



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 PM UTC

PDB ID : 7FSW / pdb_00007fsw
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z169675004
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.14 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

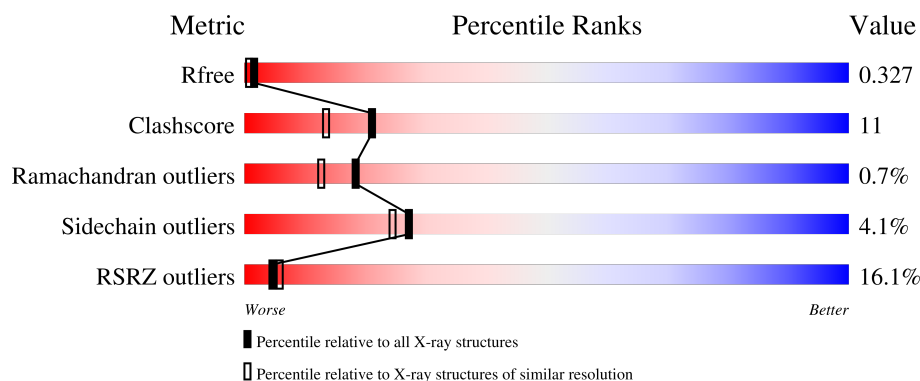
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	7% 75% 21% ..
1	B	195	6% 81% 18% .
1	C	195	16% 80% 18% ..
1	D	195	34% 59% 35% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6357 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.

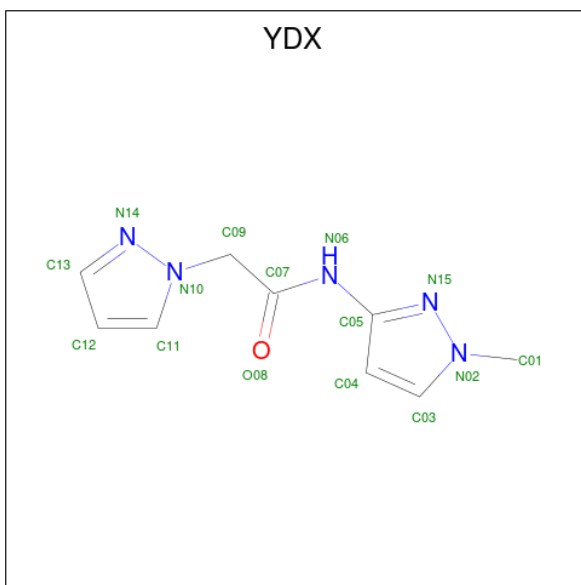
- Molecule 1 is a protein called Syntenin-1.

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:

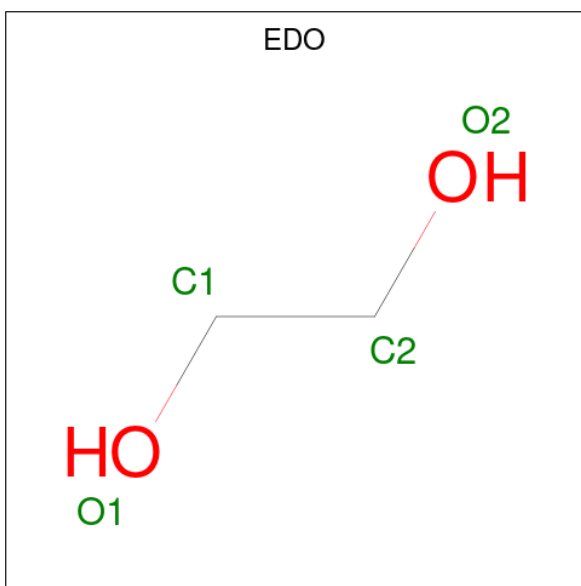
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

- Molecule 2 is N-(1-methyl-1H-pyrazol-3-yl)-2-(1H-pyrazol-1-yl)acetamide (CCD ID: YDX) (formula: C₉H₁₁N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



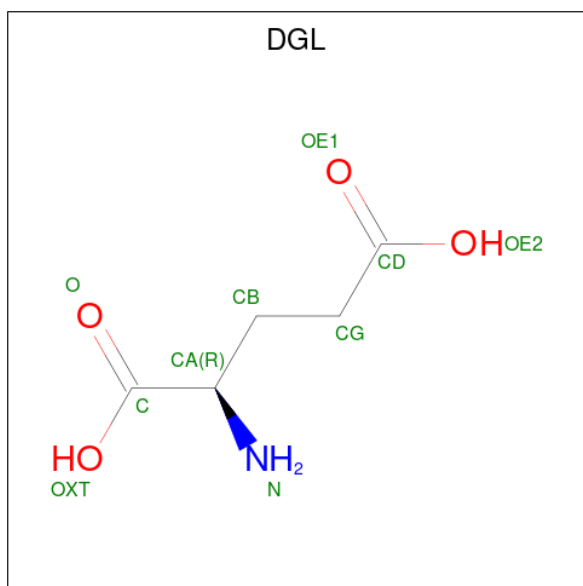
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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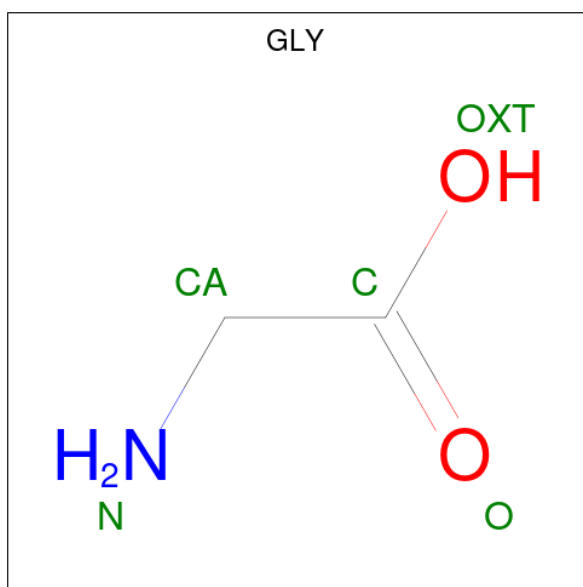
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



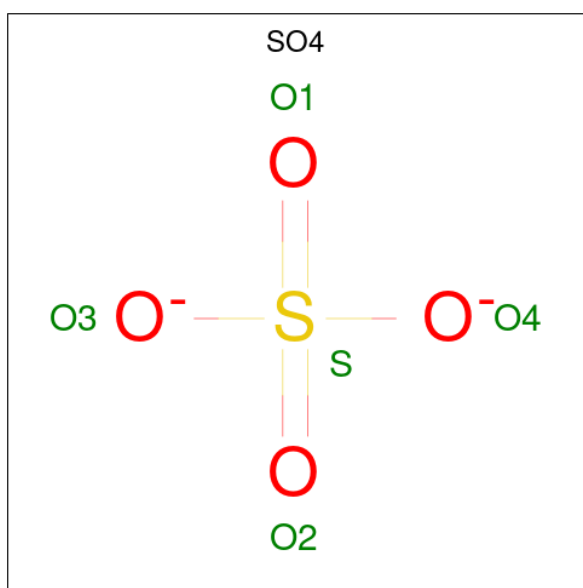
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

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



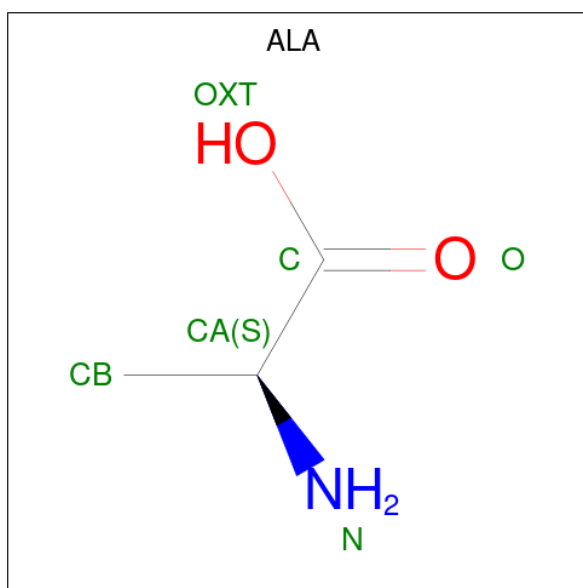
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

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



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		

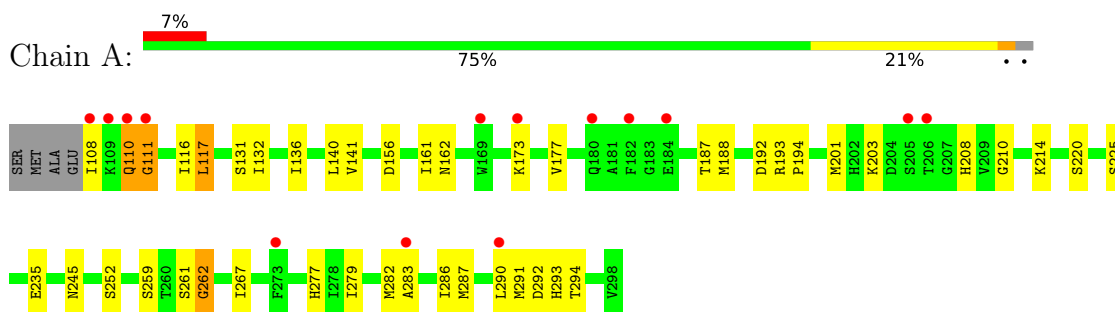
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	51	Total	O	0	0
			51	51		
8	B	100	Total	O	0	0
			100	100		
8	C	63	Total	O	0	1
			64	64		
8	D	74	Total	O	0	1
			74	74		

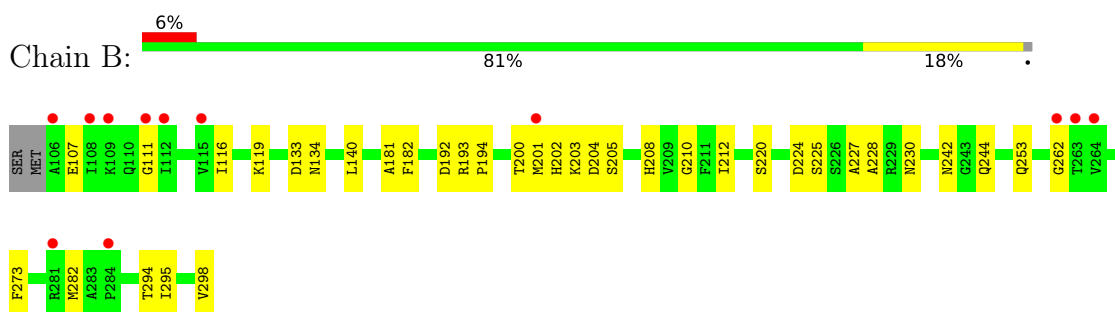
3 Residue-property plots [i](#)

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.

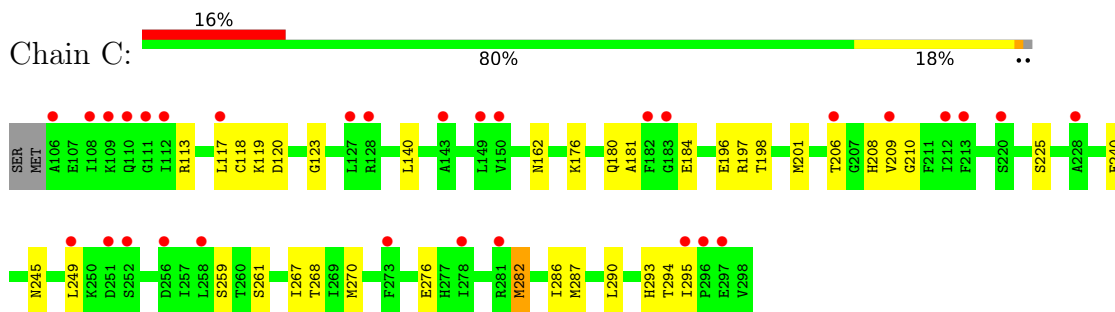
• Molecule 1: Syntenin-1



• Molecule 1: Syntenin-1

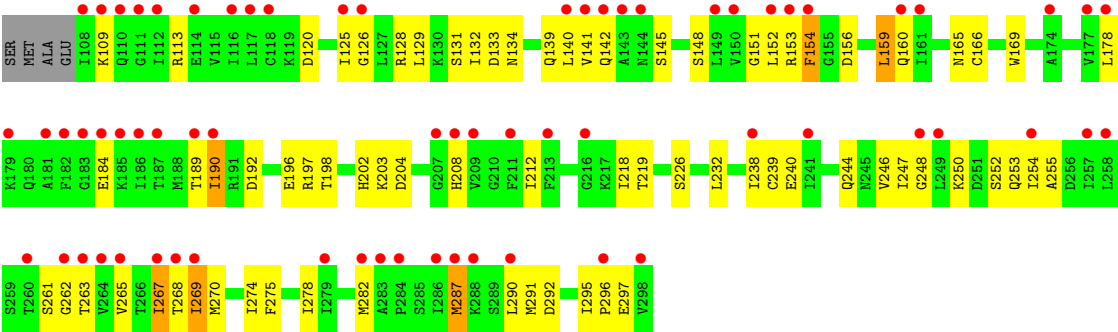


• Molecule 1: Syntenin-1



• 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	80.42Å 49.68Å 116.28Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	115.85 – 2.14 115.84 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.7 (115.85-2.14) 99.9 (115.84-2.14)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.247 , 0.325 0.252 , 0.327	Depositor DCC
R_{free} test set	2518 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.7	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	0.94	EDS
Total number of atoms	6357	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 32.19 % 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 9.7870e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, YDX, DGL, 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	0.57	0/1502	1.02	2/2019 (0.1%)
1	B	0.56	0/1516	1.07	2/2038 (0.1%)
1	C	0.55	0/1535	1.01	1/2063 (0.0%)
1	D	0.60	0/1502	1.09	2/2019 (0.1%)
All	All	0.57	0/6055	1.05	7/8139 (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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	120	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	133	ASP	CA-CB-CG	6.09	118.69	112.60
1	D	292	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	194	PRO	CB-CA-C	-5.60	103.93	112.11
1	B	194	PRO	CB-CA-C	-5.47	103.68	112.21
1	B	295	ILE	CB-CA-C	5.41	115.97	110.94

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	GLY	Peptide
1	C	113	ARG	Sidechain

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	32	0
1	B	1495	0	1541	24	0
1	C	1514	0	1558	24	0
1	D	1481	0	1530	58	0
2	A	15	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	2	0
3	C	12	0	18	0	0
3	D	12	0	18	0	0
4	B	10	0	7	0	0
4	D	10	0	7	0	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0
6	D	10	0	0	1	0
7	D	6	0	4	0	0
8	A	51	0	0	3	0
8	B	100	0	0	12	0
8	C	64	0	0	5	0
8	D	74	0	0	9	0
All	All	6357	0	6235	136	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 11.

All (136) 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:287:MET:SD	8:D:473:HOH:O	2.09	1.08
1:B:133:ASP:OD1	8:B:401:HOH:O	1.80	0.99
1:C:276:GLU:HG2	8:C:431:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:O	1:D:166:CYS:SG	2.37	0.81
1:C:261:SER:HB2	8:C:421:HOH:O	1.79	0.81
1:D:204:ASP:OD2	8:D:401:HOH:O	2.02	0.78
1:D:152:LEU:HD22	1:D:190:ILE:HD12	1.68	0.75
1:A:173:LYS:O	1:A:177:VAL:HG23	1.86	0.75
1:D:198:THR:HG22	1:D:268:THR:OG1	1.87	0.74
1:D:255:ALA:O	8:D:402:HOH:O	2.06	0.72
1:A:287:MET:SD	1:A:291:MET:HE2	2.29	0.72
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.73	0.70
1:A:286:ILE:HG23	1:A:290:LEU:HD12	1.73	0.70
1:B:208:HIS:O	8:B:402:HOH:O	2.09	0.69
1:D:152:LEU:O	8:D:403:HOH:O	2.12	0.68
1:B:202:HIS:HD2	8:B:444:HOH:O	1.76	0.67
1:B:228:ALA:O	8:B:403:HOH:O	2.13	0.66
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.78	0.65
1:D:142:GLN:HB2	8:D:457:HOH:O	1.95	0.65
1:A:140:LEU:HD12	1:A:287:MET:HE2	1.79	0.65
1:A:235:GLU:OE1	8:A:401:HOH:O	2.14	0.65
1:B:107:GLU:HA	8:B:424:HOH:O	1.97	0.65
1:A:290:LEU:CD1	1:B:182:PHE:HB2	2.27	0.64
1:A:140:LEU:HD23	1:A:141:VAL:N	2.12	0.63
1:A:108:ILE:HA	1:A:192:ASP:OD2	1.98	0.63
1:C:118:CYS:SG	1:C:184:GLU:O	2.56	0.63
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.79	0.62
1:D:226:SER:OG	6:D:304:SO4:O2	2.12	0.61
1:B:202:HIS:CD2	8:B:444:HOH:O	2.52	0.61
1:D:139:GLN:HG2	1:D:282:MET:CE	2.31	0.60
1:B:204:ASP:HB2	8:B:436:HOH:O	2.03	0.59
1:C:198:THR:HG22	1:C:268:THR:OG1	2.03	0.58
1:D:261:SER:OG	1:D:265:VAL:HG22	2.03	0.58
1:D:270:MET:SD	1:D:275:PHE:HA	2.43	0.58
1:D:198:THR:HA	1:D:267:ILE:O	2.05	0.57
1:D:131:SER:O	1:D:132:ILE:HD13	2.04	0.57
1:D:218:ILE:HD13	1:D:232:LEU:HD11	1.86	0.56
1:D:141:VAL:HG21	1:D:153:ARG:HA	1.88	0.56
1:A:111:GLY:HA3	8:A:414:HOH:O	2.07	0.55
1:A:117:LEU:HD13	1:A:188:MET:HE3	1.88	0.55
1:D:140:LEU:HD23	1:D:141:VAL:C	2.32	0.55
1:A:203:LYS:HA	1:A:208:HIS:O	2.07	0.55
1:D:197:ARG:NH1	8:D:408:HOH:O	2.37	0.55
1:D:153:ARG:O	1:D:156:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:THR:HG23	8:B:407:HOH:O	2.07	0.54
1:B:212:ILE:HB	1:B:220:SER:HB3	1.89	0.53
1:D:160:GLN:OE1	1:D:189:THR:HG21	2.08	0.53
1:D:142:GLN:HB3	1:D:145:SER:HB3	1.91	0.52
1:D:165:ASN:O	1:D:169:TRP:CZ2	2.63	0.52
1:A:282:MET:HG2	1:A:287:MET:HE3	1.92	0.52
1:B:253:GLN:OE1	8:B:406:HOH:O	2.19	0.52
1:D:254:ILE:O	1:D:255:ALA:C	2.53	0.52
1:D:153:ARG:HG2	8:D:404:HOH:O	2.09	0.51
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.43	0.51
1:D:126:GLY:HA3	1:D:145:SER:HB2	1.93	0.51
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.92	0.51
1:B:133:ASP:OD1	3:B:301:EDO:O2	2.28	0.51
1:C:294:THR:HG22	1:C:295:ILE:C	2.36	0.50
1:D:128:ARG:O	1:D:129:LEU:HD23	2.12	0.50
1:D:212:ILE:O	1:D:219:THR:OG1	2.25	0.50
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.26	0.50
1:C:206:THR:HG1	1:C:208:HIS:HD1	1.60	0.49
1:D:139:GLN:O	1:D:282:MET:HE1	2.12	0.49
1:A:279:ILE:C	1:A:279:ILE:HD12	2.37	0.49
1:A:283:ALA:HB3	1:A:286:ILE:HD12	1.94	0.49
1:D:148:SER:O	1:D:151:GLY:N	2.40	0.49
1:A:210:GLY:HA3	1:A:225:SER:CB	2.43	0.49
1:B:244:GLN:OE1	8:B:405:HOH:O	2.18	0.49
1:A:161:ILE:O	1:A:162:ASN:C	2.55	0.49
1:B:242:ASN:ND2	8:B:416:HOH:O	2.45	0.49
1:C:210:GLY:HA3	1:C:225:SER:CB	2.42	0.49
1:B:201:MET:SD	1:B:227:ALA:HA	2.53	0.48
1:D:261:SER:CB	1:D:265:VAL:HG22	2.43	0.48
1:C:282:MET:CE	1:C:287:MET:HB2	2.43	0.48
1:C:210:GLY:HA3	1:C:225:SER:HB2	1.96	0.48
1:C:197[A]:ARG:NH2	8:C:401:HOH:O	2.09	0.48
1:D:244:GLN:O	1:D:246:VAL:HG13	2.14	0.48
1:B:210:GLY:HA3	1:B:225:SER:CB	2.43	0.47
1:C:176:LYS:O	1:C:180:GLN:HG3	2.14	0.47
1:D:203:LYS:HG3	1:D:263:THR:O	2.14	0.47
1:D:154:PHE:C	1:D:154:PHE:CD1	2.92	0.47
1:C:249:LEU:HD21	1:C:293:HIS:CE1	2.49	0.47
1:A:214:LYS:O	8:A:402:HOH:O	2.20	0.47
1:C:286:ILE:HG22	1:C:290:LEU:HD12	1.97	0.47
1:A:140:LEU:HD23	1:A:140:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:HD23	1:D:140:LEU:C	2.40	0.46
1:D:203:LYS:HA	1:D:208:HIS:O	2.15	0.46
1:C:119:LYS:NZ	1:C:181:ALA:O	2.41	0.46
1:B:203:LYS:HD3	1:B:262:GLY:O	2.15	0.46
1:C:119:LYS:HB3	1:C:123:GLY:HA2	1.98	0.46
1:D:142:GLN:HG3	1:D:290:LEU:HD22	1.98	0.46
1:D:113:ARG:HH11	1:D:113:ARG:HB3	1.82	0.45
1:D:152:LEU:HD22	1:D:190:ILE:CD1	2.42	0.45
1:D:154:PHE:CE1	1:D:247:ILE:HD13	2.51	0.45
1:B:119:LYS:NZ	1:B:181:ALA:O	2.35	0.45
1:A:131:SER:HA	1:A:136:ILE:HD13	1.99	0.45
1:B:200:THR:O	1:B:230:ASN:OD1	2.34	0.45
1:D:274:ILE:O	1:D:278:ILE:HG13	2.17	0.44
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.98	0.44
1:D:120:ASP:OD1	1:D:120:ASP:C	2.59	0.44
1:A:116:ILE:HD12	1:A:187:THR:HG22	1.98	0.44
1:A:245:ASN:O	1:A:293:HIS:HD2	2.01	0.43
1:A:287:MET:SD	1:A:291:MET:CE	3.03	0.43
1:A:132:ILE:HD13	1:A:277:HIS:CE1	2.54	0.43
1:B:210:GLY:HA3	1:B:225:SER:HB2	1.99	0.43
1:D:196:GLU:HA	1:D:269:ILE:O	2.18	0.43
1:B:273[B]:PHE:CE2	3:B:301:EDO:H12	2.54	0.43
1:C:249:LEU:HD21	1:C:293:HIS:ND1	2.34	0.42
1:A:140:LEU:HD23	1:A:141:VAL:C	2.44	0.42
1:C:196:GLU:HG2	1:C:270:MET:HB2	2.01	0.42
1:D:154:PHE:CZ	1:D:247:ILE:HD13	2.55	0.42
1:C:245:ASN:OD1	1:C:245:ASN:C	2.62	0.42
1:B:192:ASP:O	1:B:193:ARG:C	2.62	0.42
1:D:139:GLN:HG2	1:D:282:MET:HE2	2.01	0.42
1:A:110:GLN:O	1:A:111:GLY:C	2.62	0.42
1:C:201:MET:HE1	1:C:267:ILE:HG13	2.02	0.42
1:D:139:GLN:HG2	1:D:282:MET:HE1	2.02	0.42
1:D:203:LYS:HD2	1:D:262:GLY:O	2.19	0.42
1:D:291:MET:HE2	1:D:291:MET:HB2	1.84	0.42
1:A:192:ASP:O	1:A:193:ARG:C	2.62	0.41
1:D:152:LEU:CD2	1:D:190:ILE:HD12	2.43	0.41
1:A:261:SER:C	1:A:262:GLY:O	2.64	0.41
1:B:204:ASP:HA	8:B:412:HOH:O	2.19	0.41
1:C:240:GLU:HB2	1:C:268:THR:HB	2.03	0.41
1:D:126:GLY:HA2	8:D:457:HOH:O	2.20	0.41
1:A:279:ILE:O	1:A:282:MET:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:LYS:N	1:D:192:ASP:OD2	2.49	0.41
1:D:240:GLU:OE2	8:D:404:HOH:O	2.21	0.41
1:C:176:LYS:HB2	8:C:420:HOH:O	2.20	0.41
1:D:113:ARG:HH11	1:D:113:ARG:CB	2.34	0.41
1:D:250:LYS:HD2	1:D:253:GLN:NE2	2.36	0.41
1:D:282:MET:HE3	1:D:287:MET:HG3	2.01	0.41
1:D:196:GLU:OE1	1:D:239:CYS:SG	2.72	0.41
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.21	0.40
1:C:276:GLU:CG	8:C:431:HOH:O	2.52	0.40
1:D:248:GLY:HA2	1:D:287: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%)	179 (94%)	9 (5%)	2 (1%)	11	6
1	B	192/195 (98%)	186 (97%)	6 (3%)	0	100	100
1	C	194/195 (100%)	180 (93%)	13 (7%)	1 (0%)	24	19
1	D	190/195 (97%)	169 (89%)	19 (10%)	2 (1%)	11	6
All	All	766/780 (98%)	714 (93%)	47 (6%)	5 (1%)	18	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLY
1	A	262	GLY
1	D	184	GLU
1	C	162	ASN
1	D	159	LEU

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%)	161 (97%)	5 (3%)	36	37
1	B	167/168 (99%)	160 (96%)	7 (4%)	26	23
1	C	169/168 (101%)	164 (97%)	5 (3%)	36	37
1	D	166/168 (99%)	156 (94%)	10 (6%)	17	12
All	All	668/672 (99%)	641 (96%)	27 (4%)	27	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	117	LEU
1	A	220	SER
1	A	252	SER
1	A	259	SER
1	B	116	ILE
1	B	134	ASN
1	B	140	LEU
1	B	205	SER
1	B	224	ASP
1	B	282	MET
1	B	298	VAL
1	C	117	LEU
1	C	140	LEU
1	C	209	VAL
1	C	259	SER
1	C	282	MET
1	D	134	ASN
1	D	154	PHE
1	D	190	ILE
1	D	202	HIS
1	D	238	ILE
1	D	252	SER
1	D	267	ILE

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Mol	Chain	Res	Type
1	D	269	ILE
1	D	287	MET
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	215	ASN
1	A	230	ASN
1	A	293	HIS
1	B	121	GLN
1	B	139	GLN
1	B	142	GLN
1	B	202	HIS
1	B	215	ASN
1	C	139	GLN
1	C	157	GLN
1	C	230	ASN
1	C	253	GLN
1	D	157	GLN
1	D	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
3	EDO	A	302	-	3,3,3	0.10	0	2,2,2	0.07	0
3	EDO	B	301	-	3,3,3	0.30	0	2,2,2	0.22	0
5	GLY	D	308	-	4,4,4	0.96	0	3,4,4	1.30	0
4	DGL	D	307	-	8,9,9	1.07	0	8,11,11	0.90	0
3	EDO	B	302	-	3,3,3	0.30	0	2,2,2	0.40	0
6	SO4	D	304	-	4,4,4	0.29	0	6,6,6	0.08	0
7	ALA	D	306	-	5,5,5	0.98	0	6,6,6	0.93	0
3	EDO	D	302	-	3,3,3	0.13	0	2,2,2	0.12	0
3	EDO	D	301	-	3,3,3	0.26	0	2,2,2	0.23	0
3	EDO	C	302	-	3,3,3	0.07	0	2,2,2	0.14	0
3	EDO	C	301	-	3,3,3	0.17	0	2,2,2	0.04	0
3	EDO	D	303	-	3,3,3	0.15	0	2,2,2	0.12	0
5	GLY	C	304	-	4,4,4	0.83	0	3,4,4	1.17	0
3	EDO	C	303	-	3,3,3	0.47	0	2,2,2	0.61	0
6	SO4	D	305	-	4,4,4	0.31	0	6,6,6	0.12	0
4	DGL	B	303	-	8,9,9	1.09	1 (12%)	8,11,11	0.83	0
2	YDX	A	301	-	16,16,16	1.80	2 (12%)	16,21,21	2.59	5 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-
5	GLY	D	308	-	-	2/2/2/2	-
4	DGL	D	307	-	-	1/9/9/9	-
3	EDO	B	302	-	-	0/1/1/1	-
7	ALA	D	306	-	-	0/4/4/4	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	C	301	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	303	-	-	1/1/1/1	-
5	GLY	C	304	-	-	2/2/2/2	-
3	EDO	C	303	-	-	1/1/1/1	-
4	DGL	B	303	-	-	2/9/9/9	-
2	YDX	A	301	-	-	0/8/8/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	YDX	C07-N06	4.32	1.45	1.37
2	A	301	YDX	C05-N06	3.93	1.45	1.39
4	B	303	DGL	OE2-CD	-2.02	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	YDX	C03-N02-N15	-6.31	108.43	112.01
2	A	301	YDX	C01-N02-N15	4.69	124.34	119.57
2	A	301	YDX	C09-N10-C11	-3.44	124.52	127.78
2	A	301	YDX	C13-N14-N10	2.39	106.70	104.19
2	A	301	YDX	C12-C13-N14	-2.30	107.04	111.72

There are no chirality outliers.

All (11) torsion outliers are listed below:

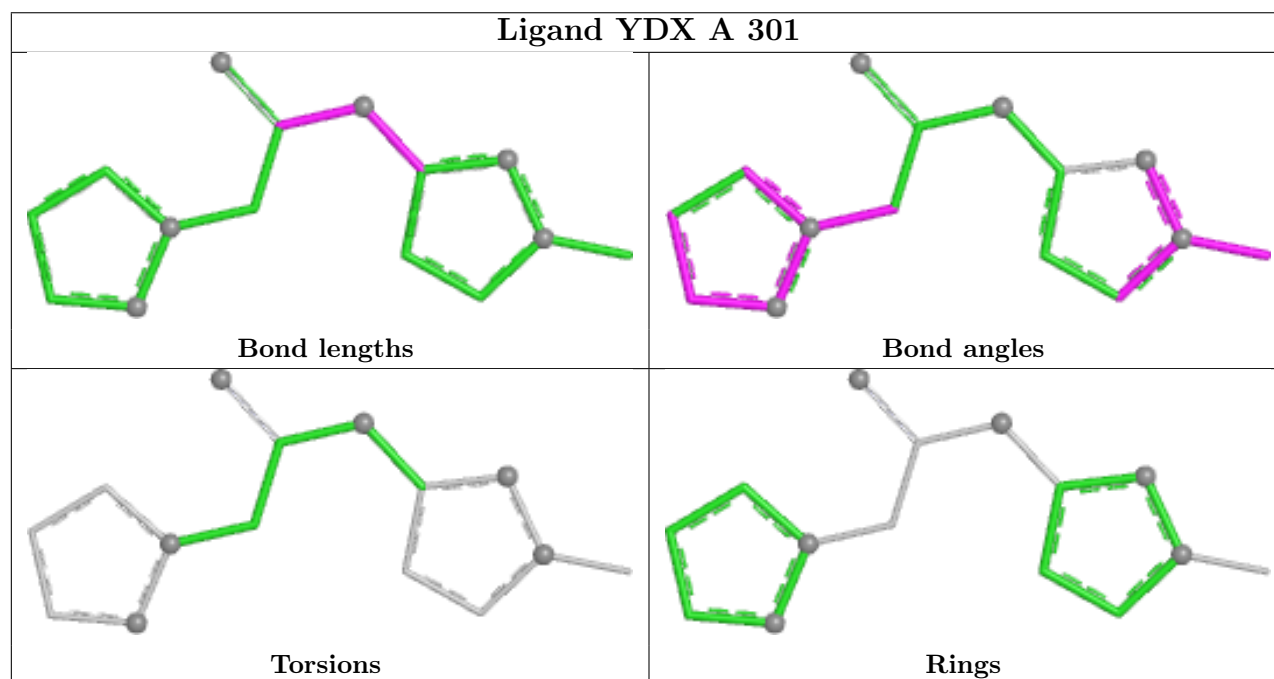
Mol	Chain	Res	Type	Atoms
5	C	304	GLY	O-C-CA-N
5	C	304	GLY	OXT-C-CA-N
5	D	308	GLY	OXT-C-CA-N
3	C	301	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
3	C	302	EDO	O1-C1-C2-O2
5	D	308	GLY	O-C-CA-N
4	B	303	DGL	OXT-C-CA-CB
4	B	303	DGL	O-C-CA-CB
4	D	307	DGL	O-C-CA-N
3	D	303	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	EDO	2	0
6	D	304	SO4	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%)	0.63	14 (7%)	21 24	17, 47, 71, 93	1 (0%)
1	B	193/195 (98%)	0.56	12 (6%)	26 30	14, 44, 67, 95	1 (0%)
1	C	193/195 (98%)	1.08	31 (16%)	4 6	18, 50, 82, 117	3 (1%)
1	D	191/195 (97%)	1.70	67 (35%)	1 1	17, 53, 79, 128	1 (0%)
All	All	768/780 (98%)	0.99	124 (16%)	4 6	14, 49, 77, 128	6 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	254	ILE	6.3
1	D	182	PHE	5.9
1	D	149	LEU	5.6
1	D	178	LEU	5.5
1	C	106	ALA	5.5
1	D	177	VAL	5.1
1	A	182	PHE	5.1
1	D	258	LEU	5.0
1	D	183	GLY	5.0
1	C	110	GLN	4.8
1	C	108	ILE	4.6
1	D	108	ILE	4.6
1	D	125	ILE	4.5
1	C	109	LYS	4.3
1	D	265	VAL	4.1
1	A	108	ILE	4.0
1	D	117	LEU	4.0
1	D	284	PRO	3.9
1	D	140	LEU	3.9
1	D	190	ILE	3.8
1	D	241	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	267	ILE	3.7
1	D	141	VAL	3.7
1	D	186	ILE	3.7
1	B	106	ALA	3.6
1	C	209	VAL	3.5
1	D	150	VAL	3.5
1	D	116	ILE	3.5
1	C	182	PHE	3.5
1	D	153	ARG	3.5
1	D	112	ILE	3.4
1	C	296	PRO	3.4
1	D	152	LEU	3.3
1	B	281	ARG	3.2
1	B	111	GLY	3.2
1	D	238	ILE	3.1
1	D	260	THR	3.1
1	C	183	GLY	3.1
1	D	187	THR	3.1
1	C	112	ILE	3.1
1	D	286	ILE	3.0
1	D	288	LYS	3.0
1	D	213	PHE	3.0
1	D	184	GLU	2.9
1	D	283	ALA	2.9
1	B	115	VAL	2.9
1	D	298	VAL	2.8
1	B	263	THR	2.8
1	D	126	GLY	2.8
1	D	109	LYS	2.8
1	B	264	VAL	2.7
1	C	117	LEU	2.7
1	C	249	LEU	2.7
1	D	209	VAL	2.7
1	D	264	VAL	2.7
1	D	257	ILE	2.7
1	D	179	LYS	2.7
1	C	111	GLY	2.6
1	C	213	PHE	2.6
1	B	108	ILE	2.5
1	C	212	ILE	2.5
1	A	109	LYS	2.5
1	D	263	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	161	ILE	2.5
1	D	144	ASN	2.5
1	C	251	ASP	2.5
1	C	127	LEU	2.5
1	D	189	THR	2.5
1	B	109	LYS	2.5
1	C	273[A]	PHE	2.5
1	D	208	HIS	2.5
1	D	216	GLY	2.5
1	B	201	MET	2.4
1	C	143	ALA	2.4
1	A	169	TRP	2.4
1	D	282	MET	2.4
1	A	283	ALA	2.4
1	D	181	ALA	2.4
1	D	290	LEU	2.4
1	A	111	GLY	2.4
1	D	269	ILE	2.4
1	C	206	THR	2.4
1	D	142	GLN	2.4
1	D	174	ALA	2.3
1	C	220	SER	2.3
1	D	279	ILE	2.3
1	C	297	GLU	2.3
1	C	281	ARG	2.3
1	D	111	GLY	2.3
1	D	207	GLY	2.3
1	C	228	ALA	2.3
1	B	262	GLY	2.3
1	C	149	LEU	2.2
1	D	249	LEU	2.2
1	A	205	SER	2.2
1	C	252	SER	2.2
1	D	114	GLU	2.2
1	C	258	LEU	2.2
1	D	110	GLN	2.2
1	D	154	PHE	2.2
1	D	211	PHE	2.2
1	D	118	CYS	2.2
1	D	287	MET	2.2
1	B	284	PRO	2.1
1	A	273[A]	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	112	ILE	2.1
1	C	278	ILE	2.1
1	A	180	GLN	2.1
1	D	248	GLY	2.1
1	D	268	THR	2.1
1	D	160	GLN	2.1
1	C	128	ARG	2.1
1	D	143	ALA	2.1
1	A	173	LYS	2.1
1	D	262	GLY	2.1
1	A	290	LEU	2.1
1	C	256	ASP	2.1
1	A	110	GLN	2.1
1	D	185	LYS	2.1
1	A	184	GLU	2.0
1	C	295	ILE	2.0
1	C	150	VAL	2.0
1	A	206	THR	2.0
1	D	296	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.

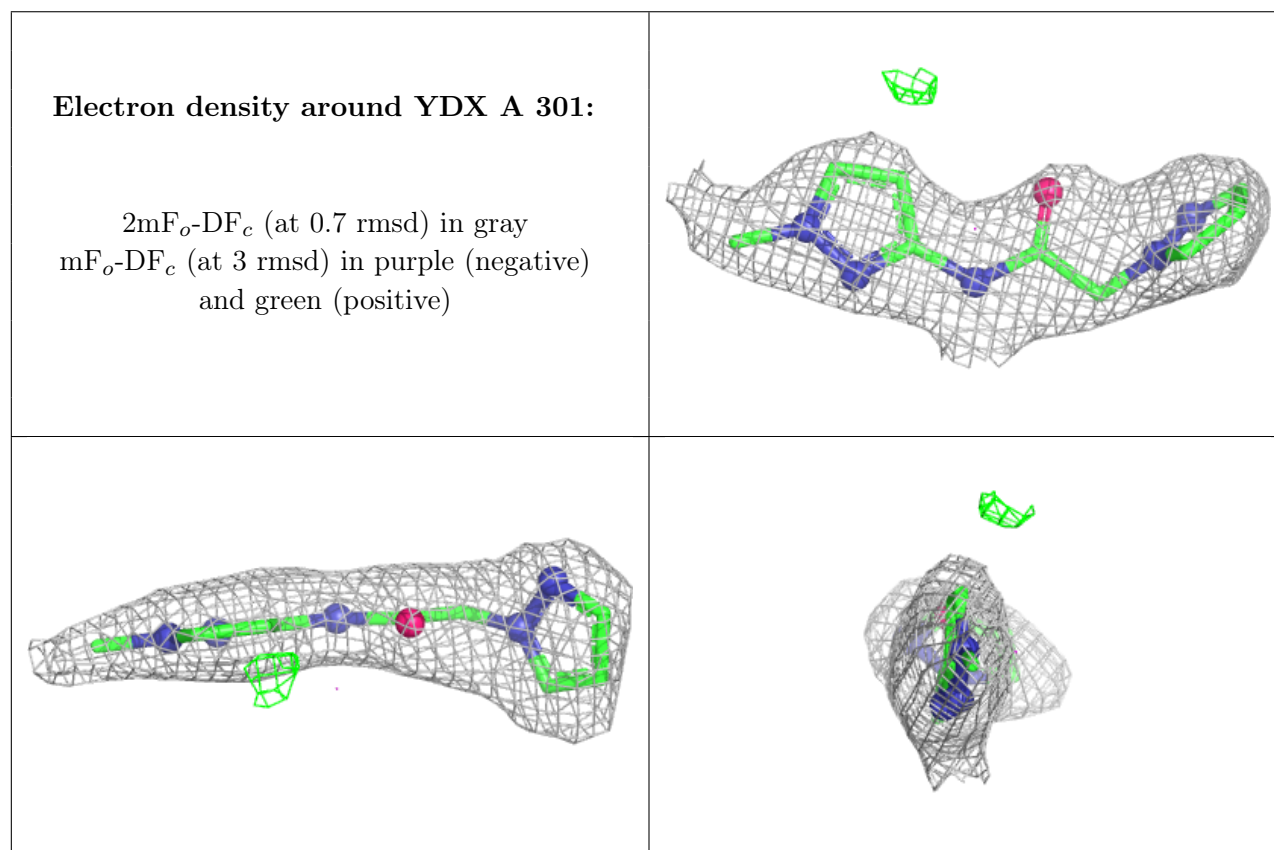
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	D	305	5/5	0.60	0.14	101,101,116,123	0
4	DGL	D	307	10/10	0.69	0.18	65,77,84,85	0
3	EDO	D	303	4/4	0.70	0.20	54,62,63,64	0
7	ALA	D	306	6/6	0.70	0.18	64,68,68,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DGL	B	303	10/10	0.76	0.15	46,77,81,92	0
5	GLY	C	304	5/5	0.77	0.12	56,58,60,62	0
6	SO4	D	304	5/5	0.79	0.11	83,85,92,94	0
3	EDO	C	301	4/4	0.85	0.13	50,50,51,56	0
3	EDO	D	302	4/4	0.86	0.13	41,46,49,49	0
5	GLY	D	308	5/5	0.87	0.13	55,59,61,65	0
2	YDX	A	301	15/15	0.87	0.13	51,58,66,67	0
3	EDO	D	301	4/4	0.88	0.15	37,44,50,55	0
3	EDO	C	303	4/4	0.89	0.16	43,50,50,51	0
3	EDO	C	302	4/4	0.93	0.10	43,45,46,47	0
3	EDO	A	302	4/4	0.93	0.13	51,51,52,52	0
3	EDO	B	301	4/4	0.94	0.10	34,39,41,46	0
3	EDO	B	302	4/4	0.97	0.06	32,39,41,41	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 ⓘ

There are no such residues in this entry.