1.32
2	B	1000	25L	CAT-NBF	9.40	1.47	1.32
2	B	1000	25L	C2-N3	9.83	1.48	1.32
2	D	1000	25L	CAU-NBG	9.87	1.48	1.32
2	C	1000	25L	CAU-NBG	10.48	1.49	1.32

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	25L	NBF-CAT-NBC	-21.18	110.41	128.86
2	C	1000	25L	NBF-CAT-NBC	-17.98	113.20	128.86
2	A	1000	25L	NBG-CAU-NBD	-16.56	114.43	128.86
2	C	1000	25L	N3-C2-N1	-16.19	114.76	128.86
2	B	1000	25L	N3-C2-N1	-16.12	114.82	128.86
2	D	1000	25L	NBG-CAU-NBD	-16.11	114.83	128.86
2	B	1000	25L	NBF-CAT-NBC	-15.53	115.33	128.86
2	A	1000	25L	N3-C2-N1	-15.48	115.38	128.86
2	D	1000	25L	N3-C2-N1	-15.37	115.48	128.86
2	B	1000	25L	NBG-CAU-NBD	-15.06	115.74	128.86
2	D	1000	25L	NBF-CAT-NBC	-14.66	116.09	128.86
2	C	1000	25L	NBG-CAU-NBD	-13.90	116.75	128.86
2	A	1000	25L	CCN-NCQ-CCB	-4.56	118.75	126.64
2	C	1000	25L	CCN-NCQ-CCB	-4.16	119.44	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	25L	CCC-CBZ-NBJ	-4.05	105.50	109.41
2	A	1000	25L	C4-C5-N7	-3.97	105.58	109.41
2	A	1000	25L	OBK-PCT-OAE	-3.85	93.70	109.25
2	D	1000	25L	C4-C5-N7	-3.52	106.01	109.41
2	C	1000	25L	C4-C5-N7	-3.37	106.15	109.41
2	A	1000	25L	C4'-O4'-C1'	-3.22	106.34	109.77
2	D	1000	25L	OBR-CCL-CCG	-3.10	100.16	111.63
2	C	1000	25L	CCC-CBZ-NBJ	-2.97	106.54	109.41
2	D	1000	25L	CCB-CBY-NBI	-2.92	106.59	109.41
2	B	1000	25L	CCC-CBZ-NBJ	-2.69	106.81	109.41
2	D	1000	25L	C1'-N9-C4	-2.62	122.10	126.64
2	A	1000	25L	C5'-C4'-C3'	-2.45	105.93	115.29
2	B	1000	25L	OBO-CCN-CCK	-2.24	102.67	106.59
2	B	1000	25L	CAY-CCI-CCF	-2.24	106.76	115.29
2	B	1000	25L	C4-C5-N7	-2.18	107.30	109.41
2	B	1000	25L	CCJ-OBP-CCO	-2.10	107.53	109.77
2	B	1000	25L	CBY-CBV-NAB	-2.01	116.38	120.47
2	D	1000	25L	OBK-CAY-CCI	2.01	116.13	109.00
2	A	1000	25L	O2'-C2'-C1'	2.01	117.91	111.61
2	B	1000	25L	OBP-CCO-CCL	2.04	110.17	106.59
2	D	1000	25L	OAQ-PCV-OAG	2.09	123.08	112.28
2	A	1000	25L	OAP-PCU-OAF	2.09	123.09	112.28
2	C	1000	25L	OAO-PCS-OAD	2.15	118.92	110.50
2	B	1000	25L	C2-N1-C6	2.19	122.59	118.77
2	A	1000	25L	CCJ-OBP-CCO	2.23	112.14	109.77
2	A	1000	25L	OAO-PCS-OAD	2.23	119.24	110.50
2	A	1000	25L	OAM-PCT-OAE	2.25	123.94	112.28
2	B	1000	25L	OAM-PCT-OAE	2.33	124.33	112.28
2	B	1000	25L	CAU-NBD-CBW	2.38	122.94	118.77
2	B	1000	25L	OBP-CCJ-CCG	2.40	109.94	105.17
2	C	1000	25L	CCG-CCL-CCO	2.42	107.49	102.75
2	A	1000	25L	OAK-CCF-CCK	2.43	118.09	111.18
2	C	1000	25L	NAC-CBW-NBD	2.43	123.58	118.77
2	A	1000	25L	O4'-C4'-C3'	2.45	110.04	105.17
2	C	1000	25L	CCJ-OBP-CCO	2.51	112.44	109.77
2	B	1000	25L	OBO-CCI-CAY	2.62	118.25	109.40
2	B	1000	25L	OAO-PCS-OAD	2.69	121.03	110.50
2	C	1000	25L	CCO-NCR-CCC	2.76	131.40	126.64
2	B	1000	25L	OBQ-PCV-OAG	2.78	120.38	109.46
2	D	1000	25L	CAU-NBD-CBW	2.84	123.75	118.77
2	B	1000	25L	CAT-NBC-CBV	2.99	123.99	118.77
2	B	1000	25L	NAB-CBV-NBC	3.11	124.93	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	25L	OAK-CCF-CCK	3.22	120.34	111.18
2	D	1000	25L	C2-N1-C6	3.23	124.43	118.77
2	A	1000	25L	CAU-NBD-CBW	3.29	124.52	118.77
2	C	1000	25L	C2-N1-C6	3.33	124.60	118.77
2	B	1000	25L	OBM-CBA-CCJ	3.51	121.46	109.00
2	D	1000	25L	CAT-NBC-CBV	3.67	125.20	118.77
2	A	1000	25L	CAT-NBC-CBV	4.75	127.09	118.77
2	C	1000	25L	CAT-NBC-CBV	4.78	127.13	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	25L	4	0
2	C	1000	25L	3	0
2	D	1000	25L	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	672/717 (93%)	0.03	18 (2%) 55 52	51, 99, 141, 177	0
1	B	672/717 (93%)	0.12	20 (2%) 51 48	52, 98, 150, 217	0
1	C	671/717 (93%)	0.85	119 (17%) 2 1	88, 152, 208, 260	0
1	D	672/717 (93%)	0.98	145 (21%) 1 1	94, 152, 213, 285	0
All	All	2687/2868 (93%)	0.50	302 (11%) 6 5	51, 128, 197, 285	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	ALA	16.2
1	C	498	LEU	13.6
1	C	146	GLY	12.0
1	D	72	LEU	10.9
1	C	607	GLN	10.7
1	D	622	LEU	10.4
1	D	75	LEU	10.2
1	B	619	THR	9.9
1	D	48	ASP	9.8
1	C	590	TYR	9.5
1	B	622	LEU	9.4
1	D	321	HIS	9.3
1	B	618	GLY	9.3
1	D	320	LEU	9.2
1	D	625	SER	9.2
1	C	230	VAL	9.0
1	D	47	ALA	8.1
1	D	714	LYS	7.9
1	D	678	GLY	7.6
1	C	510	ASP	7.5
1	C	499	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	C	177	GLY	7.3
1	D	710	TYR	7.0
1	C	642	ASN	6.9
1	D	422	GLU	6.9
1	D	38	GLN	6.9
1	D	152	HIS	6.6
1	C	109	LEU	6.6
1	D	626	PHE	6.6
1	D	319	ARG	6.5
1	D	187	HIS	6.4
1	C	697	SER	6.3
1	C	258	GLU	6.3
1	C	643	ALA	6.0
1	C	667	LEU	5.8
1	D	105	LEU	5.8
1	D	106	LEU	5.8
1	D	713	THR	5.8
1	D	333	ASN	5.7
1	C	579	ALA	5.7
1	D	668	GLY	5.7
1	D	563	LEU	5.7
1	C	264	VAL	5.6
1	C	125	THR	5.6
1	D	485	PRO	5.6
1	C	130	ALA	5.6
1	C	606	ASN	5.5
1	D	232	VAL	5.5
1	C	169	ALA	5.5
1	C	81	ALA	5.3
1	D	253	VAL	5.3
1	D	495	GLY	5.1
1	D	186	LEU	5.1
1	B	59	SER	5.1
1	D	261	GLN	5.1
1	D	37	GLU	4.9
1	D	249	ASN	4.9
1	C	696	PRO	4.8
1	C	497	PHE	4.8
1	D	600	SER	4.7
1	D	182	VAL	4.7
1	B	76	LEU	4.7
1	C	592	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	281	LEU	4.6
1	D	431	CYS	4.6
1	D	252	LEU	4.6
1	C	245	VAL	4.6
1	D	619	THR	4.6
1	C	112	ASN	4.5
1	D	722	LYS	4.5
1	D	181	VAL	4.5
1	C	507	TRP	4.4
1	C	282	ARG	4.4
1	D	282	ARG	4.4
1	D	311	ASP	4.3
1	D	564	PHE	4.3
1	D	219	ILE	4.3
1	C	91	ALA	4.2
1	D	684	GLN	4.2
1	D	230	VAL	4.1
1	D	179	VAL	4.1
1	D	544	PHE	4.0
1	D	93	PRO	4.0
1	C	663	TYR	4.0
1	D	49	ALA	4.0
1	D	679	GLU	4.0
1	C	353	ARG	4.0
1	D	511	PRO	4.0
1	D	515	LYS	4.0
1	D	707	LEU	3.9
1	D	80	GLY	3.9
1	C	238	LYS	3.8
1	D	260	GLU	3.8
1	D	514	ILE	3.8
1	C	474	HIS	3.8
1	C	141	PHE	3.8
1	C	544	PHE	3.7
1	C	184	ILE	3.7
1	C	488	ILE	3.7
1	C	90	GLY	3.7
1	C	668	GLY	3.7
1	C	431	CYS	3.7
1	C	545	GLU	3.6
1	D	361	ILE	3.6
1	C	134	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	254	GLN	3.6
1	D	512	GLN	3.6
1	D	163	ARG	3.6
1	D	220	THR	3.6
1	C	664	GLN	3.6
1	B	50	ASN	3.6
1	D	183	THR	3.6
1	C	534	ILE	3.5
1	B	431	CYS	3.5
1	C	578	LEU	3.5
1	D	380	GLY	3.5
1	D	723	HIS	3.5
1	D	601	ASP	3.5
1	C	259	GLN	3.5
1	D	493	LYS	3.5
1	C	175	GLU	3.4
1	C	256	LEU	3.4
1	D	241	LEU	3.4
1	C	608	ASN	3.4
1	D	429	HIS	3.4
1	C	489	LEU	3.4
1	D	73	VAL	3.4
1	C	145	ASN	3.4
1	C	680	HIS	3.3
1	D	35	ASP	3.3
1	D	250	LEU	3.3
1	C	283	LEU	3.3
1	C	512	GLN	3.3
1	D	728	HIS	3.3
1	D	149	VAL	3.3
1	D	85	LEU	3.2
1	D	484	GLN	3.2
1	C	593	LEU	3.2
1	D	74	ALA	3.2
1	D	336	PRO	3.2
1	C	379	LEU	3.2
1	D	284	GLU	3.1
1	C	341	TRP	3.1
1	D	335	LYS	3.1
1	D	51	PHE	3.1
1	D	430	VAL	3.1
1	C	301	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	278	ALA	3.1
1	C	463	LEU	3.1
1	B	663	TYR	3.1
1	C	504	SER	3.1
1	D	231	ASN	3.0
1	D	82	ASP	3.0
1	D	225	ASP	3.0
1	C	274	ALA	3.0
1	C	370	ALA	3.0
1	D	518	LEU	3.0
1	D	297	THR	3.0
1	C	351	ILE	3.0
1	A	728	HIS	3.0
1	D	685	LYS	3.0
1	C	496	THR	3.0
1	C	509	GLU	3.0
1	C	47	ALA	2.9
1	C	86	ARG	2.9
1	A	49	ALA	2.9
1	C	257	LEU	2.9
1	C	559	LEU	2.9
1	D	213	ASP	2.8
1	D	204	LEU	2.8
1	C	248	LYS	2.8
1	D	602	ILE	2.8
1	D	102	ASN	2.8
1	C	565	HIS	2.8
1	D	565	HIS	2.8
1	C	262	ILE	2.8
1	D	524	LEU	2.8
1	A	433	ALA	2.7
1	D	26	MET	2.7
1	A	341	TRP	2.7
1	D	76	LEU	2.7
1	C	354	PRO	2.7
1	D	640	GLU	2.7
1	B	351	ILE	2.7
1	C	519	GLU	2.7
1	D	110	LEU	2.7
1	C	128	MET	2.7
1	C	321	HIS	2.7
1	C	406	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	50	ASN	2.7
1	D	492	SER	2.7
1	C	115	ASP	2.6
1	C	116	VAL	2.6
1	D	403	VAL	2.6
1	A	593	LEU	2.6
1	D	280	GLU	2.6
1	C	243	LEU	2.6
1	C	632	LYS	2.6
1	D	78	LYS	2.6
1	D	287	ALA	2.6
1	C	514	ILE	2.6
1	C	76	LEU	2.6
1	C	108	LEU	2.6
1	C	366	GLU	2.6
1	C	525	VAL	2.6
1	D	709	MET	2.6
1	C	369	ILE	2.6
1	C	227	GLY	2.6
1	A	256	LEU	2.6
1	C	470	ILE	2.6
1	A	608	ASN	2.6
1	C	208	LEU	2.6
1	D	379	LEU	2.6
1	C	168	THR	2.6
1	D	428	LEU	2.5
1	A	43	LEU	2.5
1	D	109	LEU	2.5
1	D	143	TYR	2.5
1	C	640	GLU	2.5
1	C	503	LYS	2.5
1	D	708	VAL	2.5
1	D	494	ASN	2.5
1	A	100	THR	2.5
1	C	666	THR	2.5
1	D	317	PHE	2.5
1	D	690	LYS	2.5
1	C	304	ALA	2.5
1	C	215	LYS	2.5
1	D	234	GLY	2.4
1	D	704	PHE	2.4
1	C	508	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	728	HIS	2.4
1	B	49	ALA	2.4
1	A	193	VAL	2.4
1	D	150	ASN	2.4
1	D	23	LEU	2.4
1	D	83	PRO	2.4
1	D	682	ASN	2.4
1	C	58	TRP	2.4
1	C	479	SER	2.4
1	C	459	ALA	2.4
1	C	639	GLU	2.4
1	C	209	LEU	2.4
1	A	262	ILE	2.3
1	B	167	ALA	2.3
1	D	706	ASP	2.3
1	D	505	ILE	2.3
1	D	663	TYR	2.3
1	D	683	GLU	2.3
1	D	577	LEU	2.3
1	C	631	THR	2.3
1	D	334	TRP	2.3
1	C	383	GLU	2.3
1	D	267	THR	2.3
1	D	641	MET	2.3
1	C	191	ALA	2.3
1	C	466	LEU	2.3
1	D	217	LYS	2.3
1	A	76	LEU	2.2
1	B	42	LEU	2.2
1	D	427	CYS	2.2
1	D	290	LEU	2.2
1	A	116	VAL	2.2
1	C	129	GLU	2.2
1	D	283	LEU	2.2
1	A	434	LEU	2.2
1	C	669	ASP	2.2
1	D	95	ILE	2.2
1	D	341	TRP	2.2
1	B	60	PRO	2.2
1	B	671	LEU	2.2
1	C	26	MET	2.1
1	D	269	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	133	TYR	2.1
1	A	99	ILE	2.1
1	D	396	SER	2.1
1	C	188	ALA	2.1
1	D	700	PHE	2.1
1	B	400	GLN	2.1
1	B	420	GLY	2.1
1	B	707	LEU	2.1
1	D	268	ASP	2.1
1	D	534	ILE	2.1
1	A	439	LEU	2.1
1	A	379	LEU	2.1
1	C	224	LEU	2.1
1	B	334	TRP	2.1
1	D	185	LEU	2.1
1	D	399	GLY	2.0
1	C	515	LYS	2.0
1	D	69	SER	2.0
1	D	216	ALA	2.0
1	C	140	ARG	2.0
1	C	467	PHE	2.0
1	D	502	ASP	2.0
1	A	492	SER	2.0
1	C	148	ASP	2.0
1	D	615	LEU	2.0
1	B	544	PHE	2.0
1	D	358	LYS	2.0
1	C	432	LEU	2.0
1	D	42	LEU	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
2	25L	A	1000	75/75	0.94	0.21	-0.28	62,86,117,126	0
2	25L	D	1000	75/75	0.85	0.18	-0.59	85,138,168,212	0
2	25L	B	1000	75/75	0.95	0.18	-0.85	49,79,110,130	0
2	25L	C	1000	75/75	0.83	0.18	-1.02	88,137,230,247	0

## 6.5 Other polymers

There are no such residues in this entry.