



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 12:22 PM EDT

PDB ID : 7FSZ / pdb_00007fsz
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z3006151474
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.05 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

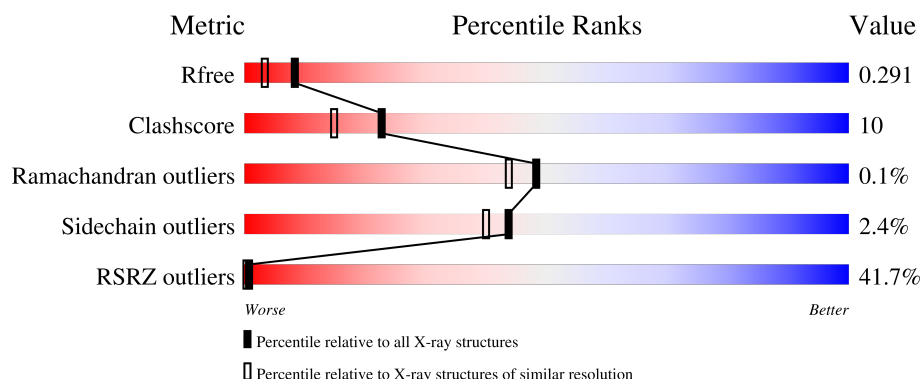
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	<div> <div>38%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
1	B	195	<div> <div>26%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	C	195	<div> <div>37%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
1	D	195	<div> <div>63%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>

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	LQ3	D	301	X	-	-	-
6	SO4	D	306	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6375 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:

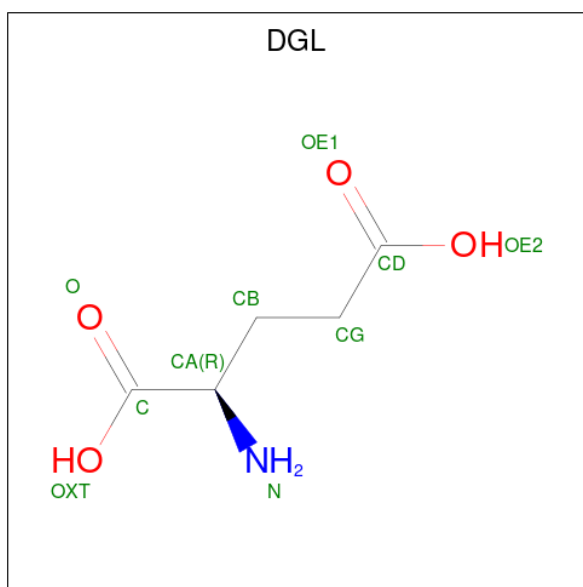
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



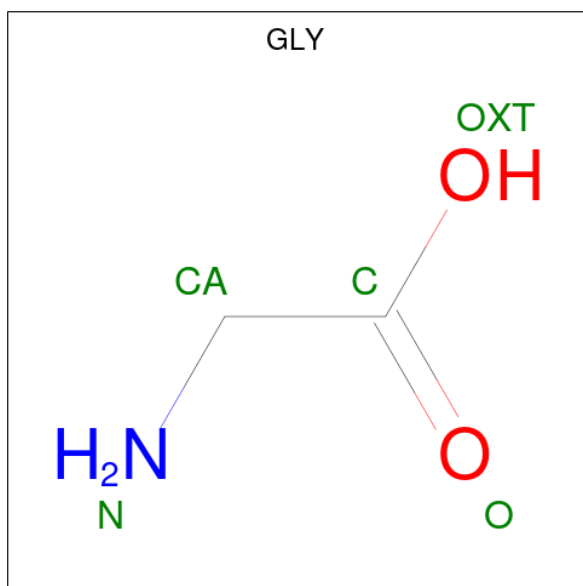
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is D-GLUTAMIC ACID (CCD ID: DGL) (formula: $C_5H_9NO_4$).



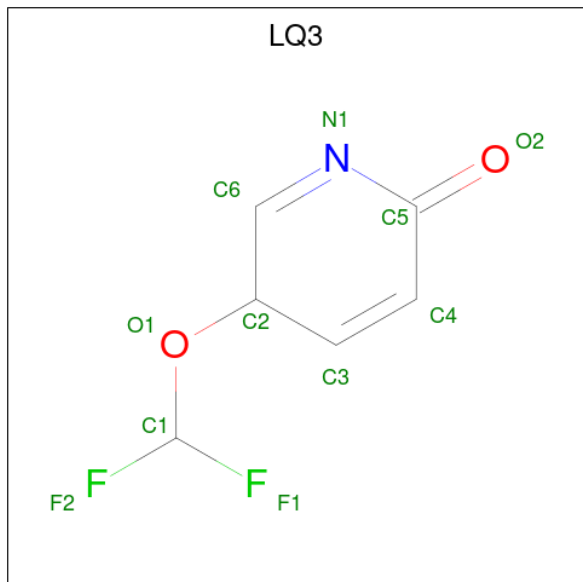
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



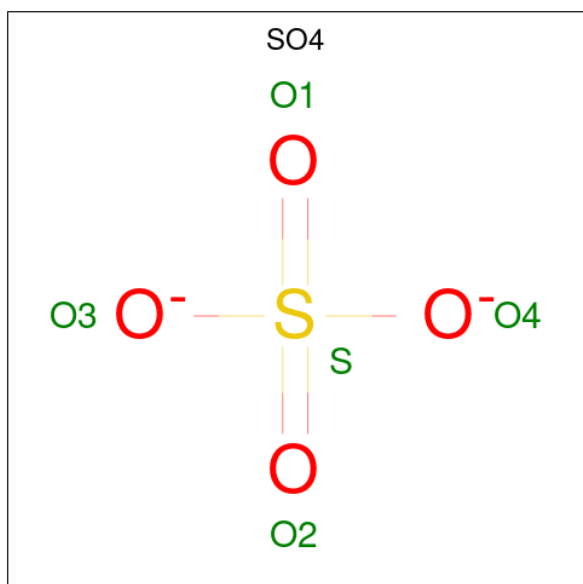
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			5	2	1	2		
4	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 5 is (5S)-5-(difluoromethoxy)pyridin-2(5H)-one (CCD ID: LQ3) (formula: $C_6H_5F_2NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	F	N	O	0	0
			11	6	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		

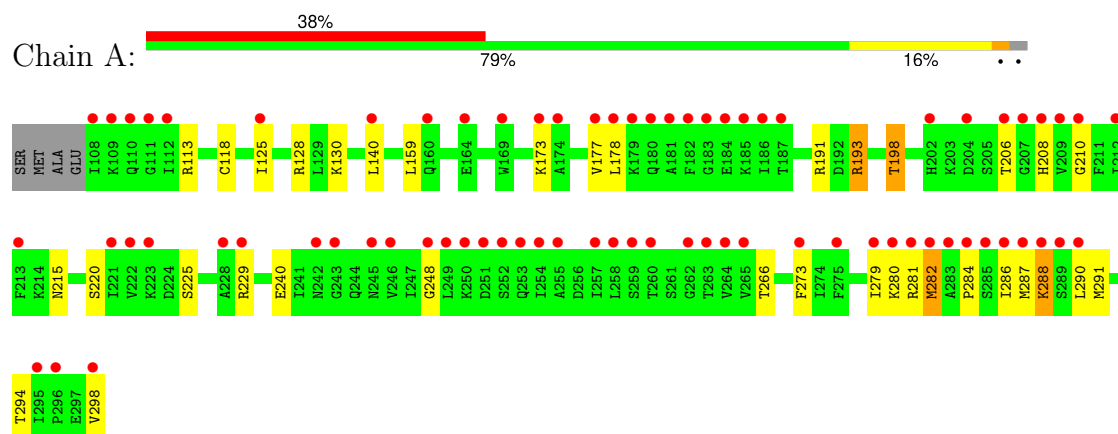
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	48	Total	O	0	0
			48	48		
7	B	102	Total	O	0	1
			102	102		
7	C	71	Total	O	0	1
			72	72		
7	D	94	Total	O	0	0
			94	94		

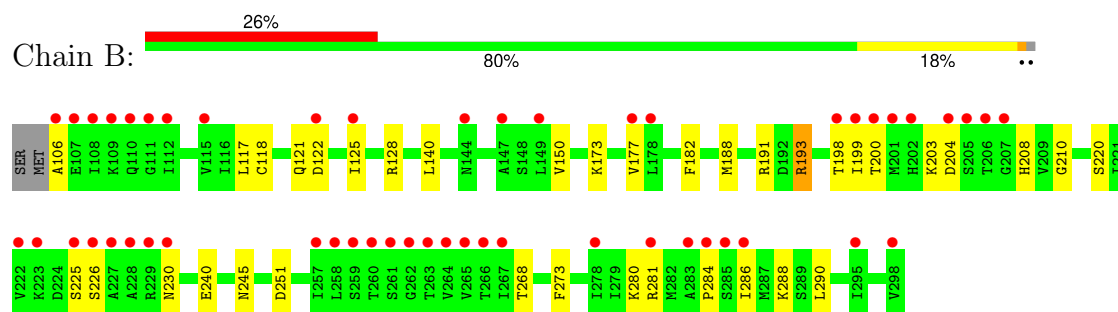
3 Residue-property plots [i](#)

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.

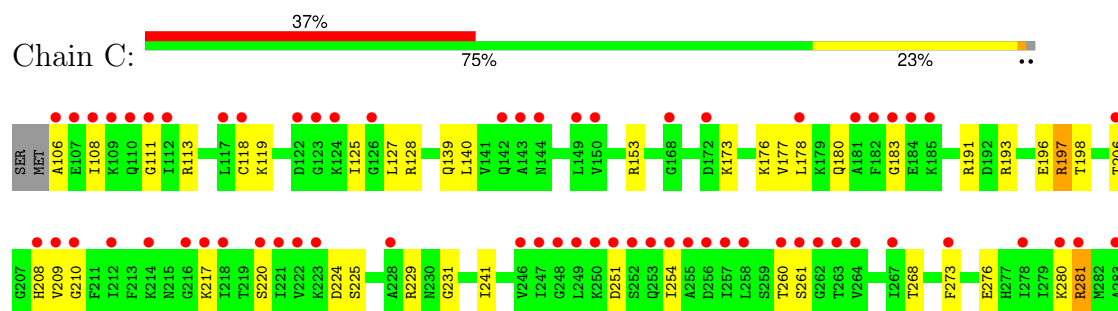
• Molecule 1: Syntenin-1

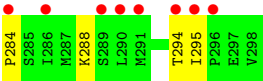


• Molecule 1: Syntenin-1

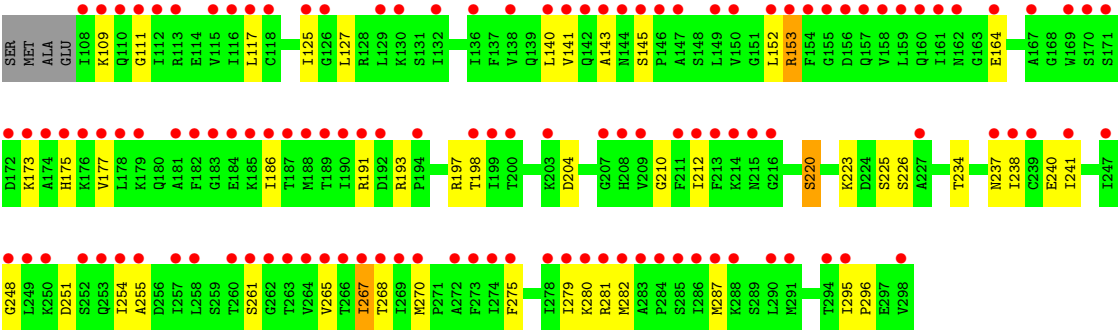


• Molecule 1: Syntenin-1





● 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	80.27Å 49.40Å 115.54Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	68.34 – 2.05 68.34 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.34-2.05) 91.6 (68.34-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.285 , 0.340 0.292 , 0.291	Depositor DCC
R_{free} test set	2797 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6375	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 36.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9364e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DGL, EDO, LQ3

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	0.42	0/1502	0.77	0/2019
1	B	0.42	0/1516	0.75	0/2038
1	C	0.41	0/1535	0.73	0/2063
1	D	0.49	0/1502	0.77	0/2019
All	All	0.43	0/6055	0.75	0/8139

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	4
1	B	0	3
1	C	0	9
1	D	0	4
All	All	0	20

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	191	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	229	ARG	Sidechain
1	B	128	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	191	ARG	Sidechain
1	B	193	ARG	Sidechain
1	C	111	GLY	Peptide
1	C	113	ARG	Sidechain
1	C	127	LEU	Peptide
1	C	128	ARG	Sidechain
1	C	191	ARG	Sidechain
1	C	193	ARG	Sidechain
1	C	197[A]	ARG	Sidechain
1	C	229	ARG	Sidechain
1	C	281	ARG	Sidechain
1	D	111	GLY	Peptide
1	D	153	ARG	Sidechain
1	D	191	ARG	Sidechain
1	D	281	ARG	Sidechain

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	34	0
1	B	1495	0	1541	30	0
1	C	1514	0	1558	28	0
1	D	1481	0	1530	40	1
2	A	4	0	6	0	0
2	B	8	0	12	0	0
2	C	12	0	18	2	0
2	D	8	0	12	1	0
3	B	10	0	7	0	0
3	D	10	0	7	0	0
4	C	5	0	2	0	0
4	D	5	0	2	0	0
5	D	11	0	0	0	0
6	D	15	0	0	3	1
7	A	48	0	0	6	0
7	B	102	0	0	10	1
7	C	72	0	0	9	0
7	D	94	0	0	16	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6375	0	6225	126	2

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 10.

All (126) 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:197:ARG:NH2	7:D:401:HOH:O	1.69	1.23
1:B:200:THR:O	1:B:230:ASN:ND2	1.97	0.98
1:C:206:THR:HG1	1:C:208:HIS:HD1	1.04	0.95
1:C:261:SER:HB2	7:C:434:HOH:O	1.71	0.89
1:C:251:ASP:OD1	7:C:401:HOH:O	1.94	0.85
1:A:248:GLY:O	1:A:288:LYS:HB3	1.77	0.83
1:A:206:THR:HG1	1:A:208:HIS:HD1	1.09	0.83
1:B:208:HIS:O	7:B:402:HOH:O	1.97	0.83
1:A:281:ARG:O	1:A:282:MET:SD	2.38	0.82
1:B:203:LYS:O	7:B:403:HOH:O	2.00	0.79
1:C:217:LYS:HD3	7:C:439:HOH:O	1.84	0.76
1:C:260:THR:OG1	7:C:402:HOH:O	2.01	0.76
1:A:273[B]:PHE:HD1	7:A:412:HOH:O	1.69	0.74
1:B:226:SER:N	7:B:401:HOH:O	1.91	0.73
1:D:204:ASP:OD2	7:D:403:HOH:O	2.07	0.73
1:D:197:ARG:NH1	7:D:408:HOH:O	2.20	0.72
1:D:255:ALA:O	7:D:404:HOH:O	2.08	0.71
1:A:125:ILE:HD11	1:A:178:LEU:HD13	1.73	0.70
1:C:118:CYS:HA	7:C:404:HOH:O	1.93	0.69
1:A:140:LEU:HD11	1:A:282:MET:CG	2.24	0.68
1:A:298:VAL:HG12	7:A:423:HOH:O	1.93	0.68
1:A:286:ILE:HG23	1:A:290:LEU:HD12	1.75	0.68
1:B:150:VAL:O	7:B:405:HOH:O	2.12	0.67
1:D:251:ASP:HB2	6:D:305:SO4:O2	1.95	0.67
1:B:204:ASP:OD2	7:B:404:HOH:O	2.11	0.66
1:A:281:ARG:HG2	1:B:122:ASP:HA	1.77	0.66
1:D:125:ILE:HD11	1:D:186:ILE:HD13	1.79	0.64
1:A:290:LEU:HD13	1:B:182:PHE:HB2	1.80	0.63
1:D:143:ALA:HB3	7:D:444:HOH:O	2.00	0.62
1:C:125:ILE:HD11	1:C:178:LEU:HD13	1.82	0.62
1:D:198:THR:HG22	1:D:268:THR:OG1	2.01	0.61
1:A:282:MET:HA	1:A:282:MET:CE	2.31	0.61
2:D:303:EDO:O1	7:D:405:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ILE:HD11	1:D:186:ILE:CD1	2.33	0.59
1:A:140:LEU:HD11	1:A:282:MET:HG3	1.85	0.59
1:B:204:ASP:HB2	7:B:427:HOH:O	2.01	0.59
1:C:276:GLU:OE1	7:C:403:HOH:O	2.16	0.58
1:D:164:GLU:HG3	7:D:436:HOH:O	2.02	0.58
1:A:140:LEU:HD11	1:A:282:MET:HG2	1.84	0.58
1:D:117:LEU:HD22	1:D:125:ILE:HG23	1.85	0.58
1:D:175:HIS:CE1	6:D:306:SO4:O1	2.56	0.58
1:A:281:ARG:HB3	1:B:121:GLN:O	2.04	0.57
1:D:226:SER:OG	6:D:304:SO4:O2	2.12	0.57
1:D:109:LYS:NZ	1:D:153:ARG:HH22	2.02	0.56
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.12	0.56
1:A:279:ILE:HG13	1:A:280:LYS:N	2.21	0.56
1:A:284:PRO:O	1:A:288:LYS:HG2	2.05	0.56
1:C:153:ARG:CZ	7:C:427:HOH:O	2.54	0.55
1:C:284:PRO:O	1:C:288:LYS:HG3	2.07	0.54
1:D:145:SER:HA	7:D:443:HOH:O	2.08	0.54
1:B:198:THR:HG22	1:B:268:THR:OG1	2.07	0.54
1:D:140:LEU:C	1:D:140:LEU:HD23	2.28	0.54
1:C:273[A]:PHE:CE2	2:C:302:EDO:H11	2.44	0.53
1:A:281:ARG:CG	1:B:122:ASP:HA	2.39	0.53
1:C:153:ARG:HD3	7:C:428:HOH:O	2.09	0.53
1:D:117:LEU:HD22	1:D:125:ILE:CG2	2.39	0.53
1:C:198:THR:HG22	1:C:268:THR:OG1	2.09	0.52
1:D:117:LEU:CD2	1:D:125:ILE:HG23	2.39	0.52
1:A:173:LYS:O	1:A:177:VAL:HG23	2.09	0.52
1:A:140:LEU:HD23	1:A:291:MET:CE	2.41	0.51
1:D:234:THR:OG1	7:D:406:HOH:O	2.19	0.51
1:B:117:LEU:HD22	1:B:125:ILE:CG2	2.40	0.51
1:B:173:LYS:O	1:B:177:VAL:HG23	2.10	0.51
1:A:130:LYS:HE2	1:A:281:ARG:HD2	1.93	0.50
1:A:198:THR:HG23	1:A:266:THR:HG23	1.93	0.50
1:C:173:LYS:O	1:C:177:VAL:HG23	2.12	0.50
1:C:280:LYS:O	1:C:281:ARG:HB2	2.12	0.49
1:D:173:LYS:O	1:D:177:VAL:HG23	2.12	0.49
1:B:251:ASP:OD1	7:B:407:HOH:O	2.20	0.49
1:C:273[A]:PHE:CD2	2:C:302:EDO:H11	2.47	0.49
1:D:282:MET:HE3	1:D:287:MET:HG3	1.95	0.49
1:D:223:LYS:HA	7:D:454:HOH:O	2.12	0.49
1:D:212:ILE:HD12	1:D:220:SER:OG	2.12	0.49
1:D:237:ASN:ND2	7:D:402:HOH:O	2.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:HB3	1:B:122:ASP:HA	1.95	0.48
1:A:206:THR:OG1	1:A:208:HIS:ND1	2.12	0.48
1:B:273[A]:PHE:HD2	7:B:486[A]:HOH:O	1.96	0.48
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.96	0.48
1:D:241:ILE:HD11	1:D:254:ILE:HG23	1.95	0.48
1:D:220:SER:HB3	7:D:465:HOH:O	2.14	0.47
1:B:284:PRO:O	1:B:288:LYS:HG3	2.15	0.47
1:D:248:GLY:O	7:D:407:HOH:O	2.20	0.47
1:A:215:ASN:HA	7:A:409:HOH:O	2.13	0.47
1:C:108:ILE:HD12	1:C:197[B]:ARG:HA	1.95	0.47
1:C:119:LYS:N	7:C:404:HOH:O	2.21	0.47
1:A:287:MET:O	1:A:291:MET:HB3	2.15	0.47
1:B:280:LYS:O	1:B:281:ARG:HB2	2.15	0.46
1:B:117:LEU:HD22	1:B:125:ILE:HG23	1.96	0.46
1:B:117:LEU:HD13	1:B:188:MET:CE	2.46	0.46
1:A:273[B]:PHE:CD1	7:A:412:HOH:O	2.55	0.46
1:B:117:LEU:CD2	1:B:125:ILE:HG23	2.47	0.45
1:D:295:ILE:HB	1:D:296:PRO:HD2	1.97	0.45
1:C:106:ALA:O	1:C:198:THR:HG21	2.15	0.45
1:D:140:LEU:HD23	1:D:141:VAL:C	2.37	0.44
1:C:139:GLN:NE2	1:C:280:LYS:O	2.47	0.44
1:D:261:SER:OG	1:D:265:VAL:HG22	2.17	0.44
1:B:210:GLY:HA3	1:B:225:SER:HB2	1.99	0.44
1:C:176:LYS:HE2	1:C:180:GLN:HE22	1.82	0.44
1:D:270:MET:SD	1:D:275:PHE:HA	2.57	0.44
1:A:281:ARG:CB	1:B:121:GLN:O	2.66	0.44
1:C:210:GLY:HA3	1:C:225:SER:HB2	1.98	0.43
1:D:279:ILE:HG13	7:D:422:HOH:O	2.18	0.43
1:B:193:ARG:NH1	1:B:240:GLU:OE1	2.51	0.43
1:A:210:GLY:HA3	1:A:225:SER:HB2	2.01	0.43
1:A:140:LEU:HD23	1:A:291:MET:HE1	2.00	0.43
1:D:193:ARG:NH1	1:D:240:GLU:OE1	2.52	0.42
1:A:128:ARG:HD2	7:A:437:HOH:O	2.19	0.42
1:D:140:LEU:HD23	1:D:141:VAL:N	2.34	0.42
1:C:210:GLY:HA3	1:C:225:SER:CB	2.50	0.42
1:D:204:ASP:HB2	7:D:467:HOH:O	2.18	0.42
1:D:127:LEU:HD21	1:D:152:LEU:HD13	2.02	0.42
1:B:106:ALA:O	1:B:198:THR:HG21	2.19	0.42
1:A:193:ARG:NH1	1:A:240:GLU:OE1	2.52	0.41
1:B:245:ASN:HB2	7:B:433:HOH:O	2.20	0.41
1:D:238:ILE:HG12	1:D:267:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:C	7:B:403:HOH:O	2.54	0.41
1:B:286:ILE:HG23	1:B:290:LEU:HD12	2.02	0.41
1:C:241:ILE:HD11	1:C:254:ILE:HG23	2.03	0.41
1:D:210:GLY:HA3	1:D:225:SER:CB	2.50	0.41
1:A:294:THR:HB	7:A:448:HOH:O	2.20	0.40
1:B:210:GLY:HA3	1:B:225:SER:CB	2.51	0.40
1:D:164:GLU:CG	7:D:436:HOH:O	2.66	0.40
1:A:159:LEU:HD22	1:C:231:GLY:HA3	2.03	0.40
1:C:108:ILE:CD1	1:C:196:GLU:O	2.70	0.40
1:C:294:THR:HG22	1:C:295:ILE:C	2.42	0.40
1:A:210:GLY:HA3	1:A:225:SER:CB	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ILE:O	6:D:306:SO4:O2[2_555]	2.04	0.16
7:B:437:HOH:O	7:D:461:HOH:O[1_455]	2.08	0.12

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%)	185 (97%)	5 (3%)	0	100	100
1	B	192/195 (98%)	187 (97%)	5 (3%)	0	100	100
1	C	194/195 (100%)	186 (96%)	7 (4%)	1 (0%)	25	17
1	D	190/195 (97%)	185 (97%)	5 (3%)	0	100	100
All	All	766/780 (98%)	743 (97%)	22 (3%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	GLY

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%)	161 (97%)	5 (3%)	36	31
1	B	167/168 (99%)	163 (98%)	4 (2%)	44	40
1	C	169/168 (101%)	165 (98%)	4 (2%)	44	40
1	D	166/168 (99%)	163 (98%)	3 (2%)	54	52
All	All	668/672 (99%)	652 (98%)	16 (2%)	44	40

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	CYS
1	A	198	THR
1	A	220	SER
1	A	282	MET
1	A	288	LYS
1	B	118	CYS
1	B	140	LEU
1	B	199	ILE
1	B	220	SER
1	C	140	LEU
1	C	209	VAL
1	C	220	SER
1	C	224	ASP
1	D	220	SER
1	D	267	ILE
1	D	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	180	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
4	GLY	D	308	-	4,4,4	1.04	0	3,4,4	1.02	0
2	EDO	C	302	-	3,3,3	0.16	0	2,2,2	0.16	0
2	EDO	B	301	-	3,3,3	0.58	0	2,2,2	0.35	0
6	SO4	D	306	-	4,4,4	0.31	0	6,6,6	0.15	0
6	SO4	D	304	-	4,4,4	0.31	0	6,6,6	0.12	0
2	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	B	302	-	3,3,3	0.25	0	2,2,2	0.61	0
6	SO4	D	305	-	4,4,4	0.33	0	6,6,6	0.18	0
2	EDO	C	303	-	3,3,3	0.45	0	2,2,2	0.61	0
2	EDO	A	301	-	3,3,3	0.22	0	2,2,2	0.09	0
2	EDO	D	303	-	3,3,3	0.21	0	2,2,2	0.54	0
3	DGL	B	303	-	8,9,9	1.11	1 (12%)	8,11,11	1.05	0
4	GLY	C	304	-	4,4,4	0.81	0	3,4,4	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DGL	D	307	-	8,9,9	1.17	1 (12%)	8,11,11	1.10	0
5	LQ3	D	301	-	10,11,11	6.72	4 (40%)	7,14,14	2.74	3 (42%)
2	EDO	C	301	-	3,3,3	0.22	0	2,2,2	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLY	D	308	-	-	0/2/2/2	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	D	302	-	-	0/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-
3	DGL	D	307	-	-	3/9/9/9	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	D	303	-	-	0/1/1/1	-
3	DGL	B	303	-	-	3/9/9/9	-
4	GLY	C	304	-	-	2/2/2/2	-
5	LQ3	D	301	-	1/1/3/6	1/3/14/14	0/1/1/1
2	EDO	C	301	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	LQ3	C6-N1	17.58	1.50	1.28
5	D	301	LQ3	C4-C3	8.88	1.50	1.33
5	D	301	LQ3	C5-N1	6.48	1.50	1.38
5	D	301	LQ3	C4-C5	3.78	1.52	1.44
3	B	303	DGL	O-C	2.21	1.28	1.22
3	D	307	DGL	O-C	2.06	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	301	LQ3	O1-C2-C6	5.97	123.20	109.28
5	D	301	LQ3	O2-C5-N1	2.92	124.13	119.37
5	D	301	LQ3	O2-C5-C4	-2.41	118.54	122.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	301	LQ3	C2

All (13) torsion outliers are listed below:

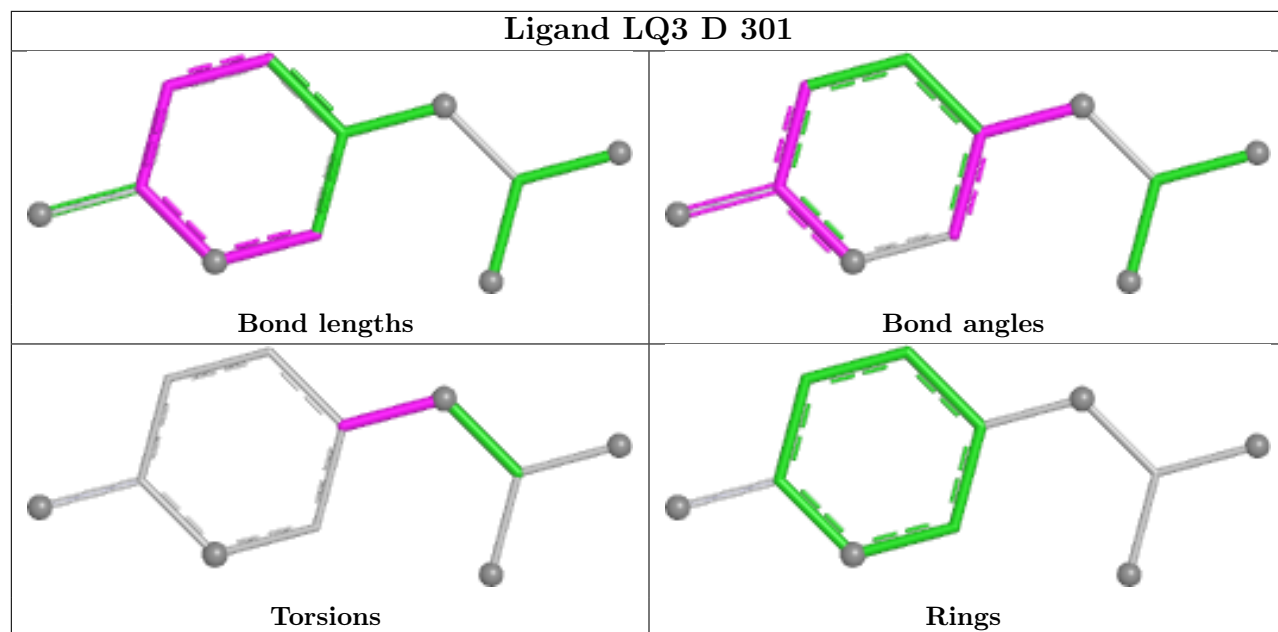
Mol	Chain	Res	Type	Atoms
4	C	304	GLY	O-C-CA-N
5	D	301	LQ3	C3-C2-O1-C1
4	C	304	GLY	OXT-C-CA-N
2	A	301	EDO	O1-C1-C2-O2
2	C	303	EDO	O1-C1-C2-O2
2	B	302	EDO	O1-C1-C2-O2
3	B	303	DGL	C-CA-CB-CG
3	B	303	DGL	N-CA-CB-CG
3	D	307	DGL	OXT-C-CA-CB
2	C	301	EDO	O1-C1-C2-O2
3	D	307	DGL	O-C-CA-CB
3	B	303	DGL	OE2-CD-CG-CB
3	D	307	DGL	CA-CB-CG-CD

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	EDO	2	0
6	D	306	SO4	1	1
6	D	304	SO4	1	0
6	D	305	SO4	1	0
2	D	303	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%)	1.77	74 (38%) 1 0	16, 49, 92, 131	1 (0%)
1	B	193/195 (98%)	1.35	51 (26%) 2 1	14, 46, 73, 95	1 (0%)
1	C	193/195 (98%)	1.83	72 (37%) 1 0	15, 51, 79, 121	3 (1%)
1	D	191/195 (97%)	2.67	123 (64%) 0 0	17, 50, 79, 113	1 (0%)
All	All	768/780 (98%)	1.90	320 (41%) 1 0	14, 49, 81, 131	6 (0%)

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	182	PHE	7.8
1	D	190	ILE	6.4
1	A	286	ILE	6.3
1	D	177	VAL	6.2
1	A	283	ALA	6.2
1	D	178	LEU	6.1
1	B	264	VAL	6.0
1	A	290	LEU	6.0
1	D	117	LEU	6.0
1	A	287	MET	6.0
1	A	182	PHE	6.0
1	C	110	GLN	5.9
1	B	106	ALA	5.9
1	A	282	MET	5.8
1	D	111	GLY	5.5
1	D	249	LEU	5.3
1	C	108	ILE	5.3
1	A	284	PRO	5.2
1	D	213	PHE	5.2
1	C	106	ALA	5.1
1	D	267	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	254	ILE	5.0
1	D	265	VAL	5.0
1	D	207	GLY	5.0
1	D	149	LEU	4.9
1	D	284	PRO	4.9
1	C	249	LEU	4.9
1	A	108	ILE	4.8
1	A	280	LYS	4.7
1	D	108	ILE	4.7
1	D	150	VAL	4.6
1	D	288	LYS	4.6
1	D	263	THR	4.6
1	D	158	VAL	4.6
1	B	227	ALA	4.6
1	D	248	GLY	4.5
1	D	153	ARG	4.5
1	C	182	PHE	4.4
1	D	161	ILE	4.3
1	B	263	THR	4.3
1	D	186	ILE	4.3
1	D	154	PHE	4.3
1	D	183	GLY	4.2
1	C	112	ILE	4.2
1	D	152	LEU	4.2
1	C	143	ALA	4.2
1	D	112	ILE	4.2
1	D	116	ILE	4.2
1	D	141	VAL	4.2
1	D	125	ILE	4.1
1	D	212	ILE	4.1
1	D	269	ILE	4.1
1	D	275	PHE	4.1
1	D	174	ALA	4.1
1	A	298	VAL	4.1
1	C	212	ILE	4.1
1	A	281	ARG	4.0
1	A	285	SER	4.0
1	C	123	GLY	4.0
1	B	281	ARG	3.9
1	D	286	ILE	3.9
1	A	109	LYS	3.9
1	B	125	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	115	VAL	3.9
1	A	288	LYS	3.8
1	A	202	HIS	3.8
1	D	273[A]	PHE	3.8
1	D	216	GLY	3.8
1	B	205	SER	3.8
1	D	189	THR	3.7
1	D	209	VAL	3.7
1	C	184	GLU	3.7
1	D	113	ARG	3.7
1	A	279	ILE	3.7
1	A	210	GLY	3.7
1	D	155	GLY	3.7
1	C	296	PRO	3.6
1	D	171	SER	3.6
1	C	258	LEU	3.6
1	D	283	ALA	3.6
1	D	175	HIS	3.6
1	B	199	ILE	3.6
1	A	206	THR	3.6
1	C	263	THR	3.6
1	C	109	LYS	3.6
1	B	108	ILE	3.5
1	C	251	ASP	3.5
1	D	260	THR	3.5
1	B	109	LYS	3.5
1	A	253	GLN	3.5
1	D	169	TRP	3.5
1	D	241	ILE	3.5
1	D	181	ALA	3.5
1	C	111	GLY	3.5
1	A	204	ASP	3.4
1	D	147	ALA	3.4
1	A	177	VAL	3.4
1	D	109	LYS	3.4
1	D	238	ILE	3.4
1	D	257	ILE	3.4
1	A	295	ILE	3.3
1	B	111	GLY	3.3
1	B	207	GLY	3.3
1	C	118	CYS	3.3
1	B	228	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	202	HIS	3.3
1	B	149	LEU	3.3
1	C	117	LEU	3.3
1	D	118	CYS	3.2
1	D	298	VAL	3.2
1	D	136	ILE	3.2
1	C	273[A]	PHE	3.2
1	B	261	SER	3.2
1	B	262	GLY	3.2
1	C	223	LYS	3.2
1	A	259	SER	3.1
1	C	286	ILE	3.1
1	A	222	VAL	3.1
1	B	206	THR	3.1
1	A	140	LEU	3.1
1	A	112	ILE	3.1
1	B	110	GLN	3.1
1	B	265	VAL	3.1
1	C	150	VAL	3.1
1	D	179	LYS	3.1
1	C	262	GLY	3.1
1	A	184	GLU	3.1
1	D	262	GLY	3.0
1	D	191	ARG	3.0
1	B	225	SER	3.0
1	C	228	ALA	3.0
1	A	257	ILE	3.0
1	B	112	ILE	3.0
1	D	214	LYS	3.0
1	A	262	GLY	3.0
1	B	115	VAL	3.0
1	D	199	ILE	3.0
1	D	294	THR	3.0
1	C	216	GLY	3.0
1	D	110	GLN	3.0
1	D	160	GLN	3.0
1	D	290	LEU	3.0
1	C	254	ILE	2.9
1	D	247	ILE	2.9
1	B	226	SER	2.9
1	C	206	THR	2.9
1	C	185	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	172	ASP	2.9
1	C	257	ILE	2.9
1	D	162	ASN	2.9
1	A	185	LYS	2.9
1	D	140	LEU	2.9
1	B	283	ALA	2.9
1	D	156	ASP	2.9
1	B	222	VAL	2.9
1	D	287	MET	2.8
1	D	261	SER	2.8
1	A	242	ASN	2.8
1	D	268	THR	2.8
1	C	264	VAL	2.8
1	D	280	LYS	2.8
1	A	263	THR	2.8
1	D	200	THR	2.8
1	D	237	ASN	2.8
1	B	200	THR	2.8
1	B	107	GLU	2.8
1	D	194	PRO	2.7
1	A	249	LEU	2.7
1	C	214	LYS	2.7
1	D	143	ALA	2.7
1	D	198	THR	2.7
1	D	279	ILE	2.7
1	C	253	GLN	2.7
1	B	284	PRO	2.7
1	C	290	LEU	2.7
1	A	289	SER	2.7
1	C	220	SER	2.7
1	D	252	SER	2.7
1	B	298	VAL	2.7
1	C	283	ALA	2.7
1	B	229	ARG	2.7
1	B	258	LEU	2.7
1	C	261	SER	2.7
1	C	181	ALA	2.7
1	C	209	VAL	2.7
1	C	142	GLN	2.7
1	D	157	GLN	2.7
1	A	251	ASP	2.7
1	B	257	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	159	LEU	2.6
1	D	258	LEU	2.6
1	D	285	SER	2.6
1	C	126	GLY	2.6
1	A	260	THR	2.6
1	B	198	THR	2.6
1	B	266	THR	2.6
1	A	179	LYS	2.6
1	C	267	ILE	2.6
1	D	282	MET	2.6
1	C	252	SER	2.6
1	A	228	ALA	2.6
1	A	243	GLY	2.6
1	D	208	HIS	2.6
1	D	272	ALA	2.6
1	D	187	THR	2.6
1	D	291	MET	2.6
1	C	107	GLU	2.6
1	C	183	GLY	2.6
1	C	124	LYS	2.6
1	D	185	LYS	2.6
1	C	178	LEU	2.6
1	A	207	GLY	2.5
1	D	126	GLY	2.5
1	D	176	LYS	2.5
1	B	295	ILE	2.5
1	D	164	GLU	2.5
1	C	149	LEU	2.5
1	C	255	ALA	2.5
1	D	167	ALA	2.5
1	C	222	VAL	2.5
1	D	184	GLU	2.5
1	A	250	LYS	2.5
1	C	122	ASP	2.5
1	D	270	MET	2.5
1	D	264	VAL	2.5
1	D	250	LYS	2.5
1	C	168	GLY	2.5
1	A	258	LEU	2.5
1	C	144[A]	ASN	2.5
1	C	278	ILE	2.4
1	C	295	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	132	ILE	2.4
1	A	265	VAL	2.4
1	C	246	VAL	2.4
1	A	296	PRO	2.4
1	D	203	LYS	2.4
1	A	212	ILE	2.4
1	D	278	ILE	2.4
1	C	210	GLY	2.4
1	D	281	ARG	2.4
1	D	144	ASN	2.4
1	D	227	ALA	2.4
1	D	255	ALA	2.4
1	B	177	VAL	2.4
1	C	284	PRO	2.4
1	C	289	SER	2.4
1	D	145	SER	2.4
1	A	186	ILE	2.4
1	C	218	ILE	2.4
1	A	252	SER	2.4
1	C	281	ARG	2.4
1	A	110	GLN	2.4
1	A	180	GLN	2.4
1	A	183	GLY	2.4
1	C	248	GLY	2.4
1	A	254	ILE	2.4
1	C	250	LYS	2.3
1	D	146	PRO	2.3
1	A	248	GLY	2.3
1	A	273[A]	PHE	2.3
1	A	164	GLU	2.3
1	A	221	ILE	2.3
1	C	247	ILE	2.3
1	C	260	THR	2.3
1	D	239	CYS	2.3
1	C	291	MET	2.3
1	B	285	SER	2.3
1	A	213	PHE	2.3
1	A	223	LYS	2.3
1	B	286	ILE	2.3
1	C	280	LYS	2.3
1	D	274	ILE	2.3
1	D	266	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	169	TRP	2.3
1	B	230	ASN	2.3
1	D	173	LYS	2.2
1	D	211	PHE	2.2
1	D	129	LEU	2.2
1	D	188	MET	2.2
1	B	259	SER	2.2
1	A	245	ASN	2.2
1	C	221	ILE	2.2
1	D	138	VAL	2.2
1	D	142	GLN	2.2
1	A	174	ALA	2.2
1	D	170	SER	2.2
1	B	122	ASP	2.2
1	A	111	GLY	2.2
1	A	275	PHE	2.1
1	A	125	ILE	2.1
1	B	267	ILE	2.1
1	B	260	THR	2.1
1	B	144	ASN	2.1
1	D	215	ASN	2.1
1	A	246	VAL	2.1
1	A	173	LYS	2.1
1	B	278	ILE	2.1
1	C	172	ASP	2.1
1	D	192	ASP	2.1
1	A	181	ALA	2.1
1	B	201	MET	2.1
1	A	160	GLN	2.1
1	B	223	LYS	2.1
1	C	217	LYS	2.1
1	D	130	LYS	2.1
1	B	204	ASP	2.1
1	C	256	ASP	2.1
1	B	178	LEU	2.1
1	A	187	THR	2.1
1	C	294	THR	2.1
1	A	255	ALA	2.0
1	B	147	ALA	2.0
1	A	209	VAL	2.0
1	A	264	VAL	2.0
1	A	208	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	2.0
1	D	253	GLN	2.0
1	D	295	ILE	2.0
1	A	229	ARG	2.0
1	C	208	HIS	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 monosaccharides in this entry.

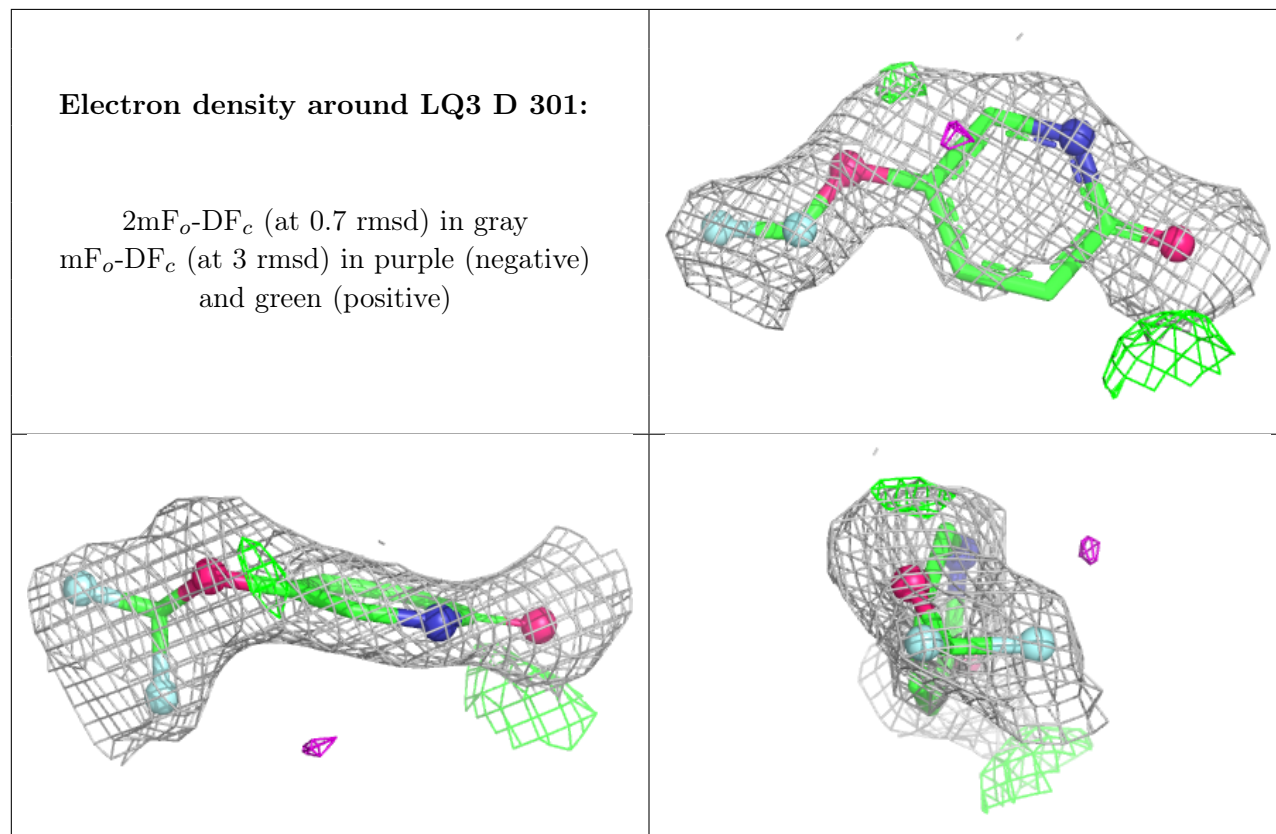
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	305	5/5	0.46	0.20	84,98,116,120	0
4	GLY	D	308	5/5	0.71	0.19	56,63,66,68	0
3	DGL	B	303	10/10	0.72	0.18	46,59,66,71	0
3	DGL	D	307	10/10	0.72	0.19	48,80,96,97	0
2	EDO	C	301	4/4	0.73	0.21	45,51,51,54	0
6	SO4	D	306	5/5	0.74	0.23	128,129,141,141	0
6	SO4	D	304	5/5	0.76	0.15	85,108,127,130	0
4	GLY	C	304	5/5	0.78	0.15	50,60,61,63	0
5	LQ3	D	301	11/11	0.81	0.20	39,42,51,51	11
2	EDO	C	303	4/4	0.82	0.23	52,58,59,62	0
2	EDO	D	303	4/4	0.89	0.14	40,41,44,45	0
2	EDO	C	302	4/4	0.89	0.15	37,42,46,46	0
2	EDO	B	301	4/4	0.89	0.16	32,39,40,57	0
2	EDO	D	302	4/4	0.91	0.12	34,34,35,37	0
2	EDO	A	301	4/4	0.93	0.10	42,47,48,50	0
2	EDO	B	302	4/4	0.95	0.08	29,34,35,38	0

The following is a graphical depiction of the model fit to experimental electron density of all

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



6.5 Other polymers [i](#)

There are no such residues in this entry.