



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:04 PM UTC

PDB ID : 7FSJ / pdb_00007fsj
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z57744712
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

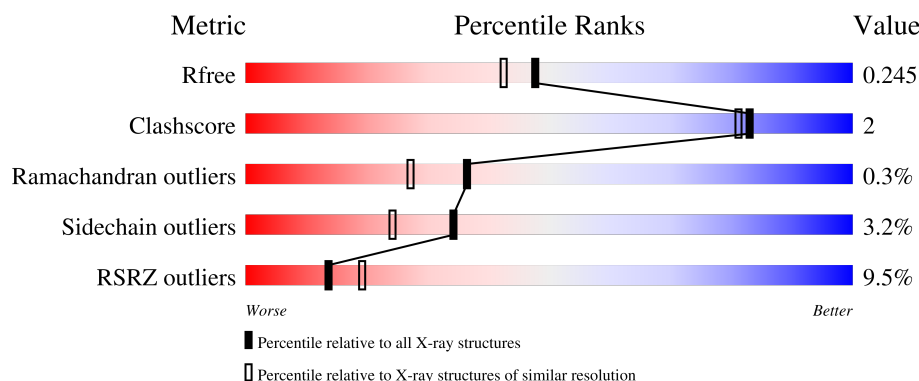
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	195	16% 90% 8% ..
1	B	195	5% 91% 8% .
1	C	195	10% 86% 13% ..
1	D	195	7% 90% 7% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6469 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

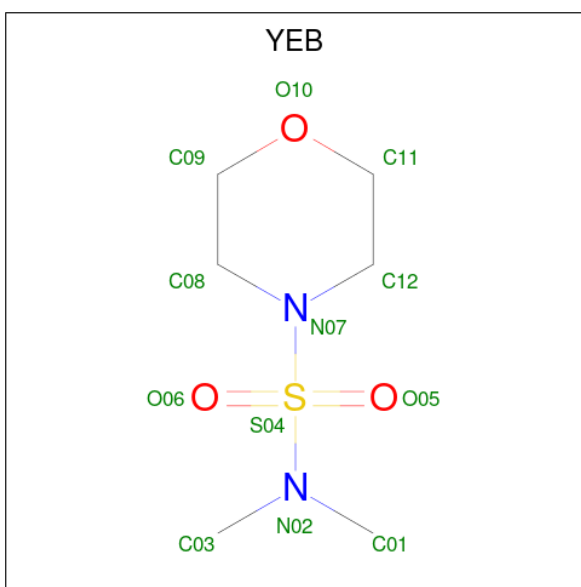
- Molecule 1 is a protein called Syntenin-1.

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is N,N-dimethylmorpholine-4-sulfonamide (CCD ID: YEB) (formula: $C_6H_{14}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

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



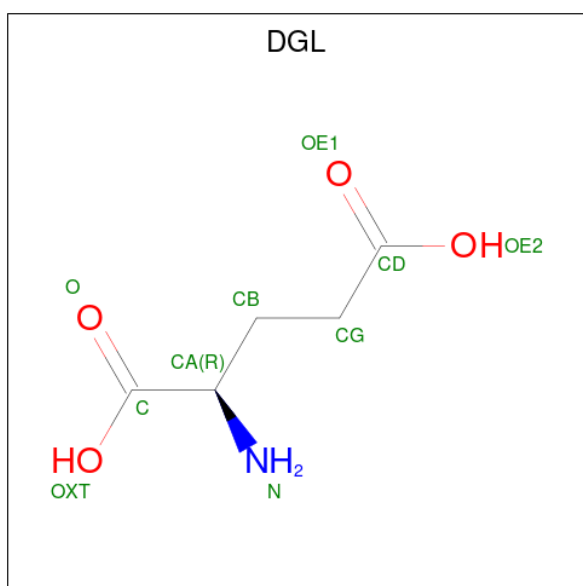
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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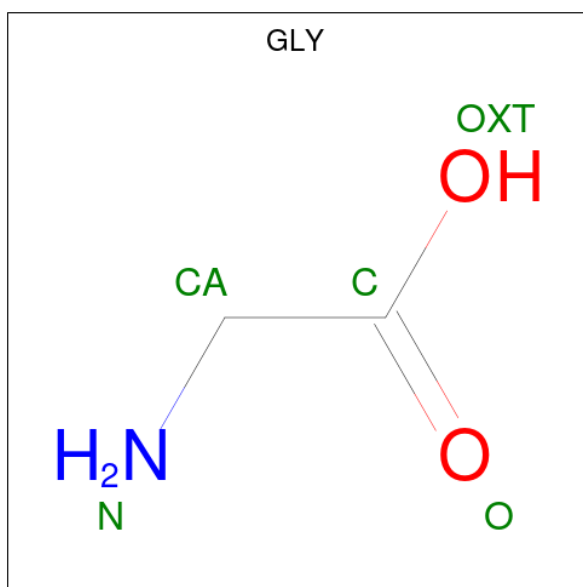
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



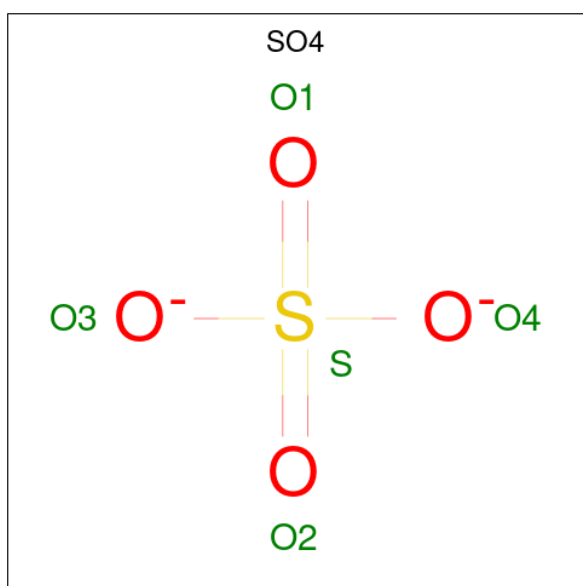
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

- 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).



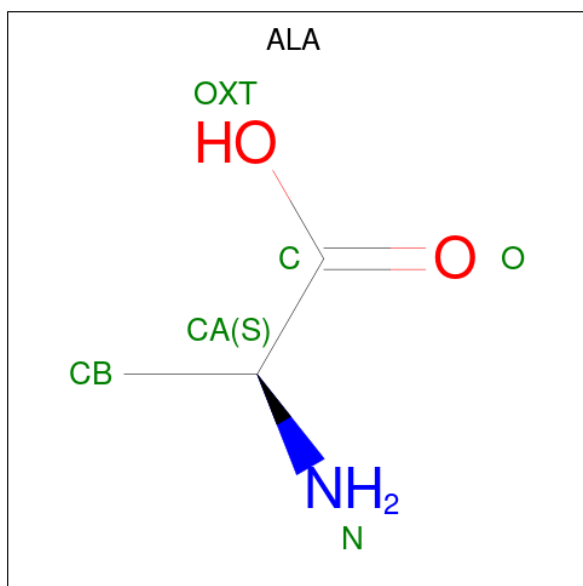
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

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

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

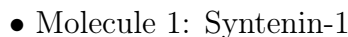
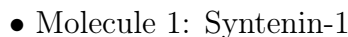
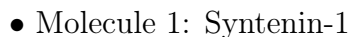


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total	O	0	0
			62	62		
8	B	114	Total	O	0	1
			114	114		
8	C	93	Total	O	0	1
			94	94		
8	D	125	Total	O	0	1
			125	125		

- 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	81.16Å 49.54Å 114.91Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	114.49 – 1.97 114.49 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (114.49-1.97) 99.5 (114.49-1.97)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.260 (Not available) , 0.245	Depositor DCC
R_{free} test set	3136 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.7	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	0.95	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5386e-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: YEB, EDO, 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	1.16	0/1502	1.41	1/2019 (0.0%)
1	B	1.14	1/1516 (0.1%)	1.41	2/2038 (0.1%)
1	C	1.18	0/1535	1.43	3/2063 (0.1%)
1	D	1.18	0/1510	1.46	3/2030 (0.1%)
All	All	1.17	1/6063 (0.0%)	1.43	9/8150 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	HIS	CE1-NE2	5.50	1.38	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	THR	CA-CB-OG1	-6.98	99.12	109.60
1	D	198	THR	CA-CB-OG1	-6.08	100.48	109.60
1	C	266	THR	CA-CB-OG1	-5.86	100.81	109.60
1	B	263	THR	CA-CB-OG1	-5.50	101.35	109.60
1	C	235	GLU	N-CA-CB	-5.39	104.11	112.30
1	C	278	ILE	CA-C-O	-5.35	115.39	120.95
1	B	125	ILE	N-CA-C	-5.31	107.60	111.90
1	D	271	PRO	CA-C-N	5.01	127.32	120.46
1	D	271	PRO	C-N-CA	5.01	127.32	120.46

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	7	0
1	B	1495	0	1541	5	0
1	C	1514	0	1558	11	1
1	D	1489	0	1533	9	0
2	A	12	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	12	0	18	0	0
3	D	8	0	12	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	15	0	0	0	0
7	D	6	0	4	0	0
8	A	62	0	0	0	0
8	B	114	0	0	2	0
8	C	94	0	0	3	0
8	D	125	0	0	2	0
All	All	6469	0	6232	30	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 2.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.72	0.72
1:B:177:VAL:O	8:B:401:HOH:O	2.13	0.66
1:A:109:LYS:N	1:A:192:ASP:OD2	2.30	0.65
1:D:125:ILE:HD11	1:D:127:LEU:HD12	1.81	0.62
1:D:154:PHE:CD1	1:D:247:ILE:CD1	2.83	0.60
1:C:192:ASP:OD1	8:C:401:HOH:O	2.17	0.59
1:A:140:LEU:CD1	1:A:282:MET:SD	2.92	0.57
1:C:121:GLN:HG3	8:C:460:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD11	1:A:282:MET:SD	2.45	0.56
1:A:286:ILE:HG23	1:A:290:LEU:HD12	1.88	0.55
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.89	0.54
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.41	0.54
1:C:108:ILE:CD1	1:C:198:THR:HG23	2.40	0.52
1:C:108:ILE:HD12	1:C:198:THR:HG23	1.92	0.52
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.95	0.49
1:D:154:PHE:CE1	1:D:247:ILE:CD1	2.96	0.49
1:D:197:ARG:NH2	8:D:401:HOH:O	2.17	0.48
1:C:229:ARG:NH2	8:C:404:HOH:O	2.46	0.48
1:D:154:PHE:CE1	1:D:247:ILE:HD13	2.49	0.48
1:D:182:PHE:HB3	1:D:184:GLU:OE1	2.14	0.47
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.96	0.47
1:A:197:ARG:HD3	1:C:194:PRO:O	2.15	0.45
1:C:226:SER:HA	1:C:229:ARG:NH2	2.32	0.44
1:B:137:PHE:CE2	1:B:157:GLN:HB2	2.53	0.44
1:B:133:ASP:OD1	8:B:402:HOH:O	2.21	0.44
1:C:240:GLU:HA	1:C:244:GLN:O	2.17	0.43
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.01	0.42
1:D:202:HIS:CE1	8:D:451:HOH:O	2.72	0.42
1:C:140:LEU:HD12	1:C:291:MET:HE2	2.03	0.41
1:D:154:PHE:CZ	1:D:247:ILE:HD13	2.56	0.41

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)
1:C:124:LYS:NZ	1:C:297:GLU:OE2[2_544]	2.18	0.02

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	14
1	B	192/195 (98%)	189 (98%)	3 (2%)	0	100	100
1	C	194/195 (100%)	184 (95%)	9 (5%)	1 (0%)	24	14
1	D	191/195 (98%)	186 (97%)	5 (3%)	0	100	100
All	All	767/780 (98%)	740 (96%)	25 (3%)	2 (0%)	36	27

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/168 (99%)	160 (96%)	6 (4%)	31	20
1	B	167/168 (99%)	162 (97%)	5 (3%)	36	27
1	C	169/168 (101%)	163 (96%)	6 (4%)	31	20
1	D	167/168 (99%)	163 (98%)	4 (2%)	43	35
All	All	669/672 (100%)	648 (97%)	21 (3%)	34	26

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	140	LEU
1	A	171	SER
1	A	184	GLU
1	A	206	THR
1	A	259	SER
1	B	110	GLN
1	B	140	LEU
1	B	205	SER

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Mol	Chain	Res	Type
1	B	266	THR
1	B	284	PRO
1	C	109	LYS
1	C	132	ILE
1	C	150	VAL
1	C	214	LYS
1	C	288	LYS
1	C	297	GLU
1	D	121	GLN
1	D	125	ILE
1	D	286	ILE
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	B	139	GLN
1	B	165	ASN
1	C	110	GLN
1	C	180	GLN
1	C	215	ASN
1	C	230	ASN
1	D	157	GLN

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$
3	EDO	D	301	-	3,3,3	0.28	0	2,2,2	0.14	0
3	EDO	B	302	-	3,3,3	0.49	0	2,2,2	0.32	0
4	DGL	D	307	-	8,9,9	1.33	1 (12%)	8,11,11	0.99	0
3	EDO	A	302	-	3,3,3	0.12	0	2,2,2	0.32	0
7	ALA	D	306	-	5,5,5	1.12	1 (20%)	6,6,6	0.82	0
3	EDO	B	301	-	3,3,3	0.29	0	2,2,2	0.19	0
3	EDO	C	302	-	3,3,3	0.49	0	2,2,2	0.04	0
4	DGL	B	303	-	8,9,9	0.87	0	8,11,11	1.54	2 (25%)
2	YEB	A	301	-	11,12,12	2.36	3 (27%)	15,17,17	2.83	5 (33%)
3	EDO	C	303	-	3,3,3	0.53	0	2,2,2	0.64	0
6	SO4	D	304	-	4,4,4	0.28	0	6,6,6	0.11	0
6	SO4	D	305	-	4,4,4	0.32	0	6,6,6	0.32	0
3	EDO	D	302	-	3,3,3	0.28	0	2,2,2	0.18	0
6	SO4	D	303	-	4,4,4	0.26	0	6,6,6	0.10	0
5	GLY	C	304	-	4,4,4	0.88	0	3,4,4	1.01	0
3	EDO	C	301	-	3,3,3	0.24	0	2,2,2	0.15	0
5	GLY	D	308	-	4,4,4	1.32	1 (25%)	3,4,4	1.01	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
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
4	DGL	D	307	-	-	2/9/9/9	-
3	EDO	A	302	-	-	0/1/1/1	-
7	ALA	D	306	-	-	0/4/4/4	-
3	EDO	B	301	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	302	-	-	0/1/1/1	-
4	DGL	B	303	-	-	0/9/9/9	-
2	YEB	A	301	-	-	4/12/20/20	0/1/1/1
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	D	302	-	-	1/1/1/1	-
5	GLY	C	304	-	-	0/2/2/2	-
3	EDO	C	301	-	-	0/1/1/1	-
5	GLY	D	308	-	-	2/2/2/2	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	YEB	S04-N02	6.42	1.71	1.60
2	A	301	YEB	O06-S04	3.00	1.48	1.42
4	D	307	DGL	O-C	2.91	1.30	1.22
2	A	301	YEB	O05-S04	2.63	1.47	1.42
5	D	308	GLY	OXT-C	-2.55	1.22	1.30
7	D	306	ALA	OXT-C	-2.06	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	YEB	O06-S04-O05	-6.93	107.97	121.67
2	A	301	YEB	C09-C08-N07	6.01	112.55	108.27
2	A	301	YEB	C12-N07-C08	-3.55	108.04	112.12
2	A	301	YEB	C03-N02-C01	2.88	120.46	114.75
4	B	303	DGL	OXT-C-O	-2.85	117.62	124.08
2	A	301	YEB	C11-C12-N07	2.83	110.28	108.27
4	B	303	DGL	OE1-CD-CG	-2.03	116.66	123.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	YEB	C12-N07-S04-O06
5	D	308	GLY	O-C-CA-N
5	D	308	GLY	OXT-C-CA-N
2	A	301	YEB	C03-N02-S04-O05
3	C	303	EDO	O1-C1-C2-O2
3	D	302	EDO	O1-C1-C2-O2
2	A	301	YEB	C08-N07-S04-O06

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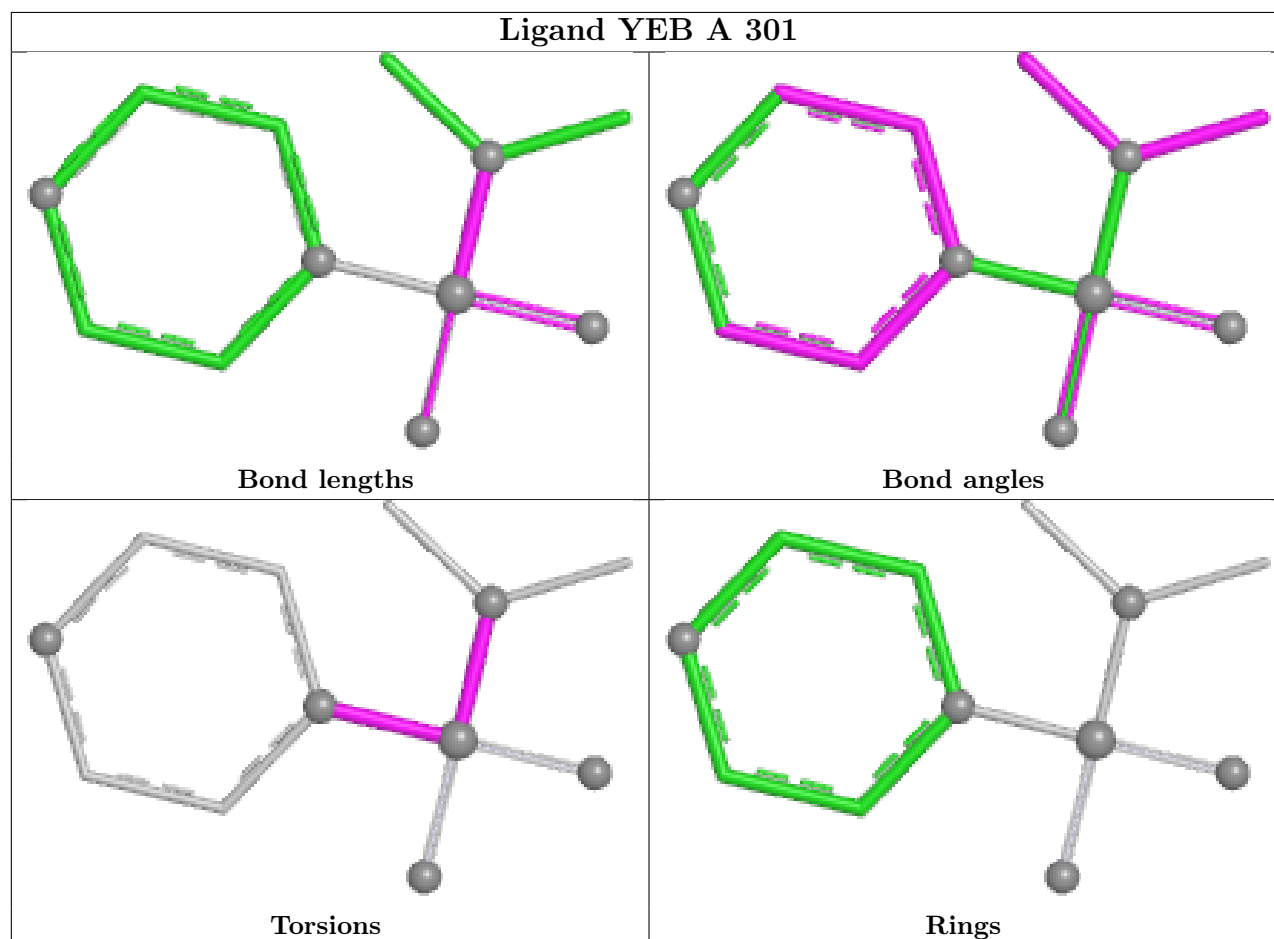
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Mol	Chain	Res	Type	Atoms
4	D	307	DGL	O-C-CA-CB
4	D	307	DGL	OXT-C-CA-CB
2	A	301	YEB	C03-N02-S04-N07

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [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%)	1.64	31 (16%) 4 6	8, 39, 66, 87	17 (8%)
1	B	193/195 (98%)	0.50	9 (4%) 36 46	7, 39, 61, 84	1 (0%)
1	C	193/195 (98%)	0.87	20 (10%) 11 16	7, 38, 66, 106	6 (3%)
1	D	191/195 (97%)	0.48	13 (6%) 23 31	7, 36, 60, 94	2 (1%)
All	All	768/780 (98%)	0.87	73 (9%) 14 19	7, 38, 64, 106	26 (3%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	PHE	17.2
1	C	298	VAL	15.1
1	D	273[A]	PHE	14.7
1	A	181	ALA	14.7
1	A	186	ILE	14.7
1	A	183	GLY	14.2
1	A	178	LEU	13.8
1	A	111	GLY	13.7
1	A	112	ILE	13.0
1	A	108	ILE	12.7
1	A	273[A]	PHE	12.1
1	A	109	LYS	11.7
1	B	273[A]	PHE	11.4
1	A	179	LYS	11.3
1	C	197[A]	ARG	11.2
1	A	298	VAL	11.2
1	C	273[A]	PHE	11.1
1	C	296	PRO	11.1
1	D	256[A]	ASP	10.3
1	A	185	LYS	9.9
1	A	180	GLN	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	113	ARG	8.9
1	C	297	GLU	8.8
1	A	184	GLU	8.5
1	C	144[A]	ASN	8.3
1	A	110	GLN	7.4
1	C	108	ILE	6.0
1	C	110	GLN	5.7
1	C	106	ALA	5.2
1	B	109	LYS	4.8
1	B	118	CYS	4.8
1	A	283	ALA	4.6
1	D	182	PHE	4.5
1	A	286	ILE	4.1
1	A	281	ARG	4.1
1	A	282	MET	3.7
1	B	111	GLY	3.7
1	C	209	VAL	3.7
1	C	182	PHE	3.7
1	C	118	CYS	3.5
1	D	108	ILE	3.4
1	D	109	LYS	3.2
1	A	117	LEU	3.2
1	C	109	LYS	3.2
1	A	118	CYS	3.1
1	C	107	GLU	3.1
1	B	110	GLN	3.0
1	C	295	ILE	3.0
1	C	111	GLY	2.8
1	A	125	ILE	2.8
1	C	281	ARG	2.7
1	D	118	CYS	2.7
1	D	144	ASN	2.7
1	D	111	GLY	2.6
1	A	280	LYS	2.6
1	B	108	ILE	2.6
1	D	110	GLN	2.6
1	A	140	LEU	2.6
1	A	290	LEU	2.5
1	C	151	GLY	2.4
1	D	184	GLU	2.4
1	A	284	PRO	2.3
1	D	125	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	ILE	2.2
1	D	112	ILE	2.2
1	C	206	THR	2.2
1	A	289	SER	2.2
1	D	288	LYS	2.1
1	A	121	GLN	2.1
1	B	286	ILE	2.1
1	A	163	GLY	2.0
1	B	106	ALA	2.0
1	C	112	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.

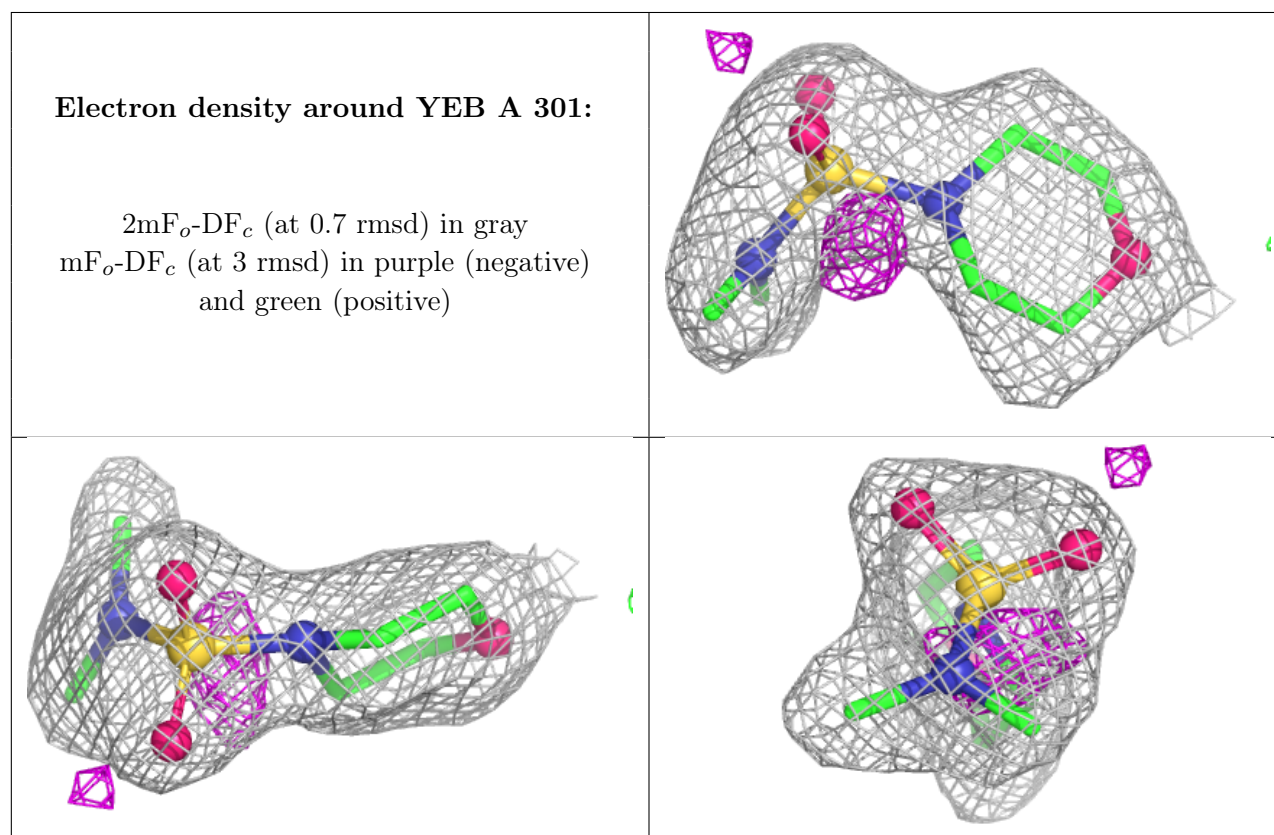
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DGL	D	307	10/10	0.77	0.18	47,76,84,86	0
4	DGL	B	303	10/10	0.86	0.13	44,57,67,68	0
6	SO4	D	304	5/5	0.86	0.11	64,84,89,102	0
2	YEB	A	301	12/12	0.87	0.15	52,54,59,59	0
6	SO4	D	303	5/5	0.88	0.12	66,72,85,92	0
5	GLY	C	304	5/5	0.88	0.10	44,49,52,56	0
6	SO4	D	305	5/5	0.90	0.13	67,69,83,94	0
3	EDO	C	303	4/4	0.91	0.19	58,61,65,66	0
5	GLY	D	308	5/5	0.93	0.13	56,58,72,81	0
3	EDO	C	302	4/4	0.93	0.12	38,42,43,43	0
7	ALA	D	306	6/6	0.93	0.11	54,60,62,67	0
3	EDO	A	302	4/4	0.94	0.13	38,43,44,45	0
3	EDO	C	301	4/4	0.95	0.10	36,37,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	301	4/4	0.95	0.08	28,30,31,34	0
3	EDO	B	301	4/4	0.96	0.07	33,37,37,40	0
3	EDO	B	302	4/4	0.97	0.06	27,37,39,41	0
3	EDO	D	302	4/4	0.97	0.08	42,43,45,46	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.