



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:16 AM UTC

PDB ID : 7FTA / pdb_00007fta
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z228589380
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.03 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)
Xtrriage (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

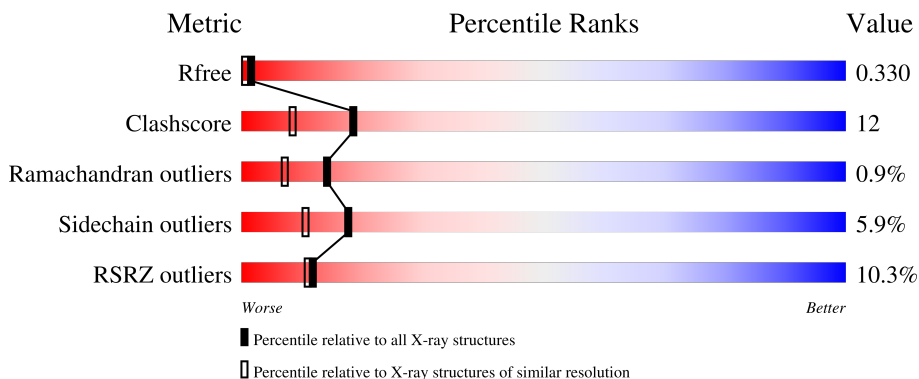
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	 5% 74% 22% ..
1	B	195	 4% 77% 21% ..
1	C	195	 6% 69% 29% ..
1	D	195	 25% 57% 37% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6303 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
			Total	C	N	O	S			
1	A	191	1481	935	262	275	9	0	1	0
1	B	193	1495	943	264	279	9	0	1	0
1	C	193	1514	953	270	282	9	0	3	0
1	D	191	1481	935	262	275	9	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

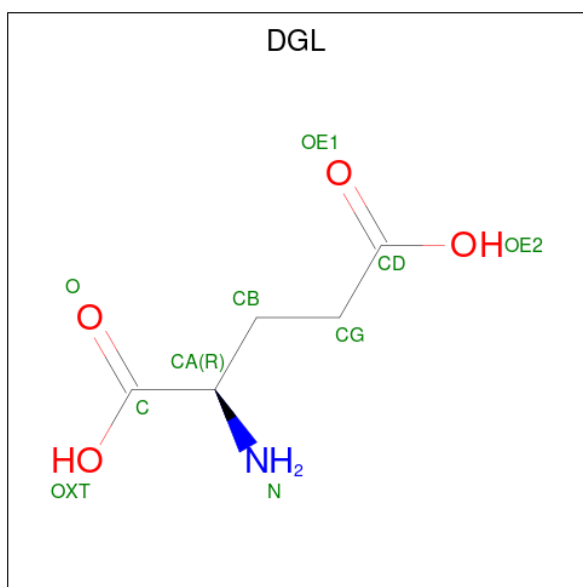
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



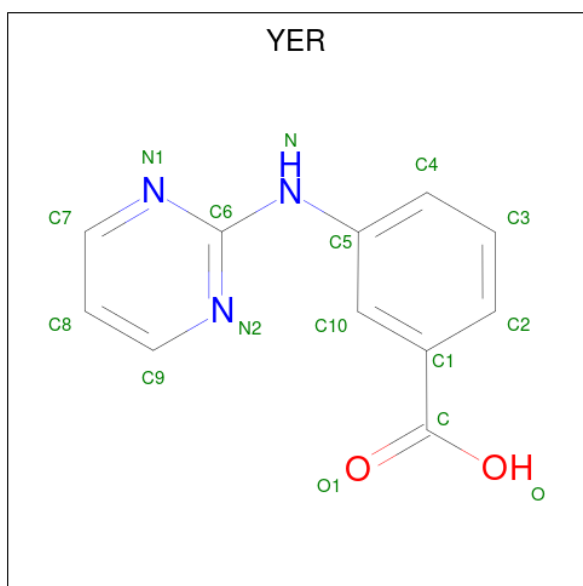
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

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



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

- Molecule 4 is 3-[(pyrimidin-2-yl)amino]benzoic acid (CCD ID: YER) (formula: C₁₁H₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



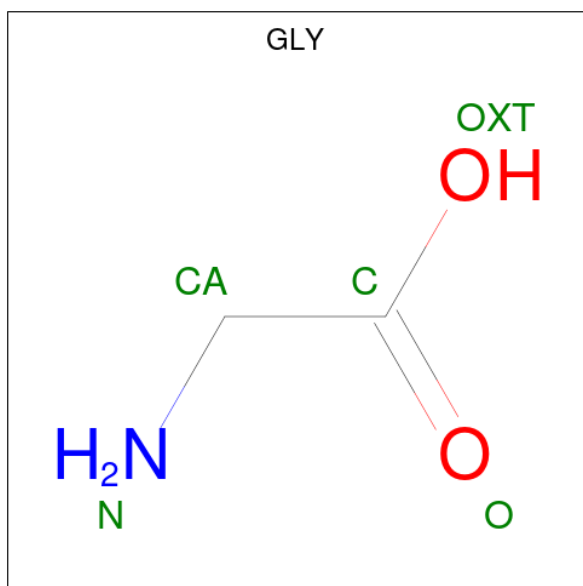
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	16	11	3	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	D	1	16	11	3	2	0	0

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



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

- 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		

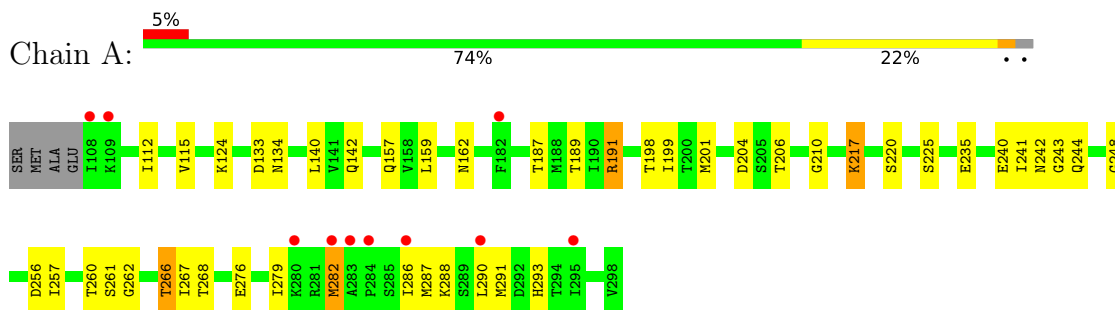
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	33	Total	O	0	0
			33	33		
7	B	86	Total	O	0	0
			86	86		
7	C	57	Total	O	0	0
			57	57		
7	D	56	Total	O	0	1
			57	57		

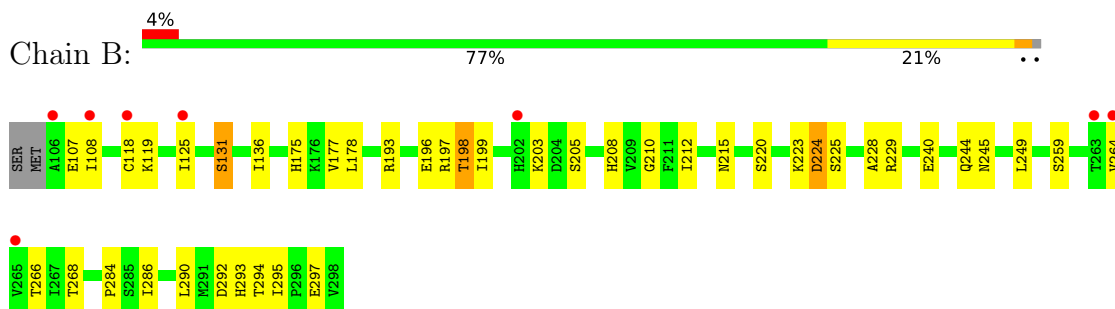
3 Residue-property plots [i](#)

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.

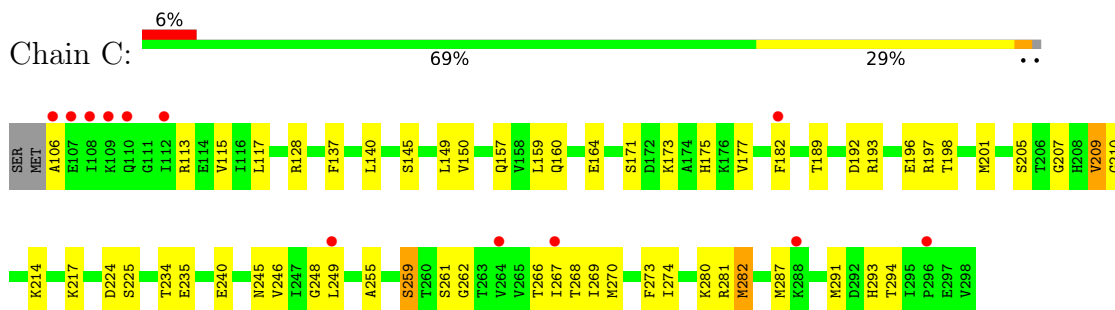
- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1

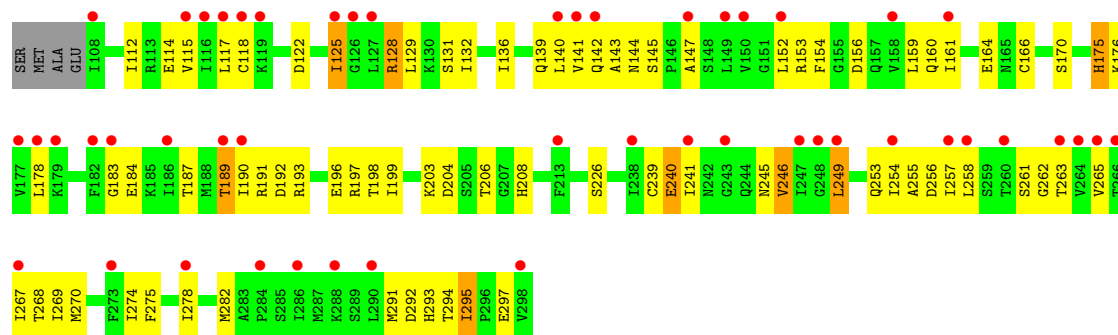


- Molecule 1: Syntenin-1



- 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	80.18Å 49.71Å 115.74Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	57.67 – 2.03 57.67 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.5 (57.67-2.03) 97.7 (57.67-2.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.244 , 0.330 0.251 , 0.330	Depositor DCC
R_{free} test set	2907 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6303	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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 34.24 % 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 $7.0384e-04$. 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/1502	1.20	2/2019 (0.1%)
1	B	0.66	0/1516	1.22	3/2038 (0.1%)
1	C	0.68	0/1535	1.16	4/2063 (0.2%)
1	D	0.71	0/1502	1.32	3/2019 (0.1%)
All	All	0.68	0/6055	1.23	12/8139 (0.1%)

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	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	THR	CB-CA-C	7.46	121.46	110.26
1	B	292	ASP	CA-CB-CG	6.07	118.67	112.60
1	C	294	THR	CB-CA-C	-5.93	100.24	109.61
1	C	189	THR	CA-CB-OG1	-5.89	100.76	109.60
1	B	198	THR	CA-CB-OG1	-5.85	100.82	109.60
1	D	240	GLU	CB-CG-CD	5.65	122.21	112.60
1	C	274	ILE	N-CA-C	-5.51	104.99	111.00
1	A	134	ASN	CA-CB-CG	-5.44	107.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	HIS	CA-CB-CG	-5.38	108.42	113.80
1	D	245	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	293	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	175	HIS	CA-CB-CG	-5.06	108.74	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ARG	Sidechain
1	B	197	ARG	Sidechain
1	C	113	ARG	Sidechain
1	D	128	ARG	Sidechain
1	D	191	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1481	0	1530	27	0
1	B	1495	0	1541	21	0
1	C	1514	0	1558	36	0
1	D	1481	0	1530	64	0
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	12	0	18	1	0
2	D	8	0	12	1	0
3	B	10	0	7	0	0
3	D	10	0	7	0	0
4	C	16	0	0	2	0
4	D	16	0	0	0	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0
6	D	5	0	0	0	0
7	A	33	0	0	3	0
7	B	86	0	0	6	1
7	C	57	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	57	0	0	10	1
All	All	6303	0	6225	148	1

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 12.

All (148) 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:D:198:THR:HG22	1:D:268:THR:OG1	1.71	0.91
1:B:229:ARG:NH1	7:B:403:HOH:O	2.03	0.89
1:B:228:ALA:O	7:B:401:HOH:O	1.89	0.89
1:B:208:HIS:O	7:B:402:HOH:O	1.97	0.82
1:C:235:GLU:OE2	7:C:401:HOH:O	1.97	0.81
1:D:114:GLU:OE1	7:D:401:HOH:O	2.02	0.77
1:B:107:GLU:HA	7:B:407:HOH:O	1.83	0.77
1:D:240:GLU:HB2	1:D:268:THR:HB	1.70	0.74
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.71	0.73
1:D:293:HIS:NE2	7:D:403:HOH:O	2.23	0.71
1:D:197:ARG:NH2	7:D:402:HOH:O	2.20	0.70
1:D:153:ARG:HD2	1:D:240:GLU:OE2	1.91	0.69
1:D:261:SER:OG	1:D:265:VAL:HG22	1.94	0.68
1:D:128:ARG:O	1:D:129:LEU:HD23	1.94	0.68
1:A:282:MET:SD	1:A:287:MET:HG2	2.34	0.67
1:B:177:VAL:O	7:B:404:HOH:O	2.13	0.66
1:A:276:GLU:HG3	7:A:424:HOH:O	1.96	0.65
1:C:273[B]:PHE:CZ	7:C:457:HOH:O	2.50	0.65
1:D:161:ILE:O	1:D:164:GLU:N	2.26	0.65
1:C:240:GLU:HB2	1:C:268:THR:HB	1.79	0.64
1:A:276:GLU:CG	7:A:424:HOH:O	2.45	0.63
1:C:282:MET:HE3	1:C:287:MET:HB2	1.80	0.63
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.81	0.62
1:C:115:VAL:HB	1:C:150:VAL:HG11	1.82	0.62
1:D:261:SER:CB	1:D:265:VAL:HG22	2.29	0.62
1:D:193:ARG:NH1	1:D:240:GLU:OE1	2.33	0.61
1:C:201:MET:HE1	1:C:267:ILE:HG13	1.83	0.61
1:A:217:LYS:HD3	1:A:235:GLU:HA	1.83	0.60
1:D:295:ILE:HD12	1:D:295:ILE:O	2.02	0.60
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.02	0.60
1:D:240:GLU:HB2	1:D:268:THR:CB	2.32	0.60
1:C:245:ASN:N	2:C:302:EDO:O2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:HD23	1:D:141:VAL:C	2.27	0.59
1:D:254:ILE:O	1:D:255:ALA:C	2.45	0.59
1:C:246:VAL:HG12	1:C:249:LEU:HD12	1.85	0.58
1:C:137:PHE:CE2	1:C:157:GLN:HB2	2.39	0.58
1:B:212:ILE:HB	1:B:220:SER:HB3	1.85	0.58
1:D:203:LYS:HG3	1:D:263:THR:O	2.03	0.58
1:D:239:CYS:HB2	1:D:268:THR:HG22	1.87	0.57
1:D:203:LYS:HD2	1:D:262:GLY:O	2.05	0.57
1:D:183:GLY:N	7:D:409:HOH:O	2.37	0.56
1:A:157:GLN:HG2	1:A:159:LEU:HD23	1.87	0.56
1:D:147:ALA:HB1	1:D:152:LEU:HD12	1.87	0.55
1:C:248:GLY:O	1:C:249:LEU:C	2.50	0.54
1:D:204:ASP:OD1	1:D:204:ASP:C	2.49	0.54
1:A:142:GLN:HE21	1:A:290:LEU:HD22	1.73	0.54
1:C:145:SER:O	1:C:149:LEU:HG	2.09	0.53
1:A:210:GLY:HA3	1:A:225:SER:CB	2.40	0.52
1:C:182:PHE:C	7:C:405:HOH:O	2.53	0.51
1:D:203:LYS:HA	1:D:208:HIS:O	2.11	0.51
1:C:201:MET:HE1	1:C:267:ILE:CG1	2.39	0.51
1:B:245:ASN:OD1	1:B:245:ASN:C	2.53	0.51
1:D:141:VAL:HG21	1:D:153:ARG:HA	1.90	0.51
1:D:198:THR:HA	1:D:267:ILE:O	2.11	0.51
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.75	0.51
1:B:210:GLY:HA3	1:B:225:SER:CB	2.41	0.51
1:D:241:ILE:HG13	1:D:246:VAL:HG11	1.92	0.51
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.94	0.50
1:A:256:ASP:O	1:A:260:THR:HG23	2.11	0.50
1:D:131:SER:O	1:D:132:ILE:HD13	2.11	0.50
1:C:255:ALA:O	1:C:259:SER:OG	2.30	0.49
1:C:282:MET:CE	1:C:287:MET:HB2	2.41	0.49
1:B:240:GLU:HA	1:B:244:GLN:O	2.12	0.49
1:C:217:LYS:HE3	7:C:444:HOH:O	2.13	0.49
1:C:280:LYS:O	1:C:281:ARG:HB2	2.11	0.49
1:D:161:ILE:HD13	1:D:178:LEU:HD21	1.95	0.49
1:D:115:VAL:HG23	1:D:117:LEU:HD11	1.95	0.48
1:D:203:LYS:CD	1:D:263:THR:HA	2.44	0.48
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.14	0.48
1:D:160:GLN:OE1	1:D:189:THR:HB	2.14	0.48
1:D:270:MET:SD	1:D:275:PHE:HA	2.54	0.48
1:A:140:LEU:HD23	1:A:291:MET:HE2	1.94	0.48
1:B:249:LEU:HD21	1:B:293:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:VAL:H	4:C:301:YER:C	2.28	0.47
1:D:196:GLU:HA	1:D:269:ILE:O	2.14	0.47
1:D:255:ALA:O	1:D:258:LEU:HB2	2.15	0.47
1:C:291:MET:O	1:C:293:HIS:CE1	2.68	0.46
1:D:187:THR:HG22	7:D:428:HOH:O	2.14	0.46
1:D:249:LEU:HB3	1:D:253:GLN:OE1	2.16	0.46
1:C:160:GLN:HA	1:C:164:GLU:O	2.16	0.46
1:D:206:THR:HG1	1:D:208:HIS:HD1	1.61	0.46
1:A:204:ASP:OD1	1:A:204:ASP:N	2.45	0.45
1:C:150:VAL:O	1:C:150:VAL:HG12	2.17	0.45
1:D:129:LEU:HD13	1:D:136:ILE:HG21	1.97	0.45
1:D:170:SER:HB2	7:D:424:HOH:O	2.16	0.45
1:D:295:ILE:HD13	1:D:297:GLU:C	2.42	0.45
1:D:295:ILE:HD13	1:D:297:GLU:O	2.16	0.45
1:D:153:ARG:HD3	2:D:302:EDO:O1	2.17	0.45
1:A:198:THR:HA	1:A:267:ILE:O	2.17	0.45
1:D:154:PHE:CD1	1:D:154:PHE:C	2.95	0.45
1:D:156:ASP:OD1	1:D:193:ARG:HG3	2.17	0.45
1:D:142:GLN:HB3	1:D:145:SER:HB3	1.99	0.45
1:C:245:ASN:OD1	1:C:245:ASN:C	2.60	0.44
1:A:140:LEU:HD21	1:A:282:MET:SD	2.57	0.44
1:C:128:ARG:HB2	1:C:140:LEU:HB3	2.00	0.44
1:C:210:GLY:HA3	1:C:225:SER:CB	2.47	0.44
1:D:204:ASP:N	1:D:208:HIS:O	2.39	0.44
1:D:256:ASP:N	1:D:256:ASP:OD1	2.51	0.44
1:A:286:ILE:O	1:A:290:LEU:HB2	2.18	0.43
1:C:106:ALA:O	1:C:198:THR:HG21	2.18	0.43
1:D:144:ASN:HB2	7:D:422:HOH:O	2.18	0.43
1:D:293:HIS:CE1	7:D:403:HOH:O	2.69	0.43
1:D:115:VAL:HG23	1:D:117:LEU:CD1	2.49	0.43
1:D:139:GLN:HG2	1:D:282:MET:CE	2.49	0.43
1:A:241:ILE:O	1:A:242:ASN:C	2.61	0.43
1:D:192:ASP:O	1:D:193:ARG:C	2.61	0.43
1:D:197:ARG:O	1:D:268:THR:HA	2.19	0.43
1:D:291:MET:HE2	1:D:291:MET:HB2	1.87	0.43
1:B:294:THR:HG22	1:B:295:ILE:O	2.19	0.42
1:D:274:ILE:O	1:D:278:ILE:HG13	2.19	0.42
1:B:198:THR:C	1:B:199:ILE:HG13	2.44	0.42
1:A:240:GLU:HA	1:A:244:GLN:O	2.19	0.42
1:A:242:ASN:ND2	1:A:261:SER:OG	2.52	0.42
1:D:152:LEU:HD21	1:D:190:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLY:O	1:A:288:LYS:HG3	2.20	0.42
1:C:157:GLN:HG2	1:C:159:LEU:HD12	2.01	0.42
1:B:193:ARG:HB3	1:B:196:GLU:HB2	2.02	0.42
1:D:143:ALA:O	1:D:144:ASN:HB2	2.19	0.42
1:D:153:ARG:O	1:D:156:ASP:HB2	2.20	0.42
1:A:240:GLU:HB2	1:A:268:THR:HB	2.01	0.41
1:C:115:VAL:HB	1:C:150:VAL:CG1	2.48	0.41
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.90	0.41
1:B:240:GLU:HB2	1:B:268:THR:HB	2.02	0.41
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.02	0.41
1:C:267:ILE:HG22	1:C:269:ILE:HG23	2.01	0.41
1:C:273[B]:PHE:CE1	7:C:457:HOH:O	2.72	0.41
1:D:206:THR:HG23	7:D:433:HOH:O	2.20	0.41
1:A:266:THR:HG22	7:A:421:HOH:O	2.20	0.41
1:B:131:SER:HA	1:B:136:ILE:HD13	2.03	0.41
1:D:175:HIS:O	1:D:176:LYS:C	2.63	0.41
1:C:205:SER:C	1:C:207:GLY:H	2.28	0.41
4:C:301:YER:N1	4:C:301:YER:C4	2.83	0.41
1:D:175:HIS:O	1:D:178:LEU:N	2.26	0.41
1:A:112:ILE:HG23	1:A:189:THR:HG22	2.03	0.41
1:A:241:ILE:O	1:A:243:GLY:N	2.53	0.41
1:A:133:ASP:HB3	1:C:234:THR:O	2.21	0.41
1:A:162:ASN:HA	1:A:187:THR:OG1	2.21	0.41
1:A:279:ILE:O	1:A:282:MET:HB2	2.20	0.41
1:B:118:CYS:O	1:B:119:LYS:C	2.62	0.41
1:D:161:ILE:O	1:D:164:GLU:HB2	2.20	0.41
1:B:203:LYS:NZ	1:B:259:SER:O	2.54	0.41
1:B:286:ILE:HG23	1:B:290:LEU:HD12	2.02	0.41
1:C:115:VAL:O	1:C:115:VAL:HG23	2.21	0.41
1:C:173:LYS:O	1:C:177:VAL:HG23	2.20	0.41
1:B:108:ILE:N	7:B:407:HOH:O	2.36	0.40
1:C:201:MET:CE	1:C:267:ILE:HG12	2.51	0.40
1:B:223:LYS:O	1:B:224:ASP:C	2.64	0.40
1:D:153:ARG:HG2	7:D:407:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:456:HOH:O	7:D:425:HOH:O[1_455]	2.05	0.15

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%)	181 (95%)	8 (4%)	1 (0%)	24	17
1	B	192/195 (98%)	181 (94%)	10 (5%)	1 (0%)	24	17
1	C	194/195 (100%)	179 (92%)	13 (7%)	2 (1%)	12	5
1	D	190/195 (97%)	165 (87%)	22 (12%)	3 (2%)	7	2
All	All	766/780 (98%)	706 (92%)	53 (7%)	7 (1%)	14	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	184	GLU
1	D	175	HIS
1	A	262	GLY
1	C	193	ARG
1	B	284	PRO
1	D	246	VAL
1	C	262	GLY

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%)	157 (95%)	9 (5%)	20	13
1	B	167/168 (99%)	159 (95%)	8 (5%)	23	15
1	C	169/168 (101%)	158 (94%)	11 (6%)	15	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	166/168 (99%)	155 (93%)	11 (7%)	15 8
All	All	668/672 (99%)	629 (94%)	39 (6%)	18 11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	VAL
1	A	124	LYS
1	A	199	ILE
1	A	206	THR
1	A	217	LYS
1	A	220	SER
1	A	257	ILE
1	A	266	THR
1	A	282	MET
1	B	125	ILE
1	B	131	SER
1	B	205	SER
1	B	215	ASN
1	B	224	ASP
1	B	264	VAL
1	B	266	THR
1	B	297	GLU
1	C	117	LEU
1	C	171	SER
1	C	192	ASP
1	C	209	VAL
1	C	214	LYS
1	C	224	ASP
1	C	259	SER
1	C	261	SER
1	C	266	THR
1	C	270	MET
1	C	282	MET
1	D	112	ILE
1	D	118	CYS
1	D	122	ASP
1	D	125	ILE
1	D	159	LEU
1	D	166	CYS
1	D	199	ILE
1	D	226	SER

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Mol	Chain	Res	Type
1	D	249	LEU
1	D	257	ILE
1	D	295	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	230	ASN
1	A	253	GLN
1	A	293	HIS
1	B	142	GLN
1	B	157	GLN
1	B	208	HIS
1	B	253	GLN
1	C	180	GLN
1	D	157	GLN
1	D	215	ASN
1	D	244	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](#)

15 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	C	303	-	3,3,3	0.31	0	2,2,2	0.36	0
2	EDO	C	304	-	3,3,3	0.43	0	2,2,2	0.64	0
4	YER	C	301	-	17,17,17	0.40	0	22,22,22	0.32	0
2	EDO	D	303	-	3,3,3	0.09	0	2,2,2	0.44	0
6	SO4	D	304	-	4,4,4	0.28	0	6,6,6	0.05	0
4	YER	D	301	-	17,17,17	0.38	0	22,22,22	0.37	0
2	EDO	B	302	-	3,3,3	0.36	0	2,2,2	0.30	0
2	EDO	B	301	-	3,3,3	0.13	0	2,2,2	0.40	0
2	EDO	D	302	-	3,3,3	0.15	0	2,2,2	0.20	0
5	GLY	D	306	-	4,4,4	0.91	0	3,4,4	1.21	0
3	DGL	D	305	-	8,9,9	1.10	1 (12%)	8,11,11	0.87	0
2	EDO	A	301	-	3,3,3	0.26	0	2,2,2	0.17	0
3	DGL	B	303	-	8,9,9	1.11	1 (12%)	8,11,11	1.13	0
5	GLY	C	305	-	4,4,4	0.73	0	3,4,4	1.15	0
2	EDO	C	302	-	3,3,3	0.26	0	2,2,2	0.03	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	303	-	-	1/1/1/1	-
2	EDO	C	304	-	-	1/1/1/1	-
4	YER	C	301	-	-	4/8/8/8	0/2/2/2
2	EDO	D	303	-	-	1/1/1/1	-
4	YER	D	301	-	-	0/8/8/8	0/2/2/2
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	B	301	-	-	1/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
5	GLY	D	306	-	-	2/2/2/2	-
3	DGL	D	305	-	-	0/9/9/9	-
2	EDO	A	301	-	-	1/1/1/1	-
3	DGL	B	303	-	-	3/9/9/9	-
5	GLY	C	305	-	-	2/2/2/2	-
2	EDO	C	302	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	DGL	O-C	2.40	1.29	1.22
3	D	305	DGL	O-C	2.06	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	305	GLY	O-C-CA-N
5	C	305	GLY	OXT-C-CA-N
5	D	306	GLY	OXT-C-CA-N
4	C	301	YER	O-C-C1-C10
4	C	301	YER	O1-C-C1-C10
5	D	306	GLY	O-C-CA-N
4	C	301	YER	O-C-C1-C2
4	C	301	YER	O1-C-C1-C2
2	C	302	EDO	O1-C1-C2-O2
2	C	304	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
3	B	303	DGL	CA-CB-CG-CD
2	C	303	EDO	O1-C1-C2-O2
3	B	303	DGL	OE1-CD-CG-CB
2	D	303	EDO	O1-C1-C2-O2
3	B	303	DGL	OE2-CD-CG-CB
2	A	301	EDO	O1-C1-C2-O2

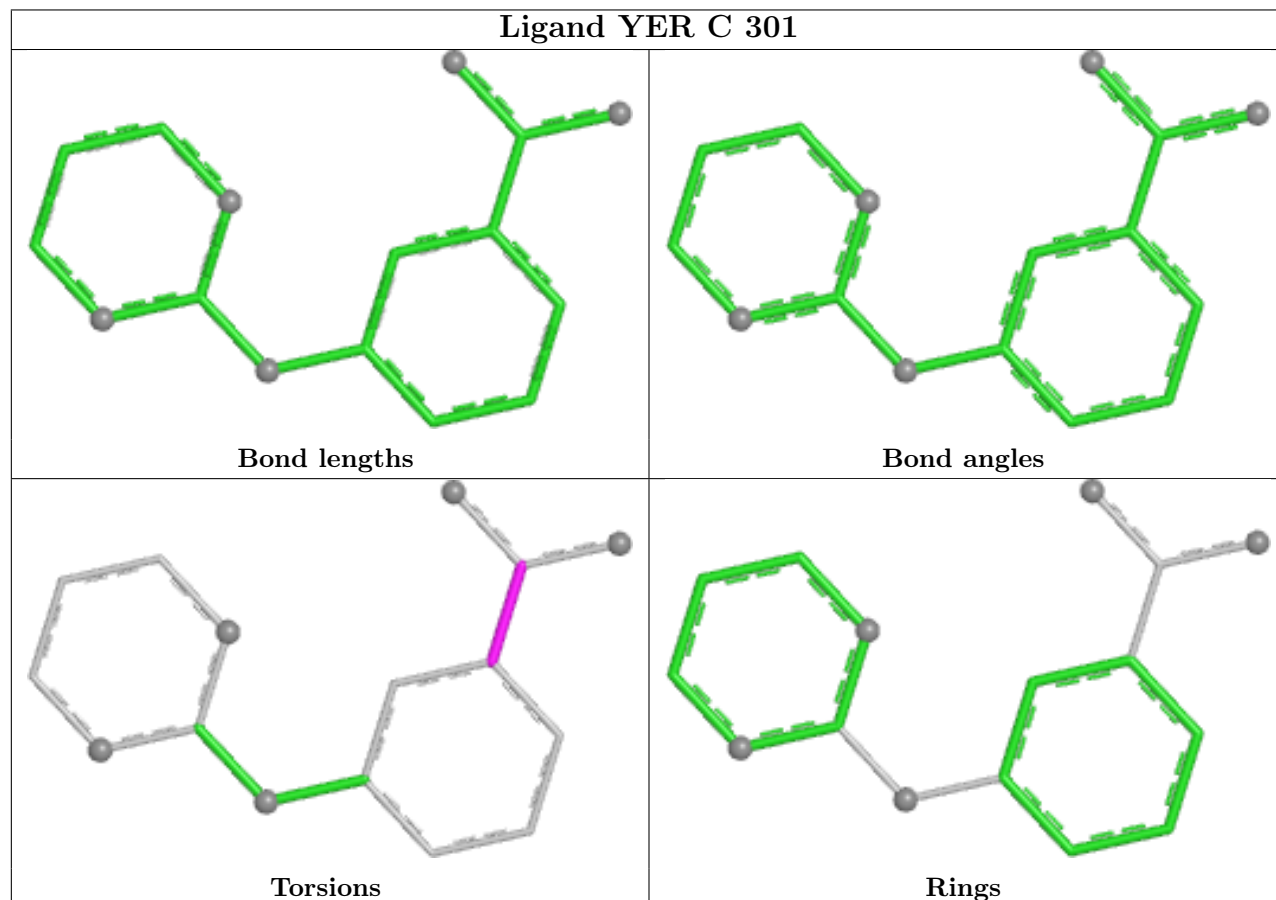
There are no ring outliers.

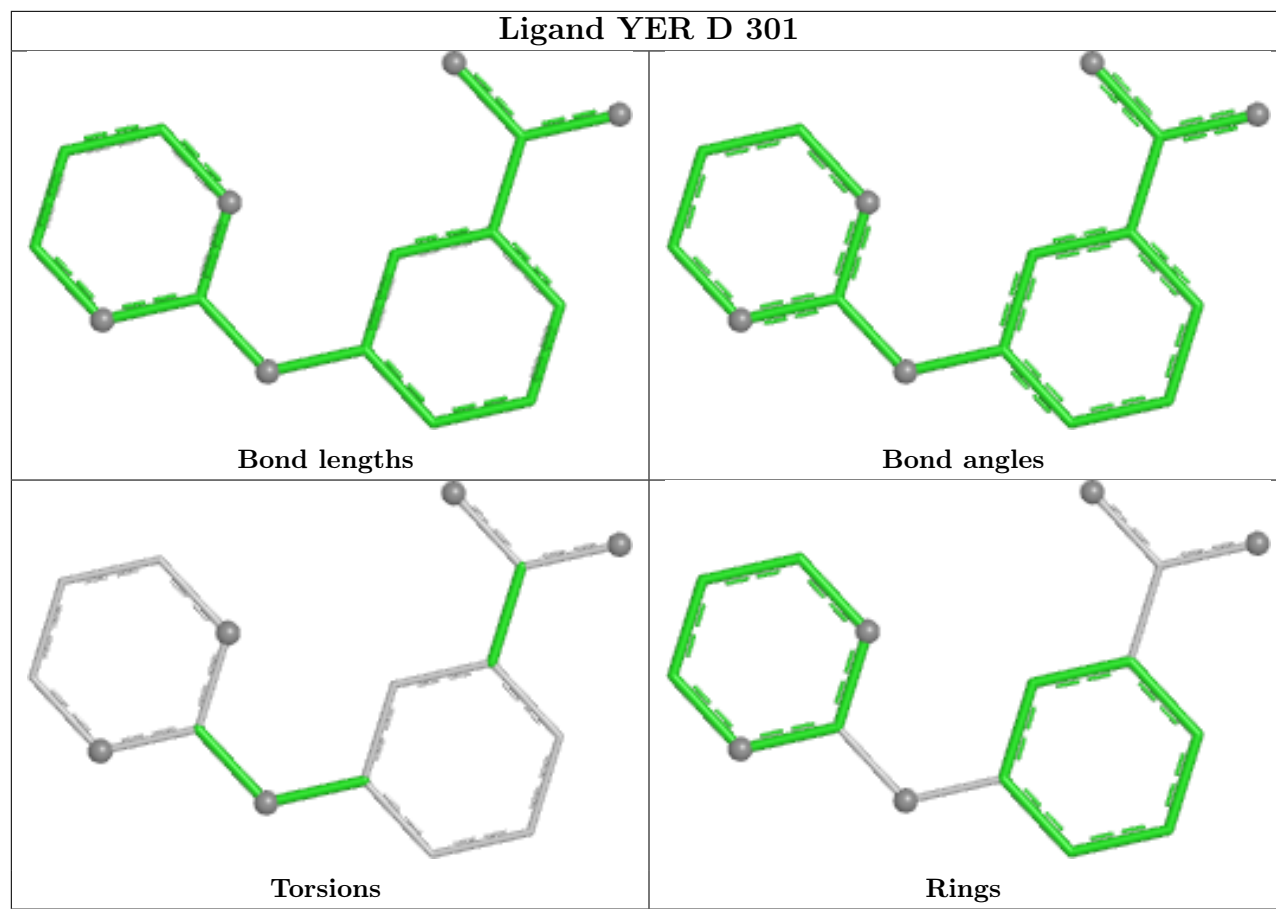
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	YER	2	0
2	D	302	EDO	1	0
2	C	302	EDO	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

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%)	0.60	10 (5%) 33 32	20, 60, 102, 118	1 (0%)
1	B	193/195 (98%)	0.39	8 (4%) 41 41	19, 56, 77, 96	1 (0%)
1	C	193/195 (98%)	0.62	12 (6%) 26 25	21, 59, 97, 130	3 (1%)
1	D	191/195 (97%)	1.37	49 (25%) 1 1	23, 66, 95, 135	1 (0%)
All	All	768/780 (98%)	0.75	79 (10%) 12 11	19, 60, 94, 135	6 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	254	ILE	5.3
1	C	108	ILE	5.1
1	D	178	LEU	5.0
1	C	109	LYS	4.9
1	D	298	VAL	4.9
1	A	182	PHE	4.3
1	D	258	LEU	4.3
1	D	190	ILE	4.3
1	D	149	LEU	4.2
1	D	125	ILE	4.1
1	C	106	ALA	4.0
1	D	273[A]	PHE	3.9
1	B	264	VAL	3.8
1	D	186	ILE	3.8
1	D	241	ILE	3.8
1	D	141	VAL	3.8
1	D	126	GLY	3.8
1	D	140	LEU	3.8
1	D	260	THR	3.8
1	A	109	LYS	3.7
1	D	117	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	263	THR	3.6
1	B	106	ALA	3.4
1	D	150	VAL	3.4
1	D	265	VAL	3.3
1	A	286	ILE	3.3
1	D	177	VAL	3.3
1	A	108	ILE	3.3
1	C	112	ILE	3.1
1	D	267	ILE	3.1
1	A	284	PRO	3.1
1	C	296	PRO	3.1
1	D	290	LEU	3.0
1	D	179	LYS	2.9
1	B	265	VAL	2.9
1	D	127	LEU	2.9
1	D	161	ILE	2.9
1	D	264	VAL	2.8
1	D	286	ILE	2.8
1	A	283	ALA	2.8
1	D	116	ILE	2.7
1	C	264	VAL	2.7
1	C	110	GLN	2.7
1	C	182	PHE	2.7
1	B	125	ILE	2.7
1	D	278	ILE	2.6
1	A	290	LEU	2.6
1	D	257	ILE	2.6
1	D	243	GLY	2.6
1	A	282	MET	2.5
1	D	183	GLY	2.5
1	D	238	ILE	2.5
1	D	266	THR	2.4
1	D	147	ALA	2.4
1	D	108	ILE	2.4
1	D	119	LYS	2.3
1	D	189	THR	2.3
1	D	142	GLN	2.3
1	C	107	GLU	2.3
1	D	118	CYS	2.3
1	D	249	LEU	2.3
1	D	115	VAL	2.2
1	D	158	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	288	LYS	2.2
1	D	248	GLY	2.2
1	B	118	CYS	2.2
1	D	182	PHE	2.2
1	C	249	LEU	2.2
1	C	267	ILE	2.1
1	A	280	LYS	2.1
1	B	263	THR	2.1
1	A	295	ILE	2.1
1	B	108	ILE	2.1
1	D	213	PHE	2.1
1	B	202	HIS	2.1
1	C	288	LYS	2.1
1	D	247	ILE	2.1
1	D	152	LEU	2.0
1	D	284	PRO	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.

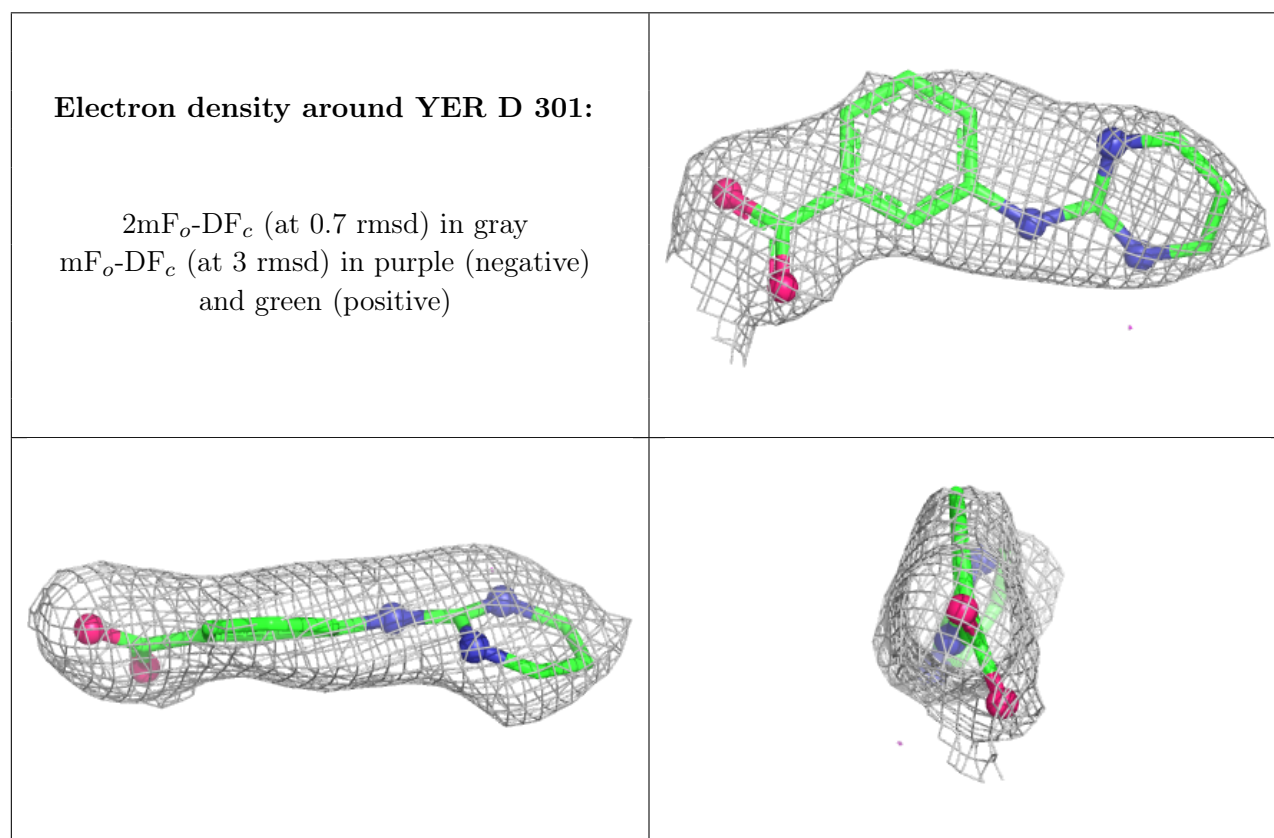
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DGL	D	305	10/10	0.73	0.16	67,99,123,123	0
3	DGL	B	303	10/10	0.75	0.14	59,94,107,113	0
6	SO4	D	304	5/5	0.80	0.10	90,103,115,122	0
5	GLY	C	305	5/5	0.83	0.11	63,69,74,79	0
4	YER	D	301	16/16	0.89	0.11	46,58,71,72	0
2	EDO	C	302	4/4	0.89	0.12	64,64,66,69	0
5	GLY	D	306	5/5	0.89	0.11	66,68,69,70	0

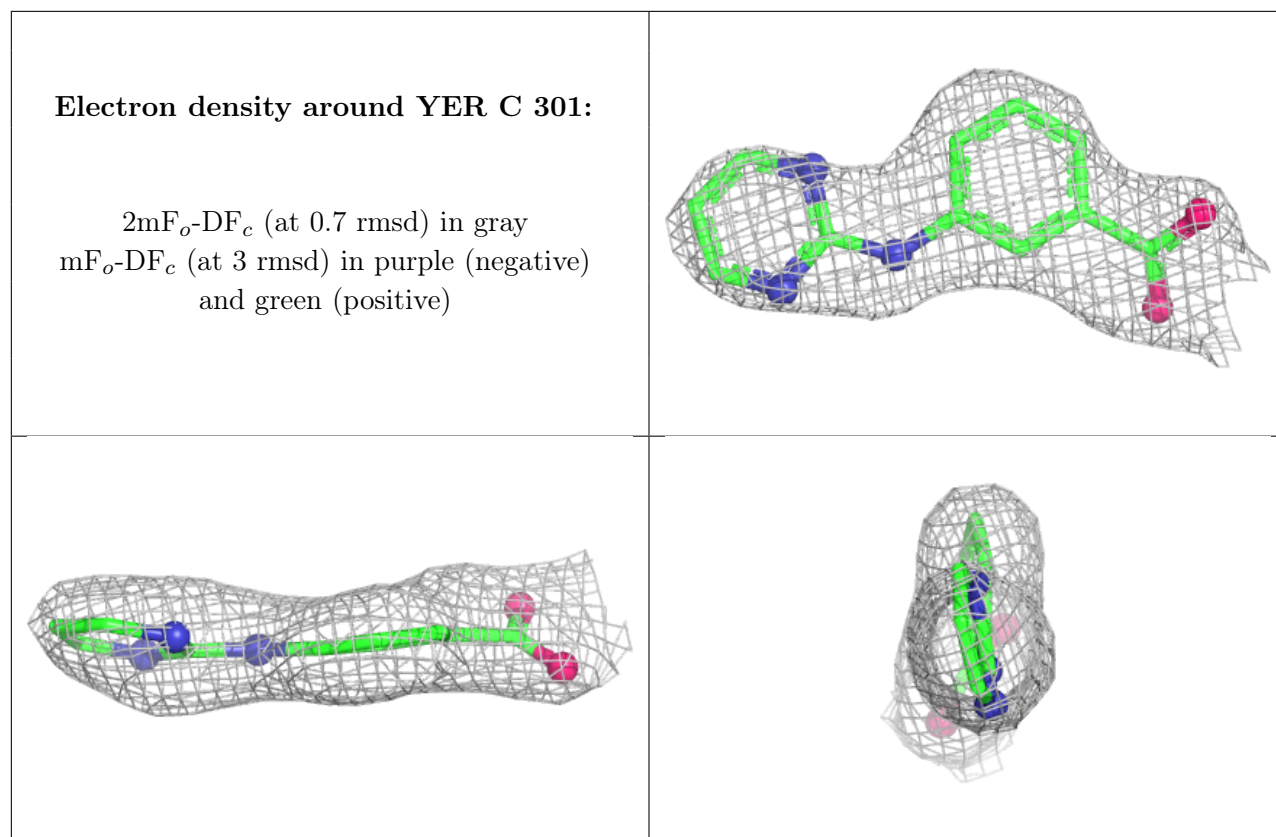
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	D	303	4/4	0.89	0.14	49,53,56,63	0
2	EDO	D	302	4/4	0.90	0.11	55,56,57,69	0
2	EDO	C	304	4/4	0.90	0.18	70,72,79,79	0
2	EDO	C	303	4/4	0.92	0.12	48,62,62,70	0
2	EDO	B	301	4/4	0.92	0.13	49,60,62,70	0
2	EDO	B	302	4/4	0.93	0.08	53,55,56,56	0
2	EDO	A	301	4/4	0.93	0.13	66,73,76,84	0
4	YER	C	301	16/16	0.94	0.09	57,66,88,90	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.