



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:10 PM UTC

PDB ID : 7FSM / pdb_00007fsm
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z763030030
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.
Deposited on : 2023-01-24
Resolution : 2.10 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

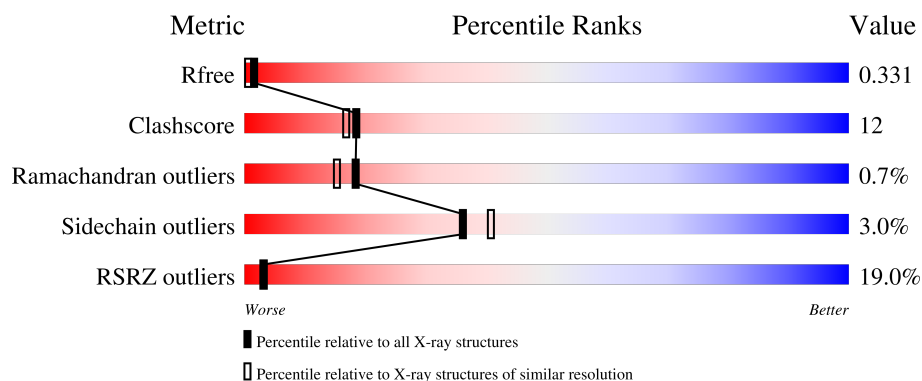
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	11% 79% 17% ..
1	B	195	7% 85% 14% ..
1	C	195	17% 75% 24% ..
1	D	195	39% 54% 39% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6384 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.

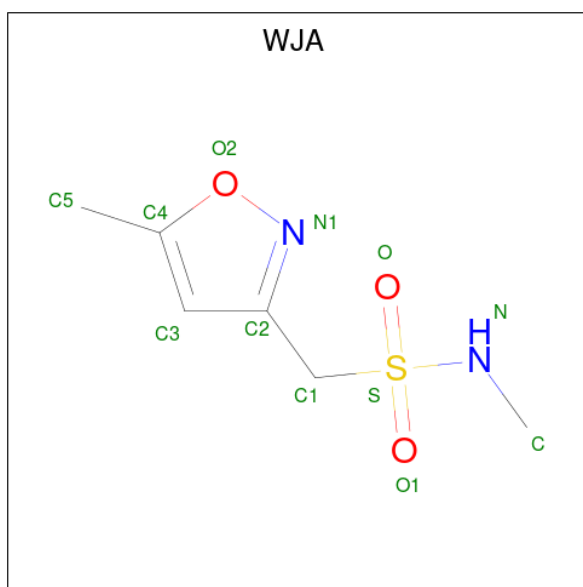
- Molecule 1 is a protein called Syntenin-1.

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-methyl-1-(5-methyl-1,2-oxazol-3-yl)methanesulfonamide (CCD ID: WJA) (formula: C₆H₁₀N₂O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

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



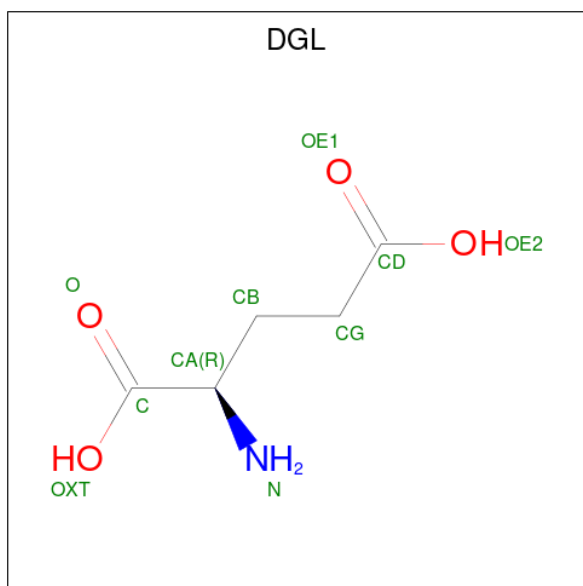
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

- 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	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

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



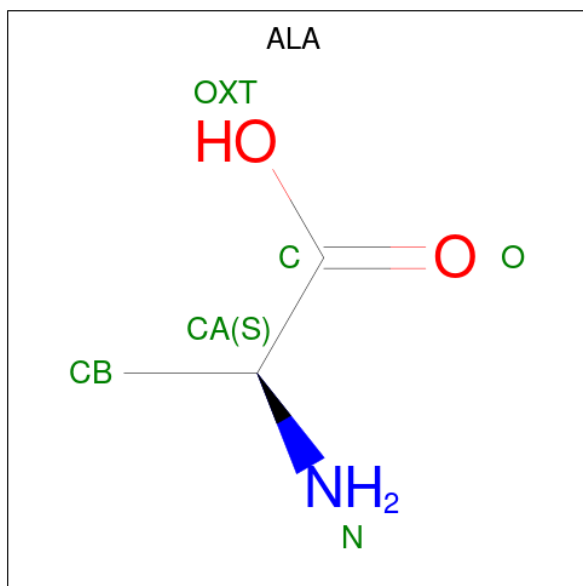
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	2	1	2		
5	D	1	Total	C	N	O	0	0
			5	2	1	2		

- 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		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



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

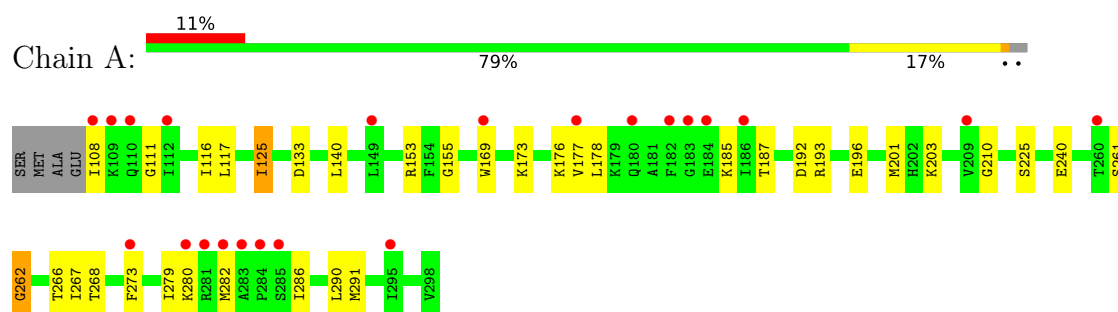
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	55	Total	O	0	0
			55	55		
8	B	110	Total	O	0	0
			110	110		
8	C	67	Total	O	0	1
			68	68		
8	D	90	Total	O	0	0
			90	90		

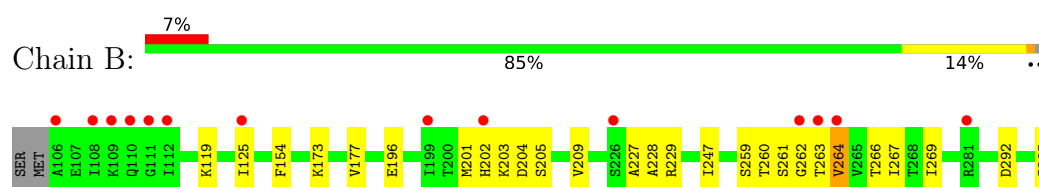
3 Residue-property plots

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.

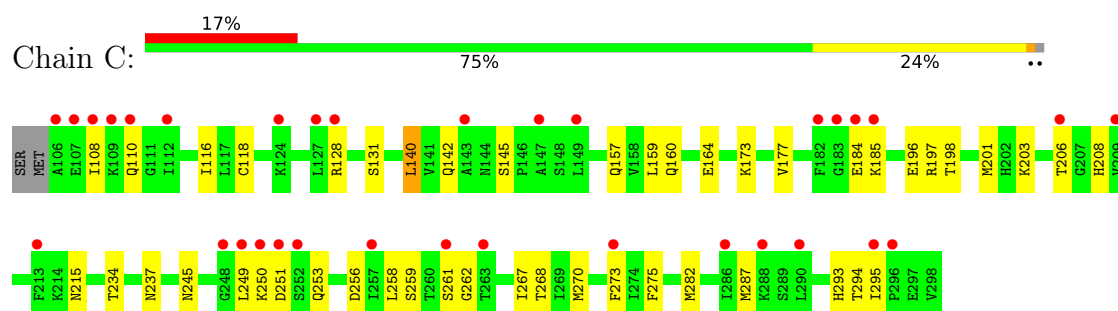
• Molecule 1: Syntenin-1



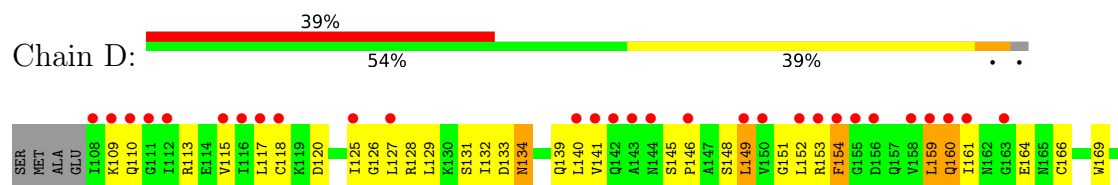
• Molecule 1: Syntenin-1

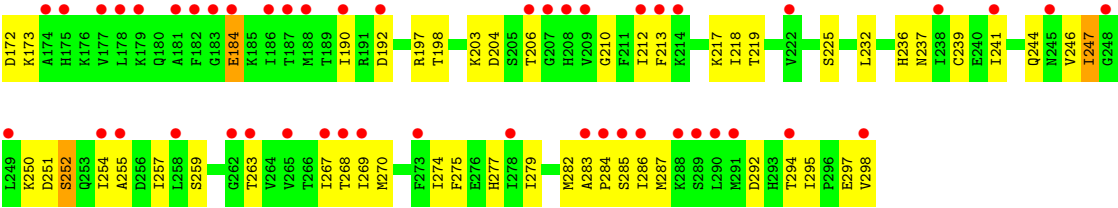


• Molecule 1: Syntenin-1



• 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	80.31Å 49.61Å 115.63Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	115.15 – 2.10 115.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (115.15-2.10) 99.9 (115.15-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.254 , 0.330 0.260 , 0.331	Depositor DCC
R_{free} test set	3250 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.150	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6384	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.94 % 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 1.2026e-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, WJA, SO4, EDO

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	0.58	0/1502	1.03	2/2019 (0.1%)
1	B	0.57	0/1516	1.07	1/2038 (0.0%)
1	C	0.58	0/1535	1.03	0/2063
1	D	0.64	0/1502	1.17	2/2019 (0.1%)
All	All	0.59	0/6055	1.08	5/8139 (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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	213	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	266	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	187	THR	CA-CB-OG1	-5.17	101.85	109.60
1	D	134	ASN	CA-CB-CG	-5.14	107.46	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	160	GLN	Peptide

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	26	0
1	B	1495	0	1541	21	0
1	C	1514	0	1558	30	0
1	D	1481	0	1530	70	0
2	A	12	0	0	0	0
3	A	4	0	6	1	0
3	B	8	0	12	0	0
3	C	12	0	18	1	0
3	D	8	0	12	1	0
4	B	10	0	7	2	0
4	D	10	0	7	0	0
5	C	5	0	2	0	0
5	D	5	0	2	0	0
6	D	10	0	0	1	0
7	D	6	0	4	0	0
8	A	55	0	0	2	0
8	B	110	0	0	9	2
8	C	68	0	0	4	0
8	D	90	0	0	14	2
All	All	6384	0	6229	148	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 12.

All (148) 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	8:D:401:HOH:O	2.00	0.94
1:D:252:SER:HB3	8:D:464:HOH:O	1.74	0.86
1:D:237:ASN:OD1	8:D:402:HOH:O	2.00	0.79
1:D:255:ALA:O	8:D:403:HOH:O	2.01	0.78
1:D:159:LEU:O	1:D:166:CYS:SG	2.42	0.77
1:D:287:MET:SD	8:D:488:HOH:O	2.44	0.75
1:D:204:ASP:OD2	8:D:404:HOH:O	2.04	0.75
1:D:279:ILE:HD11	8:D:468:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLN:HG2	1:D:282:MET:CE	2.20	0.71
1:B:196:GLU:OE1	8:B:401:HOH:O	2.09	0.70
1:D:236:HIS:NE2	8:D:401:HOH:O	2.26	0.69
1:D:212:ILE:O	1:D:219:THR:OG1	2.10	0.69
1:B:202:HIS:HA	1:B:263:THR:O	1.93	0.69
1:D:139:GLN:O	1:D:282:MET:HE1	1.95	0.67
1:D:140:LEU:HD23	1:D:141:VAL:C	2.19	0.67
1:B:228:ALA:O	8:B:403:HOH:O	2.13	0.67
1:D:218:ILE:HD13	1:D:232:LEU:HD21	1.80	0.64
1:D:118:CYS:SG	1:D:184:GLU:O	2.48	0.63
1:A:240:GLU:HB2	1:A:268:THR:HB	1.80	0.63
1:B:201:MET:SD	1:B:227:ALA:HA	2.39	0.62
1:D:203:LYS:HG3	1:D:263:THR:O	1.99	0.61
1:D:251:ASP:HB2	6:D:304:SO4:O1	2.00	0.61
1:D:244:GLN:HE22	1:D:257:ILE:HD13	1.66	0.61
1:A:111:GLY:HA2	8:A:448:HOH:O	2.01	0.60
1:C:282:MET:HE3	1:C:287:MET:HB2	1.84	0.59
1:C:237:ASN:CG	1:C:275:PHE:CD2	2.80	0.59
1:D:283:ALA:O	1:D:284:PRO:C	2.45	0.59
1:C:203:LYS:NZ	1:C:258:LEU:O	2.25	0.59
1:D:198:THR:HG22	1:D:268:THR:OG1	2.03	0.58
1:B:262:GLY:O	1:B:264:VAL:N	2.37	0.58
1:A:140:LEU:HD23	1:A:291:MET:HE2	1.85	0.58
1:B:203:LYS:NZ	1:B:259:SER:O	2.36	0.58
1:B:229:ARG:NH1	8:B:414:HOH:O	2.33	0.57
1:B:262:GLY:O	1:B:263:THR:C	2.46	0.57
1:D:270:MET:SD	1:D:275:PHE:HA	2.43	0.57
1:A:201:MET:HE1	1:A:267:ILE:HD12	1.86	0.57
1:D:153:ARG:HG2	8:D:430:HOH:O	2.04	0.57
1:B:259:SER:C	1:B:261:SER:H	2.13	0.57
1:D:120:ASP:OD1	1:D:120:ASP:C	2.47	0.56
4:B:303:DGL:N	8:B:409:HOH:O	2.28	0.56
1:C:249:LEU:HD21	1:C:293:HIS:CE1	2.41	0.56
1:B:204:ASP:HB2	8:B:433:HOH:O	2.06	0.55
1:C:198:THR:HG22	1:C:268:THR:OG1	2.06	0.55
1:D:134:ASN:O	8:D:405:HOH:O	2.17	0.55
1:B:201:MET:HE1	1:B:267:ILE:HD12	1.90	0.54
1:C:203:LYS:HD2	1:C:262:GLY:O	2.09	0.53
1:D:128:ARG:O	1:D:129:LEU:HD23	2.09	0.53
1:D:139:GLN:HG2	1:D:282:MET:HE2	1.91	0.53
1:C:253:GLN:O	1:C:256:ASP:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:O	1:B:177:VAL:HG23	2.10	0.52
1:C:196:GLU:HG2	1:C:270:MET:HB2	1.92	0.52
1:D:210:GLY:HA3	1:D:225:SER:HB2	1.91	0.52
1:A:108:ILE:HA	1:A:192:ASP:OD2	2.10	0.52
1:A:192:ASP:O	1:A:193:ARG:C	2.53	0.51
1:C:118:CYS:SG	1:C:184:GLU:O	2.67	0.51
1:C:142:GLN:O	1:C:145:SER:OG	2.24	0.51
1:D:139:GLN:HG2	1:D:282:MET:HE1	1.89	0.51
1:A:111:GLY:CA	8:A:448:HOH:O	2.58	0.51
1:A:133:ASP:HB3	1:C:234:THR:O	2.11	0.51
1:A:140:LEU:HD21	1:A:282:MET:HE1	1.93	0.50
1:B:209:VAL:HA	8:B:413:HOH:O	2.11	0.50
1:D:239:CYS:HB2	1:D:268:THR:HG22	1.94	0.50
1:C:273[A]:PHE:HD1	8:C:449:HOH:O	1.95	0.49
1:B:262:GLY:C	1:B:264:VAL:N	2.70	0.49
1:D:295:ILE:HD11	1:D:298:VAL:HG12	1.94	0.49
1:D:203:LYS:NZ	1:D:259:SER:O	2.46	0.49
1:C:173:LYS:O	1:C:177:VAL:HG23	2.12	0.49
1:D:197:ARG:O	1:D:268:THR:HA	2.13	0.49
1:C:128:ARG:HD2	1:C:140:LEU:HD22	1.93	0.49
1:B:259:SER:O	1:B:261:SER:N	2.39	0.48
1:C:160:GLN:HA	1:C:164:GLU:O	2.12	0.48
1:A:173:LYS:O	1:A:177:VAL:HG23	2.13	0.48
1:A:176:LYS:O	1:A:177:VAL:C	2.57	0.48
1:D:241:ILE:HD11	1:D:254:ILE:HG23	1.94	0.48
1:D:110:GLN:CA	8:D:417:HOH:O	2.62	0.48
1:D:160:GLN:CD	1:D:160:GLN:N	2.72	0.48
1:D:117:LEU:HD11	1:D:146:PRO:C	2.39	0.48
1:D:154:PHE:CZ	1:D:247:ILE:HD12	2.49	0.48
1:D:218:ILE:CD1	1:D:232:LEU:HD11	2.44	0.47
1:D:140:LEU:HD23	1:D:140:LEU:C	2.39	0.47
1:D:127:LEU:HD21	1:D:152:LEU:HD13	1.95	0.47
1:C:116:ILE:HG23	1:C:185:LYS:HB2	1.97	0.47
1:D:133:ASP:OD1	3:D:302:EDO:O1	2.32	0.47
1:A:210:GLY:HA3	1:A:225:SER:CB	2.45	0.47
1:B:204:ASP:HA	8:B:418:HOH:O	2.15	0.47
1:C:261:SER:OG	1:C:262:GLY:N	2.47	0.47
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.81	0.46
1:D:244:GLN:NE2	1:D:257:ILE:HD13	2.29	0.46
1:D:148:SER:O	1:D:151:GLY:N	2.38	0.46
1:D:154:PHE:C	1:D:154:PHE:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ILE:O	1:D:164:GLU:HB2	2.16	0.46
1:B:119:LYS:HG2	1:B:125:ILE:HD11	1.97	0.46
1:D:244:GLN:HE22	1:D:257:ILE:CD1	2.28	0.45
1:C:108:ILE:CD1	1:C:198:THR:HG23	2.46	0.45
1:A:279:ILE:O	1:A:280:LYS:C	2.59	0.45
1:D:131:SER:O	1:D:132:ILE:HD13	2.16	0.45
1:D:198:THR:HA	1:D:267:ILE:O	2.16	0.45
4:B:303:DGL:OE1	8:B:404:HOH:O	2.21	0.45
1:D:237:ASN:O	1:D:269:ILE:HA	2.16	0.45
1:C:253:GLN:HG2	8:C:457:HOH:O	2.17	0.45
1:D:152:LEU:HD21	1:D:190:ILE:HG13	1.99	0.45
1:D:283:ALA:O	1:D:285:SER:N	2.50	0.45
1:B:259:SER:C	1:B:261:SER:N	2.75	0.44
1:C:282:MET:HE3	1:C:287:MET:CB	2.47	0.44
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.18	0.44
1:D:244:GLN:O	1:D:246:VAL:HG13	2.18	0.44
1:A:169:TRP:CZ3	1:A:177:VAL:HG21	2.53	0.44
1:D:110:GLN:N	8:D:417:HOH:O	2.52	0.43
1:A:286:ILE:HG23	1:A:290:LEU:HD12	2.00	0.43
1:C:250:LYS:O	1:C:251:ASP:C	2.61	0.43
1:D:126:GLY:HA3	1:D:145:SER:HB2	2.01	0.43
1:D:132:ILE:HD12	1:D:277:HIS:CG	2.52	0.43
1:D:217:LYS:HB2	1:D:237:ASN:HD21	1.84	0.43
1:C:197[B]:ARG:CZ	3:C:303:EDO:H11	2.49	0.43
1:D:109:LYS:N	1:D:192:ASP:OD2	2.51	0.43
1:D:210:GLY:HA3	1:D:225:SER:CB	2.48	0.43
1:D:283:ALA:HB3	1:D:286:ILE:HD12	2.01	0.43
1:C:294:THR:HG22	1:C:295:ILE:C	2.43	0.43
1:B:119:LYS:HG2	1:B:125:ILE:CD1	2.49	0.43
1:A:282:MET:HE2	1:A:286:ILE:CG2	2.49	0.42
1:B:154:PHE:CD1	1:B:247:ILE:CD1	3.02	0.42
1:C:118:CYS:HA	8:C:401:HOH:O	2.18	0.42
1:D:274:ILE:O	1:D:275:PHE:C	2.61	0.42
1:D:287:MET:CE	8:D:488:HOH:O	2.66	0.42
1:D:117:LEU:HD11	1:D:146:PRO:O	2.19	0.42
1:A:116:ILE:HG21	1:A:185:LYS:HE2	2.01	0.42
1:D:204:ASP:OD1	1:D:204:ASP:C	2.63	0.42
1:D:140:LEU:HD23	1:D:141:VAL:N	2.34	0.42
1:A:125:ILE:HD11	1:A:178:LEU:HD13	2.02	0.41
1:A:116:ILE:CG2	1:A:185:LYS:HG2	2.50	0.41
1:A:203:LYS:HE2	1:A:262:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ASN:OD1	1:C:245:ASN:C	2.64	0.41
1:A:140:LEU:HD23	1:A:291:MET:CE	2.51	0.41
1:A:273[B]:PHE:CE2	3:A:302:EDO:H22	2.56	0.41
1:C:116:ILE:CG2	1:C:185:LYS:HB2	2.51	0.41
1:C:201:MET:HE1	1:C:267:ILE:HG12	2.03	0.41
1:C:206:THR:HB	1:C:208:HIS:ND1	2.36	0.41
1:D:166:CYS:HA	1:D:169:TRP:CE2	2.56	0.41
1:D:172:ASP:O	1:D:173:LYS:C	2.61	0.41
1:B:295:ILE:O	8:B:405:HOH:O	2.22	0.40
1:C:157:GLN:HG2	1:C:159:LEU:HD12	2.03	0.40
1:D:197:ARG:O	1:D:269:ILE:N	2.46	0.40
1:A:155:GLY:HA3	1:A:196:GLU:OE2	2.21	0.40
1:D:148:SER:O	1:D:149:LEU:C	2.64	0.40
1:A:282:MET:HE2	1:A:286:ILE:HG22	2.02	0.40
1:C:215:ASN:ND2	8:C:414:HOH:O	2.54	0.40
1:A:261:SER:C	1:A:262:GLY:O	2.64	0.40
1:D:110:GLN:HB3	8:D:417:HOH:O	2.22	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)
8:B:477:HOH:O	8:D:467:HOH:O[1_455]	1.90	0.30
8:B:446:HOH:O	8:D:469:HOH:O[1_455]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/195 (97%)	177 (93%)	12 (6%)	1 (0%)	24	22
1	B	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	24	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	194/195 (100%)	186 (96%)	8 (4%)	0	100	100
1	D	190/195 (97%)	175 (92%)	12 (6%)	3 (2%)	7	4
All	All	766/780 (98%)	721 (94%)	40 (5%)	5 (1%)	18	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	LEU
1	B	260	THR
1	D	149	LEU
1	D	184	GLU
1	A	262	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%)	164 (99%)	2 (1%)	63	72
1	B	167/168 (99%)	162 (97%)	5 (3%)	36	41
1	C	169/168 (101%)	165 (98%)	4 (2%)	43	49
1	D	166/168 (99%)	157 (95%)	9 (5%)	20	18
All	All	668/672 (99%)	648 (97%)	20 (3%)	36	41

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

Mol	Chain	Res	Type
1	A	117	LEU
1	A	125	ILE
1	B	205	SER
1	B	264	VAL
1	B	266	THR
1	B	269	ILE
1	B	298	VAL

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Mol	Chain	Res	Type
1	C	110	GLN
1	C	131	SER
1	C	140	LEU
1	C	259	SER
1	D	113	ARG
1	D	115	VAL
1	D	125	ILE
1	D	154	PHE
1	D	206	THR
1	D	247	ILE
1	D	250	LYS
1	D	252	SER
1	D	297	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	142	GLN
1	A	215	ASN
1	A	230	ASN
1	A	237	ASN
1	B	134	ASN
1	B	142	GLN
1	B	160	GLN
1	C	121	GLN
1	C	230	ASN
1	C	253	GLN
1	D	215	ASN
1	D	237	ASN
1	D	244	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 [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	DGL	B	303	-	8,9,9	0.84	0	8,11,11	1.11	0
3	EDO	C	303	-	3,3,3	0.44	0	2,2,2	0.66	0
6	SO4	D	304	-	4,4,4	0.25	0	6,6,6	0.15	0
3	EDO	A	302	-	3,3,3	0.21	0	2,2,2	0.28	0
3	EDO	D	301	-	3,3,3	0.35	0	2,2,2	0.26	0
7	ALA	D	305	-	5,5,5	0.95	0	6,6,6	0.85	0
5	GLY	D	307	-	4,4,4	0.88	0	3,4,4	1.20	0
3	EDO	C	301	-	3,3,3	0.26	0	2,2,2	0.23	0
3	EDO	B	301	-	3,3,3	0.38	0	2,2,2	0.18	0
3	EDO	D	302	-	3,3,3	0.23	0	2,2,2	0.16	0
4	DGL	D	306	-	8,9,9	1.17	0	8,11,11	0.96	0
5	GLY	C	304	-	4,4,4	0.91	0	3,4,4	1.09	0
3	EDO	B	302	-	3,3,3	0.15	0	2,2,2	0.35	0
6	SO4	D	303	-	4,4,4	0.29	0	6,6,6	0.08	0
2	WJA	A	301	-	10,12,12	2.66	5 (50%)	13,17,17	4.40	10 (76%)
3	EDO	C	302	-	3,3,3	0.07	0	2,2,2	0.18	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	DGL	B	303	-	-	2/9/9/9	-
3	EDO	C	303	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	301	-	-	0/1/1/1	-
7	ALA	D	305	-	-	0/4/4/4	-
5	GLY	D	307	-	-	2/2/2/2	-
3	EDO	C	301	-	-	1/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
4	DGL	D	306	-	-	3/9/9/9	-
5	GLY	C	304	-	-	2/2/2/2	-
3	EDO	B	302	-	-	1/1/1/1	-
2	WJA	A	301	-	-	0/6/8/8	0/1/1/1
3	EDO	C	302	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	WJA	S-N	4.83	1.71	1.60
2	A	301	WJA	O-S	3.57	1.48	1.43
2	A	301	WJA	O2-C4	-3.44	1.30	1.35
2	A	301	WJA	O2-N1	-3.25	1.36	1.42
2	A	301	WJA	O1-S	2.81	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	WJA	O1-S-O	-9.92	105.46	119.34
2	A	301	WJA	O2-C4-C5	6.04	124.20	115.89
2	A	301	WJA	O1-S-N	6.02	114.97	107.66
2	A	301	WJA	C3-C2-N1	-5.04	106.57	111.41
2	A	301	WJA	O-S-N	-3.50	103.41	107.66
2	A	301	WJA	C5-C4-C3	-3.39	128.19	134.05
2	A	301	WJA	O1-S-C1	-3.19	102.90	108.15
2	A	301	WJA	O-S-C1	2.63	112.47	108.15
2	A	301	WJA	O2-C4-C3	-2.07	107.56	109.88
2	A	301	WJA	C4-O2-N1	2.03	110.54	108.47

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	304	GLY	O-C-CA-N

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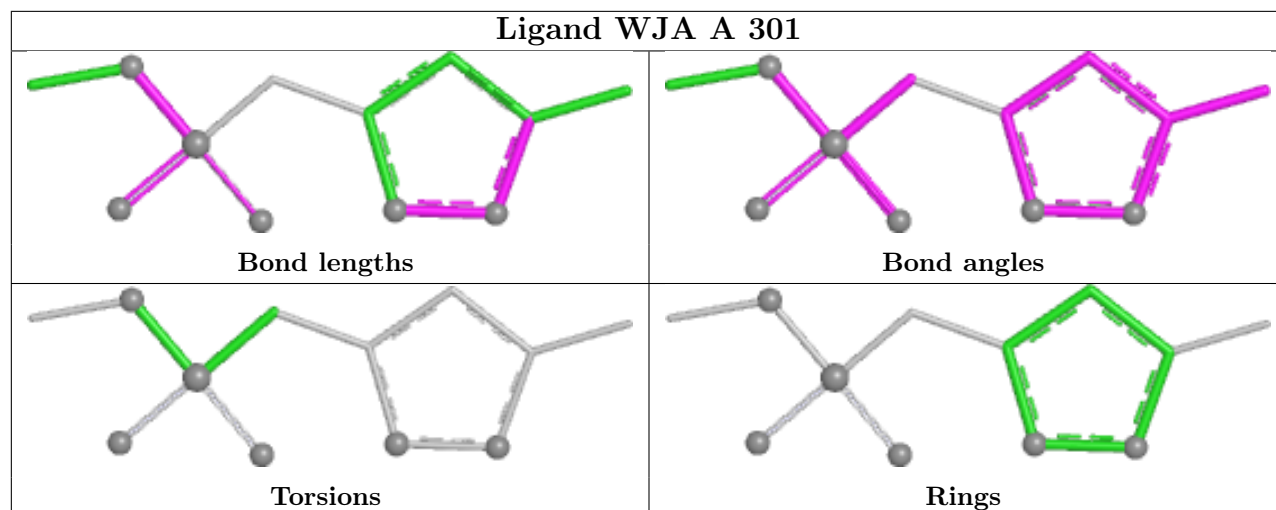
Mol	Chain	Res	Type	Atoms
5	C	304	GLY	OXT-C-CA-N
5	D	307	GLY	OXT-C-CA-N
5	D	307	GLY	O-C-CA-N
4	D	306	DGL	OXT-C-CA-CB
4	D	306	DGL	O-C-CA-CB
3	B	302	EDO	O1-C1-C2-O2
3	C	301	EDO	O1-C1-C2-O2
4	D	306	DGL	CA-CB-CG-CD
4	B	303	DGL	C-CA-CB-CG
3	C	302	EDO	O1-C1-C2-O2
4	B	303	DGL	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	DGL	2	0
3	C	303	EDO	1	0
6	D	304	SO4	1	0
3	A	302	EDO	1	0
3	D	302	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/195 (97%)	0.80	22 (11%) 9 10	14, 41, 69, 95	1 (0%)
1	B	193/195 (98%)	0.55	14 (7%) 21 22	12, 38, 59, 85	1 (0%)
1	C	193/195 (98%)	1.24	33 (17%) 4 4	15, 46, 75, 95	3 (1%)
1	D	191/195 (97%)	1.90	77 (40%) 0 1	16, 45, 70, 102	1 (0%)
All	All	768/780 (98%)	1.12	146 (19%) 3 3	12, 43, 68, 102	6 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	116	ILE	7.6
1	C	106	ALA	6.7
1	C	108	ILE	6.6
1	D	190	ILE	5.9
1	C	110	GLN	5.9
1	A	281	ARG	5.5
1	D	178	LEU	5.4
1	D	182	PHE	5.4
1	D	108	ILE	5.4
1	D	267	ILE	5.1
1	A	182	PHE	5.0
1	D	183	GLY	4.7
1	D	254	ILE	4.6
1	D	118	CYS	4.6
1	D	186	ILE	4.4
1	A	108	ILE	4.3
1	D	125	ILE	4.3
1	D	284	PRO	4.3
1	D	141	VAL	4.3
1	A	283	ALA	4.2
1	B	264	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	109	LYS	4.2
1	B	106	ALA	4.1
1	D	184	GLU	4.1
1	D	149	LEU	4.1
1	D	265	VAL	4.0
1	D	142	GLN	3.9
1	D	117	LEU	3.9
1	D	248	GLY	3.9
1	D	161	ILE	3.8
1	C	249	LEU	3.8
1	C	112	ILE	3.7
1	D	241	ILE	3.7
1	C	273[A]	PHE	3.7
1	D	112	ILE	3.7
1	B	111	GLY	3.6
1	C	182	PHE	3.6
1	D	154	PHE	3.6
1	A	284	PRO	3.6
1	D	140	LEU	3.6
1	D	153	ARG	3.5
1	D	238	ILE	3.4
1	C	286	ILE	3.4
1	B	263	THR	3.3
1	D	208	HIS	3.3
1	C	251	ASP	3.3
1	D	298	VAL	3.3
1	B	108	ILE	3.3
1	A	209	VAL	3.2
1	D	177	VAL	3.2
1	B	125	ILE	3.2
1	D	212	ILE	3.1
1	D	273[A]	PHE	3.1
1	D	209	VAL	3.1
1	D	283	ALA	3.1
1	C	288	LYS	3.1
1	D	258	LEU	3.1
1	C	252	SER	3.1
1	C	183	GLY	3.1
1	A	273[A]	PHE	3.0
1	C	149	LEU	2.9
1	D	115	VAL	2.9
1	D	158	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	150	VAL	2.9
1	D	288	LYS	2.8
1	C	296	PRO	2.8
1	D	269	ILE	2.8
1	C	107	GLU	2.8
1	B	199	ILE	2.8
1	A	282	MET	2.7
1	C	257	ILE	2.7
1	D	110	GLN	2.6
1	A	184	GLU	2.6
1	A	280	LYS	2.6
1	D	109	LYS	2.6
1	D	181	ALA	2.6
1	D	192	ASP	2.6
1	D	152	LEU	2.6
1	C	128	ARG	2.5
1	B	110	GLN	2.5
1	D	163	GLY	2.5
1	D	207	GLY	2.5
1	B	112	ILE	2.5
1	A	295	ILE	2.4
1	C	261	SER	2.4
1	B	262	GLY	2.4
1	D	245	ASN	2.4
1	B	226	SER	2.4
1	C	206	THR	2.4
1	D	222	VAL	2.4
1	D	278	ILE	2.4
1	D	286	ILE	2.4
1	B	202	HIS	2.4
1	D	291	MET	2.3
1	C	209	VAL	2.3
1	D	285	SER	2.3
1	D	187	THR	2.3
1	C	248	GLY	2.3
1	D	111	GLY	2.3
1	D	290	LEU	2.3
1	B	281	ARG	2.3
1	A	109	LYS	2.3
1	D	214	LYS	2.3
1	D	155	GLY	2.3
1	D	179	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	213	PHE	2.3
1	C	147	ALA	2.3
1	C	127	LEU	2.3
1	A	112	ILE	2.2
1	D	263	THR	2.2
1	C	250	LYS	2.2
1	D	143	ALA	2.2
1	D	174	ALA	2.2
1	D	127	LEU	2.2
1	A	110	GLN	2.2
1	C	295	ILE	2.2
1	D	160	GLN	2.2
1	B	109	LYS	2.2
1	A	186	ILE	2.2
1	D	188	MET	2.2
1	D	175	HIS	2.2
1	D	249	LEU	2.2
1	D	206	THR	2.2
1	D	294	THR	2.2
1	C	213	PHE	2.1
1	A	177	VAL	2.1
1	D	255	ALA	2.1
1	D	159	LEU	2.1
1	C	184	GLU	2.1
1	D	156	ASP	2.1
1	A	260	THR	2.1
1	D	289	SER	2.1
1	D	262	GLY	2.1
1	A	169	TRP	2.1
1	C	143	ALA	2.1
1	A	149	LEU	2.1
1	A	183	GLY	2.1
1	C	185	LYS	2.1
1	A	285	SER	2.1
1	A	180	GLN	2.0
1	C	263	THR	2.0
1	D	268	THR	2.0
1	C	124	LYS	2.0
1	D	144	ASN	2.0
1	C	290	LEU	2.0
1	D	146	PRO	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 ⓘ

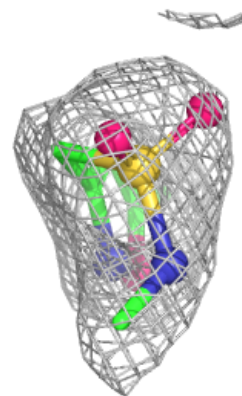
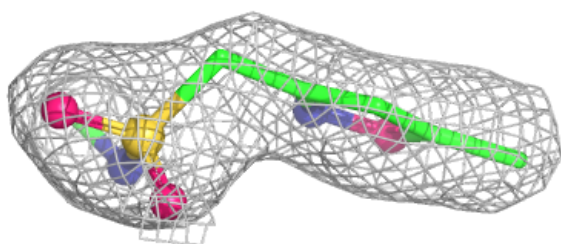
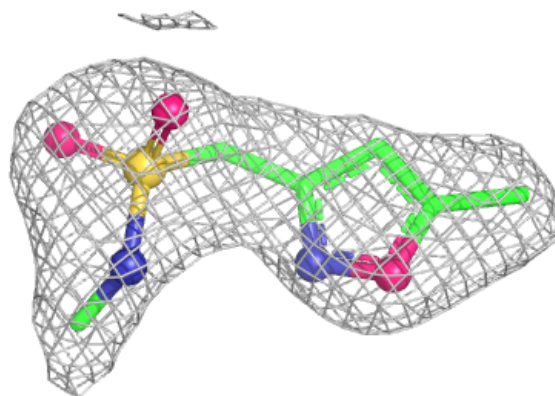
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	304	5/5	0.47	0.17	74,81,97,99	0
4	DGL	D	306	10/10	0.71	0.23	30,40,44,45	10
5	GLY	C	304	5/5	0.80	0.16	50,59,62,68	0
4	DGL	B	303	10/10	0.81	0.17	20,25,26,26	10
3	EDO	C	301	4/4	0.81	0.17	41,43,48,52	0
5	GLY	D	307	5/5	0.82	0.15	55,58,61,65	0
3	EDO	C	303	4/4	0.82	0.25	46,53,54,57	0
7	ALA	D	305	6/6	0.82	0.17	71,73,79,80	0
6	SO4	D	303	5/5	0.85	0.11	61,64,72,75	0
3	EDO	C	302	4/4	0.88	0.19	37,37,39,43	0
3	EDO	D	302	4/4	0.90	0.16	38,39,40,41	0
3	EDO	D	301	4/4	0.90	0.14	32,39,41,42	0
3	EDO	B	301	4/4	0.92	0.13	34,39,40,46	0
3	EDO	A	302	4/4	0.93	0.13	35,36,37,39	0
2	WJA	A	301	12/12	0.93	0.10	33,38,41,50	0
3	EDO	B	302	4/4	0.96	0.07	29,30,31,32	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 WJA 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.