Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2026 – 01:47 PM UTC

PDB ID	:	6M12 / pdb_00006m12
Title	:	Crystal Structure of Rnase L in complex with SU11652
Authors	:	Tang, J.; Huang, H.
Deposited on	:	2020-02-24
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

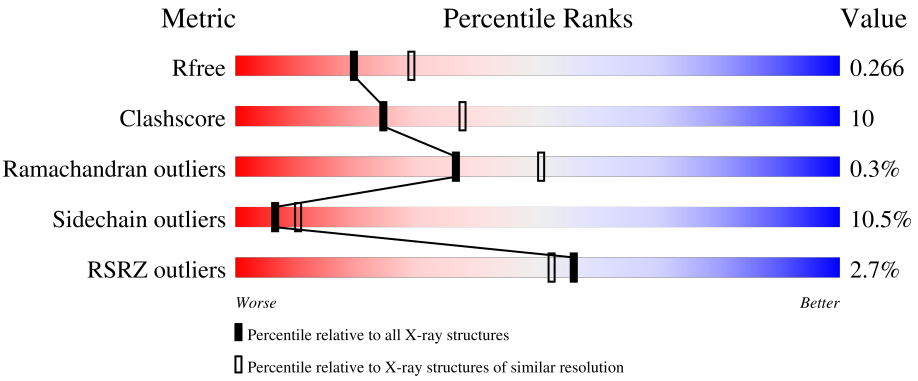
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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

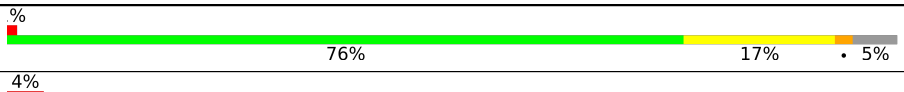
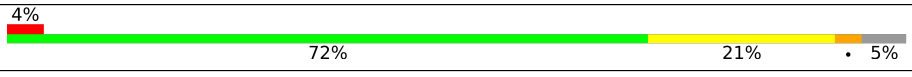
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 <=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	

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
4	PO4	a	803	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11057 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.

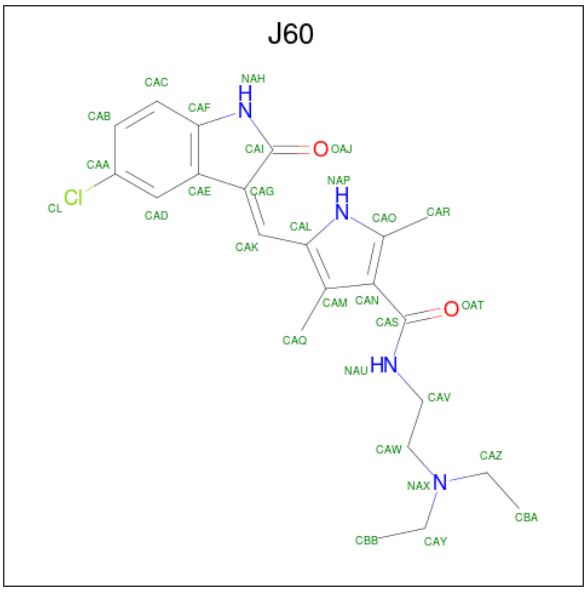
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	681	Total	C	N	O	S	0	0	0
			5418	3402	953	1041	22			
1	b	684	Total	C	N	O	S	0	0	0
			5442	3417	960	1043	22			

There are 10 discrepancies between the modelled and reference sequences:

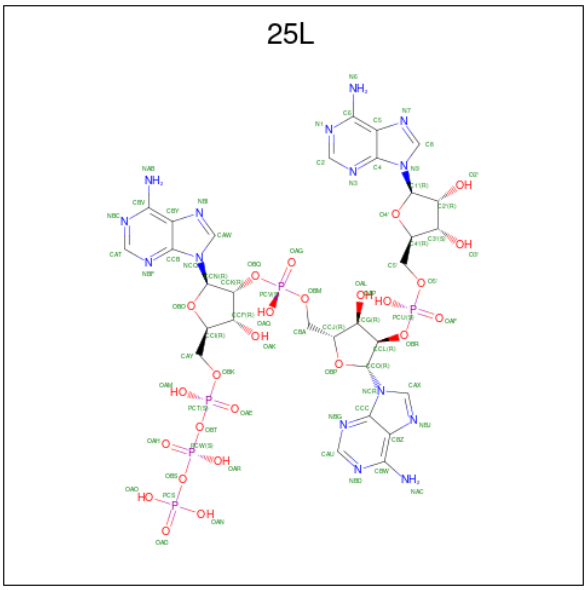
Chain	Residue	Modelled	Actual	Comment	Reference
a	16	GLY	-	expression tag	UNP A5H025
a	17	ALA	-	expression tag	UNP A5H025
a	18	MET	-	expression tag	UNP A5H025
a	19	ASP	-	expression tag	UNP A5H025
a	20	PRO	-	expression tag	UNP A5H025
b	16	GLY	-	expression tag	UNP A5H025
b	17	ALA	-	expression tag	UNP A5H025
b	18	MET	-	expression tag	UNP A5H025
b	19	ASP	-	expression tag	UNP A5H025
b	20	PRO	-	expression tag	UNP A5H025

- Molecule 2 is 5-[(E)-(5-CHLORO-2-OXO-1,2-DIHYDRO-3H-INDOL-3-YLIDENE)METHYL]-N-[2-(DIETHYLAMINO)ETHYL]-2,4-DIMETHYL-1H-PYRROLE-3-CARBOXAMIDE (CCD ID: J60) (formula: $C_{22}H_{27}ClN_4O_2$) (labeled as "Ligand of Interest" by depositor).



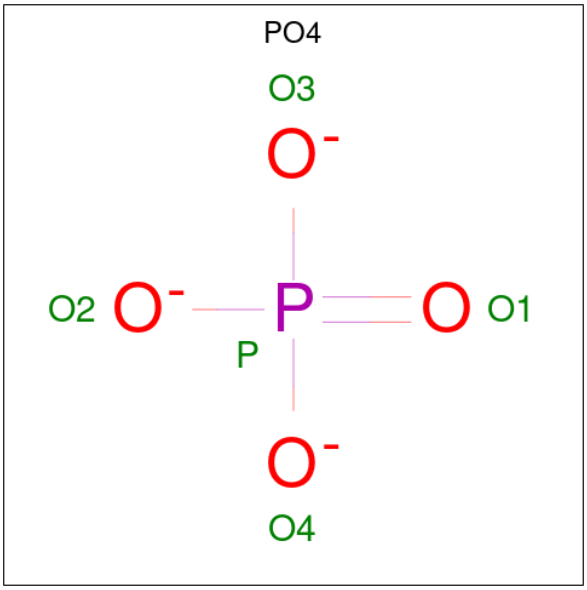
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	a	1	Total	C	Cl	N	O	0	0
			29	22	1	4	2		
2	b	1	Total	C	Cl	N	O	0	0
			29	22	1	4	2		

- Molecule 3 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: $C_{30}H_{40}N_{15}O_{25}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	a	1	Total	C	N	O	P	0	0
			67	30	15	19	3		
3	b	1	Total	C	N	O	P	0	0
			67	30	15	19	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



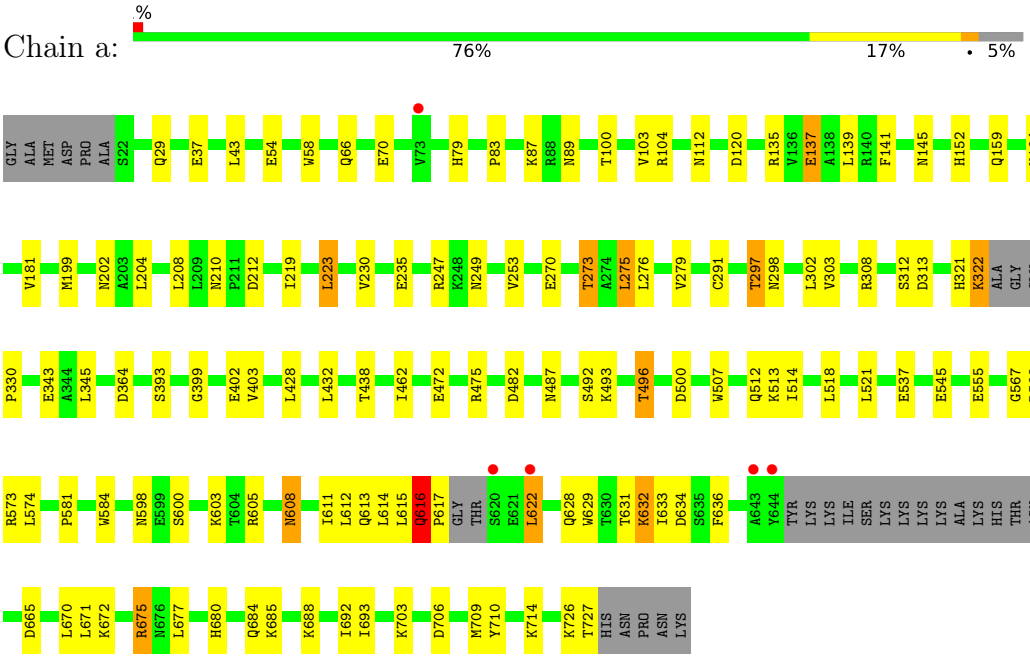
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots (i)

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.

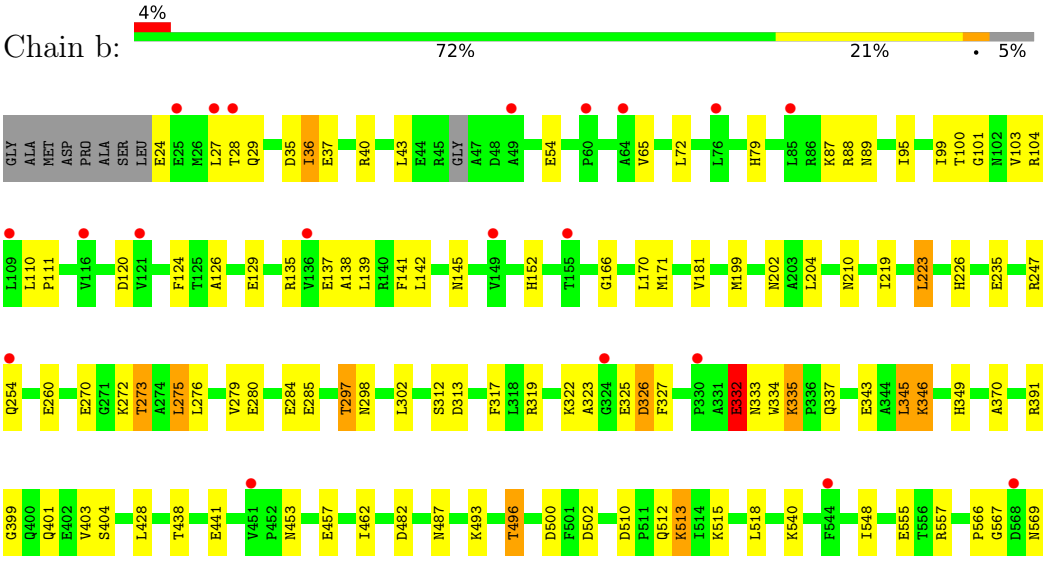
• Molecule 1: Ribonuclease L

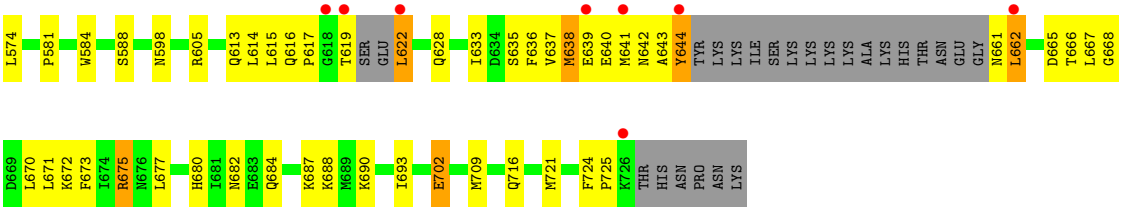
Chain a:



• Molecule 1: Ribonuclease L

Chain b:




L574
P581
W584
S588
N598
R605
Q613
L614
L615
Q616
P617
G618
T619
SER
GLU
L622
Q628
I633
D634
S635
F636
V637
M638
E639
E640
M641
N642
A643
Y644
TYR
LYS
LYS
ILE
SER
LYS
LYS
LYS
LYS
ALA
LYS
HIS
THR
ASN
GLU
GLY
N661
L662
D665
T666
L667
G668
D669
L670
L671
K672
F673
I674
R675
N676
L677
H680
I681
N682
E683
Q684
K687
K688
M689
K690
I693
E702
M709
Q716
M721
F724
P725
K726
THR
HIS
ASN
PRO
ASN
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.71Å 110.38Å 262.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.30 – 2.40 57.30 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (57.30-2.40) 99.4 (57.30-2.40)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.266 0.235 , 0.266	Depositor DCC
R_{free} test set	3336 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11057	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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, PO4, J60

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	0.83	0/5514	1.00	1/7445 (0.0%)
1	b	0.84	0/5539	1.02	6/7479 (0.1%)
All	All	0.84	0/11053	1.01	7/14924 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	333	ASN	N-CA-C	9.72	124.53	112.87
1	b	332	GLU	N-CA-C	8.22	128.30	110.80
1	b	638	MET	N-CA-C	-7.69	101.88	111.11
1	b	335	LYS	CA-C-N	-6.21	113.89	120.03
1	b	335	LYS	C-N-CA	-6.21	113.89	120.03
1	a	608	ASN	CB-CA-C	-6.03	100.43	110.68
1	b	500	ASP	N-CA-C	5.69	117.57	110.91

There are no chirality outliers.

There are no planarity outliers.

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	5418	0	5334	91	0
1	b	5442	0	5350	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	29	0	27	5	0
2	b	29	0	27	8	0
3	a	67	0	31	2	0
3	b	67	0	31	5	0
4	a	5	0	0	2	0
All	All	11057	0	10800	216	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 10.

All (216) 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)
3:b:801:25L:O4'	3:b:801:25L:C1'	1.65	1.28
3:a:802:25L:O4'	3:a:802:25L:C1'	1.66	1.27
1:b:638:MET:O	1:b:642:ASN:OD1	1.53	1.24
1:a:475:ARG:HG2	1:a:571:GLU:CB	1.75	1.16
1:b:297:THR:HB	1:b:323:ALA:CB	1.77	1.13
1:a:629:TRP:HA	1:a:632:LYS:HE3	1.23	1.08
1:a:297:THR:HB	1:a:322:LYS:HG3	1.35	1.07
1:b:637:VAL:O	1:b:641:MET:HB2	1.54	1.06
1:b:210:ASN:O	1:b:247:ARG:NH2	1.87	1.05
1:b:616:GLN:NE2	1:b:668:GLY:H	1.54	1.05
1:a:629:TRP:CA	1:a:632:LYS:HE3	1.86	1.04
1:a:632:LYS:HE2	1:a:632:LYS:H	1.24	1.01
1:b:297:THR:HB	1:b:323:ALA:HB1	1.43	1.01
1:b:584:TRP:CD2	1:b:725:PRO:HG3	1.96	1.00
1:b:635:SER:O	1:b:639:GLU:HB2	1.61	0.99
1:b:297:THR:CB	1:b:323:ALA:HB3	1.93	0.97
1:b:297:THR:HB	1:b:323:ALA:HB3	1.46	0.93
1:b:298:ASN:O	1:b:327:PHE:CD1	2.22	0.93
1:b:635:SER:O	1:b:639:GLU:CB	2.17	0.93
1:a:475:ARG:CG	1:a:571:GLU:CB	2.50	0.90
1:a:628:GLN:O	1:a:632:LYS:NZ	2.05	0.89
1:b:297:THR:CG2	1:b:323:ALA:HB3	2.01	0.89
1:a:632:LYS:HE2	1:a:632:LYS:N	1.87	0.88
1:a:297:THR:HB	1:a:322:LYS:CG	2.04	0.87
1:a:159:GLN:HE22	1:b:391:ARG:HH22	1.20	0.87
1:b:297:THR:CB	1:b:323:ALA:CB	2.52	0.86
1:a:507:TRP:CZ2	1:a:570:VAL:HG11	2.10	0.86
1:a:322:LYS:NZ	1:a:322:LYS:HA	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:617:PRO:HG3	1:a:714:LYS:HE3	1.58	0.84
1:b:613:GLN:O	1:b:617:PRO:HG3	1.78	0.84
1:b:641:MET:HG2	1:b:673:PHE:CE1	2.12	0.83
2:b:802:J60:NAP	2:b:802:J60:OAJ	2.12	0.81
1:b:584:TRP:CG	1:b:725:PRO:HG3	2.16	0.81
1:b:637:VAL:O	1:b:641:MET:CB	2.29	0.80
1:a:329:PRO:CD	1:a:330:PRO:HD3	2.13	0.78
1:b:641:MET:CG	1:b:673:PHE:CE1	2.66	0.77
1:a:514:ILE:HG21	1:a:573:ARG:HH11	1.49	0.77
1:b:298:ASN:O	1:b:327:PHE:CE1	2.38	0.77
1:b:297:THR:HG21	1:b:323:ALA:HB3	1.65	0.77
1:b:636:PHE:HA	1:b:639:GLU:HB3	1.66	0.76
1:a:629:TRP:C	1:a:632:LYS:HE3	2.12	0.75
1:b:616:GLN:NE2	1:b:666:THR:HB	2.01	0.75
1:a:500:ASP:OD1	2:a:801:J60:CL	2.42	0.75
1:a:514:ILE:HD13	1:a:570:VAL:HG13	1.70	0.74
3:b:801:25L:OAF	3:b:801:25L:HCO	1.87	0.74
1:b:724:PHE:HB3	1:b:725:PRO:HD2	1.69	0.73
1:b:635:SER:O	1:b:639:GLU:N	2.21	0.73
1:b:584:TRP:CE2	1:b:725:PRO:CG	2.74	0.70
1:a:432:LEU:HD13	2:a:801:J60:HAB	1.74	0.69
1:a:514:ILE:CD1	1:a:570:VAL:HG13	2.22	0.69
1:b:616:GLN:NE2	1:b:668:GLY:N	2.36	0.69
1:b:605:ARG:NH2	1:b:662:LEU:O	2.25	0.69
1:a:329:PRO:N	1:a:330:PRO:HD3	2.07	0.69
1:a:631:THR:OG1	1:a:632:LYS:NZ	2.25	0.68
1:b:27:LEU:O	1:b:28:THR:C	2.37	0.68
1:a:615:LEU:O	1:a:617:PRO:HD2	1.94	0.68
1:a:159:GLN:HE22	1:b:391:ARG:NH2	1.91	0.67
1:b:584:TRP:CE2	1:b:725:PRO:HG3	2.29	0.67
1:b:298:ASN:O	1:b:327:PHE:HD1	1.75	0.67
1:b:636:PHE:O	1:b:640:GLU:N	2.25	0.67
1:a:605:ARG:NH2	1:a:662:LEU:O	2.28	0.66
2:a:801:J60:OAJ	2:a:801:J60:NAP	2.26	0.66
1:a:329:PRO:N	1:a:330:PRO:CD	2.58	0.66
1:b:567:GLY:O	1:b:570:VAL:HB	1.97	0.65
1:b:628:GLN:HA	1:b:665:ASP:CG	2.23	0.64
1:a:629:TRP:O	1:a:632:LYS:HE2	1.96	0.64
1:a:628:GLN:HA	1:a:665:ASP:CG	2.23	0.63
1:a:297:THR:CB	1:a:322:LYS:HG3	2.19	0.63
1:a:629:TRP:O	1:a:632:LYS:CE	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:629:TRP:C	1:a:632:LYS:CE	2.71	0.62
1:a:617:PRO:HG3	1:a:714:LYS:CE	2.30	0.62
1:a:632:LYS:N	1:a:632:LYS:CE	2.62	0.61
1:a:629:TRP:HA	1:a:632:LYS:CE	2.16	0.61
1:b:636:PHE:CA	1:b:639:GLU:HB3	2.30	0.61
1:b:637:VAL:O	1:b:641:MET:N	2.34	0.61
1:b:641:MET:HG3	1:b:673:PHE:CE1	2.35	0.60
1:b:622:LEU:HG	1:b:622:LEU:O	1.99	0.60
1:b:641:MET:CG	1:b:673:PHE:HE1	2.11	0.60
1:a:297:THR:HG21	1:a:322:LYS:HB2	1.84	0.60
1:a:329:PRO:HD2	1:a:330:PRO:HD3	1.83	0.58
1:a:297:THR:CB	1:a:322:LYS:CG	2.78	0.58
1:b:398:ARG:NH2	1:b:502:ASP:OD2	2.36	0.58
1:a:58:TRP:CZ2	1:a:87:LYS:HE2	2.38	0.58
1:b:584:TRP:CD2	1:b:725:PRO:CG	2.80	0.58
1:a:514:ILE:CG2	1:a:573:ARG:HH11	2.16	0.58
1:b:332:GLU:OE1	1:b:349:HIS:HD2	1.85	0.58
1:b:616:GLN:HE22	1:b:668:GLY:H	1.44	0.58
1:b:110:LEU:N	1:b:111:PRO:HD2	2.19	0.57
1:a:603:LYS:HA	1:a:672:LYS:HD3	1.86	0.57
1:a:514:ILE:HG21	1:a:573:ARG:NH1	2.20	0.56
1:b:462:ILE:HA	1:b:496:THR:HG21	1.87	0.56
1:b:570:VAL:HG23	1:b:573:ARG:HG2	1.85	0.56
1:a:612:LEU:O	1:a:616:GLN:HB2	2.05	0.56
1:b:616:GLN:HE21	1:b:668:GLY:H	1.47	0.56
1:a:598:ASN:OD1	1:a:675:ARG:HD2	2.06	0.56
1:b:677:LEU:HD11	1:b:693:ILE:CD1	2.36	0.55
1:b:616:GLN:HE21	1:b:667:LEU:N	2.04	0.55
1:b:141:PHE:O	1:b:145:ASN:ND2	2.40	0.55
1:a:680:HIS:HE1	4:a:803:PO4:O3	1.90	0.54
1:a:432:LEU:CD1	2:a:801:J60:HAB	2.36	0.54
1:b:702:GLU:HA	1:b:702:GLU:OE1	2.05	0.54
1:b:334:TRP:HH2	1:b:345:LEU:HB3	1.73	0.54
1:b:598:ASN:OD1	1:b:675:ARG:HD2	2.07	0.53
1:b:635:SER:O	1:b:639:GLU:CA	2.56	0.53
1:a:677:LEU:HD11	1:a:693:ILE:CD1	2.38	0.53
1:a:208:LEU:O	1:a:247:ARG:NH2	2.39	0.53
1:b:566:PRO:HB2	1:b:570:VAL:HG21	1.90	0.53
1:b:584:TRP:CZ2	1:b:725:PRO:HD2	2.43	0.53
1:a:322:LYS:HA	1:a:322:LYS:HZ3	1.72	0.53
1:a:322:LYS:HA	1:a:322:LYS:HZ2	1.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:441:GLU:OE2	2:b:802:J60:HBA3	2.09	0.52
1:a:628:GLN:O	1:a:632:LYS:CE	2.57	0.52
1:a:615:LEU:O	1:a:617:PRO:CD	2.58	0.52
1:b:642:ASN:OD1	1:b:642:ASN:N	2.43	0.52
1:a:555:GLU:HA	1:a:709:MET:HE3	1.92	0.52
1:b:570:VAL:CG2	1:b:573:ARG:HG2	2.40	0.52
1:a:159:GLN:NE2	1:b:391:ARG:HH22	2.00	0.51
1:a:507:TRP:CH2	1:a:570:VAL:HG11	2.45	0.51
3:b:801:25L:CBV	3:b:801:25L:CBW	2.89	0.51
1:b:644:TYR:CD2	1:b:644:TYR:N	2.78	0.51
1:a:482:ASP:O	1:a:487:ASN:ND2	2.44	0.50
1:a:322:LYS:HA	1:a:322:LYS:CE	2.40	0.50
1:a:581:PRO:HD2	1:a:709:MET:HE1	1.93	0.50
1:a:29:GLN:HE21	1:a:29:GLN:HA	1.77	0.50
1:b:370:ALA:CB	2:b:802:J60:HAQ3	2.40	0.50
1:b:124:PHE:CE2	3:b:801:25L:CBY	2.94	0.49
2:a:801:J60:OAT	2:a:801:J60:HAW2	2.12	0.49
1:a:364:ASP:OD2	1:b:88:ARG:NH1	2.46	0.49
1:b:343:GLU:CD	1:b:346:LYS:NZ	2.71	0.49
1:b:581:PRO:HD2	1:b:709:MET:HE1	1.93	0.49
3:b:801:25L:HAW	3:b:801:25L:HAYA	1.94	0.49
1:b:370:ALA:CB	2:b:802:J60:CAQ	2.91	0.48
1:a:611:ILE:HG13	1:a:615:LEU:HD12	1.95	0.48
1:b:616:GLN:HE22	1:b:668:GLY:N	2.08	0.48
1:a:581:PRO:HB2	1:a:709:MET:HE2	1.94	0.48
1:b:319:ARG:O	1:b:322:LYS:CG	2.62	0.48
1:a:139:LEU:HD22	1:a:181:VAL:HG13	1.96	0.48
1:b:139:LEU:HD22	1:b:181:VAL:HG13	1.96	0.47
1:b:584:TRP:CE2	1:b:725:PRO:CD	2.97	0.47
1:b:441:GLU:OE1	2:b:802:J60:HAR1	2.14	0.47
1:a:569:ASN:ND2	1:a:572:ASP:HB2	2.29	0.47
1:b:343:GLU:OE2	1:b:346:LYS:NZ	2.47	0.47
1:b:555:GLU:HA	1:b:709:MET:HE3	1.95	0.47
1:a:137:GLU:CD	1:a:137:GLU:H	2.21	0.47
1:a:291:CYS:HB3	1:a:321:HIS:CE1	2.50	0.47
1:a:462:ILE:HA	1:a:496:THR:HG21	1.97	0.47
1:b:101:GLY:O	1:b:138:ALA:HB2	2.15	0.46
1:b:584:TRP:CZ2	1:b:725:PRO:CD	2.98	0.46
1:b:284:GLU:OE2	1:b:313:ASP:HB3	2.15	0.46
1:b:482:ASP:O	1:b:487:ASN:ND2	2.48	0.46
1:a:275:LEU:HD13	1:a:302:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:370:ALA:HB1	2:b:802:J60:HAQ3	1.97	0.46
1:b:510:ASP:OD2	1:b:513:LYS:HE2	2.16	0.46
1:a:622:LEU:HD22	1:a:622:LEU:HA	1.78	0.45
1:b:219:ILE:HG22	1:b:223:LEU:HD22	1.99	0.45
1:b:584:TRP:CD1	1:b:725:PRO:HG3	2.52	0.45
1:b:616:GLN:N	1:b:617:PRO:HD3	2.31	0.45
1:a:43:LEU:HB3	1:a:79:HIS:CD2	2.52	0.45
1:b:65:VAL:O	1:b:100:THR:HG21	2.16	0.45
1:a:617:PRO:CG	1:a:710:TYR:OH	2.65	0.44
1:b:641:MET:HG3	1:b:673:PHE:HE1	1.79	0.44
1:a:634:ASP:OD2	1:a:692:ILE:HD13	2.16	0.44
1:b:326:ASP:OD1	1:b:326:ASP:N	2.50	0.44
1:b:441:GLU:OE2	2:b:802:J60:HAR3	2.17	0.44
1:a:249:ASN:O	1:a:253:VAL:HG23	2.17	0.44
1:b:202:ASN:OD1	1:b:204:LEU:HB3	2.18	0.44
1:b:43:LEU:HB3	1:b:79:HIS:CD2	2.52	0.44
1:b:716:GLN:O	1:b:721:MET:SD	2.76	0.44
1:b:106:LEU:HD22	1:b:142:LEU:HD21	1.99	0.44
1:b:275:LEU:HD13	1:b:302:LEU:HD11	1.99	0.44
1:b:319:ARG:O	1:b:322:LYS:HG3	2.18	0.44
1:b:89:ASN:O	1:b:120:ASP:HB2	2.18	0.43
1:b:171:MET:HE2	1:b:202:ASN:HA	2.00	0.43
1:b:399:GLY:O	1:b:403:VAL:HG12	2.17	0.43
1:b:636:PHE:C	1:b:639:GLU:HB3	2.43	0.43
1:a:399:GLY:O	1:a:403:VAL:HG12	2.18	0.43
1:b:36:ILE:HD11	1:b:72:LEU:HG	2.00	0.43
1:b:95:ILE:HA	1:b:126:ALA:HB2	2.00	0.43
1:b:581:PRO:HB2	1:b:709:MET:HE2	2.00	0.43
1:a:636:PHE:HE2	1:a:688:LYS:HB3	1.83	0.43
3:a:802:25L:HAX	3:a:802:25L:OBM	2.19	0.43
1:b:249:ASN:O	1:b:253:VAL:HG23	2.19	0.43
1:b:152:HIS:HB3	1:b:166:GLY:HA2	2.01	0.43
1:a:219:ILE:HG22	1:a:223:LEU:HD22	2.01	0.43
1:a:83:PRO:HG3	1:a:112:ASN:HB2	2.01	0.42
1:a:202:ASN:OD1	1:a:204:LEU:HB3	2.19	0.42
1:a:581:PRO:HB2	1:a:709:MET:CE	2.49	0.42
1:b:273:THR:HG22	1:b:276:LEU:H	1.84	0.42
1:a:273:THR:HG22	1:a:276:LEU:H	1.83	0.42
1:b:279:VAL:HG21	1:b:302:LEU:HD22	2.01	0.42
1:b:615:LEU:C	1:b:617:PRO:HD3	2.44	0.42
1:b:605:ARG:HH12	1:b:661:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:677:LEU:HD11	1:a:693:ILE:HD13	2.01	0.42
1:b:588:SER:HB3	1:b:725:PRO:HB3	2.01	0.42
1:b:682:ASN:OD1	1:b:690:LYS:HE2	2.20	0.42
1:b:99:ILE:HG13	1:b:129:GLU:HB3	2.02	0.42
1:a:567:GLY:O	1:a:568:ASP:OD1	2.37	0.42
1:b:145:ASN:N	1:b:145:ASN:HD22	2.18	0.42
1:a:89:ASN:O	1:a:120:ASP:HB2	2.19	0.42
1:a:581:PRO:HA	1:a:584:TRP:CG	2.55	0.42
1:b:548:ILE:HG23	1:b:557:ARG:HG3	2.01	0.41
1:a:152:HIS:HB3	1:a:166:GLY:HA2	2.02	0.41
4:a:803:PO4:O2	1:b:680:HIS:NE2	2.53	0.41
1:b:555:GLU:HG3	1:b:709:MET:HE3	2.02	0.41
1:a:210:ASN:HD22	1:a:212:ASP:H	1.66	0.41
1:a:66:GLN:O	1:b:312:SER:OG	2.38	0.41
1:a:279:VAL:HG21	1:a:302:LEU:HD22	2.03	0.41
1:a:628:GLN:O	1:a:632:LYS:HE3	2.19	0.41
1:a:141:PHE:O	1:a:145:ASN:ND2	2.43	0.41
1:b:317:PHE:CD1	1:b:317:PHE:C	2.99	0.40
1:b:110:LEU:N	1:b:111:PRO:CD	2.84	0.40
1:b:272:LYS:HE2	1:b:280:GLU:OE2	2.21	0.40
1:b:548:ILE:CG2	1:b:557:ARG:HG3	2.52	0.40
2:b:802:J60:NAP	2:b:802:J60:CAI	2.76	0.40
1:a:475:ARG:HG3	1:a:571:GLU:CB	2.46	0.40
1:a:706:ASP:OD1	1:a:706:ASP:N	2.50	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	673/717 (94%)	639 (95%)	32 (5%)	2 (0%)	36 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	b	676/717 (94%)	636 (94%)	38 (6%)	2 (0%)	36 50
All	All	1349/1434 (94%)	1275 (94%)	70 (5%)	4 (0%)	36 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	570	VAL
1	b	643	ALA
1	a	616	GLN
1	b	332	GLU

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	585/617 (95%)	525 (90%)	60 (10%)	7 11
1	b	585/617 (95%)	522 (89%)	63 (11%)	6 9
All	All	1170/1234 (95%)	1047 (90%)	123 (10%)	6 10

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	37	GLU
1	a	54	GLU
1	a	70	GLU
1	a	100	THR
1	a	103	VAL
1	a	104	ARG
1	a	135	ARG
1	a	137	GLU
1	a	164	LYS
1	a	170	LEU
1	a	199	MET
1	a	223	LEU

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Mol	Chain	Res	Type
1	a	230	VAL
1	a	235	GLU
1	a	270	GLU
1	a	273	THR
1	a	275	LEU
1	a	297	THR
1	a	298	ASN
1	a	303	VAL
1	a	308	ARG
1	a	312	SER
1	a	313	ASP
1	a	322	LYS
1	a	343	GLU
1	a	345	LEU
1	a	393	SER
1	a	402	GLU
1	a	428	LEU
1	a	438	THR
1	a	472	GLU
1	a	492	SER
1	a	493	LYS
1	a	496	THR
1	a	512	GLN
1	a	513	LYS
1	a	518	LEU
1	a	521	LEU
1	a	537	GLU
1	a	545	GLU
1	a	569	ASN
1	a	572	ASP
1	a	574	LEU
1	a	600	SER
1	a	608	ASN
1	a	613	GLN
1	a	614	LEU
1	a	616	GLN
1	a	622	LEU
1	a	632	LYS
1	a	633	ILE
1	a	662	LEU
1	a	670	LEU
1	a	671	LEU

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Mol	Chain	Res	Type
1	a	675	ARG
1	a	684	GLN
1	a	685	LYS
1	a	703	LYS
1	a	726	LYS
1	a	727	THR
1	b	24	GLU
1	b	29	GLN
1	b	35	ASP
1	b	36	ILE
1	b	37	GLU
1	b	40	ARG
1	b	54	GLU
1	b	87	LYS
1	b	103	VAL
1	b	104	ARG
1	b	108	LEU
1	b	135	ARG
1	b	137	GLU
1	b	170	LEU
1	b	199	MET
1	b	223	LEU
1	b	226	HIS
1	b	235	GLU
1	b	254	GLN
1	b	260	GLU
1	b	270	GLU
1	b	273	THR
1	b	275	LEU
1	b	285	GLU
1	b	297	THR
1	b	325	GLU
1	b	326	ASP
1	b	335	LYS
1	b	337	GLN
1	b	345	LEU
1	b	346	LYS
1	b	393	SER
1	b	401	GLN
1	b	404	SER
1	b	428	LEU
1	b	438	THR

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Mol	Chain	Res	Type
1	b	453	ASN
1	b	457	GLU
1	b	493	LYS
1	b	496	THR
1	b	512	GLN
1	b	513	LYS
1	b	515	LYS
1	b	518	LEU
1	b	540	LYS
1	b	569	ASN
1	b	572	ASP
1	b	573	ARG
1	b	574	LEU
1	b	614	LEU
1	b	619	THR
1	b	622	LEU
1	b	633	ILE
1	b	644	TYR
1	b	662	LEU
1	b	670	LEU
1	b	671	LEU
1	b	672	LYS
1	b	675	ARG
1	b	684	GLN
1	b	687	LYS
1	b	688	LYS
1	b	702	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	29	GLN
1	a	38	GLN
1	a	107	GLN
1	a	159	GLN
1	a	198	ASN
1	a	210	ASN
1	a	254	GLN
1	a	292	HIS
1	a	401	GLN
1	a	664	GLN
1	a	680	HIS

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Mol	Chain	Res	Type
1	b	52	GLN
1	b	107	GLN
1	b	145	ASN
1	b	198	ASN
1	b	349	HIS
1	b	565	HIS
1	b	607	GLN
1	b	616	GLN
1	b	664	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\| > 2$
4	PO4	a	803	-	4,4,4	1.32	1 (25%)	6,6,6	0.64	0
2	J60	a	801	-	31,31,31	3.56	14 (45%)	42,44,44	2.92	17 (40%)
2	J60	b	802	-	31,31,31	3.48	16 (51%)	42,44,44	2.38	14 (33%)
3	25L	b	801	-	75,75,83	3.16	29 (38%)	111,116,130	2.23	39 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	25L	a	802	-	75,75,83	3.15	28 (37%)	111,116,130	2.27	37 (33%)

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	J60	b	802	-	-	4/18/30/30	0/3/3/3
2	J60	a	801	-	-	3/18/30/30	0/3/3/3
3	25L	a	802	-	-	11/40/88/100	0/9/9/9
3	25L	b	801	-	-	18/40/88/100	0/9/9/9

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	802	J60	CAG-CAI	-11.28	1.34	1.50
2	a	801	J60	CAG-CAI	-10.80	1.35	1.50
3	a	802	25L	O4'-C1'	10.39	1.66	1.42
3	b	801	25L	O4'-C1'	10.29	1.65	1.42
3	a	802	25L	OBO-CCN	9.03	1.62	1.42
3	b	801	25L	OBO-CCN	9.02	1.62	1.42
3	a	802	25L	OBP-CCO	8.37	1.61	1.42
3	b	801	25L	CCK-CCN	-7.59	1.34	1.53
2	b	802	J60	CAE-CAG	-7.59	1.32	1.45
2	a	801	J60	CAE-CAG	-7.43	1.32	1.45
2	b	802	J60	CAN-CAS	-7.03	1.34	1.48
3	a	802	25L	CCL-CCO	-7.00	1.35	1.53
3	b	801	25L	CCL-CCO	-6.93	1.36	1.53
3	b	801	25L	OBP-CCO	6.91	1.58	1.42
3	b	801	25L	OBO-CCI	-6.43	1.30	1.45
3	a	802	25L	CCK-CCN	-6.41	1.37	1.53
3	a	802	25L	O4'-C4'	-6.35	1.30	1.45
3	a	802	25L	C2'-C1'	-6.20	1.34	1.53
3	b	801	25L	O4'-C4'	-6.14	1.31	1.45
2	a	801	J60	CAN-CAS	-6.03	1.36	1.48
3	b	801	25L	C6-N6	5.76	1.48	1.34
3	a	802	25L	CBW-NAC	5.75	1.48	1.34
3	a	802	25L	OBO-CCI	-5.48	1.32	1.45
2	a	801	J60	CAC-CAF	-5.34	1.31	1.39
2	a	801	J60	CAA-CL	5.24	1.86	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	802	25L	OBP-CCJ	-5.16	1.33	1.45
3	b	801	25L	CBW-NAC	4.98	1.46	1.34
3	b	801	25L	C2'-C1'	-4.96	1.37	1.53
3	a	802	25L	C6-N6	4.64	1.46	1.34
3	a	802	25L	C5-N7	-4.60	1.30	1.39
3	b	801	25L	OBP-CCJ	-4.53	1.34	1.45
2	b	802	J60	CAL-CAM	-4.38	1.31	1.41
2	a	801	J60	CAI-NAH	-4.33	1.31	1.36
3	b	801	25L	O3'-C3'	-4.21	1.32	1.43
3	b	801	25L	OAK-CCF	-3.89	1.33	1.43
2	a	801	J60	CAK-CAL	-3.87	1.31	1.40
3	a	802	25L	O3'-C3'	-3.84	1.33	1.43
3	b	801	25L	CBY-CCB	-3.84	1.32	1.39
2	a	801	J60	CAE-CAF	-3.83	1.36	1.41
2	b	802	J60	CAD-CAE	-3.80	1.33	1.39
2	a	801	J60	CAR-CAO	3.78	1.56	1.49
3	b	801	25L	O2'-C2'	3.77	1.52	1.43
3	a	802	25L	CBY-NBI	-3.64	1.32	1.39
3	b	801	25L	C5-N7	-3.61	1.32	1.39
2	b	802	J60	CAA-CL	-3.59	1.66	1.74
3	b	801	25L	CBY-NBI	-3.58	1.32	1.39
2	a	801	J60	CAL-CAM	-3.46	1.33	1.41
2	a	801	J60	CAF-NAH	-3.45	1.32	1.38
3	b	801	25L	CBZ-CCC	-3.39	1.33	1.39
3	a	802	25L	C5-C4	-3.38	1.33	1.39
3	b	801	25L	OAL-CCG	-3.31	1.34	1.43
2	b	802	J60	CAK-CAL	-3.30	1.32	1.40
3	a	802	25L	CBY-CCB	-3.26	1.33	1.39
3	a	802	25L	OAL-CCG	-3.22	1.35	1.43
3	b	801	25L	CBZ-NBJ	-3.22	1.33	1.39
2	a	801	J60	CAQ-CAM	3.18	1.57	1.50
3	b	801	25L	PCT-OBT	3.14	1.66	1.54
3	a	802	25L	C8-N9	-3.12	1.32	1.37
2	b	802	J60	CAI-NAH	-3.07	1.32	1.36
3	a	802	25L	CCG-CCJ	3.03	1.60	1.53
2	b	802	J60	CAC-CAF	-3.02	1.34	1.39
2	b	802	J60	CAN-CAO	-3.01	1.33	1.39
2	b	802	J60	CAF-NAH	-2.99	1.33	1.38
3	a	802	25L	PCT-OBT	2.96	1.65	1.54
2	b	802	J60	CAO-NAP	-2.75	1.29	1.37
3	a	802	25L	CBV-NAB	2.74	1.41	1.34
3	a	802	25L	CCF-CCI	2.72	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	802	J60	CAE-CAF	-2.71	1.38	1.41
3	b	801	25L	PCV-OBQ	2.66	1.67	1.59
3	b	801	25L	CBV-NAB	2.60	1.40	1.34
3	b	801	25L	CCF-CCI	2.51	1.59	1.53
2	b	802	J60	CAQ-CAM	2.51	1.55	1.50
3	a	802	25L	CAW-NCQ	-2.51	1.33	1.37
3	a	802	25L	OAK-CCF	-2.50	1.36	1.43
3	a	802	25L	O2'-C2'	2.49	1.49	1.43
3	b	801	25L	CCG-CCJ	2.48	1.59	1.53
2	a	801	J60	CAL-NAP	-2.47	1.33	1.37
2	a	801	J60	CAO-NAP	-2.43	1.30	1.37
3	a	802	25L	CBZ-CCC	-2.34	1.34	1.39
3	a	802	25L	CCB-NBF	2.27	1.38	1.34
2	b	802	J60	CAS-NAU	2.26	1.37	1.33
3	a	802	25L	CAX-NBJ	2.26	1.36	1.31
3	b	801	25L	C8-N7	2.18	1.35	1.31
2	b	802	J60	CAR-CAO	-2.13	1.46	1.49
3	b	801	25L	PCT-OBK	2.04	1.66	1.60
3	b	801	25L	C5-C4	-2.04	1.35	1.39
3	b	801	25L	CAW-NCQ	-2.02	1.34	1.37
4	a	803	PO4	P-O4	-2.00	1.48	1.54

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	801	J60	CAF-NAH-CAI	-9.81	105.30	111.35
2	b	802	J60	CAF-NAH-CAI	-7.51	106.72	111.35
3	b	801	25L	OAM-PCT-OBK	6.41	123.39	106.67
2	a	801	J60	CAE-CAG-CAI	6.36	108.83	105.31
2	b	802	J60	CAG-CAI-NAH	5.94	110.16	106.91
3	b	801	25L	NAC-CBW-NBD	-5.92	105.20	118.38
3	b	801	25L	NBG-CAU-NBD	-5.88	119.68	128.58
3	a	802	25L	N3-C2-N1	-5.88	119.69	128.58
3	a	802	25L	NBF-CAT-NBC	-5.82	119.77	128.58
3	a	802	25L	NAC-CBW-NBD	-5.80	105.47	118.38
3	a	802	25L	C5-C4-N3	-5.57	119.04	126.72
3	b	801	25L	NBF-CAT-NBC	-5.52	120.22	128.58
3	a	802	25L	CBY-CCB-NBF	-5.49	119.15	126.72
2	a	801	J60	CAG-CAI-NAH	5.41	109.88	106.91
3	b	801	25L	CBZ-CCC-NBG	-5.34	119.36	126.72
3	a	802	25L	NBG-CAU-NBD	-5.18	120.74	128.58
3	b	801	25L	C5-C4-N3	-5.03	119.79	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	801	25L	N3-C2-N1	-4.96	121.08	128.58
2	a	801	J60	CAC-CAB-CAA	4.62	123.89	119.24
2	a	801	J60	CAD-CAE-CAF	4.60	123.87	119.39
2	a	801	J60	CAB-CAA-CAD	-4.57	115.56	121.53
2	b	802	J60	CAL-NAP-CAO	-4.44	107.47	110.31
3	b	801	25L	CBZ-CBW-NAC	4.24	133.78	123.29
3	a	802	25L	CBZ-CBW-NAC	4.18	133.64	123.29
3	a	802	25L	N9-C8-N7	-4.17	108.02	113.94
2	a	801	J60	CAD-CAA-CL	4.14	124.36	119.17
3	a	802	25L	NCR-CAX-NBJ	-4.08	108.15	113.94
2	a	801	J60	CAL-NAP-CAO	-3.95	107.78	110.31
2	b	802	J60	CAG-CAK-CAL	-3.94	120.84	133.34
3	b	801	25L	C5-C4-N9	3.93	110.09	105.81
2	b	802	J60	CAE-CAG-CAI	3.91	107.47	105.31
3	a	802	25L	CBZ-CCC-NBG	-3.91	121.34	126.72
2	a	801	J60	CAF-CAE-CAG	-3.71	104.25	106.62
3	b	801	25L	CBY-CCB-NBF	-3.68	121.65	126.72
3	a	802	25L	N6-C6-N1	-3.63	110.28	118.38
3	a	802	25L	C2-N3-C4	3.62	120.68	111.83
3	a	802	25L	NBF-CCB-NCQ	3.62	133.32	127.17
2	b	802	J60	CAN-CAO-NAP	3.52	110.10	107.48
3	b	801	25L	OBQ-CCK-CCF	-3.51	99.10	111.68
3	a	802	25L	OBQ-PCV-OAG	-3.46	98.73	109.81
3	a	802	25L	NCQ-CAW-NBI	-3.45	109.05	113.94
3	a	802	25L	N3-C4-N9	3.44	133.03	127.17
3	a	802	25L	CBV-CBY-CCB	3.40	121.82	117.18
3	b	801	25L	CAU-NBG-CCC	3.37	120.07	111.83
3	a	802	25L	C5-N7-C8	3.31	108.65	103.45
3	b	801	25L	CCG-CCL-CCO	3.25	109.02	102.81
3	b	801	25L	NAB-CBV-NBC	-3.21	111.23	118.38
3	a	802	25L	CCK-CCN-NCQ	3.17	118.97	113.75
2	a	801	J60	CAG-CAK-CAL	-3.14	123.37	133.34
2	a	801	J60	CAE-CAF-NAH	3.11	111.73	108.23
3	a	802	25L	CCC-NCR-CAX	3.11	109.00	105.74
3	b	801	25L	C2-N3-C4	3.09	119.38	111.83
3	b	801	25L	NCQ-CAW-NBI	-3.04	109.63	113.94
3	a	802	25L	NAB-CBV-NBC	-3.01	111.67	118.38
3	a	802	25L	CAT-NBF-CCB	2.99	119.12	111.83
2	b	802	J60	CAQ-CAM-CAL	-2.97	121.30	125.62
3	b	801	25L	NBG-CCC-NCR	2.95	132.19	127.17
3	a	802	25L	CAU-NBG-CCC	2.93	119.00	111.83
3	b	801	25L	C6-C5-C4	2.88	121.11	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	802	25L	CCG-CCL-CCO	2.85	108.27	102.81
3	a	802	25L	OBQ-CCK-CCF	-2.85	101.45	111.68
3	a	802	25L	CBY-NBI-CAW	2.82	107.89	103.45
3	a	802	25L	NBG-CCC-NCR	2.75	131.85	127.17
3	b	801	25L	NCR-CAX-NBJ	-2.71	110.09	113.94
3	b	801	25L	N6-C6-N1	-2.69	112.38	118.38
3	b	801	25L	O4'-C4'-C3'	-2.67	99.85	105.15
2	a	801	J60	CAW-NAX-CAY	-2.61	100.74	111.79
2	b	802	J60	CAW-NAX-CAZ	2.58	122.72	111.79
2	b	802	J60	CAO-CAN-CAM	-2.57	106.07	107.83
2	a	801	J60	CAE-CAG-CAK	-2.54	119.25	133.19
2	b	802	J60	CAD-CAE-CAF	2.53	121.85	119.39
2	a	801	J60	CAN-CAO-NAP	2.52	109.36	107.48
3	b	801	25L	C2'-C1'-N9	2.52	119.56	113.30
3	a	802	25L	OBP-CCJ-CCG	2.51	110.14	105.15
3	b	801	25L	CBY-CBV-NAB	2.50	129.47	123.29
3	b	801	25L	C3'-C2'-C1'	2.49	106.17	101.46
3	a	802	25L	OBR-CCL-CCO	-2.49	101.29	110.05
3	b	801	25L	CAT-NBF-CCB	2.48	117.90	111.83
3	a	802	25L	CBY-CBV-NAB	2.47	129.40	123.29
2	a	801	J60	CAC-CAF-CAE	-2.47	119.80	122.19
3	b	801	25L	OBO-CCN-NCQ	-2.45	103.38	108.09
3	a	802	25L	C6-C5-C4	2.45	120.52	117.18
3	b	801	25L	CBZ-CCC-NCR	2.42	108.45	105.81
3	b	801	25L	CBW-CBZ-CCC	2.39	120.44	117.18
3	b	801	25L	OBR-CCL-CCG	-2.39	103.11	111.68
2	b	802	J60	CAV-CAW-NAX	2.38	118.65	112.84
3	b	801	25L	N9-C8-N7	-2.38	110.57	113.94
2	a	801	J60	CAO-CAN-CAM	-2.37	106.20	107.83
3	b	801	25L	CBZ-NBJ-CAX	2.37	107.18	103.45
3	b	801	25L	CBY-CCB-NCQ	2.35	108.37	105.81
3	b	801	25L	C4-C5-N7	-2.28	107.97	110.58
2	a	801	J60	OAJ-CAI-NAH	-2.27	122.68	126.30
3	a	802	25L	C5-C6-N6	2.27	128.90	123.29
3	b	801	25L	C5-C6-N6	2.24	128.83	123.29
3	b	801	25L	O2'-C2'-C1'	2.23	117.78	110.10
3	a	802	25L	OAQ-PCV-OAG	2.21	122.72	112.44
3	b	801	25L	C4'-O4'-C1'	-2.20	104.60	109.47
3	a	802	25L	OBO-CCI-CCF	2.17	109.46	105.15
3	b	801	25L	CBV-CBY-CCB	2.17	120.14	117.18
2	b	802	J60	CAD-CAA-CL	-2.16	116.45	119.17
3	b	801	25L	OAL-CCG-CCL	2.11	117.08	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	b	801	25L	OBP-CCO-CCL	-2.09	102.98	106.59
3	a	802	25L	C4-C5-N7	-2.09	108.20	110.58
3	a	802	25L	OAM-PCT-OBK	2.07	112.06	106.67
3	a	802	25L	CCC-NCR-CCO	-2.03	121.89	126.63
2	b	802	J60	OAJ-CAI-NAH	-2.02	123.08	126.30
2	b	802	J60	CAC-CAB-CAA	-2.02	117.21	119.24

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	801	J60	CAW-CAV-NAU-CAS
3	a	802	25L	CBA-OBM-PCV-OAG
3	b	801	25L	C5'-O5'-PCU-OAF
3	b	801	25L	C5'-O5'-PCU-OAP
3	b	801	25L	CAY-OBK-PCT-OAM
3	b	801	25L	CAY-OBK-PCT-OBT
2	a	801	J60	CAV-CAW-NAX-CAZ
3	b	801	25L	O4'-C4'-C5'-O5'
3	b	801	25L	OBK-CAY-CCI-OBO
3	b	801	25L	OBK-CAY-CCI-CCF
3	b	801	25L	OBM-CBA-CCJ-OBP
3	b	801	25L	OBM-CBA-CCJ-CCG
2	b	802	J60	NAU-CAV-CAW-NAX
3	a	802	25L	OBK-CAY-CCI-OBO
2	b	802	J60	CAV-CAW-NAX-CAZ
2	b	802	J60	CBB-CAY-NAX-CAW
3	a	802	25L	CCK-CCN-NCQ-CAW
3	a	802	25L	O4'-C4'-C5'-O5'
3	b	801	25L	CAY-OBK-PCT-OAE
2	a	801	J60	CBB-CAY-NAX-CAZ
3	a	802	25L	C3'-C4'-C5'-O5'
3	a	802	25L	OBK-CAY-CCI-CCF
2	b	802	J60	CBB-CAY-NAX-CAZ
3	b	801	25L	C3'-C4'-C5'-O5'
3	b	801	25L	CCO-CCL-OBR-PCU
3	a	802	25L	C2'-C1'-N9-C8
3	b	801	25L	C5'-O5'-PCU-OBR
3	b	801	25L	CBA-OBM-PCV-OAG
3	b	801	25L	CBA-OBM-PCV-OAQ
3	b	801	25L	CBA-OBM-PCV-OBQ
3	a	802	25L	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
3	a	802	25L	CCK-CCN-NCQ-CCB
3	a	802	25L	O4'-C1'-N9-C8
3	b	801	25L	CCG-CCL-OBR-PCU
3	b	801	25L	CCL-OBR-PCU-OAP
3	a	802	25L	OBO-CCN-NCQ-CAW

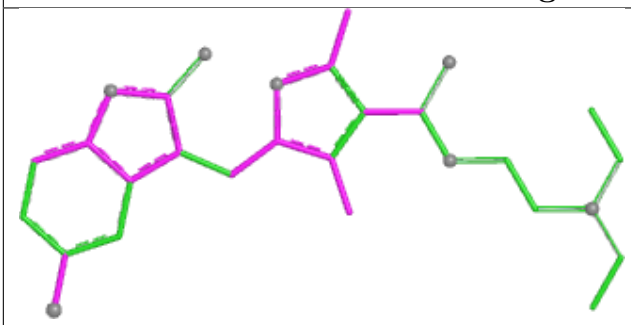
There are no ring outliers.

5 monomers are involved in 22 short contacts:

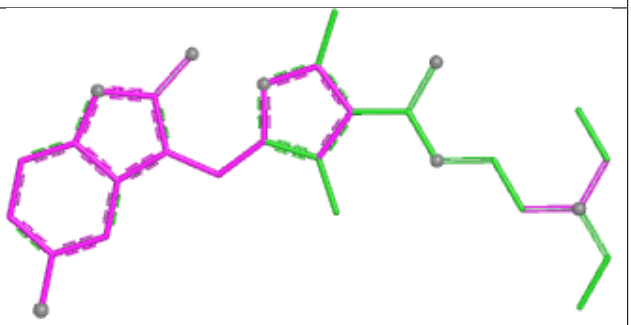
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	a	803	PO4	2	0
2	a	801	J60	5	0
2	b	802	J60	8	0
3	b	801	25L	5	0
3	a	802	25L	2	0

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 then 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.

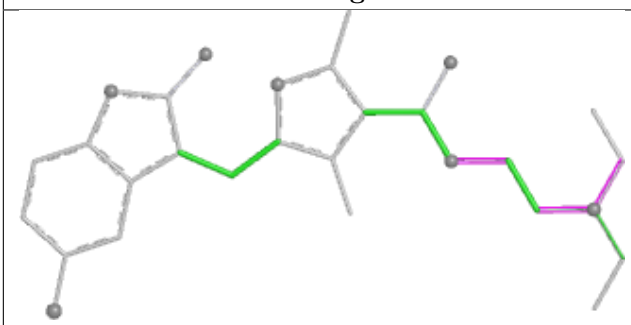
Ligand J60 a 801



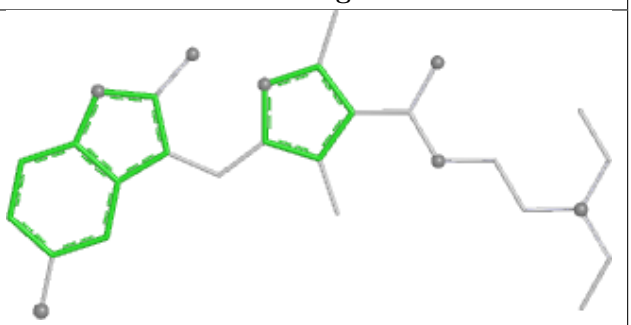
Bond lengths



Bond angles

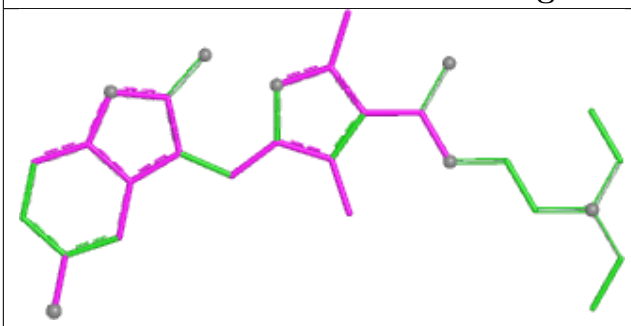


Torsions

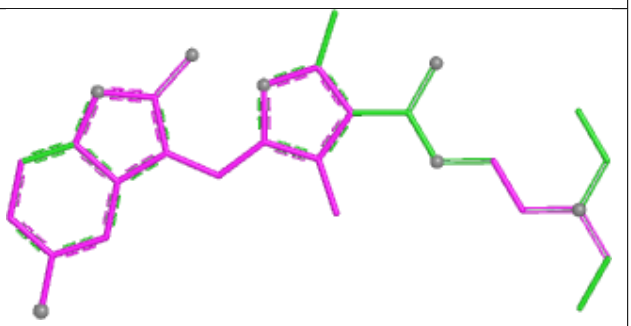


Rings

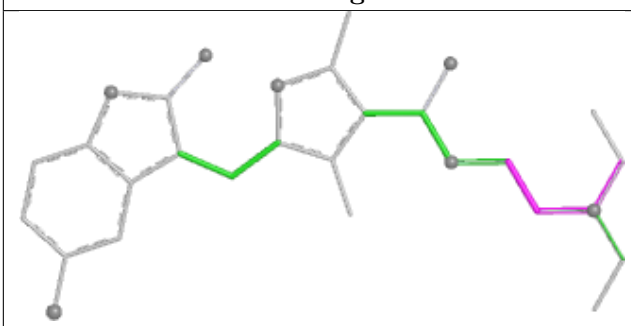
Ligand J60 b 802



Bond lengths



Bond angles



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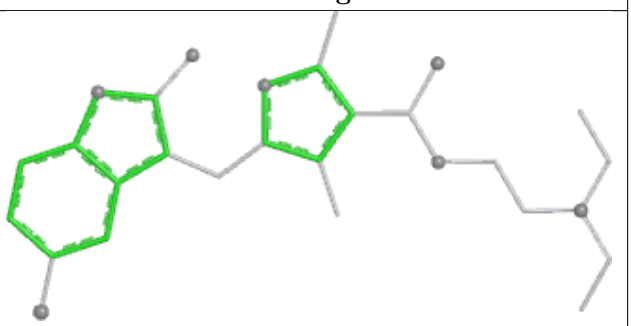
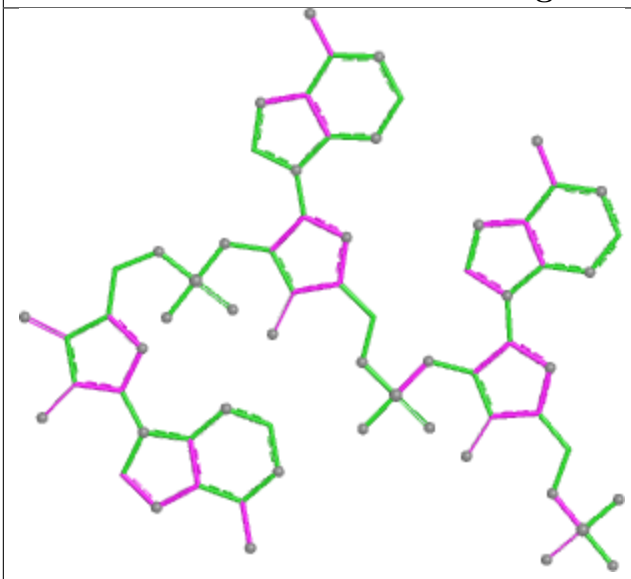
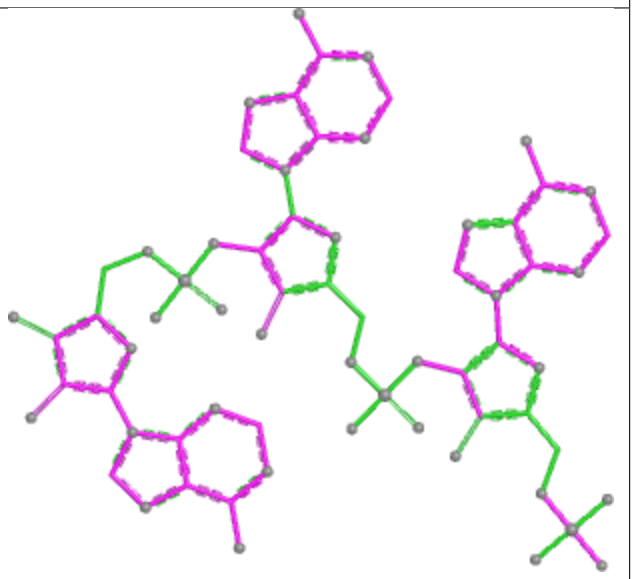


Rings

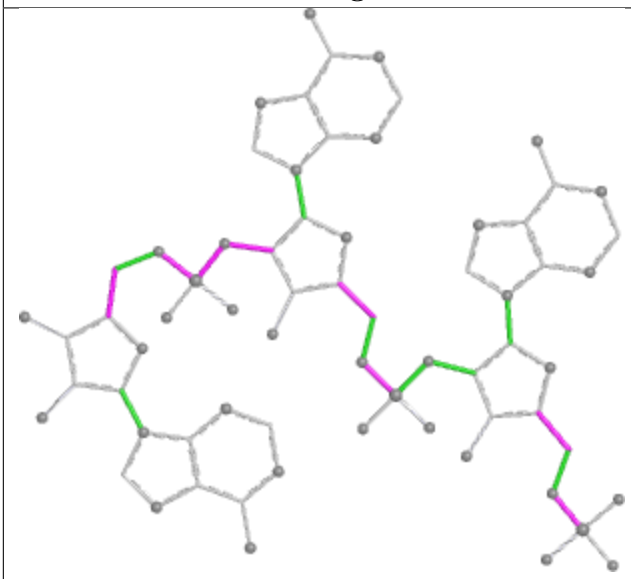
Ligand 25L b 801



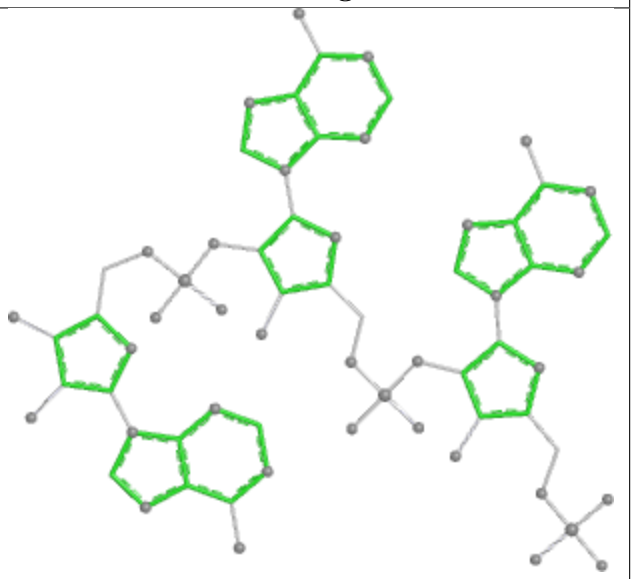
Bond lengths



Bond angles

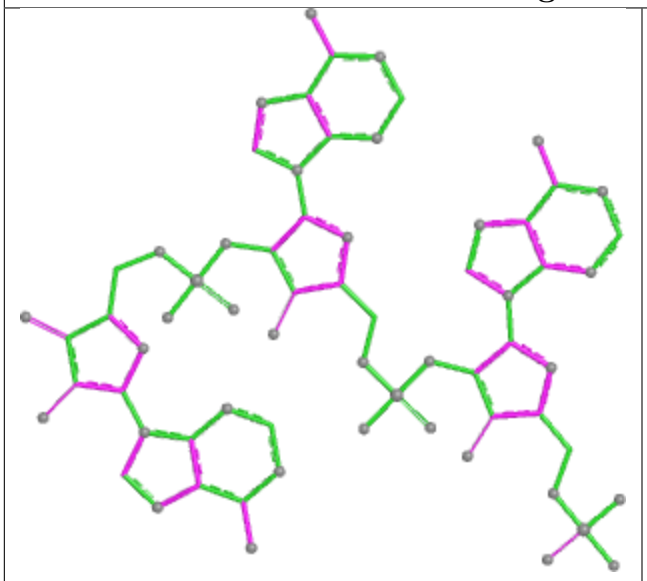


Torsions



Rings

Ligand 25L a 802



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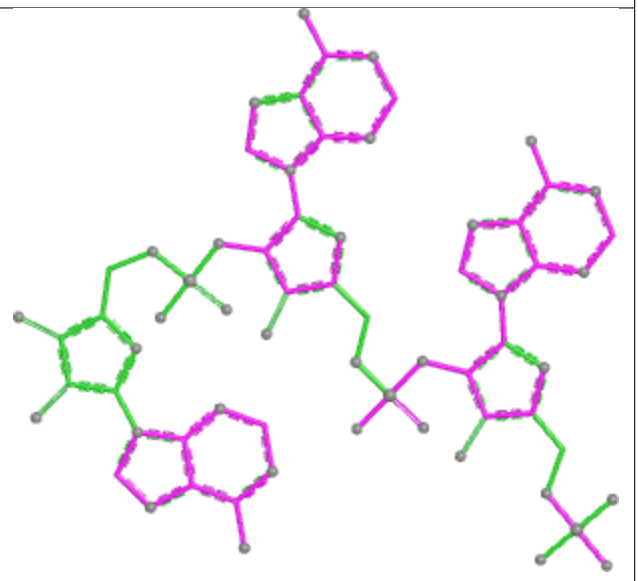

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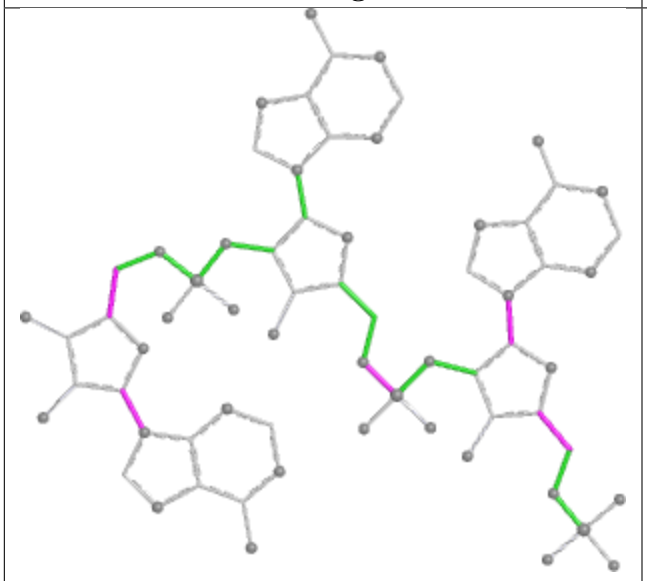
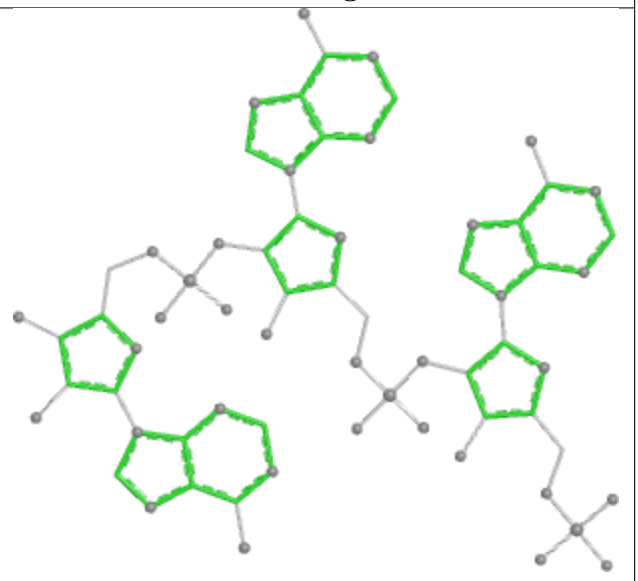


Torsions



Rings

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, 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	681/717 (94%)	0.24	7 (1%) 79 76	43, 81, 121, 163	0
1	b	684/717 (95%)	0.40	30 (4%) 39 34	46, 84, 133, 161	0
All	All	1365/1434 (95%)	0.32	37 (2%) 56 52	43, 83, 127, 163	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	622	LEU	3.6
1	b	726	LYS	3.4
1	a	643	ALA	3.1
1	a	622	LEU	3.1
1	b	155	THR	3.0
1	b	49	ALA	3.0
1	a	329	PRO	3.0
1	b	25	GLU	2.9
1	b	28	THR	2.9
1	b	64	ALA	2.9
1	b	662	LEU	2.9
1	b	121	VAL	2.8
1	a	662	LEU	2.8
1	a	644	TYR	2.8
1	b	639	GLU	2.8
1	b	568	ASP	2.8
1	b	619	THR	2.7
1	b	570	VAL	2.7
1	b	644	TYR	2.6
1	b	451	VAL	2.6
1	b	76	LEU	2.5
1	b	330	PRO	2.5
1	b	109	LEU	2.5
1	b	149	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	b	641	MET	2.4
1	b	136	VAL	2.3
1	b	618	GLY	2.2
1	a	620	SER	2.2
1	b	60	PRO	2.2
1	b	544	PHE	2.2
1	b	254	GLN	2.2
1	b	116	VAL	2.1
1	b	85	LEU	2.1
1	b	324	GLY	2.1
1	b	27	LEU	2.0
1	a	73	VAL	2.0
1	b	108	LEU	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 oligosaccharides in this entry.

6.4 Ligands (i)

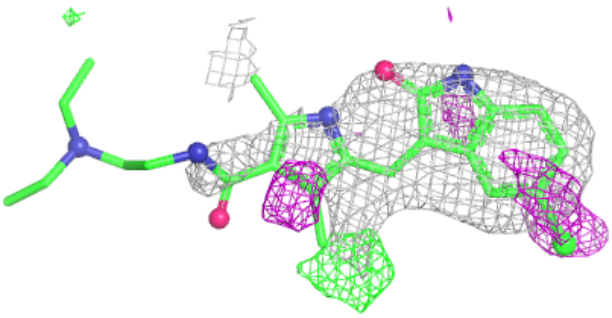
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

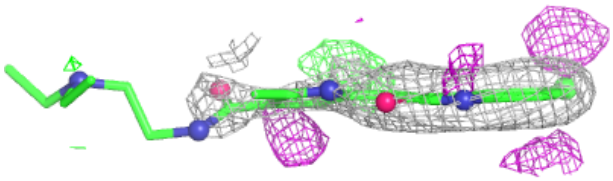
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	J60	b	802	29/29	0.68	0.21	76,155,183,188	0
2	J60	a	801	29/29	0.73	0.24	80,114,169,177	0
3	25L	b	801	67/75	0.92	0.10	60,93,118,134	0
3	25L	a	802	67/75	0.95	0.07	50,68,76,92	0
4	PO4	a	803	5/5	0.96	0.06	68,69,71,82	0

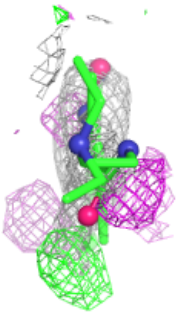
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J60 b 802:

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

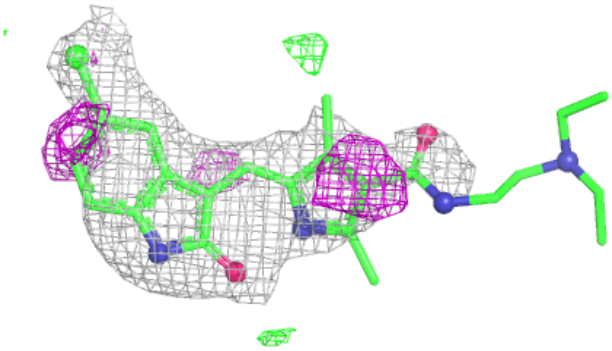


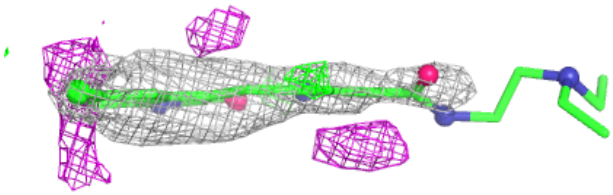


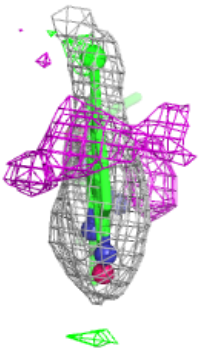


Electron density around J60 a 801:

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

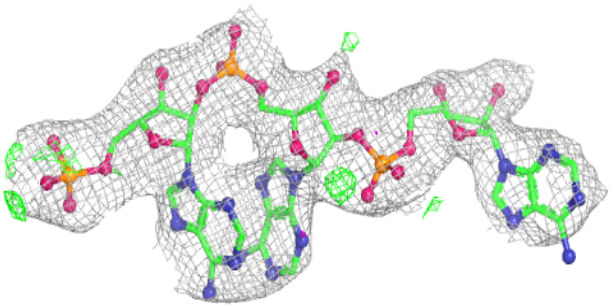


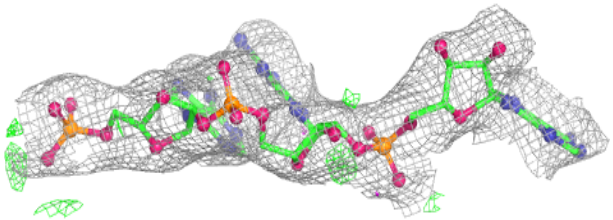


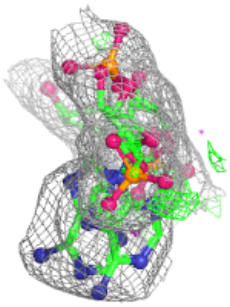


Electron density around 25L b 801:

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

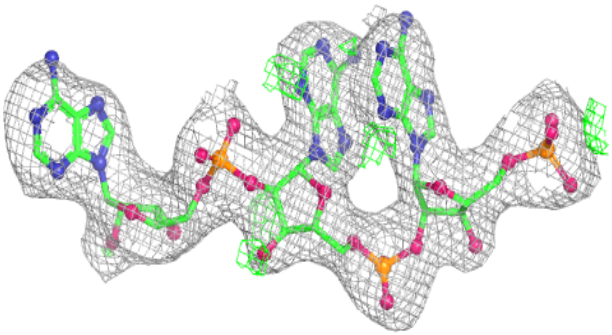


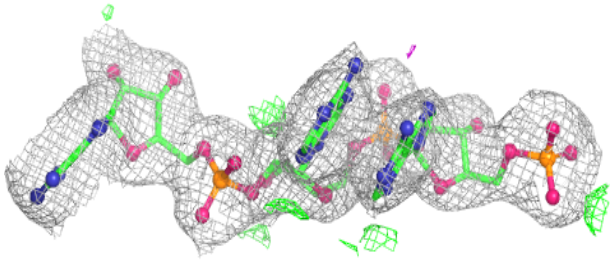


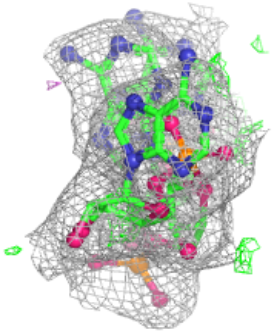


Electron density around 25L a 802:

$2mF_o$-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.