



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:42 PM UTC

PDB ID : 7FSP / pdb_00007fsp
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z1650168321
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 1.86 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

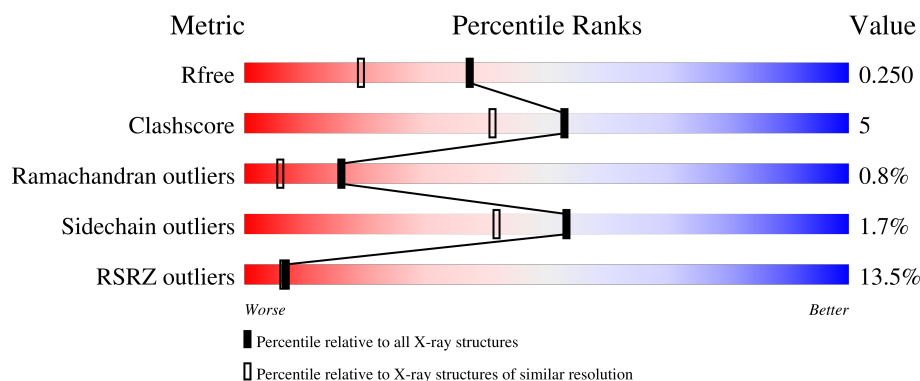
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	18% 81% 15% ..
1	B	195	6% 88% 10% ...
1	C	195	15% 90% 9% ..
1	D	195	13% 78% 18% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Syntenin-1.

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

There are 8 discrepancies between the modelled and reference sequences:

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

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



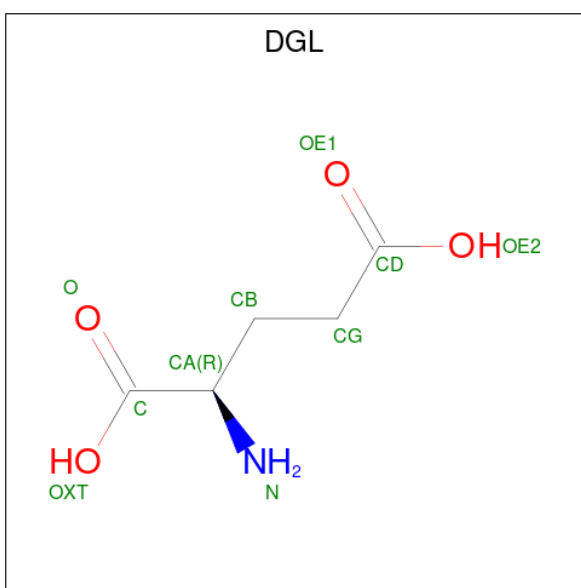
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



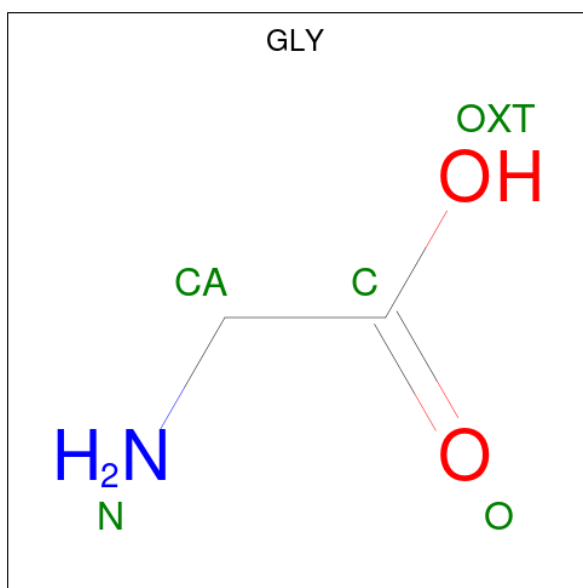
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: C₅H₉NO₄).



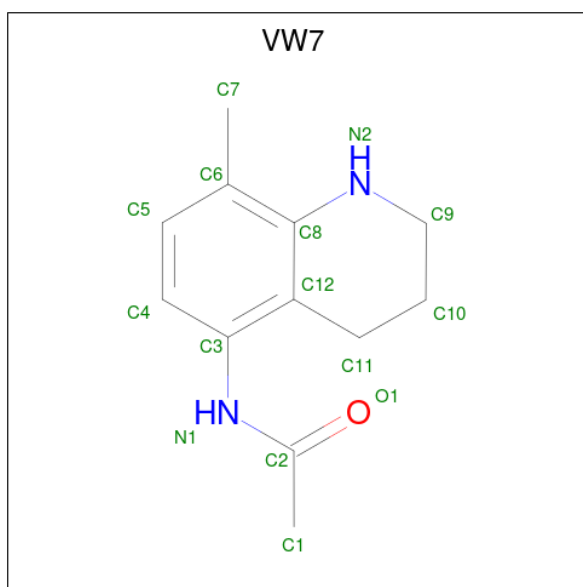
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

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



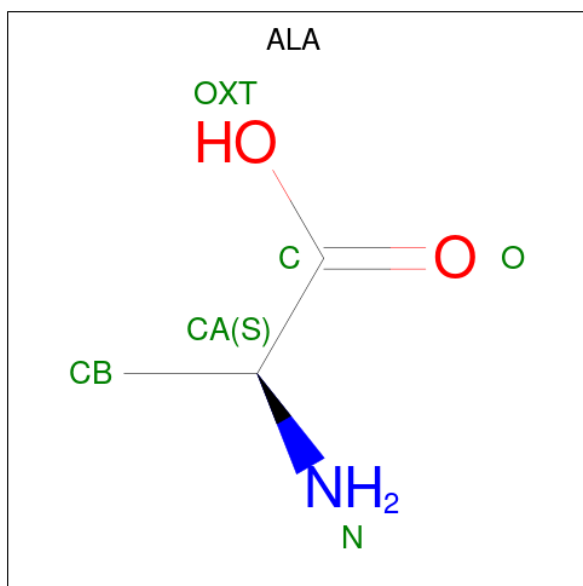
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 6 is N-(8-methyl-1,2,3,4-tetrahydroquinolin-5-yl)acetamide (CCD ID: VW7) (formula: $C_{12}H_{16}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			15	12	2	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		

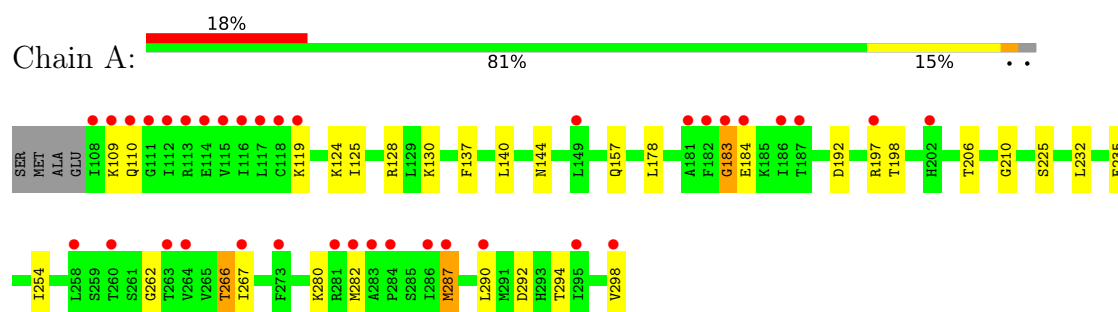
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	52	Total	O	0	0
			52	52		
8	B	108	Total	O	0	1
			108	108		
8	C	82	Total	O	0	1
			83	83		
8	D	129	Total	O	0	1
			129	129		

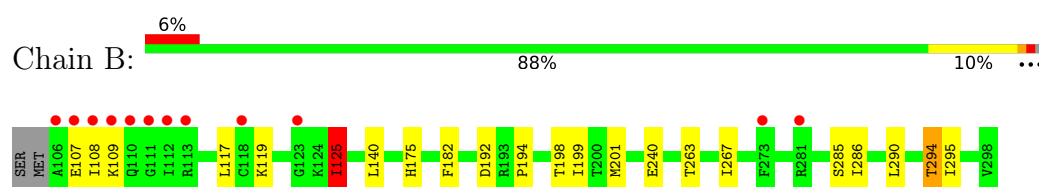
3 Residue-property plots [i](#)

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.

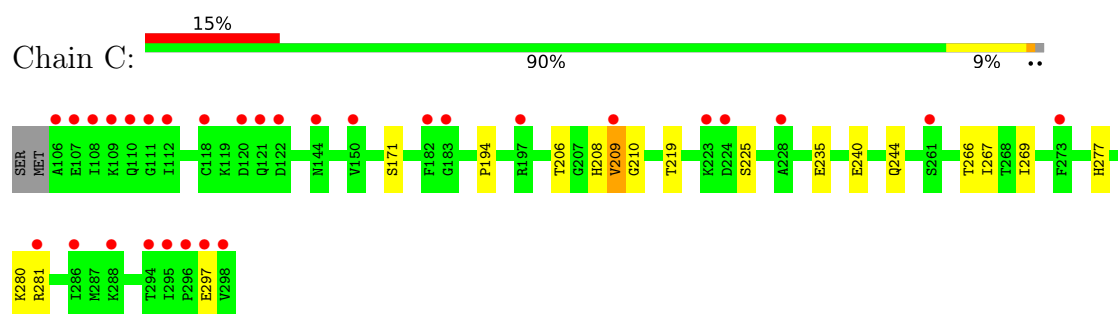
• Molecule 1: Syntenin-1



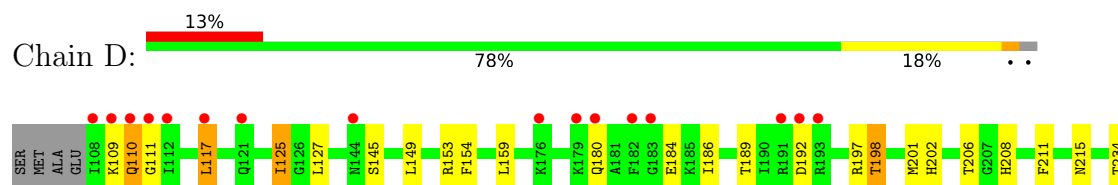
• Molecule 1: Syntenin-1

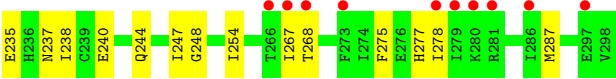


• Molecule 1: Syntenin-1



• 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	80.44Å 49.50Å 114.42Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	80.09 – 1.86 80.09 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.09-1.86) 99.8 (80.09-1.86)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.239 0.211 , 0.250	Depositor DCC
R_{free} test set	3723 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6441	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 21.07 % 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 7.5880e-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: EDO, VW7, SO4, DGL

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	1.47	5/2019 (0.2%)
1	B	1.24	2/1516 (0.1%)	1.45	7/2038 (0.3%)
1	C	1.25	2/1535 (0.1%)	1.45	4/2063 (0.2%)
1	D	1.29	5/1502 (0.3%)	1.47	4/2019 (0.2%)
All	All	1.24	9/6055 (0.1%)	1.46	20/8139 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	HIS	CE1-NE2	7.29	1.39	1.32
1	C	277	HIS	CE1-NE2	7.09	1.39	1.32
1	C	209	VAL	C-O	6.39	1.31	1.23
1	D	235	GLU	C-O	6.12	1.31	1.23
1	D	237	ASN	C-O	5.88	1.31	1.23
1	D	215	ASN	C-O	-5.50	1.16	1.23
1	D	277	HIS	CE1-NE2	5.45	1.38	1.32
1	D	234	THR	C-O	5.25	1.30	1.23
1	B	240	GLU	C-O	5.20	1.30	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	THR	CA-CB-OG1	-8.85	96.32	109.60
1	B	294	THR	CB-CA-C	-7.99	95.50	109.64
1	B	263	THR	CA-CB-OG1	-7.23	98.75	109.60
1	D	198	THR	CA-CB-OG1	-6.90	99.25	109.60
1	C	266	THR	CA-CB-OG1	-6.17	100.35	109.60
1	C	171	SER	CA-C-N	5.89	128.49	120.54
1	C	171	SER	C-N-CA	5.89	128.49	120.54
1	A	266	THR	CA-CB-OG1	-5.78	100.93	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ILE	N-CA-C	-5.75	107.25	111.90
1	D	153	ARG	CG-CD-NE	-5.70	99.47	112.00
1	D	189	THR	CB-CA-C	5.43	118.99	110.19
1	D	254	ILE	N-CA-C	-5.39	105.28	110.72
1	A	110	GLN	N-CA-C	-5.30	107.35	112.97
1	B	285	SER	N-CA-C	-5.23	105.64	112.23
1	B	199	ILE	CA-C-O	-5.17	114.97	120.39
1	A	130	LYS	CA-C-N	5.08	128.56	121.24
1	A	130	LYS	C-N-CA	5.08	128.56	121.24
1	B	194	PRO	CB-CA-C	-5.06	104.30	111.68
1	A	254	ILE	N-CA-C	-5.04	105.79	110.53
1	C	219	THR	N-CA-C	-5.04	107.80	114.04

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	19	0
1	B	1495	0	1541	11	0
1	C	1514	0	1558	10	0
1	D	1481	0	1530	24	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	B	5	0	0	0	0
3	C	5	0	0	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	10	0	4	2	0
6	D	15	0	0	0	0
7	D	6	0	4	1	0
8	A	52	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	108	0	0	1	0
8	C	83	0	0	2	0
8	D	129	0	0	3	0
All	All	6441	0	6231	62	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 5.

All (62) 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:125:ILE:HD11	1:D:127:LEU:HD12	1.68	0.76
1:A:140:LEU:HD11	1:A:282:MET:SD	2.31	0.71
1:C:209:VAL:HG23	8:C:408:HOH:O	1.90	0.71
1:D:109:LYS:N	1:D:192:ASP:OD2	2.19	0.71
1:B:107:GLU:HB2	1:B:109:LYS:NZ	2.07	0.70
1:B:107:GLU:HB2	1:B:109:LYS:HZ2	1.60	0.67
1:D:117:LEU:HD12	1:D:117:LEU:H	1.61	0.66
1:A:109:LYS:N	1:A:192:ASP:OD2	2.30	0.62
1:A:198:THR:CG2	1:A:266:THR:HG23	2.30	0.60
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.35	0.59
1:D:117:LEU:HD12	1:D:117:LEU:N	2.20	0.57
1:D:198:THR:HG22	1:D:268:THR:OG1	2.05	0.57
1:A:128:ARG:HB2	1:A:140:LEU:HB2	1.87	0.56
1:A:232:LEU:HD11	1:A:267:ILE:HD11	1.89	0.55
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.88	0.55
1:A:197:ARG:HD3	1:C:194:PRO:O	2.07	0.55
1:A:140:LEU:CD1	1:A:282:MET:SD	2.95	0.53
1:B:109:LYS:N	1:B:192:ASP:OD2	2.41	0.53
1:D:154:PHE:CD1	1:D:247:ILE:HD13	2.45	0.52
1:D:145:SER:O	1:D:149:LEU:HG	2.09	0.52
1:D:275:PHE:CZ	5:D:307:GLY:HA3	2.45	0.51
1:A:119:LYS:HD2	1:A:183:GLY:HA2	1.94	0.50
1:D:197:ARG:NH2	8:D:403:HOH:O	2.26	0.50
1:B:294:THR:HG22	1:B:295:ILE:O	2.12	0.50
1:B:117:LEU:HD12	1:B:117:LEU:N	2.26	0.49
1:A:298:VAL:HG13	8:A:418:HOH:O	2.13	0.48
1:C:280:LYS:O	1:C:281:ARG:HB2	2.13	0.48
1:D:197:ARG:NH1	8:D:405:HOH:O	2.29	0.48
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.24	0.47
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:PHE:CD1	1:D:247:ILE:CD1	2.97	0.47
1:C:240:GLU:HA	1:C:244:GLN:O	2.14	0.47
1:D:109:LYS:HE3	1:D:109:LYS:HB2	1.75	0.46
1:C:235:GLU:OE2	8:C:401:HOH:O	2.21	0.45
1:D:238:ILE:O	5:D:307:GLY:N	2.49	0.45
1:C:267:ILE:HG22	1:C:269:ILE:HG23	1.98	0.44
1:A:198:THR:CG2	1:A:266:THR:CG2	2.95	0.44
1:D:248:GLY:HA2	1:D:287:MET:HE3	2.00	0.44
1:D:206:THR:OG1	1:D:208:HIS:ND1	2.49	0.44
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.99	0.44
1:D:248:GLY:CA	1:D:287:MET:HE3	2.47	0.43
1:D:109:LYS:C	1:D:110:GLN:O	2.61	0.43
1:A:124:LYS:HD3	8:B:410:HOH:O	2.19	0.43
1:D:240:GLU:HA	1:D:244:GLN:O	2.19	0.43
1:D:202:HIS:CE1	8:D:472:HOH:O	2.71	0.43
1:B:286:ILE:HG23	1:B:290:LEU:HD12	2.01	0.43
1:A:125:ILE:HD11	1:A:178:LEU:HD13	2.01	0.43
1:C:206:THR:OG1	1:C:208:HIS:CE1	2.73	0.42
1:B:294:THR:HG22	1:B:295:ILE:N	2.33	0.42
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.02	0.41
1:D:117:LEU:CD1	1:D:186:ILE:HB	2.50	0.41
1:D:180:GLN:NE2	1:D:180:GLN:HA	2.34	0.41
1:A:137:PHE:CE2	1:A:157:GLN:HB2	2.55	0.41
1:B:107:GLU:HB2	1:B:109:LYS:HZ3	1.83	0.41
1:D:201:MET:HE1	1:D:267:ILE:HD12	2.03	0.41
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.20	0.41
1:C:210:GLY:HA3	1:C:225:SER:CB	2.50	0.41
1:A:210:GLY:HA3	1:A:225:SER:CB	2.51	0.41
1:B:119:LYS:HE3	1:B:125:ILE:HD11	2.03	0.41
1:D:211:PHE:O	7:D:304:ALA:N	2.53	0.41
1:D:275:PHE:O	1:D:278:ILE:HG22	2.21	0.41
1:A:282:MET:HE3	1:A:287:MET:HG3	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%)	181 (95%)	6 (3%)	3 (2%)	7	2
1	B	192/195 (98%)	189 (98%)	2 (1%)	1 (0%)	24	13
1	C	194/195 (100%)	186 (96%)	8 (4%)	0	100	100
1	D	190/195 (97%)	182 (96%)	6 (3%)	2 (1%)	11	3
All	All	766/780 (98%)	738 (96%)	22 (3%)	6 (1%)	16	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	D	110	GLN
1	A	183	GLY
1	A	262	GLY
1	D	111	GLY
1	B	108	ILE

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%)	162 (98%)	4 (2%)	43	28
1	B	167/168 (99%)	165 (99%)	2 (1%)	63	55
1	C	169/168 (101%)	168 (99%)	1 (1%)	78	73
1	D	166/168 (99%)	162 (98%)	4 (2%)	43	28
All	All	668/672 (99%)	657 (98%)	11 (2%)	53	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	206	THR
1	A	280	LYS
1	A	287	MET
1	B	125	ILE
1	B	140	LEU
1	C	297	GLU
1	D	117	LEU
1	D	125	ILE
1	D	159	LEU
1	D	184	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	139	GLN
1	A	237	ASN
1	A	244	GLN
1	B	142	GLN
1	B	180	GLN
1	C	215	ASN
1	D	180	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	$\# Z > 2$
2	EDO	B	302	-	3,3,3	0.33	0	2,2,2	0.39	0
4	DGL	D	305	-	8,9,9	1.03	0	8,11,11	1.16	1 (12%)
2	EDO	A	302	-	3,3,3	0.45	0	2,2,2	0.49	0
5	GLY	D	306	-	4,4,4	1.34	1 (25%)	3,4,4	1.38	0
6	VW7	D	301	-	16,16,16	2.41	5 (31%)	20,22,22	1.95	5 (25%)
2	EDO	C	301	-	3,3,3	0.23	0	2,2,2	0.42	0
2	EDO	C	302	-	3,3,3	0.24	0	2,2,2	0.41	0
2	EDO	D	302	-	3,3,3	0.19	0	2,2,2	0.20	0
5	GLY	D	307	-	4,4,4	1.11	1 (25%)	3,4,4	1.40	0
3	SO4	B	303	-	4,4,4	0.34	0	6,6,6	0.15	0
2	EDO	D	303	-	3,3,3	0.51	0	2,2,2	0.66	0
5	GLY	C	304	-	4,4,4	0.79	0	3,4,4	1.53	1 (33%)
3	SO4	C	303	-	4,4,4	0.31	0	6,6,6	0.11	0
7	ALA	D	304	-	5,5,5	1.04	0	6,6,6	0.97	0
2	EDO	A	301	-	3,3,3	0.14	0	2,2,2	0.08	0
2	EDO	B	301	-	3,3,3	0.24	0	2,2,2	0.22	0
4	DGL	B	304	-	8,9,9	1.08	1 (12%)	8,11,11	1.22	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	302	-	-	0/1/1/1	-
4	DGL	D	305	-	-	3/9/9/9	-
2	EDO	A	302	-	-	1/1/1/1	-
5	GLY	D	306	-	-	0/2/2/2	-
6	VW7	D	301	-	-	0/4/11/11	0/2/2/2
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
5	GLY	D	307	-	-	0/2/2/2	-

Continued on next page...

Continued from previous page...

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	VW7	C2-N1	4.85	1.45	1.36
6	D	301	VW7	C8-N2	4.41	1.45	1.37
6	D	301	VW7	C11-C12	4.27	1.58	1.51
6	D	301	VW7	C3-N1	3.14	1.47	1.41
6	D	301	VW7	C8-C6	2.77	1.44	1.40
5	D	306	GLY	OXT-C	-2.62	1.22	1.30
4	B	304	DGL	OXT-C	-2.22	1.23	1.30
5	D	307	GLY	OXT-C	-2.09	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301	VW7	C11-C12-C3	-5.75	117.58	120.55
6	D	301	VW7	C3-N1-C2	-3.07	120.10	127.50
6	D	301	VW7	C1-C2-N1	2.56	118.80	114.95
6	D	301	VW7	C10-C9-N2	2.35	116.28	111.48
6	D	301	VW7	C4-C5-C6	-2.16	118.75	121.98
5	C	304	GLY	OXT-C-CA	2.09	121.70	113.38
4	D	305	DGL	OXT-C-O	-2.08	119.36	124.08
4	B	304	DGL	OE1-CD-CG	-2.06	116.54	123.09

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
2	A	302	EDO	O1-C1-C2-O2
2	D	303	EDO	O1-C1-C2-O2
4	D	305	DGL	OXT-C-CA-CB
4	D	305	DGL	O-C-CA-CB

Continued on next page...

Continued from previous page...

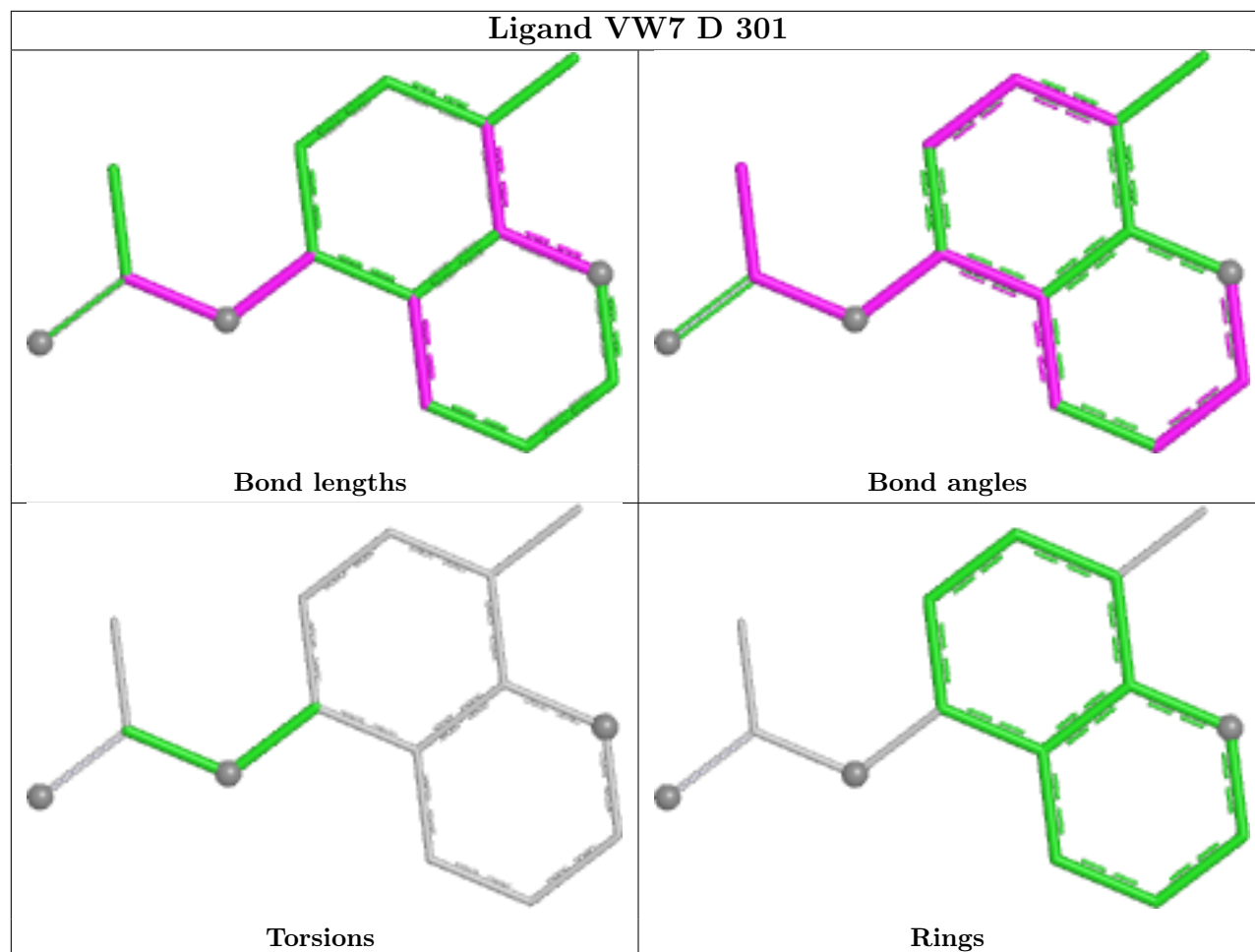
Mol	Chain	Res	Type	Atoms
2	C	302	EDO	O1-C1-C2-O2
4	B	304	DGL	OXT-C-CA-CB
4	D	305	DGL	N-CA-CB-CG
4	B	304	DGL	OE1-CD-CG-CB
4	B	304	DGL	OE2-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	307	GLY	2	0
7	D	304	ALA	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%)	1.41	36 (18%) 3 3	12, 47, 79, 109	15 (7%)
1	B	193/195 (98%)	0.59	12 (6%) 26 29	10, 39, 55, 68	9 (4%)
1	C	193/195 (98%)	0.91	30 (15%) 5 5	10, 38, 68, 99	13 (6%)
1	D	191/195 (97%)	0.79	26 (13%) 7 6	9, 32, 54, 77	21 (10%)
All	All	768/780 (98%)	0.92	104 (13%) 7 6	9, 39, 69, 109	58 (7%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	12.3
1	A	267	ILE	11.2
1	C	261	SER	9.9
1	D	108	ILE	9.9
1	A	117	LEU	9.8
1	A	116	ILE	9.2
1	D	111	GLY	9.2
1	D	109	LYS	8.5
1	B	108	ILE	8.5
1	A	273[A]	PHE	8.2
1	A	115	VAL	7.9
1	D	112	ILE	7.9
1	B	112	ILE	7.6
1	A	112	ILE	7.5
1	B	106	ALA	7.5
1	D	191	ARG	7.4
1	D	192	ASP	7.3
1	B	111	GLY	7.3
1	C	298	VAL	7.1
1	A	111	GLY	7.0
1	D	117	LEU	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	294	THR	6.9
1	A	108	ILE	6.7
1	D	193	ARG	6.7
1	A	118	CYS	6.6
1	C	150	VAL	6.4
1	D	182	PHE	6.2
1	A	109	LYS	6.1
1	C	108	ILE	6.0
1	D	279	ILE	5.9
1	C	110	GLN	5.8
1	A	110	GLN	5.8
1	D	273[A]	PHE	5.7
1	B	109	LYS	5.7
1	C	106	ALA	5.4
1	C	144[A]	ASN	5.4
1	D	110	GLN	5.3
1	C	121	GLN	5.2
1	C	296	PRO	5.0
1	D	278	ILE	5.0
1	A	119	LYS	4.9
1	A	182	PHE	4.8
1	A	286	ILE	4.8
1	D	266	THR	4.8
1	D	179	LYS	4.8
1	C	273[A]	PHE	4.8
1	B	273[A]	PHE	4.7
1	C	197[A]	ARG	4.7
1	C	120	ASP	4.6
1	B	110	GLN	4.6
1	D	267	ILE	4.4
1	C	288	LYS	4.3
1	D	121	GLN	4.2
1	A	290	LEU	4.2
1	A	114	GLU	4.2
1	A	113	ARG	4.2
1	D	183	GLY	4.1
1	D	180	GLN	4.0
1	C	109	LYS	3.9
1	D	144	ASN	3.9
1	B	118	CYS	3.9
1	C	297	GLU	3.8
1	A	282	MET	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	268	THR	3.6
1	A	283	ALA	3.5
1	C	122	ASP	3.5
1	C	182	PHE	3.5
1	B	113	ARG	3.5
1	B	107	GLU	3.5
1	D	176	LYS	3.4
1	C	209	VAL	3.3
1	A	184	GLU	3.3
1	A	287	MET	3.3
1	C	112	ILE	3.2
1	C	111	GLY	3.1
1	D	280	LYS	3.1
1	C	295	ILE	3.0
1	A	284	PRO	2.9
1	C	107	GLU	2.9
1	A	186	ILE	2.7
1	A	202	HIS	2.6
1	A	183	GLY	2.6
1	C	224	ASP	2.6
1	A	263	THR	2.6
1	D	297	GLU	2.5
1	A	281	ARG	2.5
1	C	286	ILE	2.4
1	A	260	THR	2.4
1	C	118	CYS	2.4
1	C	183	GLY	2.4
1	C	223	LYS	2.3
1	B	123	GLY	2.2
1	C	228	ALA	2.2
1	D	286	ILE	2.2
1	A	197	ARG	2.2
1	A	181	ALA	2.2
1	A	187	THR	2.2
1	A	258	LEU	2.1
1	A	295	ILE	2.1
1	D	281	ARG	2.1
1	A	149	LEU	2.1
1	A	264	VAL	2.0
1	C	281	ARG	2.0
1	B	281	ARG	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](#)

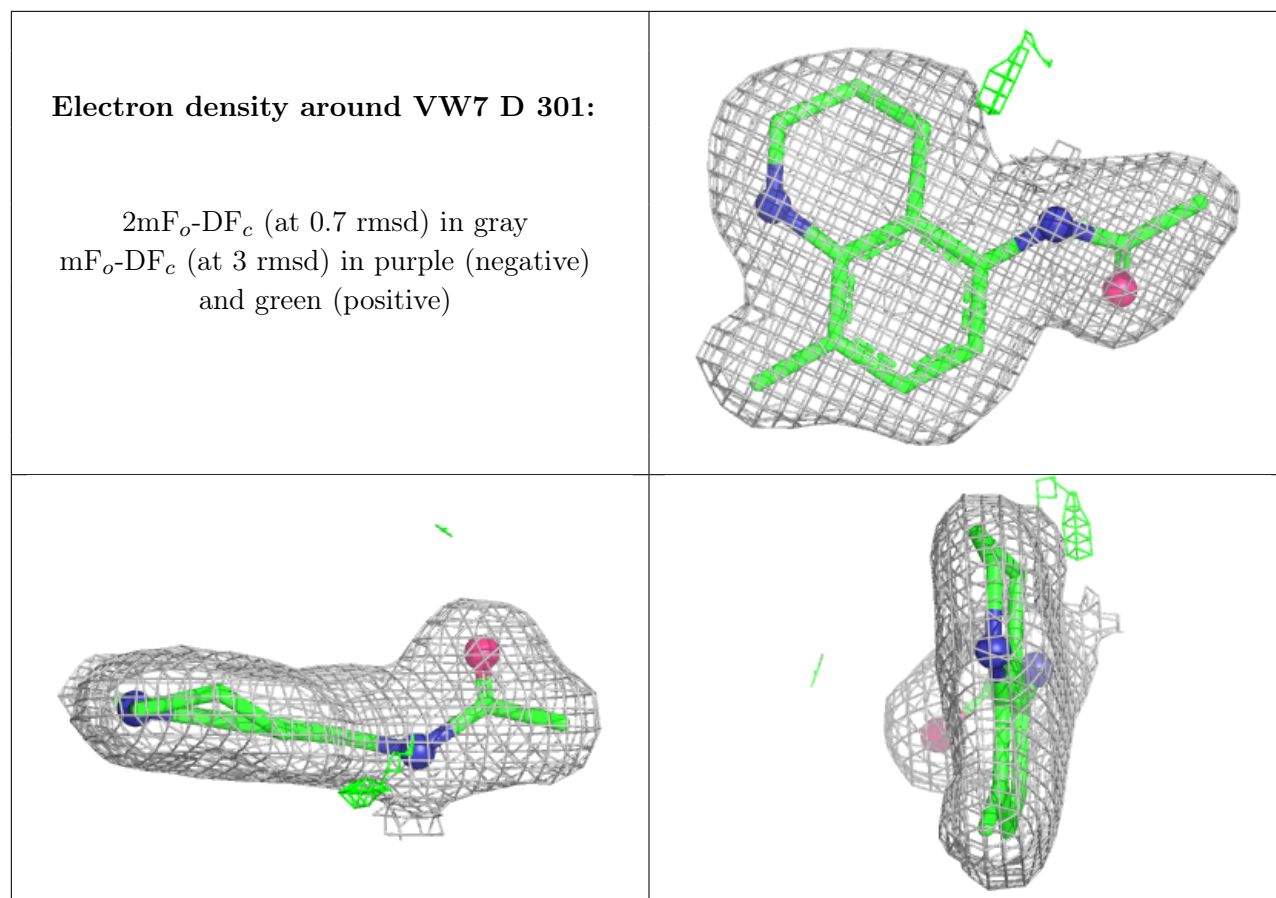
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	EDO	A	302	4/4	0.81	0.28	61,65,70,74	0
3	SO4	C	303	5/5	0.83	0.11	75,81,86,86	0
4	DGL	B	304	10/10	0.83	0.13	42,55,63,64	0
3	SO4	B	303	5/5	0.84	0.14	67,76,80,86	0
5	GLY	D	306	5/5	0.88	0.16	56,64,69,77	0
4	DGL	D	305	10/10	0.90	0.12	34,52,64,79	0
5	GLY	D	307	5/5	0.90	0.14	43,44,46,51	0
5	GLY	C	304	5/5	0.91	0.10	46,52,55,59	0
7	ALA	D	304	6/6	0.91	0.13	49,62,68,69	0
2	EDO	B	301	4/4	0.92	0.12	36,36,39,40	0
2	EDO	C	302	4/4	0.95	0.12	40,44,45,46	0
2	EDO	A	301	4/4	0.95	0.09	38,39,40,44	0
6	VW7	D	301	15/15	0.95	0.07	33,34,36,36	0
2	EDO	C	301	4/4	0.95	0.10	35,35,35,40	0
2	EDO	D	302	4/4	0.96	0.07	24,24,27,30	0
2	EDO	D	303	4/4	0.97	0.06	33,33,35,35	0
2	EDO	B	302	4/4	0.97	0.07	31,34,37,40	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.