



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:01 AM UTC

PDB ID : 1FML / pdb_00001fml
Title : CRYSTAL STRUCTURE OF RETINOL DEHYDRATASE IN A COMPLEX WITH RETINOL AND PAP
Authors : Pakhomova, S.; Kobayashi, M.; Buck, J.; Newcomer, M.E.
Deposited on : 2000-08-17
Resolution : 2.75 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)
Xtrriage (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

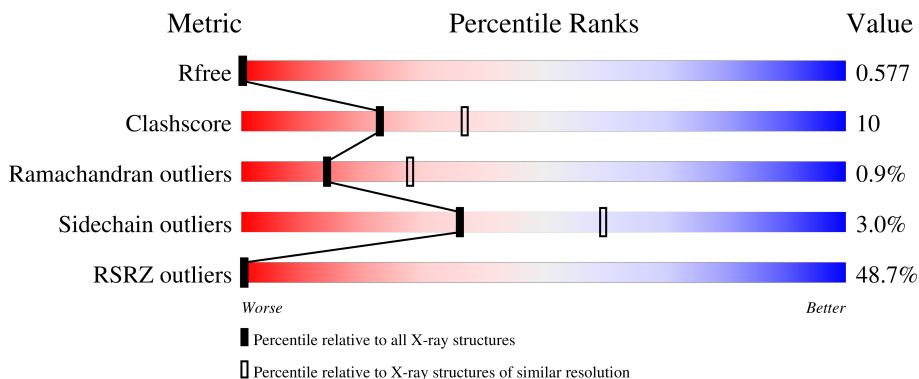
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	351	
1	B	351	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5859 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 RETINOL DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2838	1837	470	515	16	0	1	0
1	B	341	2832	1833	468	515	16	0	0	0

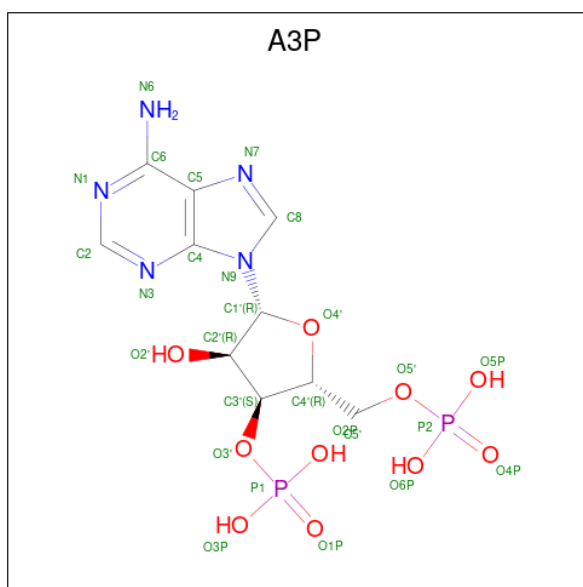
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	PHE	SEE REMARK 999	UNP Q26490
B	142	SER	PHE	SEE REMARK 999	UNP Q26490

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

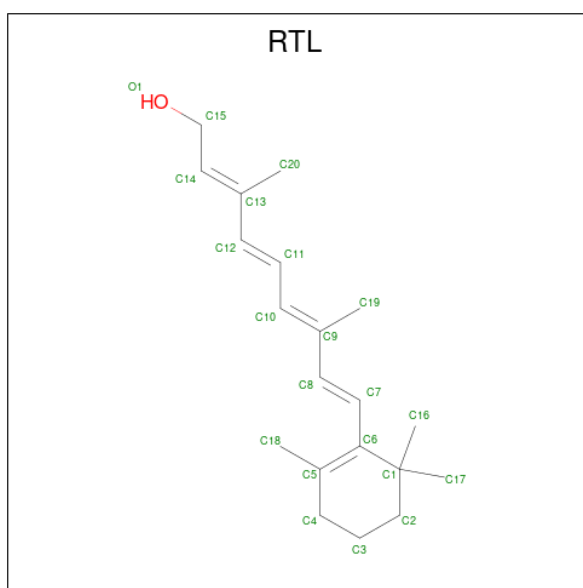
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is RETINOL (CCD ID: RTL) (formula: $C_{20}H_{30}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	O			
4	A	1	Total	C	O	0	0
			21	20	1		
4	B	1	Total	C	O	0	0
			21	20	1		

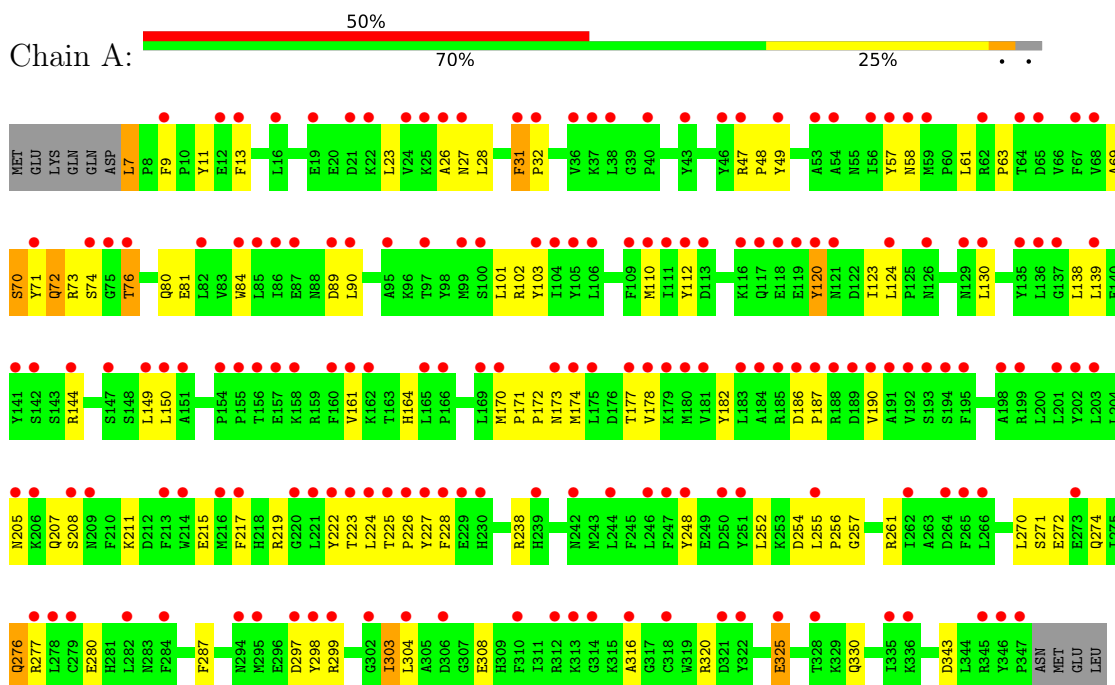
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0
5	B	45	Total 45	O 45	0	0

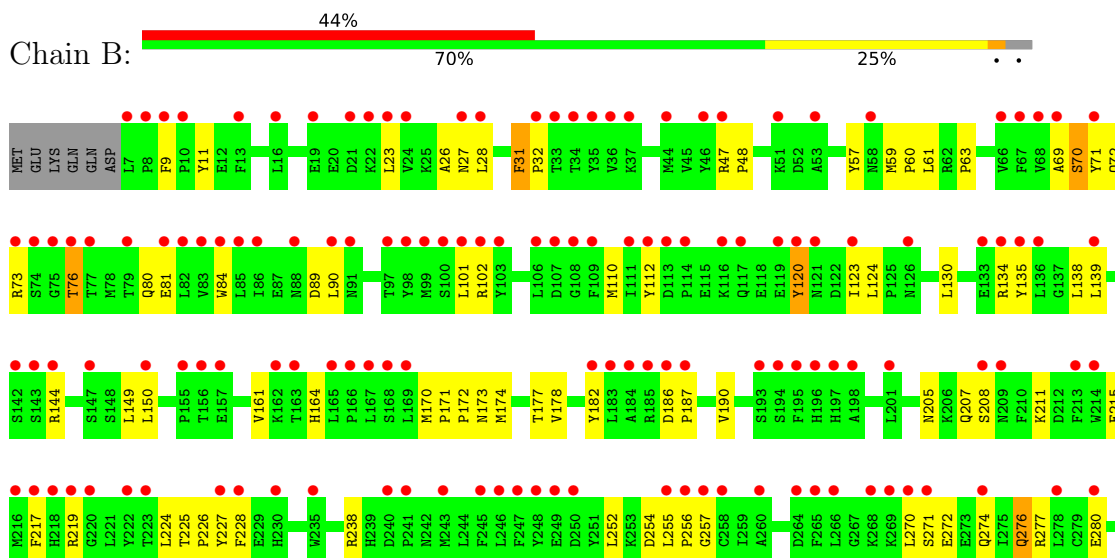
3 Residue-property plots i

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: RETINOL DEHYDRATASE



• Molecule 1: RETINOL DEHYDRATASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.05Å 66.61Å 84.90Å 90.00° 111.29° 90.00°	Depositor
Resolution (Å)	38.45 – 2.75 38.45 – 2.75	Depositor EDS
% Data completeness (in resolution range)	87.8 (38.45-2.75) 29.2 (38.45-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.55 (at 2.22Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.273 0.553 , 0.577	Depositor DCC
R_{free} test set	330 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtrriage
Anisotropy	1.382	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 394.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.036 for l,-k,h	Xtrriage
F_o, F_c correlation	0.31	EDS
Total number of atoms	5859	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: RTL, CA, A3P

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	0.46	0/2924	0.96	13/3960 (0.3%)
1	B	0.46	0/2913	0.96	13/3945 (0.3%)
All	All	0.46	0/5837	0.96	26/7905 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	TYR	N-CA-C	-8.65	96.53	110.20
1	B	71	TYR	N-CA-C	-8.22	97.21	110.20
1	B	217	PHE	N-CA-C	6.29	117.83	110.97
1	A	217	PHE	N-CA-C	6.18	117.70	110.97
1	A	225	THR	N-CA-C	-6.04	101.16	110.58
1	A	7	LEU	CA-C-N	-5.98	112.98	120.51
1	A	7	LEU	C-N-CA	-5.98	112.98	120.51
1	B	225	THR	N-CA-C	-5.89	101.39	110.58
1	A	120	TYR	N-CA-C	5.67	117.26	111.14
1	B	120	TYR	N-CA-C	5.59	117.17	111.14
1	A	211	LYS	N-CA-C	-5.58	105.10	111.07
1	B	297	ASP	N-CA-C	-5.50	105.44	111.82
1	B	72	GLN	N-CA-C	5.48	117.36	110.24
1	B	110	MET	N-CA-C	5.39	119.35	112.34
1	A	110	MET	N-CA-C	5.38	119.33	112.34
1	A	228	PHE	N-CA-C	5.37	118.04	111.82
1	A	72	GLN	N-CA-C	5.31	117.15	110.24
1	B	31	PHE	CA-C-N	5.31	125.12	119.28
1	B	31	PHE	C-N-CA	5.31	125.12	119.28
1	B	228	PHE	N-CA-C	5.30	117.96	111.82
1	A	31	PHE	CA-C-N	5.28	124.91	119.05
1	A	31	PHE	C-N-CA	5.28	124.91	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	TRP	N-CA-C	-5.17	106.23	112.54
1	B	211	LYS	N-CA-C	-5.15	105.56	111.07
1	B	303	ILE	N-CA-C	5.10	117.07	111.77
1	A	303	ILE	N-CA-C	5.01	116.98	111.77

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	2838	0	2765	60	0
1	B	2832	0	2762	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	11	1	0
3	B	27	0	11	1	0
4	A	21	0	30	0	0
4	B	21	0	30	0	0
5	A	46	0	0	1	0
5	B	45	0	0	2	0
All	All	5859	0	5609	118	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 (118) 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:120:TYR:O	1:A:123:ILE:HG12	1.84	0.77
1:B:120:TYR:O	1:B:123:ILE:HG12	1.85	0.77
1:A:187:PRO:HG3	1:A:227:TYR:CE2	2.28	0.69
1:B:187:PRO:HG3	1:B:227:TYR:CE2	2.31	0.65
1:A:272:GLU:O	1:A:276:GLN:HB2	1.98	0.63
1:B:272:GLU:O	1:B:276:GLN:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD21	1:A:161:VAL:HG22	1.82	0.61
1:A:255:LEU:HB3	1:A:256:PRO:HD3	1.84	0.60
1:B:81:GLU:OE2	1:B:81:GLU:HA	2.02	0.60
1:A:298:TYR:HD2	1:A:303:ILE:HD11	1.69	0.58
1:A:238:ARG:NH2	1:A:343:ASP:OD2	2.37	0.58
1:B:150:LEU:HD21	1:B:161:VAL:HG22	1.84	0.58
1:B:238:ARG:NH2	1:B:343:ASP:OD2	2.36	0.58
1:A:69:ALA:O	1:A:70:SER:HB3	2.04	0.58
1:A:252:LEU:HD12	1:A:316:ALA:HB2	1.84	0.57
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.87	0.57
1:B:298:TYR:HD2	1:B:303:ILE:HD11	1.69	0.56
1:B:252:LEU:HD12	1:B:316:ALA:HB2	1.86	0.56
1:B:69:ALA:O	1:B:70:SER:HB3	2.04	0.56
1:B:254:ASP:OD2	1:B:257:GLY:HA3	2.06	0.56
1:B:270:LEU:HA	1:B:274:GLN:OE1	2.07	0.55
1:B:299:ARG:HB2	1:B:304:LEU:HD12	1.88	0.55
1:B:144:ARG:HD3	1:B:149:LEU:HD21	1.88	0.55
1:A:81:GLU:OE2	1:A:81:GLU:HA	2.07	0.55
1:B:47:ARG:HB3	1:B:48:PRO:HD3	1.89	0.54
1:A:325:GLU:H	1:A:325:GLU:CD	2.16	0.54
1:A:47:ARG:HB3	1:A:48:PRO:HD3	1.90	0.54
1:A:72:GLN:HG2	5:A:475:HOH:O	2.08	0.54
1:A:270:LEU:HA	1:A:274:GLN:OE1	2.07	0.54
1:A:299:ARG:HB2	1:A:304:LEU:HD12	1.89	0.54
1:B:76:THR:HG22	1:B:80:GLN:HE21	1.71	0.54
1:A:144:ARG:HD3	1:A:149:LEU:HD21	1.89	0.54
1:B:325:GLU:H	1:B:325:GLU:CD	2.16	0.54
1:A:76:THR:HG22	1:A:80:GLN:HE21	1.72	0.54
1:A:254:ASP:OD2	1:A:257:GLY:HA3	2.08	0.54
1:A:270:LEU:HB3	1:A:274:GLN:HB2	1.91	0.53
1:A:277:ARG:HA	1:A:280:GLU:OE1	2.09	0.53
1:B:112:TYR:CE1	1:B:139:LEU:HD22	2.43	0.53
1:A:112:TYR:CE1	1:A:139:LEU:HD22	2.45	0.52
1:B:277:ARG:HA	1:B:280:GLU:OE1	2.10	0.52
1:B:270:LEU:HB3	1:B:274:GLN:HB2	1.91	0.52
1:A:205:ASN:C	1:A:207:GLN:N	2.67	0.51
1:B:73:ARG:CZ	3:B:500:A3P:H5'1	2.41	0.51
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.11	0.50
1:A:7:LEU:HB2	1:A:58:ASN:OD1	2.11	0.50
1:B:308:GLU:OE1	1:B:308:GLU:HA	2.11	0.50
1:A:73:ARG:CZ	3:A:400:A3P:H5'1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASN:C	1:B:207:GLN:N	2.67	0.49
1:A:9:PHE:CE2	1:A:11:TYR:HB2	2.46	0.49
1:A:27:ASN:HB2	1:A:28:LEU:HD12	1.94	0.49
1:A:90:LEU:HD21	1:A:274:GLN:HB3	1.94	0.49
1:B:9:PHE:CE2	1:B:11:TYR:HB2	2.47	0.49
1:B:320:ARG:HG2	1:B:320:ARG:NH1	2.28	0.49
1:A:320:ARG:HG2	1:A:320:ARG:NH1	2.28	0.48
1:A:124:LEU:CD1	1:A:130:LEU:HD21	2.44	0.48
1:B:27:ASN:HB2	1:B:28:LEU:HD12	1.94	0.48
1:B:205:ASN:C	1:B:207:GLN:H	2.21	0.48
1:A:215:GLU:O	1:A:219:ARG:HB2	2.13	0.48
1:B:90:LEU:HD21	1:B:274:GLN:HB3	1.96	0.48
1:B:124:LEU:CD1	1:B:130:LEU:HD21	2.44	0.47
1:B:47:ARG:HG3	1:B:47:ARG:HH11	1.79	0.47
1:B:63:PRO:HA	1:B:177:THR:O	2.15	0.47
1:B:81:GLU:HG2	1:B:287:PHE:HE1	1.79	0.47
1:B:215:GLU:O	1:B:219:ARG:HB2	2.14	0.47
1:A:172:PRO:O	1:A:173:ASN:HB2	2.15	0.46
1:A:205:ASN:C	1:A:207:GLN:H	2.22	0.46
1:B:70:SER:O	1:B:164:HIS:HA	2.16	0.46
1:B:172:PRO:O	1:B:173:ASN:HB2	2.16	0.46
1:A:61:LEU:CD1	1:A:174:MET:HB2	2.46	0.46
1:B:61:LEU:CD1	1:B:174:MET:HB2	2.46	0.45
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.80	0.45
1:A:63:PRO:HA	1:A:177:THR:O	2.17	0.45
1:A:23:LEU:O	1:A:26:ALA:HB3	2.17	0.45
1:A:271:SER:O	1:A:272:GLU:C	2.60	0.45
1:B:271:SER:O	1:B:272:GLU:C	2.59	0.45
1:A:70:SER:O	1:A:164:HIS:HA	2.17	0.45
1:A:299:ARG:NH2	1:A:308:GLU:O	2.50	0.44
1:A:81:GLU:HG2	1:A:287:PHE:HE1	1.80	0.44
1:A:90:LEU:N	1:A:90:LEU:HD12	2.33	0.44
1:B:285:GLU:HG2	5:B:592:HOH:O	2.16	0.44
1:A:320:ARG:HG2	1:A:320:ARG:HH11	1.82	0.44
1:B:286:LYS:NZ	5:B:585:HOH:O	2.51	0.43
1:B:299:ARG:NH2	1:B:308:GLU:O	2.49	0.43
1:B:320:ARG:HG2	1:B:320:ARG:HH11	1.82	0.43
1:A:61:LEU:HD11	1:A:174:MET:HB2	2.00	0.43
1:A:186:ASP:O	1:A:190:VAL:HG23	2.18	0.43
1:A:170:MET:O	1:A:171:PRO:C	2.62	0.42
1:A:257:GLY:O	1:A:261:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:LEU:O	1:B:26:ALA:HB3	2.19	0.42
1:B:90:LEU:HD12	1:B:90:LEU:N	2.35	0.42
1:B:47:ARG:HG3	1:B:47:ARG:NH1	2.34	0.42
1:B:57:TYR:O	1:B:171:PRO:HG3	2.19	0.42
1:B:89:ASP:O	1:B:90:LEU:C	2.62	0.42
1:A:80:GLN:HB3	1:A:103:TYR:CE1	2.54	0.42
1:A:89:ASP:O	1:A:90:LEU:C	2.61	0.42
1:A:57:TYR:O	1:A:171:PRO:HG3	2.20	0.41
1:B:61:LEU:HD11	1:B:174:MET:HB2	2.02	0.41
1:B:186:ASP:O	1:B:190:VAL:HG23	2.20	0.41
1:A:76:THR:HG22	1:A:80:GLN:NE2	2.34	0.41
1:A:48:PRO:O	1:A:49:TYR:C	2.63	0.41
1:A:31:PHE:HA	1:A:32:PRO:HD3	1.83	0.41
1:A:222:TYR:O	1:A:223:THR:C	2.63	0.41
1:B:324:ASP:OD2	1:B:324:ASP:C	2.64	0.41
1:A:74:SER:O	1:A:248:TYR:HB2	2.21	0.41
1:B:124:LEU:HD12	1:B:130:LEU:HD11	2.03	0.41
1:A:13:PHE:CD1	1:A:13:PHE:C	2.99	0.41
1:A:47:ARG:HG3	1:A:47:ARG:NH1	2.36	0.41
1:A:255:LEU:N	1:A:256:PRO:CD	2.84	0.41
1:B:59:MET:HA	1:B:60:PRO:HD3	1.93	0.41
1:B:69:ALA:O	1:B:182:TYR:HA	2.21	0.41
1:B:76:THR:HG22	1:B:80:GLN:NE2	2.34	0.41
1:A:84:TRP:CE2	1:A:102:ARG:HD2	2.56	0.40
1:B:134:ARG:O	1:B:135:TYR:C	2.63	0.40
1:B:84:TRP:CE2	1:B:102:ARG:HD2	2.56	0.40
1:B:170:MET:O	1:B:171:PRO:C	2.64	0.40
1:A:69:ALA:O	1:A:182:TYR:HA	2.22	0.40
1:B:31:PHE:HA	1:B:32:PRO:HD3	1.83	0.40
1:B:339:LEU:C	1:B:342:THR:HG22	2.47	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	340/351 (97%)	315 (93%)	22 (6%)	3 (1%)	14	28
1	B	339/351 (97%)	311 (92%)	25 (7%)	3 (1%)	14	28
All	All	679/702 (97%)	626 (92%)	47 (7%)	6 (1%)	14	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	B	208	SER
1	A	70	SER
1	B	70	SER
1	B	226	PRO
1	A	226	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	305/316 (96%)	296 (97%)	9 (3%)	36	60
1	B	304/316 (96%)	295 (97%)	9 (3%)	36	60
All	All	609/632 (96%)	591 (97%)	18 (3%)	36	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	101	LEU
1	A	138	LEU
1	A	178	VAL
1	A	224	LEU
1	A	276	GLN
1	A	297	ASP

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Mol	Chain	Res	Type
1	A	325	GLU
1	A	330	GLN
1	B	76	THR
1	B	101	LEU
1	B	138	LEU
1	B	178	VAL
1	B	224	LEU
1	B	276	GLN
1	B	297	ASP
1	B	325	GLU
1	B	330	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	GLN
1	A	117	GLN
1	A	276	GLN
1	A	330	GLN
1	A	338	ASN
1	B	72	GLN
1	B	80	GLN
1	B	276	GLN
1	B	330	GLN
1	B	338	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	RTL	B	501	-	21,21,21	1.40	2 (9%)	28,28,28	4.01	16 (57%)
3	A3P	B	500	-	29,29,29	1.33	4 (13%)	44,45,45	0.81	1 (2%)
4	RTL	A	401	-	21,21,21	1.45	2 (9%)	28,28,28	4.03	16 (57%)
3	A3P	A	400	-	29,29,29	1.42	5 (17%)	44,45,45	0.79	1 (2%)

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
4	RTL	B	501	-	-	6/14/31/31	0/1/1/1
3	A3P	B	500	-	-	3/15/31/31	0/3/3/3
4	RTL	A	401	-	-	4/14/31/31	0/1/1/1
3	A3P	A	400	-	-	3/15/31/31	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	A3P	C4-N3	4.07	1.42	1.34
3	A	400	A3P	C4-N3	3.98	1.41	1.34
3	A	400	A3P	C2-N3	3.21	1.39	1.33
4	A	401	RTL	C5-C6	3.08	1.39	1.34
4	B	501	RTL	C5-C6	3.01	1.39	1.34
4	B	501	RTL	C1-C6	2.90	1.57	1.53
4	A	401	RTL	C1-C6	2.88	1.57	1.53
3	A	400	A3P	C6-N1	2.73	1.43	1.35
3	B	500	A3P	C2-N3	2.71	1.38	1.33
3	A	400	A3P	C2-N1	2.58	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	A3P	C5-C4	2.43	1.43	1.39
3	B	500	A3P	C6-N1	2.21	1.41	1.35
3	B	500	A3P	C2-N1	2.06	1.37	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	RTL	C12-C13-C14	10.93	133.71	118.49
4	A	401	RTL	C12-C13-C14	10.92	133.69	118.49
4	A	401	RTL	C2-C3-C4	10.38	134.11	111.28
4	B	501	RTL	C2-C3-C4	10.24	133.80	111.28
4	A	401	RTL	C20-C13-C12	-7.53	106.59	118.09
4	B	501	RTL	C20-C13-C12	-7.52	106.60	118.09
4	A	401	RTL	C15-C14-C13	-5.34	117.94	126.61
4	B	501	RTL	C15-C14-C13	-5.13	118.28	126.61
4	B	501	RTL	C4-C5-C6	4.81	129.21	122.70
4	A	401	RTL	C4-C5-C6	4.78	129.16	122.70
4	A	401	RTL	C3-C4-C5	-4.77	105.56	114.06
4	B	501	RTL	C3-C4-C5	-4.66	105.74	114.06
4	B	501	RTL	C10-C11-C12	-4.25	110.89	123.20
4	A	401	RTL	C2-C1-C6	4.17	116.49	110.44
4	B	501	RTL	C2-C1-C6	4.09	116.39	110.44
4	A	401	RTL	C10-C11-C12	-3.98	111.67	123.20
4	B	501	RTL	C11-C12-C13	3.56	136.14	126.36
4	A	401	RTL	C11-C12-C13	3.50	135.96	126.36
4	A	401	RTL	C7-C8-C9	-3.01	121.78	126.23
4	A	401	RTL	C17-C1-C6	2.87	114.75	110.24
4	B	501	RTL	C17-C1-C6	2.78	114.59	110.24
4	B	501	RTL	C18-C5-C6	-2.76	121.47	124.48
4	A	401	RTL	C18-C5-C6	-2.62	121.63	124.48
4	B	501	RTL	C7-C8-C9	-2.58	122.41	126.23
4	B	501	RTL	C16-C1-C2	-2.42	99.64	108.95
4	B	501	RTL	C20-C13-C14	-2.33	119.69	123.73
4	B	501	RTL	C16-C1-C6	2.32	113.89	110.24
4	A	401	RTL	C20-C13-C14	-2.32	119.71	123.73
3	A	400	A3P	O2'-C2'-C3'	2.32	117.68	111.19
4	A	401	RTL	C16-C1-C2	-2.30	100.14	108.95
3	B	500	A3P	O2'-C2'-C3'	2.19	117.31	111.19
4	A	401	RTL	C16-C1-C6	2.13	113.59	110.24
4	A	401	RTL	C18-C5-C4	-2.06	109.20	113.60
4	B	501	RTL	C18-C5-C4	-2.01	109.30	113.60

There are no chirality outliers.

All (16) torsion outliers are listed below:

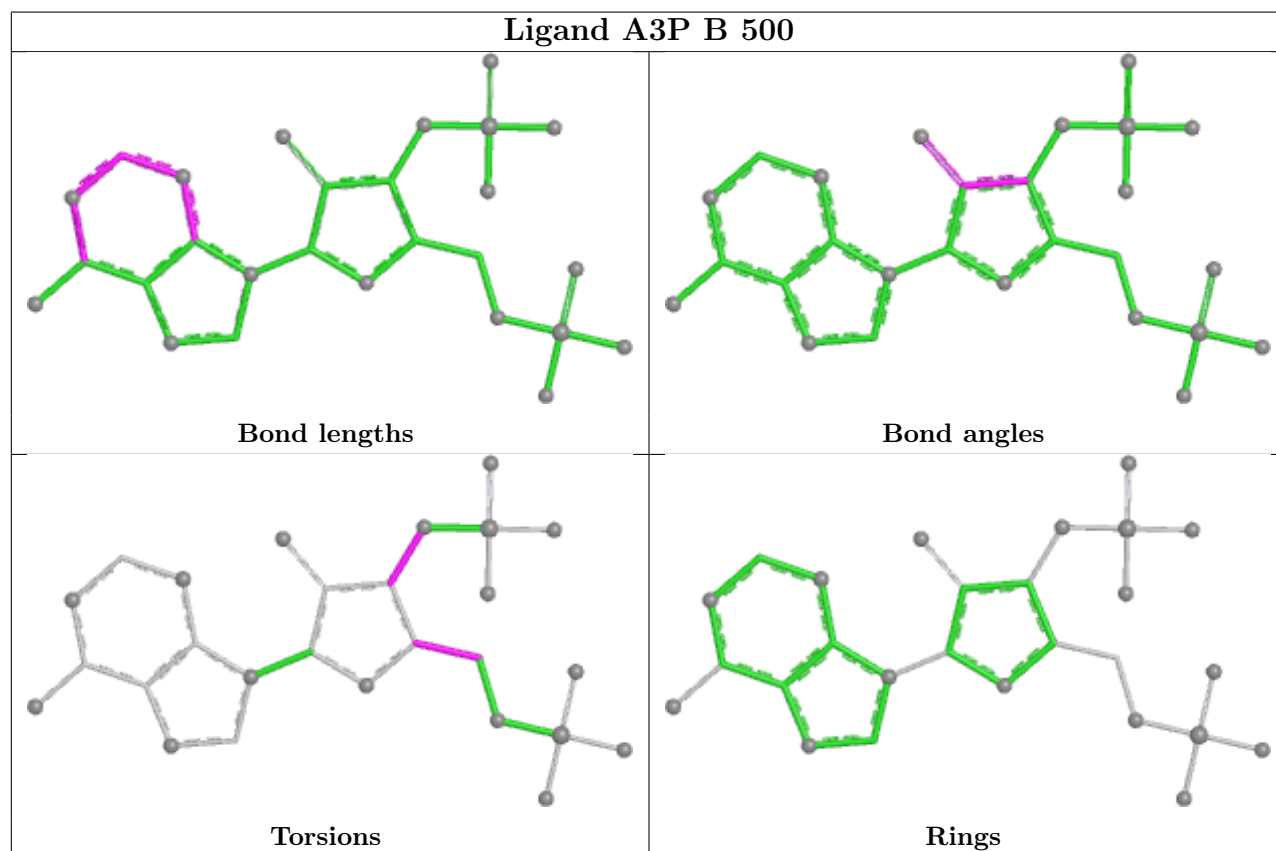
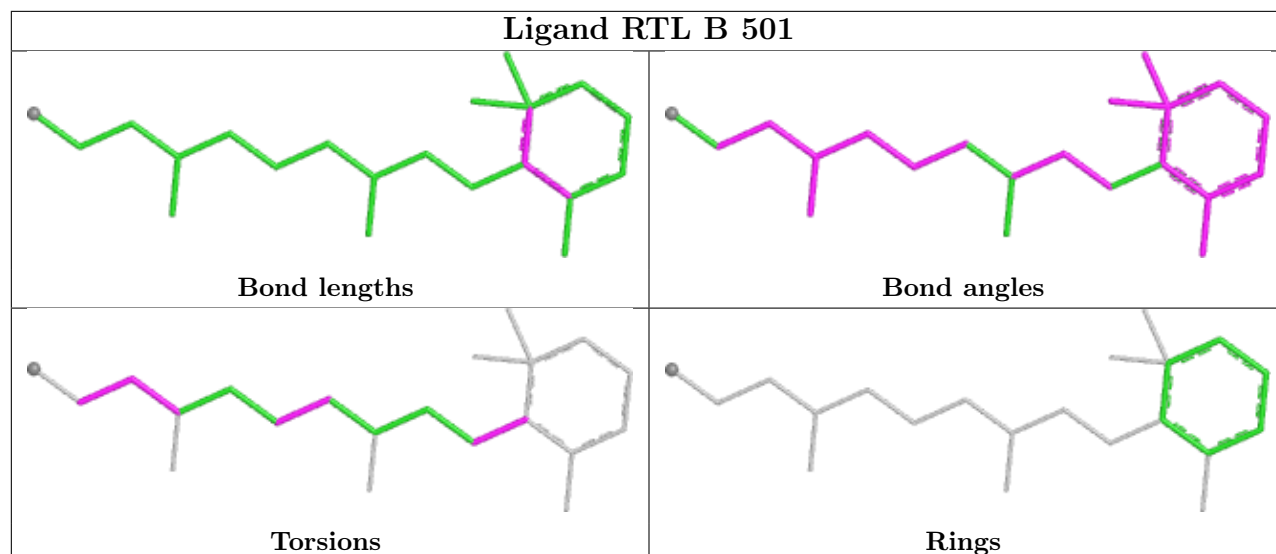
Mol	Chain	Res	Type	Atoms
4	A	401	RTL	C12-C13-C14-C15
4	A	401	RTL	C20-C13-C14-C15
4	B	501	RTL	C12-C13-C14-C15
4	B	501	RTL	C20-C13-C14-C15
4	A	401	RTL	C9-C10-C11-C12
4	B	501	RTL	C9-C10-C11-C12
4	B	501	RTL	C1-C6-C7-C8
4	A	401	RTL	C13-C14-C15-O1
3	A	400	A3P	C3'-C4'-C5'-O5'
3	B	500	A3P	C3'-C4'-C5'-O5'
4	B	501	RTL	C5-C6-C7-C8
4	B	501	RTL	C13-C14-C15-O1
3	B	500	A3P	C2'-C3'-O3'-P1
3	B	500	A3P	C4'-C3'-O3'-P1
3	A	400	A3P	C2'-C3'-O3'-P1
3	A	400	A3P	C4'-C3'-O3'-P1

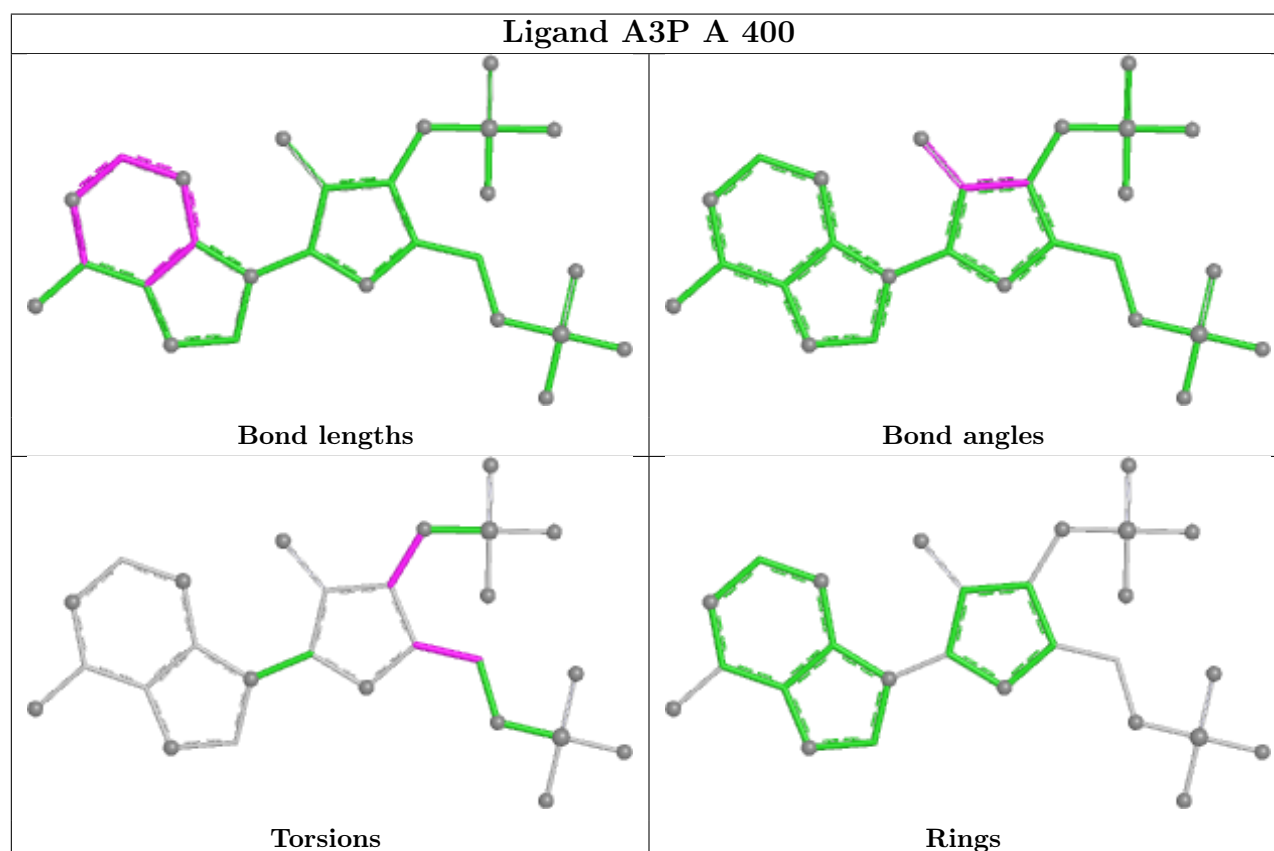
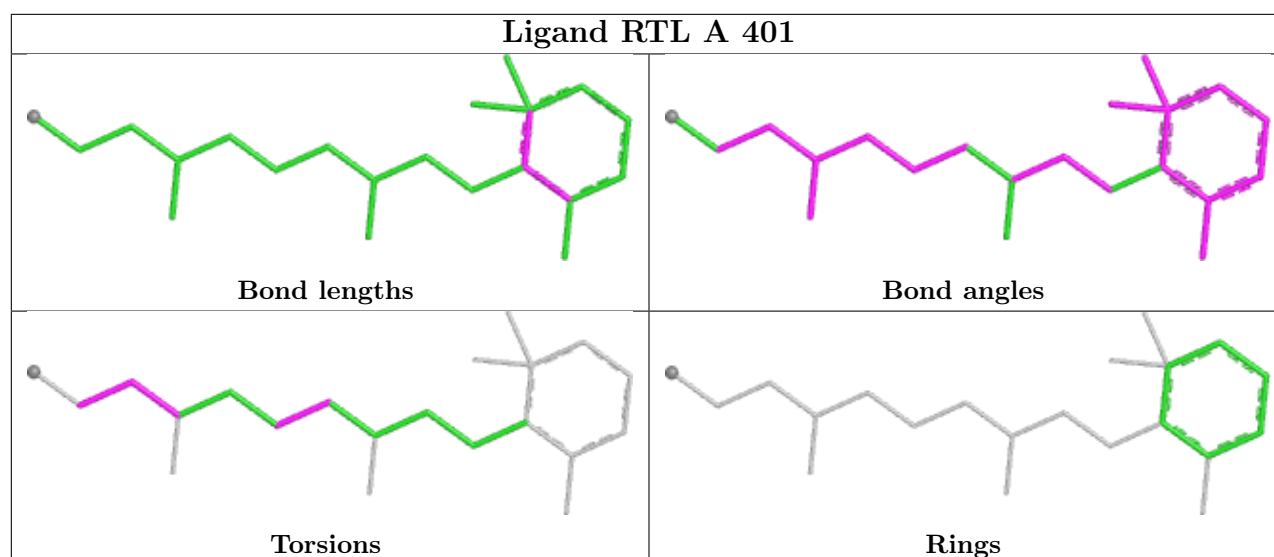
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	A3P	1	0
3	A	400	A3P	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.





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	341/351 (97%)	2.60	176 (51%) 0 0	8, 31, 58, 83	1 (0%)
1	B	341/351 (97%)	2.34	156 (45%) 0 0	11, 31, 55, 71	0
All	All	682/702 (97%)	2.47	332 (48%) 0 0	8, 31, 57, 83	1 (0%)

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	VAL	24.5
1	B	86	ILE	20.8
1	B	183	LEU	19.8
1	A	142	SER	16.0
1	A	86	ILE	12.4
1	A	192	VAL	11.4
1	A	230	HIS	11.4
1	A	189	ASP	10.9
1	B	23	LEU	10.9
1	B	74	SER	10.3
1	A	99	MET	9.7
1	B	147	SER	9.5
1	A	105	TYR	8.9
1	B	35	TYR	8.6
1	A	214	TRP	8.5
1	A	190	VAL	8.3
1	A	57	TYR	7.7
1	B	71	TYR	7.6
1	A	250	ASP	7.6
1	B	182	TYR	7.5
1	A	203	LEU	7.4
1	A	316	ALA	7.3
1	A	177	THR	7.3
1	B	248	TYR	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	193	SER	7.1
1	B	83	VAL	6.8
1	A	185	ARG	6.7
1	A	151	ALA	6.7
1	A	54	ALA	6.7
1	B	230	HIS	6.4
1	B	278	LEU	6.2
1	A	56	ILE	6.0
1	B	88	ASN	6.0
1	A	46	TYR	6.0
1	A	139	LEU	5.9
1	A	147	SER	5.9
1	A	187	PRO	5.7
1	A	248	TYR	5.7
1	A	175	LEU	5.6
1	A	201	LEU	5.6
1	B	76	THR	5.6
1	B	228	PHE	5.5
1	B	28	LEU	5.5
1	A	279	CYS	5.5
1	A	318	CYS	5.5
1	A	112	TYR	5.5
1	A	229	GLU	5.4
1	B	321	ASP	5.4
1	B	347	PRO	5.4
1	A	130	LEU	5.4
1	A	22	LYS	5.3
1	A	194	SER	5.3
1	B	165	LEU	5.3
1	B	217	PHE	5.2
1	A	178	VAL	5.2
1	B	112	TYR	5.1
1	B	346	TYR	5.1
1	A	206	LYS	5.1
1	A	84	TRP	5.1
1	A	150	LEU	5.0
1	A	100	SER	5.0
1	B	47	ARG	5.0
1	B	100	SER	5.0
1	B	107	ASP	5.0
1	B	117	GLN	5.0
1	A	302	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	73	ARG	4.9
1	A	137	GLY	4.9
1	A	166	PRO	4.9
1	A	222	TYR	4.9
1	B	335	ILE	4.8
1	B	119	GLU	4.8
1	A	135	TYR	4.8
1	B	75	GLY	4.8
1	B	163	THR	4.8
1	A	75	GLY	4.7
1	A	346	TYR	4.7
1	A	209	ASN	4.7
1	B	344	LEU	4.7
1	B	250	ASP	4.6
1	B	336	LYS	4.6
1	B	34	THR	4.6
1	B	240	ASP	4.6
1	B	9	PHE	4.5
1	B	97	THR	4.5
1	B	134	ARG	4.5
1	B	68	VAL	4.5
1	A	136	LEU	4.5
1	B	106	LEU	4.4
1	B	81	GLU	4.4
1	B	67	PHE	4.4
1	A	36	VAL	4.4
1	B	85	LEU	4.3
1	B	316	ALA	4.3
1	B	213	PHE	4.3
1	B	223	THR	4.3
1	A	264	ASP	4.3
1	A	336	LYS	4.3
1	B	51	LYS	4.2
1	A	89	ASP	4.2
1	A	345	ARG	4.2
1	A	85	LEU	4.2
1	B	222	TYR	4.2
1	A	82	LEU	4.2
1	A	183	LEU	4.2
1	A	188	ARG	4.2
1	B	10	PRO	4.2
1	A	273	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	ILE	4.1
1	A	71	TYR	4.1
1	B	19	GLU	4.1
1	A	299	ARG	4.1
1	A	220	GLY	4.1
1	A	242	ASN	4.1
1	A	31	PHE	4.0
1	B	24	VAL	4.0
1	B	270	LEU	4.0
1	B	310	PHE	4.0
1	B	247	PHE	4.0
1	A	158	LYS	4.0
1	A	202	TYR	4.0
1	A	67	PHE	4.0
1	A	32	PRO	3.9
1	A	53	ALA	3.9
1	B	268	LYS	3.9
1	A	282	LEU	3.9
1	A	297	ASP	3.9
1	B	46	TYR	3.9
1	A	116	LYS	3.8
1	A	295	MET	3.8
1	B	82	LEU	3.8
1	B	338	ASN	3.7
1	A	162	LYS	3.7
1	B	258	CYS	3.7
1	B	216	MET	3.7
1	A	199	ARG	3.6
1	A	120	TYR	3.6
1	B	142	SER	3.6
1	B	111	ILE	3.6
1	A	298	TYR	3.6
1	A	109	PHE	3.6
1	A	117	GLN	3.6
1	A	74	SER	3.6
1	B	101	LEU	3.6
1	B	69	ALA	3.5
1	B	187	PRO	3.5
1	A	12	GLU	3.5
1	B	196	HIS	3.5
1	A	347	PRO	3.5
1	B	269	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	208	SER	3.5
1	A	225	THR	3.5
1	A	129	ASN	3.5
1	B	53	ALA	3.5
1	B	241	PRO	3.5
1	B	245	PHE	3.5
1	A	24	VAL	3.5
1	A	179	LYS	3.5
1	A	40	PRO	3.4
1	A	284	PHE	3.4
1	A	174	MET	3.4
1	A	65	ASP	3.4
1	A	313	LYS	3.4
1	A	95	ALA	3.4
1	B	66	VAL	3.4
1	A	43	TYR	3.4
1	B	114	PRO	3.4
1	B	201	LEU	3.4
1	A	21	ASP	3.4
1	A	68	VAL	3.3
1	B	139	LEU	3.3
1	A	110	MET	3.3
1	A	58	ASN	3.3
1	A	310	PHE	3.3
1	A	76	THR	3.3
1	A	97	THR	3.3
1	B	120	TYR	3.3
1	A	198	ALA	3.3
1	A	335	ILE	3.3
1	A	19	GLU	3.2
1	A	180	MET	3.2
1	B	300	GLU	3.2
1	B	77	THR	3.2
1	A	247	PHE	3.2
1	B	280	GLU	3.2
1	B	311	ILE	3.2
1	A	170	MET	3.2
1	B	162	LYS	3.2
1	B	13	PHE	3.2
1	A	255	LEU	3.1
1	B	157	GLU	3.1
1	A	37	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	SER	3.1
1	A	165	LEU	3.1
1	B	58	ASN	3.1
1	B	167	LEU	3.1
1	B	257	GLY	3.1
1	B	144	ARG	3.1
1	A	26	ALA	3.0
1	A	322	TYR	3.0
1	A	213	PHE	3.0
1	A	217	PHE	3.0
1	B	195	PHE	3.0
1	B	266	LEU	3.0
1	B	289	ASN	3.0
1	A	277	ARG	3.0
1	A	266	LEU	3.0
1	A	64	THR	3.0
1	A	126	ASN	2.9
1	A	314	GLY	2.9
1	A	154	PRO	2.9
1	A	226	PRO	2.9
1	B	294	ASN	2.9
1	B	337	ASP	2.9
1	A	118	GLU	2.9
1	B	168	SER	2.9
1	B	185	ARG	2.9
1	B	21	ASP	2.9
1	A	223	THR	2.9
1	B	197	HIS	2.9
1	A	87	GLU	2.8
1	B	264	ASP	2.8
1	A	149	LEU	2.8
1	B	218	HIS	2.8
1	A	59	MET	2.8
1	B	169	LEU	2.8
1	A	191	ALA	2.8
1	A	304	LEU	2.8
1	B	136	LEU	2.8
1	A	119	GLU	2.8
1	A	25	LYS	2.7
1	B	108	GLY	2.7
1	A	328	THR	2.7
1	A	103	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	251	TYR	2.7
1	B	246	LEU	2.7
1	B	220	GLY	2.7
1	B	116	LYS	2.7
1	B	123	ILE	2.7
1	A	106	LEU	2.7
1	A	228	PHE	2.7
1	A	141	TYR	2.6
1	B	27	ASN	2.6
1	B	184	ALA	2.6
1	A	13	PHE	2.6
1	B	8	PRO	2.6
1	B	260	ALA	2.6
1	B	22	LYS	2.6
1	B	133	GLU	2.6
1	B	36	VAL	2.6
1	A	306	ASP	2.6
1	B	113	ASP	2.6
1	A	224	LEU	2.6
1	A	49	TYR	2.6
1	A	121	ASN	2.6
1	A	173	ASN	2.6
1	A	184	ALA	2.6
1	B	150	LEU	2.5
1	A	325	GLU	2.5
1	B	32	PRO	2.5
1	B	155	PRO	2.5
1	A	156	THR	2.5
1	A	38	LEU	2.5
1	B	227	TYR	2.5
1	B	249	GLU	2.5
1	B	121	ASN	2.5
1	A	221	LEU	2.5
1	A	278	LEU	2.5
1	B	102	ARG	2.5
1	B	109	PHE	2.5
1	B	126	ASN	2.5
1	B	219	ARG	2.5
1	B	255	LEU	2.5
1	B	302	GLY	2.5
1	B	288	LYS	2.4
1	A	27	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	91	ASN	2.4
1	A	169	LEU	2.4
1	B	7	LEU	2.4
1	B	143	SER	2.4
1	B	186	ASP	2.4
1	B	99	MET	2.4
1	A	195	PHE	2.4
1	B	166	PRO	2.4
1	B	265	PHE	2.4
1	A	244	LEU	2.4
1	A	113	ASP	2.4
1	A	186	ASP	2.4
1	A	9	PHE	2.4
1	A	262	ILE	2.4
1	B	235	TRP	2.4
1	B	37	LYS	2.4
1	A	155	PRO	2.4
1	A	160	PHE	2.4
1	B	209	ASN	2.3
1	B	243	MET	2.3
1	B	79	THR	2.3
1	A	205	ASN	2.3
1	B	84	TRP	2.3
1	B	214	TRP	2.3
1	B	312	ARG	2.3
1	B	16	LEU	2.3
1	B	156	THR	2.3
1	A	144	ARG	2.3
1	A	124	LEU	2.3
1	A	246	LEU	2.3
1	A	181	VAL	2.3
1	A	111	ILE	2.2
1	B	198	ALA	2.2
1	A	227	TYR	2.2
1	B	256	PRO	2.2
1	A	16	LEU	2.2
1	A	90	LEU	2.2
1	B	98	TYR	2.2
1	A	321	ASP	2.2
1	A	239[A]	HIS	2.2
1	B	135	TYR	2.1
1	B	44	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	265	PHE	2.1
1	A	62	ARG	2.1
1	A	193	SER	2.1
1	A	208	SER	2.1
1	A	47	ARG	2.1
1	A	312	ARG	2.1
1	B	33	THR	2.1
1	A	216	MET	2.1
1	A	294	ASN	2.1
1	A	157	GLU	2.0
1	B	271	SER	2.0
1	B	90	LEU	2.0
1	B	274	GLN	2.0
1	B	103	TYR	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.

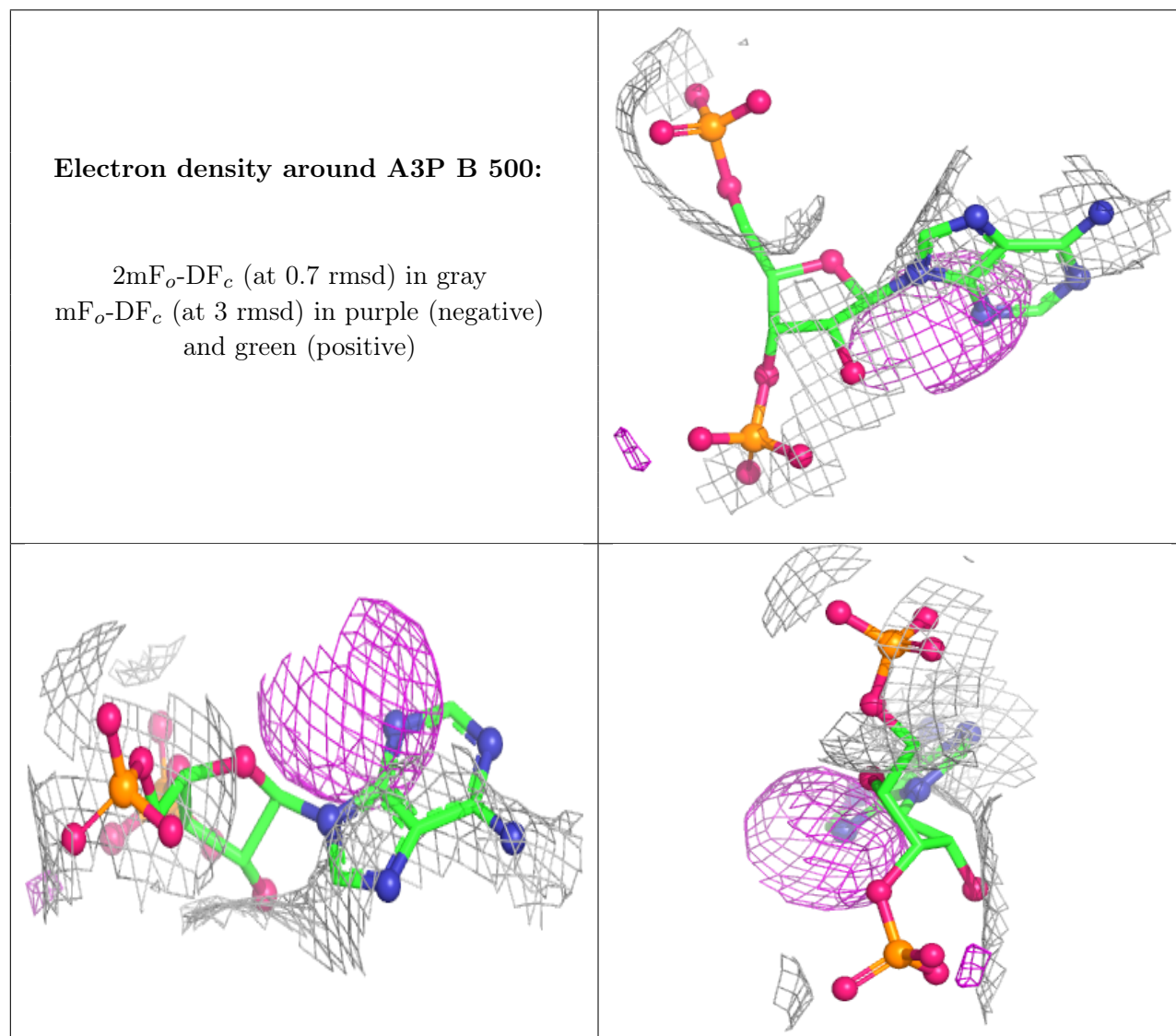
6.4 Ligands [i](#)

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
3	A3P	B	500	27/27	0.26	0.30	25,25,25,25	0
2	CA	A	450	1/1	0.48	0.08	83,83,83,83	0
3	A3P	A	400	27/27	0.57	0.13	6,6,6,6	0
2	CA	B	550	1/1	0.61	0.21	85,85,85,85	0
4	RTL	A	401	21/21	0.72	0.24	53,53,53,53	0
4	RTL	B	501	21/21	0.84	0.18	65,65,65,65	0

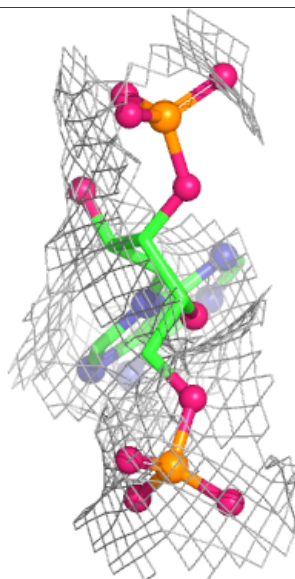
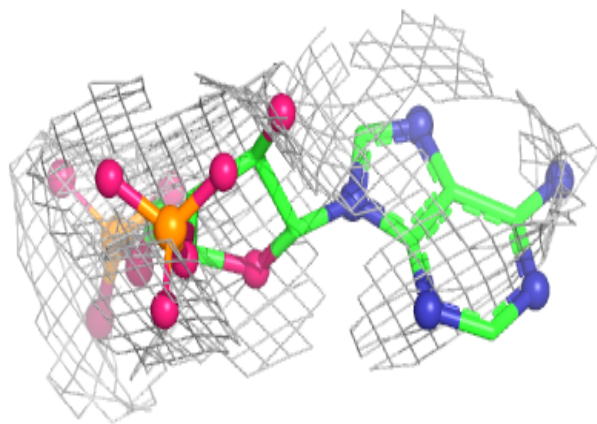
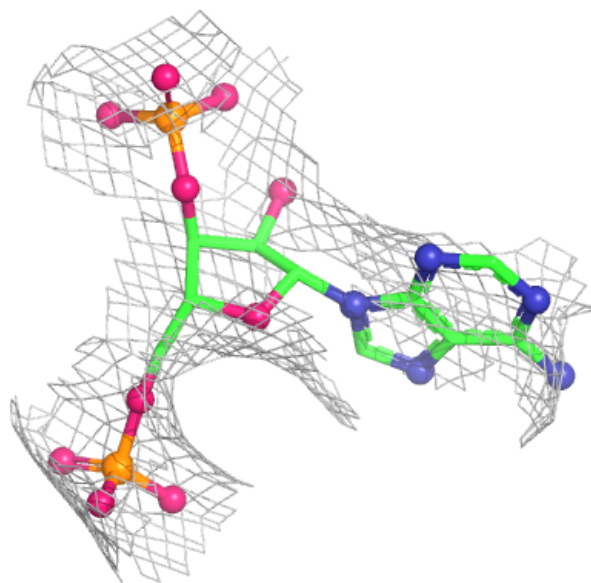
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



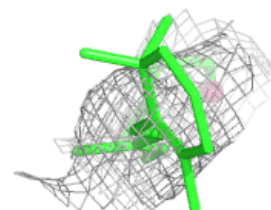
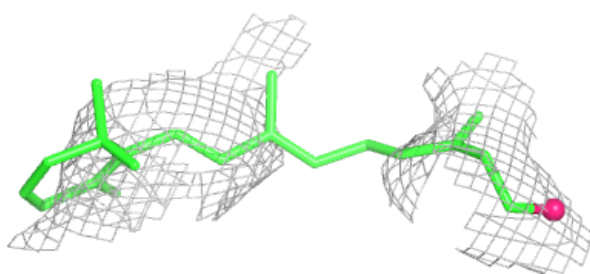
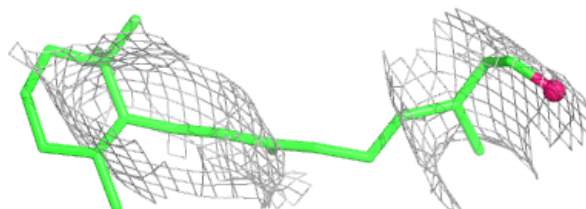
Electron density around A3P A 400:

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

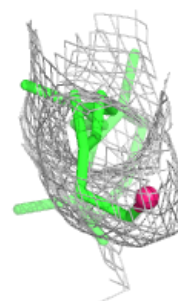
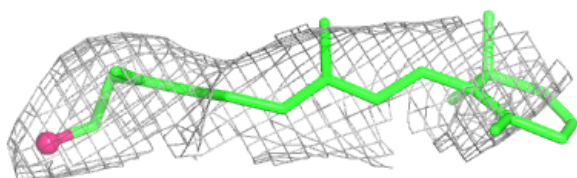
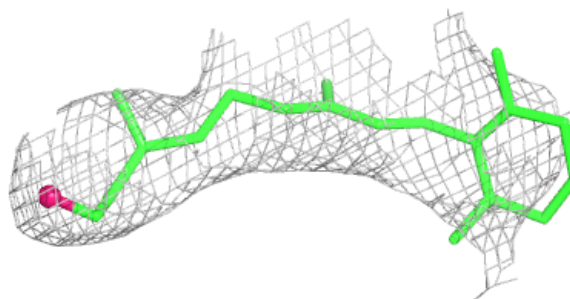


Electron density around RTL A 401:

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

**Electron density around RTL B 501:**

$2mF_o-DF_c$ (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.