



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 7, 2023 – 04:33 PM EST

PDB ID : 7FT5  
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with POB0093  
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.  
Deposited on : 2023-01-24  
Resolution : 1.77 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

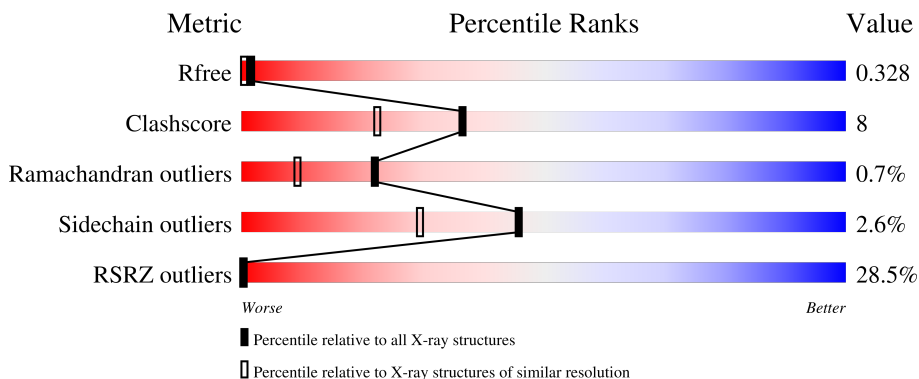
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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))
$R_{free}$	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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  $\geq 3$ , 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	 22% 81% 14% ..
1	B	195	 16% 82% 16% ..
1	C	195	 39% 76% 19% ...
1	D	195	 35% 78% 19% .

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6417 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.

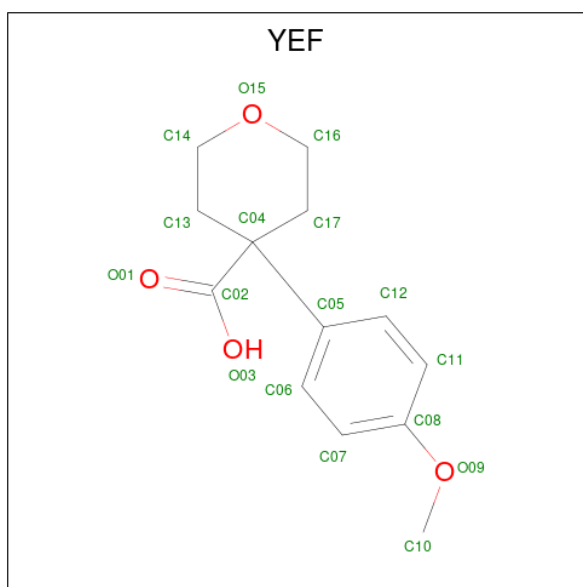
- Molecule 1 is a protein called Syntenin-1.

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	1517	955	272	281	9	0	3	0
1	D	191	1489	939	263	278	9	0	2	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 4-(4-methoxyphenyl)oxane-4-carboxylic acid (three-letter code: YEF) (formula: C<sub>13</sub>H<sub>16</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	13	4		
2	C	1	Total	C	O	0	0
			17	13	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



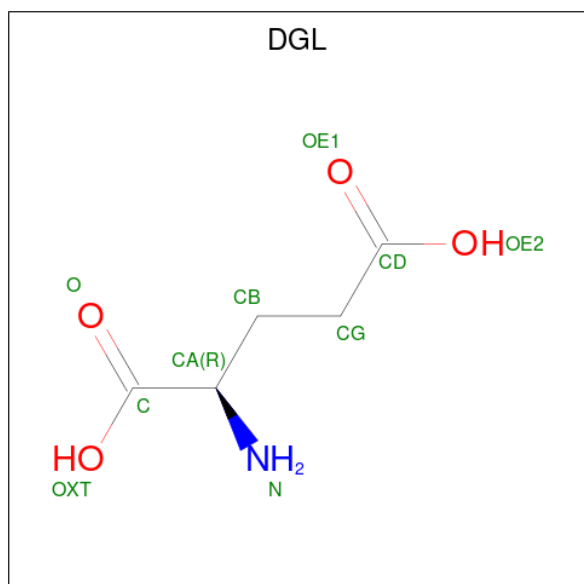
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	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	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 (three-letter code: DGL) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



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 (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



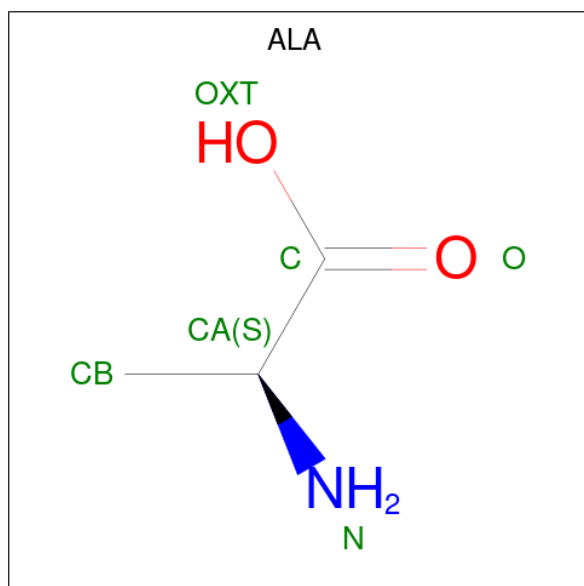
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	O			S
6	D	1	5	4	1	0	0
6	D	1	5	4	1	0	0

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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 (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



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

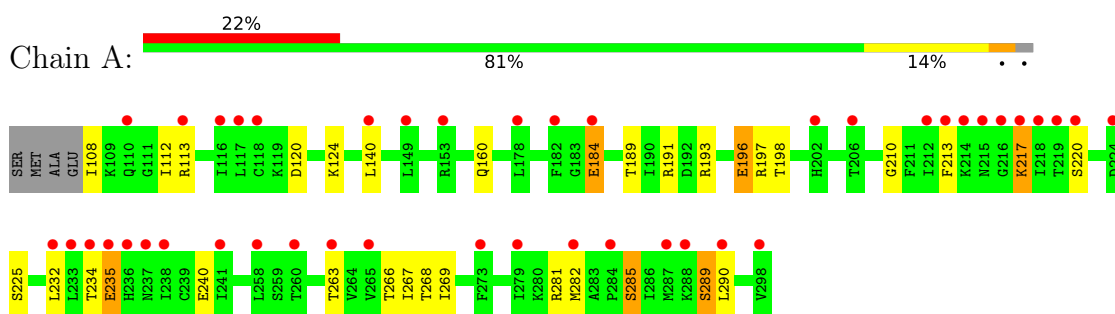
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total	O	0	0
			50	50		
8	B	101	Total	O	0	1
			101	101		
8	C	74	Total	O	0	0
			74	74		
8	D	93	Total	O	0	1
			93	93		

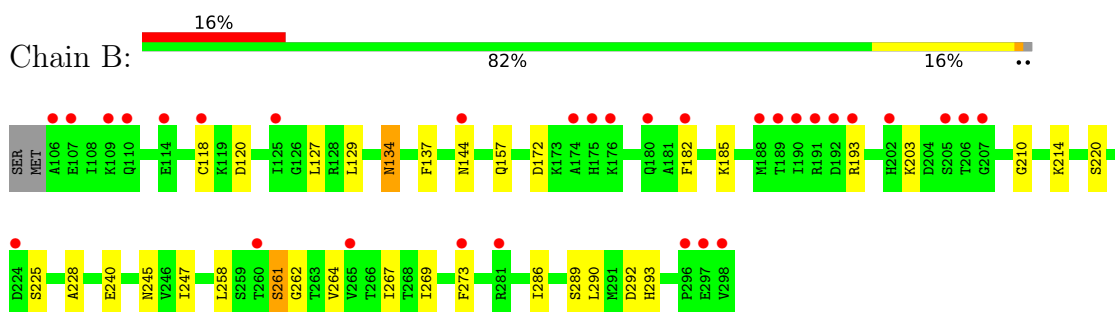
### 3 Residue-property plots [i](#)

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.

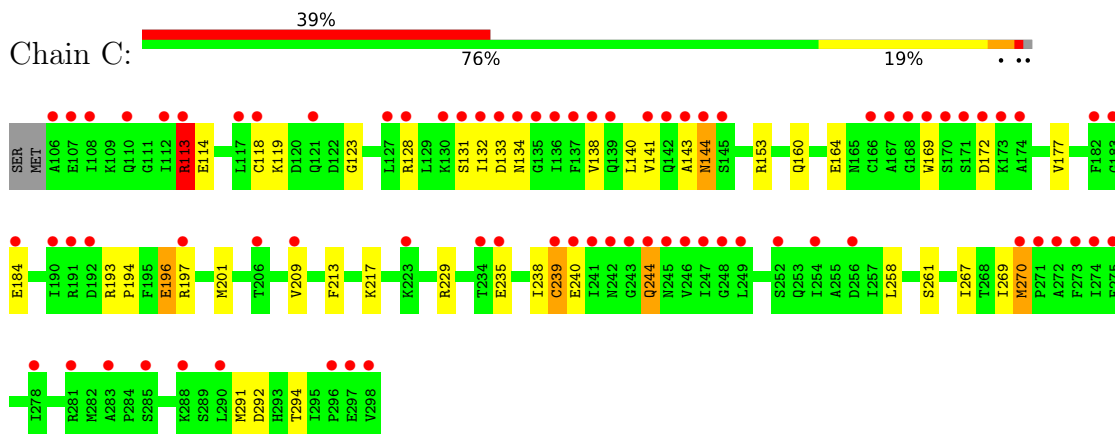
- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1




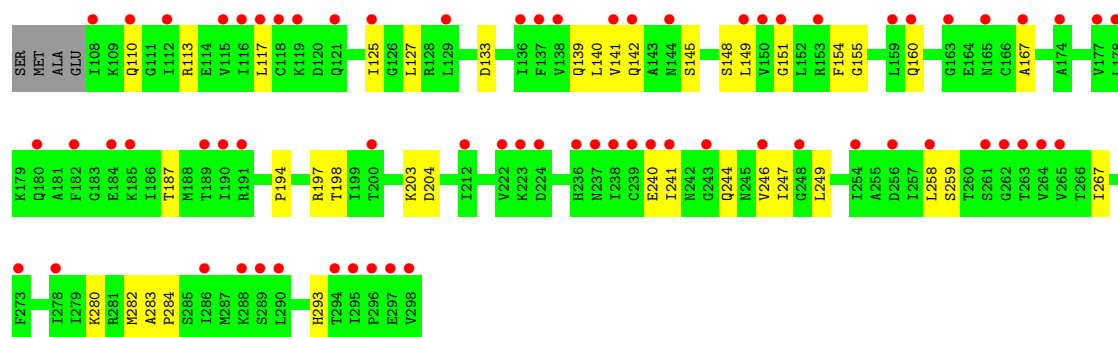
- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1



Chain D:  35% 78% 19%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.34Å 49.17Å 116.22Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	80.04 – 1.77 80.03 – 1.77	Depositor EDS
% Data completeness (in resolution range)	96.8 (80.04-1.77) 96.9 (80.03-1.77)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 1.77Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.256 , 0.299 0.291 , 0.328	Depositor DCC
$R_{free}$ test set	4212 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.9	Xtrriage
Anisotropy	0.403	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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 35.29 % 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 5.9723e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DGL, EDO, YEF, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.17	9/1502 (0.6%)	1.02	2/2019 (0.1%)
1	B	0.80	3/1516 (0.2%)	0.88	0/2038
1	C	1.53	15/1538 (1.0%)	1.17	8/2066 (0.4%)
1	D	0.84	0/1510	0.88	0/2030
All	All	1.13	27/6066 (0.4%)	0.99	10/8153 (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
1	D	0	1
All	All	0	3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	239	CYS	CB-SG	22.95	2.21	1.82
1	A	235	GLU	CD-OE2	20.48	1.48	1.25
1	A	235	GLU	CD-OE1	18.22	1.45	1.25
1	C	113[A]	ARG	CA-CB	17.20	1.91	1.53
1	C	113[B]	ARG	CA-CB	17.20	1.91	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	GLU	OE1-CD-OE2	18.85	145.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113[A]	ARG	CA-C-O	-15.33	87.90	120.10
1	C	113[B]	ARG	CA-C-O	-15.33	87.90	120.10
1	C	113[A]	ARG	CB-CA-C	12.28	134.96	110.40
1	C	113[B]	ARG	CB-CA-C	12.28	134.96	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	ASN	Mainchain
1	C	113[A]	ARG	Mainchain
1	D	160	GLN	Peptide

## 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	21	0
1	B	1495	0	1541	19	0
1	C	1517	0	1565	36	0
1	D	1489	0	1533	26	0
2	A	17	0	0	0	0
2	C	17	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	1	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	50	0	0	1	0
8	B	101	0	0	5	0
8	C	74	0	0	3	0
8	D	93	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6417	0	6239	98	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 8.

The worst 5 of 98 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:C:113[A]:ARG:CB	1:C:113[A]:ARG:CA	1.91	1.45
1:C:113[A]:ARG:CA	1:C:113[A]:ARG:C	1.90	1.38
1:C:270:MET:CG	1:C:270:MET:SD	2.13	1.36
1:C:239:CYS:SG	1:C:239:CYS:CB	2.21	1.29
1:B:273[A]:PHE:HE2	8:B:494:HOH:O	1.28	1.14

There are no symmetry-related clashes.

## 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%)	179 (94%)	9 (5%)	2 (1%)	14	4
1	B	192/195 (98%)	186 (97%)	5 (3%)	1 (0%)	29	14
1	C	194/195 (100%)	185 (95%)	8 (4%)	1 (0%)	29	14
1	D	191/195 (98%)	183 (96%)	7 (4%)	1 (0%)	29	14
All	All	767/780 (98%)	733 (96%)	29 (4%)	5 (1%)	22	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU

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Mol	Chain	Res	Type
1	A	281	ARG
1	D	167	ALA
1	B	261	SER
1	C	144	ASN

### 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%)	158 (95%)	8 (5%)	25	10
1	B	167/168 (99%)	162 (97%)	5 (3%)	41	24
1	C	169/168 (101%)	167 (99%)	2 (1%)	71	62
1	D	167/168 (99%)	164 (98%)	3 (2%)	59	45
All	All	669/672 (100%)	651 (97%)	18 (3%)	46	28

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	113[B]	ARG
1	D	280	LYS
1	D	117	LEU
1	B	144	ASN
1	C	113[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	C	142	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 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
7	ALA	D	306	-	5,5,5	1.03	1 (20%)	6,6,6	1.36	1 (16%)
3	EDO	C	304	-	3,3,3	0.33	0	2,2,2	0.47	0
3	EDO	D	302	-	3,3,3	0.08	0	2,2,2	0.33	0
6	SO4	D	305	-	4,4,4	0.37	0	6,6,6	0.09	0
3	EDO	B	302	-	3,3,3	0.13	0	2,2,2	0.18	0
5	GLY	C	305	-	4,4,4	0.96	0	3,4,4	1.40	0
2	YEF	C	301	-	18,18,18	2.12	3 (16%)	22,25,25	1.23	2 (9%)
4	DGL	B	303	-	8,9,9	0.98	0	10,11,11	1.38	2 (20%)
3	EDO	C	303	-	3,3,3	0.11	0	2,2,2	0.26	0
5	GLY	D	308	-	4,4,4	1.12	1 (25%)	3,4,4	1.52	0
3	EDO	A	402	-	3,3,3	0.09	0	2,2,2	0.23	0
4	DGL	D	307	-	8,9,9	1.02	0	10,11,11	1.20	2 (20%)
2	YEF	A	401	-	18,18,18	2.15	3 (16%)	22,25,25	0.83	0
3	EDO	D	301	-	3,3,3	0.12	0	2,2,2	0.33	0
6	SO4	D	304	-	4,4,4	0.38	0	6,6,6	0.05	0
3	EDO	C	302	-	3,3,3	0.15	0	2,2,2	0.22	0
3	EDO	B	301	-	3,3,3	0.16	0	2,2,2	0.19	0
6	SO4	D	303	-	4,4,4	0.37	0	6,6,6	0.06	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
7	ALA	D	306	-	-	0/4/4/4	-
3	EDO	C	304	-	-	1/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
5	GLY	C	305	-	-	2/2/2/2	-
2	YEF	C	301	-	-	0/14/24/24	0/2/2/2
4	DGL	B	303	-	-	2/9/9/9	-
3	EDO	C	303	-	-	1/1/1/1	-
5	GLY	D	308	-	-	2/2/2/2	-
3	EDO	A	402	-	-	1/1/1/1	-
4	DGL	D	307	-	-	1/9/9/9	-
2	YEF	A	401	-	-	0/14/24/24	0/2/2/2
3	EDO	D	301	-	-	0/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	YEF	C04-C05	5.92	1.62	1.53
2	A	401	YEF	C04-C05	5.56	1.62	1.53
2	A	401	YEF	C13-C04	-4.89	1.48	1.55
2	C	301	YEF	C13-C04	-4.66	1.48	1.55
2	A	401	YEF	C17-C04	-3.81	1.49	1.55

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	306	ALA	OXT-C-O	-2.75	117.83	124.09
4	B	303	DGL	OXT-C-O	-2.61	118.16	124.09
2	C	301	YEF	O15-C16-C17	2.52	114.22	111.56
2	C	301	YEF	C17-C04-C13	2.49	110.54	107.82
4	B	303	DGL	OXT-C-CA	2.44	121.69	113.38

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	305	GLY	O-C-CA-N

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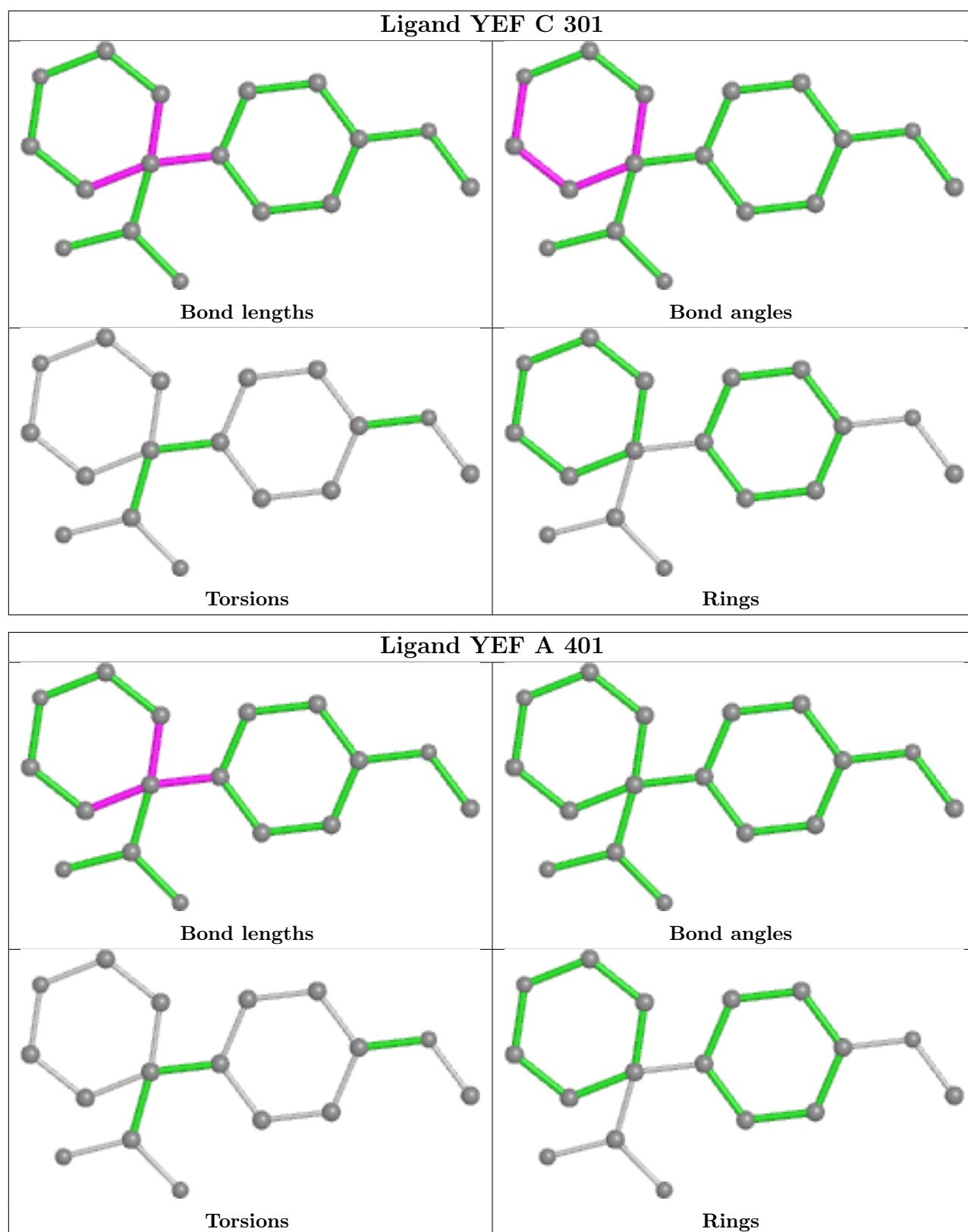
Mol	Chain	Res	Type	Atoms
5	D	308	GLY	OXT-C-CA-N
5	D	308	GLY	O-C-CA-N
5	C	305	GLY	OXT-C-CA-N
3	C	303	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	191/195 (97%)	1.63	43 (22%) 0 0	31, 48, 75, 85	23 (12%)
1	B	193/195 (98%)	1.23	31 (16%) 1 1	34, 47, 65, 70	18 (9%)
1	C	193/195 (98%)	2.58	76 (39%) 0 0	35, 48, 68, 89	55 (28%)
1	D	191/195 (97%)	1.97	69 (36%) 0 0	37, 50, 71, 80	20 (10%)
All	All	768/780 (98%)	1.85	219 (28%) 0 0	31, 48, 69, 89	116 (15%)

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	274	ILE	11.0
1	C	169	TRP	10.7
1	D	239	CYS	10.2
1	D	182	PHE	10.2
1	C	138	VAL	9.9

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

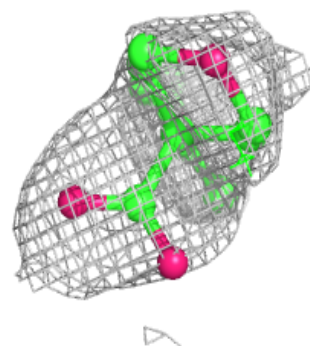
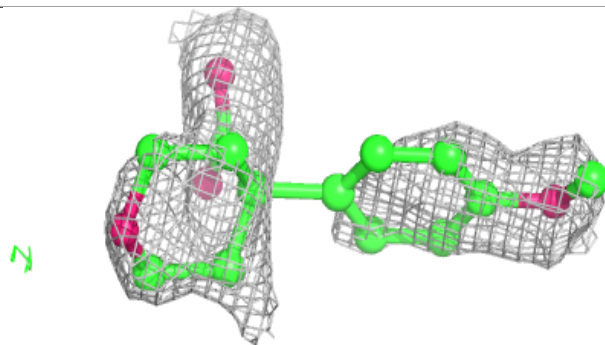
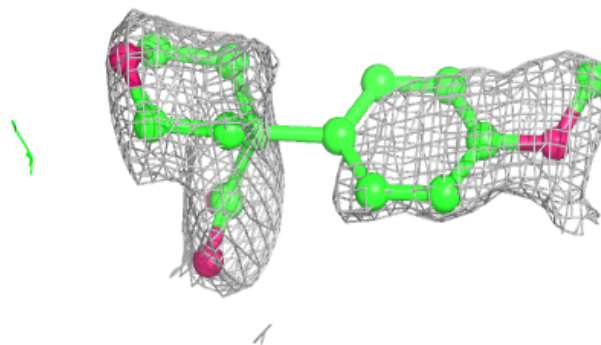
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	304	4/4	0.42	0.30	47,54,54,55	0
4	DGL	D	307	10/10	0.44	0.28	85,99,106,107	0
7	ALA	D	306	6/6	0.53	0.31	75,79,80,81	0
5	GLY	C	305	5/5	0.78	0.27	50,58,64,67	0
2	YEF	A	401	17/17	0.78	0.24	48,50,52,52	17
3	EDO	A	402	4/4	0.79	0.13	56,60,61,63	0
2	YEF	C	301	17/17	0.79	0.24	73,75,78,78	0
4	DGL	B	303	10/10	0.79	0.30	52,68,81,84	0
6	SO4	D	305	5/5	0.80	0.39	103,106,108,116	0
3	EDO	D	301	4/4	0.80	0.19	31,34,35,41	0
5	GLY	D	308	5/5	0.83	0.27	69,72,74,75	0
6	SO4	D	303	5/5	0.83	0.23	69,77,84,84	0
3	EDO	C	303	4/4	0.85	0.14	50,58,59,61	0
3	EDO	C	302	4/4	0.85	0.12	29,31,32,35	0
3	EDO	D	302	4/4	0.87	0.19	48,54,58,61	0
6	SO4	D	304	5/5	0.88	0.13	114,115,117,120	0
3	EDO	B	301	4/4	0.89	0.14	52,55,57,58	0
3	EDO	B	302	4/4	0.93	0.09	37,37,38,38	0

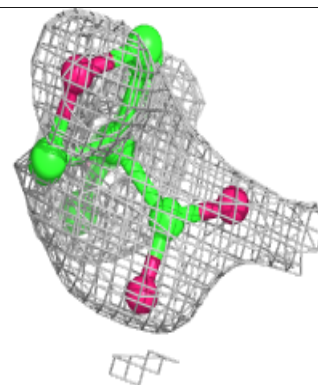
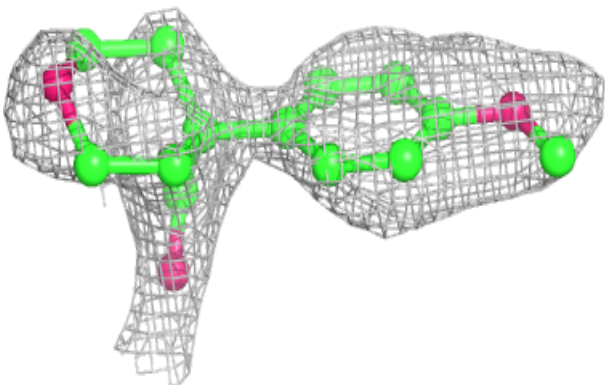
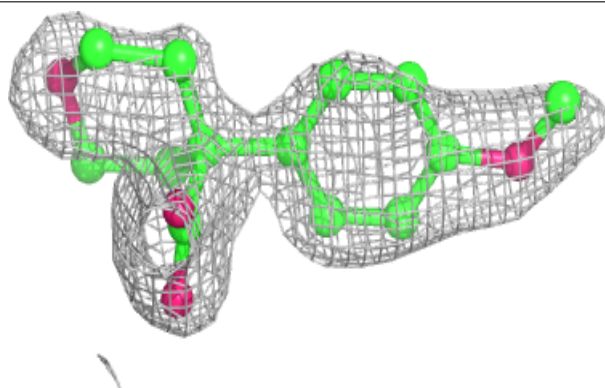
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around YEF A 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around YEF C 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.