Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:26 PM EDT

PDB ID	:	8ECF
Title	:	Cryo structure of Mycobacterium tuberculosis beta lactamase microcrystals mixed with sulbactam for 3 hours
Authors	:	Malla, T.N.; Schmidt, M.
Deposited on	:	2022-09-01
Resolution	:	2.74 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:

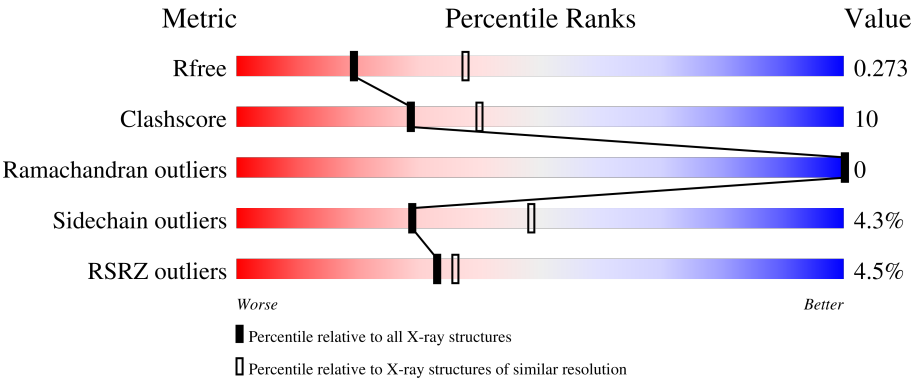
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	267	2% 81% 16%
1	B	267	3% 79% 19%
1	C	267	7% 76% 21%
1	D	267	5% 79% 19%

2 Entry composition (i)

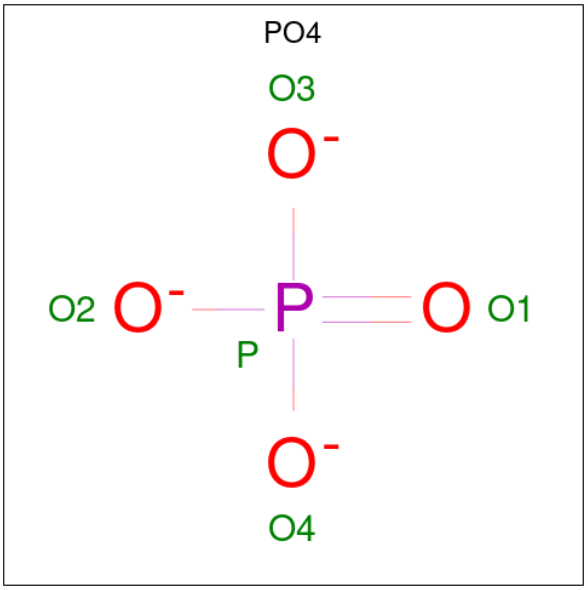
There are 4 unique types of molecules in this entry. The entry contains 16072 atoms, of which 7884 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	265	Total	C	H	N	O	S	115	0	0
			3948	1243	1960	352	387	6			
1	B	265	Total	C	H	N	O	S	115	0	0
			3948	1243	1960	352	387	6			
1	C	265	Total	C	H	N	O	S	115	0	0
			3948	1243	1960	352	387	6			
1	D	265	Total	C	H	N	O	S	115	0	0
			3948	1243	1960	352	387	6			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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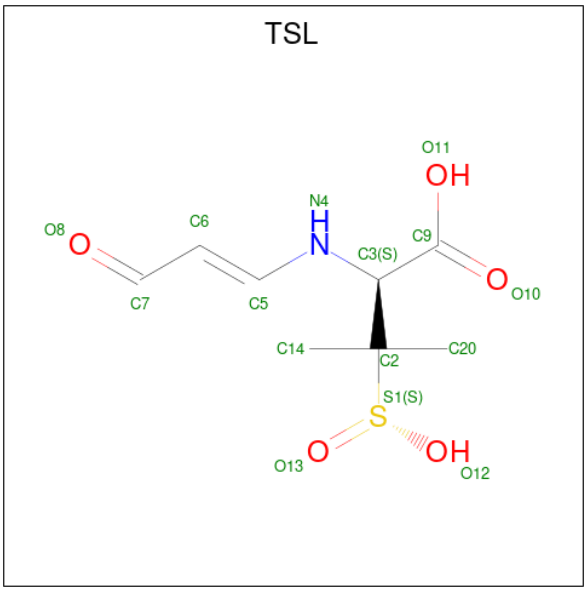
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is TRANS-ENAMINE INTERMEDIATE OF SULBACTAM (three-letter code: TSL) (formula: $C_8H_{13}NO_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O S 26 8 11 1 5 1	1	0
3	B	1	Total C H N O S 26 8 11 1 5 1	1	0
3	C	1	Total C H N O S 26 8 11 1 5 1	1	0
3	D	1	Total C H N O S 26 8 11 1 5 1	1	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0
4	B	43	Total O 43 43	0	0
4	C	28	Total O 28 28	0	0

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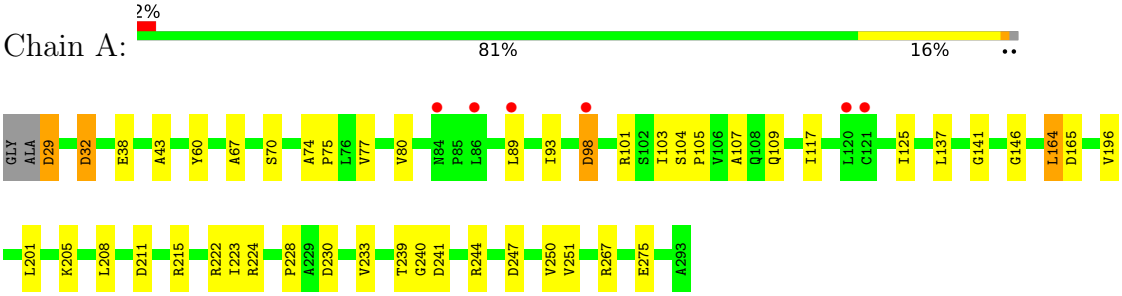
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	45	Total O 45 45	0	0

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.

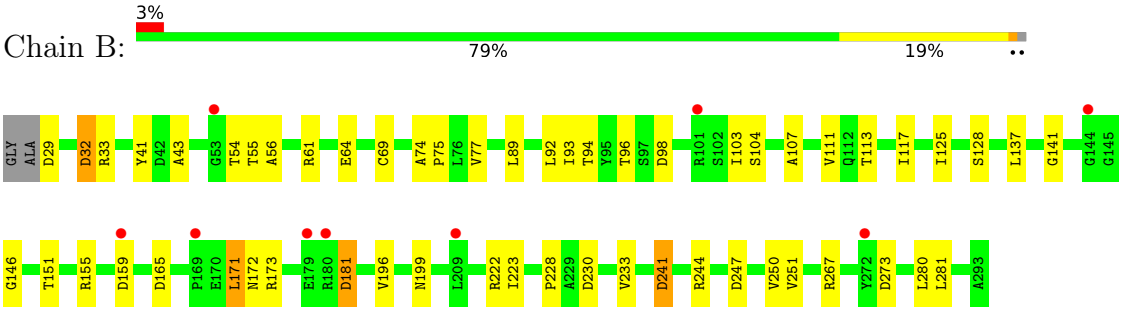
• Molecule 1: Beta-lactamase

Chain A:



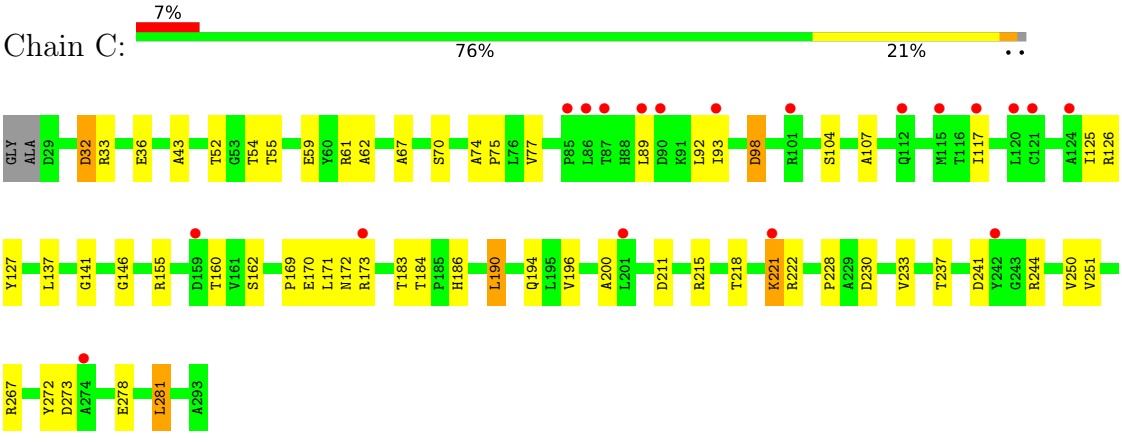
• Molecule 1: Beta-lactamase

Chain B:



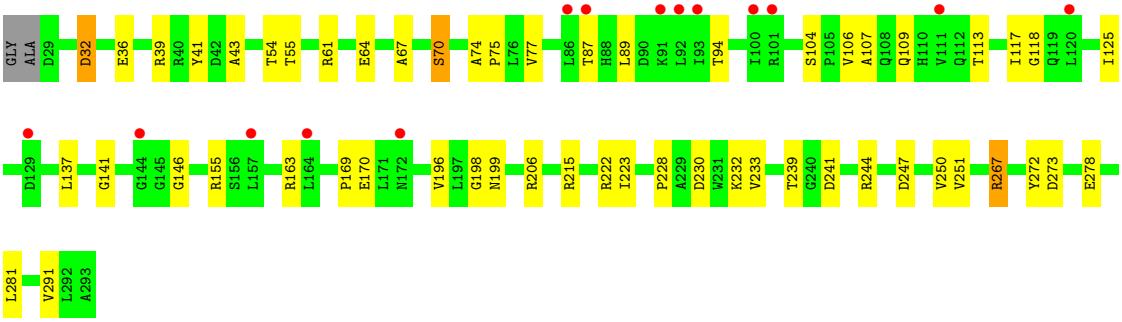
• Molecule 1: Beta-lactamase

Chain C:



• Molecule 1: Beta-lactamase

Chain D:


GLY ALA D29 D32 E36 R39 R40 Y41 D42 A43 T54 T55 R61 E64 A67 S70 A74 P75 L76 V77 L86 T87 H88 L89 D90 K91 L92 I93 T94 I100 R101 S104 P105 V106 A107 Q108 Q109 H110 V111 Q112 T113 I117 G118 Q119 L120 I125
D129 L137 G141 G144 G145 G146 R155 S156 L157 R163 L164 P169 E170 L171 N172 V196 L197 G198 N199 R206 R215 R222 I223 P228 A229 D230 W231 K232 V233 T239 G240 D241 R244 D247 V250 V251 R267 Y272 D273 E278
L281 V291 L292 A293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.44Å 96.67Å 111.03Å 90.00° 108.08° 90.00°	Depositor
Resolution (Å)	48.33 – 2.74 48.33 – 2.74	Depositor EDS
% Data completeness (in resolution range)	60.0 (48.33-2.74) 60.1 (48.33-2.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.211 , 0.268 0.216 , 0.273	Depositor DCC
R_{free} test set	1322 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16072	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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: PO4, TSL

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	0.34	1/2027 (0.0%)	0.64	0/2767
1	B	0.34	0/2027	0.65	0/2767
1	C	0.34	1/2027 (0.0%)	0.63	0/2767
1	D	0.37	1/2027 (0.0%)	0.63	0/2767
All	All	0.35	3/8108 (0.0%)	0.64	0/11068

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	SER	CB-OG	7.87	1.52	1.42
1	C	70	SER	CB-OG	5.37	1.49	1.42
1	A	70	SER	CB-OG	5.33	1.49	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	163	ARG	Sidechain
1	D	267	ARG	Sidechain

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	1988	1960	1955	37	0
1	B	1988	1960	1955	35	0
1	C	1988	1960	1955	49	0
1	D	1988	1960	1955	35	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	15	11	11	2	0
3	B	15	11	11	0	0
3	C	15	11	11	0	0
3	D	15	11	11	1	0
4	A	40	0	0	6	0
4	B	43	0	0	7	0
4	C	28	0	0	9	0
4	D	45	0	0	5	0
All	All	8188	7884	7864	154	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 (154) 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:B:54:THR:HG22	4:B:419:HOH:O	1.52	1.06
1:C:170:GLU:O	4:C:402:HOH:O	1.78	0.98
1:D:215:ARG:NH1	4:D:401:HOH:O	1.95	0.98
1:A:29:ASP:N	4:A:401:HOH:O	2.04	0.89
1:D:41:TYR:O	1:D:267:ARG:NH1	2.09	0.86
1:C:172:ASN:ND2	4:C:401:HOH:O	1.66	0.85
1:C:52:THR:HG22	1:C:55:THR:OG1	1.77	0.84
1:D:198:GLY:O	1:D:206:ARG:NH1	2.13	0.81
1:C:194:GLN:HG3	1:C:200:ALA:HB2	1.63	0.79
1:A:98:ASP:O	4:A:402:HOH:O	2.06	0.74
1:A:101:ARG:HG2	4:A:402:HOH:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:HB3	4:C:402:HOH:O	1.87	0.74
1:A:74:ALA:HB3	1:A:75:PRO:HD3	1.75	0.68
1:B:54:THR:CG2	4:B:419:HOH:O	2.23	0.68
1:C:162:SER:OG	1:C:183:THR:HG23	1.93	0.68
1:C:186:HIS:O	1:C:190:LEU:HD22	1.95	0.67
1:C:74:ALA:HB3	1:C:75:PRO:HD3	1.76	0.67
1:C:241:ASP:O	1:C:244:ARG:HG3	1.96	0.66
1:D:74:ALA:HB3	1:D:75:PRO:HD3	1.77	0.66
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.77	0.65
1:B:69:CYS:HA	4:B:429:HOH:O	1.95	0.65
1:C:218:THR:OG1	4:C:403:HOH:O	2.14	0.65
1:A:241:ASP:O	1:A:244:ARG:HG3	1.97	0.65
1:C:169:PRO:HA	4:C:401:HOH:O	1.96	0.64
1:C:173:ARG:HG3	1:C:272:TYR:HE2	1.62	0.64
1:B:241:ASP:O	1:B:244:ARG:HG3	1.98	0.62
1:C:222:ARG:NH1	1:C:237:THR:HB	2.16	0.61
1:C:92:LEU:HD13	1:C:93:ILE:N	2.18	0.59
1:D:241:ASP:O	1:D:244:ARG:HG3	2.02	0.59
1:C:221:LYS:HD3	1:C:221:LYS:H	1.68	0.59
1:C:74:ALA:HB3	1:C:75:PRO:CD	2.34	0.58
1:A:224:ARG:NH2	4:A:405:HOH:O	2.29	0.58
1:A:74:ALA:HB3	1:A:75:PRO:CD	2.34	0.58
1:C:221:LYS:HE2	1:C:278:GLU:OE2	2.04	0.58
1:C:59:GLU:HG2	1:C:62:ALA:HB3	1.86	0.58
1:D:67:ALA:HB3	1:D:244:ARG:HD3	1.86	0.57
1:B:74:ALA:HB3	1:B:75:PRO:CD	2.36	0.56
1:B:41:TYR:O	1:B:267:ARG:NH1	2.38	0.56
1:D:54:THR:OG1	1:D:55:THR:HG23	2.05	0.56
1:D:74:ALA:HB3	1:D:75:PRO:CD	2.35	0.56
1:A:275:GLU:HB3	1:B:113:THR:HG22	1.87	0.56
1:B:89:LEU:HA	1:B:117:ILE:HB	1.88	0.56
1:A:67:ALA:HB3	1:A:244:ARG:HD3	1.88	0.55
1:A:77:VAL:O	1:A:80:VAL:HG22	2.06	0.55
1:D:199:ASN:ND2	4:D:404:HOH:O	2.39	0.54
1:D:61:ARG:HD3	1:D:64:GLU:OE2	2.07	0.54
1:C:52:THR:CG2	1:C:55:THR:OG1	2.52	0.54
1:A:240:GLY:HA2	3:A:302:TSL:H203	1.89	0.54
1:B:61:ARG:HD3	1:B:64:GLU:OE2	2.08	0.54
1:B:98:ASP:OD1	1:B:98:ASP:N	2.40	0.54
1:C:54:THR:OG1	1:C:55:THR:HG23	2.07	0.53
1:B:222:ARG:HD3	1:B:281:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HG11	1:B:250:VAL:HG21	1.91	0.52
1:D:155:ARG:NH1	4:D:405:HOH:O	2.42	0.52
1:C:126:ARG:NH2	1:C:127:TYR:OH	2.42	0.52
1:C:183:THR:HG22	1:C:184:THR:N	2.25	0.52
1:D:196:VAL:HG11	1:D:250:VAL:HG21	1.91	0.52
1:B:93:ILE:HD11	1:B:117:ILE:HD11	1.92	0.52
1:C:222:ARG:HD3	1:C:281:LEU:HD12	1.92	0.52
1:A:196:VAL:HG11	1:A:250:VAL:HG21	1.93	0.51
1:A:77:VAL:O	1:A:80:VAL:CG2	2.59	0.51
1:C:98:ASP:N	1:C:98:ASP:OD1	2.43	0.51
1:C:196:VAL:HG11	1:C:250:VAL:HG21	1.93	0.51
1:A:222:ARG:NH2	1:A:239:THR:OG1	2.45	0.50
1:D:169:PRO:HD2	1:D:170:GLU:OE1	2.10	0.50
1:B:155:ARG:HD2	1:B:159:ASP:O	2.11	0.50
1:B:241:ASP:N	1:B:241:ASP:OD1	2.45	0.50
1:B:33:ARG:NH2	4:B:401:HOH:O	2.23	0.50
1:B:128:SER:HB2	4:B:411:HOH:O	2.13	0.49
1:B:141:GLY:O	1:B:146:GLY:HA2	2.12	0.49
1:C:170:GLU:HA	4:C:402:HOH:O	2.13	0.48
1:C:141:GLY:O	1:C:146:GLY:HA2	2.14	0.48
1:B:33:ARG:HH12	1:C:33:ARG:HH22	1.60	0.48
1:A:141:GLY:O	1:A:146:GLY:HA2	2.14	0.48
1:C:222:ARG:HH11	1:C:237:THR:CG2	2.27	0.48
1:A:77:VAL:HG21	1:A:125:ILE:HD11	1.95	0.48
1:D:141:GLY:O	1:D:146:GLY:HA2	2.14	0.48
1:A:224:ARG:HG3	4:A:433:HOH:O	2.14	0.47
1:A:233:VAL:HG22	1:A:251:VAL:HG12	1.95	0.47
1:C:67:ALA:HB3	1:C:244:ARG:HD3	1.95	0.47
1:D:233:VAL:HG22	1:D:251:VAL:HG12	1.96	0.47
1:D:222:ARG:NH2	1:D:239:THR:OG1	2.44	0.47
1:D:89:LEU:HA	1:D:117:ILE:HB	1.96	0.47
1:C:89:LEU:HA	1:C:117:ILE:HB	1.95	0.47
1:C:273:ASP:OD1	1:C:273:ASP:N	2.46	0.47
1:B:233:VAL:HG22	1:B:251:VAL:HG12	1.96	0.47
1:C:77:VAL:HG21	1:C:125:ILE:HD11	1.97	0.47
1:A:223:ILE:HG13	1:A:247:ASP:HB3	1.97	0.47
1:D:199:ASN:HD22	1:D:199:ASN:N	2.12	0.47
1:D:241:ASP:N	1:D:241:ASP:OD1	2.47	0.47
1:C:221:LYS:H	1:C:221:LYS:CD	2.27	0.46
3:A:302:TSL:C5	3:A:302:TSL:H201	2.45	0.46
1:B:77:VAL:HG21	1:B:125:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ASP:OD1	1:D:273:ASP:N	2.45	0.46
1:A:164:LEU:HD23	1:A:165:ASP:H	1.81	0.46
1:A:164:LEU:HD23	1:A:165:ASP:N	2.31	0.46
1:C:233:VAL:HG22	1:C:251:VAL:HG12	1.97	0.46
1:D:223:ILE:HG13	1:D:247:ASP:HB3	1.98	0.46
1:C:59:GLU:HG2	1:C:62:ALA:CB	2.46	0.45
1:A:105:PRO:HB2	1:B:103:ILE:HD13	1.99	0.45
1:B:55:THR:HG22	1:B:56:ALA:O	2.17	0.45
1:D:113:THR:HG21	4:D:412:HOH:O	2.16	0.45
1:A:93:ILE:HD11	1:A:117:ILE:CD1	2.46	0.45
1:B:32:ASP:N	1:B:32:ASP:OD1	2.50	0.45
1:D:32:ASP:N	1:D:32:ASP:OD1	2.49	0.45
1:A:211:ASP:O	1:A:215:ARG:HG3	2.17	0.45
1:C:32:ASP:N	1:C:32:ASP:OD1	2.49	0.45
1:C:222:ARG:HH12	1:C:237:THR:HB	1.80	0.45
1:A:32:ASP:N	1:A:32:ASP:OD1	2.50	0.44
1:A:93:ILE:HD12	1:A:93:ILE:N	2.31	0.44
1:D:77:VAL:HG21	1:D:125:ILE:HD11	1.99	0.44
1:B:171:LEU:HB2	1:B:181:ASP:OD2	2.17	0.44
1:C:211:ASP:O	1:C:215:ARG:HG3	2.18	0.44
1:C:104:SER:HB3	1:C:107:ALA:HB3	2.00	0.44
1:D:43:ALA:HB2	1:D:267:ARG:HG2	2.00	0.44
1:C:54:THR:OG1	1:C:55:THR:N	2.51	0.43
1:B:172:ASN:HB3	4:B:429:HOH:O	2.17	0.43
1:C:170:GLU:C	4:C:402:HOH:O	2.45	0.43
1:A:89:LEU:HA	1:A:117:ILE:HB	1.99	0.43
1:A:104:SER:HB3	1:A:107:ALA:HB3	2.01	0.43
1:A:228:PRO:HB2	1:A:230:ASP:OD1	2.19	0.43
1:B:96:THR:HB	4:B:418:HOH:O	2.17	0.43
1:D:36:GLU:OE2	1:D:39:ARG:NH2	2.50	0.43
1:C:43:ALA:HB2	1:C:267:ARG:HG2	2.00	0.43
1:B:273:ASP:OD1	1:B:273:ASP:N	2.45	0.43
1:D:228:PRO:HB2	1:D:230:ASP:OD1	2.19	0.43
1:D:104:SER:HB3	1:D:107:ALA:HB3	2.02	0.42
1:A:103:ILE:HG22	1:A:105:PRO:HD3	2.02	0.42
1:A:267:ARG:NH1	1:A:275:GLU:O	2.52	0.42
1:C:146:GLY:HA2	4:C:410:HOH:O	2.19	0.42
1:C:61:ARG:HH11	1:C:61:ARG:HG3	1.85	0.42
1:D:118:GLY:HA3	4:D:406:HOH:O	2.19	0.42
1:B:137:LEU:O	1:B:146:GLY:HA3	2.19	0.42
1:D:54:THR:OG1	1:D:55:THR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:O	1:D:109:GLN:HG2	2.20	0.42
1:D:239:THR:O	3:D:302:TSL:H6	2.20	0.42
1:C:170:GLU:CA	4:C:402:HOH:O	2.67	0.42
1:A:38:GLU:OE1	1:A:60:TYR:OH	2.37	0.41
1:B:89:LEU:CD1	1:B:117:ILE:HG22	2.51	0.41
1:A:201:LEU:N	4:A:406:HOH:O	2.47	0.41
1:C:228:PRO:HB2	1:C:230:ASP:OD1	2.20	0.41
1:D:241:ASP:OD2	1:D:272:TYR:CZ	2.73	0.41
1:C:137:LEU:O	1:C:146:GLY:HA3	2.20	0.41
1:A:137:LEU:O	1:A:146:GLY:HA3	2.20	0.41
1:D:137:LEU:O	1:D:146:GLY:HA3	2.20	0.41
1:B:228:PRO:HB2	1:B:230:ASP:OD1	2.20	0.41
1:A:77:VAL:HA	1:A:80:VAL:HG22	2.02	0.41
1:B:104:SER:HB3	1:B:107:ALA:HB3	2.02	0.41
1:B:223:ILE:HG13	1:B:247:ASP:HB3	2.02	0.41
1:D:241:ASP:OD2	1:D:272:TYR:CE1	2.74	0.41
1:C:221:LYS:CE	1:C:278:GLU:OE2	2.69	0.40
1:A:205:LYS:O	1:A:208:LEU:HB2	2.22	0.40
1:B:43:ALA:HB2	1:B:267:ARG:HG2	2.04	0.40
1:A:43:ALA:HB2	1:A:267:ARG:HG2	2.02	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	263/267 (98%)	252 (96%)	11 (4%)	0	100	100
1	B	263/267 (98%)	252 (96%)	11 (4%)	0	100	100
1	C	263/267 (98%)	251 (95%)	12 (5%)	0	100	100
1	D	263/267 (98%)	251 (95%)	12 (5%)	0	100	100
All	All	1052/1068 (98%)	1006 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	202/202 (100%)	197 (98%)	5 (2%)	47	67
1	B	202/202 (100%)	189 (94%)	13 (6%)	17	31
1	C	202/202 (100%)	193 (96%)	9 (4%)	27	47
1	D	202/202 (100%)	194 (96%)	8 (4%)	31	52
All	All	808/808 (100%)	773 (96%)	35 (4%)	29	48

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	32	ASP
1	A	98	ASP
1	A	109	GLN
1	A	164	LEU
1	B	29	ASP
1	B	32	ASP
1	B	92	LEU
1	B	94	THR
1	B	111	VAL
1	B	151	THR
1	B	165	ASP
1	B	171	LEU
1	B	173	ARG
1	B	181	ASP
1	B	199	ASN
1	B	241	ASP
1	B	280	LEU
1	C	32	ASP
1	C	36	GLU
1	C	98	ASP
1	C	155	ARG

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Mol	Chain	Res	Type
1	C	160	THR
1	C	171	LEU
1	C	190	LEU
1	C	221	LYS
1	C	281	LEU
1	D	32	ASP
1	D	70	SER
1	D	87	THR
1	D	94	THR
1	D	232	LYS
1	D	278	GLU
1	D	281	LEU
1	D	291	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	C	108	GLN
1	D	199	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	TSL	A	302	1	9,14,14	0.85	0	9,19,19	0.70	0
2	PO4	D	301	-	4,4,4	0.53	0	6,6,6	0.51	0
2	PO4	C	301	-	4,4,4	1.01	0	6,6,6	0.34	0
2	PO4	A	301	-	4,4,4	0.84	0	6,6,6	0.44	0
3	TSL	B	302	1	9,14,14	0.90	0	9,19,19	0.48	0
3	TSL	D	302	1	9,14,14	0.91	0	9,19,19	0.93	1 (11%)
3	TSL	C	302	1	9,14,14	0.92	0	9,19,19	1.05	1 (11%)
2	PO4	B	301	-	4,4,4	0.67	0	6,6,6	0.53	0

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
3	TSL	C	302	1	-	5/17/21/21	-
3	TSL	A	302	1	-	6/17/21/21	-
3	TSL	B	302	1	-	5/17/21/21	-
3	TSL	D	302	1	-	7/17/21/21	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	TSL	C5-C6-C7	2.47	129.25	121.80
3	D	302	TSL	O8-C7-C6	-2.21	118.14	125.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	TSL	C14-C2-S1-O13
3	A	302	TSL	C20-C2-S1-O13
3	A	302	TSL	C6-C5-N4-C3

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Mol	Chain	Res	Type	Atoms
3	A	302	TSL	C5-C6-C7-O8
3	B	302	TSL	C6-C5-N4-C3
3	B	302	TSL	N4-C5-C6-C7
3	B	302	TSL	C5-C6-C7-O8
3	C	302	TSL	C14-C2-S1-O13
3	C	302	TSL	C20-C2-S1-O13
3	C	302	TSL	C6-C5-N4-C3
3	C	302	TSL	C5-C6-C7-O8
3	D	302	TSL	C2-C3-C9-O11
3	D	302	TSL	C9-C3-N4-C5
3	D	302	TSL	C6-C5-N4-C3
3	D	302	TSL	C5-C6-C7-O8
3	D	302	TSL	N4-C3-C9-O10
3	D	302	TSL	N4-C3-C9-O11
3	B	302	TSL	C2-C3-N4-C5
3	C	302	TSL	C2-C3-N4-C5
3	A	302	TSL	N4-C3-C9-O11
3	A	302	TSL	N4-C3-C9-O10
3	B	302	TSL	C2-C3-C9-O10
3	D	302	TSL	C2-C3-C9-O10

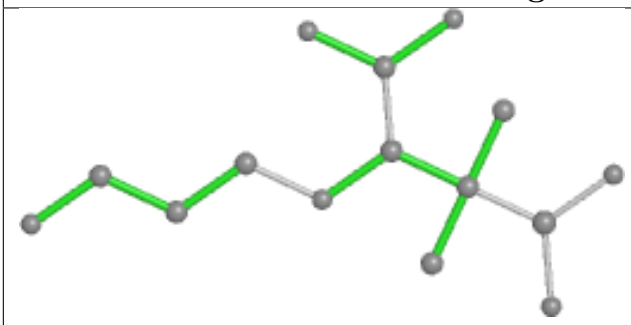
There are no ring outliers.

2 monomers are involved in 3 short contacts:

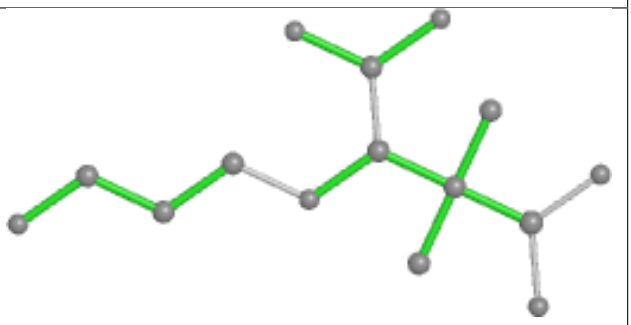
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	TSL	2	0
3	D	302	TSL	1	0

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.

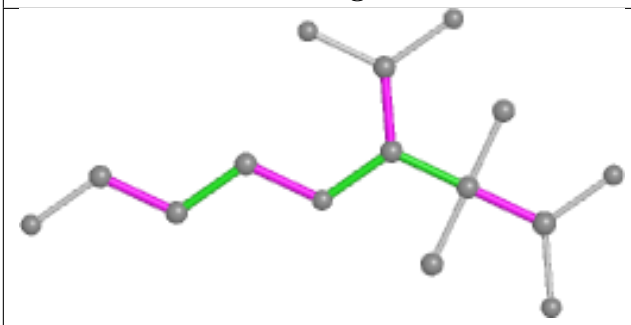
Ligand TSL A 302



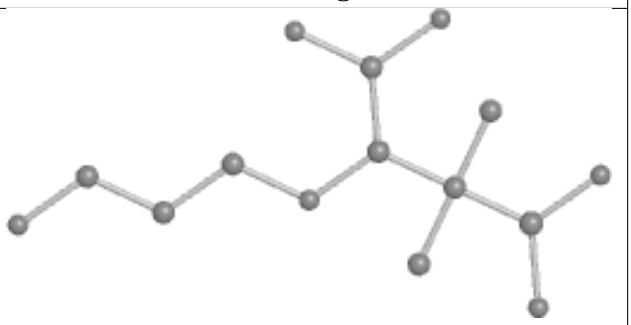
Bond lengths



Bond angles

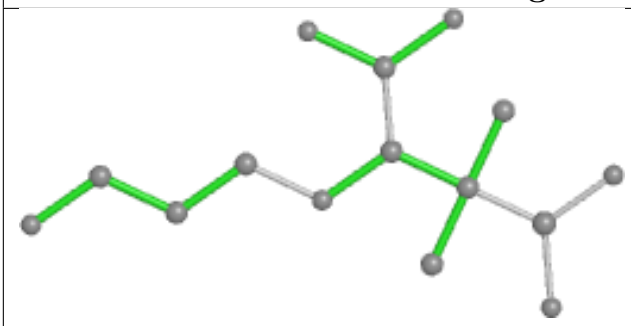


Torsions

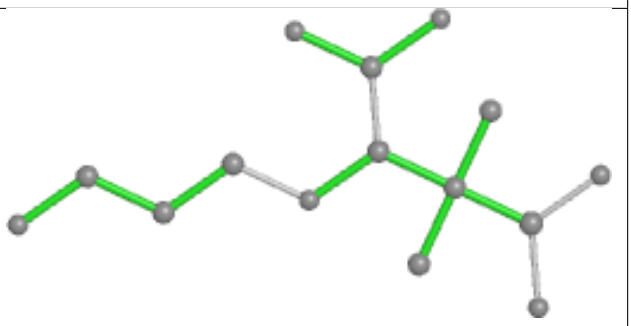


Rings

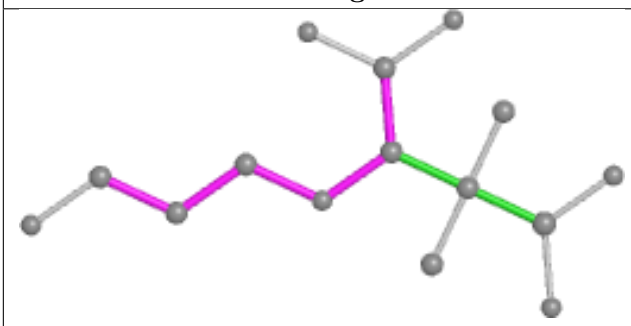
Ligand TSL B 302



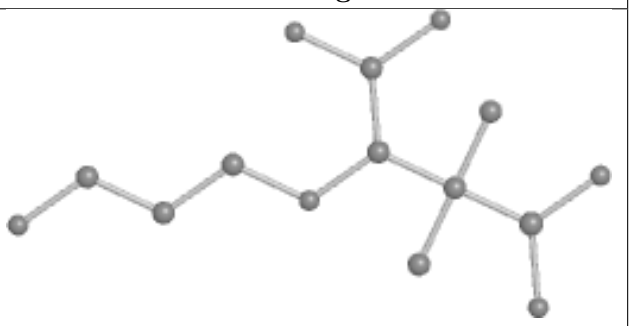
Bond lengths



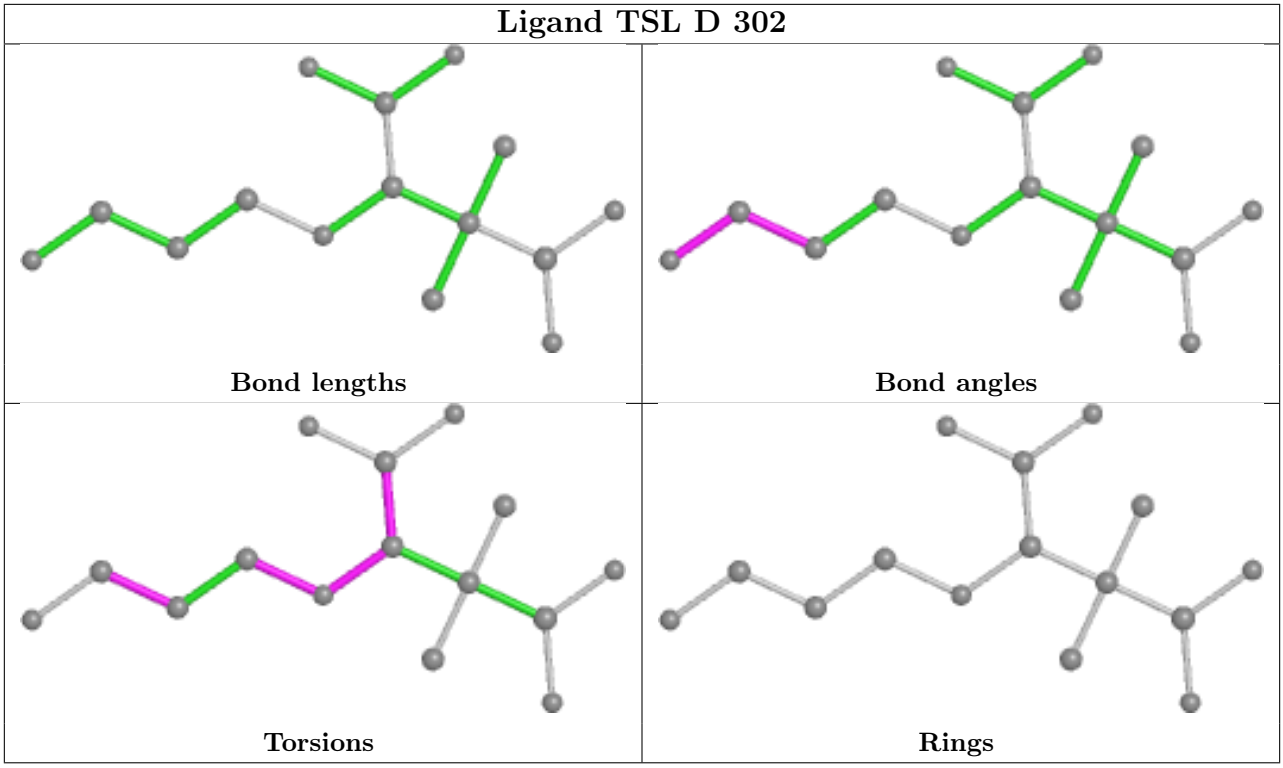
Bond angles

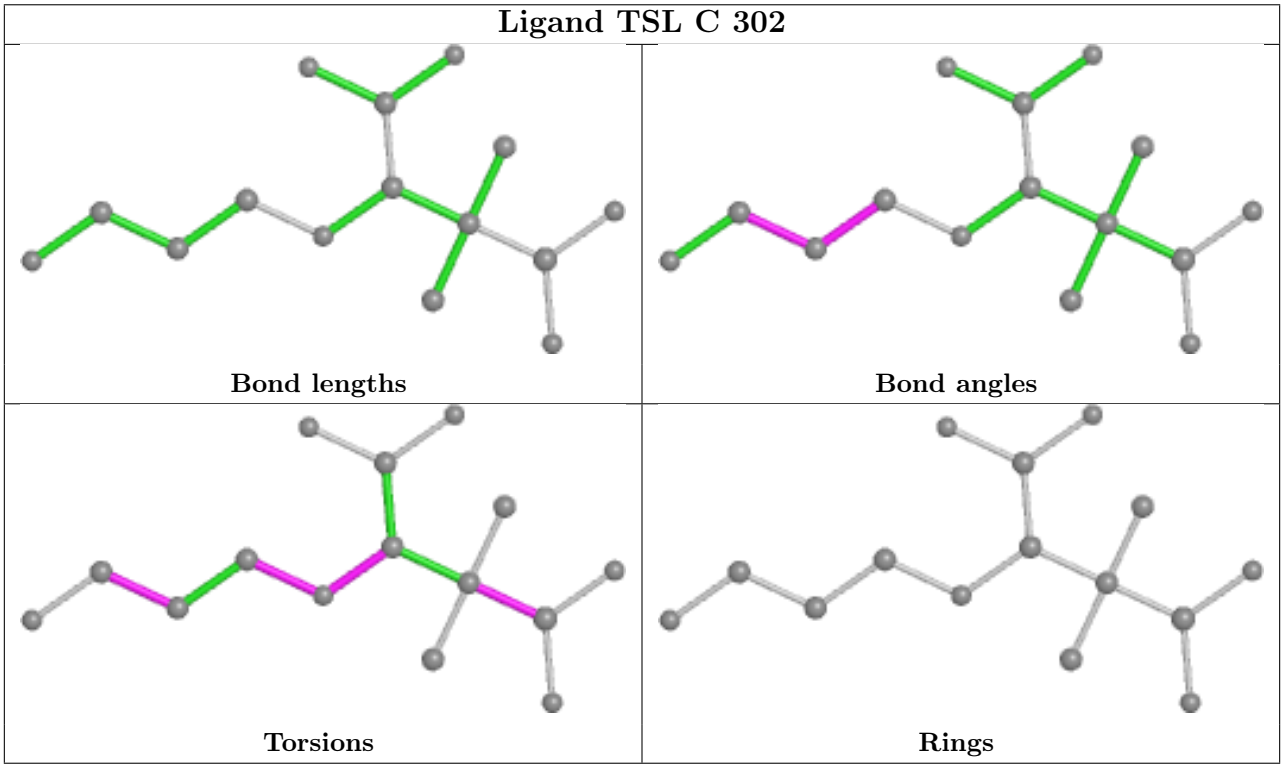


Torsions



Rings





5.7 Other polymers

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, 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	265/267 (99%)	0.40	6 (2%)	60	67	32, 54, 83, 98	0
1	B	265/267 (99%)	0.51	9 (3%)	45	50	33, 57, 94, 125	0
1	C	265/267 (99%)	0.60	19 (7%)	15	17	44, 64, 95, 117	0
1	D	265/267 (99%)	0.46	14 (5%)	26	29	34, 54, 85, 108	0
All	All	1060/1068 (99%)	0.49	48 (4%)	33	36	32, 57, 90, 125	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	LEU	7.0
1	D	93	ILE	5.7
1	B	159	ASP	5.0
1	C	159	ASP	4.0
1	B	101	ARG	3.6
1	C	93	ILE	3.6
1	B	53	GLY	3.4
1	C	89	LEU	3.3
1	A	98	ASP	3.3
1	C	90	ASP	3.0
1	A	89	LEU	3.0
1	D	87	THR	3.0
1	D	111	VAL	3.0
1	D	86	LEU	3.0
1	C	121	CYS	2.9
1	C	242	TYR	2.9
1	A	86	LEU	2.9
1	B	179	GLU	2.8
1	D	164	LEU	2.8
1	B	272	TYR	2.8
1	C	120	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	172	ASN	2.7
1	C	173	ARG	2.7
1	C	112	GLN	2.7
1	A	84	ASN	2.7
1	C	85	PRO	2.6
1	B	180	ARG	2.6
1	B	144	GLY	2.6
1	C	115	MET	2.5
1	C	101	ARG	2.4
1	D	101	ARG	2.4
1	D	129	ASP	2.4
1	C	87	THR	2.4
1	C	221	LYS	2.4
1	A	120	LEU	2.4
1	D	157	LEU	2.3
1	C	274	ALA	2.3
1	D	92	LEU	2.2
1	D	100	ILE	2.2
1	B	169	PRO	2.2
1	D	120	LEU	2.1
1	C	124	ALA	2.1
1	B	209	LEU	2.1
1	D	91	LYS	2.1
1	D	144	GLY	2.1
1	C	201	LEU	2.1
1	C	117	ILE	2.1
1	A	121	CYS	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,

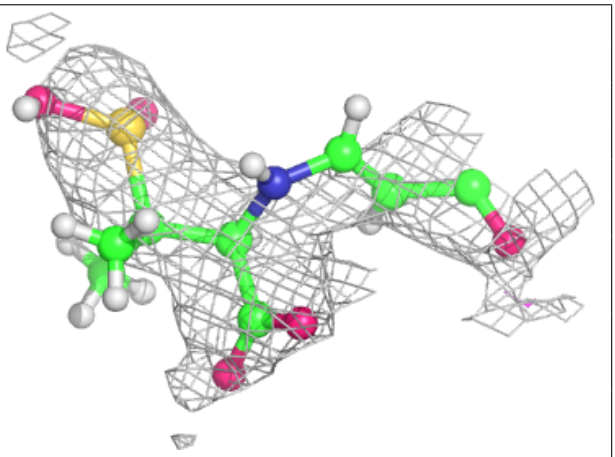
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

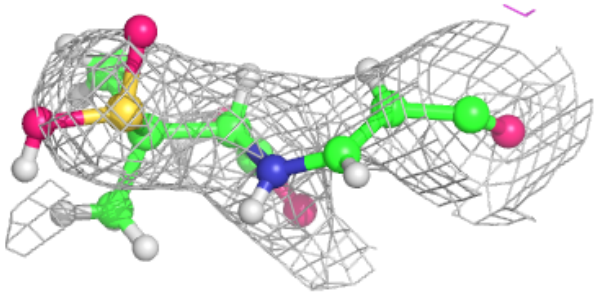
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TSL	B	302	15/15	0.85	0.35	69,114,121,125	1
3	TSL	A	302	15/15	0.86	0.36	62,121,142,146	1
3	TSL	C	302	15/15	0.86	0.46	74,136,152,167	1
3	TSL	D	302	15/15	0.88	0.32	69,118,129,138	1
2	PO4	C	301	5/5	0.93	0.20	73,75,80,88	0
2	PO4	D	301	5/5	0.95	0.24	73,76,84,88	0
2	PO4	B	301	5/5	0.96	0.22	57,62,65,67	0
2	PO4	A	301	5/5	0.98	0.19	46,49,52,54	0

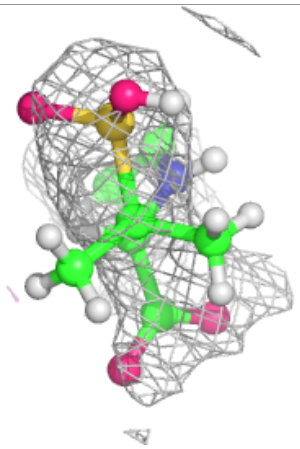
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TSL B 302:

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

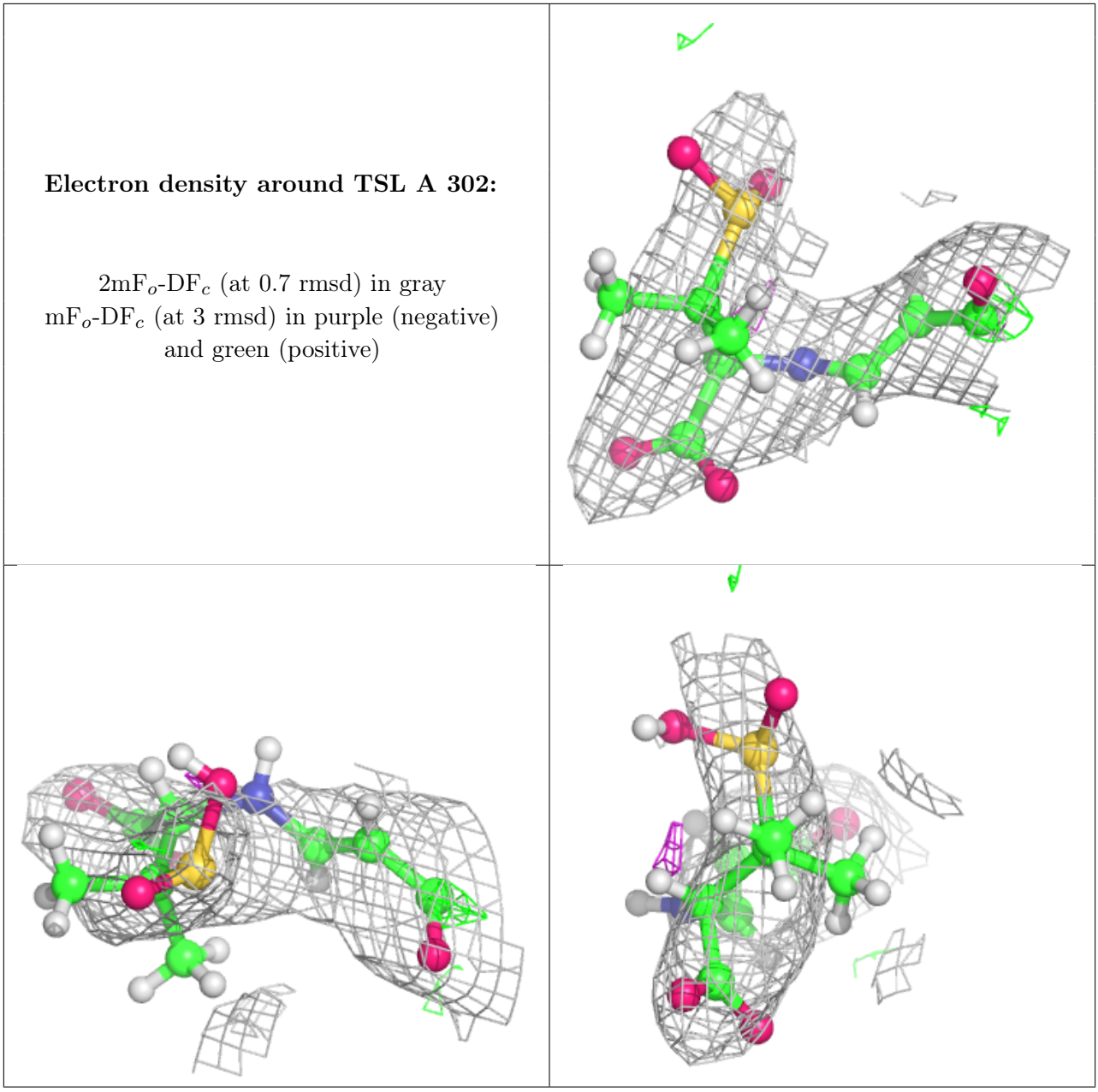






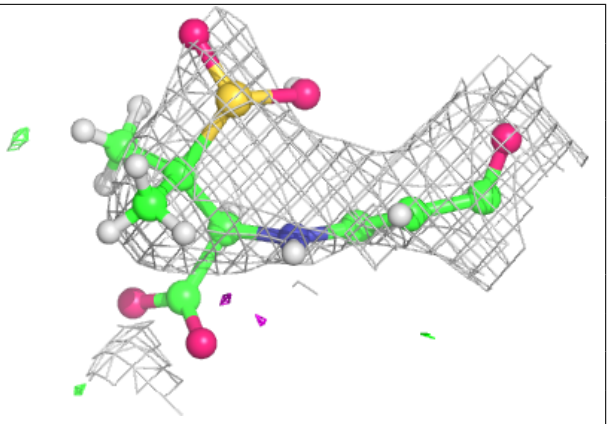
Electron density around TSL A 302:

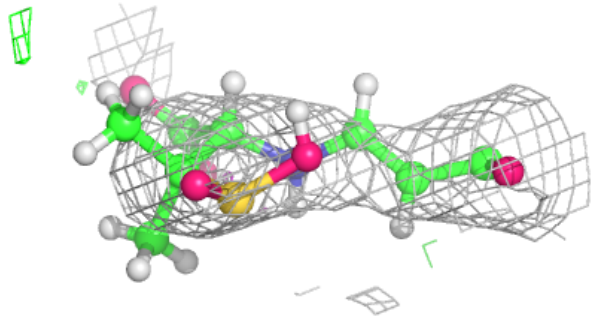
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

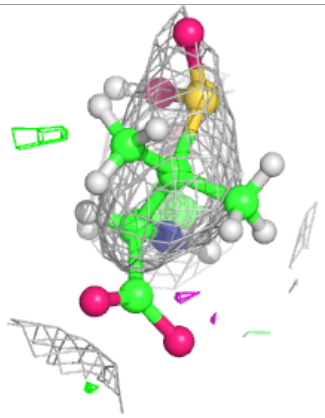


Electron density around TSL C 302:

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

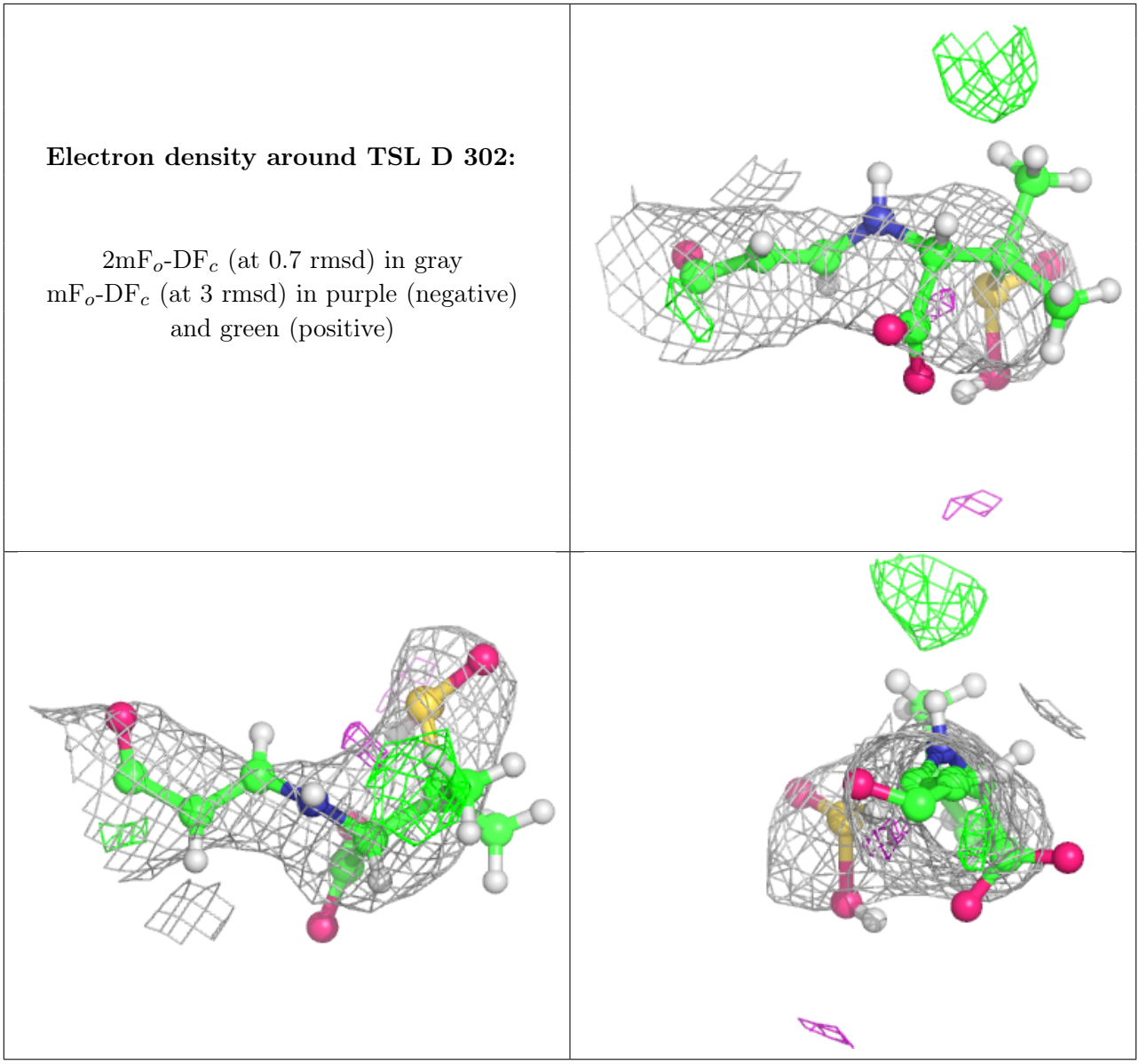






Electron density around TSL D 302:

$2mF_o$-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.