



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 PM UTC

PDB ID : 6M13 / pdb_00006m13
Title : Crystal structure of Rnase L in complex with Toceranib
Authors : Tang, J.; Huang, H.
Deposited on : 2020-02-24
Resolution : 2.56 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

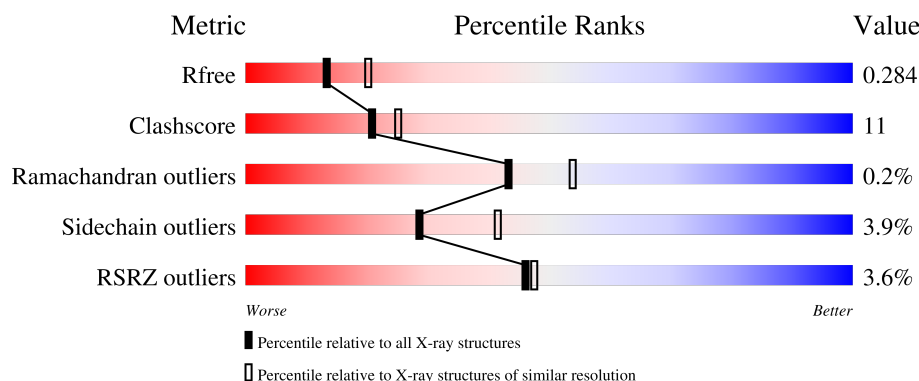
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	2% 76% 17% • 5%
1	b	717	5% 70% 25% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11078 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.

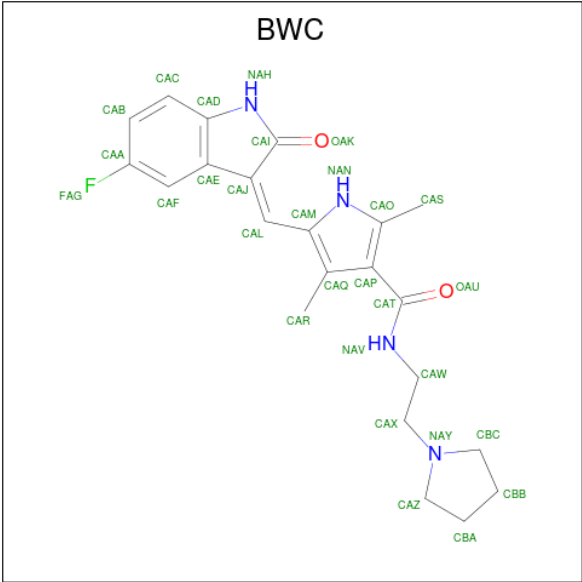
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	681	Total	C	N	O	S	0	0	0
			5408	3395	953	1038	22			
1	b	688	Total	C	N	O	S	0	0	0
			5463	3425	968	1049	21			

There are 10 discrepancies between the modelled and reference sequences:

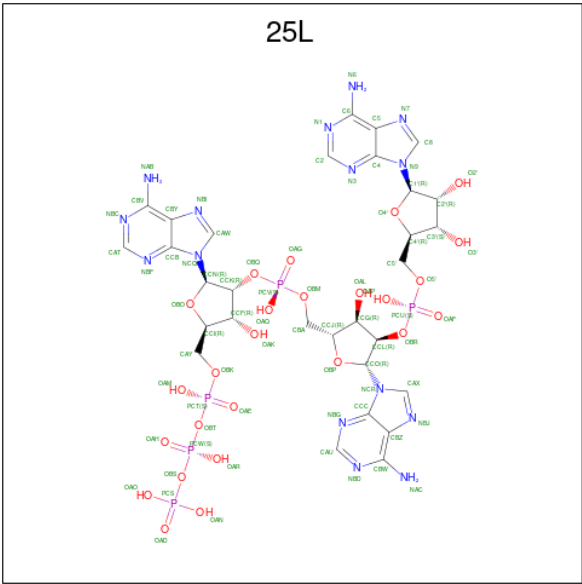
Chain	Residue	Modelled	Actual	Comment	Reference
a	16	GLY	-	expression tag	UNP A5H025
a	17	ALA	-	expression tag	UNP A5H025
a	18	MET	-	expression tag	UNP A5H025
a	19	ASP	-	expression tag	UNP A5H025
a	20	PRO	-	expression tag	UNP A5H025
b	16	GLY	-	expression tag	UNP A5H025
b	17	ALA	-	expression tag	UNP A5H025
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-[(Z)-(5-fluoranyl-2-oxidanylidene-1H-indol-3-ylidene)methyl]-2,4-dimethyl-N-(2-pyrrolidin-1-ylethyl)-1H-pyrrole-3-carboxamide (CCD ID: BWC) (formula: C₂₂H₂₅FN₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	a	1	Total	C	F	N	O	0	0
			29	22	1	4	2		
2	b	1	Total	C	F	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: C₃₀H₄₀N₁₅O₂₅P₅).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

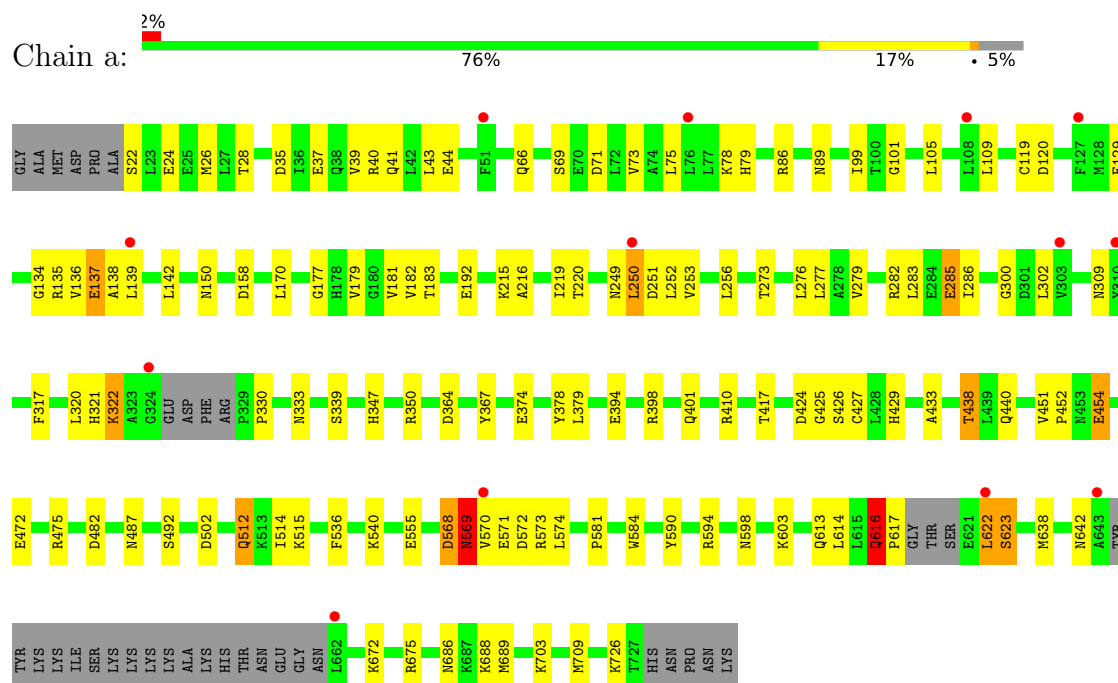
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	a	7	Total	O		
			7	7	0	0
5	b	3	Total	O		
			3	3	0	0

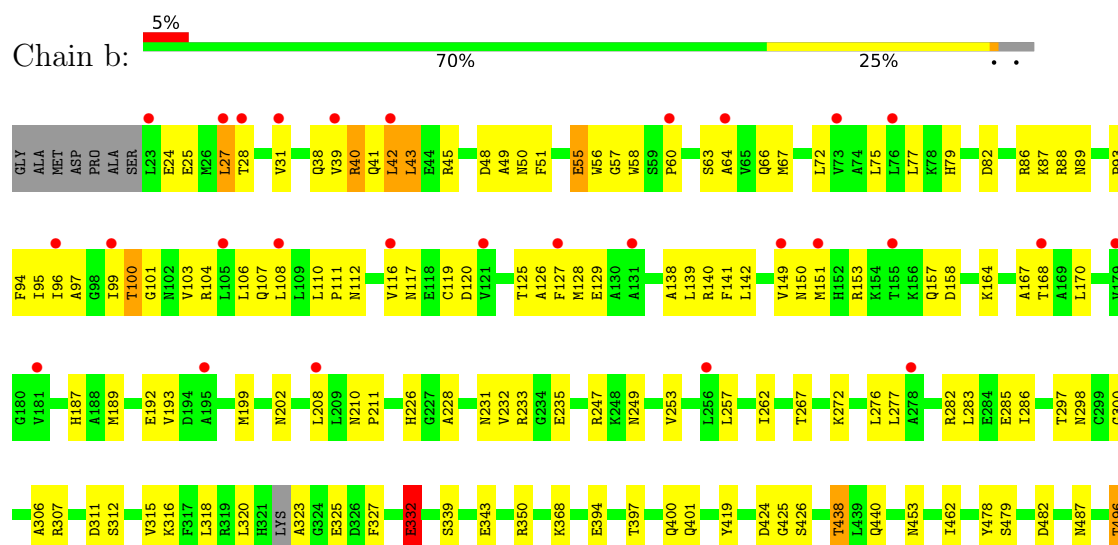
3 Residue-property plots

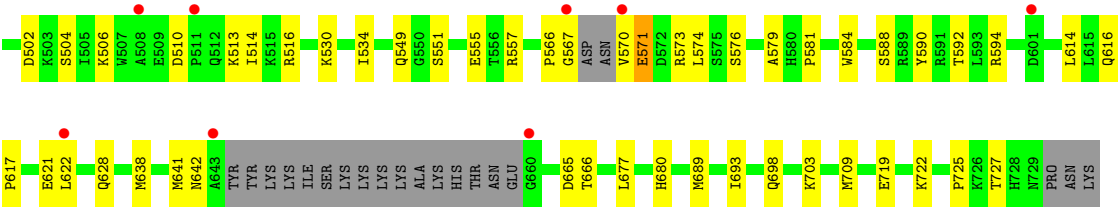
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.45Å 111.36Å 263.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.02 – 2.56 69.02 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (69.02-2.56) 99.3 (69.02-2.56)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.286 0.232 , 0.284	Depositor DCC
R_{free} test set	2883 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: BWC, 25L, PO4

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	0.77	0/5503	0.87	4/7430 (0.1%)
1	b	0.74	0/5560	0.84	0/7508
All	All	0.76	0/11063	0.86	4/14938 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	333	ASN	N-CA-C	6.96	118.86	111.28
1	a	616	GLN	N-CA-C	6.47	124.11	109.81
1	a	569	ASN	N-CA-C	5.54	118.22	108.75
1	a	572	ASP	N-CA-C	-5.06	107.66	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5408	0	5325	95	0
1	b	5463	0	5360	150	0
2	a	29	0	0	1	0
2	b	29	0	0	0	0
3	a	67	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	b	67	0	31	4	0
4	a	5	0	0	1	0
5	a	7	0	0	1	0
5	b	3	0	0	0	0
All	All	11078	0	10747	242	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 11.

All (242) 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:902:25L:O4'	3:b:902:25L:C1'	1.64	1.30
3:a:802:25L:O4'	3:a:802:25L:C1'	1.63	1.29
1:b:566:PRO:O	1:b:573:ARG:NH2	1.68	1.24
1:b:616:GLN:CB	1:b:621:GLU:OE2	1.87	1.21
1:b:616:GLN:CA	1:b:621:GLU:OE2	1.90	1.20
1:b:43:LEU:HD13	1:b:79:HIS:CD2	1.81	1.15
1:b:616:GLN:HA	1:b:621:GLU:OE2	1.49	1.11
1:a:569:ASN:HB2	1:a:573:ARG:HG3	1.24	1.10
1:a:638:MET:O	1:a:642:ASN:ND2	1.86	1.09
1:b:43:LEU:CD1	1:b:79:HIS:HD2	1.66	1.08
1:b:332:GLU:OE2	1:b:350:ARG:HD3	1.54	1.08
1:b:43:LEU:HD13	1:b:79:HIS:HD2	0.88	1.05
1:b:638:MET:O	1:b:642:ASN:ND2	1.88	1.05
1:b:125:THR:HG21	1:b:151:MET:HE1	1.33	1.04
1:a:569:ASN:CB	1:a:573:ARG:HG3	1.88	1.03
1:a:569:ASN:HB2	1:a:573:ARG:CG	1.98	0.94
1:b:616:GLN:HB2	1:b:621:GLU:OE2	1.69	0.89
1:b:332:GLU:CD	1:b:350:ARG:HD3	1.99	0.85
1:a:99:ILE:O	1:a:135:ARG:NH1	2.11	0.83
1:a:514:ILE:HG21	1:a:573:ARG:HH22	1.44	0.82
1:b:106:LEU:CD2	1:b:142:LEU:HD11	2.10	0.82
1:b:616:GLN:HE22	1:b:666:THR:HB	1.46	0.79
1:b:125:THR:HG21	1:b:151:MET:CE	2.14	0.78
1:a:512:GLN:O	1:a:515:LYS:HG2	1.83	0.78
1:b:86:ARG:NH1	1:b:119:CYS:O	2.18	0.77
1:b:43:LEU:CD1	1:b:79:HIS:CD2	2.54	0.77
1:b:106:LEU:HD23	1:b:142:LEU:HD11	1.67	0.75
1:b:551:SER:HB2	1:b:557:ARG:HG3	1.69	0.73
1:b:104:ARG:O	1:b:108:LEU:HG	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:298:ASN:O	1:b:327:PHE:CD1	2.43	0.72
1:a:514:ILE:HG21	1:a:573:ARG:NH2	2.04	0.71
1:b:48:ASP:OD1	1:b:49:ALA:N	2.23	0.70
1:a:249:ASN:HD22	1:a:252:LEU:H	1.39	0.70
1:b:38:GLN:O	1:b:42:LEU:HB2	1.91	0.70
1:a:279:VAL:HG21	1:a:302:LEU:HD12	1.75	0.69
1:b:566:PRO:C	1:b:573:ARG:HH22	2.00	0.69
1:a:321:HIS:O	1:a:321:HIS:ND1	2.26	0.69
1:b:677:LEU:HD11	1:b:693:ILE:CD1	2.24	0.68
1:a:170:LEU:HD11	1:a:182:VAL:HG23	1.75	0.68
1:b:27:LEU:HD11	1:b:51:PHE:CD2	2.29	0.67
1:b:141:PHE:HD1	1:b:142:LEU:HD12	1.60	0.67
1:b:282:ARG:NH1	1:b:311:ASP:CG	2.52	0.67
1:b:27:LEU:CD2	1:b:28:THR:HG23	2.25	0.67
1:a:398:ARG:NH1	1:a:502:ASP:OD2	2.28	0.67
1:b:210:ASN:HD22	1:b:211:PRO:HD2	1.60	0.66
1:a:613:GLN:O	1:a:616:GLN:HB2	1.94	0.66
1:b:66:GLN:HB3	1:b:96:ILE:HD11	1.77	0.66
1:b:616:GLN:CB	1:b:621:GLU:CD	2.69	0.66
1:a:283:LEU:HB3	1:a:286:ILE:HD13	1.78	0.65
1:a:622:LEU:O	1:a:623:SER:C	2.39	0.65
1:b:99:ILE:HG23	1:b:129:GLU:HB3	1.78	0.65
1:b:510:ASP:HB3	1:b:513:LYS:HD2	1.78	0.65
1:b:332:GLU:OE2	1:b:350:ARG:CD	2.41	0.64
1:b:125:THR:CG2	1:b:151:MET:HE1	2.18	0.64
1:b:28:THR:HA	1:b:31:VAL:HG12	1.79	0.64
1:a:300:GLY:O	1:a:302:LEU:HD22	1.99	0.63
1:a:536:PHE:HE2	1:a:540:LYS:NZ	1.97	0.63
1:a:451:VAL:HG22	1:a:454:GLU:HG2	1.80	0.63
1:b:555:GLU:HA	1:b:709:MET:HE3	1.81	0.62
1:b:43:LEU:HD22	1:b:79:HIS:CD2	2.34	0.62
1:b:588:SER:O	1:b:592:THR:HG23	1.99	0.62
1:a:555:GLU:HA	1:a:709:MET:HE3	1.82	0.62
1:a:150:ASN:ND2	1:a:192:GLU:HG3	2.15	0.62
1:b:127:PHE:CZ	1:b:149:VAL:HG12	2.36	0.61
1:b:592:THR:HG21	1:b:725:PRO:HD3	1.83	0.61
1:b:616:GLN:HB3	1:b:621:GLU:OE2	1.93	0.61
1:a:536:PHE:CE2	1:a:540:LYS:HE3	2.36	0.60
1:b:566:PRO:C	1:b:573:ARG:NH2	2.56	0.60
1:b:567:GLY:CA	1:b:570:VAL:HG22	2.31	0.60
1:a:482:ASP:O	1:a:487:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:28:THR:HG22	1:b:60:PRO:HG3	1.82	0.60
1:b:96:ILE:O	1:b:99:ILE:HG13	2.02	0.59
1:b:253:VAL:O	1:b:257:LEU:HD12	2.02	0.59
1:b:168:THR:HG22	1:b:170:LEU:H	1.67	0.59
1:b:641:MET:HE1	1:b:689:MET:SD	2.43	0.58
1:a:66:GLN:NE2	1:b:307:ARG:O	2.37	0.58
1:a:569:ASN:HB3	1:a:573:ARG:HG3	1.81	0.58
1:b:50:ASN:HD21	1:b:82:ASP:H	1.52	0.58
1:b:482:ASP:O	1:b:487:ASN:ND2	2.36	0.58
1:a:536:PHE:HE2	1:a:540:LYS:CE	2.17	0.57
1:b:231:ASN:HD21	1:b:262:ILE:HA	1.69	0.57
1:a:249:ASN:ND2	1:a:252:LEU:H	2.01	0.57
1:a:427:CYS:HG	1:a:429:HIS:CE1	2.22	0.57
1:b:283:LEU:HB3	1:b:286:ILE:HD13	1.85	0.57
1:b:513:LYS:O	1:b:516:ARG:HG2	2.04	0.56
1:b:210:ASN:HD22	1:b:211:PRO:CD	2.18	0.56
1:a:475:ARG:NH1	1:a:571:GLU:O	2.39	0.55
1:b:616:GLN:HB3	1:b:621:GLU:CD	2.31	0.55
1:b:27:LEU:HG	1:b:28:THR:HG23	1.89	0.55
1:b:453:ASN:O	1:b:698:GLN:NE2	2.39	0.55
1:b:567:GLY:HA2	1:b:570:VAL:HG22	1.89	0.55
1:b:530:LYS:HG3	1:b:534:ILE:HD12	1.88	0.55
1:b:43:LEU:CD2	1:b:79:HIS:CD2	2.90	0.55
1:b:55:GLU:HG2	1:b:56:TRP:CD1	2.42	0.55
1:b:106:LEU:HD22	1:b:142:LEU:HD11	1.87	0.54
1:a:101:GLY:HA3	1:a:135:ARG:HD2	1.88	0.54
1:b:187:HIS:NE2	1:b:226:HIS:CE1	2.75	0.54
1:b:298:ASN:O	1:b:327:PHE:HD1	1.90	0.54
1:a:536:PHE:CE2	1:a:540:LYS:CE	2.90	0.54
1:a:216:ALA:O	1:a:220:THR:HG23	2.07	0.54
1:b:63:SER:HA	1:b:66:GLN:HG2	1.90	0.54
1:a:249:ASN:HD21	1:a:251:ASP:HB2	1.72	0.54
1:a:603:LYS:HA	1:a:672:LYS:HD3	1.90	0.54
1:a:279:VAL:CG2	1:a:302:LEU:HD12	2.38	0.53
1:b:43:LEU:HD21	1:b:79:HIS:HB3	1.90	0.53
1:a:89:ASN:O	1:a:120:ASP:HB2	2.09	0.53
1:b:397:THR:O	1:b:400:GLN:HG3	2.08	0.53
1:b:57:GLY:O	1:b:87:LYS:HB3	2.10	0.52
1:b:87:LYS:NZ	3:b:902:25L:OAP	2.42	0.52
1:b:93:PRO:HA	1:b:96:ILE:HG22	1.91	0.52
1:a:182:VAL:HG11	1:a:219:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:27:LEU:HD23	1:b:28:THR:N	2.24	0.52
1:a:613:GLN:HA	1:a:616:GLN:HG2	1.91	0.52
1:b:202:ASN:ND2	1:b:232:VAL:HG21	2.25	0.52
1:b:40:ARG:HB3	1:b:75:LEU:HD11	1.91	0.52
1:b:43:LEU:CG	1:b:79:HIS:CD2	2.93	0.52
1:a:69:SER:O	1:a:73:VAL:HG23	2.11	0.51
1:a:581:PRO:HA	1:a:584:TRP:CG	2.46	0.51
1:b:581:PRO:HA	1:b:584:TRP:CG	2.46	0.51
1:a:279:VAL:HG21	1:a:302:LEU:CD1	2.41	0.51
1:b:285:GLU:HB2	1:b:286:ILE:HD12	1.90	0.51
1:a:137:GLU:CD	1:a:137:GLU:H	2.19	0.51
1:b:549:GLN:O	1:b:557:ARG:NH2	2.43	0.51
1:a:37:GLU:O	1:a:41:GLN:HG3	2.11	0.51
1:b:140:ARG:HG2	1:b:189:MET:CE	2.40	0.51
1:b:64:ALA:O	1:b:67:MET:HG2	2.11	0.51
1:b:89:ASN:O	1:b:120:ASP:HB2	2.11	0.51
1:b:99:ILE:HD12	1:b:100:THR:N	2.27	0.50
1:a:347:HIS:O	1:a:350:ARG:HG2	2.11	0.50
4:a:803:PO4:O3	1:b:680:HIS:NE2	2.43	0.50
1:b:394:GLU:HG2	1:b:426:SER:HA	1.93	0.50
1:a:282:ARG:HD3	1:a:309:ASN:HB3	1.92	0.50
1:b:99:ILE:CG2	1:b:129:GLU:HB3	2.40	0.50
1:b:462:ILE:HA	1:b:496:THR:HG21	1.94	0.50
1:a:250:LEU:H	1:a:250:LEU:HD23	1.76	0.50
1:a:273:THR:O	1:a:277:LEU:HD12	2.12	0.50
1:a:364:ASP:OD2	1:b:88:ARG:NH1	2.44	0.50
1:a:40:ARG:O	1:a:44:GLU:HG2	2.12	0.50
1:a:598:ASN:OD1	1:a:675:ARG:HD2	2.12	0.50
1:b:233:ARG:NH1	1:b:267:THR:O	2.41	0.49
1:a:37:GLU:CD	1:a:40:ARG:HH12	2.19	0.49
1:a:374:GLU:HG2	1:a:398:ARG:HH21	1.76	0.49
1:a:105:LEU:O	1:a:109:LEU:HD12	2.12	0.49
1:b:110:LEU:N	1:b:111:PRO:HD2	2.28	0.49
1:b:153:ARG:NH2	1:b:167:ALA:HB3	2.27	0.49
1:b:323:ALA:N	1:b:325:GLU:OE1	2.46	0.49
1:a:273:THR:HG22	1:a:276:LEU:HB2	1.94	0.48
1:a:367:TYR:HA	1:a:379:LEU:HD12	1.95	0.48
1:a:24:GLU:O	1:a:28:THR:HG23	2.14	0.48
2:a:801:BWC:OAU	2:a:801:BWC:CAZ	2.61	0.48
1:b:298:ASN:O	1:b:327:PHE:CE1	2.66	0.48
1:b:297:THR:HG22	1:b:297:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:249:ASN:O	1:a:253:VAL:HG23	2.13	0.48
1:a:378:TYR:OH	1:b:158:ASP:OD2	2.24	0.48
1:b:438:THR:HG22	1:b:440:GLN:H	1.78	0.47
1:b:677:LEU:HD11	1:b:693:ILE:HD12	1.96	0.47
1:b:300:GLY:HA2	1:b:327:PHE:CE2	2.50	0.47
1:a:536:PHE:HE2	1:a:540:LYS:HE3	1.76	0.47
1:b:150:ASN:ND2	1:b:192:GLU:HG3	2.29	0.47
1:b:571:GLU:OE2	1:b:571:GLU:N	2.48	0.47
1:a:394:GLU:HG2	1:a:426:SER:HA	1.96	0.47
1:b:438:THR:HG22	1:b:440:GLN:N	2.29	0.47
1:b:312:SER:O	1:b:315:VAL:HG22	2.15	0.47
1:a:179:VAL:HA	1:a:182:VAL:HG12	1.97	0.47
1:a:179:VAL:O	1:a:183:THR:HG23	2.15	0.47
1:a:410:ARG:HD3	1:b:419:TYR:CE2	2.51	0.46
1:b:424:ASP:O	1:b:425:GLY:C	2.57	0.46
1:a:590:TYR:CZ	1:a:594:ARG:HD2	2.50	0.46
1:b:590:TYR:CZ	1:b:594:ARG:HD2	2.51	0.46
1:b:616:GLN:N	1:b:617:PRO:CD	2.78	0.46
1:a:71:ASP:O	1:a:75:LEU:HG	2.15	0.46
1:b:478:TYR:CZ	1:b:506:LYS:HD3	2.51	0.46
1:a:252:LEU:O	1:a:256:LEU:HG	2.15	0.46
1:a:35:ASP:O	1:a:39:VAL:HG23	2.16	0.46
1:a:568:ASP:OD1	1:a:568:ASP:N	2.47	0.46
1:b:282:ARG:NH1	1:b:311:ASP:OD2	2.48	0.45
1:a:581:PRO:HD2	1:a:709:MET:HE1	1.98	0.45
1:b:27:LEU:CG	1:b:28:THR:HG23	2.47	0.45
1:b:581:PRO:HA	1:b:584:TRP:CD1	2.51	0.45
1:a:581:PRO:HA	1:a:584:TRP:CD1	2.52	0.45
1:b:93:PRO:HA	1:b:96:ILE:CG2	2.46	0.45
1:a:99:ILE:HG13	1:a:129:GLU:HB3	1.98	0.45
1:a:374:GLU:CG	1:a:398:ARG:HH21	2.29	0.45
1:b:43:LEU:HD22	1:b:79:HIS:CG	2.51	0.45
1:b:628:GLN:HA	1:b:665:ASP:CG	2.42	0.45
1:a:158:ASP:OD2	1:b:368:LYS:NZ	2.44	0.45
1:a:574:LEU:HB2	5:a:907:HOH:O	2.16	0.45
1:b:104:ARG:HB2	1:b:107:GLN:HE21	1.82	0.45
1:b:479:SER:HB2	1:b:514:ILE:HG22	1.99	0.45
1:b:502:ASP:OD1	1:b:502:ASP:N	2.31	0.44
1:b:77:LEU:HD11	1:b:112:ASN:ND2	2.32	0.44
1:b:199:MET:HE3	1:b:199:MET:HA	1.98	0.44
1:b:316:LYS:O	1:b:320:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:438:THR:HG22	1:a:440:GLN:N	2.32	0.44
1:b:39:VAL:HG21	1:b:72:LEU:HD21	1.99	0.44
1:b:153:ARG:HG3	1:b:153:ARG:HH11	1.82	0.44
1:b:616:GLN:NE2	1:b:666:THR:HB	2.23	0.44
1:b:138:ALA:O	1:b:142:LEU:HD13	2.17	0.44
1:b:579:ALA:HA	1:b:727:THR:HG21	1.99	0.44
1:b:719:GLU:O	1:b:722:LYS:HG2	2.17	0.44
1:a:424:ASP:O	1:a:425:GLY:C	2.57	0.43
1:b:140:ARG:HG2	1:b:189:MET:HE3	2.00	0.43
1:a:138:ALA:O	1:a:142:LEU:HD12	2.19	0.43
1:a:285:GLU:H	1:a:285:GLU:CD	2.27	0.43
1:b:58:TRP:CE2	3:b:902:25L:N7	2.86	0.43
1:a:417:THR:HB	1:a:433:ALA:HB2	2.01	0.43
1:a:616:GLN:HA	1:a:616:GLN:OE1	2.19	0.42
1:a:686:ASN:HB3	1:a:689:MET:HE2	2.01	0.42
1:b:77:LEU:HD23	1:b:77:LEU:O	2.19	0.42
1:b:120:ASP:OD2	3:b:902:25L:HAT	2.19	0.42
1:a:43:LEU:HB3	1:a:79:HIS:CD2	2.54	0.42
1:b:318:LEU:O	1:b:323:ALA:HB2	2.19	0.42
1:b:97:ALA:HB1	1:b:106:LEU:CD1	2.49	0.42
1:b:581:PRO:HD2	1:b:709:MET:HE1	2.02	0.42
1:a:134:GLY:HA2	1:a:181:VAL:HG21	2.02	0.42
1:b:101:GLY:O	1:b:138:ALA:HB2	2.20	0.42
1:a:22:SER:O	1:a:26:MET:HE2	2.20	0.41
1:a:177:GLY:O	1:a:215:LYS:HD3	2.20	0.41
1:a:179:VAL:HG12	1:a:215:LYS:NZ	2.35	0.41
1:a:322:LYS:HE3	1:a:322:LYS:HA	2.02	0.41
1:a:438:THR:HG22	1:a:440:GLN:H	1.84	0.41
1:b:193:VAL:HG22	1:b:228:ALA:HB2	2.02	0.41
1:b:249:ASN:O	1:b:253:VAL:HG23	2.19	0.41
1:a:86:ARG:NH2	1:a:119:CYS:O	2.49	0.41
1:a:616:GLN:HB3	1:a:617:PRO:HD3	2.02	0.41
1:a:317:PHE:HA	1:a:320:LEU:HG	2.02	0.41
1:b:27:LEU:HD11	1:b:51:PHE:HD2	1.82	0.41
1:b:401:GLN:HG2	1:b:504:SER:O	2.20	0.41
1:a:570:VAL:O	1:a:570:VAL:HG12	2.20	0.41
1:b:128:MET:HE1	1:b:153:ARG:HG2	2.02	0.41
1:a:75:LEU:O	1:a:78:LYS:HB3	2.21	0.41
1:b:139:LEU:HD23	1:b:189:MET:HE1	2.01	0.41
1:b:306:ALA:HB3	1:b:315:VAL:HG12	2.02	0.41
1:b:567:GLY:HA3	1:b:570:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:66:GLN:O	1:b:312:SER:OG	2.39	0.41
1:b:272:LYS:HB3	1:b:276:LEU:HD23	2.03	0.41
1:b:574:LEU:HD23	1:b:574:LEU:HA	1.85	0.41
1:a:136:VAL:O	1:a:139:LEU:HG	2.21	0.40
1:b:103:VAL:HG22	1:b:138:ALA:HA	2.02	0.40
1:b:94:PHE:CZ	1:b:116:VAL:HG23	2.56	0.40
1:b:208:LEU:O	1:b:247:ARG:NH2	2.54	0.40
1:b:95:ILE:HA	1:b:126:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	673/717 (94%)	643 (96%)	28 (4%)	2 (0%)	36	44
1	b	680/717 (95%)	649 (95%)	30 (4%)	1 (0%)	48	60
All	All	1353/1434 (94%)	1292 (96%)	58 (4%)	3 (0%)	43	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	623	SER
1	b	332	GLU
1	a	330	PRO

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	582/617 (94%)	562 (97%)	20 (3%)	32	47
1	b	586/617 (95%)	561 (96%)	25 (4%)	26	38
All	All	1168/1234 (95%)	1123 (96%)	45 (4%)	28	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	137	GLU
1	a	250	LEU
1	a	285	GLU
1	a	322	LYS
1	a	339	SER
1	a	401	GLN
1	a	438	THR
1	a	452	PRO
1	a	454	GLU
1	a	472	GLU
1	a	492	SER
1	a	512	GLN
1	a	568	ASP
1	a	569	ASN
1	a	614	LEU
1	a	616	GLN
1	a	622	LEU
1	a	688	LYS
1	a	703	LYS
1	a	726	LYS
1	b	24	GLU
1	b	25	GLU
1	b	27	LEU
1	b	40	ARG
1	b	41	GLN
1	b	42	LEU
1	b	43	LEU
1	b	45	ARG
1	b	55	GLU
1	b	100	THR
1	b	117	ASN
1	b	157	GLN
1	b	164	LYS

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Mol	Chain	Res	Type
1	b	235	GLU
1	b	277	LEU
1	b	332	GLU
1	b	339	SER
1	b	343	GLU
1	b	438	THR
1	b	496	THR
1	b	571	GLU
1	b	576	SER
1	b	614	LEU
1	b	622	LEU
1	b	703	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	41	GLN
1	a	50	ASN
1	a	107	GLN
1	a	145	ASN
1	a	198	ASN
1	a	249	ASN
1	a	400	GLN
1	a	407	GLN
1	a	442	HIS
1	a	608	ASN
1	a	642	ASN
1	a	698	GLN
1	b	79	HIS
1	b	107	GLN
1	b	157	GLN
1	b	198	ASN
1	b	210	ASN
1	b	226	HIS
1	b	333	ASN
1	b	453	ASN
1	b	512	GLN
1	b	562	HIS
1	b	616	GLN
1	b	716	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	1.00	0	6,6,6	0.97	1 (16%)
2	BWC	b	901	-	32,32,32	2.47	9 (28%)	44,46,46	2.07	11 (25%)
3	25L	b	902	-	75,75,83	3.19	27 (36%)	111,116,130	2.17	35 (31%)
3	25L	a	802	-	75,75,83	3.17	27 (36%)	111,116,130	2.13	34 (30%)
2	BWC	a	801	-	32,32,32	2.36	9 (28%)	44,46,46	2.32	15 (34%)

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	BWC	b	901	-	-	4/14/33/33	0/4/4/4
2	BWC	a	801	-	-	7/14/33/33	0/4/4/4
3	25L	b	902	-	-	16/40/88/100	0/9/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	25L	a	802	-	-	8/40/88/100	0/9/9/9

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	902	25L	O4'-C1'	9.91	1.64	1.42
3	a	802	25L	O4'-C1'	9.44	1.63	1.42
3	a	802	25L	OBO-CCN	9.23	1.63	1.42
3	b	902	25L	OBP-CCO	8.66	1.62	1.42
3	a	802	25L	OBP-CCO	8.62	1.61	1.42
2	b	901	BWC	CAJ-CAI	-8.55	1.38	1.50
3	b	902	25L	OBO-CCN	8.53	1.61	1.42
3	a	802	25L	CCL-CCO	-8.02	1.33	1.53
3	b	902	25L	CCK-CCN	-7.90	1.33	1.53
2	a	801	BWC	CAJ-CAI	-7.60	1.39	1.50
3	b	902	25L	CCL-CCO	-7.29	1.35	1.53
3	a	802	25L	CCK-CCN	-6.90	1.36	1.53
3	b	902	25L	OBO-CCI	-6.78	1.29	1.45
3	a	802	25L	C2'-C1'	-6.38	1.33	1.53
3	b	902	25L	O4'-C4'	-6.17	1.31	1.45
3	a	802	25L	OBP-CCJ	-6.08	1.31	1.45
3	b	902	25L	C2'-C1'	-5.72	1.35	1.53
3	a	802	25L	C6-N6	5.69	1.48	1.34
3	a	802	25L	CBW-NAC	5.63	1.48	1.34
3	b	902	25L	C6-N6	5.60	1.48	1.34
3	b	902	25L	CBW-NAC	5.45	1.48	1.34
3	a	802	25L	O4'-C4'	-5.43	1.32	1.45
3	a	802	25L	OBO-CCI	-5.39	1.33	1.45
3	b	902	25L	OBP-CCJ	-4.97	1.33	1.45
2	b	901	BWC	CAS-CAO	4.85	1.58	1.49
2	a	801	BWC	CAS-CAO	4.19	1.56	1.49
3	a	802	25L	OAL-CCG	-4.16	1.32	1.43
2	a	801	BWC	CAE-CAJ	-4.03	1.38	1.45
3	b	902	25L	OAL-CCG	-4.01	1.33	1.43
2	a	801	BWC	CAP-CAT	-4.01	1.40	1.48
3	a	802	25L	PCT-OBT	3.87	1.69	1.54
2	b	901	BWC	CAP-CAT	-3.80	1.40	1.48
2	a	801	BWC	CAT-NAV	3.78	1.40	1.33
2	b	901	BWC	CAE-CAJ	-3.69	1.39	1.45
3	b	902	25L	CBY-CCB	-3.54	1.32	1.39
2	b	901	BWC	CAL-CAJ	3.53	1.41	1.35
3	b	902	25L	OAK-CCF	-3.47	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	902	25L	O3'-C3'	-3.43	1.34	1.43
3	b	902	25L	CBV-NAB	3.42	1.42	1.34
3	b	902	25L	PCT-OBT	3.40	1.67	1.54
3	a	802	25L	C5-N7	-3.39	1.32	1.39
3	b	902	25L	C5-N7	-3.32	1.33	1.39
3	a	802	25L	O3'-C3'	-3.28	1.34	1.43
3	a	802	25L	CBV-NAB	3.27	1.42	1.34
2	b	901	BWC	CAT-NAV	3.19	1.39	1.33
2	a	801	BWC	CAL-CAJ	3.15	1.40	1.35
3	b	902	25L	CBZ-CCC	-3.05	1.33	1.39
3	a	802	25L	CCF-CCI	3.04	1.60	1.53
2	a	801	BWC	CAR-CAQ	2.96	1.56	1.50
3	a	802	25L	CBZ-CCC	-2.90	1.33	1.39
3	a	802	25L	C8-N9	-2.76	1.32	1.37
3	a	802	25L	CBY-NBI	-2.72	1.34	1.39
3	b	902	25L	PCU-O5'	2.68	1.69	1.59
3	a	802	25L	CBY-CCB	-2.67	1.34	1.39
3	a	802	25L	OAK-CCF	-2.66	1.36	1.43
2	b	901	BWC	CAE-CAD	-2.66	1.38	1.41
3	a	802	25L	C5-C4	-2.64	1.34	1.39
3	b	902	25L	PCV-OBQ	2.64	1.67	1.59
3	b	902	25L	CBY-NBI	-2.63	1.34	1.39
3	b	902	25L	O2'-C2'	2.60	1.49	1.43
3	b	902	25L	C2-N3	2.55	1.38	1.33
2	a	801	BWC	CAC-CAD	-2.55	1.35	1.39
2	b	901	BWC	CAR-CAQ	2.54	1.56	1.50
3	b	902	25L	C5-C4	-2.48	1.34	1.39
3	a	802	25L	C2-N3	2.31	1.38	1.33
3	a	802	25L	O2'-C2'	2.27	1.48	1.43
3	b	902	25L	C8-N9	-2.13	1.33	1.37
2	b	901	BWC	CAC-CAD	-2.13	1.36	1.39
3	a	802	25L	PCU-O5'	2.06	1.67	1.59
3	a	802	25L	CCG-CCJ	2.05	1.58	1.53
2	a	801	BWC	CAE-CAD	-2.03	1.38	1.41
3	b	902	25L	CCG-CCJ	2.02	1.58	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	901	BWC	CAX-NAY-CBC	-6.60	97.62	113.25
3	a	802	25L	N3-C2-N1	-5.95	119.58	128.58
3	b	902	25L	NBG-CAU-NBD	-5.65	120.03	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	902	25L	N3-C2-N1	-5.52	120.23	128.58
2	a	801	BWC	CAO-CAP-CAQ	-5.51	104.06	107.83
3	a	802	25L	CBY-CCB-NBF	-5.43	119.24	126.72
3	b	902	25L	C5-C4-N3	-5.40	119.28	126.72
3	b	902	25L	CBZ-CCC-NBG	-5.34	119.36	126.72
3	a	802	25L	NBG-CAU-NBD	-5.31	120.54	128.58
3	b	902	25L	NBF-CAT-NBC	-5.29	120.57	128.58
2	a	801	BWC	CAD-NAH-CAI	-5.22	108.13	111.35
3	a	802	25L	NBF-CAT-NBC	-5.15	120.78	128.58
3	b	902	25L	CBY-CCB-NBF	-5.11	119.68	126.72
2	a	801	BWC	CAX-NAY-CBC	-5.07	101.23	113.25
3	a	802	25L	NAC-CBW-NBD	-5.05	107.12	118.38
3	a	802	25L	C5-C4-N3	-4.90	119.96	126.72
2	b	901	BWC	CAO-CAP-CAQ	-4.81	104.54	107.83
3	b	902	25L	NAC-CBW-NBD	-4.72	107.86	118.38
2	a	801	BWC	CAX-NAY-CAZ	4.59	124.12	113.25
2	b	901	BWC	CAJ-CAI-NAH	4.47	109.36	106.91
3	a	802	25L	CBZ-CCC-NBG	-4.46	120.57	126.72
3	b	902	25L	NAB-CBV-NBC	-4.32	108.75	118.38
2	a	801	BWC	CAJ-CAI-NAH	4.15	109.18	106.91
3	b	902	25L	C3'-C2'-C1'	4.08	109.18	101.46
3	a	802	25L	CBZ-CBW-NAC	4.05	133.32	123.29
3	a	802	25L	C3'-C2'-C1'	3.99	109.02	101.46
2	b	901	BWC	CAD-NAH-CAI	-3.95	108.91	111.35
3	b	902	25L	NCQ-CAW-NBI	-3.94	108.34	113.94
2	a	801	BWC	CAP-CAO-NAN	3.90	110.39	107.48
3	b	902	25L	N9-C8-N7	-3.81	108.54	113.94
3	a	802	25L	NCR-CAX-NBJ	-3.74	108.64	113.94
3	a	802	25L	NAB-CBV-NBC	-3.64	110.27	118.38
3	b	902	25L	CAU-NBG-CCC	3.53	120.46	111.83
3	a	802	25L	C2-N3-C4	3.48	120.32	111.83
3	b	902	25L	N3-C4-N9	3.46	133.05	127.17
3	a	802	25L	N9-C8-N7	-3.37	109.16	113.94
2	a	801	BWC	CAB-CAA-CAF	-3.36	118.80	123.23
3	b	902	25L	C2-N3-C4	3.35	120.02	111.83
3	b	902	25L	CBZ-CBW-NAC	3.33	131.53	123.29
3	b	902	25L	NCR-CAX-NBJ	-3.31	109.24	113.94
3	b	902	25L	CBY-CBV-NAB	3.30	131.46	123.29
3	a	802	25L	CBV-CBY-CCB	3.26	121.63	117.18
3	a	802	25L	OBQ-CKK-CCF	-3.23	100.08	111.68
3	b	902	25L	CAT-NBF-CCB	3.22	119.69	111.83
2	b	901	BWC	CAB-CAA-CAF	-3.18	119.03	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	802	25L	CBY-CBV-NAB	3.14	131.07	123.29
3	b	902	25L	NBG-CCC-NCR	3.13	132.50	127.17
3	b	902	25L	C6-C5-C4	3.09	121.40	117.18
3	a	802	25L	NCQ-CAW-NBI	-3.08	109.56	113.94
2	b	901	BWC	OAK-CAI-NAH	-3.08	121.39	126.30
3	b	902	25L	OAM-PCT-OBK	3.00	114.49	106.67
3	b	902	25L	C5-N7-C8	2.99	108.15	103.45
3	a	802	25L	CAT-NBF-CCB	2.97	119.09	111.83
3	a	802	25L	CAU-NBG-CCC	2.91	118.94	111.83
2	a	801	BWC	OAU-CAT-CAP	-2.89	117.19	121.53
3	b	902	25L	NBF-CCB-NCQ	2.89	132.08	127.17
3	b	902	25L	CBY-NBI-CAW	2.88	107.98	103.45
3	a	802	25L	NBF-CCB-NCQ	2.84	132.00	127.17
2	a	801	BWC	OAK-CAI-NAH	-2.82	121.81	126.30
2	a	801	BWC	CAM-NAN-CAO	-2.81	108.52	110.31
2	b	901	BWC	CAD-CAE-CAJ	2.73	108.38	106.62
3	a	802	25L	CBY-CCB-NCQ	2.71	108.76	105.81
3	a	802	25L	OBT-PCT-OAM	2.68	117.86	107.80
3	a	802	25L	C5-C4-N9	2.68	108.73	105.81
3	a	802	25L	NBG-CCC-NCR	2.66	131.70	127.17
2	b	901	BWC	CAP-CAQ-CAM	2.63	110.73	106.73
3	a	802	25L	C5-N7-C8	2.60	107.53	103.45
3	b	902	25L	OBT-PCT-OBK	-2.53	100.07	106.67
3	a	802	25L	N6-C6-N1	-2.50	112.81	118.38
3	a	802	25L	CCG-CCL-CCO	2.48	107.56	102.81
2	a	801	BWC	CAP-CAQ-CAM	2.46	110.47	106.73
3	a	802	25L	CBZ-NBJ-CAX	2.44	107.28	103.45
3	a	802	25L	N3-C4-N9	2.43	131.30	127.17
3	b	902	25L	CBW-CBZ-CCC	2.42	120.49	117.18
3	b	902	25L	CBV-CBY-CCB	2.42	120.48	117.18
2	b	901	BWC	CBA-CBB-CBC	-2.40	98.45	105.10
3	a	802	25L	C2'-C1'-N9	2.39	119.24	113.30
3	b	902	25L	C5'-C4'-C3'	-2.37	106.67	115.21
3	a	802	25L	C4-C5-N7	-2.36	107.89	110.58
2	a	801	BWC	CAE-CAJ-CAL	-2.33	120.38	133.19
3	a	802	25L	CBY-NBI-CAW	2.31	107.09	103.45
2	a	801	BWC	CBA-CBB-CBC	-2.31	98.70	105.10
3	a	802	25L	C6-C5-C4	2.30	120.33	117.18
2	a	801	BWC	CAW-NAV-CAT	2.27	127.45	122.47
3	b	902	25L	C2'-C1'-N9	2.27	118.94	113.30
3	b	902	25L	CBY-CCB-NCQ	2.22	108.23	105.81
3	b	902	25L	CBZ-CCC-NCR	2.14	108.14	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	902	25L	OBR-CCL-CCG	-2.13	104.04	111.68
4	a	803	PO4	O4-P-O1	-2.13	103.42	110.95
2	a	801	BWC	CAR-CAQ-CAM	-2.10	122.56	125.62
3	b	902	25L	CBZ-NBJ-CAX	2.09	106.74	103.45
3	a	802	25L	OBP-CCO-NCR	2.08	112.08	108.09
2	b	901	BWC	CAE-CAJ-CAL	-2.07	121.81	133.19
2	b	901	BWC	CAP-CAO-NAN	2.06	109.02	107.48
3	b	902	25L	C4-C5-N7	-2.02	108.28	110.58
3	b	902	25L	CCG-CCL-CCO	2.01	106.65	102.81

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	801	BWC	CAW-CAX-NAY-CAZ
2	b	901	BWC	CAQ-CAP-CAT-NAV
3	b	902	25L	O4'-C4'-C5'-O5'
3	b	902	25L	CBA-OBM-PCV-OAG
3	b	902	25L	CBA-OBM-PCV-OBQ
3	b	902	25L	CCL-OBP-PCU-O5'
3	b	902	25L	CCL-OBP-PCU-OAF
2	a	801	BWC	NAV-CAW-CAX-NAY
3	b	902	25L	OBM-CBA-CCJ-OBP
3	b	902	25L	OBM-CBA-CCJ-CCG
2	b	901	BWC	NAV-CAW-CAX-NAY
3	b	902	25L	C3'-C4'-C5'-O5'
3	b	902	25L	CCO-CCL-OBP-PCU
3	a	802	25L	CCK-CCN-NCQ-CAW
2	a	801	BWC	CAX-CAW-NAV-CAT
2	b	901	BWC	CAQ-CAP-CAT-OAU
2	a	801	BWC	CAO-CAP-CAT-OAU
2	a	801	BWC	CAO-CAP-CAT-NAV
3	a	802	25L	C2'-C1'-N9-C8
3	b	902	25L	CCK-CCN-NCQ-CAW
3	a	802	25L	C3'-C4'-C5'-O5'
3	b	902	25L	C5'-O5'-PCU-OAF
3	b	902	25L	C5'-O5'-PCU-OAP
3	b	902	25L	C5'-O5'-PCU-OBP
3	b	902	25L	CCG-CCL-OBP-PCU
3	a	802	25L	C2'-C1'-N9-C4
3	a	802	25L	CCK-CCN-NCQ-CCB
2	a	801	BWC	CAQ-CAP-CAT-OAU

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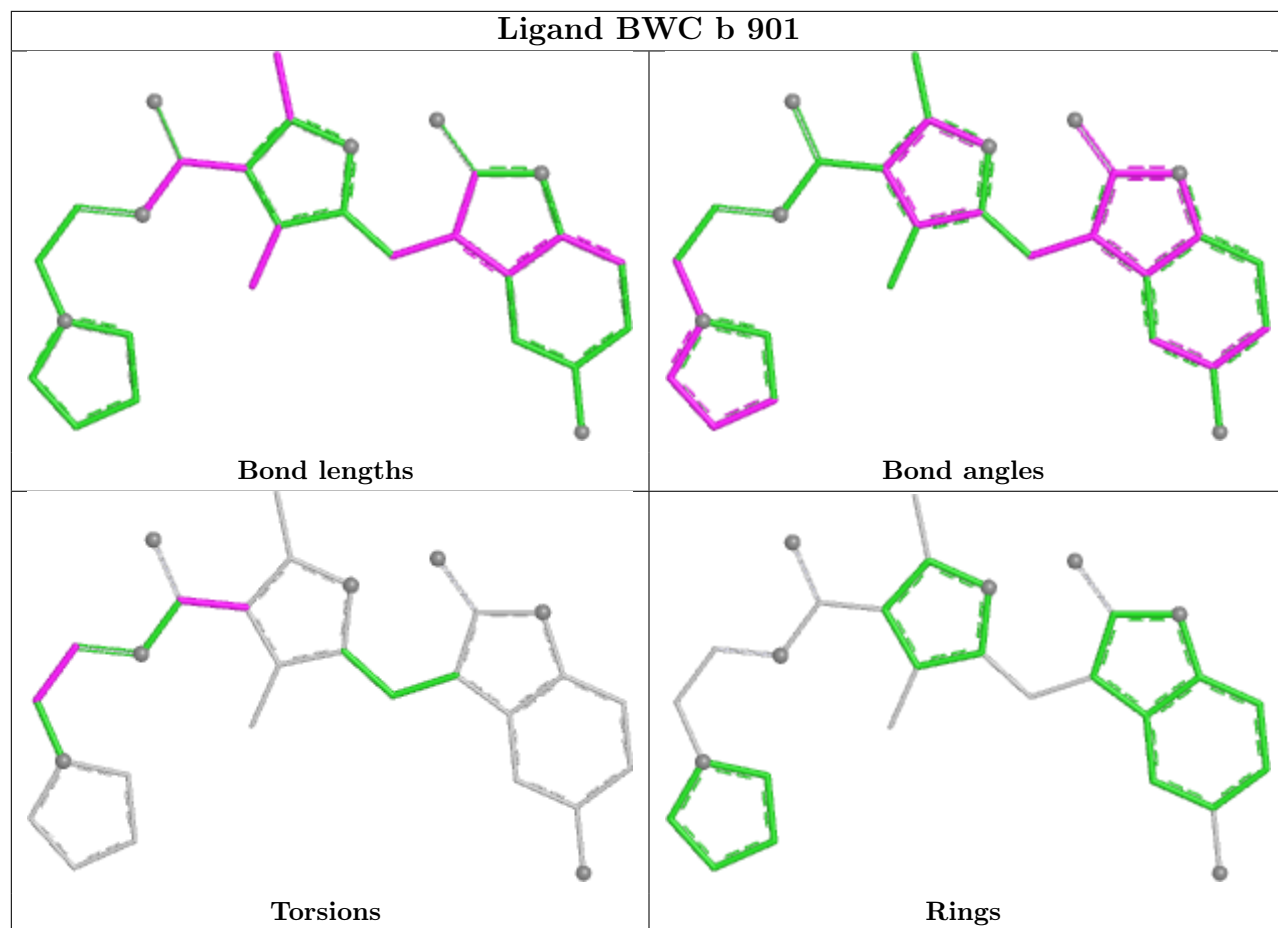
Mol	Chain	Res	Type	Atoms
2	a	801	BWC	CAQ-CAP-CAT-NAV
2	b	901	BWC	CAO-CAP-CAT-OAU
3	a	802	25L	O4'-C4'-C5'-O5'
3	a	802	25L	O4'-C1'-N9-C8
3	b	902	25L	CCL-OBR-PCU-OAP
3	a	802	25L	OBO-CCN-NCQ-CAW
3	b	902	25L	OBO-CCN-NCQ-CAW

There are no ring outliers.

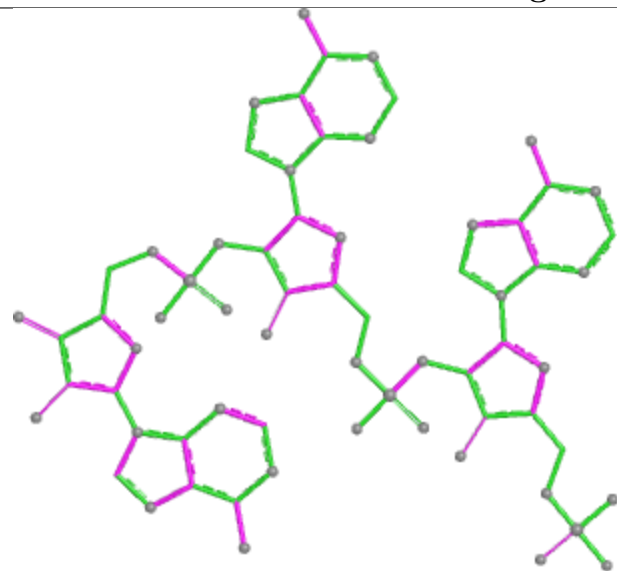
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	a	803	PO4	1	0
3	b	902	25L	4	0
3	a	802	25L	1	0
2	a	801	BWC	1	0

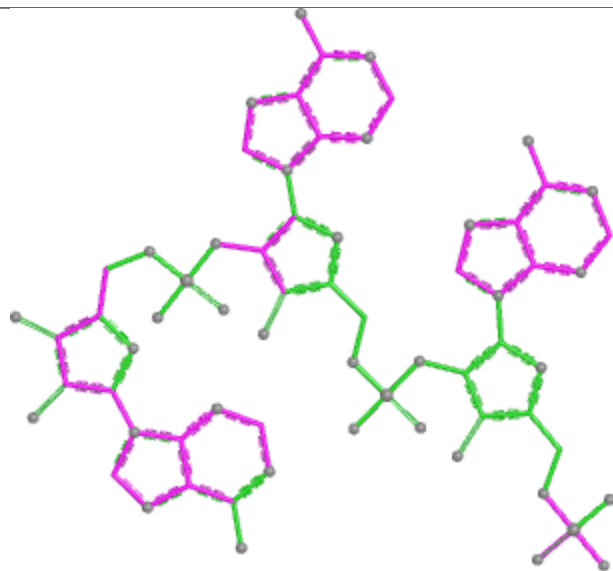
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



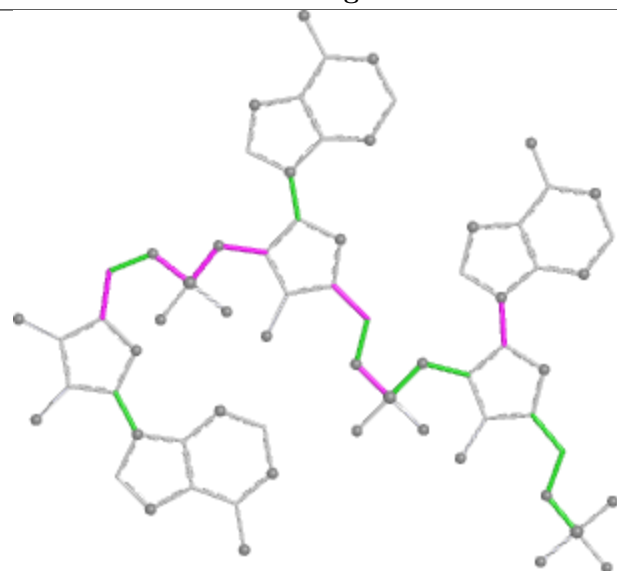
Ligand 25L b 902



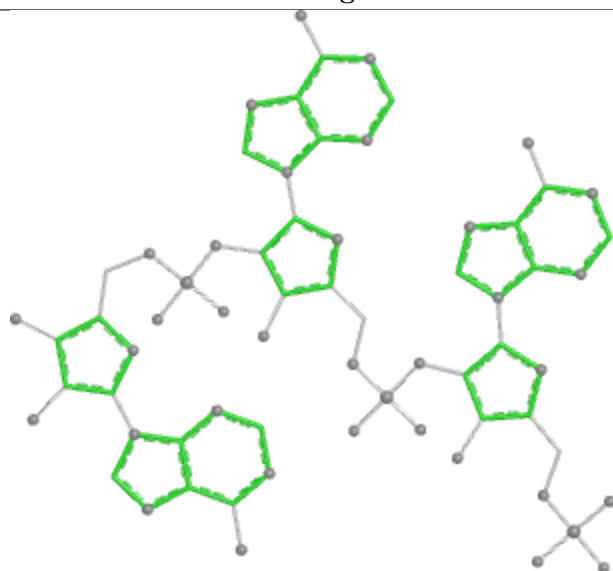
Bond lengths



Bond angles

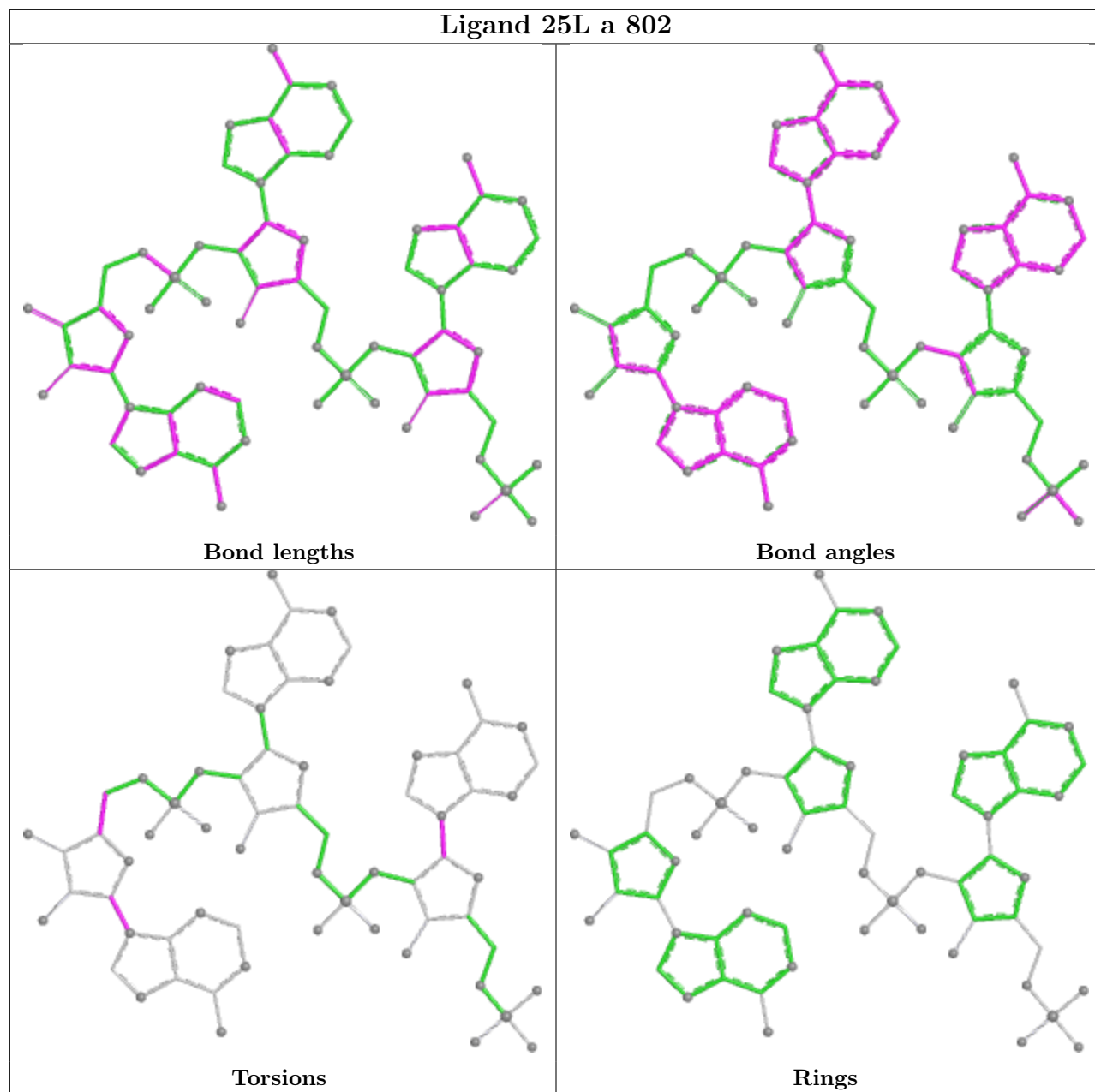


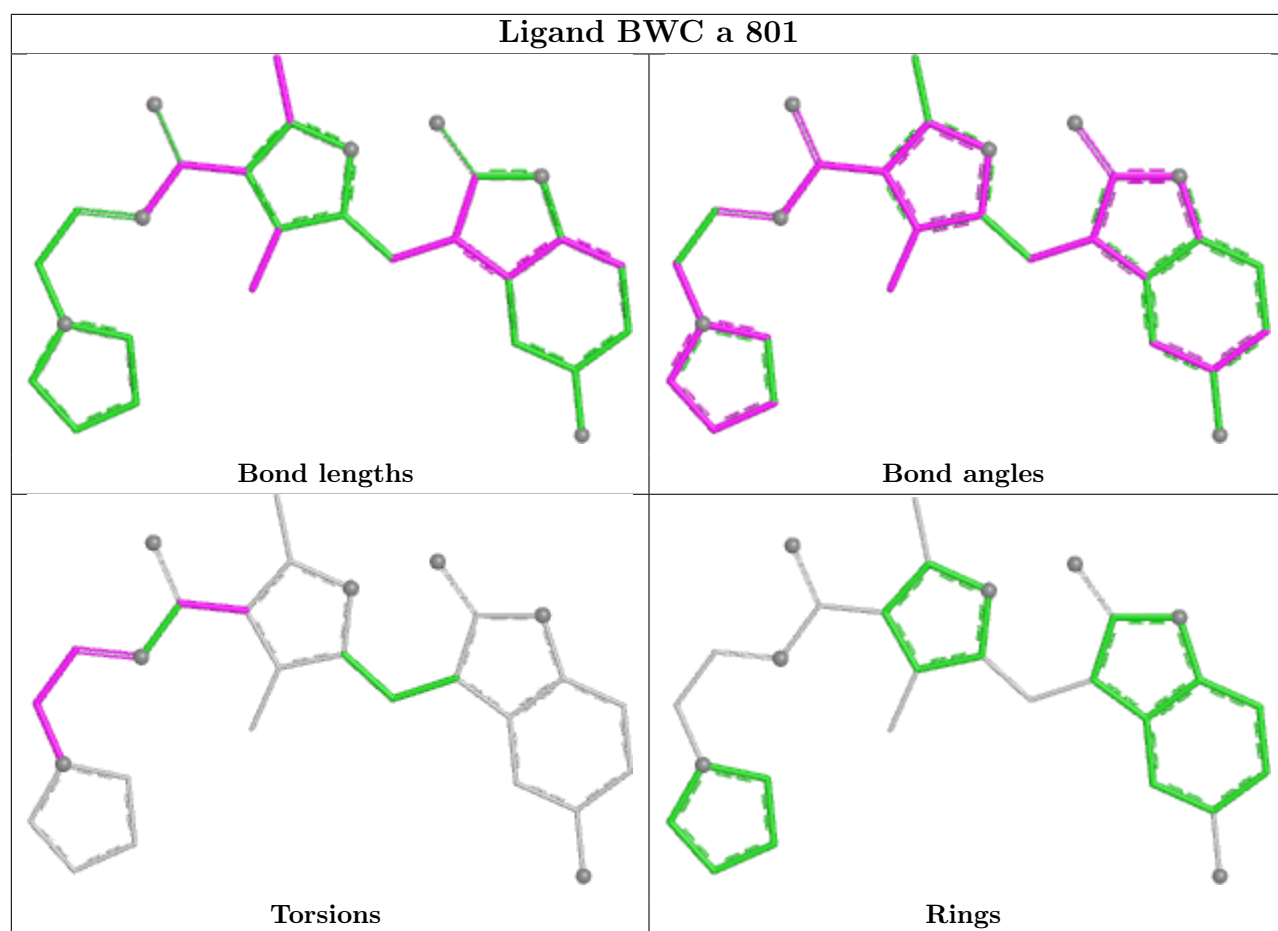
Torsions



Rings

Ligand 25L a 802





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.27	13 (1%) 66 67	50, 94, 131, 172	0
1	b	688/717 (95%)	0.41	36 (5%) 33 33	53, 98, 151, 198	0
All	All	1369/1434 (95%)	0.34	49 (3%) 46 47	50, 96, 142, 198	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	570	VAL	5.0
1	a	643	ALA	3.8
1	a	570	VAL	3.5
1	b	643	ALA	3.3
1	b	39	VAL	3.2
1	b	256	LEU	3.2
1	b	42	LEU	3.1
1	b	99	ILE	2.8
1	b	622	LEU	2.8
1	b	567	GLY	2.8
1	b	23	LEU	2.8
1	b	168	THR	2.8
1	b	208	LEU	2.7
1	b	27	LEU	2.6
1	b	179	VAL	2.6
1	b	60	PRO	2.5
1	b	96	ILE	2.5
1	a	662	LEU	2.5
1	b	73	VAL	2.4
1	a	139	LEU	2.3
1	b	108	LEU	2.3
1	a	622	LEU	2.3
1	b	76	LEU	2.3
1	b	121	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	b	116	VAL	2.3
1	a	310	TYR	2.3
1	b	155	THR	2.2
1	a	76	LEU	2.2
1	b	195	ALA	2.2
1	b	278	ALA	2.2
1	b	105	LEU	2.2
1	a	127	PHE	2.2
1	b	127	PHE	2.2
1	b	131	ALA	2.2
1	a	303	VAL	2.1
1	b	181	VAL	2.1
1	a	324	GLY	2.1
1	a	51	PHE	2.1
1	b	149	VAL	2.1
1	a	108	LEU	2.1
1	b	64	ALA	2.1
1	a	250	LEU	2.1
1	b	508	ALA	2.1
1	b	28	THR	2.1
1	b	601	ASP	2.1
1	b	511	PRO	2.1
1	b	660	GLY	2.0
1	b	151	MET	2.0
1	b	31	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

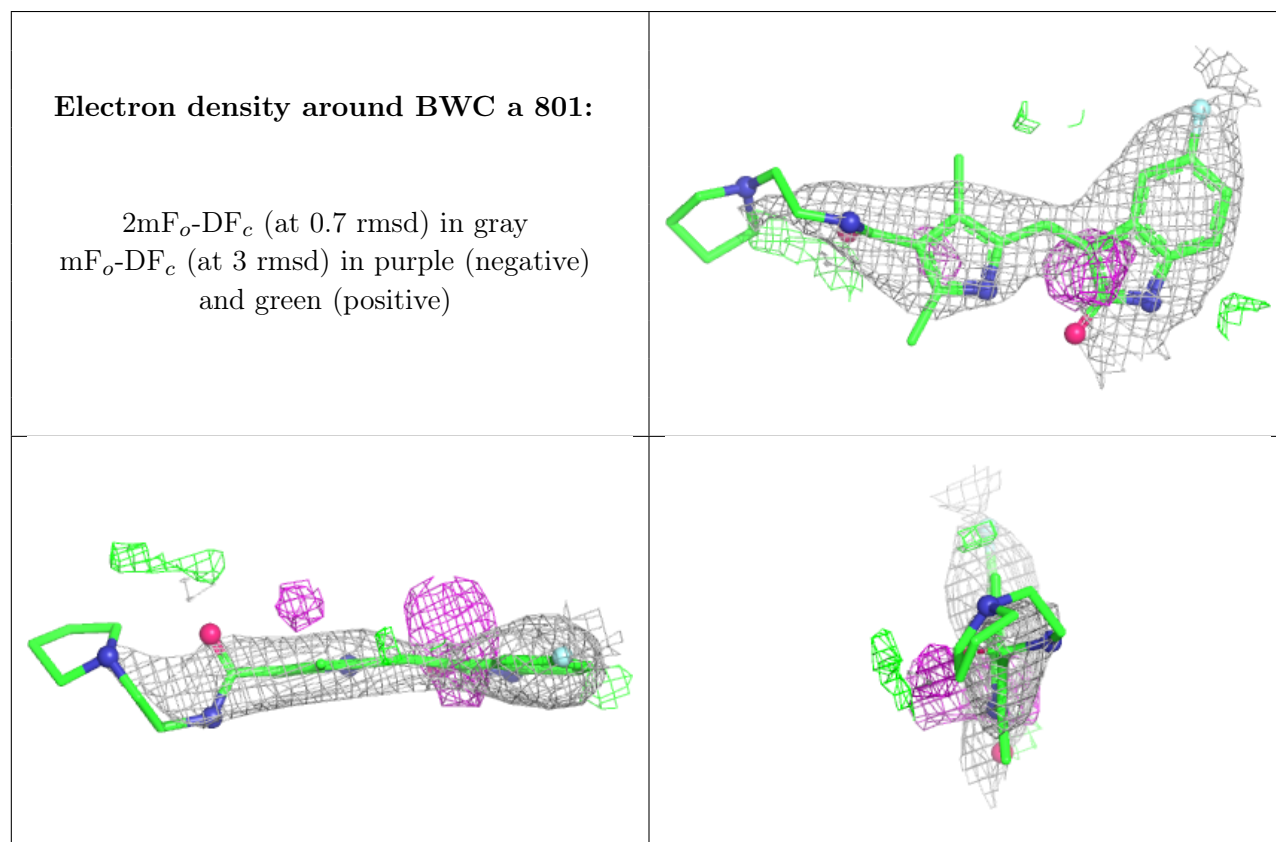
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

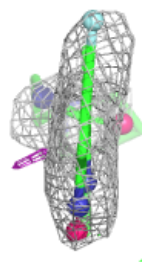
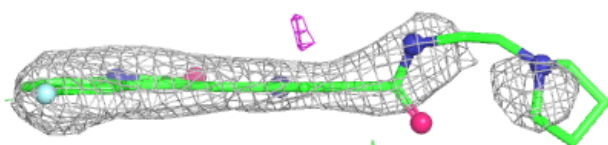
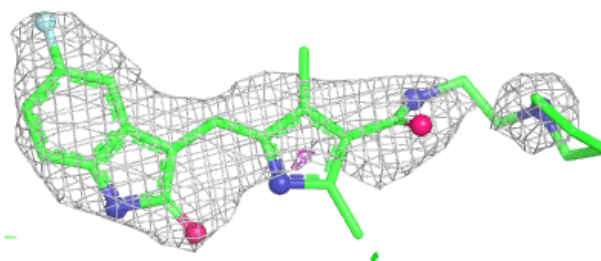
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BWC	a	801	29/29	0.82	0.20	85,102,180,181	0
2	BWC	b	901	29/29	0.84	0.16	95,134,172,174	0
3	25L	b	902	67/75	0.93	0.09	71,95,139,141	0
3	25L	a	802	67/75	0.94	0.08	62,77,91,101	0
4	PO4	a	803	5/5	0.96	0.05	68,74,84,85	0

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.

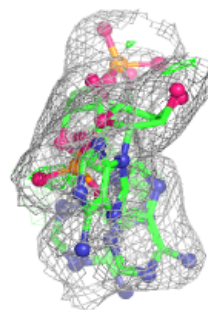
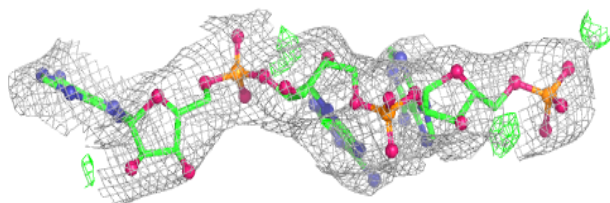
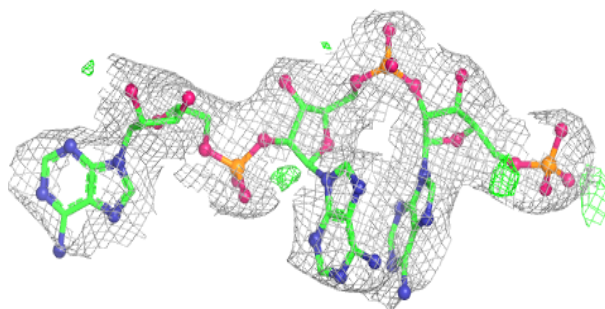


Electron density around BWC b 901:

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

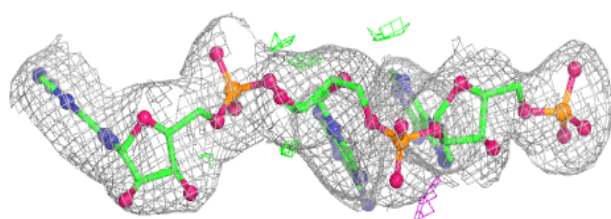
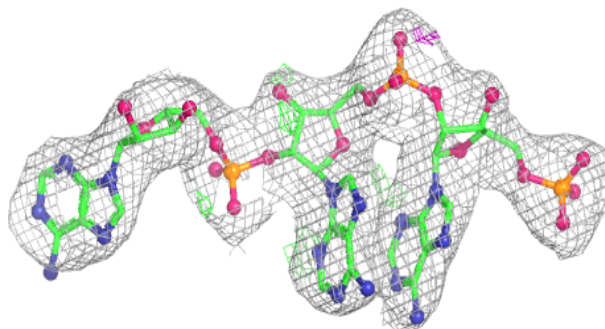
**Electron density around 25L b 902:**

$2mF_o-DF_c$ (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.