



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:42 PM UTC

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 : 4-5-2 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

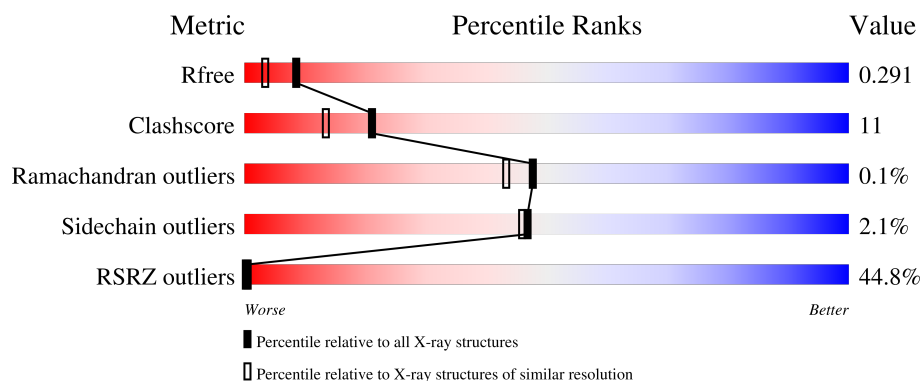
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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	45% 77% 18% ...
1	B	195	27% 78% 20% ..
1	C	195	40% 74% 24% ..
1	D	195	65% 72% 25% ..

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.

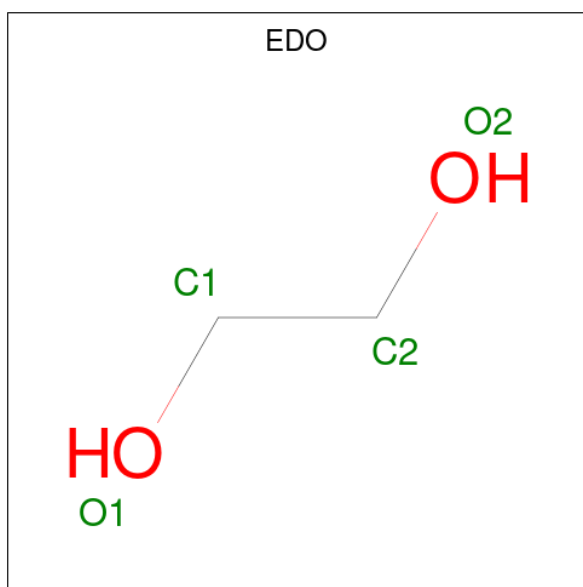
- Molecule 1 is a protein called Syntenin-1.

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:

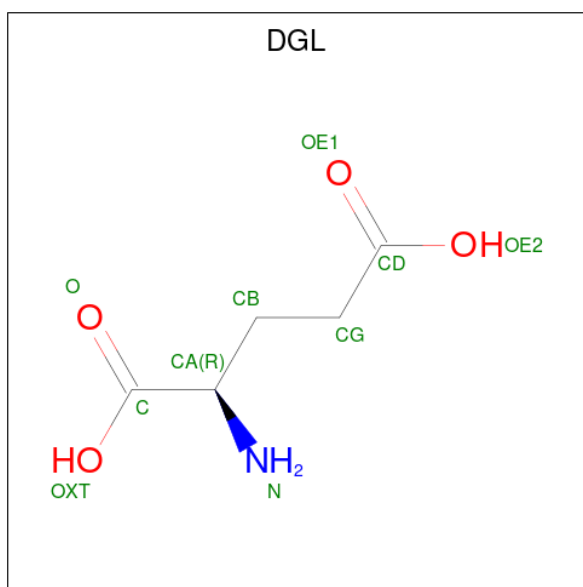
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	SER	-	expression tag	UNP O00560
A	105	MET	-	expression tag	UNP O00560
B	104	SER	-	expression tag	UNP O00560
B	105	MET	-	expression tag	UNP O00560
C	104	SER	-	expression tag	UNP O00560
C	105	MET	-	expression tag	UNP O00560
D	104	SER	-	expression tag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

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



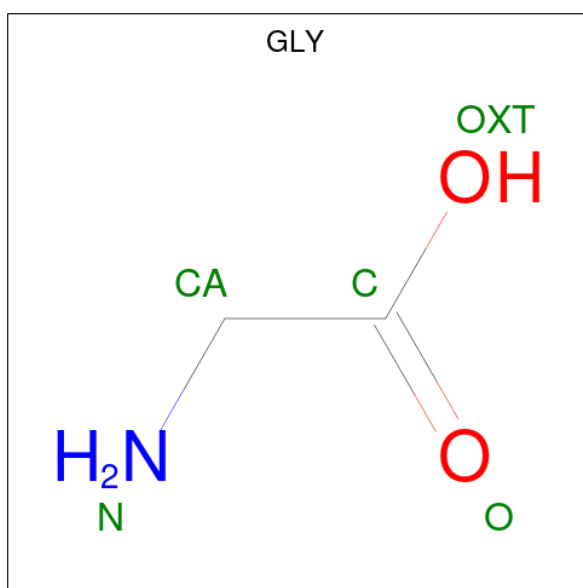
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

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



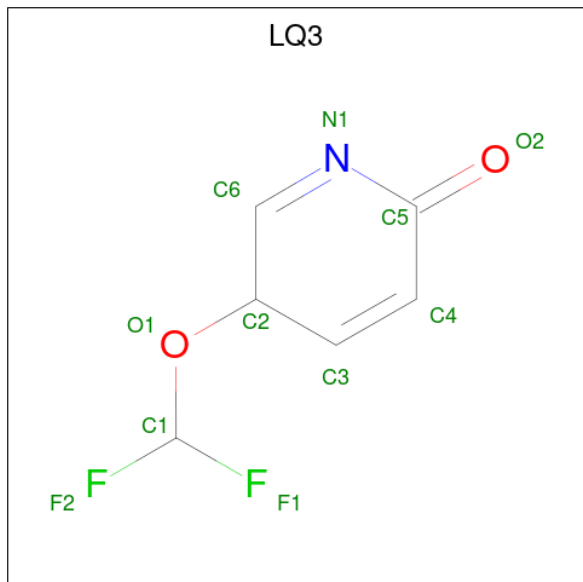
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



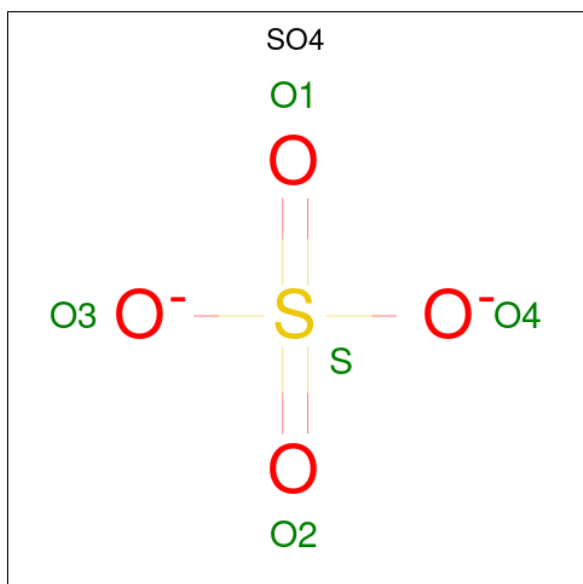
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			5	2	1	2		
4	D	1	Total	C	N	O	0	0
			5	2	1	2		

- 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		

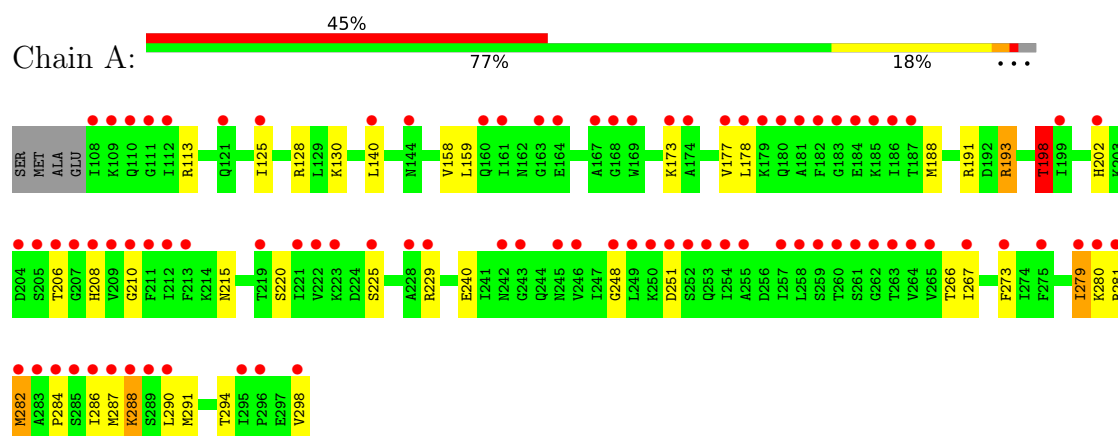
- Molecule 7 is water.

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		

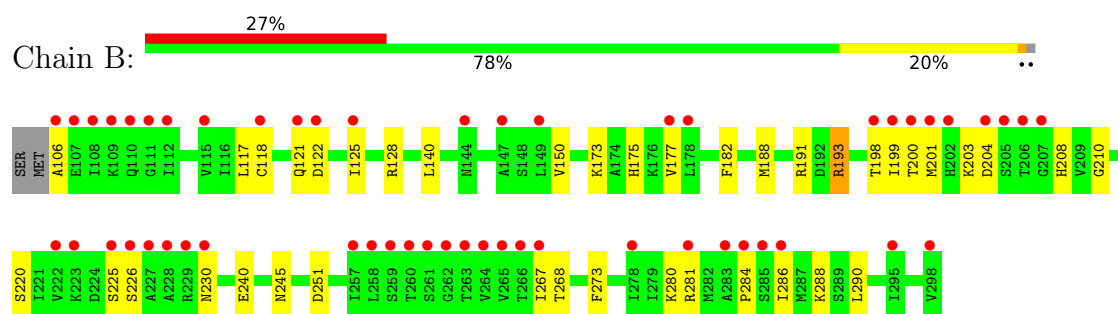
3 Residue-property plots

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.

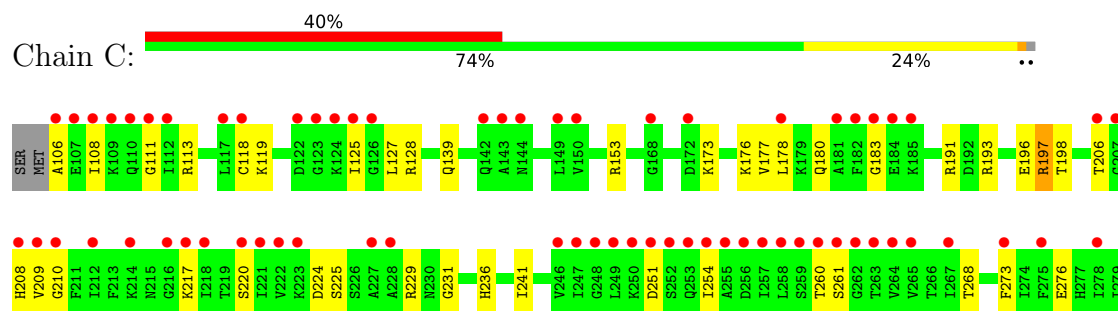
• Molecule 1: Syntenin-1

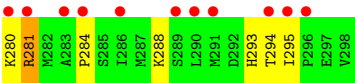


• Molecule 1: Syntenin-1

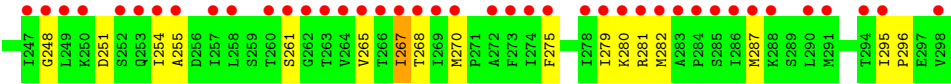
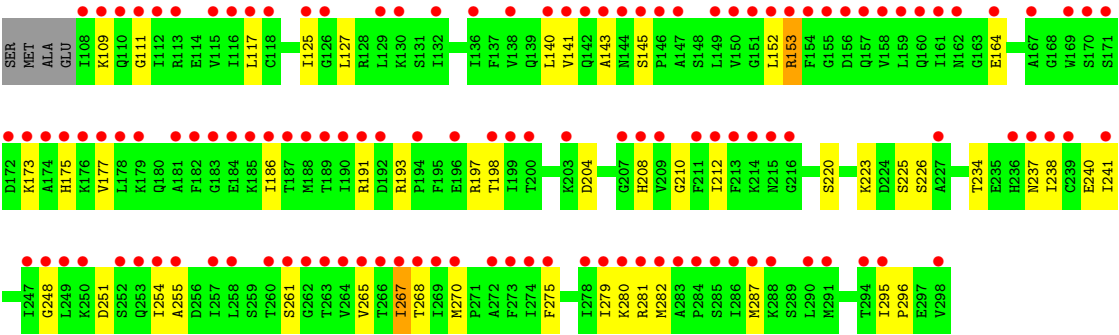


• Molecule 1: Syntenin-1





● 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	4037 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	1/1502 (0.1%)	1.06	2/2019 (0.1%)
1	B	0.66	1/1516 (0.1%)	1.04	0/2038
1	C	0.64	1/1535 (0.1%)	1.03	2/2063 (0.1%)
1	D	0.68	1/1502 (0.1%)	1.08	0/2019
All	All	0.66	4/6055 (0.1%)	1.05	4/8139 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	HIS	CE1-NE2	6.13	1.38	1.32
1	A	202	HIS	CE1-NE2	5.28	1.37	1.32
1	D	208	HIS	CE1-NE2	5.20	1.37	1.32
1	C	236	HIS	CE1-NE2	5.10	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	THR	CA-CB-OG1	-7.08	98.98	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ILE	CB-CA-C	-5.52	104.98	111.94
1	C	293	HIS	CA-C-N	5.02	127.83	120.71
1	C	293	HIS	C-N-CA	5.02	127.83	120.71

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
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	40	0
1	B	1495	0	1541	33	0
1	C	1514	0	1558	28	0
1	D	1481	0	1530	40	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	0
7	B	102	0	0	11	1
7	C	72	0	0	9	0
7	D	94	0	0	16	1
All	All	6375	0	6225	135	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 11.

All (135) 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	1.05	0.94
1:A:282:MET:HE3	1:A:282:MET:HA	1.51	0.91
1:C:261:SER:HB2	7:C:434:HOH:O	1.71	0.89
1:B:117:LEU:HD13	1:B:188:MET:HE3	1.53	0.87
1:C:251:ASP:OD1	7:C:401:HOH:O	1.94	0.85
1:A:206:THR:HG1	1:A:208:HIS:HD1	1.07	0.84
1:A:248:GLY:O	1:A:288:LYS:HB3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:303:EDO:O1	7:D:405:HOH:O	2.16	0.61
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:D:140:LEU:C	1:D:140:LEU:HD23	2.28	0.58
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:284:PRO:O	1:A:288:LYS:HG2	2.05	0.56
1:A:282:MET:HE2	7:B:466:HOH:O	2.05	0.55
1:A:279:ILE:HG13	1:A:280:LYS:N	2.21	0.55
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.88	0.55
1:A:282:MET:HA	1:A:282:MET:CE	2.31	0.55
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:C:273[A]:PHE:CE2	2:C:302:EDO:H11	2.44	0.53
1:A:158:VAL:CG1	1:A:188:MET:HE2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:140:LEU:HD23	1:D:141:VAL:C	2.37	0.50
1:C:173:LYS:O	1:C:177:VAL:HG23	2.12	0.50
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: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
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:C:280:LYS:O	1:C:281:ARG:HB2	2.12	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:A:140:LEU:HD23	1:A:291:MET:HE2	1.97	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:201:MET:HE1	1:B:267:ILE:CD1	2.45	0.46
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: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:D:282:MET:HE3	1:D:287:MET:HG3	1.98	0.45
1:C:106:ALA:O	1:C:198:THR:HG21	2.15	0.45
1:C:294:THR:HG22	1:C:295:ILE:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:158:VAL:HG11	1:A:188:MET:HE2	2.00	0.43
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: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:B:203:LYS:C	7:B:403:HOH:O	2.54	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:B:201:MET:HE3	1:B:201:MET:HB2	1.98	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:A:206:THR:HG1	1:A:208:HIS:CE1	2.29	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
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:A:251:ASP:CG	7:A:409:HOH:O	2.63	0.40
1:C:108:ILE:CD1	1:C:196:GLU:O	2.70	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%)	24	16
1	D	190/195 (97%)	185 (97%)	5 (3%)	0	100	100
All	All	766/780 (98%)	743 (97%)	22 (3%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	GLY

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%)	161 (97%)	5 (3%)	36	32
1	B	167/168 (99%)	163 (98%)	4 (2%)	43	40
1	C	169/168 (101%)	166 (98%)	3 (2%)	51	51
1	D	166/168 (99%)	164 (99%)	2 (1%)	63	65
All	All	668/672 (99%)	654 (98%)	14 (2%)	47	46

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	THR
1	A	220	SER
1	A	267	ILE
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	209	VAL
1	C	220	SER
1	C	224	ASP
1	D	267	ILE
1	D	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	142	GLN
1	B	157	GLN
1	B	160	GLN
1	B	202	HIS
1	B	215	ASN
1	C	180	GLN
1	D	160	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
6	SO4	D	305	-	4,4,4	0.33	0	6,6,6	0.18	0
2	EDO	B	302	-	3,3,3	0.25	0	2,2,2	0.61	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
2	EDO	C	302	-	3,3,3	0.16	0	2,2,2	0.16	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
4	GLY	D	308	-	4,4,4	1.04	0	3,4,4	1.02	0
5	LQ3	D	301	-	10,11,11	6.72	4 (40%)	7,14,14	2.74	3 (42%)
6	SO4	D	304	-	4,4,4	0.31	0	6,6,6	0.12	0
2	EDO	B	301	-	3,3,3	0.58	0	2,2,2	0.35	0
2	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.32	0
3	DGL	D	307	-	8,9,9	1.17	1 (12%)	8,11,11	1.10	0
6	SO4	D	306	-	4,4,4	0.31	0	6,6,6	0.15	0
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
2	EDO	B	302	-	-	1/1/1/1	-
5	LQ3	D	301	-	1/1/3/6	1/3/14/14	0/1/1/1
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	C	303	-	-	1/1/1/1	-
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	D	303	-	-	0/1/1/1	-
3	DGL	B	303	-	-	3/9/9/9	-

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

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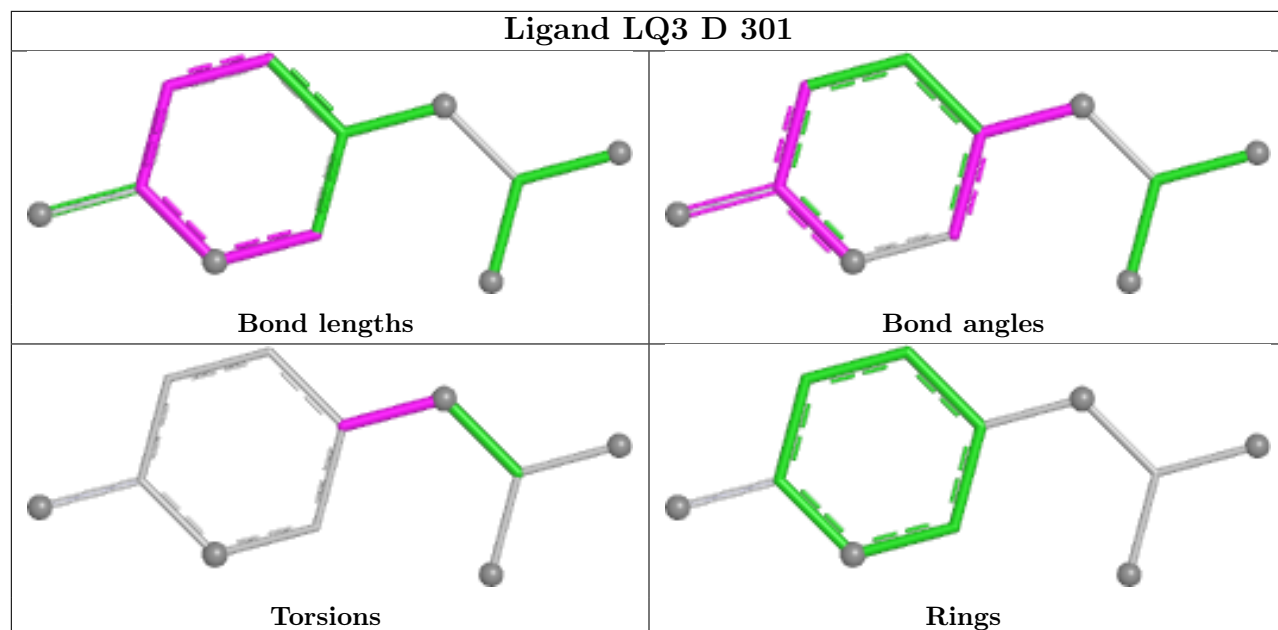
Mol	Chain	Res	Type	Atoms
2	C	301	EDO	O1-C1-C2-O2
3	D	307	DGL	O-C-CA-CB
3	B	303	DGL	OE2-CD-CG-CB
3	D	307	DGL	CA-CB-CG-CD

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	305	SO4	1	0
2	D	303	EDO	1	0
2	C	302	EDO	2	0
6	D	304	SO4	1	0
6	D	306	SO4	1	1

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.89	87 (45%) 0 0	16, 49, 92, 131	1 (0%)
1	B	193/195 (98%)	1.46	53 (27%) 1 1	14, 46, 73, 95	1 (0%)
1	C	193/195 (98%)	1.94	78 (40%) 0 0	15, 51, 79, 121	3 (1%)
1	D	191/195 (97%)	2.80	126 (65%) 0 0	17, 50, 79, 113	1 (0%)
All	All	768/780 (98%)	2.02	344 (44%) 0 0	14, 49, 81, 131	6 (0%)

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	182	PHE	8.1
1	D	190	ILE	6.6
1	A	286	ILE	6.5
1	D	177	VAL	6.4
1	A	283	ALA	6.4
1	D	178	LEU	6.3
1	B	264	VAL	6.2
1	A	290	LEU	6.2
1	D	117	LEU	6.2
1	A	182	PHE	6.2
1	A	287	MET	6.1
1	B	106	ALA	6.1
1	C	110	GLN	6.0
1	A	282	MET	6.0
1	D	111	GLY	5.7
1	D	249	LEU	5.5
1	D	213	PHE	5.5
1	C	108	ILE	5.4
1	A	284	PRO	5.4
1	C	106	ALA	5.3
1	D	267	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	254	ILE	5.2
1	D	207	GLY	5.2
1	D	265	VAL	5.2
1	D	149	LEU	5.1
1	C	249	LEU	5.1
1	D	284	PRO	5.1
1	A	108	ILE	5.0
1	D	150	VAL	4.8
1	D	108	ILE	4.8
1	D	158	VAL	4.8
1	B	227	ALA	4.8
1	D	263	THR	4.8
1	D	248	GLY	4.7
1	A	280	LYS	4.7
1	D	288	LYS	4.7
1	C	182	PHE	4.6
1	D	153	ARG	4.5
1	D	161	ILE	4.5
1	B	263	THR	4.5
1	D	154	PHE	4.5
1	D	183	GLY	4.4
1	D	186	ILE	4.4
1	C	143	ALA	4.4
1	D	152	LEU	4.4
1	C	112	ILE	4.4
1	D	141	VAL	4.3
1	D	112	ILE	4.3
1	D	116	ILE	4.3
1	D	275	PHE	4.3
1	D	125	ILE	4.3
1	D	174	ALA	4.3
1	D	212	ILE	4.3
1	D	269	ILE	4.3
1	A	298	VAL	4.2
1	C	212	ILE	4.2
1	C	123	GLY	4.1
1	A	285	SER	4.1
1	D	286	ILE	4.1
1	A	281	ARG	4.1
1	B	125	ILE	4.1
1	D	115	VAL	4.0
1	B	281	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	273[A]	PHE	4.0
1	D	216	GLY	4.0
1	A	109	LYS	4.0
1	A	202	HIS	3.9
1	D	209	VAL	3.9
1	D	189	THR	3.9
1	A	210	GLY	3.9
1	D	155	GLY	3.9
1	B	205	SER	3.9
1	A	288	LYS	3.9
1	A	279	ILE	3.8
1	D	283	ALA	3.8
1	C	258	LEU	3.8
1	C	296	PRO	3.8
1	C	184	GLU	3.8
1	D	113	ARG	3.8
1	B	199	ILE	3.7
1	D	171	SER	3.7
1	D	175	HIS	3.7
1	D	169	TRP	3.7
1	A	206	THR	3.7
1	C	263	THR	3.7
1	B	108	ILE	3.7
1	D	181	ALA	3.7
1	D	260	THR	3.7
1	C	111	GLY	3.6
1	C	251	ASP	3.6
1	D	241	ILE	3.6
1	C	109	LYS	3.6
1	D	147	ALA	3.6
1	A	253	GLN	3.6
1	A	177	VAL	3.6
1	B	109	LYS	3.6
1	D	238	ILE	3.5
1	D	257	ILE	3.5
1	A	204	ASP	3.5
1	B	111	GLY	3.5
1	B	207	GLY	3.5
1	A	295	ILE	3.5
1	B	228	ALA	3.5
1	C	118	CYS	3.5
1	D	109	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	149	LEU	3.4
1	C	117	LEU	3.4
1	B	202	HIS	3.4
1	D	118	CYS	3.4
1	D	298	VAL	3.4
1	C	273[A]	PHE	3.4
1	B	262	GLY	3.3
1	D	136	ILE	3.3
1	B	261	SER	3.3
1	A	222	VAL	3.3
1	C	286	ILE	3.3
1	A	140	LEU	3.3
1	A	259	SER	3.2
1	B	206	THR	3.2
1	C	262	GLY	3.2
1	B	265	VAL	3.2
1	C	150	VAL	3.2
1	A	112	ILE	3.2
1	D	262	GLY	3.2
1	C	223	LYS	3.2
1	C	228	ALA	3.2
1	B	110	GLN	3.2
1	A	262	GLY	3.2
1	B	115	VAL	3.1
1	A	257	ILE	3.1
1	B	112	ILE	3.1
1	B	225	SER	3.1
1	C	216	GLY	3.1
1	D	179	LYS	3.1
1	D	199	ILE	3.1
1	D	290	LEU	3.1
1	A	184	GLU	3.1
1	D	294	THR	3.1
1	D	191	ARG	3.1
1	C	254	ILE	3.1
1	D	247	ILE	3.1
1	C	206	THR	3.1
1	B	283	ALA	3.1
1	D	214	LYS	3.1
1	D	140	LEU	3.1
1	C	257	ILE	3.1
1	B	226	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	110	GLN	3.1
1	D	160	GLN	3.1
1	B	222	VAL	3.0
1	D	162	ASN	3.0
1	D	172	ASP	3.0
1	D	156	ASP	3.0
1	C	185	LYS	3.0
1	C	264	VAL	3.0
1	D	268	THR	3.0
1	A	185	LYS	3.0
1	D	287	MET	3.0
1	D	261	SER	2.9
1	A	242	ASN	2.9
1	A	263	THR	2.9
1	D	200	THR	2.9
1	B	200	THR	2.9
1	D	237	ASN	2.9
1	D	143	ALA	2.9
1	A	249	LEU	2.9
1	D	194	PRO	2.9
1	D	280	LYS	2.9
1	C	283	ALA	2.9
1	C	290	LEU	2.8
1	B	298	VAL	2.8
1	D	198	THR	2.8
1	D	279	ILE	2.8
1	B	284	PRO	2.8
1	C	181	ALA	2.8
1	B	258	LEU	2.8
1	B	107	GLU	2.8
1	C	209	VAL	2.8
1	A	289	SER	2.8
1	C	220	SER	2.8
1	D	252	SER	2.8
1	C	253	GLN	2.8
1	C	126	GLY	2.8
1	D	159	LEU	2.8
1	D	258	LEU	2.8
1	B	257	ILE	2.8
1	C	214	LYS	2.8
1	C	261	SER	2.8
1	A	243	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	228	ALA	2.8
1	D	272	ALA	2.8
1	A	260	THR	2.8
1	B	198	THR	2.8
1	B	266	THR	2.8
1	C	267	ILE	2.8
1	B	229	ARG	2.7
1	C	142	GLN	2.7
1	D	157	GLN	2.7
1	D	285	SER	2.7
1	A	251	ASP	2.7
1	C	183	GLY	2.7
1	D	187	THR	2.7
1	C	252	SER	2.7
1	D	208	HIS	2.7
1	D	282	MET	2.7
1	A	207	GLY	2.7
1	D	126	GLY	2.7
1	C	178	LEU	2.7
1	D	291	MET	2.7
1	A	179	LYS	2.7
1	C	255	ALA	2.7
1	D	167	ALA	2.7
1	C	149	LEU	2.7
1	B	295	ILE	2.7
1	C	222	VAL	2.7
1	C	107	GLU	2.6
1	C	124	LYS	2.6
1	D	185	LYS	2.6
1	D	264	VAL	2.6
1	C	168	GLY	2.6
1	A	258	LEU	2.6
1	D	176	LYS	2.6
1	D	164	GLU	2.6
1	D	270	MET	2.6
1	C	122	ASP	2.6
1	A	265	VAL	2.6
1	C	246	VAL	2.6
1	C	278	ILE	2.6
1	C	295	ILE	2.6
1	D	132	ILE	2.6
1	D	184	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	210	GLY	2.6
1	C	144[A]	ASN	2.6
1	A	250	LYS	2.6
1	D	227	ALA	2.6
1	D	255	ALA	2.6
1	A	296	PRO	2.6
1	A	212	ILE	2.5
1	B	177	VAL	2.5
1	D	278	ILE	2.5
1	D	250	LYS	2.5
1	C	284	PRO	2.5
1	A	183	GLY	2.5
1	A	186	ILE	2.5
1	C	218	ILE	2.5
1	C	248	GLY	2.5
1	D	144	ASN	2.5
1	C	289	SER	2.5
1	D	145	SER	2.5
1	A	273[A]	PHE	2.5
1	A	248	GLY	2.5
1	D	203	LYS	2.5
1	A	254	ILE	2.5
1	D	281	ARG	2.5
1	A	252	SER	2.5
1	D	146	PRO	2.5
1	A	213	PHE	2.5
1	A	169	TRP	2.5
1	A	221	ILE	2.5
1	C	247	ILE	2.5
1	A	110	GLN	2.4
1	A	180	GLN	2.4
1	D	239	CYS	2.4
1	C	260	THR	2.4
1	C	281	ARG	2.4
1	B	286	ILE	2.4
1	D	274	ILE	2.4
1	B	285	SER	2.4
1	C	291	MET	2.4
1	D	266	THR	2.4
1	C	250	LYS	2.4
1	A	164	GLU	2.4
1	D	211	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	129	LEU	2.4
1	B	230	ASN	2.4
1	A	223	LYS	2.4
1	C	280	LYS	2.4
1	D	188	MET	2.3
1	B	259	SER	2.3
1	C	221	ILE	2.3
1	D	138	VAL	2.3
1	A	174	ALA	2.3
1	A	245	ASN	2.3
1	A	111	GLY	2.3
1	D	173	LYS	2.3
1	A	275	PHE	2.3
1	D	170	SER	2.3
1	A	125	ILE	2.3
1	B	267	ILE	2.3
1	D	142	GLN	2.3
1	A	246	VAL	2.3
1	B	260	THR	2.3
1	A	181	ALA	2.3
1	B	122	ASP	2.3
1	B	278	ILE	2.2
1	B	144	ASN	2.2
1	D	215	ASN	2.2
1	B	201	MET	2.2
1	C	172	ASP	2.2
1	D	192	ASP	2.2
1	A	255	ALA	2.2
1	B	147	ALA	2.2
1	B	178	LEU	2.2
1	A	160	GLN	2.2
1	A	173	LYS	2.2
1	A	187	THR	2.2
1	C	294	THR	2.2
1	A	209	VAL	2.2
1	A	264	VAL	2.2
1	A	178	LEU	2.2
1	B	223	LYS	2.2
1	C	217	LYS	2.2
1	D	130	LYS	2.2
1	B	204	ASP	2.2
1	C	256	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	295	ILE	2.1
1	A	208	HIS	2.1
1	D	253	GLN	2.1
1	A	211	PHE	2.1
1	C	275	PHE	2.1
1	C	207	GLY	2.1
1	C	208	HIS	2.1
1	D	151	GLY	2.1
1	A	205	SER	2.1
1	C	259	SER	2.1
1	A	219	THR	2.1
1	A	168	GLY	2.1
1	A	229	ARG	2.1
1	C	265	VAL	2.1
1	B	118	CYS	2.1
1	A	144	ASN	2.1
1	A	121	GLN	2.1
1	A	199	ILE	2.1
1	C	125	ILE	2.1
1	A	225	SER	2.1
1	A	261	SER	2.1
1	B	121	GLN	2.0
1	D	236	HIS	2.0
1	A	163	GLY	2.0
1	A	161	ILE	2.0
1	A	267	ILE	2.0
1	D	196	GLU	2.0
1	A	167	ALA	2.0
1	C	227	ALA	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

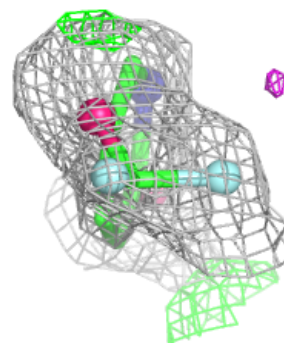
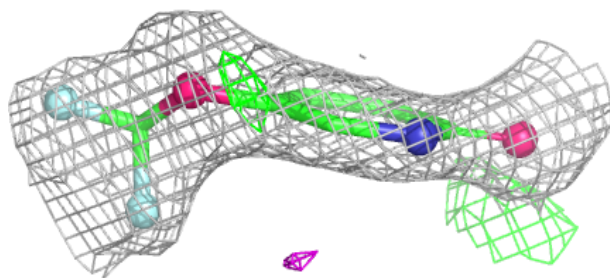
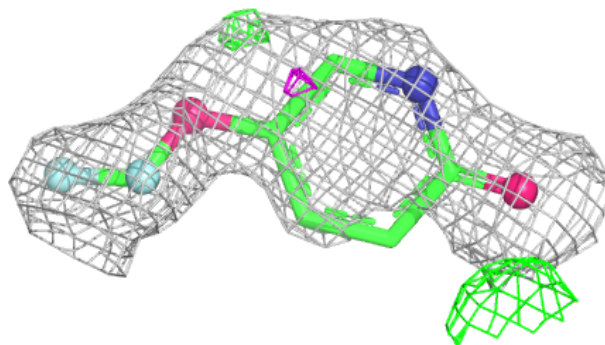
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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.

Electron density around LQ3 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.