



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:13 PM UTC

PDB ID : 7FSR / pdb_00007fsr
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z54615640
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.29 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

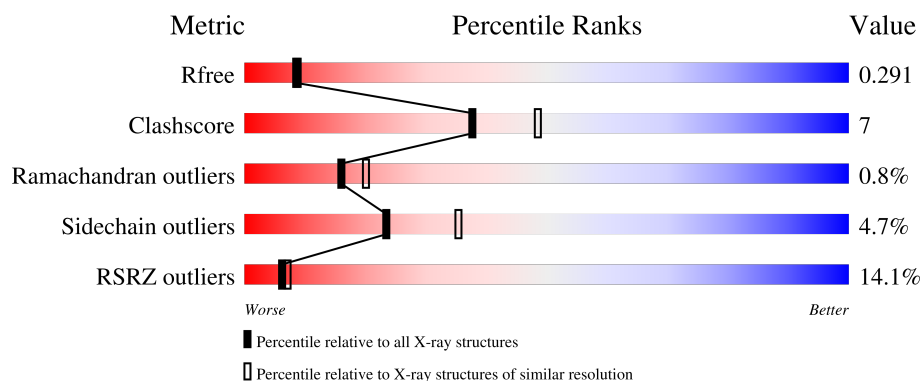
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	14% 73% 25% .
1	B	195	9% 88% 10% ..
1	C	195	15% 77% 18% ..
1	D	195	17% 77% 20% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6315 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	1	0
			1481	935	262	275	9			

There are 8 discrepancies between the modelled and reference sequences:

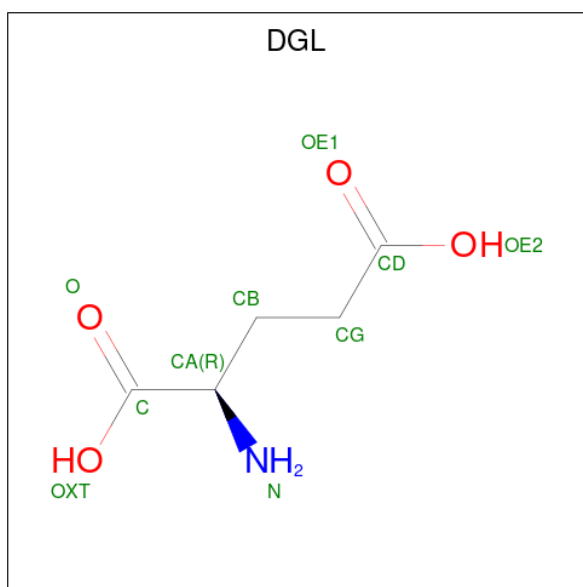
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



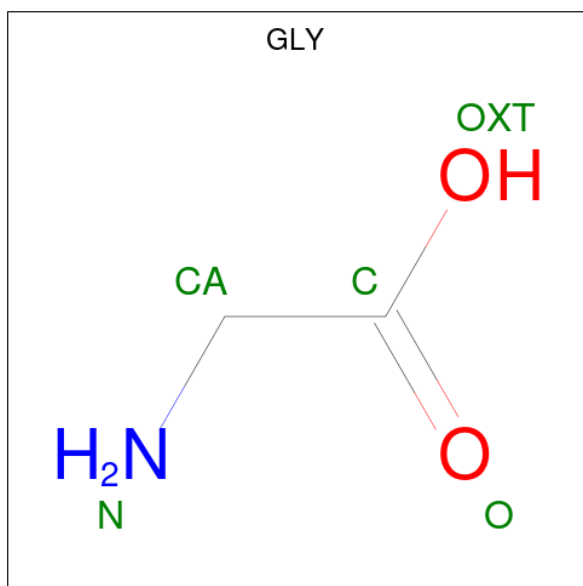
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).



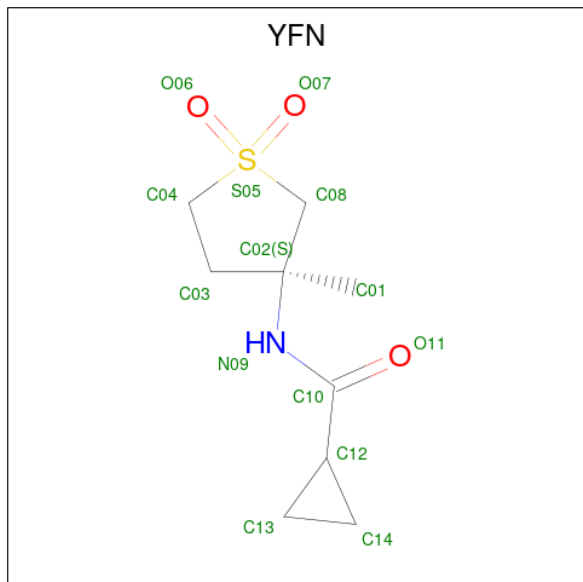
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

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



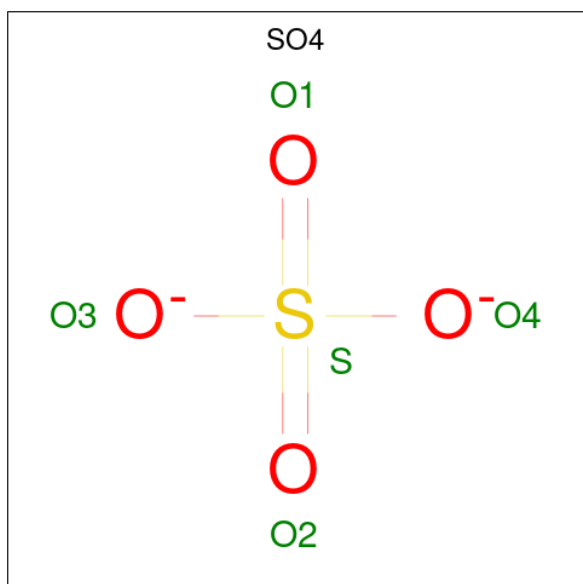
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			5	2	1	2		
4	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 5 is N-[(3S)-3-methyl-1,1-dioxo-1lambda 6 -thiolan-3-yl]cyclopropanecarboxamide (CCD ID: YFN) (formula: C₉H₁₅NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



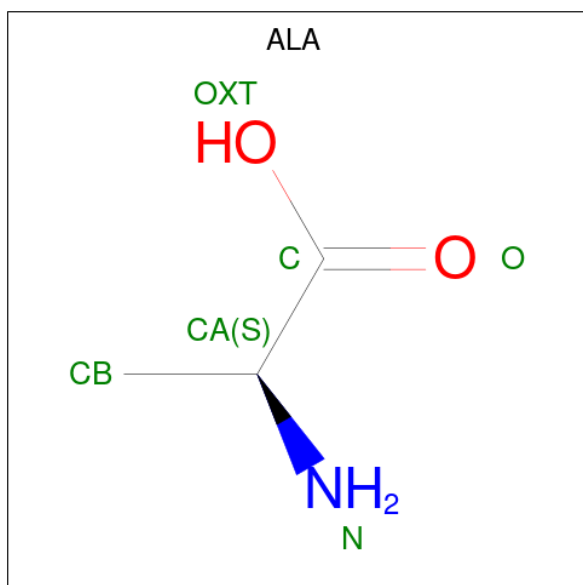
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

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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		

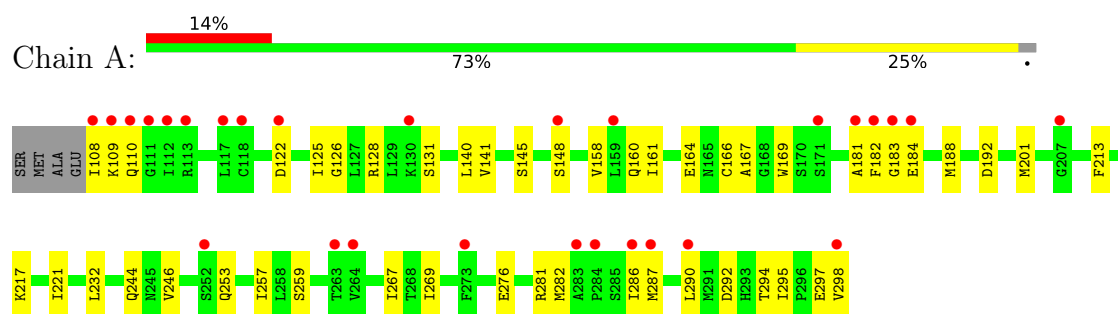
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	1
			25	25		
8	B	76	Total	O	0	1
			76	76		
8	C	59	Total	O	0	0
			59	59		
8	D	87	Total	O	0	0
			87	87		

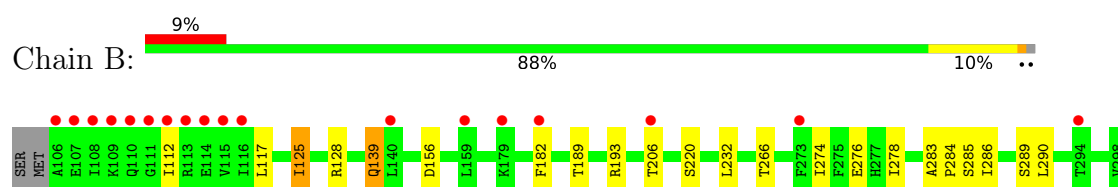
3 Residue-property plots [i](#)

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.

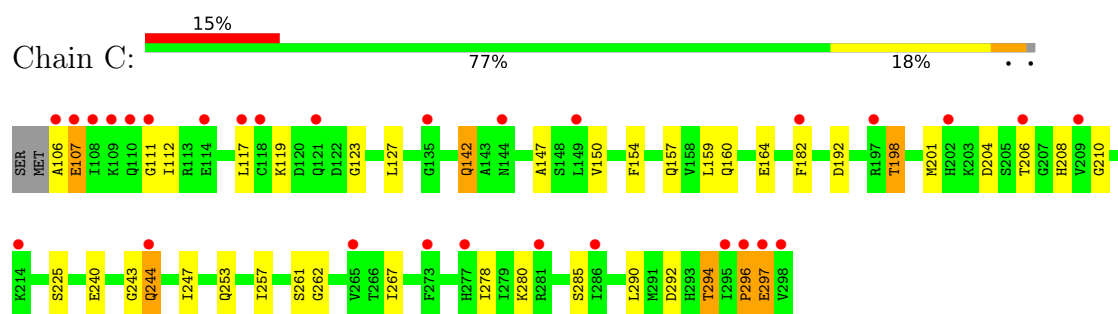
• Molecule 1: Syntenin-1



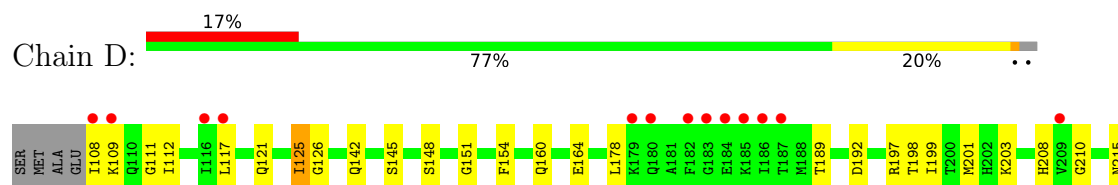
• Molecule 1: Syntenin-1

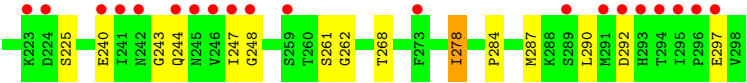


• Molecule 1: Syntenin-1



• 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	80.97Å 49.49Å 114.06Å 90.00° 95.37° 90.00°	Depositor
Resolution (Å)	113.56 – 2.29 113.56 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.1 (113.56-2.29) 99.4 (113.56-2.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.277 0.233 , 0.291	Depositor DCC
R_{free} test set	2003 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6315	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 25.71 % 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 3.0161e-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, YFN, 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	1.09	0/1502	1.47	0/2019
1	B	1.13	0/1516	1.46	0/2038
1	C	1.12	1/1535 (0.1%)	1.41	2/2063 (0.1%)
1	D	1.14	0/1502	1.45	2/2019 (0.1%)
All	All	1.12	1/6055 (0.0%)	1.45	4/8139 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	GLN	C-O	5.13	1.30	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	ILE	N-CA-CB	-5.31	103.55	112.47
1	C	192	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	204	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	112	ILE	CA-C-O	-5.00	115.85	121.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1481	0	1530	21	0
1	B	1495	0	1541	13	0
1	C	1514	0	1558	21	0
1	D	1481	0	1530	29	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	1	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	14	0	0	3	0
6	D	15	0	0	0	0
7	D	6	0	4	0	0
8	A	25	0	0	0	0
8	B	76	0	0	1	0
8	C	59	0	0	3	0
8	D	87	0	0	5	0
All	All	6315	0	6229	86	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 (86) 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)
5:D:301:YFN:C02	5:D:301:YFN:C03	1.86	1.38
1:D:197:ARG:NH1	8:D:401:HOH:O	2.14	0.81
5:D:301:YFN:C03	5:D:301:YFN:N09	2.56	0.67
1:A:161:ILE:HD12	1:A:169:TRP:HZ3	1.61	0.66
1:D:154:PHE:CD1	1:D:247:ILE:HD13	2.30	0.66
1:D:215:ASN:O	8:D:402:HOH:O	2.15	0.65
1:D:198:THR:HG22	1:D:268:THR:OG1	1.96	0.64
1:A:297:GLU:HG2	1:A:298:VAL:N	2.12	0.64
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.81	0.63
5:D:301:YFN:C03	5:D:301:YFN:C01	2.76	0.62
1:A:126:GLY:HA3	1:A:145:SER:CB	2.30	0.62
1:A:201:MET:CE	1:A:267:ILE:HD12	2.30	0.62
1:C:106:ALA:HB2	1:C:243:GLY:HA2	1.80	0.62
1:C:253:GLN:O	1:C:257:ILE:HG13	2.00	0.61
1:D:148:SER:HB2	1:D:292:ASP:OD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PHE:CD1	1:C:247:ILE:HD12	2.36	0.60
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.22	0.58
1:D:160:GLN:OE1	1:D:189:THR:HB	2.03	0.57
1:C:154:PHE:CD1	1:C:247:ILE:CD1	2.88	0.57
1:C:182:PHE:HA	8:C:422:HOH:O	2.04	0.57
1:D:142:GLN:HA	1:D:290:LEU:O	2.05	0.57
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.38	0.55
1:A:161:ILE:HD12	1:A:169:TRP:CZ3	2.42	0.54
1:D:154:PHE:CD1	1:D:247:ILE:CD1	2.91	0.54
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.89	0.53
1:C:119:LYS:HD3	1:C:123:GLY:O	2.10	0.52
1:C:111:GLY:C	1:C:112:ILE:HG13	2.35	0.51
1:C:296:PRO:HG2	1:C:297:GLU:H	1.74	0.51
1:A:109:LYS:N	1:A:192:ASP:OD2	2.38	0.51
1:A:160:GLN:HA	1:A:164:GLU:O	2.11	0.51
1:B:206:THR:HG22	1:B:206:THR:O	2.10	0.51
1:D:126:GLY:HA3	1:D:145:SER:HB2	1.92	0.51
1:A:267:ILE:HG22	1:A:269:ILE:HG23	1.92	0.51
1:C:157:GLN:HG2	1:C:159:LEU:HD12	1.93	0.50
1:C:240:GLU:HA	1:C:244:GLN:O	2.12	0.49
1:A:126:GLY:HA3	1:A:145:SER:HB2	1.94	0.49
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.43	0.49
1:A:181:ALA:C	1:A:183:GLY:H	2.20	0.49
1:C:292:ASP:OD1	1:C:294:THR:HB	2.13	0.49
1:B:283:ALA:O	1:B:285:SER:N	2.46	0.49
1:C:198:THR:HA	1:C:267:ILE:O	2.13	0.49
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.94	0.49
1:C:117:LEU:HD21	1:C:150:VAL:HG11	1.95	0.48
1:D:210:GLY:HA3	1:D:225:SER:CB	2.44	0.48
1:A:221:ILE:HD12	1:A:232:LEU:HB3	1.96	0.48
1:D:243:GLY:O	2:D:302:EDO:O1	2.32	0.48
1:D:248:GLY:HA2	1:D:287:MET:HE3	1.94	0.47
1:D:203:LYS:NZ	1:D:261:SER:O	2.48	0.47
1:B:125:ILE:HD12	1:B:125:ILE:N	2.29	0.47
1:D:154:PHE:CG	1:D:247:ILE:HD13	2.50	0.46
1:D:126:GLY:HA3	1:D:145:SER:CB	2.45	0.46
1:C:160:GLN:HA	1:C:164:GLU:O	2.15	0.46
1:B:286:ILE:HG23	1:B:290:LEU:HD12	1.98	0.46
1:D:160:GLN:HA	1:D:164:GLU:O	2.16	0.46
1:B:274:ILE:HG22	1:B:278:ILE:HD12	1.98	0.46
1:D:108:ILE:HA	1:D:192:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD12	1:D:117:LEU:C	2.42	0.45
1:B:156:ASP:OD1	1:B:193:ARG:HG3	2.17	0.45
1:A:282:MET:HE3	1:A:287:MET:HG3	1.99	0.44
1:A:166:CYS:O	1:A:167:ALA:C	2.60	0.44
1:D:154:PHE:CE1	1:D:247:ILE:HD13	2.52	0.44
1:B:128:ARG:HB2	1:B:139:GLN:HG2	2.00	0.43
1:D:240:GLU:HA	1:D:244:GLN:O	2.18	0.43
8:C:418:HOH:O	1:D:208:HIS:HE1	2.02	0.43
1:A:244:GLN:O	1:A:246:VAL:HG13	2.17	0.43
1:B:125:ILE:HD12	1:B:125:ILE:H	1.84	0.43
1:A:253:GLN:O	1:A:257:ILE:HG13	2.19	0.43
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.73	0.43
1:C:261:SER:OG	1:C:262:GLY:N	2.52	0.43
1:B:232:LEU:HD12	1:B:232:LEU:HA	1.95	0.42
1:D:151:GLY:HA2	8:D:431:HOH:O	2.19	0.42
8:C:418:HOH:O	1:D:208:HIS:CE1	2.72	0.42
1:D:197:ARG:NH2	8:D:403:HOH:O	2.27	0.42
1:A:290:LEU:HD13	1:B:182:PHE:HB2	2.02	0.41
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.02	0.41
1:C:142:GLN:HA	1:C:290:LEU:O	2.20	0.41
1:A:158:VAL:CG1	1:A:188:MET:HE2	2.51	0.41
1:C:147:ALA:O	1:C:150:VAL:HG12	2.20	0.41
1:A:128:ARG:HB2	1:A:140:LEU:HB2	2.03	0.41
1:B:276:GLU:HG2	8:B:414:HOH:O	2.21	0.41
1:D:262:GLY:HA3	8:D:434:HOH:O	2.21	0.41
1:B:117:LEU:HD12	1:B:117:LEU:N	2.36	0.40
1:C:201:MET:HE1	1:C:267:ILE:HG13	2.03	0.40
1:D:154:PHE:CZ	1:D:278:ILE:HG21	2.57	0.40
1:A:213:PHE:HA	1:A:217:LYS:O	2.22	0.40
1:D:199:ILE:HG22	1:D:201:MET:HE2	2.04	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%)	173 (91%)	15 (8%)	2 (1%)	11	13
1	B	192/195 (98%)	181 (94%)	10 (5%)	1 (0%)	24	31
1	C	194/195 (100%)	174 (90%)	18 (9%)	2 (1%)	12	15
1	D	190/195 (97%)	182 (96%)	7 (4%)	1 (0%)	24	31
All	All	766/780 (98%)	710 (93%)	50 (6%)	6 (1%)	16	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	C	296	PRO
1	C	107	GLU
1	A	182	PHE
1	B	284	PRO
1	D	111	GLY

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%)	154 (93%)	12 (7%)	13	18
1	B	167/168 (99%)	162 (97%)	5 (3%)	36	53
1	C	169/168 (101%)	161 (95%)	8 (5%)	23	35
1	D	166/168 (99%)	160 (96%)	6 (4%)	31	47
All	All	668/672 (99%)	637 (95%)	31 (5%)	23	36

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	122	ASP
1	A	125	ILE
1	A	131	SER
1	A	141	VAL
1	A	148	SER
1	A	184	GLU
1	A	259	SER
1	A	276	GLU
1	A	286	ILE
1	A	295	ILE
1	B	125	ILE
1	B	139	GLN
1	B	220	SER
1	B	266	THR
1	B	289	SER
1	C	107	GLU
1	C	142	GLN
1	C	198	THR
1	C	278	ILE
1	C	280	LYS
1	C	285	SER
1	C	294	THR
1	C	297	GLU
1	D	109	LYS
1	D	121	GLN
1	D	125	ILE
1	D	278	ILE
1	D	284	PRO
1	D	297	GLU

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

Mol	Chain	Res	Type
1	A	110	GLN
1	A	180	GLN
1	A	242	ASN
1	B	142	GLN
1	B	160	GLN
1	B	215	ASN
1	B	237	ASN
1	C	202	HIS
1	C	215	ASN

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	EDO	B	301	-	3,3,3	0.15	0	2,2,2	0.21	0
2	EDO	D	302	-	3,3,3	0.16	0	2,2,2	0.12	0
5	YFN	D	301	-	15,15,15	6.41	8 (53%)	16,24,24	2.81	5 (31%)
4	GLY	D	309	-	4,4,4	1.24	1 (25%)	3,4,4	1.43	0
6	SO4	D	306	-	4,4,4	0.36	0	6,6,6	0.18	0
2	EDO	C	303	-	3,3,3	0.19	0	2,2,2	0.35	0
6	SO4	D	304	-	4,4,4	0.33	0	6,6,6	0.05	0
6	SO4	D	305	-	4,4,4	0.36	0	6,6,6	0.08	0
4	GLY	C	304	-	4,4,4	1.04	1 (25%)	3,4,4	1.51	0
2	EDO	D	303	-	3,3,3	0.20	0	2,2,2	0.27	0
3	DGL	D	308	-	8,9,9	1.06	0	8,11,11	1.17	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	302	-	3,3,3	0.12	0	2,2,2	0.13	0
7	ALA	D	307	-	5,5,5	1.08	1 (20%)	6,6,6	1.18	1 (16%)
2	EDO	A	301	-	3,3,3	0.09	0	2,2,2	0.10	0
2	EDO	C	301	-	3,3,3	0.08	0	2,2,2	0.10	0
3	DGL	B	303	-	8,9,9	1.06	0	8,11,11	1.60	1 (12%)
2	EDO	B	302	-	3,3,3	0.41	0	2,2,2	0.45	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	302	-	-	1/1/1/1	-
5	YFN	D	301	-	-	2/9/24/24	0/2/2/2
4	GLY	D	309	-	-	2/2/2/2	-
2	EDO	C	303	-	-	1/1/1/1	-
4	GLY	C	304	-	-	0/2/2/2	-
2	EDO	D	303	-	-	0/1/1/1	-
3	DGL	D	308	-	-	4/9/9/9	-
2	EDO	C	302	-	-	1/1/1/1	-
7	ALA	D	307	-	-	0/4/4/4	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-
3	DGL	B	303	-	-	1/9/9/9	-
2	EDO	B	302	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	YFN	C03-C02	14.61	1.86	1.54
5	D	301	YFN	C02-N09	-13.90	1.33	1.48
5	D	301	YFN	C08-C02	-10.95	1.41	1.52
5	D	301	YFN	C10-N09	6.45	1.47	1.34
5	D	301	YFN	C03-C04	-4.64	1.44	1.52
5	D	301	YFN	O06-S05	2.66	1.49	1.44
4	D	309	GLY	OXT-C	-2.41	1.22	1.30
5	D	301	YFN	O11-C10	-2.38	1.18	1.23
5	D	301	YFN	O07-S05	2.30	1.48	1.44
7	D	307	ALA	OXT-C	-2.17	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	GLY	OXT-C	-2.02	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	YFN	C04-S05-C08	6.78	102.25	97.04
5	D	301	YFN	C13-C12-C10	-5.41	111.95	117.24
5	D	301	YFN	O06-S05-C08	-5.31	102.17	110.23
5	D	301	YFN	C14-C12-C10	3.65	120.81	117.24
3	B	303	DGL	OXT-C-O	-3.33	116.52	124.08
7	D	307	ALA	OXT-C-O	-2.15	119.20	124.08
3	D	308	DGL	OXT-C-O	-2.07	119.39	124.08
5	D	301	YFN	C01-C02-C03	-2.04	107.95	112.36

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	309	GLY	O-C-CA-N
5	D	301	YFN	N09-C10-C12-C13
5	D	301	YFN	O11-C10-C12-C13
4	D	309	GLY	OXT-C-CA-N
2	C	302	EDO	O1-C1-C2-O2
2	C	303	EDO	O1-C1-C2-O2
3	D	308	DGL	OXT-C-CA-CB
3	D	308	DGL	CA-CB-CG-CD
3	D	308	DGL	O-C-CA-CB
2	D	302	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
3	B	303	DGL	OXT-C-CA-CB
3	D	308	DGL	N-CA-CB-CG

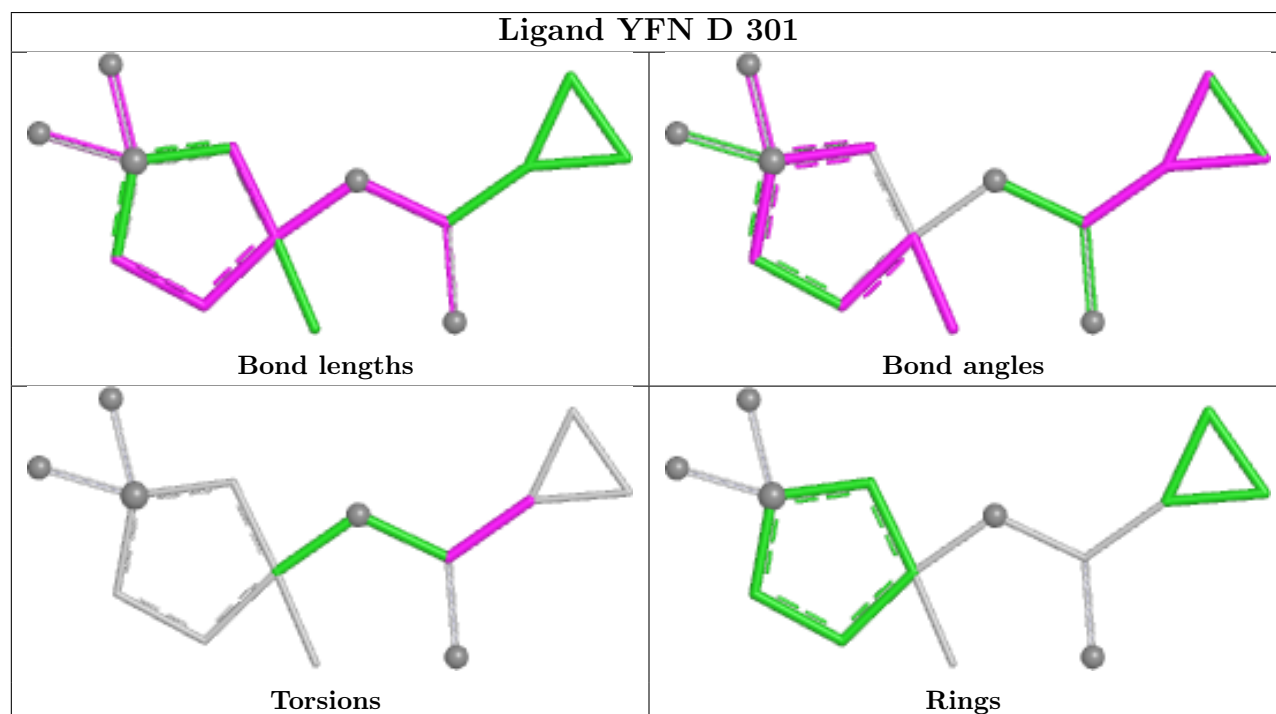
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	EDO	1	0
5	D	301	YFN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/195 (97%)	1.24	28 (14%) 6 6	16, 69, 114, 140	12 (6%)
1	B	193/195 (98%)	0.57	18 (9%) 14 16	12, 50, 73, 101	14 (7%)
1	C	193/195 (98%)	1.22	29 (15%) 5 6	16, 63, 90, 114	16 (8%)
1	D	191/195 (97%)	0.94	33 (17%) 4 4	12, 44, 63, 88	29 (15%)
All	All	768/780 (98%)	0.99	108 (14%) 6 7	12, 56, 95, 140	71 (9%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	ILE	12.6
1	A	111	GLY	11.9
1	C	108	ILE	11.8
1	C	106	ALA	11.6
1	A	108	ILE	10.7
1	D	241	ILE	9.2
1	C	296	PRO	8.6
1	A	110	GLN	8.1
1	A	109	LYS	7.9
1	C	298	VAL	7.5
1	C	295	ILE	7.5
1	A	113	ARG	7.5
1	D	247	ILE	7.3
1	D	273[A]	PHE	7.2
1	D	246	VAL	7.0
1	B	108	ILE	6.8
1	C	107	GLU	6.7
1	A	273[A]	PHE	6.7
1	D	245	ASN	6.5
1	D	295	ILE	6.4
1	D	294	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	292	ASP	6.0
1	B	111	GLY	5.9
1	B	116	ILE	5.9
1	B	112	ILE	5.7
1	D	296	PRO	5.7
1	D	186	ILE	5.6
1	D	240	GLU	5.5
1	B	140	LEU	5.5
1	D	291	MET	5.5
1	C	297	GLU	5.4
1	B	273[A]	PHE	5.4
1	C	197[A]	ARG	5.4
1	D	244	GLN	5.4
1	D	248	GLY	5.3
1	D	117	LEU	5.3
1	D	293	HIS	5.3
1	B	115	VAL	5.2
1	D	179	LYS	5.1
1	D	187	THR	5.0
1	D	289	SER	5.0
1	B	179	LYS	4.9
1	C	144[A]	ASN	4.8
1	C	273[A]	PHE	4.8
1	D	180	GLN	4.7
1	D	116	ILE	4.5
1	D	297	GLU	4.5
1	C	109	LYS	4.5
1	D	183	GLY	4.4
1	B	106	ALA	4.4
1	B	109	LYS	4.4
1	D	242	ASN	4.4
1	B	206	THR	4.3
1	C	214	LYS	4.3
1	C	111	GLY	4.3
1	A	252	SER	4.2
1	D	185	LYS	4.2
1	C	265	VAL	4.2
1	A	171	SER	4.2
1	A	118	CYS	4.2
1	D	259	SER	4.2
1	C	117	LEU	4.2
1	B	294	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	223	LYS	4.0
1	C	114	GLU	4.0
1	A	283	ALA	4.0
1	A	182	PHE	3.9
1	A	287	MET	3.8
1	A	263	THR	3.8
1	A	286	ILE	3.8
1	A	264	VAL	3.8
1	A	290	LEU	3.8
1	C	110	GLN	3.7
1	C	135	GLY	3.6
1	C	209	VAL	3.5
1	D	209	VAL	3.5
1	A	122	ASP	3.4
1	B	110	GLN	3.4
1	A	117	LEU	3.4
1	D	184	GLU	3.3
1	C	149	LEU	3.3
1	B	114	GLU	3.3
1	B	113	ARG	3.1
1	C	202	HIS	3.1
1	D	182	PHE	3.0
1	C	182	PHE	2.9
1	A	184	GLU	2.9
1	A	130	LYS	2.8
1	A	148	SER	2.8
1	A	183	GLY	2.8
1	D	224	ASP	2.7
1	A	181	ALA	2.7
1	C	118	CYS	2.6
1	D	109	LYS	2.6
1	C	244	GLN	2.6
1	B	182	PHE	2.5
1	C	206	THR	2.4
1	B	107	GLU	2.4
1	A	159	LEU	2.4
1	C	121	GLN	2.3
1	C	281	ARG	2.3
1	A	298	VAL	2.2
1	B	159	LEU	2.2
1	A	207	GLY	2.2
1	A	284	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	286	ILE	2.1
1	C	277	HIS	2.1
1	D	108	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

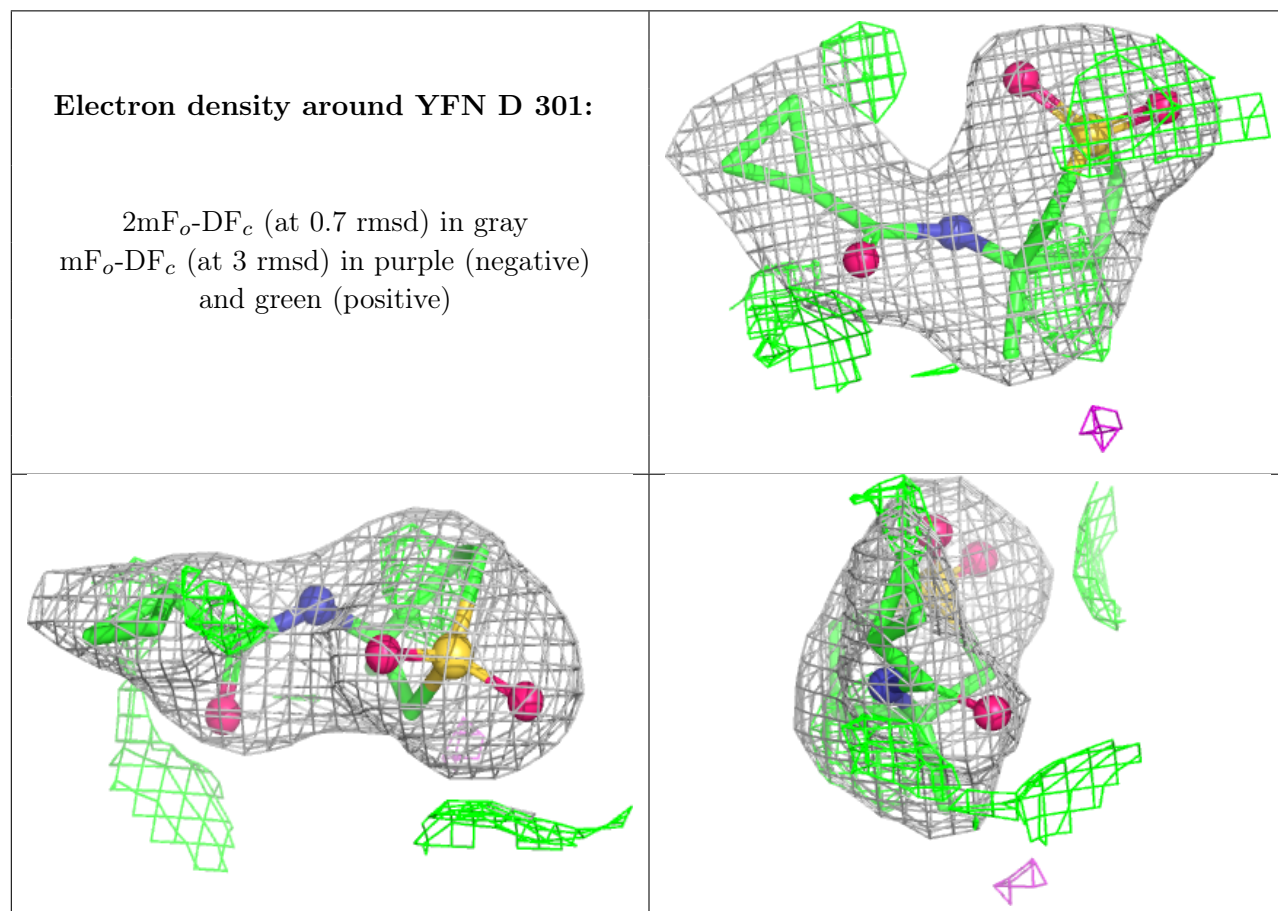
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DGL	B	303	10/10	0.80	0.13	53,73,89,93	0
6	SO4	D	305	5/5	0.81	0.17	77,79,81,84	5
6	SO4	D	304	5/5	0.82	0.12	93,99,108,111	0
3	DGL	D	308	10/10	0.82	0.15	43,62,79,81	0
4	GLY	C	304	5/5	0.85	0.12	59,60,70,75	0
2	EDO	C	303	4/4	0.86	0.25	80,81,82,83	0
6	SO4	D	306	5/5	0.89	0.14	62,69,76,93	0
2	EDO	C	301	4/4	0.91	0.12	55,55,57,59	0
2	EDO	B	302	4/4	0.91	0.11	38,44,45,48	0
2	EDO	B	301	4/4	0.92	0.10	44,45,46,46	0
2	EDO	A	301	4/4	0.92	0.11	57,61,63,64	0
2	EDO	C	302	4/4	0.93	0.12	58,61,61,65	0
2	EDO	D	302	4/4	0.93	0.09	31,31,34,35	0
7	ALA	D	307	6/6	0.93	0.11	61,68,70,70	0
4	GLY	D	309	5/5	0.94	0.11	63,67,77,82	0
5	YFN	D	301	14/14	0.94	0.13	33,34,35,36	14
2	EDO	D	303	4/4	0.95	0.08	47,47,47,48	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.