



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:28 AM UTC

PDB ID : 7FT9 / pdb_00007ft9
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z45636695
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 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

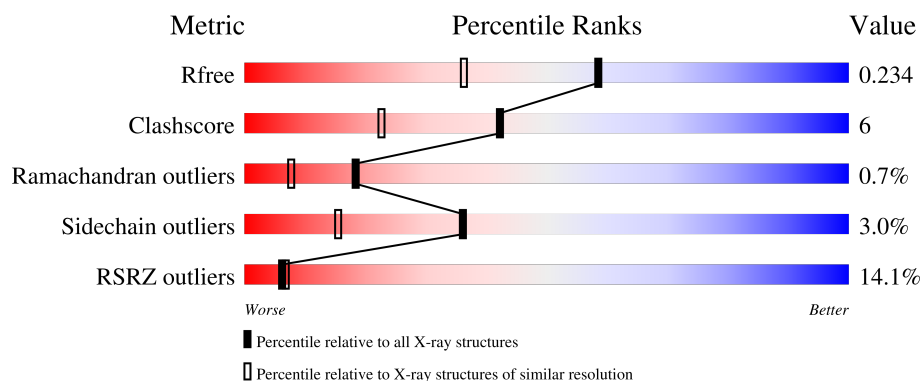
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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% 79% 17% ..
1	B	195	10% 79% 18% ..
1	C	195	14% 76% 19% ..
1	D	195	13% 76% 19% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6378 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:

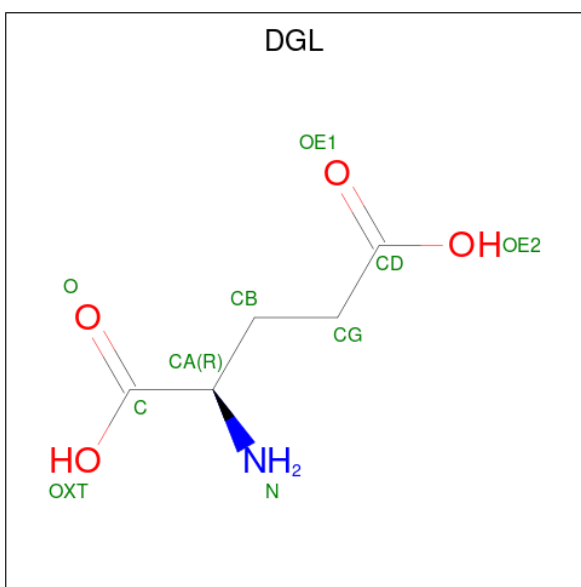
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



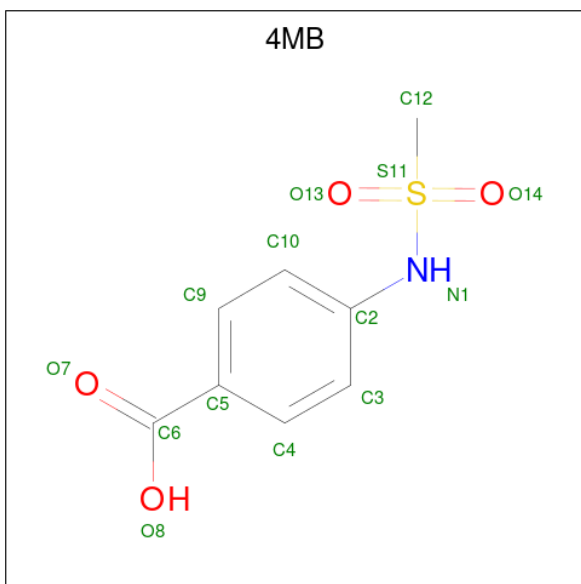
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

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



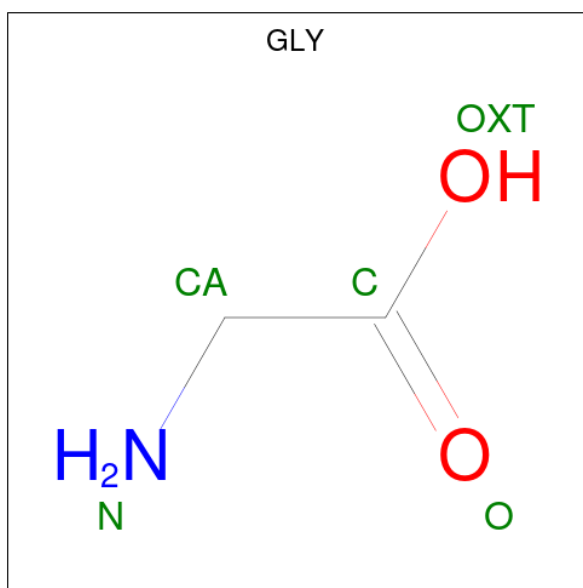
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is 4-[(METHYLSULFONYL)AMINO]BENZOIC ACID (CCD ID: 4MB) (formula: C₈H₉NO₄S) (labeled as "Ligand of Interest" by depositor).



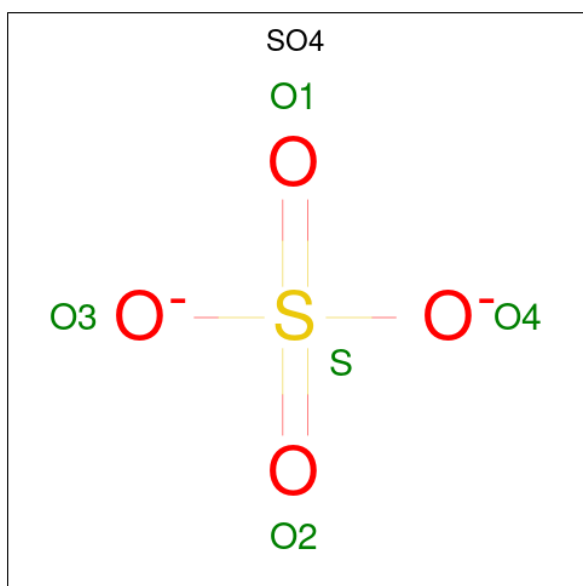
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $\text{C}_2\text{H}_5\text{NO}_2$).



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: O_4S).



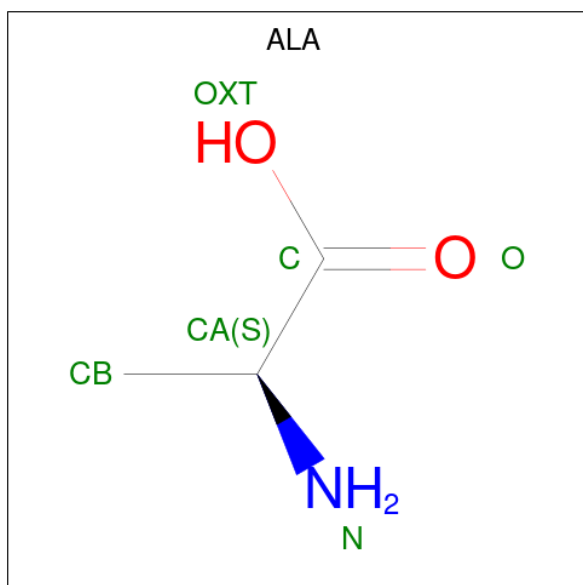
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

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

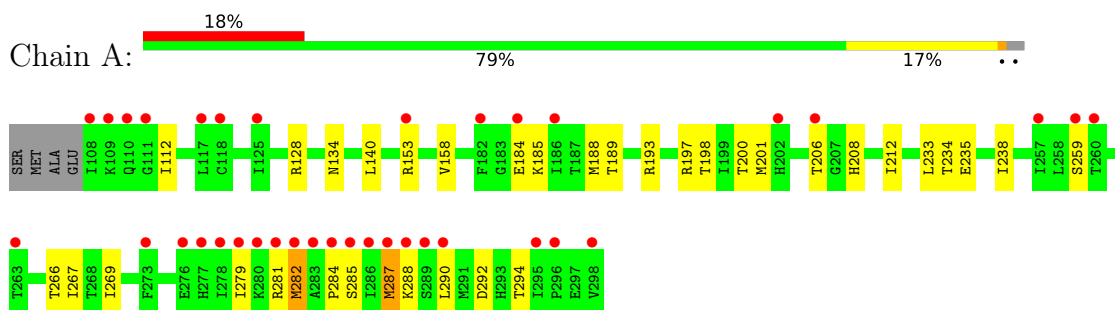
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	48	Total	O	0	0
			48	48		
8	B	86	Total	O	0	0
			86	86		
8	C	71	Total	O	0	0
			71	71		
8	D	101	Total	O	0	0
			101	101		

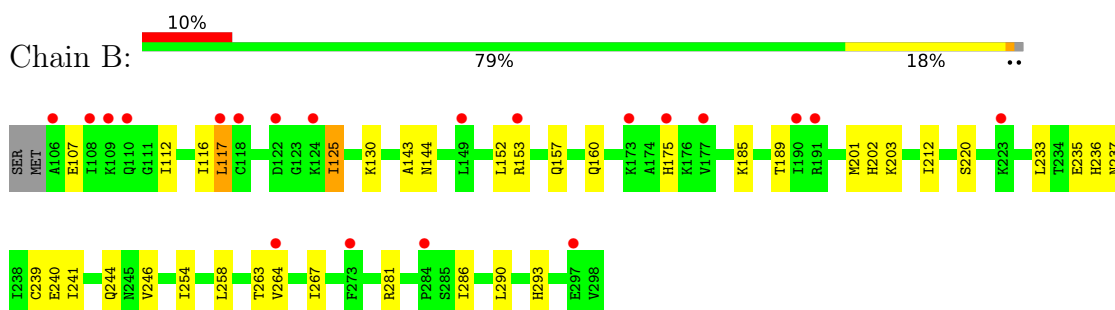
3 Residue-property plots

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.

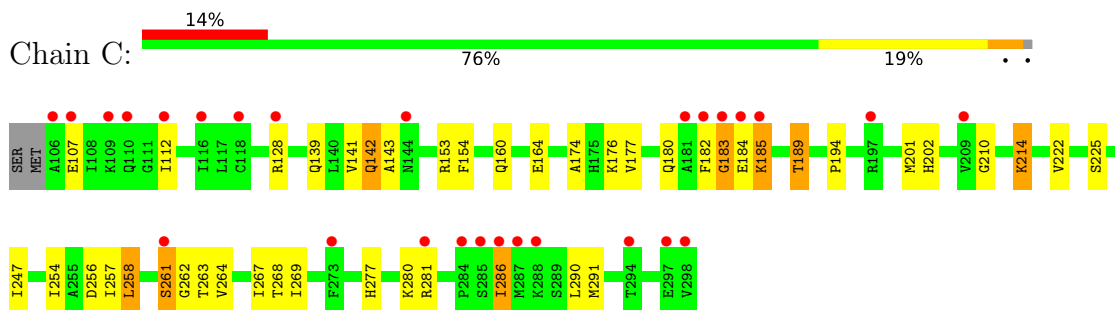
• Molecule 1: Syntenin-1



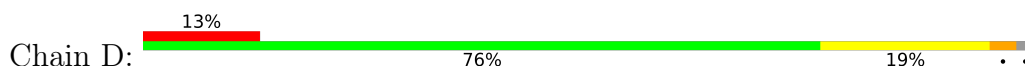
• Molecule 1: Syntenin-1

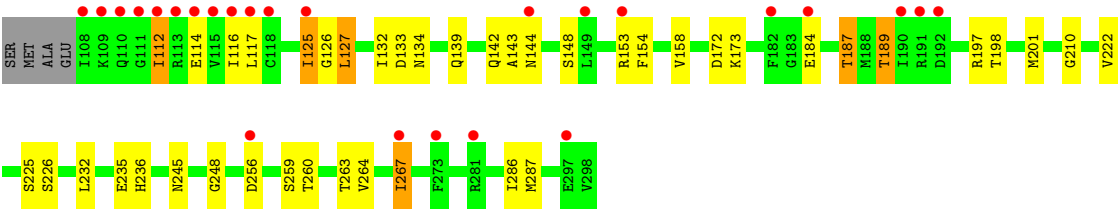


• Molecule 1: Syntenin-1



• 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	80.84Å 49.15Å 115.02Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	80.53 – 1.77 80.53 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.2 (80.53-1.77) 98.2 (80.53-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.247 0.204 , 0.234	Depositor DCC
R_{free} test set	5824 reflections (6.60%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6378	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 27.80 % 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 2.0622e-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: DGL, SO4, EDO, 4MB

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	1.26	5/1502 (0.3%)	1.53	5/2019 (0.2%)
1	B	1.39	9/1516 (0.6%)	1.54	4/2038 (0.2%)
1	C	1.36	9/1535 (0.6%)	1.50	9/2063 (0.4%)
1	D	1.43	18/1510 (1.2%)	1.60	12/2030 (0.6%)
All	All	1.36	41/6063 (0.7%)	1.54	30/8150 (0.4%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	ASN	C-O	8.03	1.33	1.23
1	D	142	GLN	C-O	7.67	1.33	1.24
1	D	267	ILE	C-O	7.53	1.31	1.24
1	D	127	LEU	C-O	7.39	1.32	1.23
1	C	142	GLN	C-O	7.13	1.32	1.23
1	B	157	GLN	C-O	7.01	1.32	1.23
1	A	212	ILE	C-O	6.50	1.30	1.24
1	D	173	LYS	C-O	6.36	1.31	1.24
1	C	177	VAL	C-O	6.36	1.31	1.24
1	A	153	ARG	C-O	6.28	1.31	1.23
1	D	172	ASP	C-O	6.03	1.31	1.24
1	D	126	GLY	C-O	5.88	1.31	1.23
1	C	277	HIS	CE1-NE2	5.88	1.38	1.32
1	C	257	ILE	C-O	5.87	1.30	1.24
1	D	139	GLN	C-O	5.86	1.31	1.24
1	A	233	LEU	C-O	5.82	1.30	1.23
1	A	193	ARG	N-CA	5.82	1.50	1.46
1	D	189	THR	C-O	5.80	1.31	1.24
1	D	154	PHE	C-O	5.70	1.30	1.23
1	C	141	VAL	C-O	5.69	1.30	1.24
1	B	152	LEU	C-O	5.66	1.30	1.23
1	B	236	HIS	CE1-NE2	5.64	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	GLN	C-O	5.64	1.30	1.24
1	B	233	LEU	C-O	5.60	1.31	1.23
1	B	240	GLU	C-O	5.56	1.30	1.23
1	A	234	THR	C-O	5.48	1.31	1.23
1	D	153	ARG	C-O	5.47	1.30	1.23
1	B	293	HIS	CE1-NE2	5.39	1.38	1.32
1	D	132	ILE	C-O	5.39	1.30	1.24
1	D	222	VAL	C-O	5.32	1.30	1.24
1	D	158	VAL	C-O	5.26	1.29	1.24
1	D	236	HIS	C-O	5.26	1.30	1.23
1	D	245	ASN	C-O	5.26	1.30	1.24
1	D	264	VAL	C-O	5.24	1.29	1.23
1	C	201	MET	C-O	5.17	1.30	1.23
1	B	239	CYS	C-O	5.17	1.30	1.24
1	D	148	SER	CA-CB	-5.09	1.45	1.53
1	C	268	THR	C-O	5.05	1.30	1.24
1	C	222	VAL	C-O	5.05	1.30	1.24
1	D	198	THR	C-O	5.03	1.30	1.24
1	C	143	ALA	C-O	5.01	1.29	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	THR	CA-CB-OG1	-7.08	98.98	109.60
1	A	193	ARG	O-C-N	-6.68	118.46	121.53
1	A	235	GLU	N-CA-CB	-6.65	102.19	112.30
1	C	256	ASP	CB-CA-C	6.57	121.70	110.79
1	B	143	ALA	CA-C-N	6.39	131.21	122.07
1	B	143	ALA	C-N-CA	6.39	131.21	122.07
1	D	134	ASN	CA-CB-CG	-6.24	106.36	112.60
1	A	200	THR	CA-CB-OG1	-6.21	100.28	109.60
1	C	261	SER	N-CA-CB	6.14	119.14	110.36
1	D	189	THR	CB-CA-C	6.09	119.80	109.75
1	D	263	THR	CA-CB-OG1	-6.02	100.58	109.60
1	D	226	SER	CA-C-O	-5.98	114.54	120.82
1	B	175	HIS	CA-CB-CG	-5.74	108.06	113.80
1	D	112	ILE	N-CA-CB	-5.62	103.65	111.41
1	D	235	GLU	N-CA-CB	-5.58	103.82	112.30
1	C	254	ILE	N-CA-C	-5.44	105.07	110.62
1	D	197	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	D	143	ALA	O-C-N	5.35	129.58	122.95
1	D	144	ASN	N-CA-C	-5.33	105.56	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	ILE	CA-C-N	5.33	127.73	120.54
1	D	286	ILE	C-N-CA	5.33	127.73	120.54
1	D	286	ILE	CA-C-O	-5.30	115.16	121.05
1	C	174	ALA	CA-C-N	5.29	127.37	120.28
1	C	174	ALA	C-N-CA	5.29	127.37	120.28
1	C	189	THR	CB-CA-C	5.25	118.69	110.19
1	A	193	ARG	N-CA-CB	-5.06	106.04	111.66
1	A	134	ASN	CA-CB-CG	-5.06	107.54	112.60
1	C	291	MET	CA-C-N	5.03	129.26	121.26
1	C	291	MET	C-N-CA	5.03	129.26	121.26
1	C	258	LEU	CA-C-O	-5.02	115.53	120.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1481	0	1530	27	0
1	B	1495	0	1541	15	0
1	C	1514	0	1558	20	0
1	D	1489	0	1533	17	0
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	1	0
3	B	10	0	7	0	0
3	D	10	0	7	0	0
4	C	14	0	8	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	48	0	0	0	0
8	B	86	0	0	2	0
8	C	71	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	101	0	0	3	0
All	All	6378	0	6234	78	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 6.

All (78) 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:A:140:LEU:HD21	1:A:282:MET:SD	1.96	1.04
1:D:125:ILE:HD11	1:D:127:LEU:HD12	1.61	0.82
1:D:187:THR:CG2	8:D:491:HOH:O	2.31	0.77
1:D:187:THR:HG22	8:D:491:HOH:O	1.85	0.76
1:A:198:THR:HG23	1:A:266:THR:CG2	2.15	0.76
1:A:198:THR:HG23	1:A:266:THR:HG23	1.69	0.75
1:A:284:PRO:O	1:A:288:LYS:HD3	1.86	0.74
1:A:128:ARG:HG3	1:A:140:LEU:HD12	1.71	0.72
1:D:248:GLY:HA2	1:D:287:MET:HE3	1.75	0.68
1:B:125:ILE:HD12	1:B:125:ILE:H	1.58	0.68
1:B:286:ILE:HG23	1:B:290:LEU:HD12	1.76	0.67
1:A:206:THR:HG22	1:A:208:HIS:CE1	2.31	0.65
1:B:125:ILE:HD12	1:B:125:ILE:N	2.12	0.65
1:D:248:GLY:CA	1:D:287:MET:HE3	2.28	0.64
1:C:184:GLU:O	1:C:185:LYS:HB3	1.98	0.64
1:A:198:THR:CG2	1:A:266:THR:HG23	2.28	0.64
1:B:241:ILE:HD11	1:B:254:ILE:HG23	1.81	0.63
1:A:284:PRO:HA	1:A:287:MET:HB2	1.85	0.58
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.86	0.58
1:C:112:ILE:CG2	1:C:189:THR:HG22	2.34	0.57
1:A:112:ILE:CG2	1:A:189:THR:CG2	2.83	0.56
1:B:125:ILE:HD11	8:B:475:HOH:O	2.05	0.56
1:D:114:GLU:OE1	1:D:116:ILE:HD11	2.06	0.56
1:A:198:THR:CG2	1:A:266:THR:CG2	2.83	0.55
1:C:153:ARG:HD3	8:C:404:HOH:O	2.05	0.54
1:D:133:ASP:OD1	2:D:302:EDO:O1	2.25	0.54
1:D:117:LEU:HD12	1:D:117:LEU:C	2.32	0.54
1:B:241:ILE:HD12	1:B:246:VAL:HG11	1.90	0.53
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.91	0.52
1:A:206:THR:HG22	1:A:206:THR:O	2.10	0.52
1:D:125:ILE:HD11	1:D:127:LEU:CD1	2.38	0.52
1:A:158:VAL:HG11	1:A:188:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:SER:OG	1:C:262:GLY:N	2.43	0.51
1:C:202:HIS:CD2	1:C:264:VAL:HG22	2.46	0.51
1:C:214:LYS:HE2	8:C:425:HOH:O	2.11	0.51
1:A:285:SER:HA	1:A:288:LYS:HD3	1.93	0.50
1:A:285:SER:HA	1:A:288:LYS:CD	2.41	0.50
1:A:140:LEU:CD2	1:A:282:MET:SD	2.86	0.50
1:A:279:ILE:HB	1:A:282:MET:CE	2.42	0.50
1:A:158:VAL:CG1	1:A:188:MET:HE2	2.42	0.49
1:B:130:LYS:HE2	1:B:281:ARG:HD3	1.96	0.48
1:B:202:HIS:O	8:B:401:HOH:O	2.20	0.47
1:C:128:ARG:NH1	1:C:281:ARG:O	2.47	0.47
1:C:280:LYS:O	1:C:281:ARG:CB	2.62	0.47
1:D:187:THR:HG23	8:D:491:HOH:O	2.07	0.47
1:A:206:THR:O	1:A:206:THR:CG2	2.63	0.47
1:C:182:PHE:O	1:C:183:GLY:O	2.33	0.46
1:D:117:LEU:HD12	1:D:117:LEU:O	2.16	0.46
1:C:112:ILE:CG2	1:C:189:THR:CG2	2.93	0.46
1:C:286:ILE:HG23	1:C:290:LEU:HD12	1.96	0.46
1:A:112:ILE:CG2	1:A:189:THR:HG22	2.46	0.45
1:B:116:ILE:HG23	1:B:185:LYS:HG3	1.98	0.45
1:C:176:LYS:O	1:C:180:GLN:HG3	2.16	0.45
1:D:232:LEU:HD11	1:D:267:ILE:HD11	1.98	0.45
1:A:197:ARG:HD3	1:C:194:PRO:O	2.16	0.45
1:C:154:PHE:CD1	1:C:247:ILE:CD1	2.99	0.45
1:B:112:ILE:CG2	1:B:189:THR:CG2	2.95	0.45
1:A:238:ILE:HG23	1:A:267:ILE:HG23	1.98	0.45
1:D:112:ILE:CG2	1:D:189:THR:CG2	2.94	0.44
1:C:210:GLY:HA3	1:C:225:SER:HB2	1.99	0.44
1:C:267:ILE:HG22	1:C:269:ILE:HG23	1.99	0.44
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.47	0.44
1:B:117:LEU:HD22	1:B:125:ILE:CG2	2.48	0.43
1:C:128:ARG:NH1	1:C:139:GLN:OE1	2.50	0.43
1:A:201:MET:HE3	1:A:201:MET:HB2	1.85	0.43
1:A:267:ILE:HG22	1:A:269:ILE:HG23	2.00	0.43
1:C:142:GLN:HA	1:C:290:LEU:O	2.19	0.43
1:D:210:GLY:HA3	1:D:225:SER:CB	2.49	0.42
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.30	0.42
1:A:279:ILE:HB	1:A:282:MET:HE3	2.01	0.42
1:B:203:LYS:NZ	1:B:258:LEU:O	2.51	0.41
1:D:201:MET:HE3	1:D:201:MET:HB2	1.95	0.41
1:D:210:GLY:HA3	1:D:225:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256[B]:ASP:O	1:D:260:THR:HG23	2.20	0.41
1:A:112:ILE:HG23	1:A:189:THR:HG22	2.03	0.41
1:C:160:GLN:HA	1:C:164:GLU:O	2.21	0.41
1:C:258:LEU:HD23	1:C:258:LEU:HA	1.94	0.40
1:B:212:ILE:HB	1:B:220:SER:HB3	2.03	0.40

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%)	8 (4%)	3 (2%)	7	1
1	B	192/195 (98%)	189 (98%)	3 (2%)	0	100	100
1	C	194/195 (100%)	184 (95%)	8 (4%)	2 (1%)	12	4
1	D	191/195 (98%)	185 (97%)	6 (3%)	0	100	100
All	All	767/780 (98%)	737 (96%)	25 (3%)	5 (1%)	18	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	282	MET
1	C	183	GLY
1	C	185	LYS
1	A	281	ARG

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%)	162 (98%)	4 (2%)	43	24
1	B	167/168 (99%)	159 (95%)	8 (5%)	23	5
1	C	169/168 (101%)	165 (98%)	4 (2%)	43	24
1	D	167/168 (99%)	163 (98%)	4 (2%)	43	24
All	All	669/672 (100%)	649 (97%)	20 (3%)	36	15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	259	SER
1	A	287	MET
1	A	290	LEU
1	B	107	GLU
1	B	117	LEU
1	B	125	ILE
1	B	144	ASN
1	B	153	ARG
1	B	160	GLN
1	B	235	GLU
1	B	264	VAL
1	C	107	GLU
1	C	214	LYS
1	C	263	THR
1	C	286	ILE
1	D	125	ILE
1	D	184	GLU
1	D	187	THR
1	D	259	SER

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

Mol	Chain	Res	Type
1	A	230	ASN
1	B	142	GLN
1	B	165	ASN

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Mol	Chain	Res	Type
1	B	180	GLN
1	B	215	ASN
1	B	230	ASN
1	C	202	HIS
1	C	277	HIS
1	D	110	GLN
1	D	208	HIS
1	D	215	ASN
1	D	230	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](#)

16 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	DGL	D	307	-	8,9,9	1.03	0	8,11,11	0.94	0
6	SO4	D	303	-	4,4,4	0.34	0	6,6,6	0.07	0
6	SO4	D	305	-	4,4,4	0.32	0	6,6,6	0.09	0
2	EDO	B	301	-	3,3,3	0.28	0	2,2,2	0.35	0
2	EDO	B	302	-	3,3,3	0.29	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DGL	B	303	-	8,9,9	1.04	0	8,11,11	1.47	1 (12%)
2	EDO	C	302	-	3,3,3	0.47	0	2,2,2	0.55	0
4	4MB	C	301	-	14,14,14	0.50	0	20,20,20	0.85	1 (5%)
2	EDO	D	302	-	3,3,3	0.07	0	2,2,2	0.24	0
7	ALA	D	306	-	5,5,5	0.94	0	6,6,6	1.04	0
2	EDO	C	303	-	3,3,3	0.52	0	2,2,2	0.56	0
6	SO4	D	304	-	4,4,4	0.31	0	6,6,6	0.09	0
2	EDO	A	301	-	3,3,3	0.09	0	2,2,2	0.06	0
2	EDO	D	301	-	3,3,3	0.40	0	2,2,2	0.15	0
5	GLY	D	308	-	4,4,4	1.22	1 (25%)	3,4,4	1.34	0
5	GLY	C	304	-	4,4,4	0.79	0	3,4,4	1.87	1 (33%)

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	DGL	D	307	-	-	1/9/9/9	-
2	EDO	B	301	-	-	1/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
3	DGL	B	303	-	-	0/9/9/9	-
2	EDO	C	302	-	-	0/1/1/1	-
4	4MB	C	301	-	-	2/9/9/9	0/1/1/1
2	EDO	D	302	-	-	1/1/1/1	-
7	ALA	D	306	-	-	0/4/4/4	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
5	GLY	D	308	-	-	2/2/2/2	-
5	GLY	C	304	-	-	0/2/2/2	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	308	GLY	OXT-C	-2.37	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	DGL	OXT-C-O	-3.08	117.09	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	304	GLY	OXT-C-CA	2.47	123.20	113.38
4	C	301	4MB	C3-C2-N1	2.19	124.63	120.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

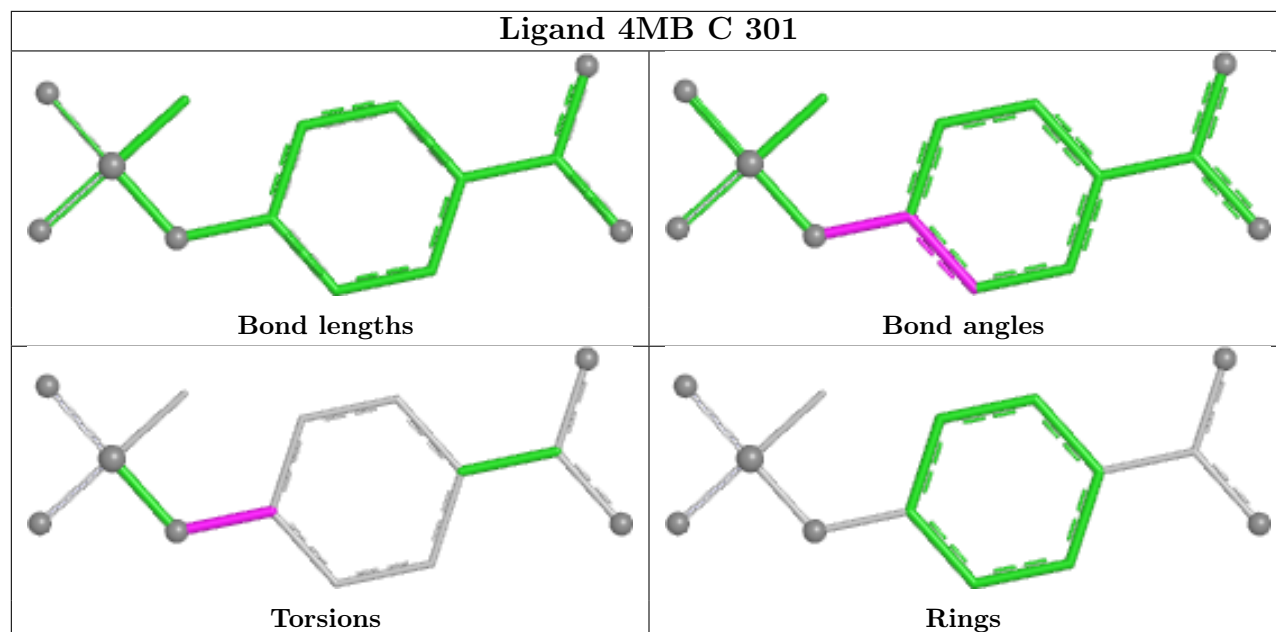
Mol	Chain	Res	Type	Atoms
5	D	308	GLY	O-C-CA-N
5	D	308	GLY	OXT-C-CA-N
2	C	303	EDO	O1-C1-C2-O2
4	C	301	4MB	C10-C2-N1-S11
4	C	301	4MB	C3-C2-N1-S11
3	D	307	DGL	O-C-CA-N
2	D	302	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	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 [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%)	1.42	36 (18%) 3 3	13, 45, 83, 128	6 (3%)
1	B	193/195 (98%)	0.83	20 (10%) 11 13	10, 40, 58, 69	6 (3%)
1	C	193/195 (98%)	1.13	27 (13%) 6 7	11, 39, 59, 68	14 (7%)
1	D	191/195 (97%)	0.94	25 (13%) 7 7	11, 35, 52, 67	13 (6%)
All	All	768/780 (98%)	1.08	108 (14%) 6 7	10, 40, 61, 128	39 (5%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ILE	12.9
1	A	273[A]	PHE	12.0
1	D	273[A]	PHE	11.7
1	C	182	PHE	10.7
1	A	286	ILE	9.7
1	A	277	HIS	9.6
1	A	276	GLU	8.5
1	C	183	GLY	8.5
1	C	181	ALA	8.3
1	D	115	VAL	8.0
1	D	256[A]	ASP	8.0
1	D	116	ILE	7.7
1	D	190	ILE	7.6
1	A	290	LEU	7.5
1	C	294	THR	7.4
1	C	185	LYS	7.1
1	B	273[A]	PHE	7.1
1	D	117	LEU	6.9
1	A	206	THR	6.4
1	C	197[A]	ARG	6.1
1	C	273[A]	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	282	MET	5.9
1	A	182	PHE	5.7
1	D	113	ARG	5.5
1	C	297	GLU	5.5
1	A	287	MET	5.5
1	C	288	LYS	5.4
1	A	259	SER	5.4
1	C	106	ALA	5.3
1	D	191	ARG	5.3
1	B	223	LYS	5.2
1	D	114	GLU	5.1
1	B	153	ARG	4.9
1	C	184	GLU	4.8
1	C	144[A]	ASN	4.8
1	B	191	ARG	4.5
1	A	283	ALA	4.5
1	D	297	GLU	4.4
1	D	153	ARG	4.3
1	A	284	PRO	4.3
1	D	192	ASP	4.2
1	A	108	ILE	4.2
1	B	109	LYS	3.9
1	D	182	PHE	3.9
1	A	279	ILE	3.8
1	A	118	CYS	3.6
1	A	111	GLY	3.5
1	B	118	CYS	3.5
1	A	184	GLU	3.5
1	C	110	GLN	3.4
1	B	149	LEU	3.4
1	C	128	ARG	3.3
1	C	287	MET	3.3
1	D	110	GLN	3.3
1	A	110	GLN	3.3
1	A	280	LYS	3.2
1	A	295	ILE	3.2
1	A	285	SER	3.2
1	D	144	ASN	3.2
1	A	288	LYS	3.2
1	C	109	LYS	3.1
1	C	107	GLU	3.1
1	B	108	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	3.1
1	A	125	ILE	3.1
1	D	125	ILE	3.0
1	A	109	LYS	2.9
1	D	108	ILE	2.9
1	A	298	VAL	2.9
1	B	297	GLU	2.7
1	C	209	VAL	2.7
1	A	117	LEU	2.7
1	D	118	CYS	2.7
1	A	257	ILE	2.7
1	B	106	ALA	2.6
1	D	112	ILE	2.6
1	C	284	PRO	2.6
1	B	284	PRO	2.5
1	C	286	ILE	2.5
1	A	263	THR	2.5
1	B	110	GLN	2.4
1	B	264	VAL	2.4
1	A	281	ARG	2.4
1	C	118	CYS	2.4
1	D	149	LEU	2.3
1	D	281	ARG	2.3
1	A	202	HIS	2.3
1	A	186	ILE	2.3
1	C	261	SER	2.3
1	D	184	GLU	2.3
1	C	298	VAL	2.3
1	D	109	LYS	2.3
1	A	260	THR	2.3
1	B	175	HIS	2.3
1	B	117	LEU	2.3
1	B	190	ILE	2.2
1	C	116	ILE	2.2
1	A	153	ARG	2.1
1	C	285	SER	2.1
1	D	111	GLY	2.1
1	A	289	SER	2.1
1	B	122	ASP	2.1
1	B	124	LYS	2.1
1	B	173	LYS	2.1
1	C	112	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	281	ARG	2.0
1	A	296	PRO	2.0
1	D	267	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](#)

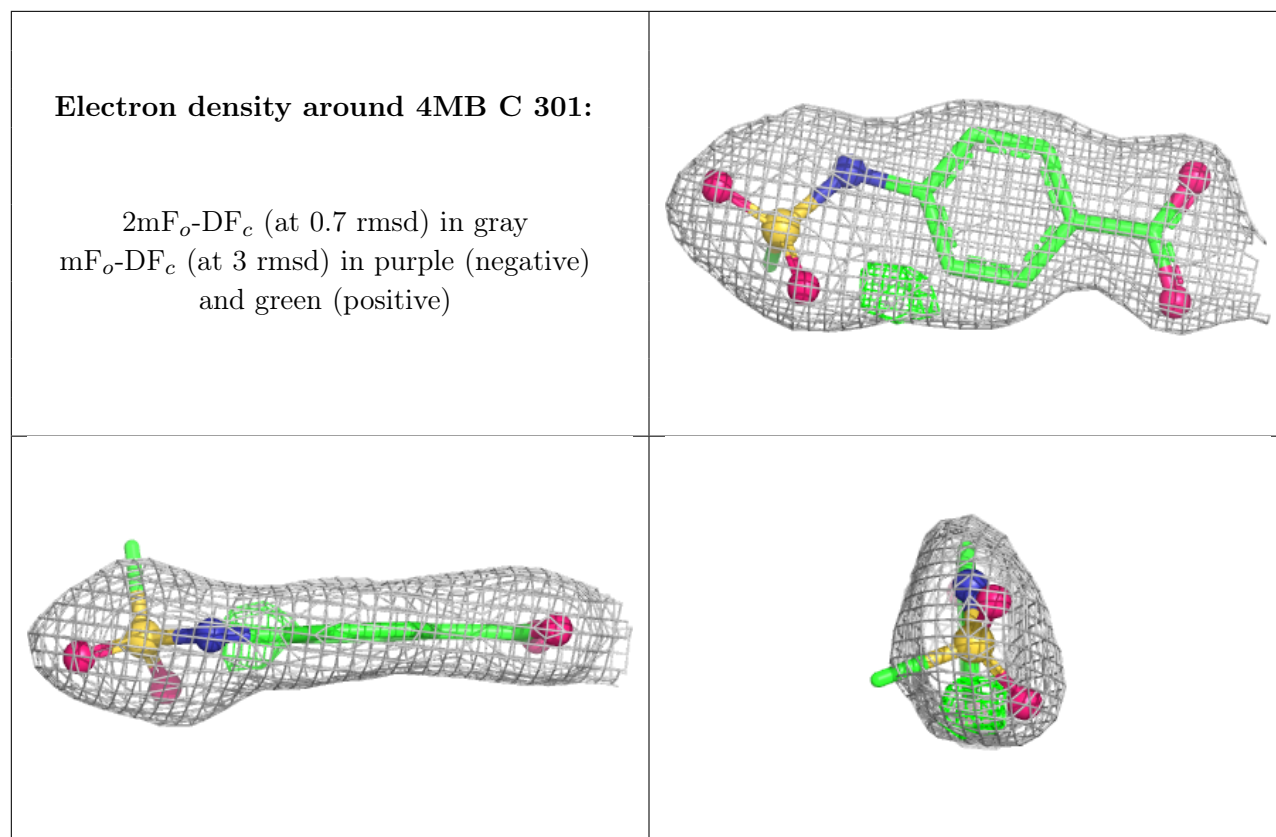
There are no oligosaccharides in this entry.

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
6	SO4	D	303	5/5	0.41	0.35	323,326,330,330	5
3	DGL	D	307	10/10	0.63	0.21	38,69,77,78	0
3	DGL	B	303	10/10	0.74	0.16	45,65,75,83	0
5	GLY	C	304	5/5	0.77	0.16	46,55,64,65	0
2	EDO	C	303	4/4	0.77	0.26	50,61,62,63	0
2	EDO	A	301	4/4	0.85	0.19	55,55,58,62	0
6	SO4	D	304	5/5	0.86	0.55	67,68,71,75	5
2	EDO	D	302	4/4	0.88	0.16	45,48,53,59	0
6	SO4	D	305	5/5	0.88	0.11	62,62,64,65	5
5	GLY	D	308	5/5	0.89	0.16	62,70,75,75	0
2	EDO	B	301	4/4	0.89	0.14	45,46,49,56	0
7	ALA	D	306	6/6	0.90	0.12	44,48,53,54	0
2	EDO	C	302	4/4	0.92	0.11	33,33,34,40	0
4	4MB	C	301	14/14	0.93	0.12	42,45,52,53	14
2	EDO	D	301	4/4	0.96	0.09	25,26,31,36	0
2	EDO	B	302	4/4	0.97	0.06	29,29,35,37	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.