



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:00 AM UTC

PDB ID : 7FSV / pdb_00007fsv
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z1454310449
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

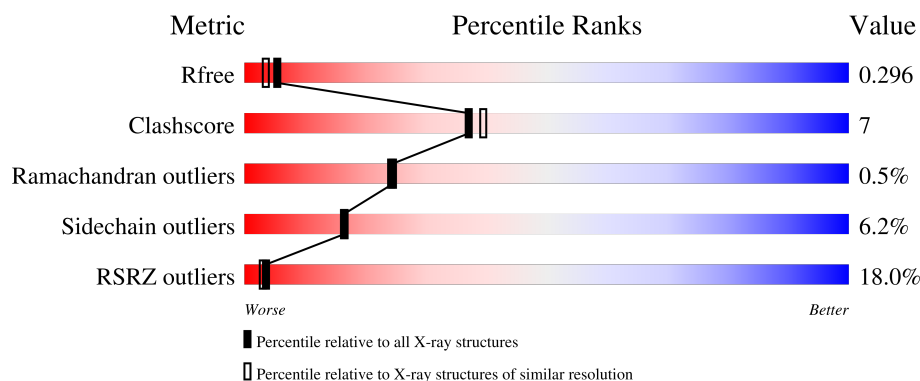
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	27% 77% 19% ..
1	B	195	12% 75% 22% ...
1	C	195	15% 80% 15% ..
1	D	195	16% 76% 21% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLY	D	307	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

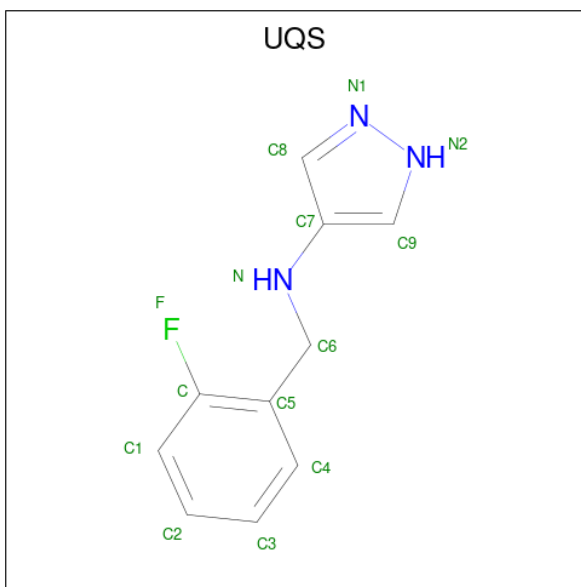
- Molecule 1 is a protein called Syntenin-1.

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

There are 8 discrepancies between the modelled and reference sequences:

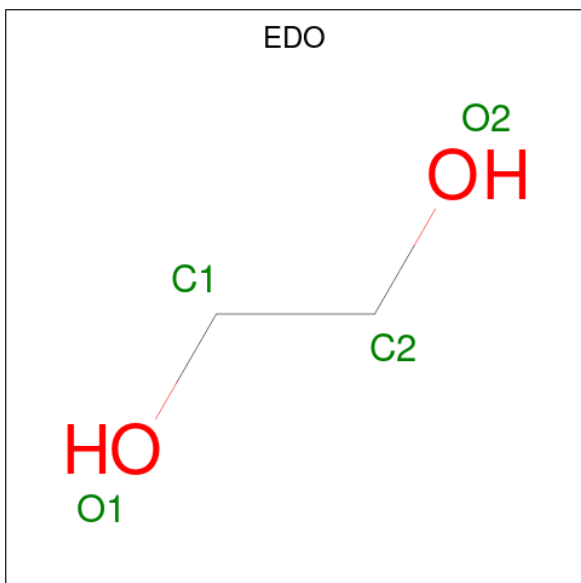
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

- Molecule 2 is N-[(2-fluorophenyl)methyl]-1H-pyrazol-4-amine (CCD ID: UQS) (formula: C₁₀H₁₀FN₃) (labeled as "Ligand of Interest" by depositor).



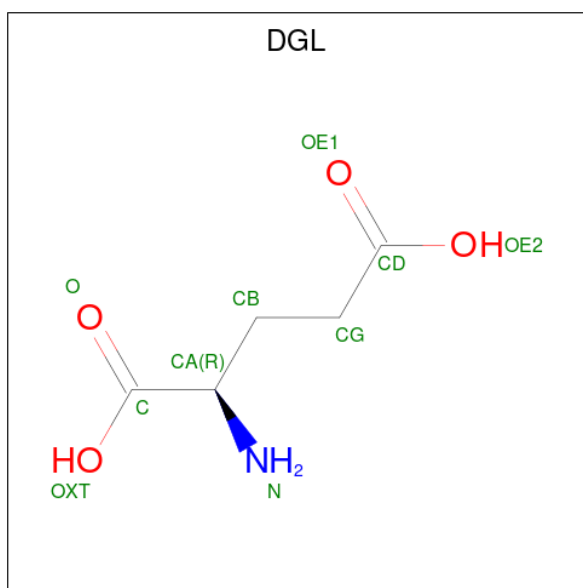
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			14	10	1	3		
2	B	1	Total	C	F	N	0	0
			14	10	1	3		
2	C	1	Total	C	F	N	0	0
			14	10	1	3		
2	D	1	Total	C	F	N	0	0
			14	10	1	3		

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



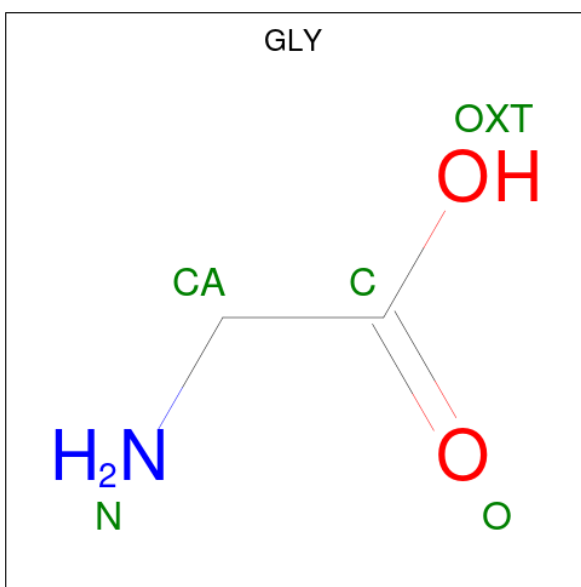
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

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



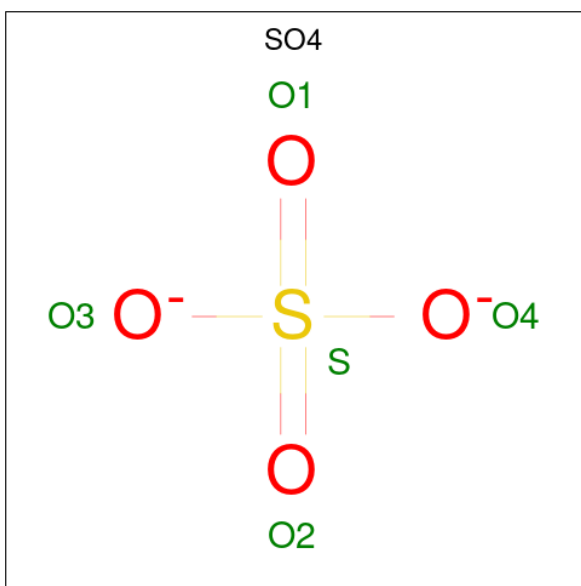
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 10 5 1 4	0	0
4	D	1	Total C N O 10 5 1 4	0	0

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



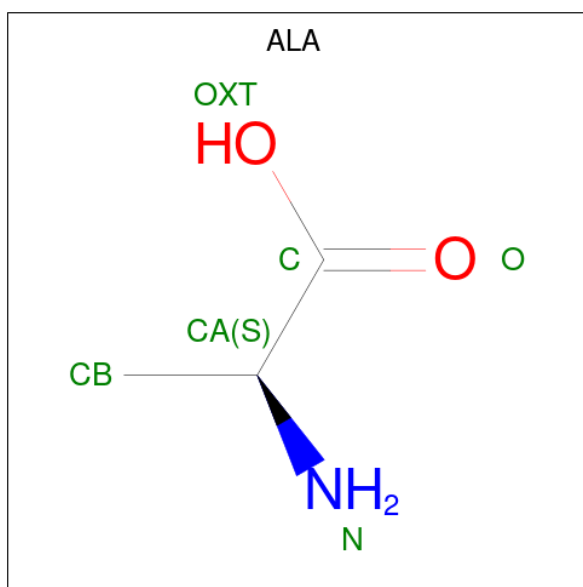
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- 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		

- Molecule 7 is ALANINE (CCD ID: ALA) (formula: C₃H₇NO₂).



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

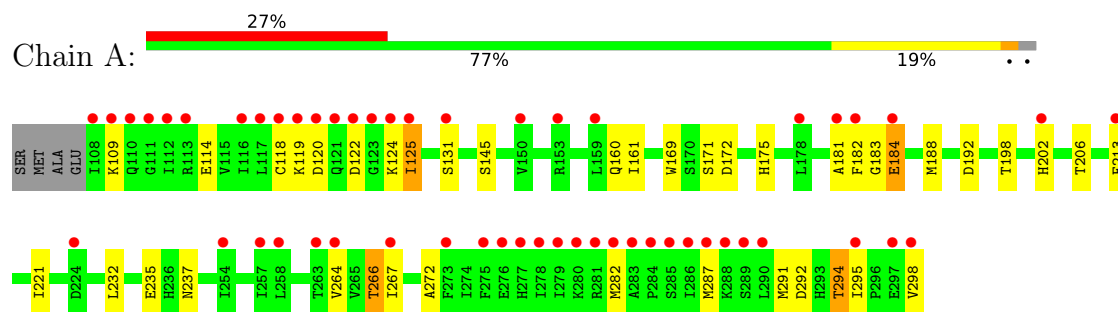
- Molecule 8 is water.

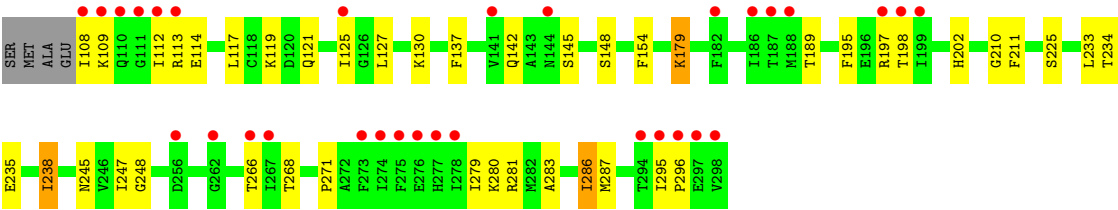
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total	O	0	0
			39	39		
8	B	73	Total	O	0	0
			73	73		
8	C	54	Total	O	0	0
			54	54		
8	D	79	Total	O	0	1
			79	79		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.91Å 49.21Å 114.40Å 90.00° 95.35° 90.00°	Depositor
Resolution (Å)	113.82 – 2.25 113.82 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (113.82-2.25) 99.7 (113.82-2.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.222 , 0.288 0.246 , 0.296	Depositor DCC
R_{free} test set	2102 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6345	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 25.85 % 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 2.9389e-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, UQS

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	3/1502 (0.2%)	1.46	0/2019
1	B	1.37	9/1516 (0.6%)	1.55	5/2038 (0.2%)
1	C	1.15	0/1535	1.47	2/2063 (0.1%)
1	D	1.27	5/1502 (0.3%)	1.46	4/2019 (0.2%)
All	All	1.24	17/6055 (0.3%)	1.48	11/8139 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	THR	C-O	10.02	1.37	1.23
1	B	273[A]	PHE	C-O	9.34	1.35	1.24
1	B	273[B]	PHE	C-O	9.34	1.35	1.24
1	B	127	LEU	C-O	8.02	1.34	1.24
1	D	233	LEU	C-O	7.87	1.33	1.23
1	B	138	VAL	C-O	7.03	1.31	1.24
1	D	238	ILE	C-O	-5.94	1.18	1.24
1	B	140	LEU	C-O	5.69	1.30	1.23
1	D	245	ASN	C-O	5.66	1.30	1.23
1	B	125	ILE	C-O	5.44	1.30	1.24
1	A	120	ASP	CB-CG	5.44	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	LEU	C-O	5.39	1.30	1.23
1	B	125	ILE	C-N	5.33	1.39	1.33
1	B	235	GLU	CG-CD	5.23	1.65	1.52
1	D	235	GLU	C-O	5.18	1.31	1.23
1	A	175	HIS	CB-CG	5.08	1.57	1.50
1	A	213	PHE	C-O	5.06	1.30	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	THR	CB-CA-C	-6.78	96.92	110.42
1	B	194	PRO	CB-CA-C	-6.70	101.77	112.21
1	B	160	GLN	CB-CG-CD	-6.51	101.53	112.60
1	B	142	GLN	CB-CA-C	-6.07	99.85	109.80
1	D	189	THR	CA-CB-OG1	-5.83	100.86	109.60
1	B	125	ILE	O-C-N	5.14	127.27	122.23
1	C	287	MET	CA-C-N	5.09	127.36	120.38
1	C	287	MET	C-N-CA	5.09	127.36	120.38
1	D	268	THR	CB-CA-C	5.08	118.43	110.19
1	D	271	PRO	CA-C-N	5.05	127.30	120.38
1	D	271	PRO	C-N-CA	5.05	127.30	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLY	Peptide
1	C	111	GLY	Peptide
1	D	127	LEU	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	19	0
1	B	1495	0	1541	22	0
1	C	1514	0	1558	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1481	0	1530	29	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	1	0
2	D	14	0	0	1	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	5	0	0	0	0
7	D	6	0	4	1	0
8	A	39	0	0	2	0
8	B	73	0	0	1	0
8	C	54	0	0	2	0
8	D	79	0	0	3	0
All	All	6345	0	6229	88	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 7.

All (88) 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:198:THR:CG2	1:D:266:THR:HG23	1.85	1.06
1:D:198:THR:HG23	1:D:266:THR:HG23	1.45	0.98
1:C:110:GLN:NE2	8:C:401:HOH:O	2.07	0.86
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.60	0.81
1:D:108:ILE:HG22	1:D:109:LYS:H	1.44	0.81
1:C:287:MET:HE1	2:C:301:UQS:C3	2.12	0.80
1:D:198:THR:CG2	1:D:266:THR:CG2	2.60	0.79
1:D:198:THR:HG23	1:D:266:THR:CG2	2.18	0.73
1:B:118:CYS:HA	1:B:183:GLY:O	1.92	0.68
1:B:292:ASP:OD1	1:B:294:THR:OG1	2.13	0.67
1:D:248:GLY:HA2	1:D:287:MET:HE3	1.77	0.65
1:C:282:MET:HE3	1:C:287:MET:SD	2.38	0.64
1:D:117:LEU:HD22	1:D:125:ILE:HG23	1.78	0.64
1:A:292:ASP:OD1	1:A:294:THR:OG1	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ILE:O	1:D:109:LYS:HG2	1.98	0.64
1:D:108:ILE:O	1:D:109:LYS:CG	2.46	0.63
1:C:246:VAL:HG12	1:C:249:LEU:HD12	1.82	0.62
1:D:108:ILE:C	1:D:109:LYS:HG3	2.25	0.61
1:D:154:PHE:CD1	1:D:247:ILE:HD13	2.37	0.60
1:D:197:ARG:NH1	8:D:401:HOH:O	2.22	0.59
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.86	0.57
1:C:128:ARG:HB2	1:C:140:LEU:HB3	1.86	0.56
1:B:136:ILE:HD11	1:B:169:TRP:O	2.06	0.56
1:D:238:ILE:O	2:D:301:UQS:N2	2.39	0.56
1:B:119:LYS:HB2	1:B:183:GLY:HA3	1.88	0.55
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.88	0.55
1:D:198:THR:HG21	1:D:266:THR:CG2	2.36	0.54
1:D:108:ILE:C	1:D:109:LYS:CG	2.80	0.54
1:A:161:ILE:HD12	1:A:169:TRP:HZ3	1.74	0.53
1:B:109:LYS:N	1:B:192:ASP:OD2	2.43	0.52
1:C:201:MET:HE1	1:C:267:ILE:HG13	1.91	0.52
1:B:274:ILE:HG22	1:B:278:ILE:CD1	2.41	0.51
1:C:116:ILE:HD12	1:C:116:ILE:N	2.26	0.50
1:C:117:LEU:HD13	1:C:150:VAL:HG11	1.93	0.50
1:A:119:LYS:NZ	1:A:181:ALA:O	2.44	0.50
1:C:108:ILE:HD12	1:C:198:THR:CG2	2.41	0.50
1:A:235:GLU:OE1	8:A:401:HOH:O	2.19	0.49
1:D:130:LYS:HE2	1:D:281:ARG:HD3	1.94	0.49
1:A:221:ILE:HD12	1:A:232:LEU:HB3	1.95	0.49
1:D:154:PHE:CD1	1:D:247:ILE:CD1	2.95	0.49
1:A:122:ASP:HB3	1:A:124:LYS:HE3	1.94	0.48
1:A:109:LYS:N	1:A:192:ASP:OD2	2.46	0.48
1:D:112:ILE:HG22	1:D:113:ARG:N	2.29	0.48
1:A:118:CYS:SG	1:A:184:GLU:O	2.65	0.47
1:C:282:MET:CE	1:C:287:MET:SD	3.02	0.47
1:C:282:MET:HE3	1:C:287:MET:CG	2.45	0.47
1:D:137:PHE:CE2	1:D:195:PHE:CE2	3.02	0.47
1:A:287:MET:O	1:A:291:MET:HB3	2.14	0.47
1:B:245:ASN:OD1	1:B:245:ASN:C	2.57	0.47
1:C:182:PHE:O	1:C:183:GLY:C	2.59	0.46
1:C:286:ILE:HG23	1:C:290:LEU:HD12	1.96	0.46
1:C:159:LEU:HD12	1:C:159:LEU:N	2.31	0.46
1:D:283:ALA:HB3	1:D:286:ILE:HG13	1.96	0.46
1:B:119:LYS:HB2	1:B:183:GLY:CA	2.45	0.46
1:B:173:LYS:O	1:B:177:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:CYS:O	1:B:119:LYS:C	2.59	0.45
1:B:274:ILE:HG22	1:B:278:ILE:HD11	1.99	0.45
1:D:287:MET:HE2	1:D:287:MET:HB3	1.86	0.45
1:A:292:ASP:OD1	1:A:292:ASP:C	2.60	0.44
1:A:172:ASP:OD1	1:B:121:GLN:HB3	2.18	0.44
1:A:125:ILE:O	1:A:145:SER:HB2	2.17	0.44
1:A:237:ASN:HD22	1:A:272:ALA:HA	1.83	0.44
1:A:198:THR:CG2	1:A:266:THR:HG23	2.48	0.44
1:D:280:LYS:HE3	8:D:434:HOH:O	2.17	0.44
1:B:159:LEU:O	1:B:160:GLN:HG3	2.18	0.43
1:C:142:GLN:HA	1:C:290:LEU:O	2.18	0.43
1:C:209:VAL:HG23	8:C:416:HOH:O	2.17	0.43
1:C:128:ARG:HB3	1:C:139:GLN:HG3	2.00	0.43
1:C:160:GLN:HA	1:C:164:GLU:O	2.19	0.43
1:B:119:LYS:NZ	1:B:181:ALA:O	2.41	0.43
1:B:126:GLY:HA3	1:B:145:SER:CB	2.49	0.43
1:B:115:VAL:HG21	1:B:152:LEU:HD21	2.01	0.42
1:D:119:LYS:NZ	1:D:179:LYS:O	2.52	0.42
1:D:202:HIS:CE1	8:D:425:HOH:O	2.72	0.42
1:C:159:LEU:N	1:C:159:LEU:CD1	2.83	0.42
1:C:292:ASP:OD1	1:C:294:THR:HB	2.20	0.42
1:B:137:PHE:CE2	1:B:195:PHE:CE2	3.08	0.42
1:A:124:LYS:HE2	1:B:185:LYS:HB3	2.01	0.41
1:B:258:LEU:HA	1:B:258:LEU:HD23	1.81	0.41
1:D:211:PHE:O	7:D:305:ALA:N	2.53	0.41
1:A:266:THR:HG22	8:A:415:HOH:O	2.20	0.41
1:A:282:MET:HE1	8:B:447:HOH:O	2.19	0.41
1:B:117:LEU:HD22	1:B:125:ILE:CG2	2.51	0.41
1:A:202:HIS:ND1	1:A:264:VAL:HG22	2.35	0.40
1:B:155:GLY:HA3	1:B:196:GLU:OE2	2.20	0.40
1:D:137:PHE:CZ	1:D:195:PHE:CE2	3.10	0.40
1:A:160:GLN:O	1:A:188:MET:HA	2.22	0.40
1:D:142:GLN:HB3	1:D:145:SER:HB3	2.03	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%)	8 (4%)	1 (0%)	24	24
1	B	192/195 (98%)	177 (92%)	14 (7%)	1 (0%)	24	24
1	C	194/195 (100%)	182 (94%)	10 (5%)	2 (1%)	12	10
1	D	190/195 (97%)	181 (95%)	9 (5%)	0	100	100
All	All	766/780 (98%)	721 (94%)	41 (5%)	4 (0%)	24	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	GLY
1	A	182	PHE
1	B	110	GLN
1	C	184	GLU

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%)	155 (93%)	11 (7%)	15	14
1	B	167/168 (99%)	158 (95%)	9 (5%)	20	21
1	C	169/168 (101%)	154 (91%)	15 (9%)	9	7
1	D	166/168 (99%)	160 (96%)	6 (4%)	31	39
All	All	668/672 (99%)	627 (94%)	41 (6%)	16	17

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	125	ILE
1	A	131	SER
1	A	171	SER
1	A	184	GLU
1	A	206	THR
1	A	266	THR
1	A	267	ILE
1	A	294	THR
1	A	295	ILE
1	A	298	VAL
1	B	139	GLN
1	B	140	LEU
1	B	198	THR
1	B	205	SER
1	B	223	LYS
1	B	263	THR
1	B	266	THR
1	B	294	THR
1	B	297	GLU
1	C	108	ILE
1	C	121	GLN
1	C	128	ARG
1	C	131	SER
1	C	150	VAL
1	C	184	GLU
1	C	188	MET
1	C	198	THR
1	C	220	SER
1	C	226	SER
1	C	257	ILE
1	C	266	THR
1	C	278	ILE
1	C	280	LYS
1	C	286	ILE
1	D	114	GLU
1	D	121	GLN
1	D	148	SER
1	D	179	LYS
1	D	279	ILE
1	D	286	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	237	ASN
1	A	242	ASN
1	B	139	GLN
1	B	142	GLN
1	B	215	ASN
1	B	237	ASN
1	C	165	ASN
1	C	215	ASN
1	D	139	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](#)

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	$\# Z > 2$
3	EDO	D	303	-	3,3,3	0.12	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UQS	A	301	-	12,15,15	0.75	0	16,19,19	1.55	4 (25%)
5	GLY	D	307	-	4,4,4	1.28	1 (25%)	3,4,4	1.72	1 (33%)
6	SO4	D	304	-	4,4,4	0.35	0	6,6,6	0.06	0
3	EDO	C	303	-	3,3,3	0.09	0	2,2,2	0.16	0
3	EDO	C	302	-	3,3,3	0.12	0	2,2,2	0.08	0
3	EDO	B	303	-	3,3,3	0.20	0	2,2,2	0.32	0
2	UQS	C	301	-	12,15,15	0.88	0	16,19,19	1.37	3 (18%)
5	GLY	C	305	-	4,4,4	0.99	0	3,4,4	1.49	0
3	EDO	C	304	-	3,3,3	0.15	0	2,2,2	0.33	0
7	ALA	D	305	-	5,5,5	1.19	1 (20%)	6,6,6	1.13	0
4	DGL	D	306	-	8,9,9	1.08	0	8,11,11	0.92	0
2	UQS	D	301	-	12,15,15	0.52	0	16,19,19	1.26	2 (12%)
3	EDO	D	302	-	3,3,3	0.21	0	2,2,2	0.05	0
3	EDO	B	302	-	3,3,3	0.14	0	2,2,2	0.24	0
3	EDO	A	302	-	3,3,3	0.14	0	2,2,2	0.01	0
2	UQS	B	301	-	12,15,15	0.75	0	16,19,19	1.08	0
4	DGL	B	304	-	8,9,9	1.14	1 (12%)	8,11,11	1.30	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
3	EDO	D	303	-	-	1/1/1/1	-
2	UQS	A	301	-	-	0/3/5/5	0/2/2/2
5	GLY	D	307	-	-	2/2/2/2	-
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	B	303	-	-	0/1/1/1	-
2	UQS	C	301	-	-	0/3/5/5	0/2/2/2
5	GLY	C	305	-	-	0/2/2/2	-
3	EDO	C	304	-	-	1/1/1/1	-
7	ALA	D	305	-	-	0/4/4/4	-
4	DGL	D	306	-	-	3/9/9/9	-
2	UQS	D	301	-	-	0/3/5/5	0/2/2/2
3	EDO	D	302	-	-	1/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
2	UQS	B	301	-	-	0/3/5/5	0/2/2/2
4	DGL	B	304	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	307	GLY	OXT-C	-2.50	1.22	1.30
7	D	305	ALA	OXT-C	-2.39	1.23	1.30
4	B	304	DGL	OXT-C	-2.16	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	DGL	OXT-C-O	-2.90	117.49	124.08
2	C	301	UQS	C7-C8-N1	-2.64	107.13	111.10
2	A	301	UQS	C4-C5-C	2.62	121.12	116.62
2	A	301	UQS	C7-C8-N1	-2.59	107.21	111.10
2	C	301	UQS	C8-N1-N2	2.51	110.65	105.75
2	A	301	UQS	C1-C-C5	-2.29	119.54	123.60
2	D	301	UQS	C8-N1-N2	2.23	110.11	105.75
2	C	301	UQS	C9-N2-N1	-2.16	106.79	111.25
5	D	307	GLY	OXT-C-CA	2.13	121.84	113.38
2	D	301	UQS	C7-C8-N1	-2.10	107.95	111.10
2	A	301	UQS	C8-N1-N2	2.08	109.81	105.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

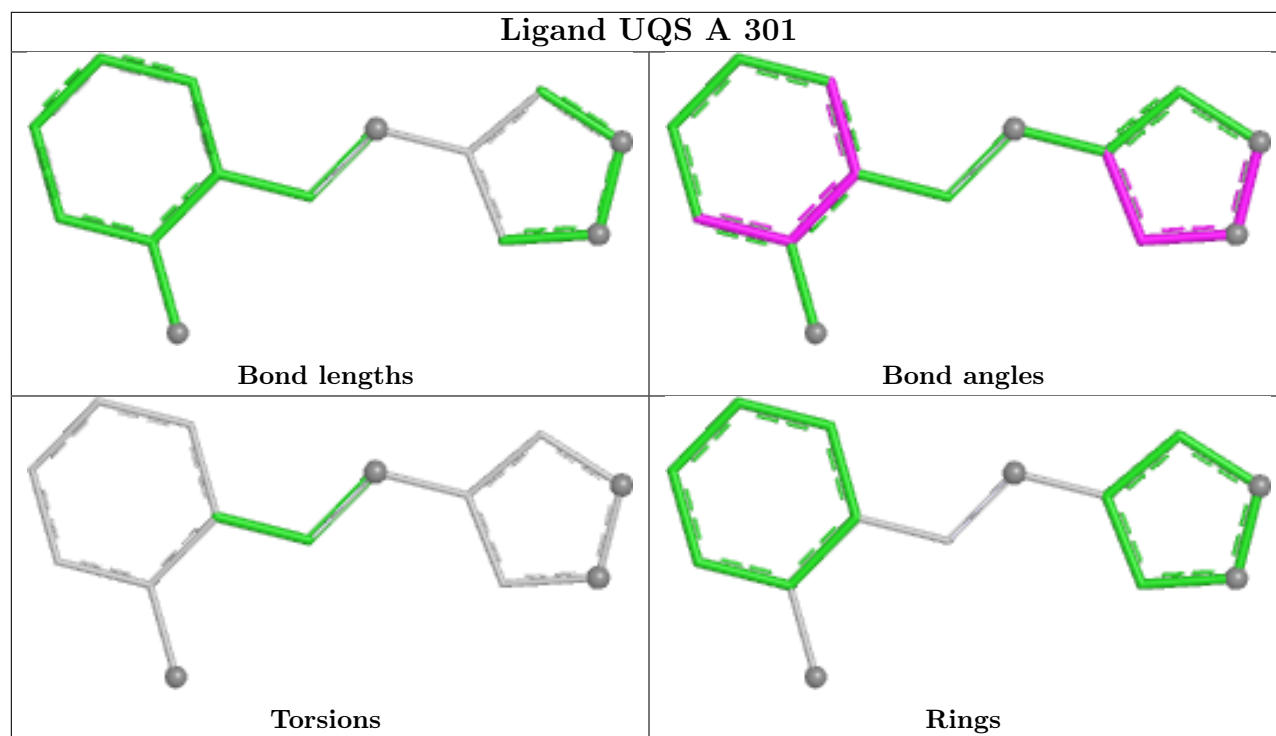
Mol	Chain	Res	Type	Atoms
5	D	307	GLY	O-C-CA-N
5	D	307	GLY	OXT-C-CA-N
3	C	304	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
4	D	306	DGL	OXT-C-CA-CB
4	D	306	DGL	O-C-CA-CB
3	B	302	EDO	O1-C1-C2-O2
3	C	302	EDO	O1-C1-C2-O2
4	D	306	DGL	CA-CB-CG-CD
3	C	303	EDO	O1-C1-C2-O2
3	D	302	EDO	O1-C1-C2-O2
3	D	303	EDO	O1-C1-C2-O2

There are no ring outliers.

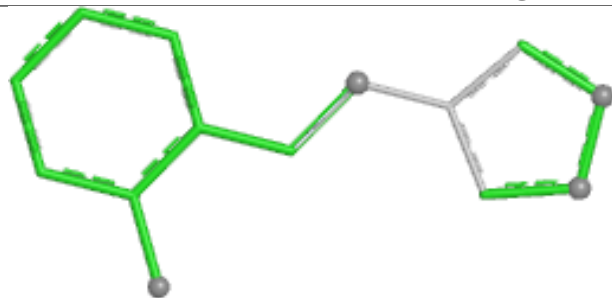
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	UQS	1	0
7	D	305	ALA	1	0
2	D	301	UQS	1	0

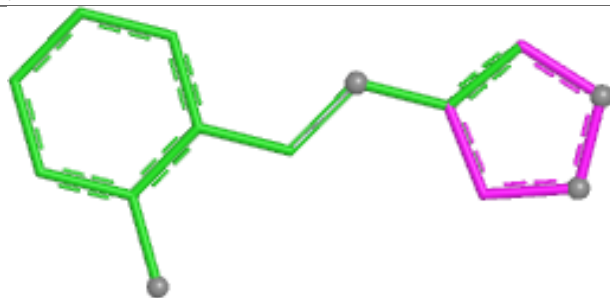
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



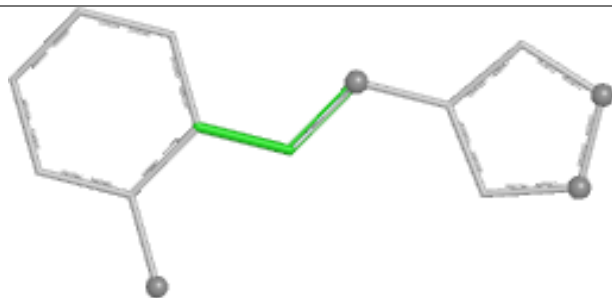
Ligand UQS C 301



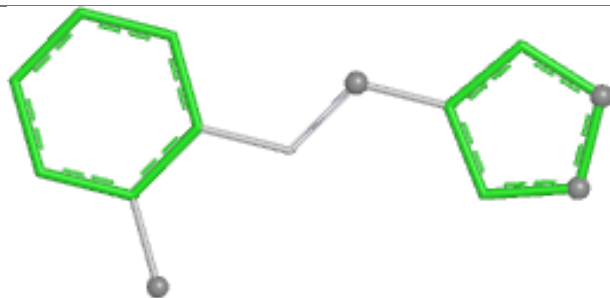
Bond lengths



Bond angles

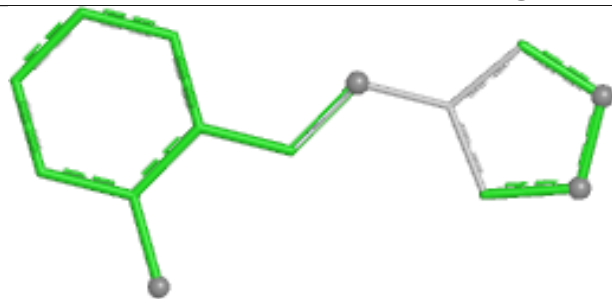


Torsions

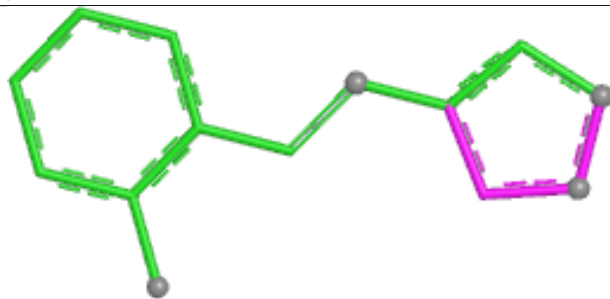


Rings

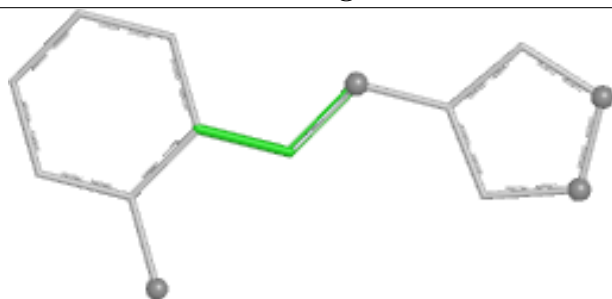
Ligand UQS D 301



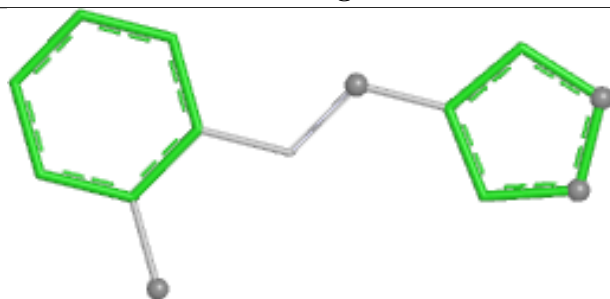
Bond lengths



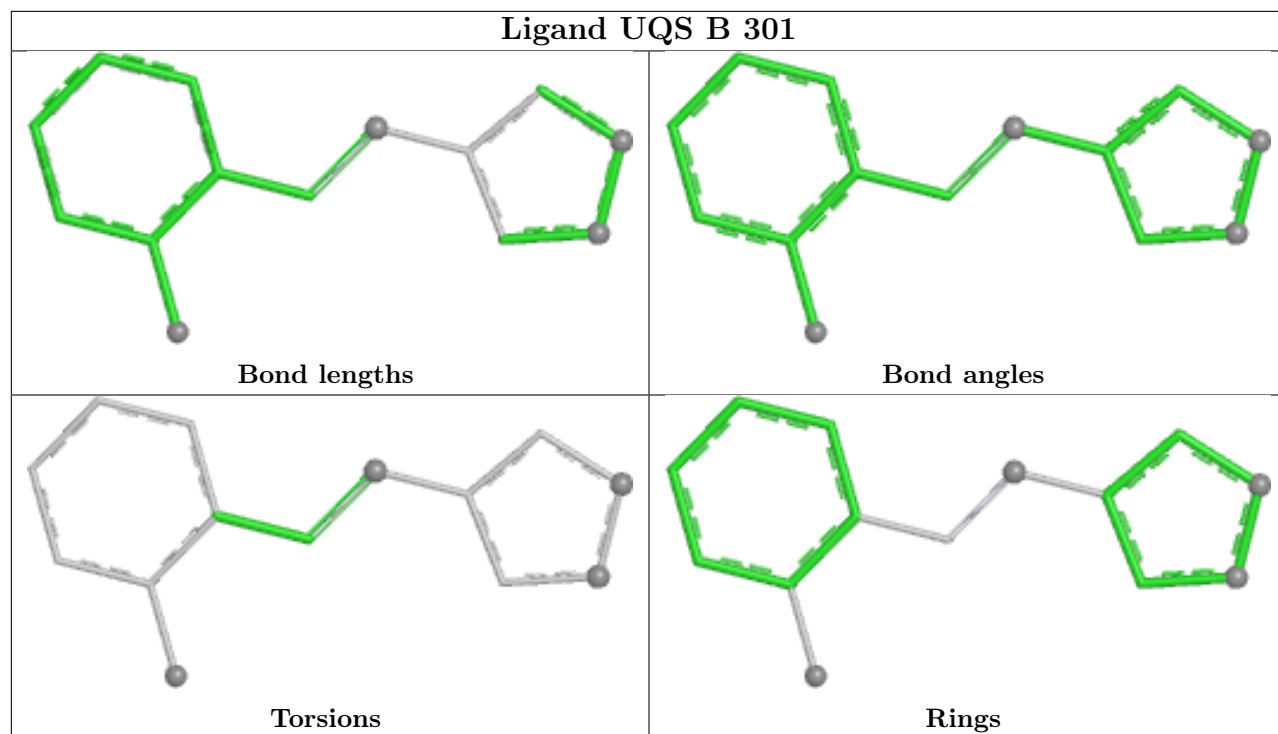
Bond angles



Torsions



Rings



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%)	2.28	53 (27%) 1 1	9, 56, 80, 104	31 (16%)
1	B	193/195 (98%)	0.96	24 (12%) 8 7	10, 51, 73, 107	10 (5%)
1	C	193/195 (98%)	1.14	30 (15%) 5 4	9, 55, 83, 130	9 (4%)
1	D	191/195 (97%)	1.18	31 (16%) 4 4	9, 44, 61, 81	26 (13%)
All	All	768/780 (98%)	1.39	138 (17%) 3 3	9, 51, 77, 130	76 (9%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273[A]	PHE	15.4
1	A	290	LEU	15.1
1	A	284	PRO	13.6
1	A	285	SER	12.7
1	A	278	ILE	12.4
1	A	283	ALA	11.9
1	A	289	SER	11.9
1	D	273[A]	PHE	11.8
1	A	275	PHE	11.5
1	C	273[A]	PHE	11.4
1	A	286	ILE	11.2
1	A	131	SER	10.9
1	A	279	ILE	10.7
1	A	288	LYS	10.6
1	A	287	MET	10.1
1	A	280	LYS	9.9
1	A	282	MET	9.7
1	D	111	GLY	9.5
1	D	275	PHE	9.3
1	A	277	HIS	9.3
1	B	273[A]	PHE	9.2

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Mol	Chain	Res	Type	RSRZ
1	D	274	ILE	9.1
1	A	276	GLU	8.9
1	B	275	PHE	8.5
1	C	116	ILE	8.1
1	B	108	ILE	8.0
1	D	112	ILE	7.6
1	A	281	ARG	7.3
1	A	111	GLY	7.3
1	B	276	GLU	7.1
1	D	108	ILE	7.1
1	B	277	HIS	7.0
1	D	277	HIS	6.6
1	B	111	GLY	6.6
1	A	109	LYS	6.3
1	A	108	ILE	6.2
1	D	109	LYS	5.9
1	C	106	ALA	5.9
1	D	276	GLU	5.9
1	B	106	ALA	5.7
1	C	209	VAL	5.6
1	D	187	THR	5.6
1	D	188	MET	5.6
1	D	125	ILE	5.5
1	B	109	LYS	5.4
1	C	108	ILE	5.3
1	A	112	ILE	5.2
1	D	295	ILE	5.2
1	D	186	ILE	5.0
1	C	188	MET	4.9
1	A	258	LEU	4.8
1	D	144	ASN	4.8
1	D	182	PHE	4.8
1	C	117	LEU	4.7
1	C	265	VAL	4.6
1	B	110	GLN	4.6
1	D	110	GLN	4.6
1	C	110	GLN	4.5
1	C	121	GLN	4.5
1	A	264	VAL	4.4
1	D	267	ILE	4.4
1	C	144[A]	ASN	4.4
1	C	197[A]	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	ASP	4.3
1	A	121	GLN	4.2
1	C	111	GLY	4.2
1	D	266	THR	4.2
1	D	113	ARG	4.1
1	D	298	VAL	4.1
1	A	117	LEU	4.1
1	A	122	ASP	4.1
1	A	124	LYS	4.1
1	D	294	THR	4.0
1	A	123	GLY	4.0
1	A	110	GLN	4.0
1	C	109	LYS	3.9
1	D	296	PRO	3.6
1	D	199	ILE	3.6
1	B	113	ARG	3.6
1	A	119	LYS	3.6
1	A	116	ILE	3.6
1	B	176	LYS	3.5
1	A	182	PHE	3.5
1	A	184	GLU	3.5
1	C	118	CYS	3.5
1	C	202	HIS	3.5
1	A	254	ILE	3.3
1	A	118	CYS	3.3
1	A	224	ASP	3.2
1	B	115	VAL	3.2
1	C	142	GLN	3.2
1	C	182	PHE	3.1
1	D	297	GLU	3.0
1	A	113	ARG	3.0
1	D	198	THR	2.9
1	D	197	ARG	2.9
1	B	287	MET	2.9
1	D	256	ASP	2.8
1	B	107	GLU	2.8
1	C	107	GLU	2.8
1	A	181	ALA	2.8
1	C	286	ILE	2.7
1	A	150	VAL	2.7
1	C	281	ARG	2.7
1	B	117	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	206	THR	2.7
1	A	298	VAL	2.6
1	A	263	THR	2.6
1	B	118	CYS	2.5
1	C	296	PRO	2.5
1	B	206	THR	2.4
1	A	178	LEU	2.4
1	A	267	ILE	2.4
1	B	278	ILE	2.3
1	A	153	ARG	2.3
1	D	141	VAL	2.3
1	B	182	PHE	2.3
1	C	287	MET	2.3
1	C	112	ILE	2.3
1	D	278	ILE	2.3
1	A	213	PHE	2.2
1	A	202	HIS	2.2
1	B	282	MET	2.2
1	A	297	GLU	2.2
1	B	123	GLY	2.2
1	A	257	ILE	2.1
1	D	262	GLY	2.1
1	A	295	ILE	2.1
1	B	112	ILE	2.1
1	B	286	ILE	2.1
1	C	284	PRO	2.1
1	C	143	ALA	2.1
1	A	159	LEU	2.1
1	A	125	ILE	2.1
1	B	186	ILE	2.0
1	C	201	MET	2.0
1	C	263	THR	2.0
1	C	285	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

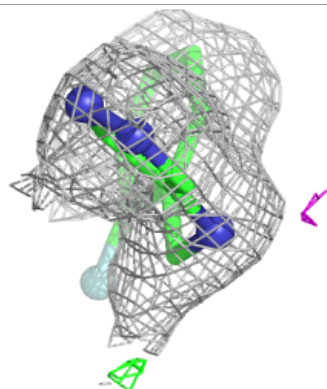
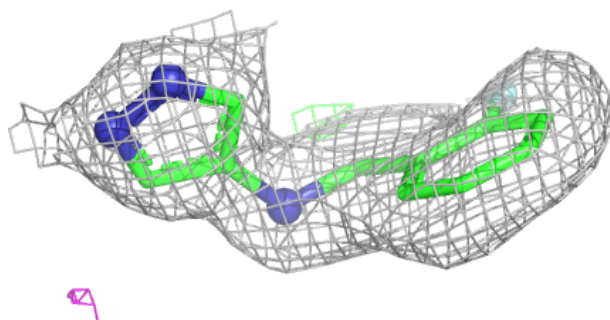
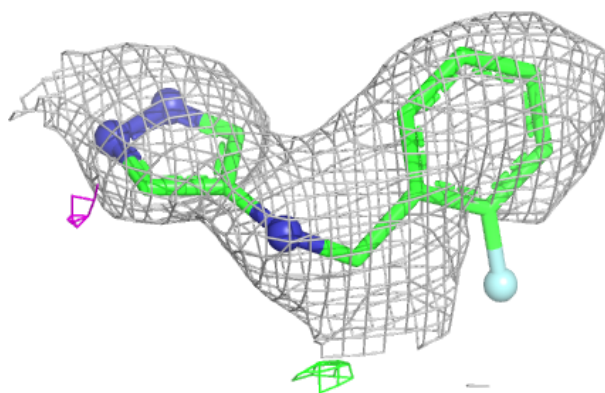
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	306	10/10	0.68	0.20	60,79,92,98	0
4	DGL	B	304	10/10	0.79	0.15	64,80,87,90	0
2	UQS	C	301	14/14	0.82	0.20	51,54,58,60	14
3	EDO	C	304	4/4	0.83	0.25	71,73,74,75	0
2	UQS	A	301	14/14	0.84	0.27	38,41,43,43	14
2	UQS	D	301	14/14	0.86	0.21	24,25,25,26	14
5	GLY	C	305	5/5	0.86	0.13	52,55,62,66	0
3	EDO	A	302	4/4	0.87	0.22	67,67,67,68	0
3	EDO	C	302	4/4	0.87	0.14	49,50,51,52	0
2	UQS	B	301	14/14	0.87	0.16	31,33,34,35	14
3	EDO	B	302	4/4	0.88	0.14	44,46,48,51	0
3	EDO	B	303	4/4	0.88	0.14	42,46,48,50	0
3	EDO	D	302	4/4	0.88	0.14	33,36,39,41	0
7	ALA	D	305	6/6	0.89	0.15	62,65,70,71	0
6	SO4	D	304	5/5	0.90	0.31	79,80,80,82	5
3	EDO	C	303	4/4	0.92	0.15	55,55,55,59	0
5	GLY	D	307	5/5	0.92	0.12	55,59,66,71	0
3	EDO	D	303	4/4	0.94	0.10	48,49,53,55	0

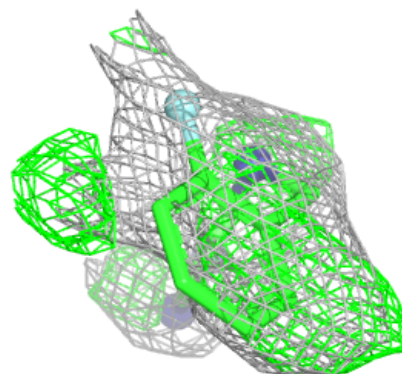
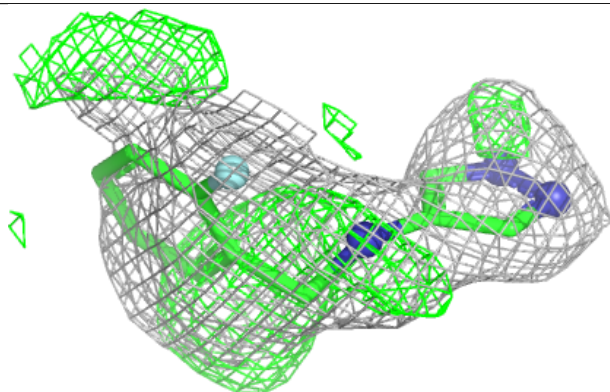
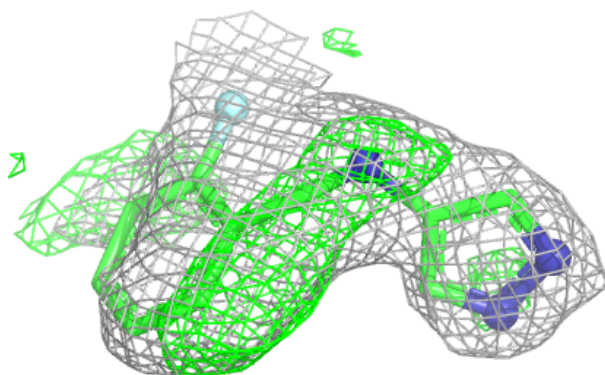
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQS 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)

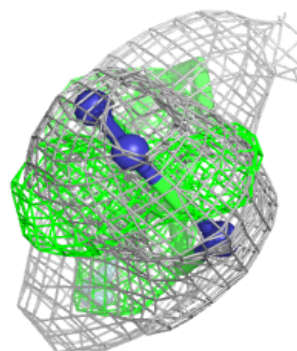
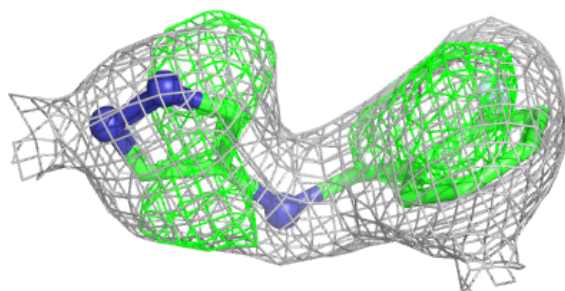
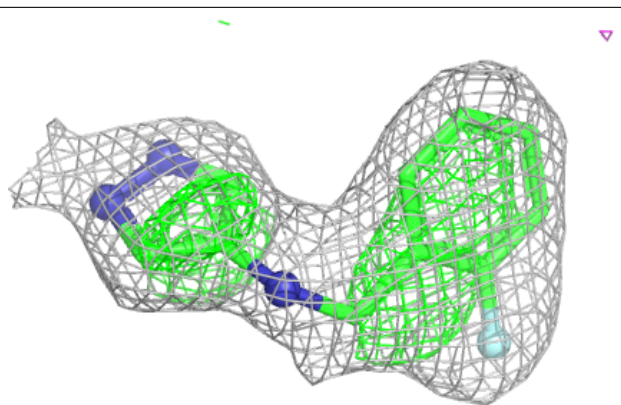
**Electron density around UQS A 301:**

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

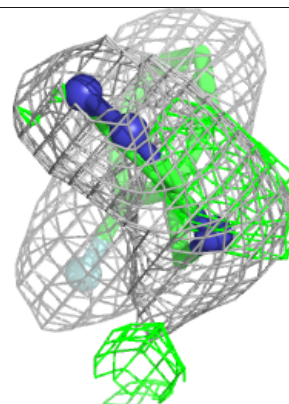
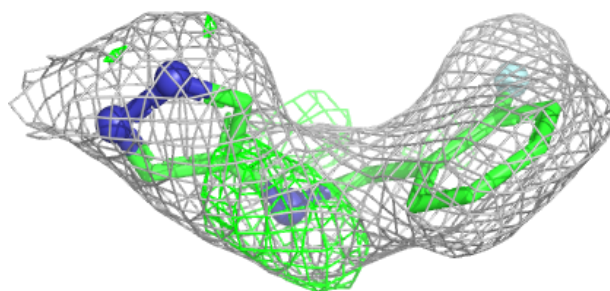
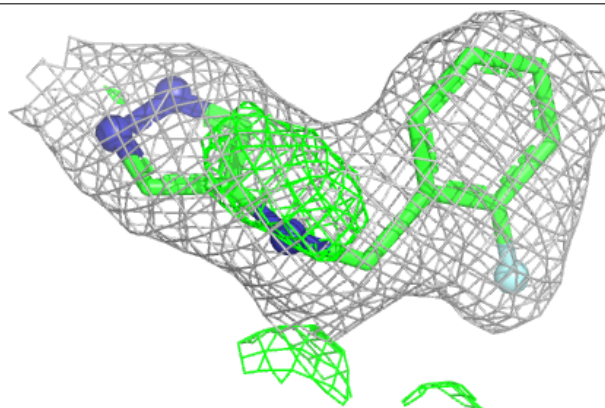


Electron density around UQS D 301:

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

**Electron density around UQS B 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.