Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2024 – 04:58 PM EDT

PDB ID	:	9BR7
Title	:	Crystal structure of human succinyl-CoA:glutarate-CoA transferase (SUGCT) in complex with Losartan carboxylic acid
Authors	:	Wu, R.; Lazarus, M.B.
Deposited on	:	2024-05-10
Resolution	:	2.08 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:

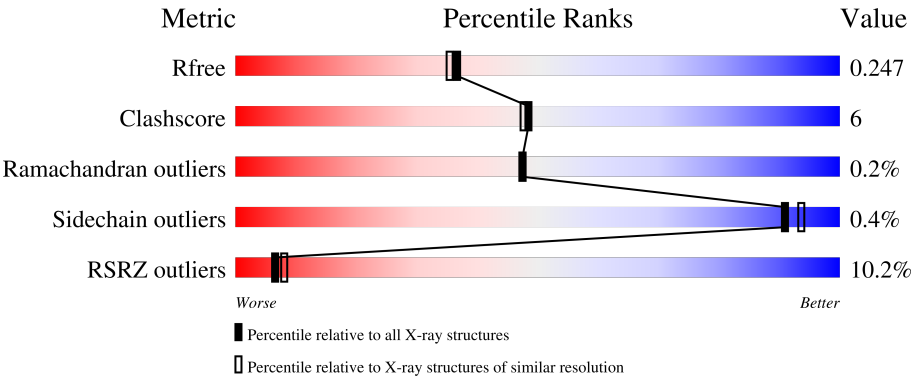
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.08 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}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	412	11% 84% 13% ·
1	B	412	7% 86% 12% ·
1	C	412	11% 81% 17% ·
1	D	412	11% 82% 15% ·

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12763 atoms, of which 69 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 Succinate--hydroxymethylglutarate CoA-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3079	1965	526	574	14			
1	B	405	Total	C	N	O	S	0	0	0
			3102	1978	530	579	15			
1	C	403	Total	C	N	O	S	0	0	0
			3086	1969	528	575	14			
1	D	402	Total	C	N	O	S	0	0	0
			3079	1965	526	574	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q9HAC7
A	28	PRO	-	expression tag	UNP Q9HAC7
A	29	GLY	-	expression tag	UNP Q9HAC7
A	30	SER	-	expression tag	UNP Q9HAC7
A	255	ALA	GLN	conflict	UNP Q9HAC7
A	256	ALA	LYS	conflict	UNP Q9HAC7
B	27	GLY	-	expression tag	UNP Q9HAC7
B	28	PRO	-	expression tag	UNP Q9HAC7
B	29	GLY	-	expression tag	UNP Q9HAC7
B	30	SER	-	expression tag	UNP Q9HAC7
B	255	ALA	GLN	conflict	UNP Q9HAC7
B	256	ALA	LYS	conflict	UNP Q9HAC7
C	27	GLY	-	expression tag	UNP Q9HAC7
C	28	PRO	-	expression tag	UNP Q9HAC7
C	29	GLY	-	expression tag	UNP Q9HAC7
C	30	SER	-	expression tag	UNP Q9HAC7
C	255	ALA	GLN	conflict	UNP Q9HAC7
C	256	ALA	LYS	conflict	UNP Q9HAC7
D	27	GLY	-	expression tag	UNP Q9HAC7
D	28	PRO	-	expression tag	UNP Q9HAC7
D	29	GLY	-	expression tag	UNP Q9HAC7

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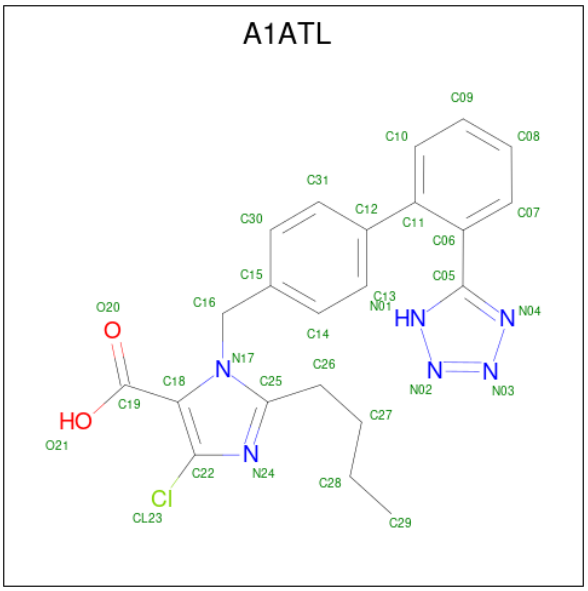
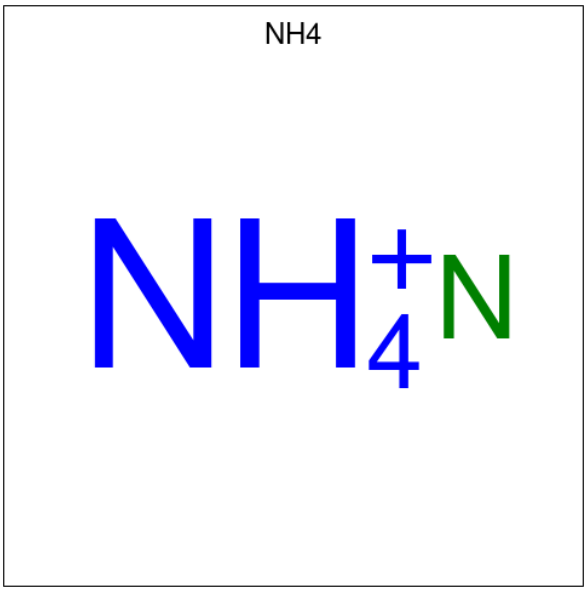
Chain	Residue	Modelled	Actual	Comment	Reference
D	30	SER	-	expression tag	UNP Q9HAC7
D	255	ALA	GLN	conflict	UNP Q9HAC7
D	256	ALA	LYS	conflict	UNP Q9HAC7

- Molecule 2 is losartan carboxylic acid (three-letter code: A1ATL) (formula: $C_{22}H_{21}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



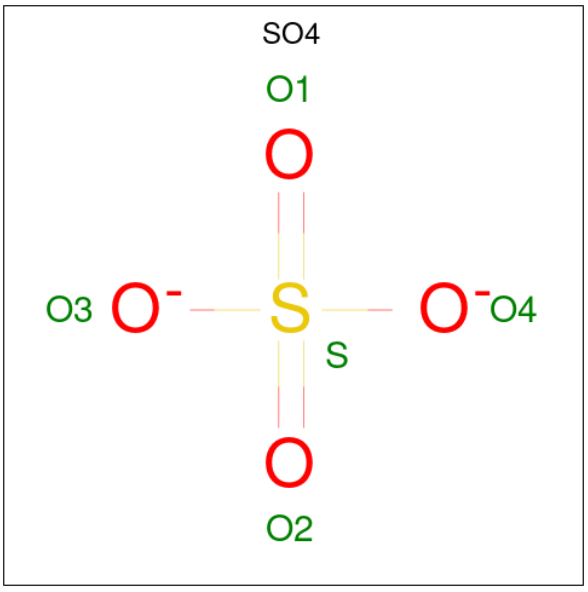
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			51	22	1	20	6	2		
2	C	1	Total	C	Cl	H	N	O	0	0
			51	22	1	20	6	2		
2	D	1	Total	C	Cl	H	N	O	0	0
			47	21	1	17	6	2		

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total H N 5 4 1	0	0
3	C	1	Total H N 5 4 1	0	0
3	D	1	Total H N 5 4 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

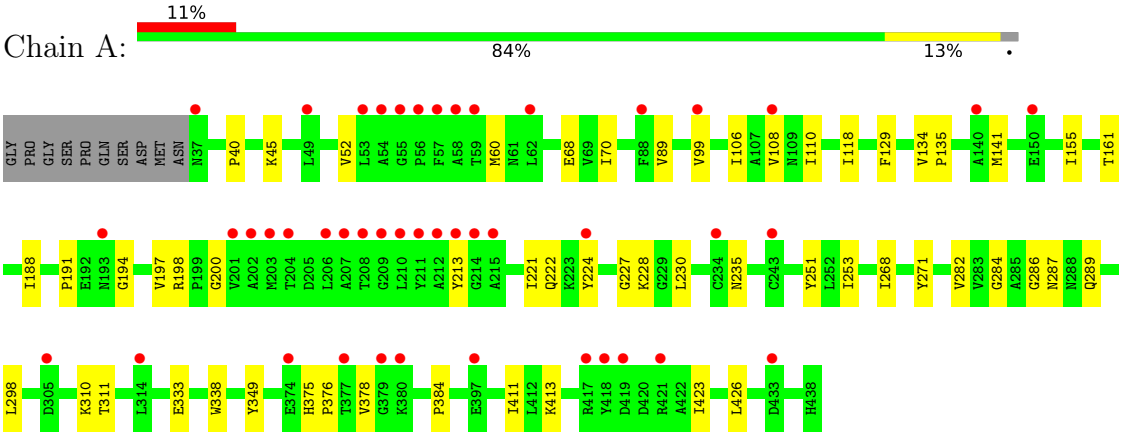
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0
5	B	62	Total O 62 62	0	0
5	C	39	Total O 39 39	0	0
5	D	48	Total O 48 48	0	0

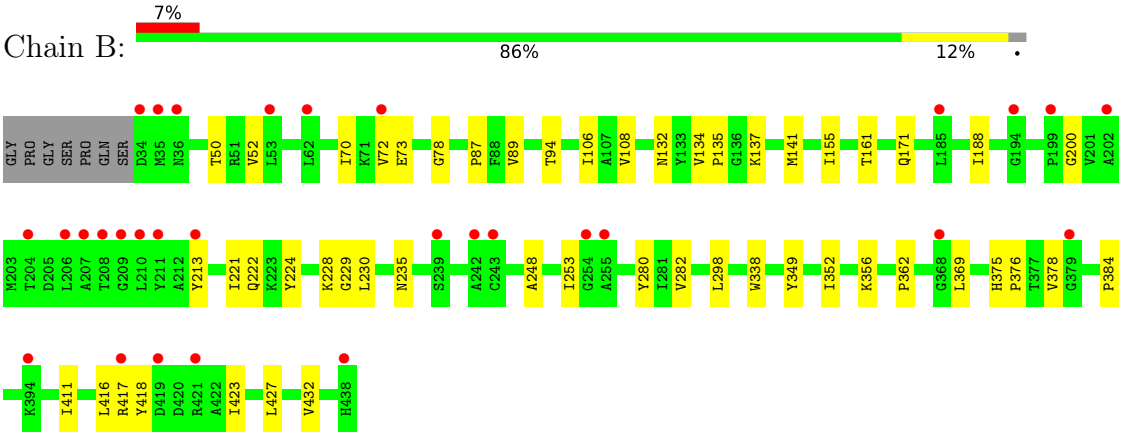
3 Residue-property plots (i)

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.

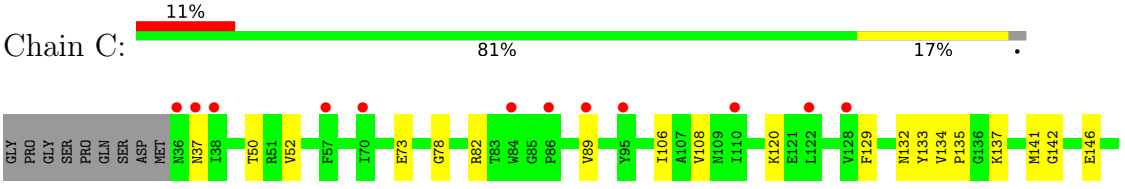
• Molecule 1: Succinate--hydroxymethylglutarate CoA-transferase

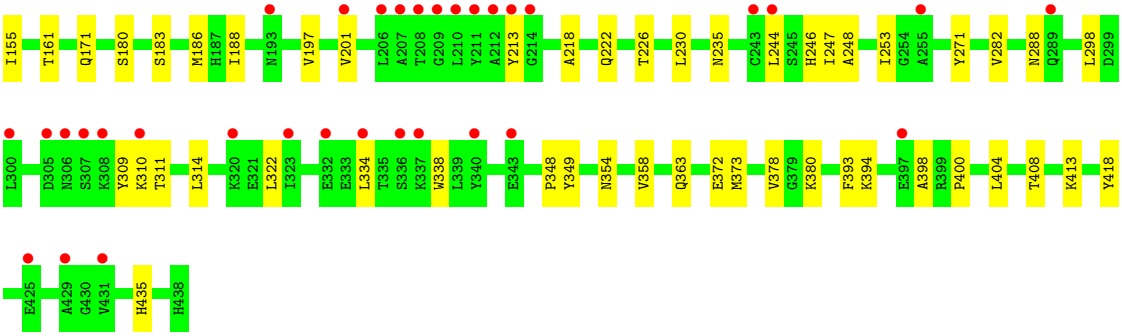


• Molecule 1: Succinate--hydroxymethylglutarate CoA-transferase

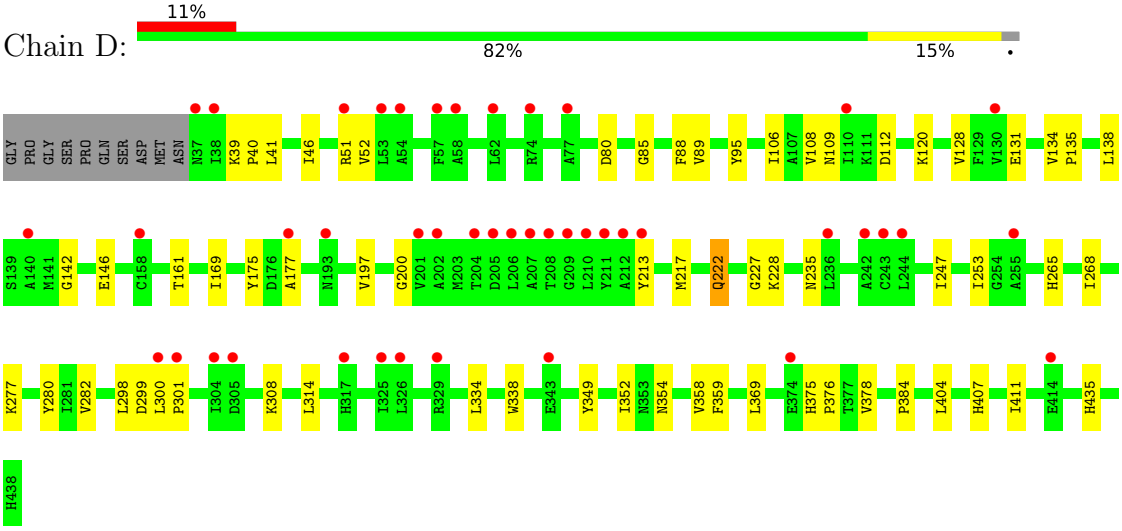


• Molecule 1: Succinate--hydroxymethylglutarate CoA-transferase





• Molecule 1: Succinate--hydroxymethylglutarate CoA-transferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.93Å 119.81Å 136.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.06 – 2.08 34.06 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.06-2.08) 99.8 (34.06-2.08)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.220 , 0.247 0.220 , 0.247	Depositor DCC
R_{free} test set	5365 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12763	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% 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: NH4, SO4, A1ATL

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	0.24	0/3147	0.46	0/4269
1	B	0.24	0/3170	0.45	0/4301
1	C	0.25	0/3154	0.45	0/4280
1	D	0.24	0/3147	0.45	0/4269
All	All	0.24	0/12618	0.45	0/17119

There are no bond length outliers.

There are no bond angle outliers.

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	3079	0	3104	39	0
1	B	3102	0	3123	35	0
1	C	3086	0	3110	53	0
1	D	3079	0	3104	46	0
2	A	31	20	0	0	0
2	C	31	20	0	0	0
2	D	30	17	0	1	0
3	A	1	4	0	0	0
3	C	1	4	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	4	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	69	0	0	0	0
5	B	62	0	0	3	0
5	C	39	0	0	2	0
5	D	48	0	0	0	0
All	All	12694	69	12441	150	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 6.

All (150) 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:268:ILE:HD11	1:A:286:GLY:HA2	1.21	1.20
1:C:197:VAL:HG21	1:D:197:VAL:HG21	1.56	0.88
1:A:268:ILE:HD11	1:A:286:GLY:CA	2.09	0.81
1:C:311:THR:OG1	1:C:314:LEU:HD23	1.86	0.75
1:C:253:ILE:HG21	1:D:89:VAL:HG21	1.69	0.75
1:B:137:LYS:HE2	1:B:141:MET:HE1	1.66	0.74
1:A:89:VAL:HG12	1:A:378:VAL:HG13	1.71	0.71
1:A:110:ILE:HG13	1:A:141:MET:HE1	1.72	0.71
1:A:221:ILE:HA	1:A:224:TYR:HD2	1.54	0.71
1:C:218:ALA:HA	1:D:217:MET:HE2	1.73	0.71
1:C:89:VAL:HG21	1:D:253:ILE:HG21	1.73	0.70
1:A:40:PRO:HB3	1:B:222:GLN:HB2	1.73	0.69
1:B:228:LYS:NZ	1:C:146:GLU:OE2	2.26	0.69
1:A:287:ASN:OD1	1:A:289:GLN:HG2	1.94	0.68
1:B:89:VAL:HG12	1:B:378:VAL:HG13	1.75	0.68
1:C:137:LYS:HE2	1:C:141:MET:HE1	1.77	0.67
1:C:373:MET:HE1	1:C:400:PRO:HA	1.79	0.65
1:D:41:LEU:HD21	1:D:217:MET:HE3	1.79	0.64
1:C:372:GLU:OE2	1:C:380:LYS:HD3	1.97	0.63
1:D:280:TYR:HB2	1:D:352:ILE:HD12	1.80	0.62
1:C:89:VAL:CG2	1:D:253:ILE:HG21	2.29	0.62
1:A:106:ILE:HG12	1:A:108:VAL:HG23	1.83	0.61
1:A:89:VAL:HG12	1:A:378:VAL:CG1	2.31	0.60
1:D:134:VAL:HG13	1:D:135:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:CG1	1:D:247:ILE:HD12	2.34	0.58
1:D:280:TYR:CB	1:D:352:ILE:HD12	2.33	0.58
1:A:191:PRO:HG2	1:A:194:GLY:HA3	1.86	0.58
1:A:282:VAL:O	1:A:349:TYR:HA	2.05	0.57
1:A:134:VAL:HG13	1:A:135:PRO:HD2	1.86	0.57
1:C:134:VAL:HG13	1:C:135:PRO:HD2	1.86	0.57
1:C:89:VAL:HG12	1:C:378:VAL:HG13	1.87	0.57
1:C:373:MET:CE	1:C:400:PRO:HA	2.35	0.57
1:C:253:ILE:HG21	1:D:89:VAL:CG2	2.35	0.56
1:D:89:VAL:HG12	1:D:378:VAL:HG13	1.87	0.56
1:D:375:HIS:CG	1:D:376:PRO:HD2	2.42	0.55
1:A:188:ILE:HG13	1:B:200:GLY:HA3	1.88	0.55
1:D:298:LEU:HD23	1:D:338:TRP:CZ3	2.42	0.55
1:B:282:VAL:O	1:B:349:TYR:HA	2.07	0.55
1:B:134:VAL:HG13	1:B:135:PRO:HD2	1.88	0.54
1:B:106:ILE:HB	1:B:411:ILE:HD12	1.90	0.54
1:C:197:VAL:CG2	1:D:197:VAL:HG21	2.35	0.54
1:A:200:GLY:HA3	1:B:188:ILE:HG13	1.90	0.54
1:A:221:ILE:HA	1:A:224:TYR:CD2	2.40	0.54
1:A:253:ILE:HG21	1:B:89:VAL:HG21	1.89	0.53
1:B:137:LYS:HE2	1:B:141:MET:CE	2.38	0.53
1:C:89:VAL:HG12	1:C:378:VAL:CG1	2.39	0.52
1:D:265:HIS:HB2	1:D:268:ILE:HG22	1.91	0.52
1:D:282:VAL:O	1:D:349:TYR:HA	2.09	0.52
1:A:375:HIS:CG	1:A:376:PRO:HD2	2.45	0.52
1:C:298:LEU:HD23	1:C:338:TRP:CZ3	2.46	0.51
1:D:146:GLU:H	1:D:146:GLU:CD	2.15	0.51
1:C:73:GLU:HB3	1:C:78:GLY:HA2	1.92	0.50
1:D:277:LYS:HB3	1:D:334:LEU:HD23	1.93	0.50
1:D:369:LEU:O	1:D:384:PRO:HA	2.11	0.50
1:C:171:GLN:HB2	5:C:633:HOH:O	2.11	0.50
1:A:298:LEU:HD23	1:A:338:TRP:CZ3	2.46	0.50
1:C:310:LYS:HG3	1:C:311:THR:HG23	1.94	0.50
1:D:46:ILE:HG12	1:D:128:VAL:HB	1.94	0.49
1:B:70:ILE:HG23	1:B:411:ILE:HD13	1.95	0.49
1:C:201:VAL:HG12	1:D:247:ILE:HD12	1.94	0.49
1:C:37:ASN:HD21	1:C:394:LYS:H	1.61	0.49
1:D:109:ASN:ND2	1:D:112:ASP:HB2	2.28	0.49
1:D:85:GLY:HA3	1:D:88:PHE:CE2	2.49	0.48
1:A:268:ILE:CD1	1:A:286:GLY:HA2	2.15	0.48
1:C:246:HIS:CE1	1:C:247:ILE:HG13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:O	1:B:235:ASN:HA	2.14	0.47
1:D:300:LEU:N	1:D:301:PRO:HD3	2.29	0.47
1:B:280:TYR:HB2	1:B:352:ILE:HD12	1.96	0.47
1:D:354:ASN:O	1:D:358:VAL:HG23	2.14	0.47
1:A:161:THR:O	1:A:235:ASN:HA	2.14	0.47
1:D:106:ILE:HG12	1:D:108:VAL:HG23	1.96	0.47
1:B:375:HIS:CG	1:B:376:PRO:HD2	2.49	0.47
1:D:222:GLN:HE21	1:D:222:GLN:HB3	1.55	0.47
1:A:106:ILE:HB	1:A:411:ILE:HD12	1.97	0.47
1:A:227:GLY:C	1:A:228:LYS:HD2	2.36	0.47
1:C:222:GLN:HE21	1:C:226:THR:HG21	1.81	0.46
1:C:188:ILE:HG13	1:D:200:GLY:HA3	1.97	0.46
1:C:288:ASN:OD1	1:C:311:THR:HA	2.15	0.46
1:D:51:ARG:NH2	1:D:80:ASP:OD1	2.49	0.46
1:B:87:PRO:HG2	1:B:94:THR:OG1	2.16	0.46
1:B:87:PRO:HD2	5:B:640:HOH:O	2.15	0.45
1:C:50:THR:HA	1:C:132:ASN:OD1	2.17	0.45
1:C:282:VAL:O	1:C:349:TYR:HA	2.16	0.45
1:D:299:ASP:C	1:D:301:PRO:HD3	2.37	0.45
1:C:222:GLN:NE2	1:C:226:THR:OG1	2.50	0.45
1:A:384:PRO:HG3	1:B:248:ALA:HB3	1.98	0.44
1:C:348:PRO:HG3	1:D:175:TYR:CZ	2.53	0.44
1:B:50:THR:HA	1:B:132:ASN:OD1	2.18	0.44
1:B:427:LEU:HD23	1:B:432:VAL:HG23	1.98	0.44
1:A:129:PHE:HB2	1:A:155:ILE:HD11	1.98	0.44
1:A:271:TYR:CD1	1:A:284:GLY:HA3	2.52	0.44
1:B:418:TYR:HB3	1:B:423:ILE:HG13	1.99	0.44
1:C:37:ASN:OD1	1:C:393:PHE:HB2	2.18	0.44
1:C:413:LYS:HG2	1:C:418:TYR:O	2.18	0.44
1:D:161:THR:O	1:D:235:ASN:HA	2.18	0.44
1:B:416:LEU:O	1:B:417:ARG:HB2	2.18	0.44
1:D:308:LYS:O	1:D:314:LEU:HB3	2.18	0.44
1:B:72:VAL:HG13	1:B:108:VAL:CG1	2.48	0.43
1:C:82:ARG:HD3	5:C:610:HOH:O	2.18	0.43
1:C:106:ILE:HG13	1:C:408:THR:HA	2.01	0.43
1:B:73:GLU:HB3	1:B:78:GLY:HA2	2.01	0.43
1:A:310:LYS:HG3	1:A:311:THR:HG23	2.01	0.43
1:D:51:ARG:HH21	1:D:80:ASP:CG	2.22	0.43
1:B:72:VAL:HG13	1:B:108:VAL:HG12	2.00	0.43
1:B:362:PRO:HG2	5:B:601:HOH:O	2.17	0.43
1:C:146:GLU:H	1:C:146:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:MET:HE3	1:C:398:ALA:HB3	2.00	0.43
1:A:70:ILE:HG23	1:A:411:ILE:HD13	2.01	0.43
1:A:230:LEU:HD12	1:A:230:LEU:C	2.39	0.43
1:C:183:SER:O	1:C:244:LEU:HD11	2.19	0.43
1:A:45:LYS:NZ	1:A:68:GLU:OE1	2.52	0.43
1:A:118:ILE:HD11	1:A:426:LEU:HD13	2.00	0.42
1:B:280:TYR:CB	1:B:352:ILE:HD12	2.48	0.42
1:C:309:TYR:CE1	1:C:322:LEU:HB2	2.53	0.42
1:C:180:SER:OG	1:C:186:MET:HG3	2.19	0.42
1:A:106:ILE:HG12	1:A:108:VAL:CG2	2.48	0.42
1:C:218:ALA:CA	1:D:217:MET:HE2	2.47	0.42
1:A:333:GLU:HB2	1:A:338:TRP:NE1	2.34	0.42
1:B:155:ILE:O	1:B:229:GLY:HA3	2.19	0.42
1:C:404:LEU:O	1:C:435:HIS:HB2	2.20	0.42
1:D:227:GLY:C	1:D:228:LYS:HD2	2.40	0.42
1:B:369:LEU:O	1:B:384:PRO:HA	2.19	0.42
1:C:161:THR:O	1:C:235:ASN:HA	2.20	0.42
1:B:221:ILE:O	1:B:224:TYR:HB2	2.19	0.42
1:C:120:LYS:HE2	1:C:142:GLY:O	2.19	0.42
1:C:248:ALA:HB1	1:D:359:PHE:CZ	2.55	0.42
1:D:407:HIS:O	1:D:411:ILE:HG12	2.20	0.41
1:A:413:LYS:HG3	1:A:423:ILE:CD1	2.50	0.41
1:C:106:ILE:HG12	1:C:108:VAL:HG23	2.02	0.41
1:D:39:LYS:HB3	1:D:40:PRO:HD2	2.03	0.41
1:A:197:VAL:HG12	1:A:198:ARG:N	2.35	0.41
1:C:334:LEU:HD12	1:C:334:LEU:N	2.35	0.41
1:A:222:GLN:OE1	1:A:230:LEU:HD23	2.20	0.41
1:C:230:LEU:HD12	1:C:230:LEU:C	2.41	0.41
1:C:271:TYR:OH	1:D:177:ALA:HB3	2.20	0.41
1:A:60:MET:SD	1:A:99:VAL:HA	2.61	0.41
1:D:95:TYR:HD1	2:D:501:A1ATL:C09	2.33	0.41
1:B:230:LEU:C	1:B:230:LEU:HD12	2.41	0.41
1:C:354:ASN:O	1:C:358:VAL:HG23	2.21	0.41
1:B:171:GLN:HB2	5:B:612:HOH:O	2.21	0.41
1:C:129:PHE:HB2	1:C:155:ILE:HD11	2.03	0.40
1:B:298:LEU:HD23	1:B:338:TRP:CH2	2.56	0.40
1:A:89:VAL:HG21	1:B:253:ILE:HG21	2.03	0.40
1:A:251:TYR:CE1	1:B:356:LYS:HG2	2.56	0.40
1:C:133:TYR:CD1	1:C:137:LYS:HD3	2.56	0.40
1:A:228:LYS:HD2	1:A:228:LYS:N	2.37	0.40
1:C:363:GLN:HB2	1:D:169:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:GLU:HG2	1:D:138:LEU:HD12	2.03	0.40
1:D:120:LYS:HE2	1:D:142:GLY:O	2.22	0.40
1:D:404:LEU:O	1:D:435:HIS:HB2	2.22	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	400/412 (97%)	394 (98%)	5 (1%)	1 (0%)	41	39
1	B	403/412 (98%)	397 (98%)	5 (1%)	1 (0%)	47	47
1	C	401/412 (97%)	395 (98%)	5 (1%)	1 (0%)	47	47
1	D	400/412 (97%)	392 (98%)	7 (2%)	1 (0%)	41	39
All	All	1604/1648 (97%)	1578 (98%)	22 (1%)	4 (0%)	47	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	B	52	VAL
1	C	52	VAL
1	D	52	VAL

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	329/337 (98%)	328 (100%)	1 (0%)	92	95
1	B	332/337 (98%)	331 (100%)	1 (0%)	92	95
1	C	330/337 (98%)	329 (100%)	1 (0%)	92	95
1	D	329/337 (98%)	327 (99%)	2 (1%)	86	89
All	All	1320/1348 (98%)	1315 (100%)	5 (0%)	91	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	TYR
1	B	213	TYR
1	C	213	TYR
1	D	213	TYR
1	D	222	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	222	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 3 are modelled with single atom - leaving 10 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	$\#\|Z\| > 2$
2	A1ATL	D	501	-	29,33,34	1.68	5 (17%)	32,46,47	2.03	10 (31%)
4	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.08	0
4	SO4	D	504	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.05	0
2	A1ATL	C	501	-	30,34,34	1.65	5 (16%)	34,47,47	1.98	9 (26%)
4	SO4	A	503	-	4,4,4	0.13	0	6,6,6	0.07	0
2	A1ATL	A	501	-	30,34,34	1.60	4 (13%)	34,47,47	2.01	10 (29%)

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	A1ATL	C	501	-	-	5/20/20/20	0/4/4/4
2	A1ATL	D	501	-	-	6/19/19/20	0/4/4/4
2	A1ATL	A	501	-	-	7/20/20/20	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	A1ATL	C05-N01	6.51	1.41	1.33
2	C	501	A1ATL	C05-N01	6.51	1.41	1.33
2	A	501	A1ATL	C05-N01	6.37	1.41	1.33
2	C	501	A1ATL	C05-N04	3.10	1.37	1.33
2	A	501	A1ATL	C05-N04	3.05	1.37	1.33
2	D	501	A1ATL	C22-CL23	-3.05	1.68	1.74
2	C	501	A1ATL	C22-CL23	-3.03	1.68	1.74
2	A	501	A1ATL	C22-CL23	-3.02	1.68	1.74
2	D	501	A1ATL	C05-N04	3.02	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	A1ATL	N01-N02	2.19	1.38	1.34
2	D	501	A1ATL	C18-C19	2.18	1.53	1.48
2	D	501	A1ATL	N01-N02	2.12	1.38	1.34
2	C	501	A1ATL	C18-C19	2.05	1.53	1.48
2	A	501	A1ATL	N01-N02	2.00	1.37	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	A1ATL	N04-C05-N01	-4.86	105.96	111.39
2	D	501	A1ATL	N04-C05-N01	-4.81	106.02	111.39
2	C	501	A1ATL	N04-C05-N01	-4.81	106.02	111.39
2	D	501	A1ATL	O20-C19-C18	-4.20	115.51	121.30
2	A	501	A1ATL	N04-N03-N02	4.04	112.17	109.53
2	C	501	A1ATL	N04-N03-N02	4.02	112.17	109.53
2	C	501	A1ATL	O20-C19-C18	-3.99	115.81	121.30
2	A	501	A1ATL	O20-C19-C18	-3.97	115.83	121.30
2	A	501	A1ATL	N01-N02-N03	-3.96	106.94	109.53
2	C	501	A1ATL	N01-N02-N03	-3.96	106.95	109.53
2	D	501	A1ATL	N04-N03-N02	3.87	112.06	109.53
2	D	501	A1ATL	N01-N02-N03	-3.82	107.04	109.53
2	A	501	A1ATL	C05-N01-N02	3.46	107.95	104.87
2	C	501	A1ATL	C05-N01-N02	3.46	107.95	104.87
2	D	501	A1ATL	C05-N01-N02	3.45	107.94	104.87
2	A	501	A1ATL	C07-C06-C11	3.00	121.65	118.67
2	A	501	A1ATL	C06-C05-N04	2.89	129.03	124.11
2	C	501	A1ATL	C07-C06-C11	2.89	121.54	118.67
2	A	501	A1ATL	C10-C11-C06	-2.79	115.90	118.67
2	D	501	A1ATL	C10-C11-C06	-2.75	115.94	118.67
2	C	501	A1ATL	C06-C05-N04	2.72	128.74	124.11
2	D	501	A1ATL	C06-C05-N04	2.69	128.69	124.11
2	D	501	A1ATL	C07-C06-C11	2.69	121.35	118.67
2	C	501	A1ATL	C10-C11-C06	-2.67	116.02	118.67
2	D	501	A1ATL	C06-C11-C12	2.40	126.66	122.82
2	A	501	A1ATL	C05-N04-N03	2.36	106.97	104.87
2	D	501	A1ATL	C05-N04-N03	2.33	106.94	104.87
2	C	501	A1ATL	C05-N04-N03	2.30	106.91	104.87
2	A	501	A1ATL	C27-C26-C25	2.04	116.69	112.16

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1ATL	C25-C26-C27-C28
2	A	501	A1ATL	C22-C18-C19-O20
2	A	501	A1ATL	C22-C18-C19-O21
2	A	501	A1ATL	N17-C18-C19-O20
2	A	501	A1ATL	N17-C18-C19-O21
2	C	501	A1ATL	C25-C26-C27-C28
2	C	501	A1ATL	C22-C18-C19-O20
2	C	501	A1ATL	C22-C18-C19-O21
2	C	501	A1ATL	N17-C18-C19-O20
2	C	501	A1ATL	N17-C18-C19-O21
2	D	501	A1ATL	C22-C18-C19-O20
2	D	501	A1ATL	C22-C18-C19-O21
2	D	501	A1ATL	N17-C18-C19-O20
2	D	501	A1ATL	N17-C18-C19-O21
2	A	501	A1ATL	N04-C05-C06-C11
2	D	501	A1ATL	C25-C26-C27-C28
2	A	501	A1ATL	C26-C27-C28-C29
2	D	501	A1ATL	N17-C25-C26-C27

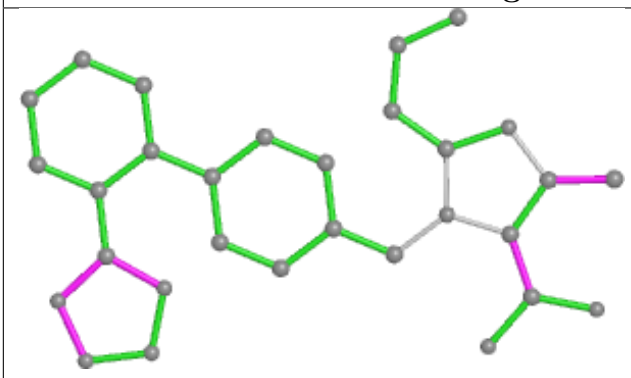
There are no ring outliers.

1 monomer is involved in 1 short contact:

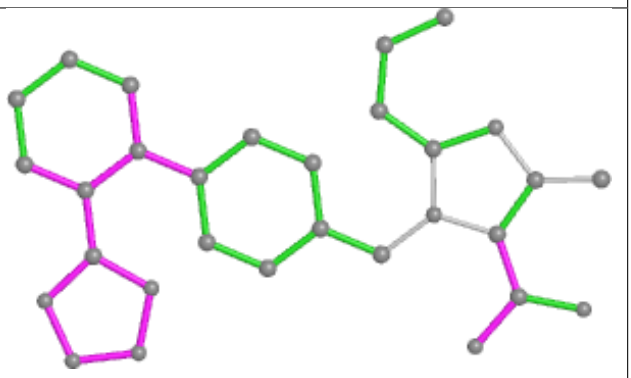
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	A1ATL	1	0

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 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.

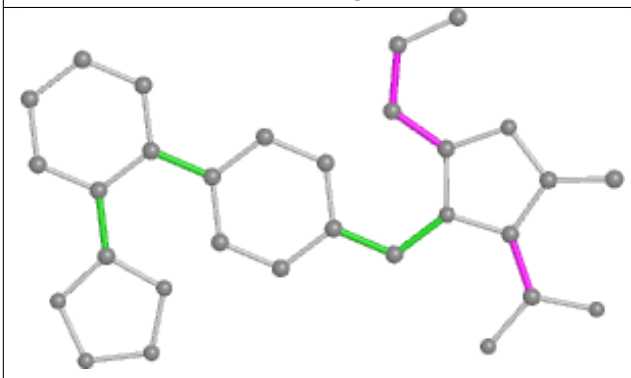
Ligand A1ATL D 501



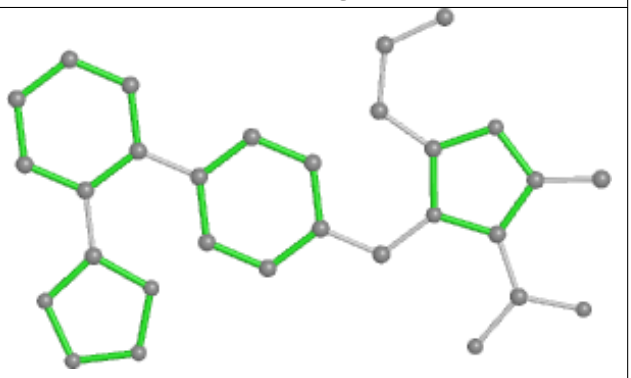
Bond lengths



Bond angles

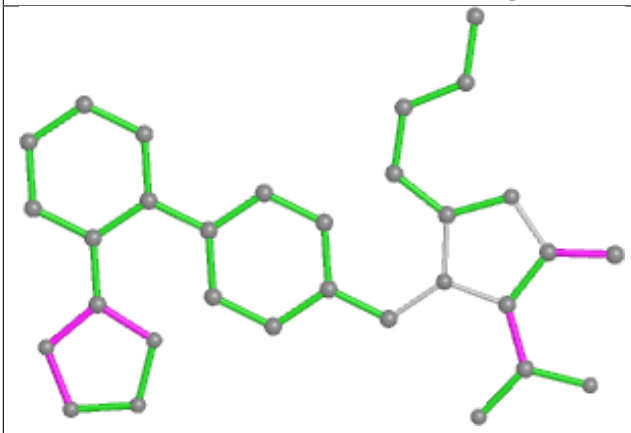


Torsions

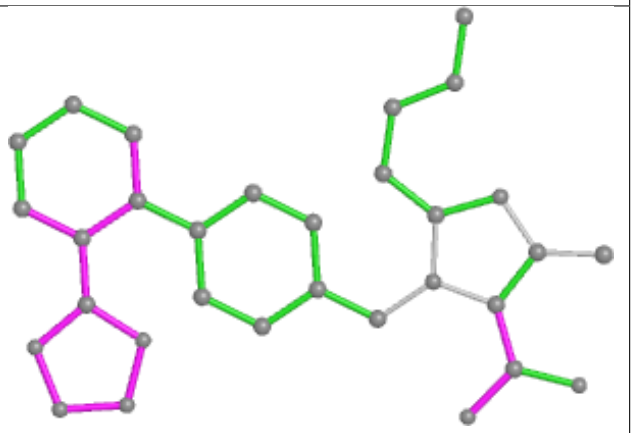


Rings

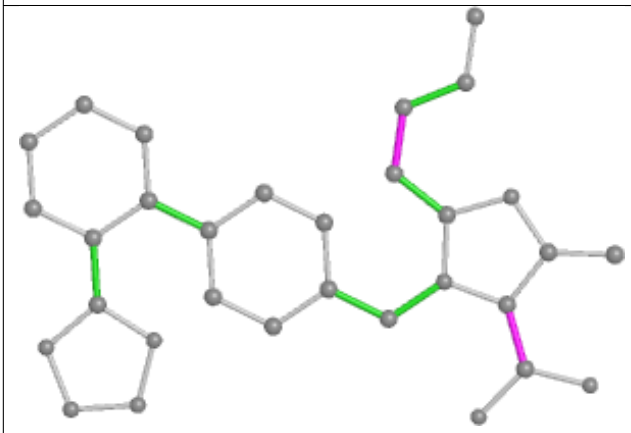
Ligand A1ATL C 501



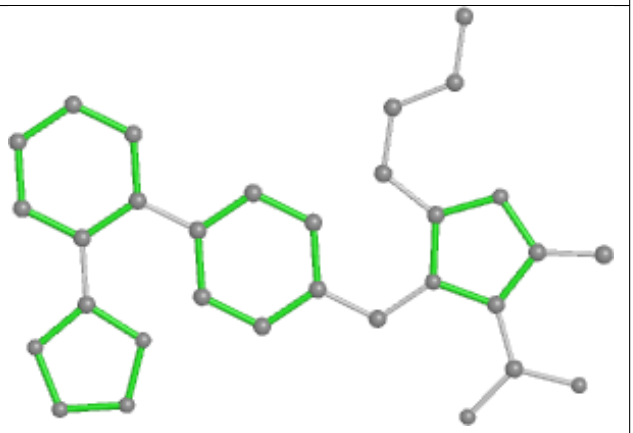
Bond lengths



Bond angles

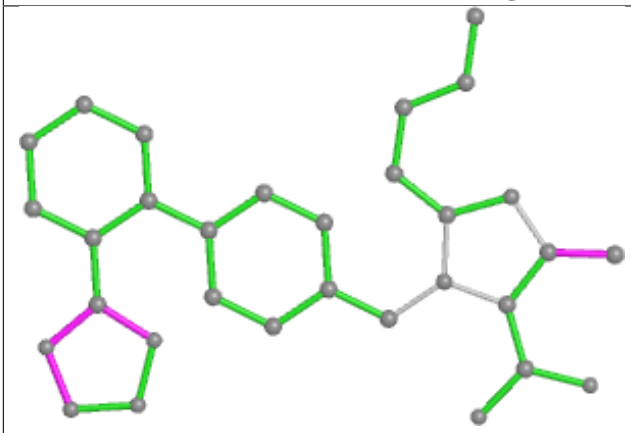


Torsions

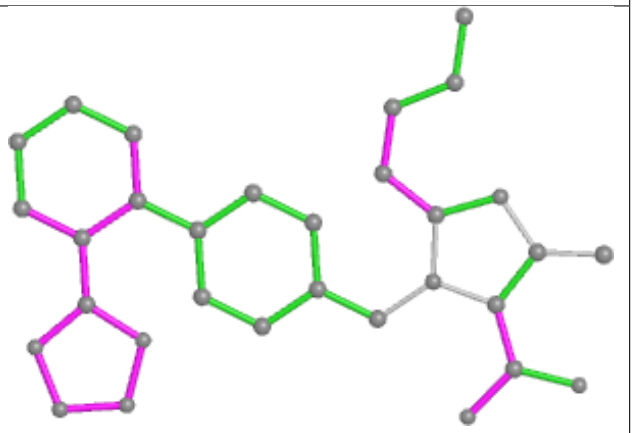


Rings

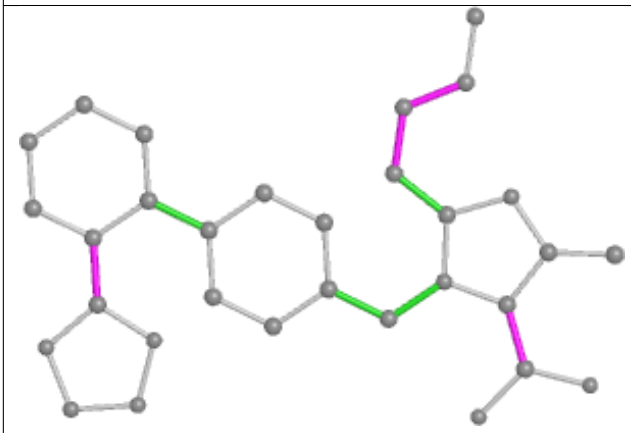
Ligand A1ATL A 501



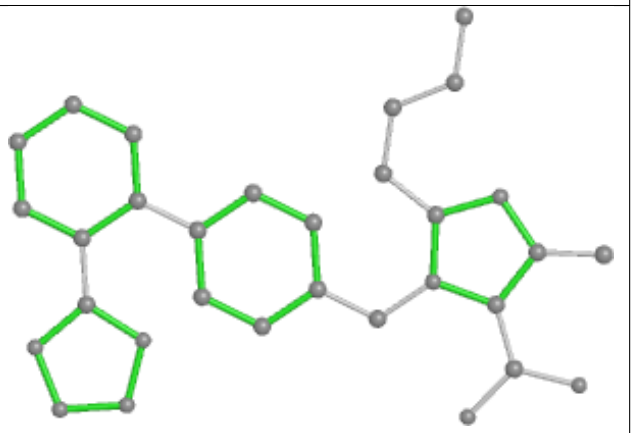
Bond lengths



Bond angles



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, 95^{th} 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	402/412 (97%)	0.65	45 (11%) 5 6	35, 47, 69, 92	0
1	B	405/412 (98%)	0.50	30 (7%) 14 18	32, 44, 61, 112	0
1	C	403/412 (97%)	0.71	45 (11%) 5 6	35, 53, 81, 117	0
1	D	402/412 (97%)	0.72	44 (10%) 5 7	37, 54, 78, 98	0
All	All	1612/1648 (97%)	0.65	164 (10%) 6 8	32, 49, 76, 117	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	ASN	9.4
1	A	58	ALA	5.2
1	A	210	LEU	5.2
1	D	37	ASN	5.1
1	A	206	LEU	5.0
1	B	35	MET	4.9
1	D	204	THR	4.7
1	C	37	ASN	4.6
1	B	34	ASP	4.3
1	A	57	PHE	4.3
1	D	209	GLY	4.3
1	D	255	ALA	4.3
1	A	207	ALA	4.2
1	D	206	LEU	4.2
1	D	57	PHE	4.1
1	C	310	LYS	4.1
1	C	320	LYS	4.1
1	D	140	ALA	4.1
1	A	204	THR	4.0
1	D	210	LEU	3.9
1	D	301	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	54	ALA	3.9
1	B	206	LEU	3.8
1	A	421	ARG	3.8
1	D	213	TYR	3.7
1	B	62	LEU	3.7
1	A	201	VAL	3.7
1	D	211	TYR	3.7
1	B	210	LEU	3.7
1	D	208	THR	3.6
1	A	55	GLY	3.6
1	A	209	GLY	3.6
1	B	243	CYS	3.5
1	C	207	ALA	3.5
1	A	417	ARG	3.5
1	D	207	ALA	3.4
1	D	236	LEU	3.4
1	B	421	ARG	3.3
1	C	307	SER	3.3
1	C	397	GLU	3.3
1	B	379	GLY	3.2
1	A	211	TYR	3.2
1	B	36	ASN	3.2
1	D	110	ILE	3.2
1	D	329	ARG	3.2
1	A	212	ALA	3.2
1	C	210	LEU	3.2
1	D	54	ALA	3.2
1	A	419	ASP	3.1
1	A	208	THR	3.1
1	D	77	ALA	3.1
1	C	343	GLU	3.1
1	B	204	THR	3.1
1	A	203	MET	3.1
1	A	56	PRO	3.1
1	B	207	ALA	3.0
1	B	438	HIS	3.0
1	C	429	ALA	3.0
1	A	213	TYR	3.0
1	C	305	ASP	3.0
1	A	243	CYS	3.0
1	A	62	LEU	3.0
1	A	374	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	213	TYR	2.9
1	C	340	TYR	2.9
1	B	255	ALA	2.9
1	C	206	LEU	2.9
1	C	89	VAL	2.8
1	C	128	VAL	2.8
1	B	209	GLY	2.8
1	A	379	GLY	2.8
1	C	431	VAL	2.8
1	D	38	ILE	2.8
1	D	158	CYS	2.8
1	D	243	CYS	2.8
1	A	380	LYS	2.7
1	D	53	LEU	2.7
1	A	59	THR	2.7
1	B	208	THR	2.7
1	D	317	HIS	2.7
1	C	214	GLY	2.7
1	D	325	ILE	2.7
1	D	212	ALA	2.7
1	D	343	GLU	2.7
1	B	213	TYR	2.7
1	A	202	ALA	2.6
1	C	334	LEU	2.6
1	A	37	ASN	2.6
1	D	374	GLU	2.6
1	C	212	ALA	2.6
1	A	214	GLY	2.6
1	D	193	ASN	2.6
1	C	211	TYR	2.6
1	D	305	ASP	2.5
1	A	215	ALA	2.5
1	C	336	SER	2.5
1	C	209	GLY	2.5
1	D	304	ILE	2.5
1	D	202	ALA	2.5
1	C	86	PRO	2.5
1	A	418	TYR	2.5
1	C	244	LEU	2.5
1	C	38	ILE	2.5
1	B	417	ARG	2.5
1	D	300	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	194	GLY	2.5
1	C	57	PHE	2.5
1	A	53	LEU	2.4
1	A	314	LEU	2.4
1	B	53	LEU	2.4
1	B	72	VAL	2.4
1	B	394	LYS	2.4
1	C	110	ILE	2.4
1	C	425	GLU	2.4
1	D	414	GLU	2.4
1	C	255	ALA	2.4
1	B	419	ASP	2.4
1	B	254	GLY	2.4
1	D	74	ARG	2.4
1	A	99	VAL	2.4
1	A	224	TYR	2.4
1	A	234	CYS	2.3
1	C	243	CYS	2.3
1	A	150	GLU	2.3
1	B	211	TYR	2.3
1	D	62	LEU	2.3
1	D	130	VAL	2.3
1	C	95	TYR	2.2
1	C	337	LYS	2.2
1	B	239	SER	2.2
1	A	49	LEU	2.2
1	B	185	LEU	2.2
1	A	88	PHE	2.2
1	D	201	VAL	2.2
1	A	305	ASP	2.2
1	C	84	TRP	2.2
1	D	58	ALA	2.2
1	D	326	LEU	2.2
1	A	433	ASP	2.2
1	A	377	THR	2.2
1	C	208	THR	2.2
1	D	244	LEU	2.2
1	A	108	VAL	2.2
1	B	202	ALA	2.2
1	C	300	LEU	2.1
1	A	193	ASN	2.1
1	D	205	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	51	ARG	2.1
1	C	201	VAL	2.1
1	B	242	ALA	2.1
1	D	177	ALA	2.1
1	C	70	ILE	2.1
1	C	122	LEU	2.1
1	A	397	GLU	2.1
1	C	306	ASN	2.1
1	C	193	ASN	2.0
1	B	199	PRO	2.0
1	C	332	GLU	2.0
1	C	308	LYS	2.0
1	C	323	ILE	2.0
1	B	368	GLY	2.0
1	A	140	ALA	2.0
1	D	242	ALA	2.0
1	C	289	GLN	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 monosaccharides 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, 95^{th} 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	A1ATL	D	501	30/31	0.76	0.29	46,57,69,70	47
2	A1ATL	C	501	31/31	0.83	0.24	39,54,66,66	51
3	NH4	A	502	1/1	0.85	0.38	38,46,46,46	5
2	A1ATL	A	501	31/31	0.88	0.21	38,46,58,58	51
3	NH4	D	502	1/1	0.90	0.24	46,56,56,56	0
4	SO4	C	504	5/5	0.90	0.16	63,66,70,93	5

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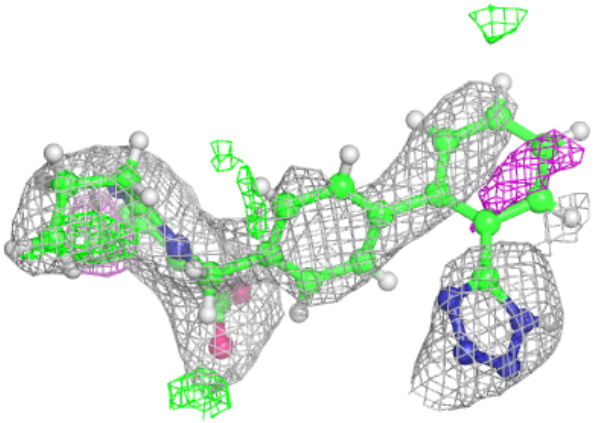
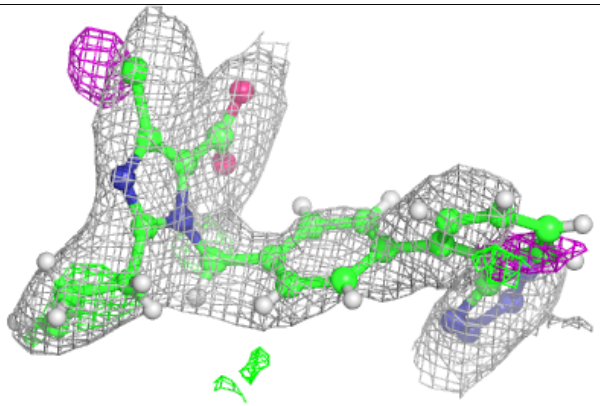
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	503	5/5	0.91	0.26	40,52,57,63	5
3	NH4	C	502	1/1	0.91	0.22	43,52,52,52	0
4	SO4	C	503	5/5	0.93	0.21	52,56,56,82	5
4	SO4	A	504	5/5	0.93	0.24	45,56,67,67	5
4	SO4	D	504	5/5	0.93	0.14	49,60,63,76	5
4	SO4	D	503	5/5	0.94	0.21	55,58,69,79	5
4	SO4	B	501	5/5	0.94	0.12	44,61,70,72	0

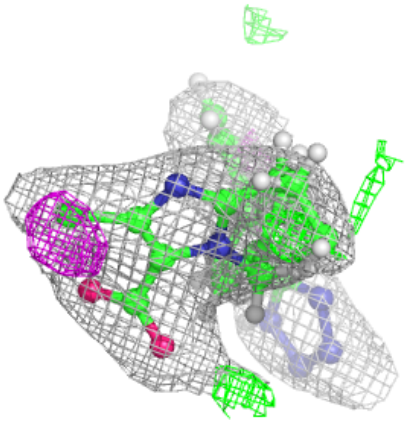
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1ATL D 501:

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

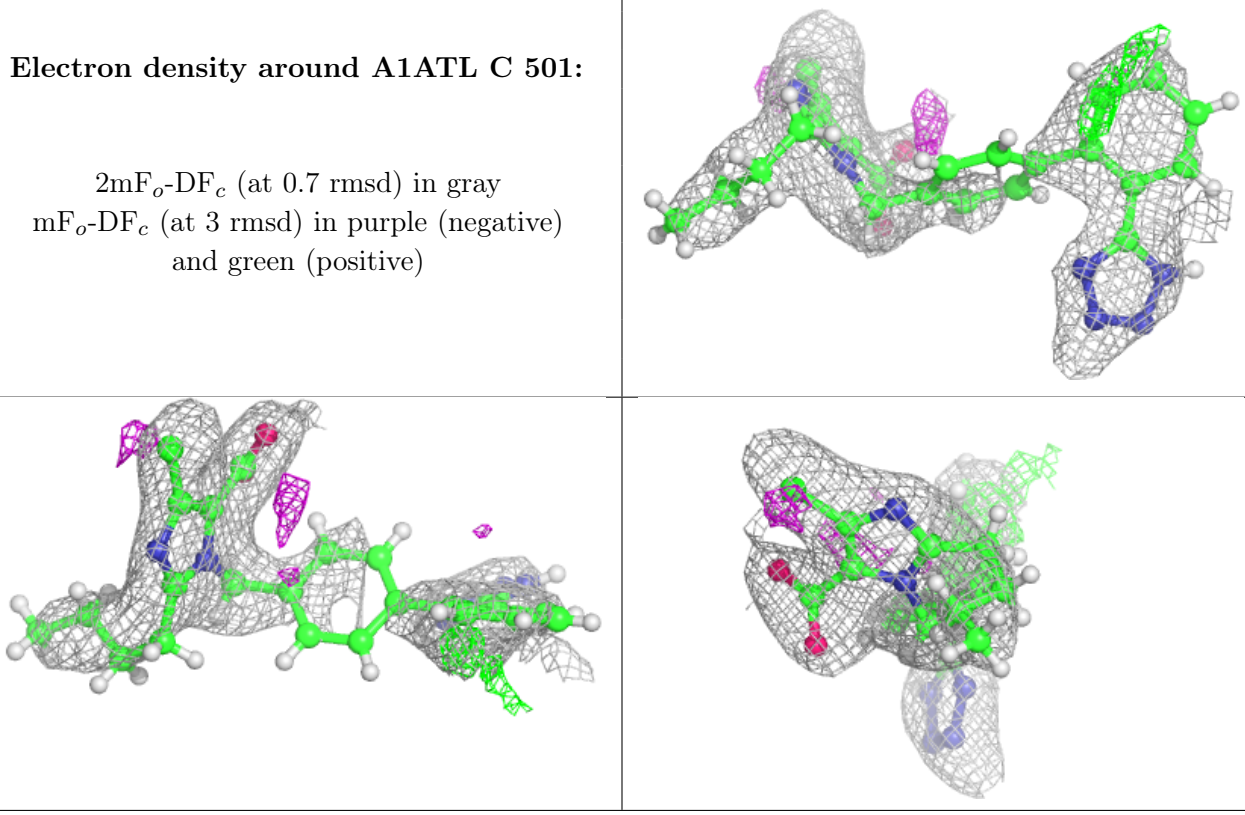






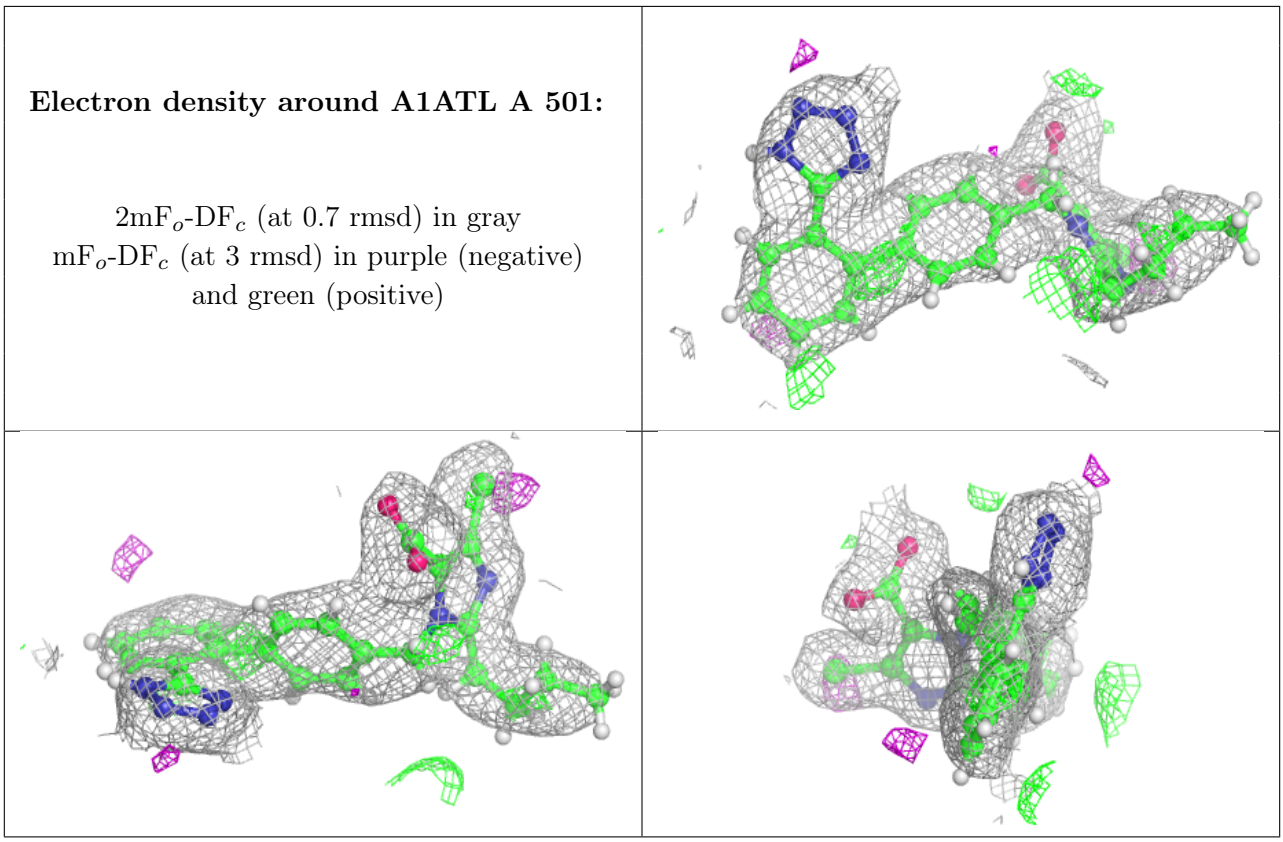
Electron density around A1ATL C 501:

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



Electron density around A1ATL A 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.