



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:12 AM UTC

PDB ID : 4O1O / pdb_00004o1o
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

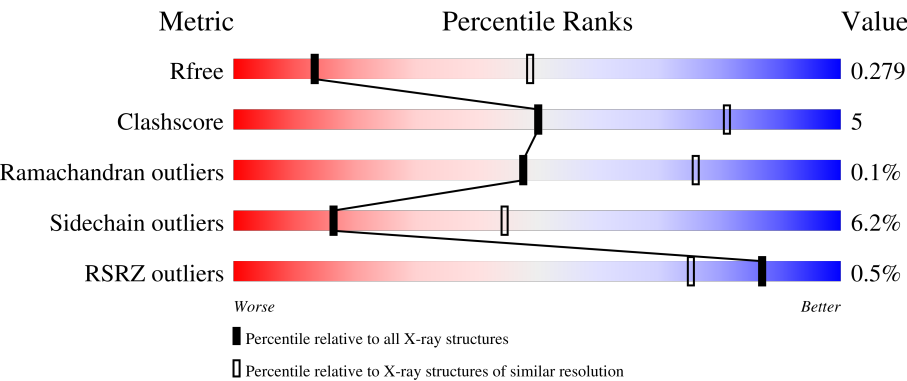
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	717	
1	C	717	
1	D	717	

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.

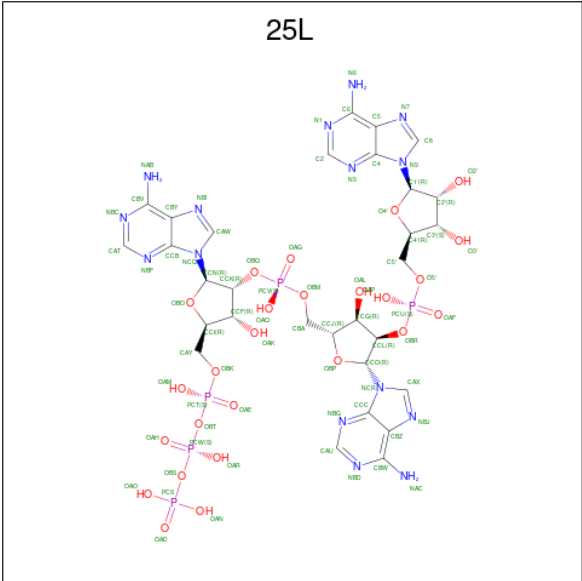
- Molecule 1 is a protein called Ribonuclease L.

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

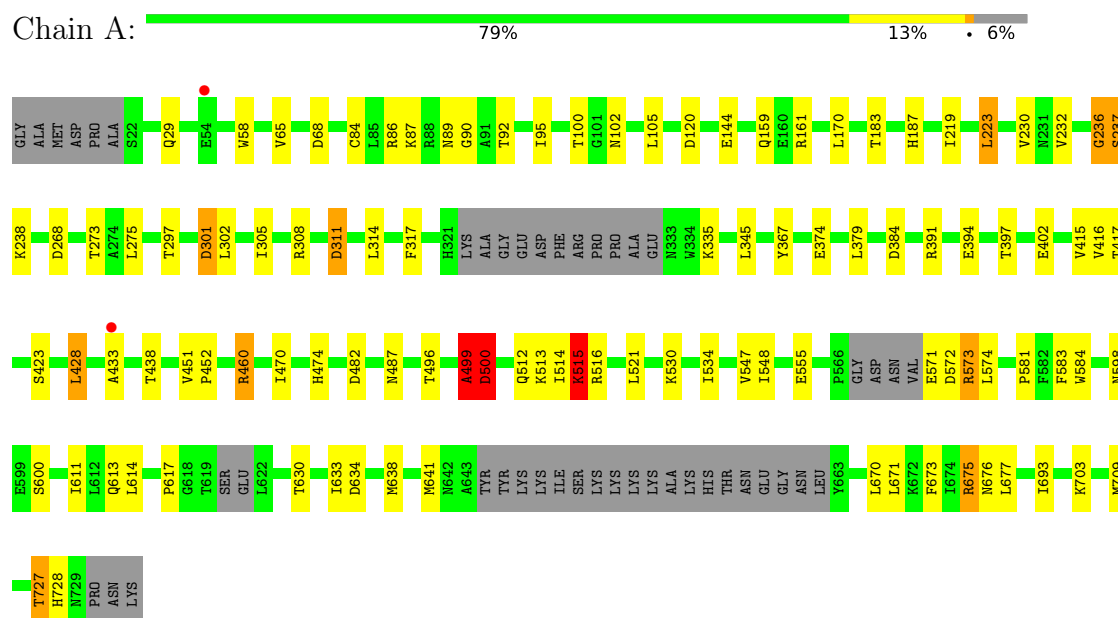
- Molecule 2 is [[[(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-4-[[[(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-4-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-3-hydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-3-hydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl] phosphono hydrogen phosphate (CCD ID: 25L) (formula: C₃₀H₄₀N₁₅O₂₅P₅).



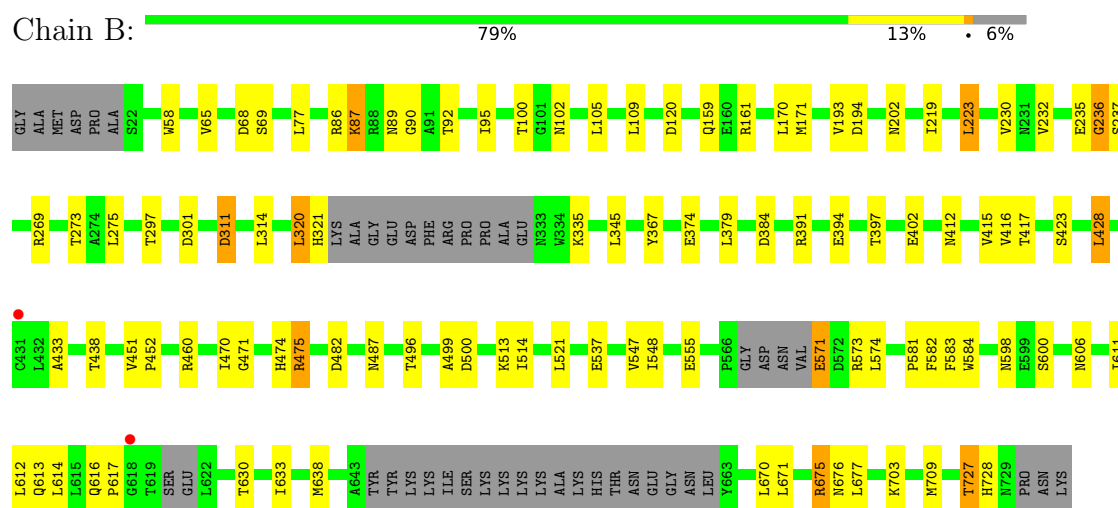
3 Residue-property plots

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

• Molecule 1: 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, α , β , γ	59.79Å 111.97Å 268.46Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	49.70 – 3.27 49.70 – 3.27	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.70-3.27) 92.9 (49.70-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.230 , 0.289 0.225 , 0.279	Depositor DCC
R_{free} test set	1596 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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	0.94	EDS
Total number of atoms	21697	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.72	0/5445	0.96	10/7349 (0.1%)
1	B	0.72	0/5445	0.94	10/7349 (0.1%)
1	C	0.63	0/5437	0.92	10/7336 (0.1%)
1	D	0.62	0/5441	0.95	12/7345 (0.2%)
All	All	0.67	0/21768	0.94	42/29379 (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 (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	LEU	N-CA-C	11.21	126.75	113.18
1	A	302	LEU	N-CA-C	-11.11	100.21	113.88
1	B	236	GLY	N-CA-C	-9.61	90.39	113.18
1	C	499	ALA	N-CA-C	9.25	127.86	114.16
1	A	236	GLY	N-CA-C	-9.03	95.75	112.37
1	C	236	GLY	N-CA-C	-8.99	96.01	111.47
1	D	499	ALA	N-CA-C	8.98	127.44	114.16
1	B	499	ALA	N-CA-C	8.73	127.08	114.16
1	D	302	LEU	N-CA-C	-8.62	103.27	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ALA	CA-C-N	-8.58	106.96	121.89
1	A	499	ALA	C-N-CA	-8.58	106.96	121.89
1	B	320	LEU	N-CA-C	-8.48	99.67	110.19
1	D	236	GLY	N-CA-C	-7.30	95.87	113.18
1	C	237	SER	N-CA-C	-7.19	93.65	108.53
1	A	500	ASP	N-CA-C	7.09	121.24	108.48
1	C	573	ARG	N-CA-C	6.73	122.16	113.88
1	D	237	SER	N-CA-C	-6.53	102.60	110.44
1	A	499	ALA	N-CA-C	6.46	120.49	112.03
1	B	68	ASP	N-CA-C	6.43	120.42	111.74
1	B	69	SER	N-CA-CB	-6.41	100.53	110.65
1	A	237	SER	N-CA-C	-6.37	97.24	110.80
1	C	617	PRO	O-C-N	-6.24	114.22	122.64
1	C	68	ASP	N-CA-C	5.75	119.58	111.52
1	C	573	ARG	N-CA-CB	-5.65	103.08	110.59
1	D	573	ARG	N-CA-C	-5.60	105.08	111.07
1	B	237	SER	N-CA-C	-5.59	99.27	109.56
1	B	236	GLY	CA-C-N	-5.54	114.53	122.67
1	B	236	GLY	C-N-CA	-5.54	114.53	122.67
1	D	69	SER	N-CA-CB	-5.44	101.71	110.69
1	D	68	ASP	N-CA-C	5.44	119.13	111.52
1	C	374	GLU	N-CA-C	5.41	122.31	110.80
1	D	541	ASN	N-CA-C	-5.40	105.31	111.14
1	D	572	ASP	N-CA-C	-5.40	103.49	111.81
1	D	541	ASN	N-CA-CB	5.40	117.89	110.07
1	C	69	SER	N-CA-CB	-5.37	101.83	110.69
1	A	68	ASP	N-CA-C	5.31	118.95	111.52
1	C	320	LEU	N-CA-C	5.29	118.20	111.69
1	A	301	ASP	CB-CA-C	5.21	117.67	110.16
1	D	301	ASP	CB-CA-C	5.21	117.66	110.16
1	A	515	LYS	CB-CA-C	-5.05	100.66	110.46
1	B	616	GLN	CA-C-N	-5.04	114.61	119.90
1	B	616	GLN	C-N-CA	-5.04	114.61	119.90

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

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Mol	Chain	Res	Type	Group
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	59	0
1	B	5352	0	5268	45	0
1	C	5345	0	5260	55	0
1	D	5348	0	5257	80	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	227	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 (227) 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:613:GLN:HE21	1:D:613:GLN:C	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:D:52:GLN:HG2	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: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
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:728:HIS:O	1:C:728:HIS:ND1	2.38	0.57
1:B:571:GLU:N	1:B:571:GLU:CD	2.62	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: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:C:311:ASP:HB3	1:C:314:LEU:HB3	1.87	0.56
1:D:164:LYS:HE3	2:D:1000:25L:OAD	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:618:GLY:C	1:C:619:THR:HG1	1.92	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:C:470:ILE:HG22	1:C:474:HIS:CE1	2.45	0.52
1:D:52:GLN:HG3	1:D:57:GLY:HA2	1.92	0.52
1:A:571:GLU:C	1:A:573:ARG:H	2.17	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:A:547:VAL:O	1:A:548:ILE:C	2.54	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:D:555:GLU:HG3	1:D:709:MET:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLY:O	1:B:475:ARG:HG3	2.12	0.50
1:B:555:GLU:HG3	1:B:709:MET:HE3	1.94	0.50
1:D:164:LYS:CE	2:D:1000:25L:OAD	2.60	0.50
1:D:587:GLU:HG2	1:D:587:GLU:O	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: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:555:GLU:HG3	1:C:709:MET:HE3	1.93	0.49
1:C:571:GLU:CD	1:C:572:ASP:H	2.20	0.49
1:C:224:LEU:HD12	1:C:255:MET:HG2	1.94	0.49
1:A:555:GLU:HG3	1:A:709:MET:HE3	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:58:TRP:CH2	1:C:87:LYS:HE3	2.49	0.47
1:C:482:ASP:O	1:C:487:ASN:ND2	2.46	0.47
1:D:630:THR:O	1:D:633:ILE:HG22	2.14	0.47
1:B:547:VAL:O	1:B:548:ILE:C	2.55	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: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:C:581:PRO:HA	1:C:584:TRP:CD1	2.50	0.47
1:D:460:ARG:HG2	1:D:583:PHE:HA	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:581:PRO:HD2	1:B:709:MET:HE1	1.97	0.46
1:C:255:MET:O	1:C:255:MET:HG3	2.15	0.46
1:C:374:GLU:O	1:D:161:ARG:HB2	2.16	0.46
1:C:417:THR:HB	1:C:433:ALA:HB2	1.98	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:B:676:ASN:O	1:B:677:LEU:C	2.59	0.45
1:D:164:LYS:HE3	2:D:1000:25L:OAR	2.16	0.45
1:B:367:TYR:HA	1:B:379:LEU:HD12	1.98	0.45
1:C:581:PRO:HD2	1:C:709:MET:HE1	1.98	0.45
1:A:581:PRO:HD2	1:A:709:MET:HE1	1.98	0.44
1:C:547:VAL:O	1:C:548:ILE:C	2.60	0.44
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:C:729:ASN:O	1:C:729:ASN:CG	2.59	0.44
1:D:727:THR:HG23	1:D:728:HIS:N	2.33	0.44
1:A:268:ASP:C	1:A:268:ASP:OD1	2.60	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:92:THR:OG1	1:D:95:ILE:HG12	2.17	0.44
1:D:616:GLN:N	1:D:617:PRO:HD3	2.33	0.44
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:A:571:GLU:C	1:A:573:ARG:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ASP:C	1:A:500:ASP:OD1	2.60	0.43
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:D:547:VAL:O	1:D:548:ILE:C	2.59	0.43
1:D:581:PRO:HD2	1:D:709:MET:HE1	2.00	0.43
1:A:86:ARG:NH1	1:A:90:GLY:O	2.51	0.43
1:D:58:TRP:CZ2	1:D:87:LYS:HE3	2.53	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
2:D:1000:25L:OAN	2:D:1000:25L:HCF	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: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:C:426:SER:HA	1:D:199:MET:HE1	2.01	0.42
1:A:530:LYS:HG3	1:A:534:ILE:HD13	2.00	0.42
1:A:641:MET:HE2	1:A:641:MET:HB2	1.97	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:391:ARG:NH2	1:D:159:GLN:HE22	2.18	0.42
1:C:727:THR:O	1:C:729:ASN:N	2.52	0.42
1:D:171:MET:HE2	1:D:202:ASN:HA	2.02	0.42
1:A:470:ILE:CG2	1:A:474:HIS:CE1	3.03	0.41
1:C:268:ASP:C	1:C:268:ASP:OD1	2.63	0.41
1:B:171:MET:HE2	1:B:202:ASN:HA	2.02	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:317:PHE:CD2	1:A:317:PHE:C	2.98	0.41
1:C:606:ASN:O	1:C:612:LEU:HD12	2.20	0.41
1:B:412:ASN:ND2	1:B:415:VAL:HG23	2.36	0.41
2:B:1000:25L:OBS	2:B:1000:25L:HAYA	2.21	0.41
1:A:676:ASN:O	1:A:677:LEU:C	2.63	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:268:ASP:OD1	1:D:268:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:676:ASN:O	1:C:677:LEU:C	2.64	0.40
1:A:512:GLN:HG3	1:A:515:LYS:HE2	2.03	0.40
1:D:77:LEU:HD11	1:D:109:LEU:HD23	2.04	0.40
1:D:104:ARG:HA	1:D:107:GLN:OE1	2.21	0.40
1:D:676:ASN:O	1:D:677:LEU:C	2.63	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%)	43	71
1	C	659/717 (92%)	630 (96%)	28 (4%)	1 (0%)	43	71
1	D	662/717 (92%)	635 (96%)	27 (4%)	0	100	100
All	All	2645/2868 (92%)	2531 (96%)	112 (4%)	2 (0%)	48	76

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%)	541 (94%)	37 (6%)	16	44
1	B	578/617 (94%)	543 (94%)	35 (6%)	17	45
1	C	577/617 (94%)	541 (94%)	36 (6%)	16	44
1	D	577/617 (94%)	542 (94%)	35 (6%)	17	45
All	All	2310/2468 (94%)	2167 (94%)	143 (6%)	16	44

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	84	CYS
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	402	GLU
1	A	423	SER
1	A	428	LEU
1	A	438	THR
1	A	460	ARG
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

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Mol	Chain	Res	Type
1	A	600	SER
1	A	611	ILE
1	A	614	LEU
1	A	670	LEU
1	A	671	LEU
1	A	675	ARG
1	A	693	ILE
1	A	703	LYS
1	A	727	THR
1	B	87	LYS
1	B	170	LEU
1	B	223	LEU
1	B	230	VAL
1	B	232	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	402	GLU
1	B	423	SER
1	B	428	LEU
1	B	438	THR
1	B	475	ARG
1	B	496	THR
1	B	500	ASP
1	B	513	LYS
1	B	514	ILE
1	B	521	LEU
1	B	537	GLU
1	B	571	GLU
1	B	573	ARG
1	B	574	LEU
1	B	600	SER
1	B	611	ILE
1	B	614	LEU
1	B	670	LEU
1	B	671	LEU
1	B	675	ARG

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Mol	Chain	Res	Type
1	B	703	LYS
1	B	727	THR
1	C	29	GLN
1	C	84	CYS
1	C	170	LEU
1	C	223	LEU
1	C	230	VAL
1	C	232	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	402	GLU
1	C	423	SER
1	C	428	LEU
1	C	438	THR
1	C	460	ARG
1	C	496	THR
1	C	500	ASP
1	C	513	LYS
1	C	514	ILE
1	C	521	LEU
1	C	537	GLU
1	C	574	LEU
1	C	600	SER
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	170	LEU
1	D	223	LEU

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Mol	Chain	Res	Type
1	D	230	VAL
1	D	232	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	402	GLU
1	D	423	SER
1	D	428	LEU
1	D	438	THR
1	D	460	ARG
1	D	496	THR
1	D	500	ASP
1	D	513	LYS
1	D	514	ILE
1	D	521	LEU
1	D	537	GLU
1	D	541	ASN
1	D	574	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	38	GLN
1	A	79	HIS
1	A	159	GLN
1	A	321	HIS
1	A	429	HIS
1	A	440	GLN

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Mol	Chain	Res	Type
1	A	486	GLN
1	A	512	GLN
1	A	542	GLN
1	A	565	HIS
1	A	608	ASN
1	A	613	GLN
1	B	32	GLN
1	B	38	GLN
1	B	79	HIS
1	B	159	GLN
1	B	337	GLN
1	B	440	GLN
1	B	486	GLN
1	B	542	GLN
1	B	565	HIS
1	B	608	ASN
1	B	613	GLN
1	C	32	GLN
1	C	38	GLN
1	C	79	HIS
1	C	159	GLN
1	C	542	GLN
1	C	565	HIS
1	C	608	ASN
1	C	613	GLN
1	C	728	HIS
1	D	32	GLN
1	D	38	GLN
1	D	79	HIS
1	D	159	GLN
1	D	321	HIS
1	D	440	GLN
1	D	486	GLN
1	D	541	ASN
1	D	542	GLN
1	D	565	HIS
1	D	608	ASN
1	D	613	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	D	1000	-	82,83,83	2.65	20 (24%)	122,130,130	2.30	32 (26%)
2	25L	B	1000	-	82,83,83	2.53	19 (23%)	122,130,130	2.42	41 (33%)
2	25L	A	1000	-	82,83,83	2.39	19 (23%)	122,130,130	2.60	38 (31%)
2	25L	C	1000	-	82,83,83	2.70	18 (21%)	122,130,130	2.43	38 (31%)

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	D	1000	-	-	17/52/100/100	0/9/9/9
2	25L	B	1000	-	-	12/52/100/100	0/9/9/9
2	25L	A	1000	-	-	13/52/100/100	0/9/9/9
2	25L	C	1000	-	-	18/52/100/100	0/9/9/9

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	25L	CAU-NBG	8.80	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	25L	CAU-NBD	8.43	1.48	1.33
2	D	1000	25L	CAT-NBC	8.40	1.48	1.33
2	D	1000	25L	CAU-NBG	8.23	1.48	1.33
2	B	1000	25L	C2-N3	8.19	1.48	1.33
2	C	1000	25L	CAT-NBC	7.98	1.48	1.33
2	D	1000	25L	C2-N1	7.92	1.48	1.33
2	D	1000	25L	CAU-NBD	7.90	1.48	1.33
2	B	1000	25L	CAT-NBF	7.80	1.47	1.33
2	A	1000	25L	CAU-NBD	7.75	1.47	1.33
2	C	1000	25L	C2-N1	7.67	1.47	1.33
2	C	1000	25L	C2-N3	7.65	1.47	1.33
2	B	1000	25L	CAT-NBC	7.55	1.47	1.33
2	D	1000	25L	C2-N3	7.52	1.47	1.33
2	D	1000	25L	CAT-NBF	7.45	1.47	1.33
2	B	1000	25L	C2-N1	7.45	1.47	1.33
2	B	1000	25L	CAU-NBD	7.24	1.46	1.33
2	A	1000	25L	C2-N3	7.11	1.46	1.33
2	B	1000	25L	CAU-NBG	7.06	1.46	1.33
2	A	1000	25L	CAU-NBG	7.04	1.46	1.33
2	C	1000	25L	CAT-NBF	6.93	1.46	1.33
2	A	1000	25L	C2-N1	6.93	1.46	1.33
2	A	1000	25L	CAT-NBC	6.72	1.45	1.33
2	A	1000	25L	PCT-OBT	5.62	1.65	1.59
2	A	1000	25L	CAT-NBF	5.58	1.43	1.33
2	C	1000	25L	CBY-CCB	5.43	1.48	1.39
2	D	1000	25L	C5-C4	5.29	1.48	1.39
2	C	1000	25L	C5-C4	5.21	1.48	1.39
2	C	1000	25L	CBZ-CCC	5.07	1.48	1.39
2	D	1000	25L	CBY-CCB	5.07	1.48	1.39
2	D	1000	25L	CBZ-CCC	4.73	1.47	1.39
2	A	1000	25L	CBZ-CCC	4.56	1.47	1.39
2	B	1000	25L	PCW-OBS	4.34	1.64	1.59
2	D	1000	25L	PCT-OBT	4.01	1.63	1.59
2	B	1000	25L	CBY-CCB	3.99	1.46	1.39
2	A	1000	25L	C5-C4	3.92	1.46	1.39
2	C	1000	25L	CBZ-NBJ	-3.83	1.32	1.39
2	B	1000	25L	CBZ-CCC	3.82	1.45	1.39
2	A	1000	25L	PCW-OBT	3.73	1.63	1.59
2	B	1000	25L	CBY-NBI	-3.72	1.32	1.39
2	B	1000	25L	C5-C4	3.53	1.45	1.39
2	C	1000	25L	PCW-OBT	3.39	1.63	1.59
2	A	1000	25L	CBZ-NBJ	-3.22	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	25L	PCW-OBT	3.19	1.62	1.59
2	D	1000	25L	C5-C6	3.12	1.49	1.41
2	A	1000	25L	CBY-CCB	3.12	1.44	1.39
2	B	1000	25L	PCW-OBT	3.07	1.62	1.59
2	C	1000	25L	CAW-NBI	3.06	1.37	1.31
2	B	1000	25L	C5-N7	-2.99	1.33	1.39
2	C	1000	25L	C5-C6	2.98	1.49	1.41
2	C	1000	25L	PCW-OBS	2.93	1.62	1.59
2	C	1000	25L	PCT-OBT	2.90	1.62	1.59
2	C	1000	25L	C8-N7	2.75	1.37	1.31
2	D	1000	25L	CBY-NBI	-2.74	1.34	1.39
2	D	1000	25L	CBZ-NBJ	-2.71	1.34	1.39
2	C	1000	25L	CBY-CBV	2.68	1.48	1.41
2	C	1000	25L	CBZ-CBW	2.68	1.48	1.41
2	B	1000	25L	C8-N7	2.66	1.36	1.31
2	A	1000	25L	CAW-NBI	2.66	1.36	1.31
2	D	1000	25L	CAX-NBJ	2.65	1.36	1.31
2	D	1000	25L	C8-N7	2.61	1.36	1.31
2	A	1000	25L	C8-N7	2.60	1.36	1.31
2	B	1000	25L	PCT-OBT	2.55	1.62	1.59
2	A	1000	25L	CAX-NBJ	2.50	1.36	1.31
2	B	1000	25L	CBZ-NBJ	-2.49	1.34	1.39
2	D	1000	25L	CBZ-CBW	2.44	1.47	1.41
2	A	1000	25L	CBY-NBI	-2.37	1.34	1.39
2	A	1000	25L	C5-C6	2.36	1.47	1.41
2	D	1000	25L	CBY-CBV	2.36	1.47	1.41
2	A	1000	25L	PCW-OBS	2.35	1.62	1.59
2	B	1000	25L	CAX-NBJ	2.29	1.36	1.31
2	D	1000	25L	CCB-NCQ	-2.26	1.33	1.37
2	A	1000	25L	C5-N7	-2.16	1.35	1.39
2	D	1000	25L	CAW-NBI	2.15	1.35	1.31
2	B	1000	25L	CCC-NCR	-2.11	1.33	1.37
2	B	1000	25L	CCB-NCQ	-2.04	1.33	1.37

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	25L	NBF-CAT-NBC	-12.00	110.41	128.58
2	C	1000	25L	NBF-CAT-NBC	-10.16	113.20	128.58
2	A	1000	25L	NBG-CAU-NBD	-9.35	114.43	128.58
2	C	1000	25L	N3-C2-N1	-9.13	114.76	128.58
2	B	1000	25L	N3-C2-N1	-9.09	114.82	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	25L	NBG-CAU-NBD	-9.09	114.83	128.58
2	B	1000	25L	NBF-CAT-NBC	-8.75	115.33	128.58
2	A	1000	25L	N3-C2-N1	-8.72	115.38	128.58
2	D	1000	25L	N3-C2-N1	-8.66	115.48	128.58
2	B	1000	25L	NBG-CAU-NBD	-8.48	115.74	128.58
2	D	1000	25L	NBF-CAT-NBC	-8.25	116.09	128.58
2	C	1000	25L	NBG-CAU-NBD	-7.81	116.75	128.58
2	C	1000	25L	CBZ-CCC-NBG	-6.89	117.23	126.72
2	A	1000	25L	C5-C4-N3	-6.25	118.11	126.72
2	B	1000	25L	C5-C4-N3	-6.24	118.13	126.72
2	D	1000	25L	CBZ-CCC-NBG	-5.99	118.47	126.72
2	C	1000	25L	NBG-CCC-NCR	5.60	136.69	127.17
2	A	1000	25L	CAT-NBF-CCB	5.35	124.91	111.83
2	A	1000	25L	C2-N3-C4	5.29	124.74	111.83
2	C	1000	25L	CAT-NBC-CBV	5.12	127.13	118.73
2	A	1000	25L	CAT-NBC-CBV	5.09	127.09	118.73
2	C	1000	25L	C5-C4-N3	-5.01	119.81	126.72
2	B	1000	25L	C2-N3-C4	4.94	123.89	111.83
2	D	1000	25L	CAU-NBG-CCC	4.85	123.69	111.83
2	C	1000	25L	C2-N3-C4	4.81	123.58	111.83
2	B	1000	25L	CBZ-CCC-NBG	-4.81	120.09	126.72
2	A	1000	25L	CBZ-CCC-NBG	-4.78	120.13	126.72
2	B	1000	25L	CBY-CCB-NBF	-4.73	120.21	126.72
2	C	1000	25L	CAU-NBG-CCC	4.72	123.35	111.83
2	B	1000	25L	N3-C4-N9	4.71	135.17	127.17
2	A	1000	25L	CAU-NBG-CCC	4.62	123.11	111.83
2	A	1000	25L	N3-C4-N9	4.57	134.94	127.17
2	D	1000	25L	NBG-CCC-NCR	4.55	134.91	127.17
2	B	1000	25L	CAU-NBG-CCC	4.45	122.70	111.83
2	D	1000	25L	CCC-CBZ-NBJ	-4.45	105.50	110.58
2	D	1000	25L	C2-N3-C4	4.40	122.56	111.83
2	A	1000	25L	C4-C5-N7	-4.38	105.58	110.58
2	C	1000	25L	CAT-NBF-CCB	4.36	122.48	111.83
2	D	1000	25L	C5-C4-N3	-4.28	120.83	126.72
2	B	1000	25L	NBF-CCB-NCQ	4.20	134.32	127.17
2	B	1000	25L	CAT-NBF-CCB	4.09	121.82	111.83
2	D	1000	25L	C4-C5-N7	-4.00	106.01	110.58
2	D	1000	25L	CAT-NBC-CBV	3.94	125.20	118.73
2	A	1000	25L	CCB-NCQ-CAW	3.90	109.83	105.74
2	C	1000	25L	C4-C5-N7	-3.87	106.15	110.58
2	A	1000	25L	OBK-PCT-OAE	-3.84	93.70	108.94
2	D	1000	25L	CBZ-NBJ-CAX	3.83	109.48	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	25L	NBG-CCC-NCR	3.83	133.68	127.17
2	C	1000	25L	N3-C4-N9	3.72	133.49	127.17
2	B	1000	25L	NBG-CCC-NCR	3.69	133.44	127.17
2	B	1000	25L	OBM-CBA-CCJ	3.66	121.46	108.99
2	D	1000	25L	CBY-CCB-NBF	-3.66	121.68	126.72
2	D	1000	25L	CAT-NBF-CCB	3.58	120.57	111.83
2	C	1000	25L	C2-N1-C6	3.57	124.60	118.73
2	C	1000	25L	CCB-NCQ-CAW	3.53	109.45	105.74
2	C	1000	25L	CCC-CBZ-NBJ	-3.53	106.54	110.58
2	A	1000	25L	CAU-NBD-CBW	3.52	124.52	118.73
2	C	1000	25L	CBW-CBZ-CCC	3.52	121.99	117.18
2	D	1000	25L	CCB-CBY-NBI	-3.49	106.59	110.58
2	D	1000	25L	C2-N1-C6	3.47	124.43	118.73
2	A	1000	25L	C5-N7-C8	3.39	108.78	103.45
2	A	1000	25L	CBY-CCB-NBF	-3.37	122.07	126.72
2	A	1000	25L	CCB-NCQ-CCN	-3.37	118.75	126.63
2	B	1000	25L	OBQ-PCV-OAG	3.31	120.38	109.81
2	B	1000	25L	CCC-CBZ-NBJ	-3.30	106.81	110.58
2	B	1000	25L	OAK-CCF-CCK	3.27	120.34	111.19
2	A	1000	25L	NBF-CCB-NCQ	3.27	132.73	127.17
2	D	1000	25L	OBR-CCL-CCG	-3.21	100.16	111.68
2	B	1000	25L	CAT-NBC-CBV	3.20	123.99	118.73
2	A	1000	25L	NCQ-CAW-NBI	-3.20	109.40	113.94
2	C	1000	25L	CBZ-NBJ-CAX	3.18	108.45	103.45
2	A	1000	25L	C4-N9-C8	3.14	109.04	105.74
2	C	1000	25L	CCB-NCQ-CCN	-3.07	119.44	126.63
2	C	1000	25L	CBY-CCB-NBF	-3.07	122.49	126.72
2	D	1000	25L	CAU-NBD-CBW	3.05	123.75	118.73
2	A	1000	25L	N9-C8-N7	-3.01	109.67	113.94
2	B	1000	25L	OAR-PCW-OBS	3.00	115.39	107.27
2	D	1000	25L	NBF-CCB-NCQ	3.00	132.26	127.17
2	D	1000	25L	N3-C4-N9	2.99	132.26	127.17
2	B	1000	25L	NAB-CBV-NBC	2.94	124.93	118.38
2	C	1000	25L	C5-N7-C8	2.93	108.05	103.45
2	B	1000	25L	CCC-NCR-CAX	2.91	108.80	105.74
2	D	1000	25L	CCB-NCQ-CAW	2.91	108.79	105.74
2	B	1000	25L	C4-C5-N7	-2.87	107.30	110.58
2	D	1000	25L	C5-N7-C8	2.86	107.95	103.45
2	C	1000	25L	CCK-CCN-NCQ	2.84	118.43	113.75
2	C	1000	25L	NBF-CCB-NCQ	2.84	131.99	127.17
2	D	1000	25L	NCR-CAX-NBJ	-2.82	109.94	113.94
2	B	1000	25L	CBY-CBV-NAB	-2.79	116.38	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	25L	OBO-CCI-CAY	2.78	118.25	109.33
2	D	1000	25L	CBY-NBI-CAW	2.76	107.79	103.45
2	B	1000	25L	CBZ-NBJ-CAX	2.74	107.75	103.45
2	C	1000	25L	CCB-CBY-NBI	-2.68	107.51	110.58
2	B	1000	25L	NCR-CAX-NBJ	-2.65	110.17	113.94
2	B	1000	25L	OAO-PCS-OAD	2.62	121.03	110.83
2	D	1000	25L	CCC-NCR-CAX	2.59	108.46	105.74
2	A	1000	25L	C5'-C4'-C3'	-2.58	105.93	115.21
2	B	1000	25L	CAU-NBD-CBW	2.56	122.94	118.73
2	B	1000	25L	OAM-PCT-OAE	2.55	124.33	112.44
2	B	1000	25L	C5-N7-C8	2.49	107.36	103.45
2	A	1000	25L	OAM-PCT-OAE	2.47	123.94	112.44
2	D	1000	25L	C4-N9-C8	2.47	108.33	105.74
2	A	1000	25L	OAK-CCF-CCK	2.47	118.09	111.19
2	A	1000	25L	O4'-C4'-C3'	2.46	110.04	105.15
2	C	1000	25L	CCG-CCL-CCO	2.45	107.49	102.81
2	C	1000	25L	CCO-NCR-CAX	-2.44	121.69	127.09
2	B	1000	25L	OBP-CCJ-CCG	2.41	109.94	105.15
2	B	1000	25L	C6-C5-C4	2.38	120.43	117.18
2	B	1000	25L	C2-N1-C6	2.35	122.59	118.73
2	B	1000	25L	CAY-CCI-CCF	-2.35	106.76	115.21
2	C	1000	25L	NAC-CBW-NBD	2.34	123.58	118.38
2	B	1000	25L	C5-C6-N6	-2.32	117.54	123.29
2	A	1000	25L	CCC-CBZ-NBJ	-2.32	107.94	110.58
2	A	1000	25L	OAP-PCU-OAF	2.29	123.09	112.44
2	D	1000	25L	OAQ-PCV-OAG	2.29	123.08	112.44
2	B	1000	25L	OBO-CCN-CCK	-2.28	102.67	106.59
2	A	1000	25L	O2'-C2'-C1'	2.27	117.91	110.10
2	D	1000	25L	NCQ-CAW-NBI	-2.24	110.76	113.94
2	C	1000	25L	NCQ-CAW-NBI	-2.23	110.77	113.94
2	C	1000	25L	C4-N9-C8	2.23	108.08	105.74
2	A	1000	25L	CCK-CCN-NCQ	2.21	117.39	113.75
2	A	1000	25L	CBY-NBI-CAW	2.21	106.93	103.45
2	D	1000	25L	N9-C8-N7	-2.21	110.80	113.94
2	C	1000	25L	CBZ-CBW-NAC	-2.21	117.82	123.29
2	B	1000	25L	CCL-CCO-NCR	-2.21	110.12	113.75
2	C	1000	25L	C3'-C2'-C1'	2.18	105.59	101.46
2	B	1000	25L	N9-C8-N7	-2.18	110.85	113.94
2	B	1000	25L	OAN-PCS-OBS	2.17	111.91	104.64
2	C	1000	25L	CBV-CBY-NBI	2.17	136.27	132.09
2	A	1000	25L	CBV-CBY-NBI	2.16	136.25	132.09
2	A	1000	25L	OAO-PCS-OAD	2.16	119.24	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	25L	CBY-CBV-NAB	-2.15	117.96	123.29
2	A	1000	25L	C2-N1-C6	2.14	122.24	118.73
2	A	1000	25L	OBS-PCS-OAD	-2.11	99.93	111.04
2	D	1000	25L	OBK-CAY-CCI	2.10	116.13	108.99
2	C	1000	25L	OBO-CCN-NCQ	-2.09	104.07	108.09
2	A	1000	25L	O4'-C4'-C5'	2.09	116.03	109.33
2	C	1000	25L	CBY-NBI-CAW	2.09	106.73	103.45
2	B	1000	25L	OBP-CCO-CCL	2.08	110.17	106.59
2	C	1000	25L	OBQ-CCK-CCF	-2.08	104.22	111.68
2	C	1000	25L	OAO-PCS-OAD	2.07	118.92	110.83
2	B	1000	25L	OBT-PCT-OAE	-2.07	104.49	110.70
2	C	1000	25L	N9-C8-N7	-2.06	111.02	113.94
2	D	1000	25L	C6-C5-N7	2.05	136.04	132.09
2	D	1000	25L	OAP-PCU-OAF	2.04	121.95	112.44
2	A	1000	25L	OBQ-CCK-CCN	-2.04	102.86	110.05
2	C	1000	25L	CCC-NCR-CCO	2.04	131.40	126.63
2	B	1000	25L	CBV-CBY-CCB	2.04	119.96	117.18
2	C	1000	25L	CAU-NBD-CBW	2.03	122.07	118.73

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	25L	CAY-OBK-PCT-OAE
2	A	1000	25L	CAY-OBK-PCT-OAM
2	A	1000	25L	CBA-OBM-PCV-OAG
2	A	1000	25L	CBA-OBM-PCV-OAQ
2	A	1000	25L	CBA-OBM-PCV-OBQ
2	B	1000	25L	C5'-O5'-PCU-OAF
2	B	1000	25L	C5'-O5'-PCU-OAP
2	B	1000	25L	CAY-OBK-PCT-OAE
2	B	1000	25L	CAY-OBK-PCT-OAM
2	C	1000	25L	C5'-O5'-PCU-OAF
2	C	1000	25L	C5'-O5'-PCU-OAP
2	C	1000	25L	C5'-O5'-PCU-OBQ
2	C	1000	25L	OBK-CAY-CCI-OBQ
2	C	1000	25L	CAY-OBK-PCT-OAE
2	C	1000	25L	CAY-OBK-PCT-OAM
2	C	1000	25L	CAY-OBK-PCT-OBT
2	C	1000	25L	CBA-OBM-PCV-OAG
2	C	1000	25L	CBA-OBM-PCV-OBQ
2	D	1000	25L	C5'-O5'-PCU-OAF

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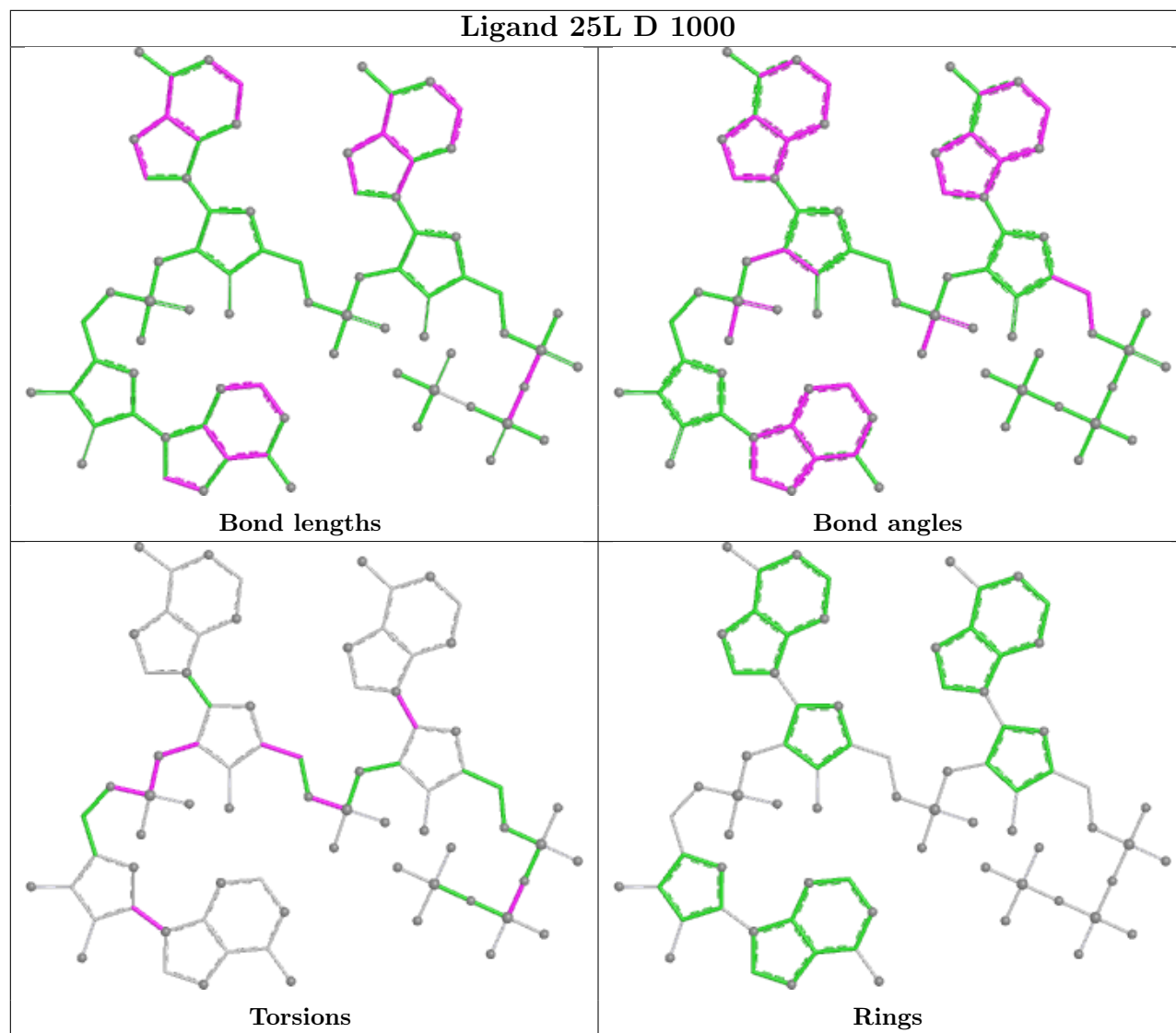
Mol	Chain	Res	Type	Atoms
2	D	1000	25L	C5'-O5'-PCU-OAP
2	D	1000	25L	CBA-OBM-PCV-OAG
2	D	1000	25L	CBA-OBM-PCV-OAQ
2	D	1000	25L	CBA-OBM-PCV-OBQ
2	B	1000	25L	OBK-CAY-CCI-OBO
2	D	1000	25L	OBM-CBA-CCJ-OBP
2	B	1000	25L	CCO-CCL-OB-R-PCU
2	C	1000	25L	OBK-CAY-CCI-CCF
2	B	1000	25L	OBK-CAY-CCI-CCF
2	B	1000	25L	CCG-CCL-OB-R-PCU
2	A	1000	25L	OBM-CBA-CCJ-OBP
2	D	1000	25L	CCO-CCL-OB-R-PCU
2	D	1000	25L	CCG-CCL-OB-R-PCU
2	D	1000	25L	OBM-CBA-CCJ-CCG
2	D	1000	25L	C2'-C1'-N9-C8
2	C	1000	25L	PCW-OBT-PCT-OAE
2	A	1000	25L	CAY-OBK-PCT-OBT
2	B	1000	25L	C5'-O5'-PCU-OB-R
2	B	1000	25L	CAY-OBK-PCT-OBT
2	C	1000	25L	CBA-OBM-PCV-OAQ
2	D	1000	25L	C5'-O5'-PCU-OB-R
2	A	1000	25L	OBM-CBA-CCJ-CCG
2	A	1000	25L	PCW-OBT-PCT-OAE
2	D	1000	25L	C2'-C1'-N9-C4
2	D	1000	25L	O4'-C1'-N9-C8
2	A	1000	25L	CCK-CCN-NCQ-CAW
2	B	1000	25L	CCK-CCN-NCQ-CAW
2	A	1000	25L	PCW-OBT-PCT-OAM
2	B	1000	25L	CCL-OB-R-PCU-OAF
2	C	1000	25L	CCL-OB-R-PCU-OAF
2	C	1000	25L	CCL-OB-R-PCU-OAP
2	C	1000	25L	PCS-OBS-PCW-OAR
2	D	1000	25L	CCL-OB-R-PCU-OAF
2	D	1000	25L	CCL-OB-R-PCU-OAP
2	A	1000	25L	C2'-C1'-N9-C8
2	C	1000	25L	CCK-CCN-NCQ-CAW
2	C	1000	25L	CCO-CCL-OB-R-PCU
2	D	1000	25L	CCK-CCN-NCQ-CAW
2	A	1000	25L	OBO-CCN-NCQ-CAW
2	C	1000	25L	PCS-OBS-PCW-OAH
2	D	1000	25L	PCT-OBT-PCW-OAR

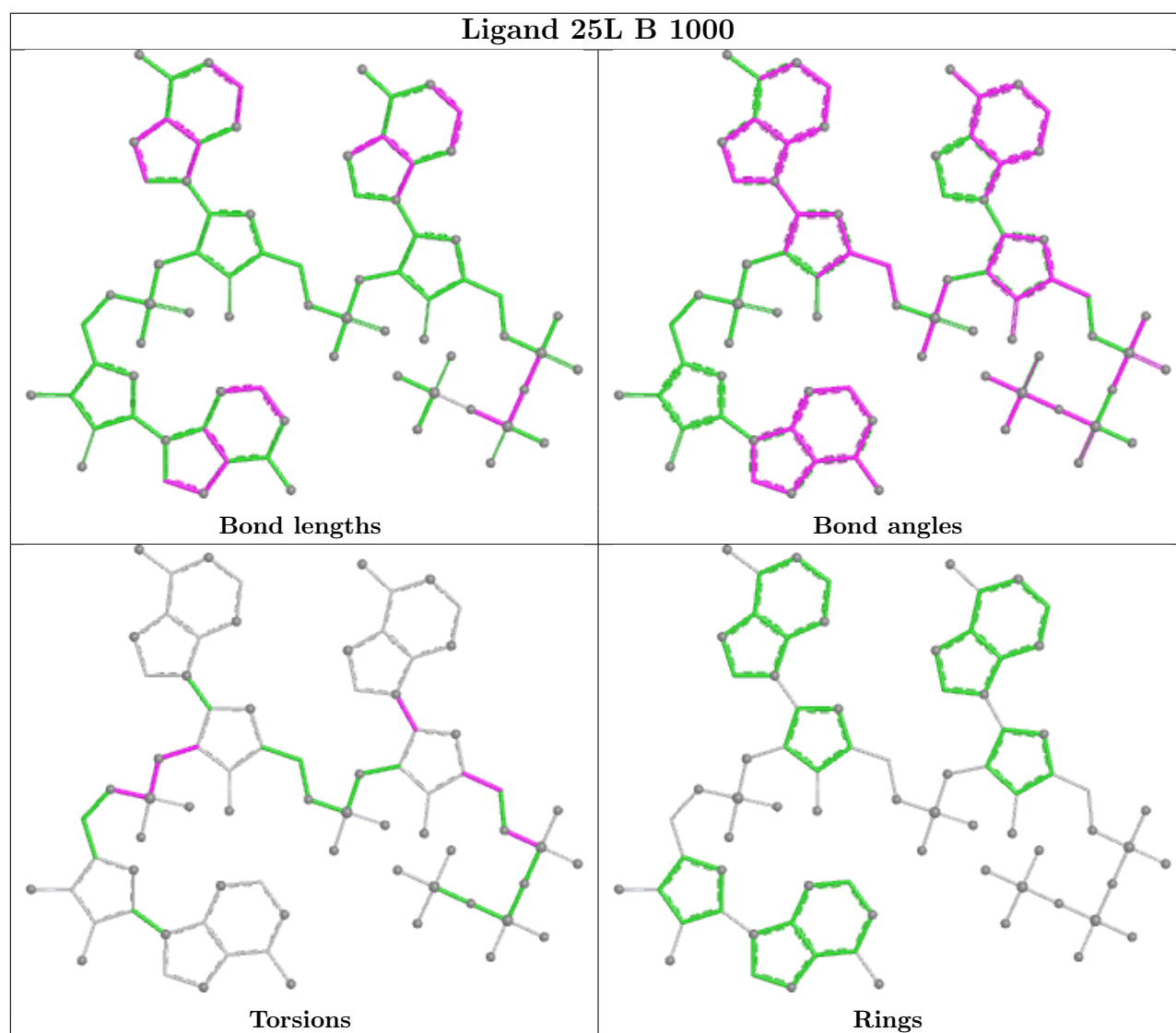
There are no ring outliers.

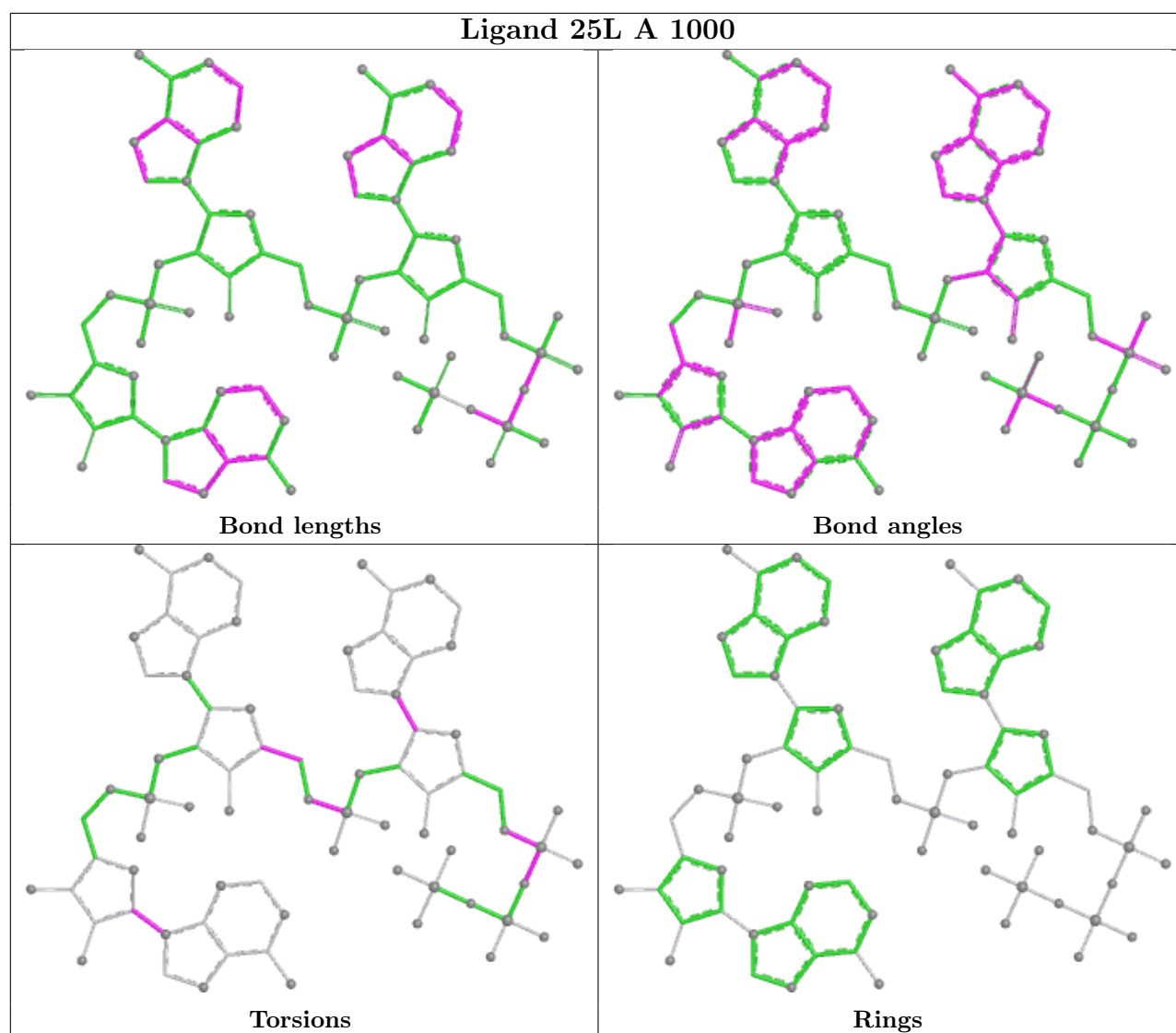
3 monomers are involved in 14 short contacts:

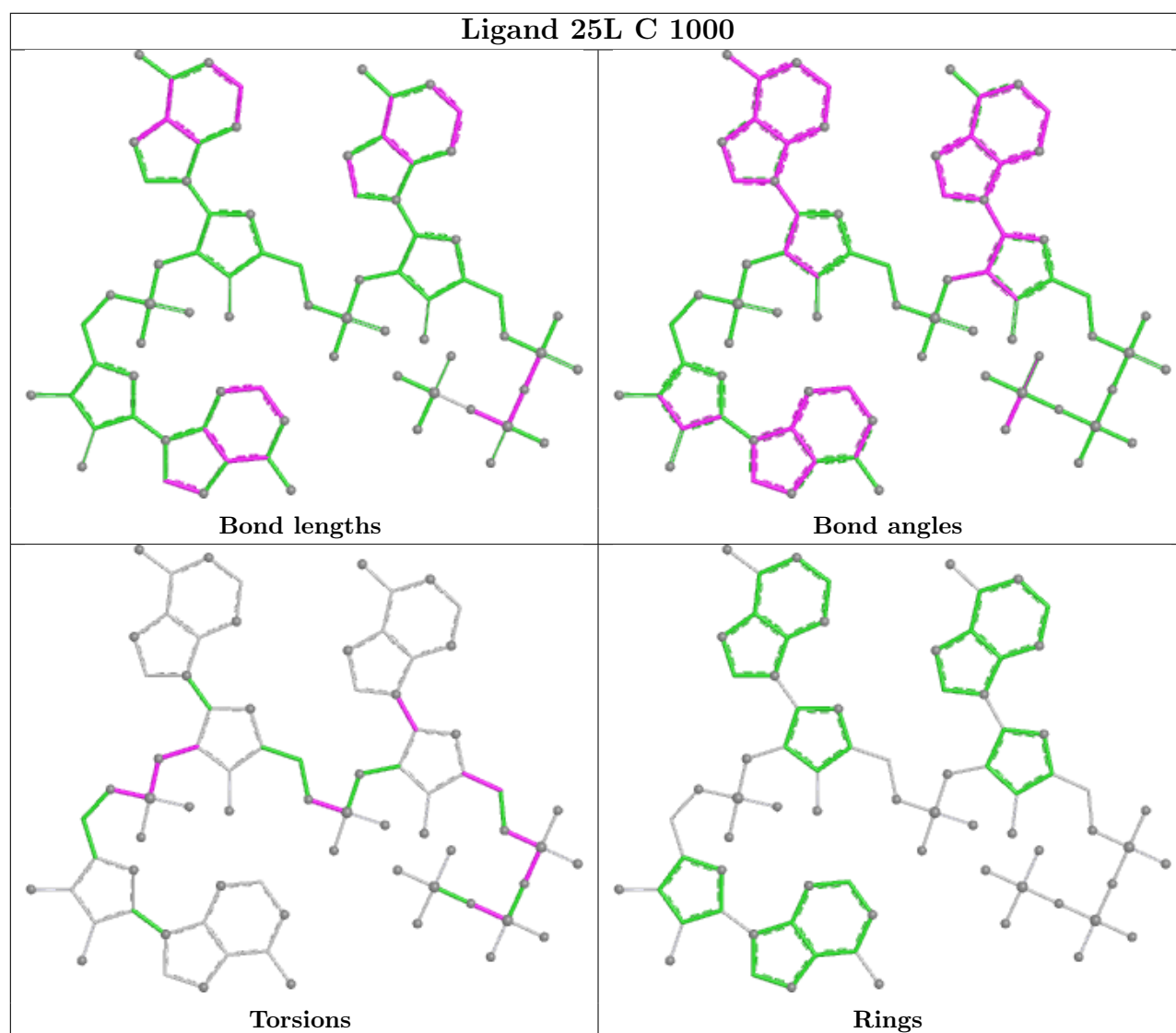
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1000	25L	7	0
2	B	1000	25L	4	0
2	C	1000	25L	3	0

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









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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	672/717 (93%)	-1.06	2 (0%) 90 82	51, 99, 141, 177	0
1	B	672/717 (93%)	-1.10	2 (0%) 90 82	52, 98, 150, 217	0
1	C	671/717 (93%)	-0.88	5 (0%) 84 70	88, 152, 208, 260	0
1	D	672/717 (93%)	-0.87	5 (0%) 84 70	94, 152, 213, 285	0
All	All	2687/2868 (93%)	-0.98	14 (0%) 87 75	51, 128, 197, 285	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	GLY	7.1
1	D	625	SER	6.5
1	C	147	ALA	5.9
1	C	370	ALA	3.7
1	D	29	GLN	3.6
1	B	618	GLY	3.0
1	D	710	TYR	2.9
1	A	54	GLU	2.7
1	C	230	VAL	2.6
1	B	431	CYS	2.6
1	D	600	SER	2.4
1	C	125	THR	2.2
1	D	320	LEU	2.1
1	A	433	ALA	2.1

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](#)

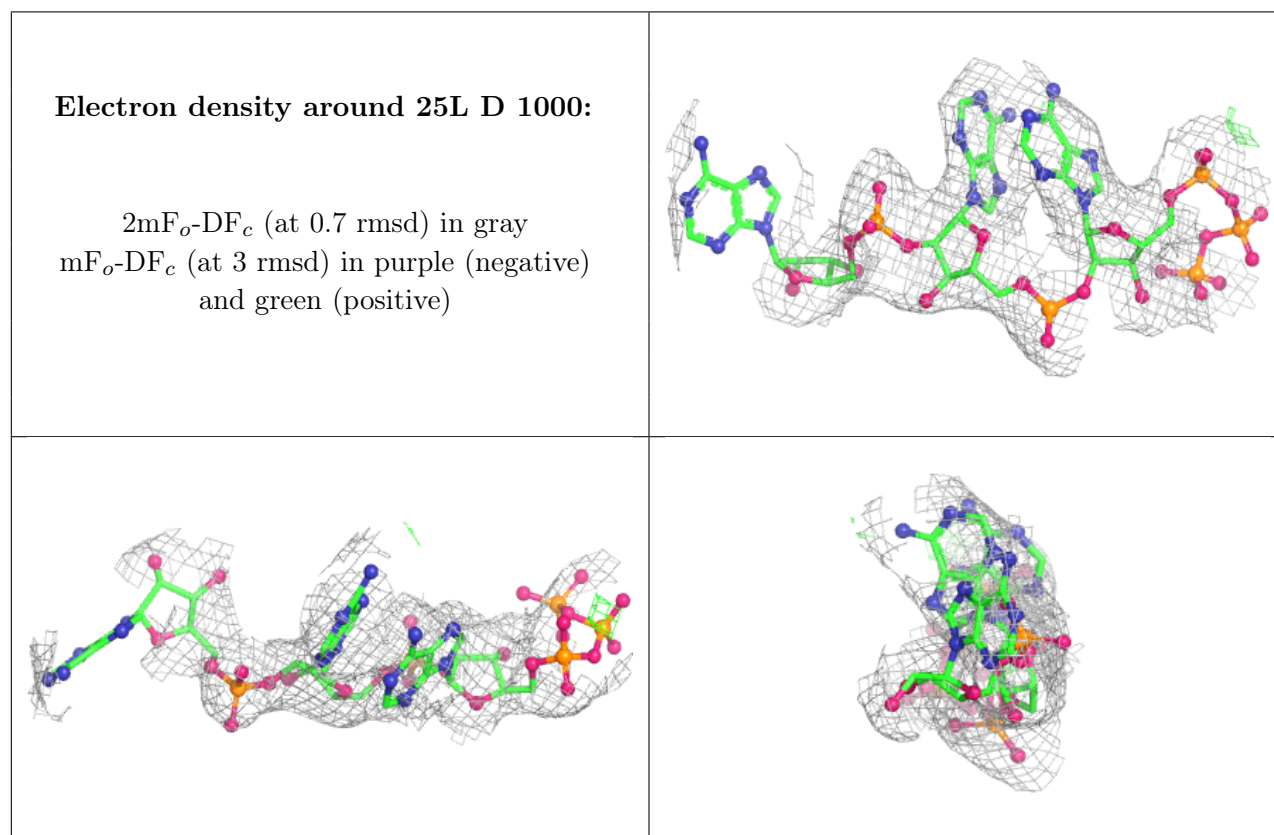
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

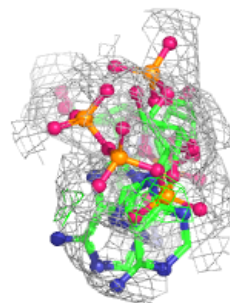
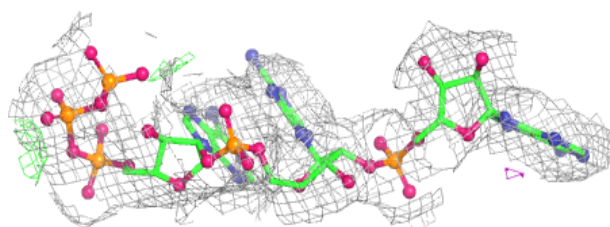
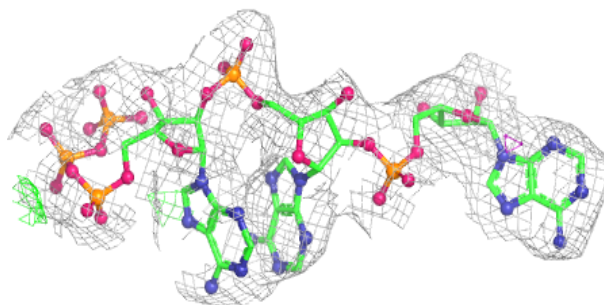
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	25L	D	1000	75/75	0.97	0.05	85,138,168,212	0
2	25L	B	1000	75/75	0.99	0.04	49,79,110,130	0
2	25L	C	1000	75/75	0.99	0.04	88,137,230,247	0
2	25L	A	1000	75/75	0.99	0.04	62,86,117,126	0

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

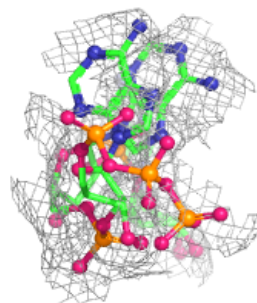
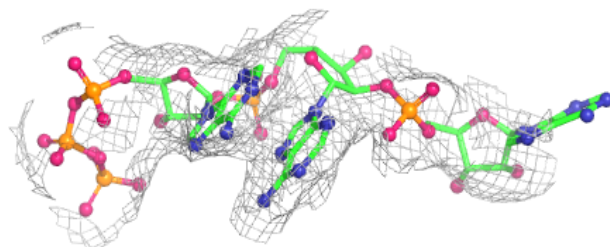
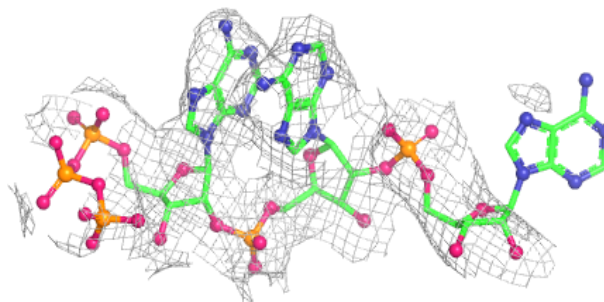


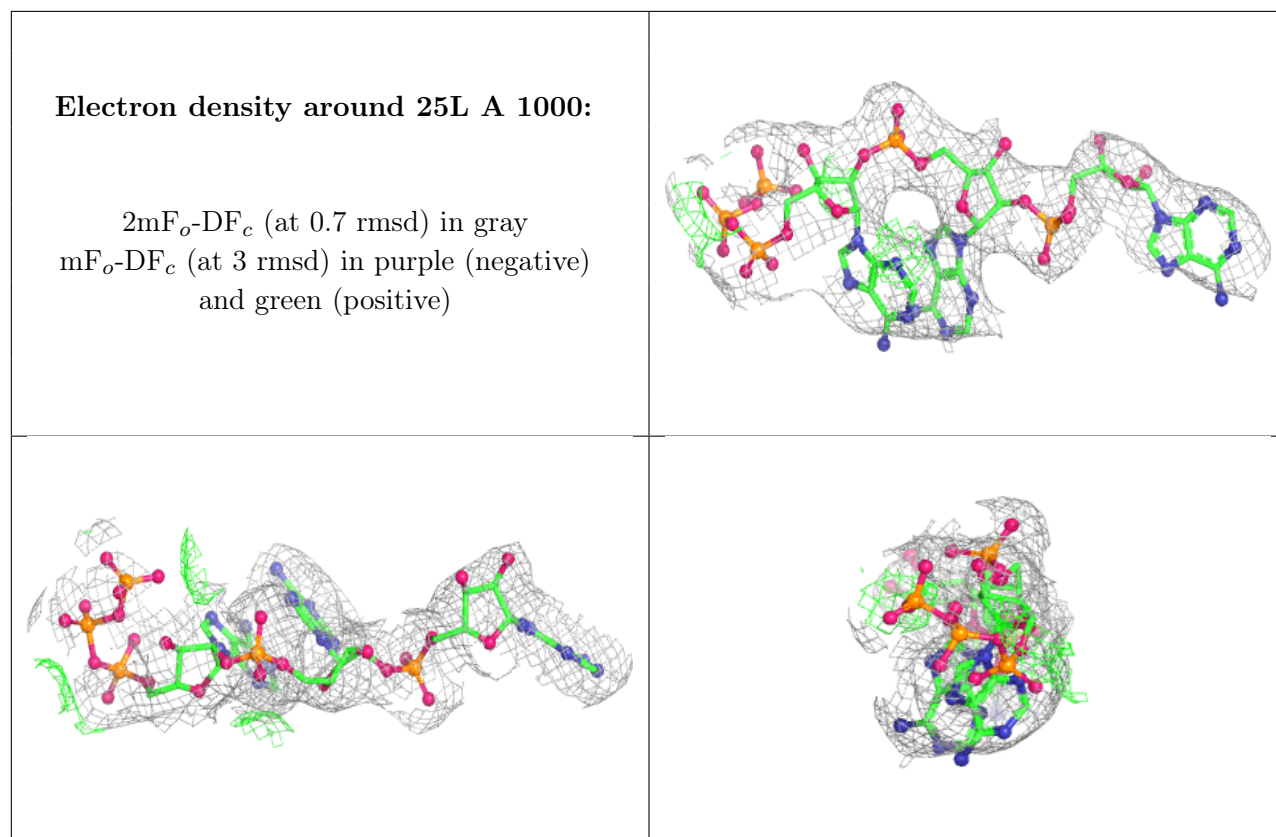
Electron density around 25L B 1000:

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

**Electron density around 25L C 1000:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.