



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:07 PM UTC

PDB ID : 7FT3 / pdb_00007ft3
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z291279160
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

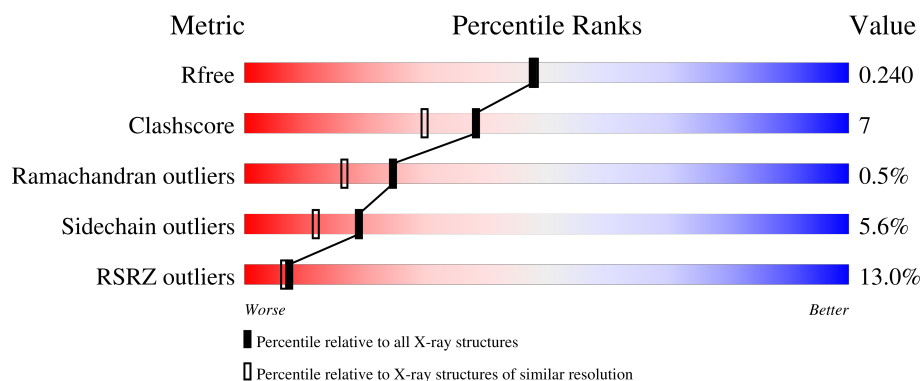
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	195	18% 77% 17% • •
1	B	195	5% 79% 17% • • •
1	C	195	15% 74% 22% • • •
1	D	195	13% 75% 20% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	D	305	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6415 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 Syntenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	1	0
			1481	935	262	275	9			
1	B	193	Total	C	N	O	S	0	1	0
			1495	943	264	279	9			
1	C	193	Total	C	N	O	S	0	3	0
			1514	953	270	282	9			
1	D	191	Total	C	N	O	S	0	2	0
			1489	939	263	278	9			

There are 8 discrepancies between the modelled and reference sequences:

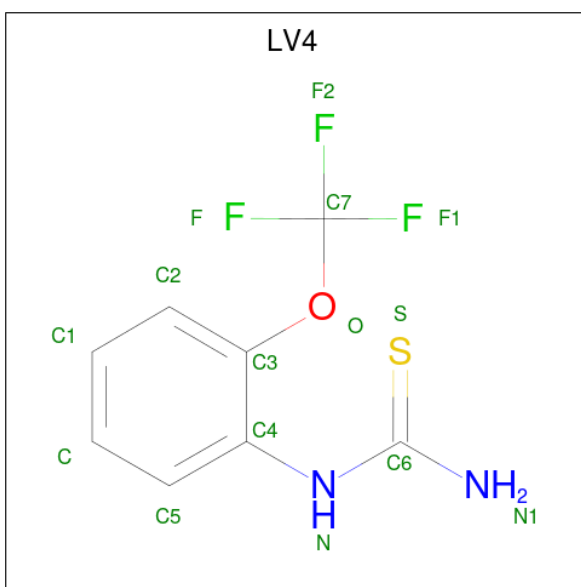
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag	UNP O00560
D	105	MET	-	expression tag	UNP O00560

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



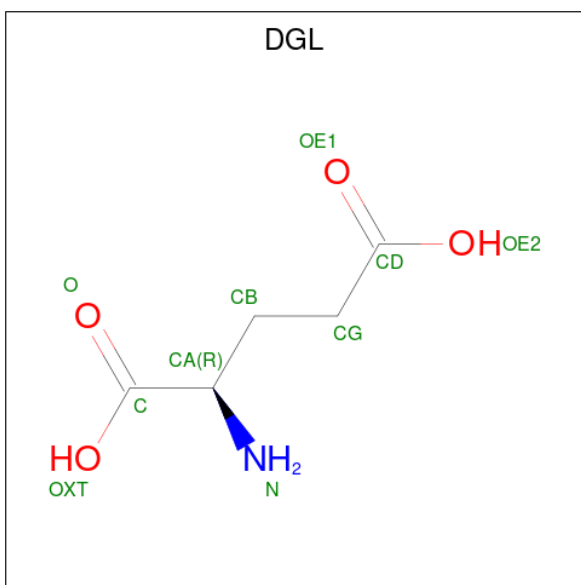
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 1-[2-(trifluoromethoxy)phenyl]thiourea (CCD ID: LV4) (formula: $C_8H_7F_3N_2OS$) (labeled as "Ligand of Interest" by depositor).



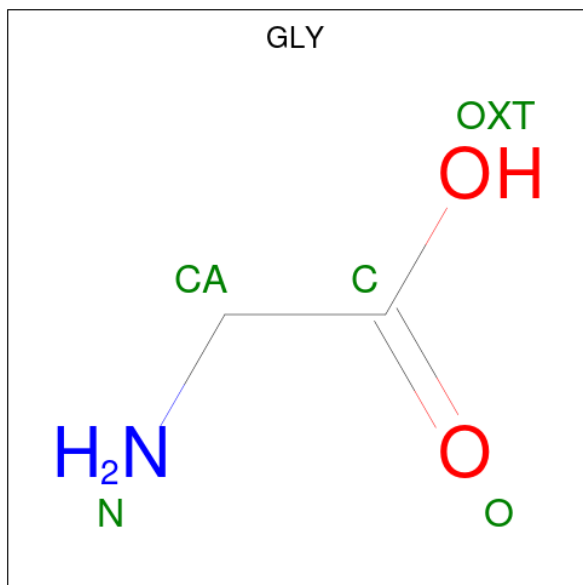
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 15	C 8	F 3	N 2	O 1	S 1	0	0
3	C	1	Total 15	C 8	F 3	N 2	O 1	S 1	0	0
3	C	1	Total 15	C 8	F 3	N 2	O 1	S 1	0	0
3	D	1	Total 15	C 8	F 3	N 2	O 1	S 1	0	0

- Molecule 4 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



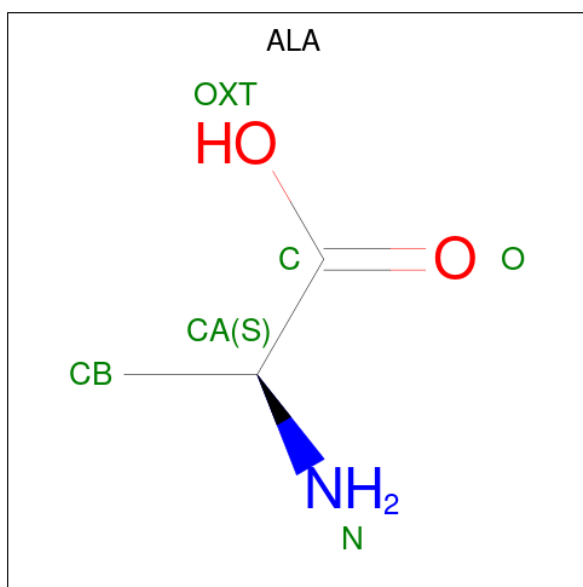
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 7 is ALANINE (CCD ID: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			6	3	1	2		

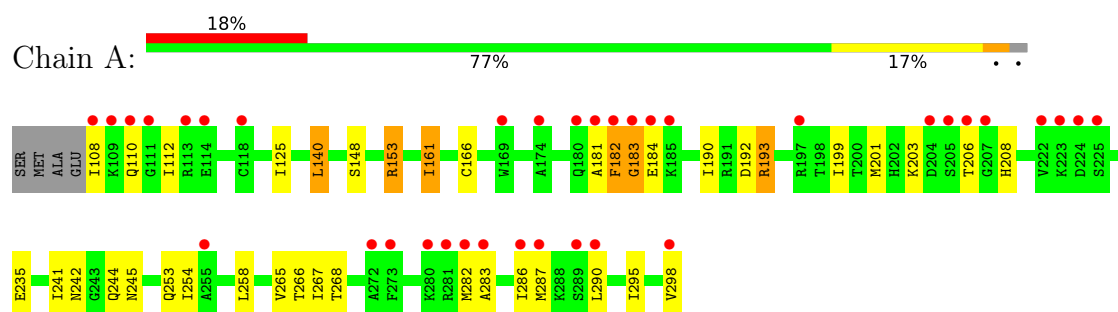
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total 44	O 44	0	0
8	B	97	Total 97	O 97	0	1
8	C	65	Total 65	O 65	0	0
8	D	87	Total 87	O 87	0	1

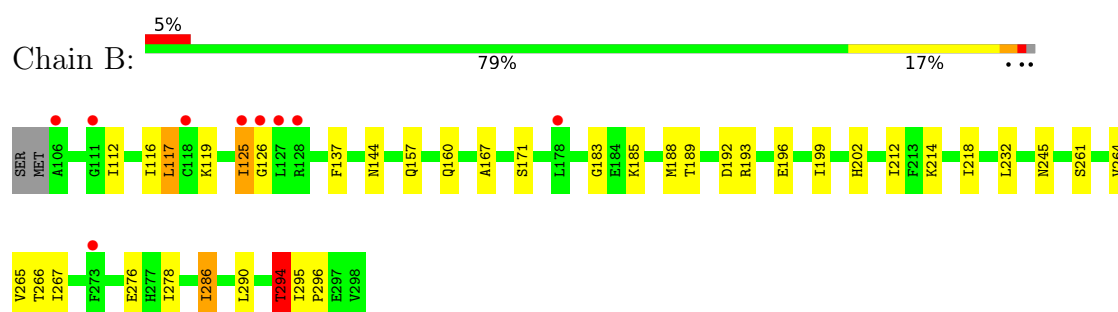
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

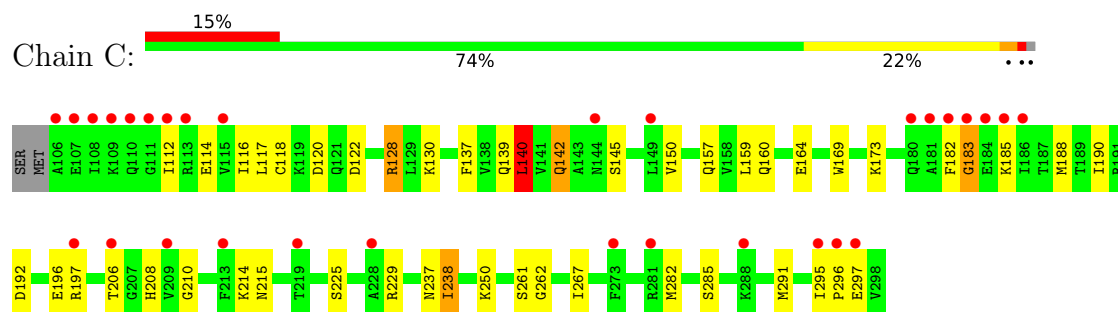
• Molecule 1: Syntenin-1



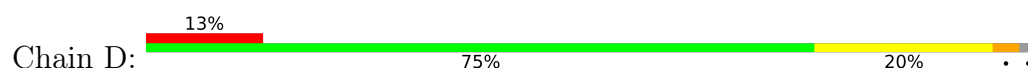
• Molecule 1: Syntenin-1

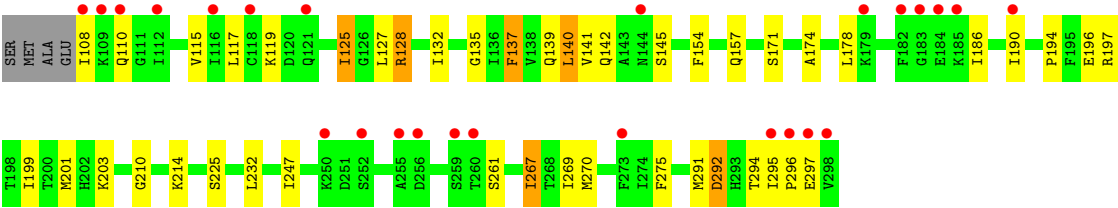


• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.55Å 49.70Å 115.89Å 90.00° 95.04° 90.00°	Depositor
Resolution (Å)	115.45 – 2.05 115.45 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (115.45-2.05) 99.6 (115.45-2.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.279 (Not available) , 0.240	Depositor DCC
R_{free} test set	2827 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5416e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, DGL, LV4, SO4

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	1.17	1/1502 (0.1%)	1.46	4/2019 (0.2%)
1	B	1.30	6/1516 (0.4%)	1.54	8/2038 (0.4%)
1	C	1.19	2/1535 (0.1%)	1.55	8/2063 (0.4%)
1	D	1.30	12/1510 (0.8%)	1.59	5/2030 (0.2%)
All	All	1.24	21/6063 (0.3%)	1.53	25/8150 (0.3%)

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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154	PHE	C-O	6.62	1.31	1.23
1	B	167	ALA	C-O	6.16	1.31	1.24
1	B	125	ILE	C-O	5.80	1.29	1.24
1	D	247	ILE	C-O	5.80	1.29	1.24
1	B	199	ILE	C-O	5.79	1.30	1.23
1	B	126	GLY	C-O	5.73	1.31	1.23
1	A	254	ILE	C-O	5.69	1.30	1.24
1	D	197	ARG	N-CA	5.64	1.53	1.45
1	D	292	ASP	CB-CG	5.62	1.66	1.52
1	D	128	ARG	C-O	5.55	1.30	1.24
1	C	130	LYS	C-O	5.54	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	ILE	C-O	5.46	1.29	1.24
1	D	135	GLY	C-O	5.34	1.29	1.23
1	D	132	ILE	C-O	5.32	1.29	1.24
1	D	141	VAL	C-O	5.27	1.29	1.24
1	D	194	PRO	C-O	-5.25	1.17	1.24
1	D	247	ILE	N-CA	5.11	1.52	1.46
1	D	137	PHE	C-O	5.08	1.30	1.23
1	C	238	ILE	N-CA	5.04	1.51	1.46
1	B	212	ILE	CA-C	5.04	1.58	1.52
1	D	190	ILE	C-O	5.02	1.29	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	ASP	CA-CB-CG	-7.24	105.36	112.60
1	D	174	ALA	N-CA-C	-6.90	103.69	111.07
1	C	237	ASN	CA-CB-CG	-6.36	106.25	112.60
1	B	294	THR	CB-CA-C	-6.24	98.45	109.62
1	B	232	LEU	CA-C-O	-6.20	114.22	121.16
1	C	192	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	268	THR	CA-CB-OG1	-6.00	100.60	109.60
1	B	266	THR	CA-CB-OG1	-5.93	100.71	109.60
1	B	192	ASP	CA-CB-CG	5.80	118.41	112.60
1	C	130	LYS	CA-C-N	5.76	129.54	121.24
1	C	130	LYS	C-N-CA	5.76	129.54	121.24
1	B	160	GLN	CB-CG-CD	-5.76	102.81	112.60
1	A	266	THR	CA-CB-OG1	-5.73	101.01	109.60
1	D	275	PHE	N-CA-C	-5.66	105.19	111.36
1	C	215	ASN	CA-C-O	-5.46	115.20	121.54
1	C	142	GLN	CA-C-O	-5.29	115.02	121.05
1	D	174	ALA	CA-C-N	5.20	127.56	120.54
1	D	174	ALA	C-N-CA	5.20	127.56	120.54
1	B	286	ILE	CA-C-N	5.19	127.66	120.29
1	B	286	ILE	C-N-CA	5.19	127.66	120.29
1	A	153	ARG	CB-CG-CD	5.18	123.22	111.30
1	A	244	GLN	CB-CG-CD	-5.16	103.83	112.60
1	B	276	GLU	CB-CA-C	5.11	119.54	110.85
1	C	140	LEU	CA-C-N	5.01	129.25	122.93
1	C	140	LEU	C-N-CA	5.01	129.25	122.93

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLN	Peptide
1	B	214	LYS	Mainchain
1	D	127	LEU	Peptide

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	1481	0	1530	24	0
1	B	1495	0	1541	17	0
1	C	1514	0	1558	25	0
1	D	1489	0	1533	19	0
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	12	0	18	0	0
2	D	8	0	12	0	0
3	B	15	0	0	0	0
3	C	30	0	0	0	0
3	D	15	0	0	0	0
4	B	10	0	7	1	0
4	D	10	0	7	0	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0
6	D	15	0	0	0	0
7	D	6	0	4	0	0
8	A	44	0	0	0	0
8	B	97	0	0	1	0
8	C	65	0	0	1	0
8	D	87	0	0	0	0
All	All	6415	0	6232	85	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 7.

All (85) 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:C:206:THR:HG1	1:C:208:HIS:HD1	1.03	0.91
1:C:137:PHE:CE2	1:C:157:GLN:HB2	2.26	0.70
1:C:229:ARG:NH2	8:C:402:HOH:O	2.28	0.67
1:C:296:PRO:HD2	1:C:297:GLU:OE1	1.95	0.66
1:A:108:ILE:HA	1:A:192:ASP:OD2	1.97	0.64
1:B:117:LEU:HD12	1:B:117:LEU:N	2.12	0.64
1:C:157:GLN:HG2	1:C:159:LEU:CD1	2.29	0.62
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.28	0.62
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.00	0.61
1:A:282:MET:HE3	1:A:287:MET:CG	2.30	0.60
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.84	0.59
1:D:128:ARG:HB2	1:D:140:LEU:HB3	1.84	0.59
1:A:286:ILE:HG23	1:A:290:LEU:HD12	1.87	0.57
1:B:119:LYS:HB2	1:B:183:GLY:HA3	1.88	0.56
1:A:282:MET:HE3	1:A:287:MET:HG3	1.87	0.55
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.91	0.53
1:C:128:ARG:HD3	1:C:140:LEU:HD22	1.89	0.53
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.91	0.53
1:C:128:ARG:CD	1:C:140:LEU:HD22	2.38	0.53
1:D:142:GLN:O	1:D:145:SER:OG	2.22	0.53
1:A:182:PHE:O	1:A:184:GLU:N	2.42	0.52
1:A:181:ALA:O	1:A:183:GLY:N	2.43	0.52
1:D:128:ARG:HH11	1:D:128:ARG:HG2	1.76	0.51
1:A:203:LYS:HA	1:A:208:HIS:O	2.11	0.51
1:C:261:SER:OG	1:C:262:GLY:N	2.42	0.51
1:C:182:PHE:C	1:C:183:GLY:O	2.53	0.51
1:D:119:LYS:CE	1:D:186:ILE:HD11	2.41	0.51
1:D:119:LYS:HE3	1:D:186:ILE:HD11	1.94	0.50
1:A:140:LEU:HD12	1:A:282:MET:SD	2.51	0.50
1:D:128:ARG:HG2	1:D:128:ARG:NH1	2.27	0.50
1:A:283:ALA:HB3	1:A:286:ILE:HD12	1.93	0.49
1:A:182:PHE:H	1:A:182:PHE:HD2	1.59	0.49
1:D:140:LEU:HD12	1:D:291:MET:HE2	1.96	0.48
1:A:206:THR:OG1	1:A:208:HIS:ND1	2.40	0.48
1:B:171:SER:OG	4:B:304:DGL:OXT	2.31	0.47
1:D:203:LYS:NZ	1:D:261:SER:O	2.39	0.47
1:B:117:LEU:HD23	1:B:125:ILE:HG23	1.98	0.46
1:B:245:ASN:OD1	1:B:245:ASN:C	2.58	0.46
1:D:196:GLU:HG3	1:D:270:MET:HE2	1.97	0.46
1:C:210:GLY:HA3	1:C:225:SER:CB	2.45	0.46
1:D:137:PHE:CE2	1:D:157:GLN:HB2	2.52	0.45
1:B:295:ILE:HA	1:B:296:PRO:HD3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASP:OD1	1:C:122:ASP:N	2.51	0.44
1:A:245:ASN:C	1:A:245:ASN:OD1	2.60	0.44
1:D:267:ILE:HG13	1:D:269:ILE:HG23	1.99	0.44
1:B:193:ARG:HB3	1:B:196:GLU:HB2	2.00	0.44
1:C:139:GLN:O	1:C:282:MET:HE1	2.18	0.44
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.82	0.44
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.99	0.44
1:C:160:GLN:HA	1:C:164:GLU:O	2.18	0.44
1:B:112:ILE:CG2	1:B:189:THR:CG2	2.96	0.43
1:B:116:ILE:HG23	1:B:185:LYS:HG2	2.00	0.43
1:C:297:GLU:O	1:C:297:GLU:HG2	2.18	0.43
1:B:125:ILE:HD12	1:B:125:ILE:N	2.34	0.43
1:B:202:HIS:CE1	1:B:264:VAL:HG22	2.53	0.43
1:A:112:ILE:HA	1:A:190:ILE:O	2.18	0.43
1:B:286:ILE:HG23	1:B:290:LEU:HD12	2.00	0.43
1:C:140:LEU:HD12	1:C:291:MET:HE2	2.01	0.43
1:A:258:LEU:CD2	1:A:265:VAL:HG11	2.49	0.43
1:D:232:LEU:HD11	1:D:267:ILE:HD11	2.00	0.43
1:C:188:MET:HE2	1:C:190:ILE:HD11	2.00	0.42
1:A:182:PHE:CD2	1:A:182:PHE:N	2.86	0.42
1:A:241:ILE:O	1:A:242:ASN:C	2.62	0.42
1:B:119:LYS:HB2	1:B:183:GLY:CA	2.49	0.42
1:B:261:SER:HB2	8:B:466:HOH:O	2.19	0.42
1:B:294:THR:HG22	1:B:295:ILE:N	2.34	0.42
1:C:128:ARG:HB2	1:C:140:LEU:HB3	2.01	0.42
1:A:140:LEU:HD11	1:A:286:ILE:HG22	2.02	0.42
1:C:295:ILE:HA	1:C:296:PRO:HD3	1.92	0.42
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.20	0.42
1:D:201:MET:HE3	1:D:201:MET:HB2	1.89	0.41
1:D:210:GLY:HA3	1:D:225:SER:CB	2.51	0.41
1:C:120:ASP:OD1	1:C:120:ASP:C	2.64	0.41
1:A:192:ASP:O	1:A:193:ARG:C	2.63	0.41
1:B:137:PHE:CE2	1:B:157:GLN:HB2	2.55	0.41
1:A:161:ILE:HG13	1:A:166:CYS:SG	2.61	0.41
1:C:169:TRP:CE2	1:C:173:LYS:HE2	2.56	0.41
1:C:142:GLN:O	1:C:145:SER:OG	2.27	0.41
1:C:238:ILE:HG23	1:C:267:ILE:HG23	2.02	0.41
1:D:128:ARG:HH11	1:D:128:ARG:CG	2.34	0.41
1:A:182:PHE:C	1:A:184:GLU:H	2.29	0.40
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.20	0.40
1:C:116:ILE:HG23	1:C:185:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.04	0.40
1:A:286:ILE:HG23	1:A:290:LEU:CD1	2.51	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	190/195 (97%)	176 (93%)	11 (6%)	3 (2%)	7	2
1	B	192/195 (98%)	184 (96%)	8 (4%)	0	100	100
1	C	194/195 (100%)	182 (94%)	11 (6%)	1 (0%)	24	16
1	D	191/195 (98%)	185 (97%)	6 (3%)	0	100	100
All	All	767/780 (98%)	727 (95%)	36 (5%)	4 (0%)	24	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	A	183	GLY
1	C	183	GLY
1	A	193	ARG

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	166/168 (99%)	158 (95%)	8 (5%)	23	16
1	B	167/168 (99%)	160 (96%)	7 (4%)	26	20
1	C	169/168 (101%)	159 (94%)	10 (6%)	18	10
1	D	167/168 (99%)	155 (93%)	12 (7%)	13	7
All	All	669/672 (100%)	632 (94%)	37 (6%)	19	12

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ILE
1	A	140	LEU
1	A	148	SER
1	A	161	ILE
1	A	199	ILE
1	A	253	GLN
1	A	295	ILE
1	A	298	VAL
1	B	117	LEU
1	B	144	ASN
1	B	188	MET
1	B	265	VAL
1	B	267	ILE
1	B	278	ILE
1	B	294	THR
1	C	112	ILE
1	C	114	GLU
1	C	117	LEU
1	C	118	CYS
1	C	128	ARG
1	C	140	LEU
1	C	150	VAL
1	C	214	LYS
1	C	250	LYS
1	C	285	SER
1	D	108	ILE
1	D	110	GLN
1	D	115	VAL
1	D	117	LEU
1	D	125	ILE
1	D	139	GLN
1	D	140	LEU
1	D	171	SER

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Mol	Chain	Res	Type
1	D	199	ILE
1	D	214	LYS
1	D	267	ILE
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	142	GLN
1	A	180	GLN
1	A	202	HIS
1	A	237	ASN
1	B	139	GLN
1	B	160	GLN
1	B	165	ASN
1	C	230	ASN
1	D	157	GLN

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 [i](#)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DGL	D	308	-	8,9,9	1.02	0	8,11,11	1.01	0
7	ALA	D	307	-	5,5,5	1.18	1 (20%)	6,6,6	1.55	1 (16%)
3	LV4	B	301	-	15,15,15	4.45	4 (26%)	20,21,21	1.69	3 (15%)
4	DGL	B	304	-	8,9,9	1.08	1 (12%)	8,11,11	1.57	1 (12%)
3	LV4	D	301	-	15,15,15	2.96	3 (20%)	20,21,21	1.00	1 (5%)
3	LV4	C	301	-	15,15,15	3.08	3 (20%)	20,21,21	1.36	4 (20%)
2	EDO	C	305	-	3,3,3	0.27	0	2,2,2	0.45	0
3	LV4	C	302	-	15,15,15	2.62	4 (26%)	20,21,21	1.03	1 (5%)
6	SO4	D	304	-	4,4,4	0.32	0	6,6,6	0.06	0
5	GLY	D	309	-	4,4,4	1.09	1 (25%)	3,4,4	1.32	0
2	EDO	D	303	-	3,3,3	0.13	0	2,2,2	0.26	0
2	EDO	C	303	-	3,3,3	0.10	0	2,2,2	0.09	0
5	GLY	C	306	-	4,4,4	1.08	1 (25%)	3,4,4	1.16	0
6	SO4	D	306	-	4,4,4	0.36	0	6,6,6	0.10	0
2	EDO	C	304	-	3,3,3	0.09	0	2,2,2	0.19	0
6	SO4	D	305	-	4,4,4	0.34	0	6,6,6	0.07	0
2	EDO	D	302	-	3,3,3	0.06	0	2,2,2	0.18	0
2	EDO	B	302	-	3,3,3	0.32	0	2,2,2	0.32	0
2	EDO	B	303	-	3,3,3	0.49	0	2,2,2	0.46	0
2	EDO	A	301	-	3,3,3	0.20	0	2,2,2	0.05	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
2	EDO	C	305	-	-	1/1/1/1	-
3	LV4	C	302	-	-	0/9/9/9	0/1/1/1
2	EDO	C	304	-	-	1/1/1/1	-
5	GLY	D	309	-	-	0/2/2/2	-
2	EDO	D	303	-	-	0/1/1/1	-
3	LV4	B	301	-	-	1/9/9/9	0/1/1/1
4	DGL	D	308	-	-	4/9/9/9	-
2	EDO	D	302	-	-	1/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
5	GLY	C	306	-	-	2/2/2/2	-
4	DGL	B	304	-	-	0/9/9/9	-
3	LV4	D	301	-	-	0/9/9/9	0/1/1/1
7	ALA	D	307	-	-	0/4/4/4	-
3	LV4	C	301	-	-	0/9/9/9	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	LV4	C6-S	-13.37	1.50	1.69
3	B	301	LV4	C6-N1	7.21	1.45	1.32
3	C	301	LV4	C6-N1	7.08	1.45	1.32
3	C	301	LV4	C6-S	-6.84	1.59	1.69
3	D	301	LV4	C6-N1	6.76	1.44	1.32
3	C	302	LV4	C6-N1	6.71	1.44	1.32
3	B	301	LV4	C6-N	6.47	1.46	1.34
3	D	301	LV4	C6-S	-6.31	1.60	1.69
3	C	302	LV4	C6-N	6.13	1.45	1.34
3	C	301	LV4	C6-N	5.90	1.45	1.34
3	D	301	LV4	C6-N	5.81	1.44	1.34
3	B	301	LV4	C4-N	4.06	1.49	1.41
3	C	302	LV4	C6-S	-2.37	1.65	1.69
7	D	307	ALA	OXT-C	-2.35	1.23	1.30
3	C	302	LV4	C4-N	2.25	1.46	1.41
4	B	304	DGL	OXT-C	-2.12	1.23	1.30
5	D	309	GLY	OXT-C	-2.03	1.24	1.30
5	C	306	GLY	OXT-C	-2.01	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	LV4	S-C6-N1	-4.40	117.26	123.14
3	B	301	LV4	N1-C6-N	3.88	124.74	117.64
4	B	304	DGL	OXT-C-O	-3.42	116.33	124.08
3	C	301	LV4	S-C6-N1	-3.35	118.67	123.14
7	D	307	ALA	OXT-C-O	-3.29	116.62	124.08
3	C	302	LV4	S-C6-N1	-2.44	119.88	123.14
3	B	301	LV4	C4-N-C6	-2.35	118.70	126.57
3	C	301	LV4	N1-C6-N	2.32	121.90	117.64
3	D	301	LV4	N1-C6-N	2.30	121.84	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	LV4	C3-C4-N	2.20	120.83	116.73
3	C	301	LV4	C4-N-C6	-2.09	119.54	126.57

There are no chirality outliers.

All (12) torsion outliers are listed below:

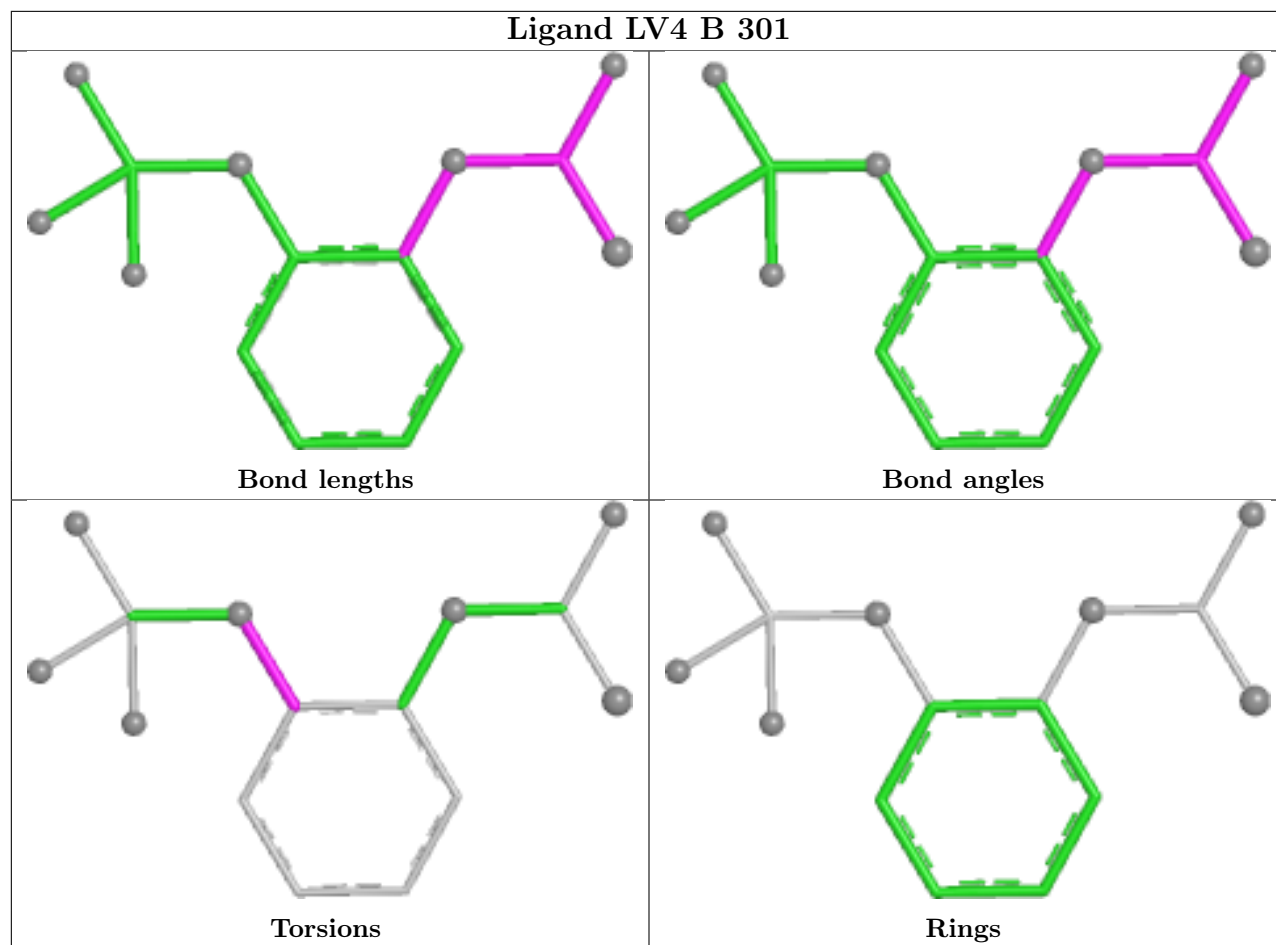
Mol	Chain	Res	Type	Atoms
5	C	306	GLY	O-C-CA-N
5	C	306	GLY	OXT-C-CA-N
2	C	305	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
3	B	301	LV4	C2-C3-O-C7
4	D	308	DGL	OXT-C-CA-CB
4	D	308	DGL	O-C-CA-CB
2	B	302	EDO	O1-C1-C2-O2
2	C	303	EDO	O1-C1-C2-O2
2	C	304	EDO	O1-C1-C2-O2
4	D	308	DGL	N-CA-CB-CG
4	D	308	DGL	CA-CB-CG-CD

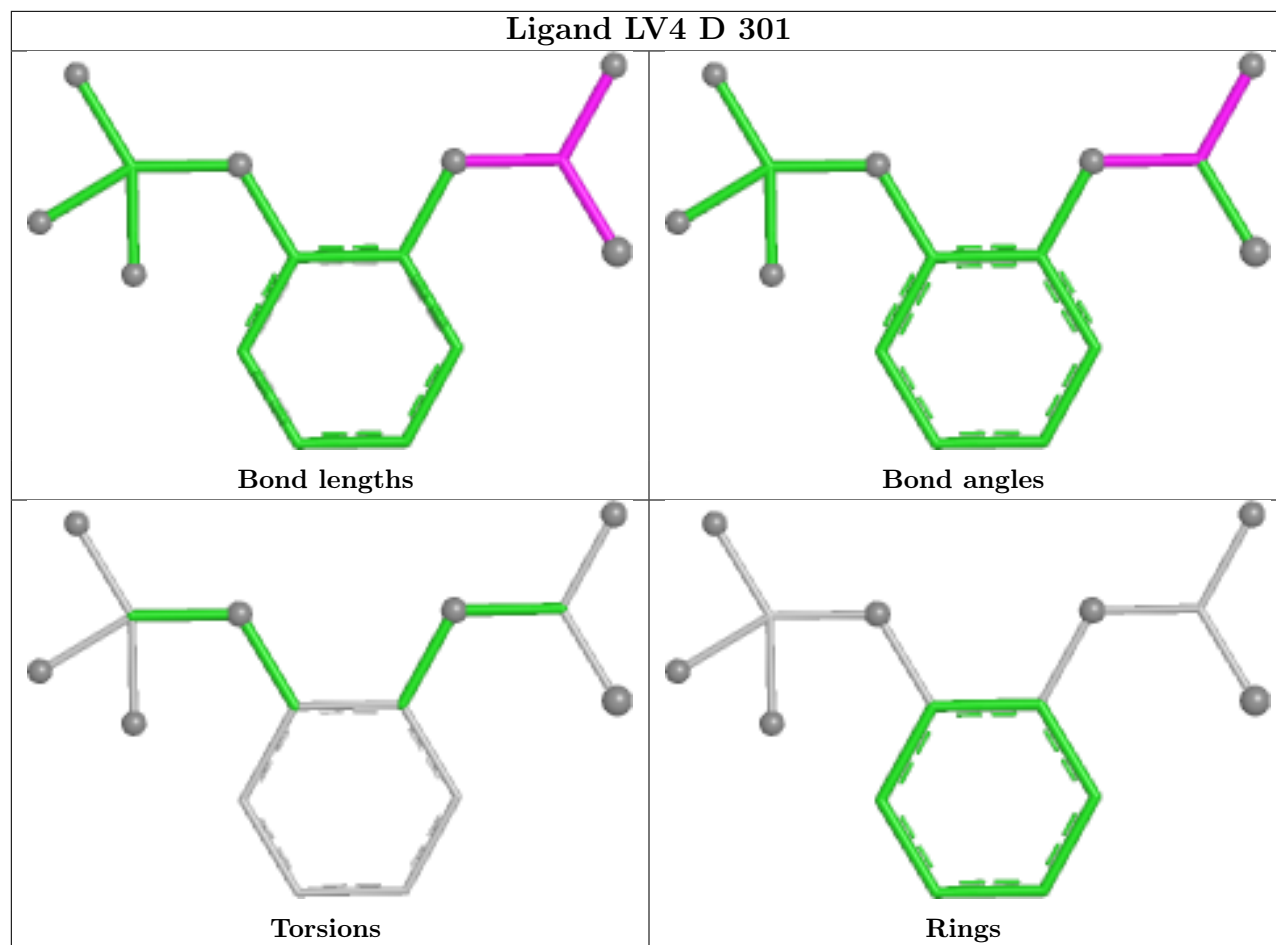
There are no ring outliers.

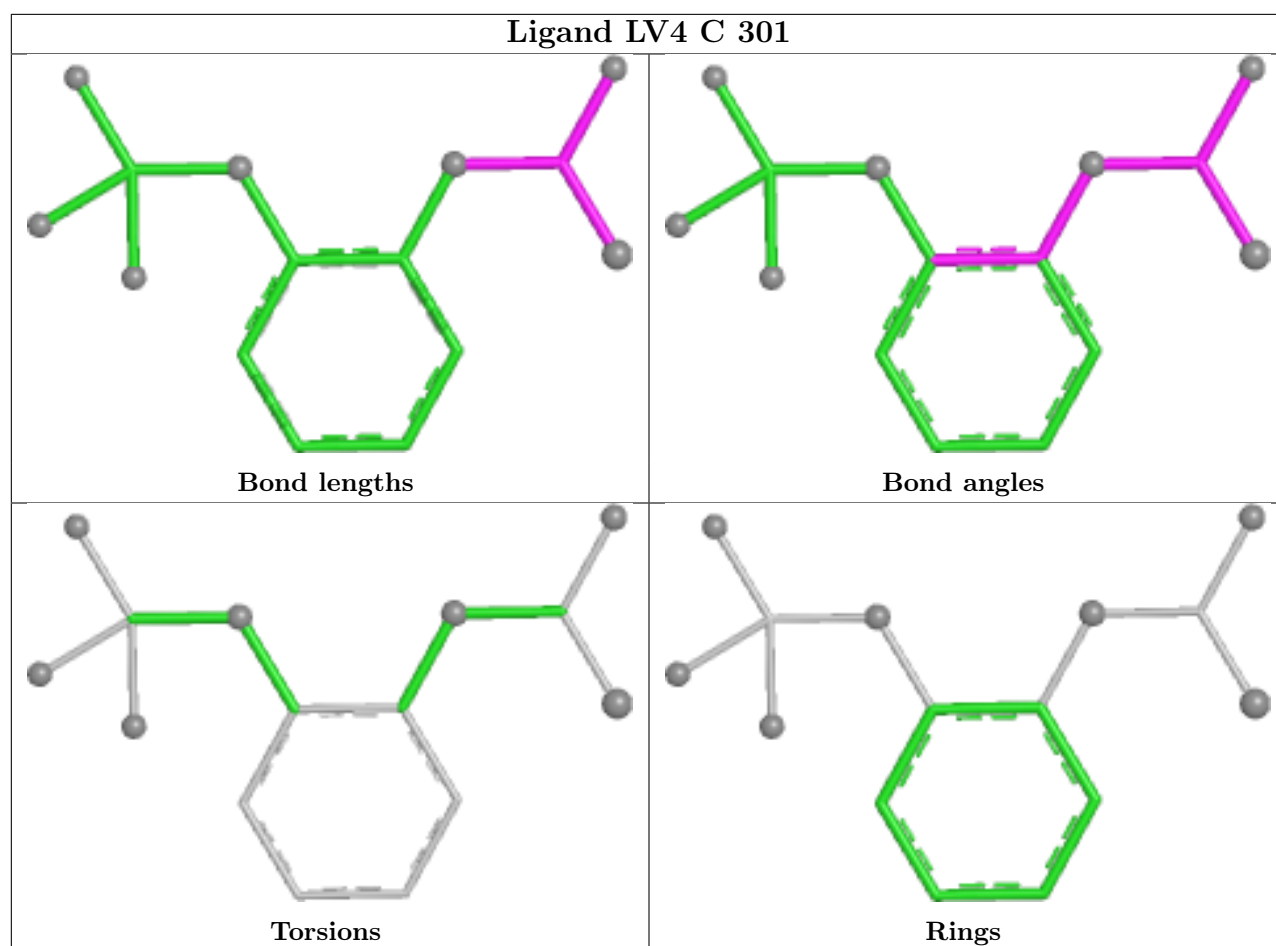
1 monomer is involved in 1 short contact:

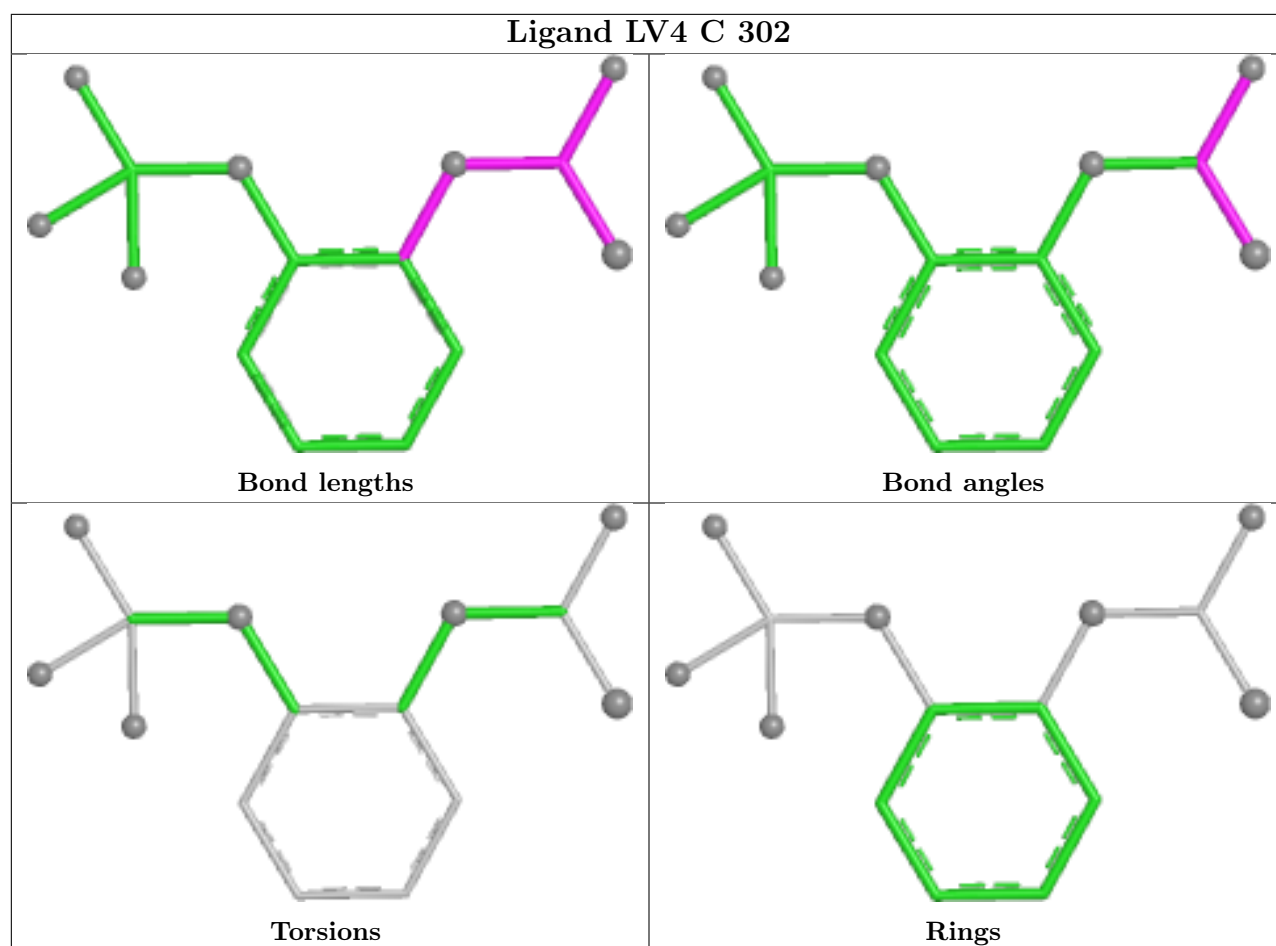
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	304	DGL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	191/195 (97%)	1.17	36 (18%) 3 2	13, 54, 81, 119	18 (9%)
1	B	193/195 (98%)	0.51	9 (4%) 36 36	14, 46, 65, 83	5 (2%)
1	C	193/195 (98%)	1.40	30 (15%) 5 4	14, 47, 66, 79	22 (11%)
1	D	191/195 (97%)	0.72	25 (13%) 7 6	12, 46, 65, 120	8 (4%)
All	All	768/780 (98%)	0.95	100 (13%) 7 6	12, 48, 71, 120	53 (6%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	ALA	13.9
1	C	112	ILE	13.3
1	C	108	ILE	11.9
1	C	111	GLY	11.1
1	C	109	LYS	10.4
1	C	113	ARG	9.0
1	C	180	GLN	8.6
1	C	182	PHE	8.0
1	A	182	PHE	7.7
1	C	181	ALA	7.5
1	C	183	GLY	7.2
1	C	107	GLU	7.0
1	C	186	ILE	6.8
1	C	110	GLN	6.7
1	A	207	GLY	5.9
1	A	206	THR	5.8
1	A	181	ALA	5.7
1	C	295	ILE	5.4
1	D	273[A]	PHE	5.4
1	A	222	VAL	5.2
1	D	260	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	182	PHE	4.7
1	C	185	LYS	4.7
1	D	259	SER	4.6
1	A	225	SER	4.5
1	B	127	LEU	4.4
1	A	273[A]	PHE	4.3
1	D	256[A]	ASP	4.3
1	C	197[A]	ARG	4.3
1	B	125	ILE	4.1
1	C	209	VAL	4.1
1	A	205	SER	4.0
1	A	183	GLY	3.9
1	C	144[A]	ASN	3.9
1	A	109	LYS	3.9
1	A	223	LYS	3.8
1	B	126	GLY	3.8
1	A	108	ILE	3.7
1	A	185	LYS	3.7
1	D	250	LYS	3.7
1	C	296	PRO	3.6
1	A	113	ARG	3.6
1	B	106	ALA	3.6
1	D	184	GLU	3.4
1	D	297	GLU	3.4
1	A	283	ALA	3.4
1	A	180	GLN	3.4
1	B	118	CYS	3.4
1	C	206	THR	3.3
1	D	118	CYS	3.3
1	B	273[A]	PHE	3.3
1	C	184	GLU	3.2
1	C	273[A]	PHE	3.2
1	A	224	ASP	3.1
1	A	280	LYS	3.1
1	D	108	ILE	3.1
1	D	112	ILE	3.1
1	D	121	GLN	3.1
1	A	184	GLU	3.0
1	D	109	LYS	3.0
1	A	204	ASP	2.9
1	C	228	ALA	2.9
1	A	114	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	282	MET	2.8
1	D	116	ILE	2.8
1	D	183	GLY	2.7
1	C	288	LYS	2.7
1	D	255	ALA	2.7
1	A	290	LEU	2.7
1	A	287	MET	2.7
1	C	115	VAL	2.7
1	C	213	PHE	2.7
1	D	296	PRO	2.7
1	D	252	SER	2.7
1	B	111	GLY	2.7
1	A	174	ALA	2.6
1	A	110	GLN	2.6
1	C	281	ARG	2.5
1	C	219	THR	2.5
1	C	297	GLU	2.5
1	A	111	GLY	2.4
1	D	190	ILE	2.4
1	D	298	VAL	2.4
1	A	255	ALA	2.3
1	A	197	ARG	2.3
1	D	185	LYS	2.3
1	A	272	ALA	2.3
1	B	178	LEU	2.3
1	D	144	ASN	2.3
1	D	179	LYS	2.3
1	A	289	SER	2.2
1	A	281	ARG	2.2
1	A	118	CYS	2.2
1	D	110	GLN	2.2
1	A	286	ILE	2.2
1	C	149	LEU	2.1
1	B	128	ARG	2.1
1	D	295	ILE	2.1
1	A	169	TRP	2.1
1	A	298	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

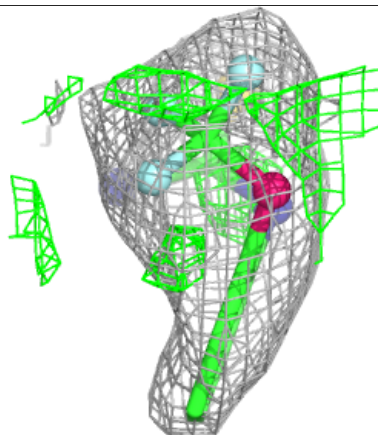
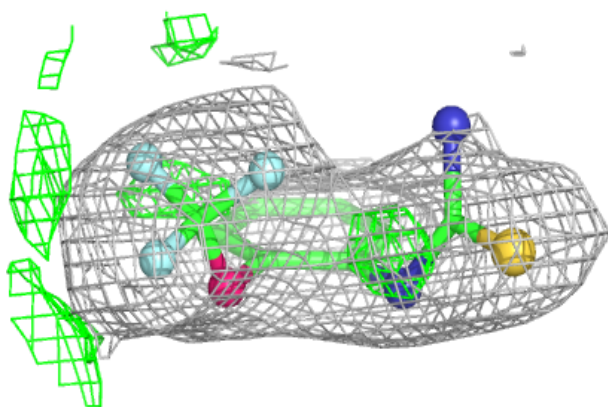
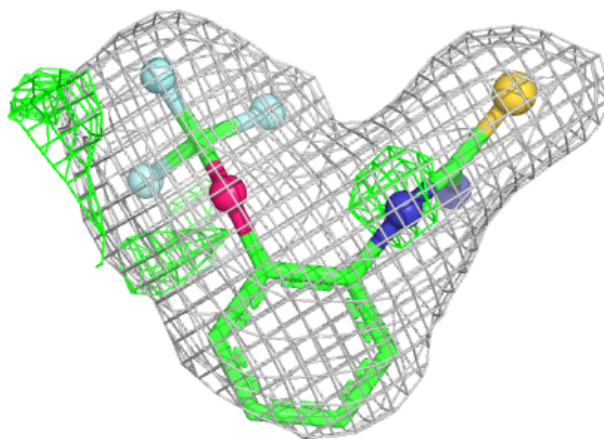
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	D	305	5/5	0.61	0.41	104,105,106,107	5
4	DGL	D	308	10/10	0.77	0.16	43,63,68,74	0
6	SO4	D	306	5/5	0.78	0.21	45,49,50,50	5
5	GLY	C	306	5/5	0.85	0.12	53,54,63,68	0
5	GLY	D	309	5/5	0.86	0.13	60,65,72,73	0
4	DGL	B	304	10/10	0.87	0.10	47,58,64,78	0
2	EDO	D	302	4/4	0.88	0.12	34,35,36,37	0
6	SO4	D	304	5/5	0.89	0.09	71,76,88,91	0
2	EDO	C	305	4/4	0.89	0.17	60,61,63,63	0
2	EDO	C	303	4/4	0.89	0.11	38,41,43,51	0
7	ALA	D	307	6/6	0.89	0.15	62,72,77,80	0
3	LV4	C	301	15/15	0.90	0.14	48,52,54,55	15
3	LV4	B	301	15/15	0.91	0.12	52,54,57,57	15
2	EDO	C	304	4/4	0.92	0.18	53,58,59,61	0
2	EDO	D	303	4/4	0.92	0.12	48,49,51,51	0
2	EDO	A	301	4/4	0.92	0.15	43,43,44,48	0
2	EDO	B	302	4/4	0.93	0.10	40,42,43,46	0
3	LV4	D	301	15/15	0.93	0.10	48,49,50,51	0
3	LV4	C	302	15/15	0.94	0.08	56,60,61,61	0
2	EDO	B	303	4/4	0.94	0.09	30,34,35,36	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.

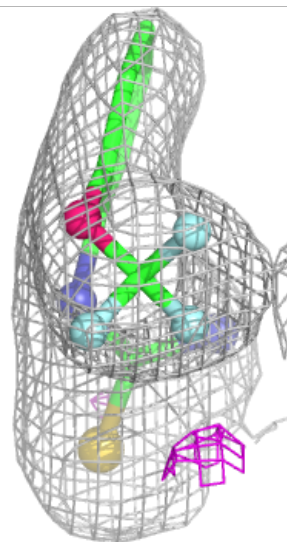
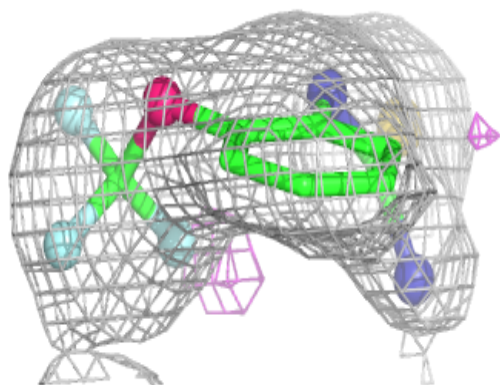
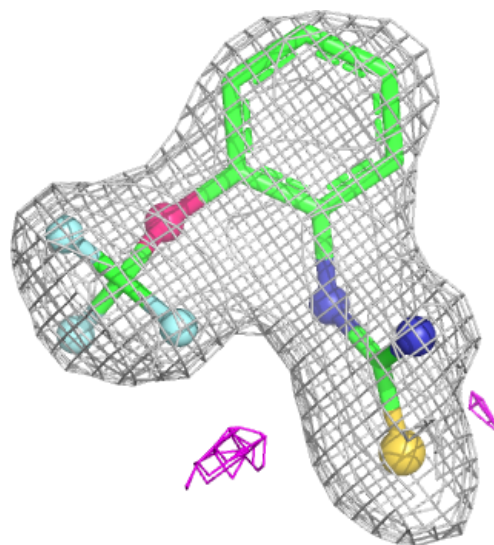
Electron density around LV4 C 301:

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



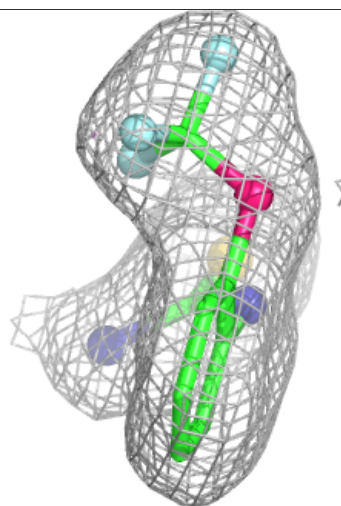
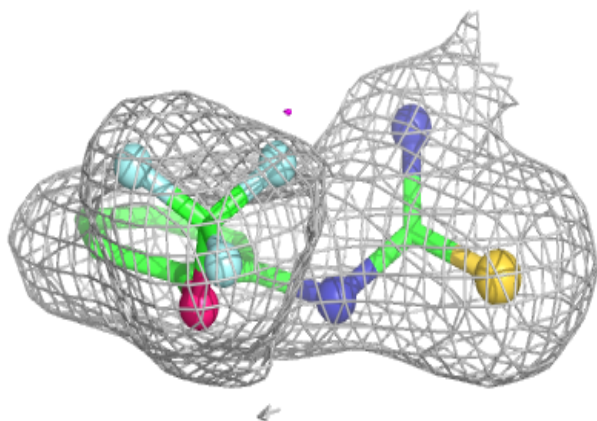
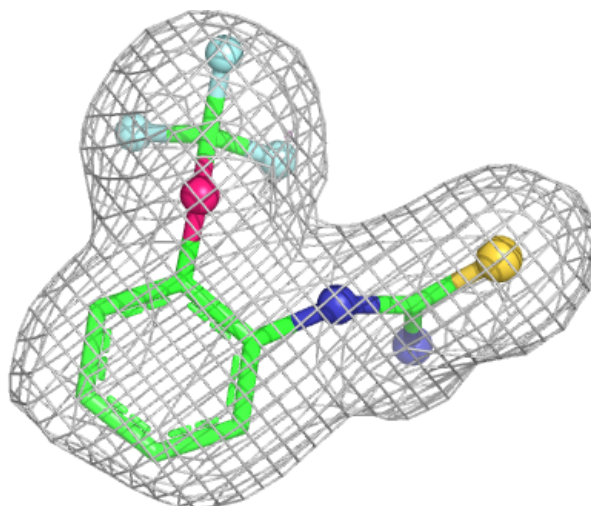
Electron density around LV4 B 301:

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



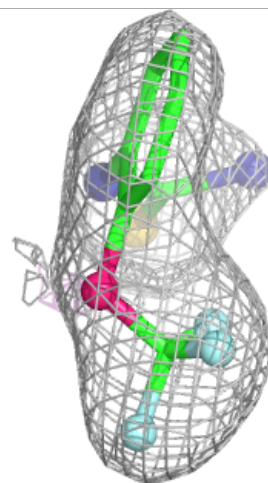
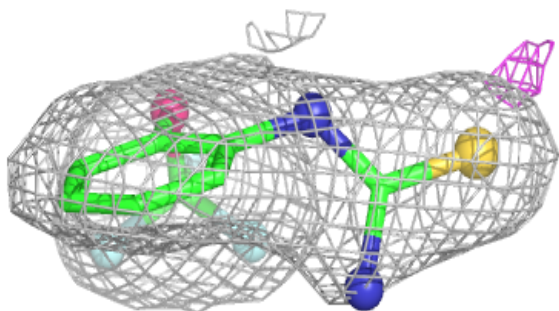
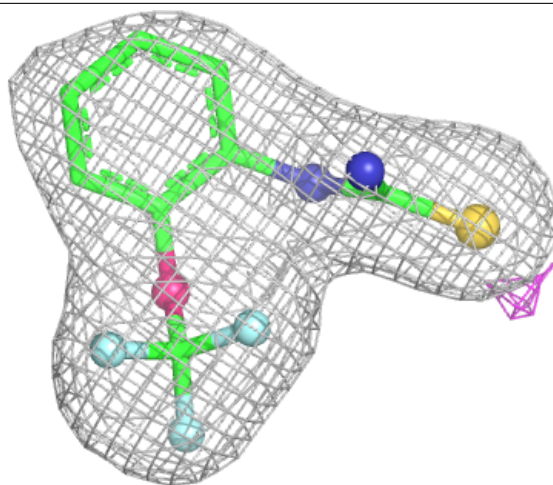
Electron density around LV4 D 301:

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



Electron density around LV4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.