



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:06 AM UTC

PDB ID : 7FSU / pdb_00007fsu
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z729726784
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 1.97 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

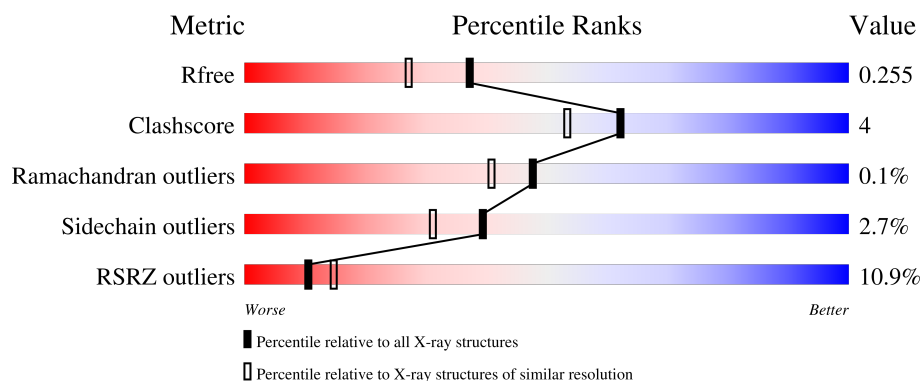
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	19% 86% 11% ..
1	B	195	9% 83% 14% ...
1	C	195	10% 86% 12% ..
1	D	195	5% 84% 13% ..

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	304	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6424 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:

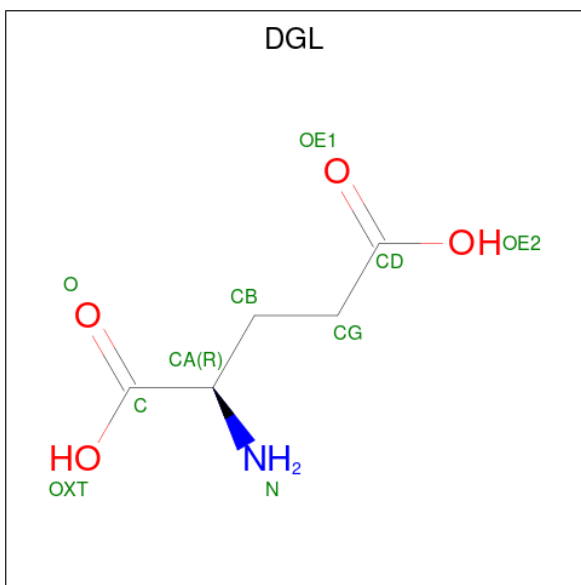
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



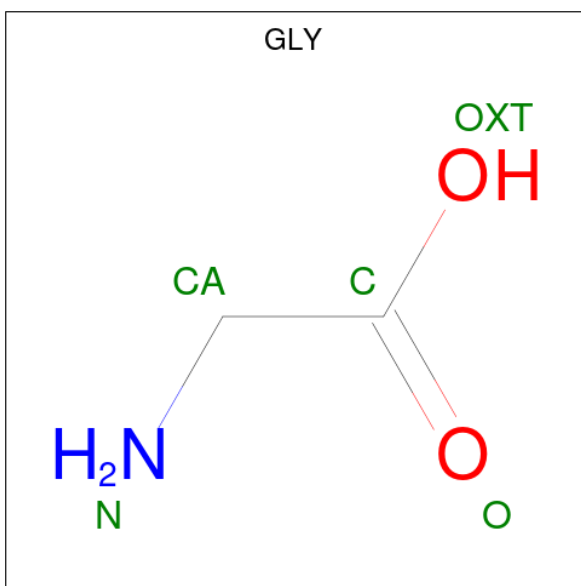
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: C₅H₉NO₄).



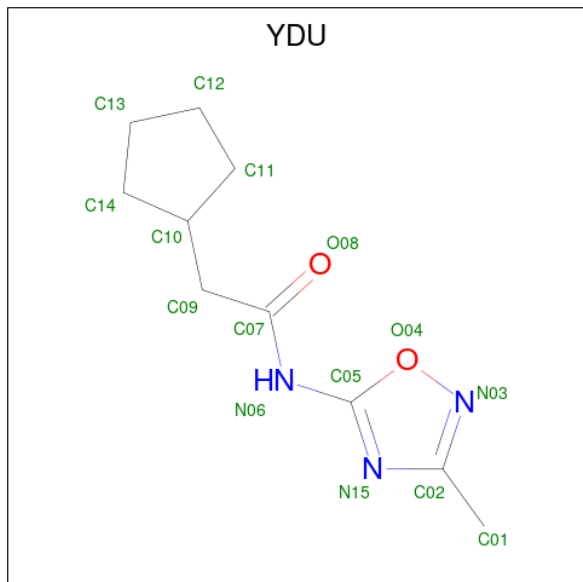
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



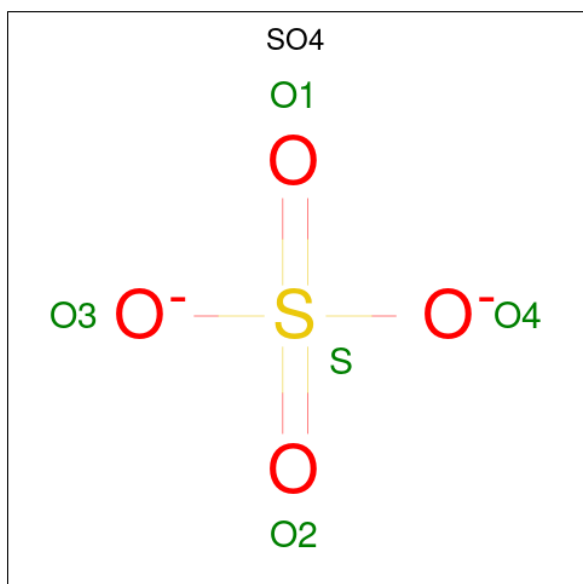
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			5	2	1	2		
4	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 5 is 2-cyclopentyl-N-(3-methyl-1,2,4-oxadiazol-5-yl)acetamide (CCD ID: YDU) (formula: $C_{10}H_{15}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			15	10	3	2		

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



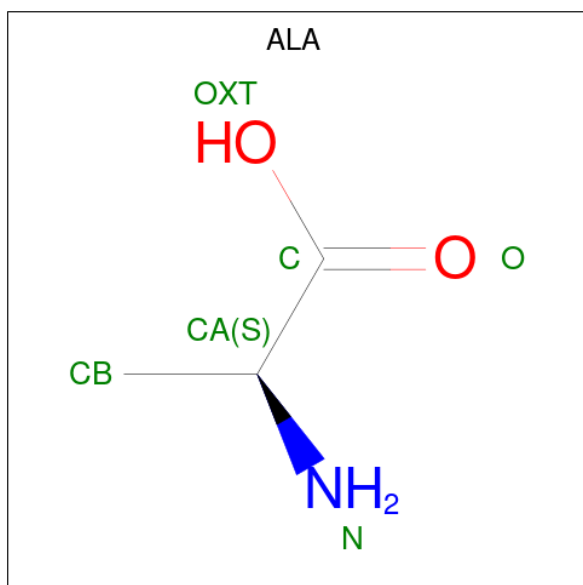
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

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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		

- Molecule 7 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



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

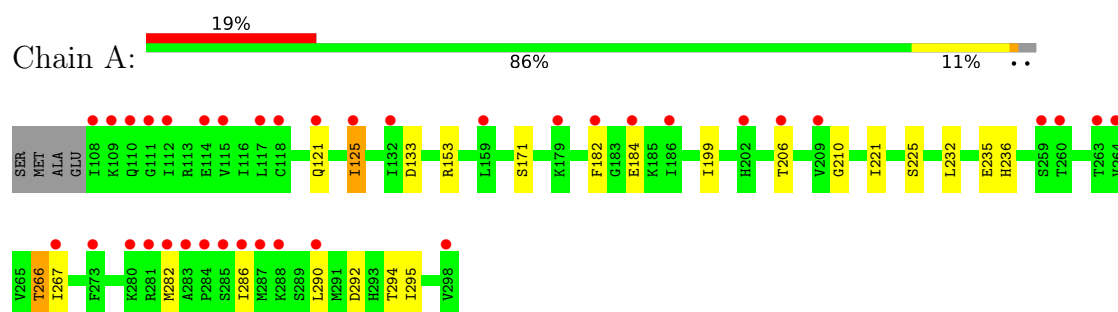
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	46	Total	O	0	0
			46	46		
8	B	105	Total	O	0	1
			105	105		
8	C	73	Total	O	0	1
			74	74		
8	D	121	Total	O	0	2
			122	122		

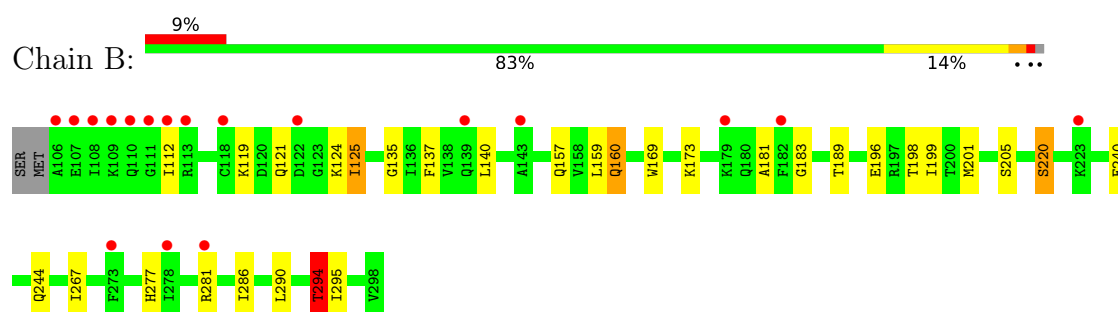
3 Residue-property plots [i](#)

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.

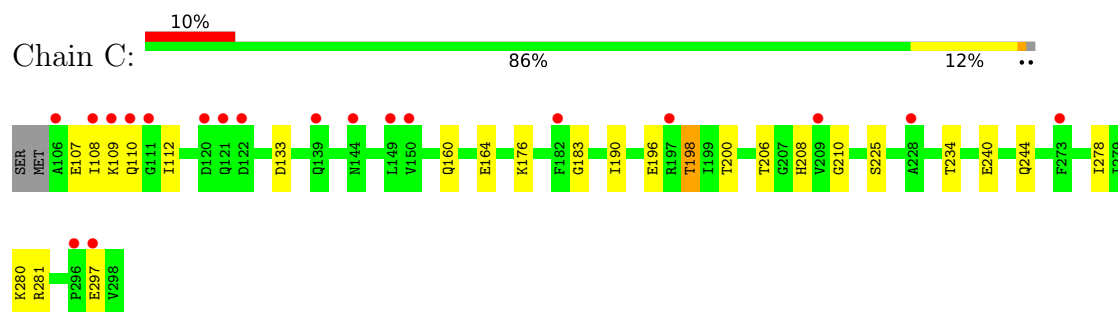
• Molecule 1: Syntenin-1



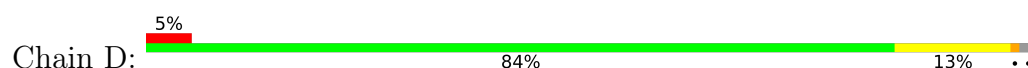
• Molecule 1: Syntenin-1

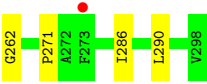
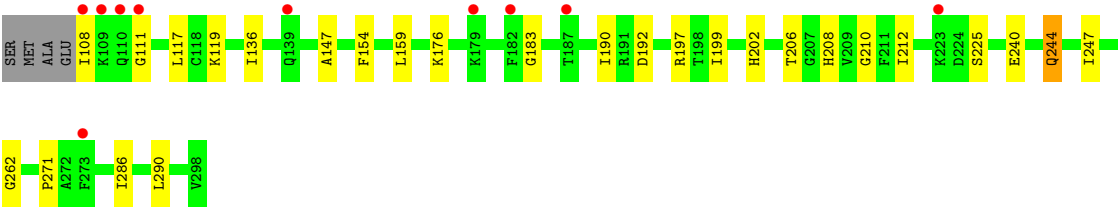


• Molecule 1: Syntenin-1



• 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	80.95Å 49.45Å 114.74Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	114.30 – 1.97 114.30 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (114.30-1.97) 99.7 (114.30-1.97)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.248 0.215 , 0.255	Depositor DCC
R_{free} test set	3127 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6424	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.81 % 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 4.3314e-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: DGL, YDU, EDO, 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	0/1502	1.49	3/2019 (0.1%)
1	B	1.24	4/1516 (0.3%)	1.50	9/2038 (0.4%)
1	C	1.19	1/1535 (0.1%)	1.47	3/2063 (0.1%)
1	D	1.29	4/1510 (0.3%)	1.51	8/2030 (0.4%)
All	All	1.22	9/6063 (0.1%)	1.49	23/8150 (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	C	0	1
1	D	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	190	ILE	C-O	7.97	1.33	1.24
1	C	196	GLU	C-O	-6.54	1.15	1.23
1	B	199	ILE	C-O	6.50	1.30	1.24
1	B	135	GLY	C-O	6.38	1.31	1.23
1	B	277	HIS	CE1-NE2	6.07	1.38	1.32
1	B	196	GLU	C-O	-5.66	1.16	1.23
1	D	136	ILE	C-O	5.62	1.30	1.24
1	D	147	ALA	C-O	5.58	1.30	1.24
1	D	212	ILE	C-O	5.36	1.30	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	THR	CA-CB-OG1	-9.19	95.82	109.60
1	C	198	THR	CA-CB-OG1	-8.14	97.39	109.60
1	B	294	THR	CB-CA-C	-7.55	96.10	109.62
1	A	266	THR	CA-CB-OG1	-7.09	98.96	109.60
1	B	295	ILE	CB-CA-C	7.01	117.46	110.94
1	B	125	ILE	N-CA-C	-6.55	106.41	112.96
1	B	160	GLN	CB-CG-CD	-6.26	101.96	112.60
1	C	200	THR	CA-CB-OG1	-6.22	100.27	109.60
1	D	199	ILE	CA-C-O	-6.22	113.86	120.39
1	D	271	PRO	CA-C-N	5.83	128.09	120.28
1	D	271	PRO	C-N-CA	5.83	128.09	120.28
1	C	278	ILE	CA-C-O	-5.38	115.36	120.95
1	B	125	ILE	CA-C-N	5.28	129.46	120.91
1	B	125	ILE	C-N-CA	5.28	129.46	120.91
1	D	244	GLN	CA-C-N	5.27	128.82	121.02
1	D	244	GLN	C-N-CA	5.27	128.82	121.02
1	B	281	ARG	CB-CA-C	-5.26	103.20	111.51
1	D	176	LYS	O-C-N	5.23	127.46	122.07
1	B	294	THR	N-CA-CB	5.22	117.72	110.04
1	A	235	GLU	N-CA-CB	-5.22	104.25	112.13
1	D	262	GLY	CA-C-N	5.07	127.38	120.54
1	D	262	GLY	C-N-CA	5.07	127.38	120.54
1	A	125	ILE	N-CA-C	-5.04	108.59	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	183	GLY	Peptide
1	D	111	GLY	Peptide

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	1481	0	1530	12	0
1	B	1495	0	1541	14	0
1	C	1514	0	1558	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1489	0	1533	11	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	10	0	7	0	0
3	D	10	0	7	0	0
4	C	5	0	2	0	0
4	D	5	0	2	0	0
5	D	15	0	0	0	0
6	D	15	0	0	0	0
7	D	6	0	4	0	0
8	A	46	0	0	1	0
8	B	105	0	0	2	0
8	C	74	0	0	0	0
8	D	122	0	0	3	0
All	All	6424	0	6232	50	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 4.

All (50) 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:201:MET:HE1	1:B:267:ILE:HD12	1.63	0.81
1:D:197:ARG:NH2	8:D:401:HOH:O	2.07	0.78
1:B:294:THR:HG22	8:B:431:HOH:O	1.92	0.70
1:A:121:GLN:HG3	8:A:441:HOH:O	1.96	0.64
1:B:286:ILE:HG23	1:B:290:LEU:HD12	1.81	0.62
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.20	0.60
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.34	0.57
1:C:206:THR:HG1	1:C:208:HIS:HD1	1.54	0.56
1:C:108:ILE:HG22	1:C:108:ILE:O	2.06	0.55
1:A:232:LEU:HD11	1:A:267:ILE:HD11	1.89	0.55
1:D:197:ARG:NH1	8:D:404:HOH:O	2.40	0.55
1:C:280:LYS:O	1:C:281:ARG:HB2	2.06	0.54
1:D:154:PHE:CD1	1:D:247:ILE:CD1	2.92	0.52
1:C:160:GLN:HA	1:C:164:GLU:O	2.08	0.52
1:D:202:HIS:CE1	8:D:414:HOH:O	2.63	0.52
1:A:206:THR:HG22	1:A:206:THR:O	2.10	0.52
1:C:108:ILE:CD1	1:C:198:THR:HG23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:HB3	1:C:234:THR:O	2.12	0.49
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.44	0.49
1:B:119:LYS:HB2	1:B:183:GLY:HA3	1.94	0.48
1:B:201:MET:HE1	1:B:267:ILE:CD1	2.37	0.48
1:A:221:ILE:HD12	1:A:232:LEU:HB3	1.95	0.48
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.96	0.47
1:B:159:LEU:O	1:B:160:GLN:HG3	2.14	0.47
1:C:210:GLY:HA3	1:C:225:SER:CB	2.45	0.47
1:B:125:ILE:HD12	1:B:125:ILE:N	2.29	0.47
1:A:282:MET:HE2	1:A:282:MET:HB3	1.84	0.47
1:B:169:TRP:CD1	1:B:173:LYS:HD3	2.51	0.46
1:B:119:LYS:NZ	1:B:181:ALA:O	2.44	0.46
1:C:240:GLU:HA	1:C:244:GLN:O	2.15	0.45
1:D:240:GLU:HA	1:D:244:GLN:O	2.17	0.44
1:D:210:GLY:HA3	1:D:225:SER:CB	2.49	0.43
1:A:232:LEU:CD1	1:A:267:ILE:HD11	2.48	0.43
1:C:108:ILE:HD12	1:C:198:THR:HG23	2.00	0.43
1:A:236:HIS:HE1	1:C:133:ASP:OD2	2.01	0.43
1:D:119:LYS:HD2	1:D:183:GLY:HA2	1.99	0.43
1:A:210:GLY:HA3	1:A:225:SER:HB2	2.01	0.42
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.01	0.42
1:A:286:ILE:HG23	1:A:290:LEU:HD12	2.02	0.42
1:C:107:GLU:HA	1:C:198:THR:HG21	2.01	0.42
1:B:125:ILE:HD12	1:B:125:ILE:H	1.84	0.42
1:D:108:ILE:HA	1:D:192:ASP:OD2	2.19	0.42
1:D:286:ILE:HG23	1:D:290:LEU:HD12	2.01	0.41
1:D:206:THR:OG1	1:D:208:HIS:ND1	2.52	0.41
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.86	0.41
1:B:220:SER:HB3	8:B:435:HOH:O	2.20	0.41
1:C:112:ILE:HA	1:C:190:ILE:O	2.21	0.41
1:B:240:GLU:HA	1:B:244:GLN:O	2.21	0.41
1:C:280:LYS:HD3	1:C:280:LYS:HA	1.89	0.41
1:B:137:PHE:CE2	1:B:157:GLN:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	181 (95%)	8 (4%)	1 (0%)	24	14
1	B	192/195 (98%)	187 (97%)	5 (3%)	0	100	100
1	C	194/195 (100%)	182 (94%)	12 (6%)	0	100	100
1	D	191/195 (98%)	186 (97%)	5 (3%)	0	100	100
All	All	767/780 (98%)	736 (96%)	30 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PHE

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	166/168 (99%)	160 (96%)	6 (4%)	31	20
1	B	167/168 (99%)	161 (96%)	6 (4%)	31	20
1	C	169/168 (101%)	165 (98%)	4 (2%)	43	35
1	D	167/168 (99%)	165 (99%)	2 (1%)	63	58
All	All	669/672 (100%)	651 (97%)	18 (3%)	39	31

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

Mol	Chain	Res	Type
1	A	125	ILE
1	A	171	SER
1	A	184	GLU
1	A	199	ILE
1	A	266	THR
1	A	295	ILE
1	B	121	GLN
1	B	124	LYS
1	B	140	LEU
1	B	205	SER
1	B	220	SER
1	B	294	THR
1	C	109	LYS
1	C	110	GLN
1	C	176	LYS
1	C	297	GLU
1	D	117	LEU
1	D	159	LEU

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	110	GLN
1	A	180	GLN
1	A	215	ASN
1	B	142	GLN
1	B	160	GLN
1	B	165	ASN
1	B	202	HIS
1	B	215	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](#)

17 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
6	SO4	D	305	-	4,4,4	0.29	0	6,6,6	0.06	0
2	EDO	B	301	-	3,3,3	0.35	0	2,2,2	0.16	0
2	EDO	D	303	-	3,3,3	0.37	0	2,2,2	0.13	0
3	DGL	B	303	-	8,9,9	1.06	0	8,11,11	1.60	1 (12%)
5	YDU	D	301	-	16,16,16	2.52	6 (37%)	19,21,21	2.30	4 (21%)
4	GLY	C	304	-	4,4,4	1.04	1 (25%)	3,4,4	1.60	0
7	ALA	D	307	-	5,5,5	1.14	1 (20%)	6,6,6	1.06	1 (16%)
2	EDO	B	302	-	3,3,3	0.45	0	2,2,2	0.28	0
6	SO4	D	304	-	4,4,4	0.34	0	6,6,6	0.07	0
2	EDO	C	303	-	3,3,3	0.16	0	2,2,2	0.35	0
2	EDO	D	302	-	3,3,3	0.12	0	2,2,2	0.12	0
4	GLY	D	309	-	4,4,4	1.24	1 (25%)	3,4,4	1.30	0
2	EDO	A	301	-	3,3,3	0.09	0	2,2,2	0.09	0
3	DGL	D	308	-	8,9,9	1.12	0	8,11,11	1.08	0
2	EDO	C	302	-	3,3,3	0.13	0	2,2,2	0.10	0
2	EDO	C	301	-	3,3,3	0.21	0	2,2,2	0.21	0
6	SO4	D	306	-	4,4,4	0.34	0	6,6,6	0.07	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	B	301	-	-	1/1/1/1	-
2	EDO	D	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DGL	B	303	-	-	3/9/9/9	-
5	YDU	D	301	-	-	0/8/15/15	0/2/2/2
4	GLY	C	304	-	-	0/2/2/2	-
7	ALA	D	307	-	-	0/4/4/4	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
4	GLY	D	309	-	-	0/2/2/2	-
2	EDO	A	301	-	-	0/1/1/1	-
3	DGL	D	308	-	-	4/9/9/9	-
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	YDU	C07-N06	5.02	1.46	1.37
5	D	301	YDU	C05-N06	4.24	1.44	1.36
5	D	301	YDU	O04-N03	-3.62	1.35	1.42
5	D	301	YDU	C13-C14	-3.50	1.37	1.51
5	D	301	YDU	C11-C10	-2.86	1.38	1.53
5	D	301	YDU	C14-C10	2.65	1.67	1.53
4	D	309	GLY	OXT-C	-2.42	1.22	1.30
7	D	307	ALA	OXT-C	-2.08	1.24	1.30
4	C	304	GLY	OXT-C	-2.02	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	YDU	N15-C02-N03	-7.63	107.93	114.91
5	D	301	YDU	O04-N03-C02	3.74	108.59	102.82
3	B	303	DGL	OXT-C-O	-3.37	116.44	124.08
5	D	301	YDU	C01-C02-N03	2.65	126.15	121.71
5	D	301	YDU	O04-C05-N06	2.25	125.07	119.24
7	D	307	ALA	OXT-C-O	-2.09	119.33	124.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	303	EDO	O1-C1-C2-O2

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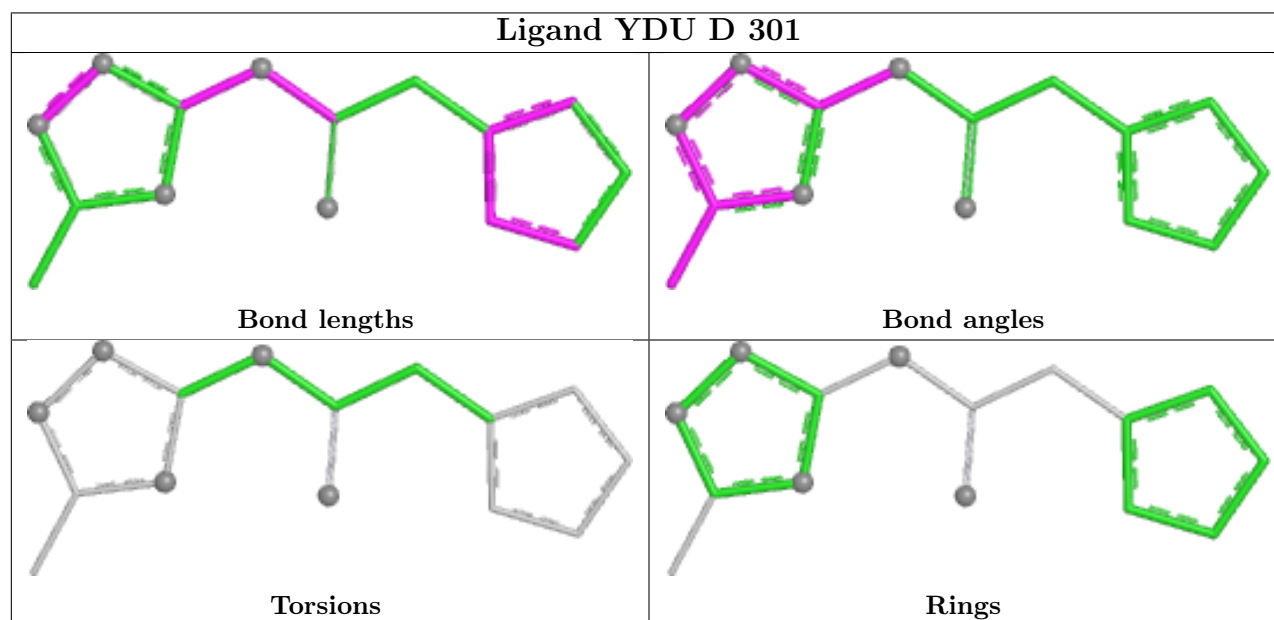
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Mol	Chain	Res	Type	Atoms
3	D	308	DGL	OXT-C-CA-CB
3	D	308	DGL	O-C-CA-CB
2	D	303	EDO	O1-C1-C2-O2
3	D	308	DGL	CA-CB-CG-CD
3	B	303	DGL	C-CA-CB-CG
2	B	301	EDO	O1-C1-C2-O2
3	B	303	DGL	N-CA-CB-CG
3	D	308	DGL	N-CA-CB-CG
3	B	303	DGL	OE2-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

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

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 [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%)	1.41	37 (19%) 3 4	12, 50, 85, 113	13 (6%)
1	B	193/195 (98%)	0.86	18 (9%) 14 20	10, 39, 56, 67	12 (6%)
1	C	193/195 (98%)	0.88	19 (9%) 13 18	12, 44, 68, 103	9 (4%)
1	D	191/195 (97%)	0.20	10 (5%) 33 42	9, 33, 51, 74	7 (3%)
All	All	768/780 (98%)	0.84	84 (10%) 10 15	9, 41, 68, 113	41 (5%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	ILE	14.6
1	A	298	VAL	14.5
1	B	106	ALA	13.5
1	B	112	ILE	12.7
1	A	267	ILE	12.0
1	B	111	GLY	10.0
1	B	113	ARG	9.5
1	C	120	ASP	9.3
1	B	109	LYS	8.3
1	C	121	GLN	8.3
1	C	122	ASP	8.0
1	A	111	GLY	7.8
1	A	108	ILE	7.5
1	A	112	ILE	7.5
1	B	107	GLU	7.5
1	C	106	ALA	7.4
1	D	273[A]	PHE	6.8
1	A	273[A]	PHE	6.8
1	C	150	VAL	6.7
1	C	273[A]	PHE	6.5
1	A	206	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	109	LYS	5.9
1	C	108	ILE	5.9
1	B	110	GLN	5.8
1	B	273[A]	PHE	5.8
1	A	286	ILE	5.8
1	D	187	THR	5.6
1	A	280	LYS	5.4
1	A	118	CYS	5.4
1	C	144[A]	ASN	5.2
1	C	197[A]	ARG	5.1
1	D	108	ILE	5.1
1	A	182	PHE	5.1
1	A	290	LEU	4.9
1	A	259	SER	4.8
1	B	223	LYS	4.7
1	B	179	LYS	4.5
1	C	297	GLU	4.5
1	A	284	PRO	4.2
1	A	282	MET	4.1
1	D	179	LYS	4.1
1	A	110	GLN	4.0
1	A	114	GLU	3.9
1	B	118	CYS	3.8
1	A	287	MET	3.7
1	A	283	ALA	3.7
1	D	110	GLN	3.6
1	D	109	LYS	3.6
1	C	110	GLN	3.5
1	A	281	ARG	3.4
1	A	263	THR	3.4
1	C	139	GLN	3.4
1	D	139	GLN	3.4
1	C	209	VAL	3.4
1	D	223	LYS	3.3
1	C	182	PHE	3.3
1	C	111	GLY	3.1
1	A	117	LEU	3.0
1	B	139	GLN	3.0
1	C	109	LYS	2.8
1	A	202	HIS	2.8
1	D	182	PHE	2.8
1	B	143	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	209	VAL	2.6
1	A	121	GLN	2.5
1	A	264	VAL	2.3
1	A	184	GLU	2.3
1	A	125	ILE	2.3
1	A	159	LEU	2.3
1	A	260	THR	2.3
1	B	281	ARG	2.2
1	A	285	SER	2.2
1	C	296	PRO	2.2
1	C	228	ALA	2.2
1	B	278	ILE	2.2
1	B	182	PHE	2.2
1	A	132	ILE	2.2
1	A	288	LYS	2.2
1	A	179	LYS	2.1
1	D	111	GLY	2.1
1	A	186	ILE	2.1
1	B	122	ASP	2.1
1	A	115	VAL	2.0
1	C	149	LEU	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	304	5/5	0.69	0.41	211,214,216,216	5
3	DGL	B	303	10/10	0.83	0.14	46,62,69,72	0

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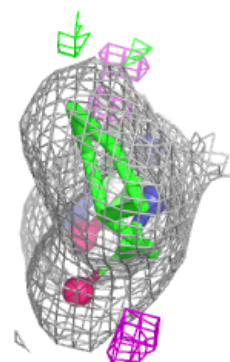
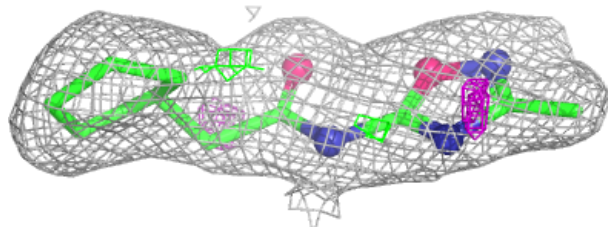
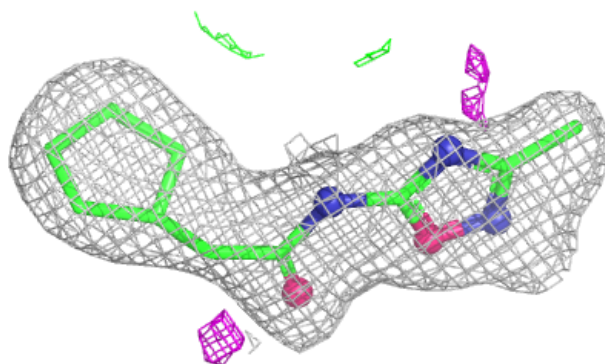
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	305	5/5	0.85	0.10	63,73,86,96	0
3	DGL	D	308	10/10	0.87	0.13	32,55,63,69	0
6	SO4	D	306	5/5	0.89	0.15	63,64,68,70	5
2	EDO	C	302	4/4	0.90	0.13	49,54,55,55	0
2	EDO	C	303	4/4	0.90	0.18	62,62,66,71	0
4	GLY	C	304	5/5	0.90	0.10	47,49,53,55	0
5	YDU	D	301	15/15	0.91	0.11	43,48,49,49	0
2	EDO	B	301	4/4	0.92	0.10	33,37,39,44	0
2	EDO	A	301	4/4	0.92	0.11	46,50,52,52	0
2	EDO	C	301	4/4	0.93	0.11	35,36,40,41	0
7	ALA	D	307	6/6	0.93	0.10	51,57,61,65	0
4	GLY	D	309	5/5	0.95	0.11	55,62,68,70	0
2	EDO	D	303	4/4	0.96	0.10	38,43,43,44	0
2	EDO	B	302	4/4	0.96	0.10	27,32,37,38	0
2	EDO	D	302	4/4	0.97	0.07	26,27,28,32	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 YDU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.