



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2023 – 04:27 PM EST

PDB ID : 7FT4  
Title : SDCBP PanDDA analysis group deposition – The PDZ domains of SDCBP in complex with Z48847594  
Authors : Bradshaw, W.J.; Katis, V.L.; Bountra, C.; von Delft, F.; Brennan, P.E.  
Deposited on : 2023-01-24  
Resolution : 2.17 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.32.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

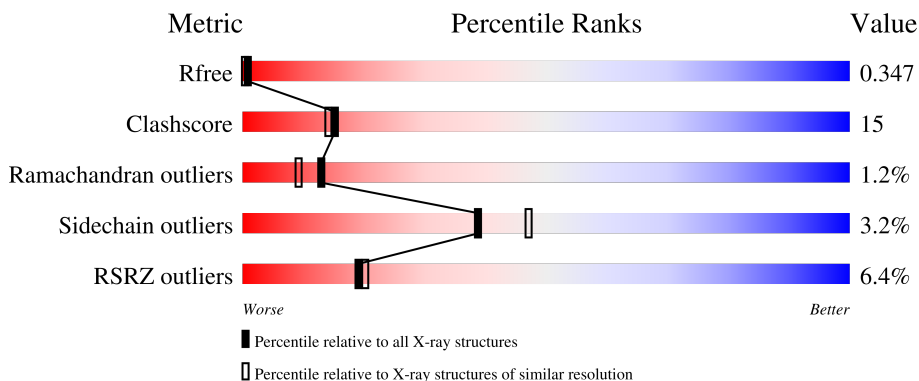
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


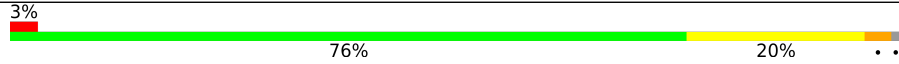
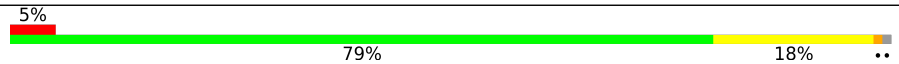

The reported resolution of this entry is 2.17 Å.

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))
$R_{free}$	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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  $\geq 3$ , 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	 3% 74% 21% ..
1	B	195	 3% 76% 20% ..
1	C	195	 5% 79% 18% ..
1	D	195	 15% 51% 44% ..

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6337 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.

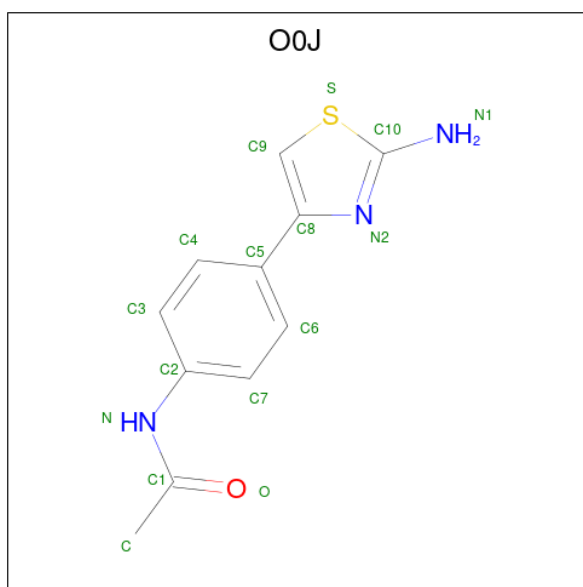
- Molecule 1 is a protein called Syntenin-1.

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

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-[4-(2-amino-1,3-thiazol-4-yl)phenyl]acetamide (three-letter code: O0J) (formula: C<sub>11</sub>H<sub>11</sub>N<sub>3</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	16	11	3	1	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



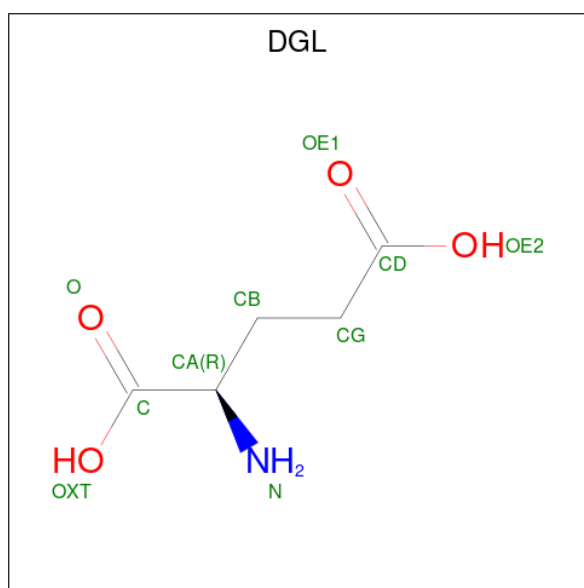
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0

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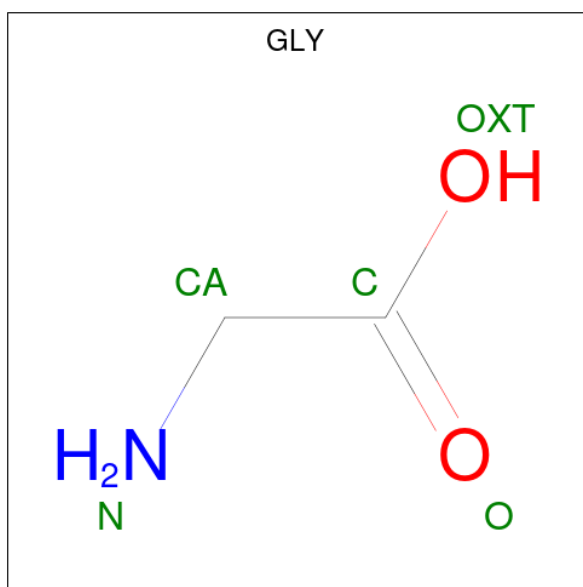
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



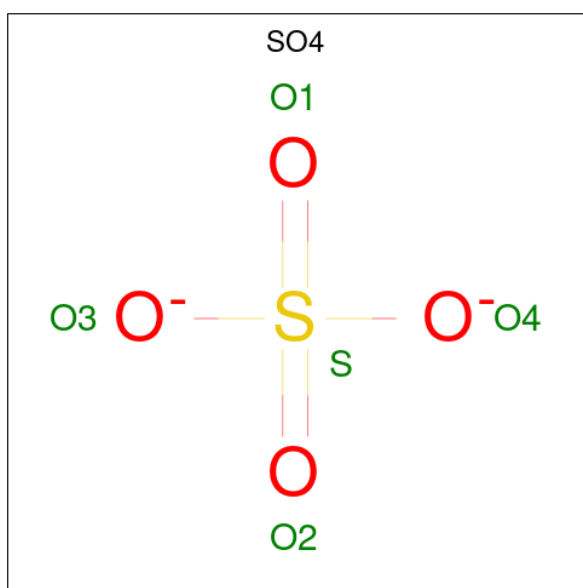
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



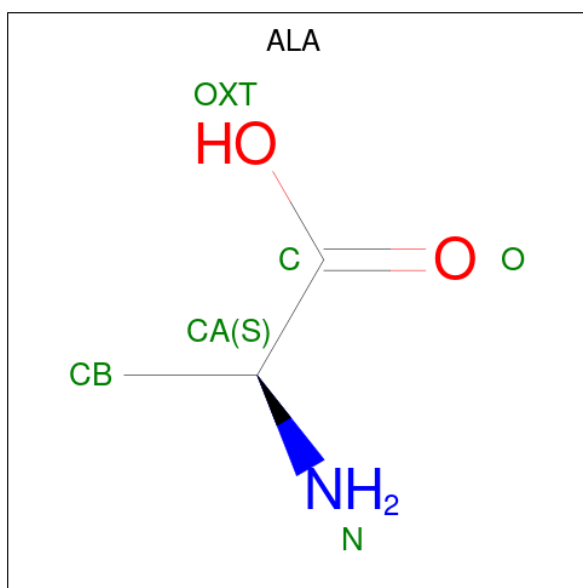
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	C	1	5	2	1	2	0	0
5	D	1	5	2	1	2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 7 is ALANINE (three-letter code: ALA) (formula:  $C_3H_7NO_2$ ).



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

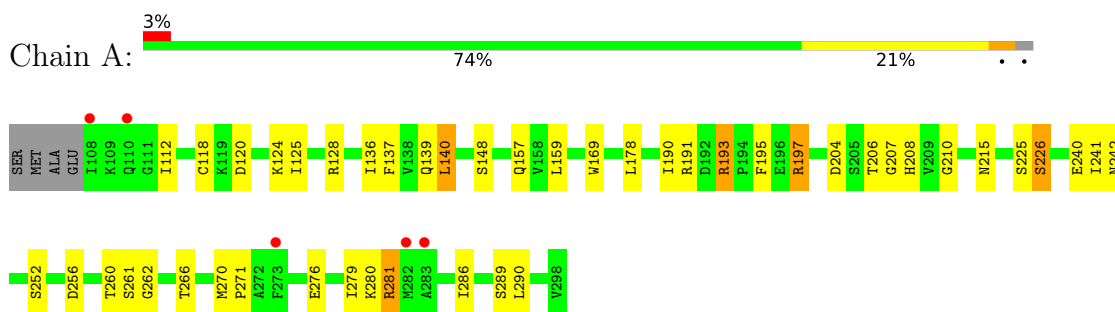
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	42	Total	O	0	0
			42	42		
8	B	90	Total	O	0	1
			90	90		
8	C	67	Total	O	0	0
			67	67		
8	D	73	Total	O	0	0
			73	73		

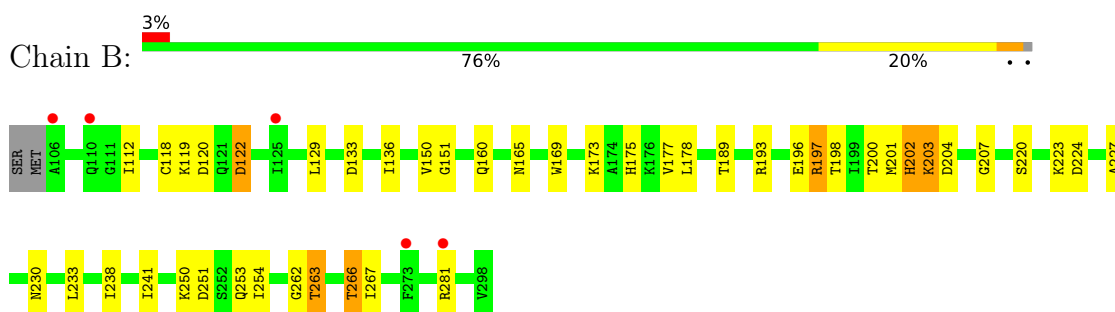
### 3 Residue-property plots [i](#)

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.

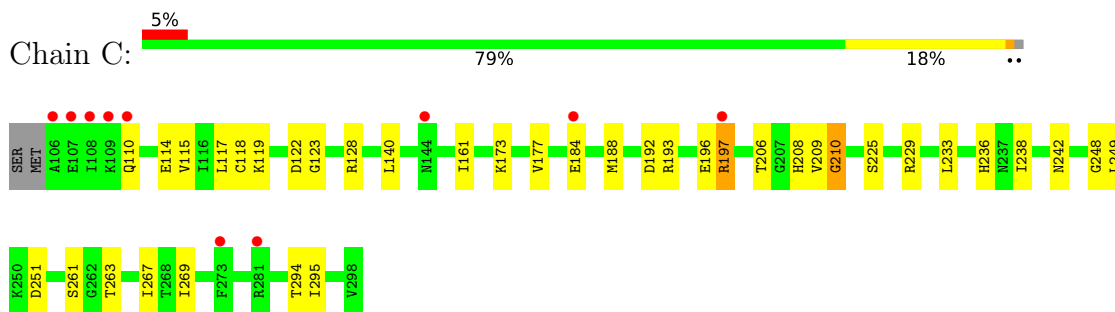
- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1



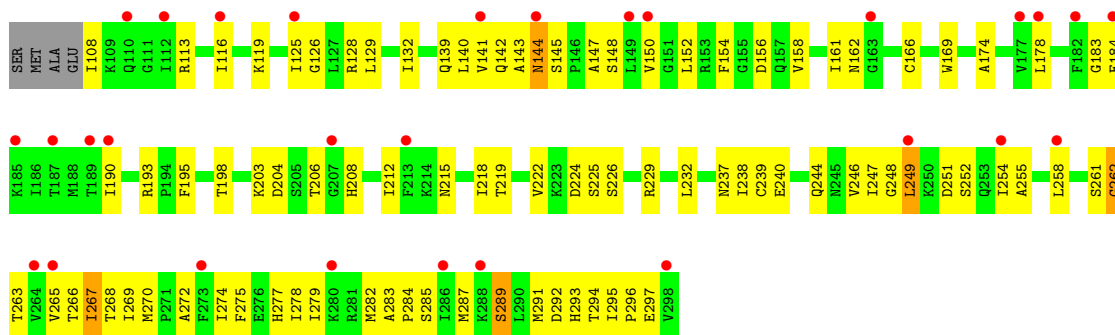
- Molecule 1: Syntenin-1



- Molecule 1: Syntenin-1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.16Å 49.09Å 115.07Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	45.16 – 2.17 45.12 – 2.17	Depositor EDS
% Data completeness (in resolution range)	80.2 (45.16-2.17) 80.2 (45.12-2.17)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, $R_{free}$	0.249 , 0.347 0.254 , 0.347	Depositor DCC
$R_{free}$ test set	1873 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 32.45 % 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 9.3739e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DGL, O0J, 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	0.39	0/1502	0.79	0/2019
1	B	0.39	0/1516	0.81	0/2038
1	C	0.39	0/1535	0.77	0/2063
1	D	0.42	0/1502	0.83	0/2019
All	All	0.40	0/6055	0.80	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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Sidechain
1	B	197	ARG	Sidechain
1	C	197[A]	ARG	Sidechain
1	D	113	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	35	0
1	B	1495	0	1541	35	0
1	C	1514	0	1558	24	0
1	D	1481	0	1530	95	0
2	A	16	0	0	4	0
3	A	4	0	6	0	0
3	B	8	0	12	1	0
3	C	12	0	18	0	0
3	D	8	0	12	0	0
4	B	10	0	7	1	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	2	0
7	D	6	0	4	0	0
8	A	42	0	0	7	0
8	B	90	0	0	8	0
8	C	67	0	0	3	0
8	D	73	0	0	19	0
All	All	6337	0	6229	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (184) 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:152:LEU:O	8:D:401:HOH:O	1.79	0.98
1:B:150:VAL:O	8:B:401:HOH:O	1.89	0.90
1:D:128:ARG:O	1:D:129:LEU:HD23	1.79	0.82
1:B:133:ASP:OD1	3:B:301:EDO:O2	1.97	0.82
1:B:173:LYS:O	1:B:177:VAL:HG23	1.81	0.80
1:C:128:ARG:HB2	1:C:140:LEU:HB3	1.65	0.79
1:A:280:LYS:HA	8:A:433:HOH:O	1.82	0.79
1:B:133:ASP:OD1	8:B:402:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:MET:SD	8:D:473:HOH:O	2.44	0.75
1:D:238:ILE:O	8:D:402:HOH:O	2.05	0.75
1:D:139:GLN:HG2	1:D:282:MET:HE1	1.68	0.75
1:D:139:GLN:O	1:D:282:MET:HE1	1.88	0.73
1:D:215:ASN:O	8:D:403:HOH:O	2.06	0.73
1:C:229:ARG:NH2	8:C:401:HOH:O	2.21	0.73
1:D:208:HIS:CG	8:D:419:HOH:O	2.41	0.72
1:A:128:ARG:HB3	1:A:140:LEU:HB3	1.72	0.70
1:D:150:VAL:O	8:D:404:HOH:O	2.09	0.70
1:D:152:LEU:C	8:D:401:HOH:O	2.27	0.69
1:D:226:SER:OG	6:D:303:SO4:O2	2.10	0.67
1:D:237:ASN:OD1	8:D:405:HOH:O	2.12	0.67
1:D:272:ALA:HB1	8:D:422:HOH:O	1.95	0.67
1:A:197:ARG:NH2	8:A:402:HOH:O	2.19	0.67
1:D:139:GLN:HG2	1:D:282:MET:CE	2.27	0.65
1:D:204:ASP:OD2	8:D:406:HOH:O	2.13	0.64
1:D:141:VAL:HG21	1:D:152:LEU:O	1.97	0.64
1:D:237:ASN:O	1:D:269:ILE:HA	1.98	0.64
1:B:160:GLN:NE2	1:B:165:ASN:OD1	2.29	0.63
1:B:202:HIS:O	1:B:203:LYS:O	2.15	0.63
1:A:128:ARG:HD3	2:A:301:O0J:C6	2.29	0.63
1:D:295:ILE:HG23	1:D:296:PRO:HD2	1.81	0.62
1:B:262:GLY:O	1:B:263:THR:C	2.39	0.61
1:D:293:HIS:NE2	8:D:408:HOH:O	2.31	0.61
1:D:203:LYS:HG3	1:D:263:THR:O	2.02	0.60
1:B:119:LYS:NZ	1:B:178:LEU:O	2.31	0.60
1:D:283:ALA:O	1:D:284:PRO:C	2.40	0.60
1:D:144:ASN:ND2	8:D:411:HOH:O	2.35	0.59
1:B:196:GLU:OE1	8:B:404:HOH:O	2.17	0.59
1:C:118:CYS:SG	1:C:184:GLU:O	2.59	0.59
1:A:204:ASP:O	1:A:207:GLY:N	2.29	0.59
1:B:204:ASP:OD2	8:B:403:HOH:O	2.16	0.59
1:A:125:ILE:HD11	1:A:178:LEU:HD13	1.85	0.58
1:A:204:ASP:OD1	1:A:208:HIS:N	2.33	0.58
1:D:108:ILE:HG12	1:D:193:ARG:CZ	2.34	0.58
1:B:200:THR:O	1:B:230:ASN:ND2	2.36	0.58
1:A:128:ARG:HB2	2:A:301:O0J:C7	2.34	0.57
1:D:252:SER:O	1:D:255:ALA:HB3	2.05	0.57
1:D:126:GLY:HA3	1:D:145:SER:HB2	1.85	0.57
1:D:254:ILE:O	1:D:255:ALA:C	2.41	0.57
2:A:301:O0J:O	1:B:118:CYS:SG	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ILE:HD13	1:D:178:LEU:HD21	1.86	0.57
1:D:252:SER:CB	8:D:410:HOH:O	2.53	0.56
1:A:128:ARG:NE	1:A:139:GLN:OE1	2.38	0.56
1:D:158:VAL:O	1:D:166:CYS:SG	2.61	0.56
1:A:157:GLN:HG2	1:A:159:LEU:HD23	1.88	0.56
1:D:142:GLN:HB3	1:D:145:SER:HB3	1.86	0.56
1:D:251:ASP:N	6:D:304:SO4:O2	2.39	0.55
1:B:202:HIS:O	1:B:203:LYS:C	2.44	0.55
1:D:261:SER:OG	1:D:265:VAL:HG22	2.07	0.55
1:D:287:MET:O	1:D:291:MET:HB2	2.06	0.55
1:B:151:GLY:HA3	8:B:401:HOH:O	2.06	0.55
1:D:292:ASP:OD1	1:D:294:THR:HG23	2.07	0.55
1:A:128:ARG:HD3	2:A:301:O0J:C5	2.38	0.54
1:B:193:ARG:HB3	1:B:196:GLU:HB2	1.89	0.54
1:D:169:TRP:HE3	1:D:174:ALA:HB2	1.73	0.54
1:D:116:ILE:O	1:D:150:VAL:HG11	2.07	0.54
1:D:206:THR:OG1	1:D:208:HIS:ND1	2.40	0.53
1:D:287:MET:HG3	1:D:291:MET:CE	2.38	0.53
1:A:112:ILE:HD11	1:A:191:ARG:NH2	2.24	0.53
1:A:215:ASN:O	8:A:401:HOH:O	2.18	0.53
1:C:206:THR:OG1	1:C:208:HIS:ND1	2.41	0.53
1:D:270:MET:SD	1:D:275:PHE:HA	2.49	0.53
1:A:286:ILE:HG23	1:A:290:LEU:CD1	2.39	0.52
1:C:196:GLU:O	1:C:197[B]:ARG:HD3	2.08	0.52
1:D:261:SER:CB	1:D:265:VAL:HG22	2.38	0.52
1:D:239:CYS:HB2	1:D:268:THR:HG22	1.91	0.52
1:D:198:THR:HA	1:D:267:ILE:O	2.10	0.52
1:C:193:ARG:HG2	1:C:196:GLU:OE1	2.10	0.52
1:D:272:ALA:C	8:D:422:HOH:O	2.48	0.52
1:B:129:LEU:H	1:B:175:HIS:CE1	2.29	0.51
1:B:136:ILE:HD11	1:B:169:TRP:O	2.11	0.51
1:D:161:ILE:HG22	1:D:162:ASN:HD22	1.74	0.51
1:A:226:SER:OG	8:A:403:HOH:O	2.19	0.51
1:A:276:GLU:OE2	8:A:404:HOH:O	2.19	0.51
1:D:195:PHE:HD2	1:D:278:ILE:HD11	1.76	0.51
1:D:203:LYS:HE3	1:D:265:VAL:CG2	2.41	0.51
1:D:119:LYS:HG3	1:D:183:GLY:HA3	1.93	0.50
1:A:136:ILE:HD11	1:A:169:TRP:O	2.12	0.50
1:A:169:TRP:O	8:A:405:HOH:O	2.20	0.50
1:D:215:ASN:CB	8:D:403:HOH:O	2.60	0.50
1:D:274:ILE:O	1:D:275:PHE:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HG2	1:C:197[B]:ARG:HH12	1.77	0.49
1:D:145:SER:OG	1:D:147:ALA:HB3	2.11	0.49
1:D:255:ALA:O	8:D:407:HOH:O	2.20	0.49
1:A:256:ASP:O	1:A:260:THR:HG23	2.11	0.49
1:A:281:ARG:CD	1:B:122:ASP:HA	2.42	0.49
1:B:241:ILE:HD11	1:B:254:ILE:HG23	1.95	0.49
1:B:281:ARG:HD2	4:B:303:DGL:HA	1.94	0.49
1:D:198:THR:HG22	1:D:268:THR:OG1	2.13	0.48
1:C:210:GLY:HA3	1:C:225:SER:CB	2.44	0.48
1:D:140:LEU:HD23	1:D:141:VAL:C	2.34	0.48
1:D:252:SER:HB3	8:D:410:HOH:O	2.14	0.48
1:A:193:ARG:NH1	1:A:240:GLU:OE1	2.46	0.48
1:A:120:ASP:OD1	1:A:124:LYS:HB2	2.14	0.48
1:D:295:ILE:HG22	1:D:297:GLU:H	1.78	0.47
1:A:266:THR:HG22	8:A:423:HOH:O	2.13	0.47
1:B:262:GLY:HA2	8:B:412:HOH:O	2.13	0.47
1:B:112:ILE:CG2	1:B:189:THR:HG22	2.44	0.47
1:C:173:LYS:O	1:C:177:VAL:HG23	2.15	0.47
1:D:132:ILE:HD12	1:D:277:HIS:ND1	2.30	0.47
1:A:128:ARG:HB3	1:A:140:LEU:CB	2.43	0.47
1:D:125:ILE:HD11	1:D:178:LEU:HD13	1.96	0.47
1:B:197:ARG:NH2	1:B:233:LEU:HD12	2.30	0.47
1:D:270:MET:SD	1:D:278:ILE:HD12	2.54	0.47
1:B:200:THR:OG1	1:B:266:THR:OG1	2.26	0.46
1:B:202:HIS:C	1:B:203:LYS:O	2.53	0.46
1:B:203:LYS:HB3	1:B:207:GLY:HA2	1.98	0.46
1:D:274:ILE:O	1:D:277:HIS:N	2.48	0.46
1:B:250:LYS:O	1:B:251:ASP:C	2.54	0.46
1:D:154:PHE:CZ	1:D:247:ILE:HD13	2.50	0.46
1:B:238:ILE:HG23	1:B:267:ILE:HG23	1.98	0.46
1:A:270:MET:O	1:A:271:PRO:C	2.54	0.46
1:D:265:VAL:HG12	1:D:267:ILE:CG2	2.46	0.46
1:B:201:MET:SD	1:B:227:ALA:HA	2.55	0.46
1:D:239:CYS:HA	1:D:247:ILE:CG1	2.45	0.45
1:D:212:ILE:O	1:D:219:THR:OG1	2.21	0.45
1:D:285:SER:O	1:D:289:SER:OG	2.27	0.45
1:D:291:MET:O	1:D:293:HIS:CD2	2.70	0.45
1:A:261:SER:OG	1:A:262:GLY:N	2.50	0.45
1:A:157:GLN:O	1:A:190:ILE:HA	2.17	0.45
1:B:224:ASP:HB3	8:B:423:HOH:O	2.16	0.45
1:A:241:ILE:O	1:A:242:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ALA:CB	8:D:422:HOH:O	2.59	0.44
1:A:281:ARG:HD2	1:B:122:ASP:HA	1.98	0.44
1:D:218:ILE:HD13	1:D:232:LEU:HD21	1.98	0.44
1:A:210:GLY:HA3	1:A:225:SER:HB2	1.99	0.44
1:D:147:ALA:O	1:D:148:SER:C	2.56	0.44
1:D:203:LYS:HD2	1:D:262:GLY:O	2.18	0.43
1:A:206:THR:HG22	1:A:206:THR:O	2.17	0.43
1:A:137:PHE:HZ	1:C:233:LEU:HD11	1.82	0.43
1:C:197[A]:ARG:NH1	8:C:405:HOH:O	2.32	0.43
1:A:286:ILE:HG23	1:A:290:LEU:HD12	2.01	0.43
1:C:192:ASP:O	1:C:193:ARG:C	2.56	0.43
1:D:193:ARG:HD2	1:D:240:GLU:OE2	2.19	0.43
1:C:236:HIS:CD2	1:C:269:ILE:HD12	2.54	0.43
1:C:242:ASN:ND2	1:C:261:SER:OG	2.51	0.43
1:D:140:LEU:HD12	1:D:282:MET:SD	2.59	0.43
1:D:283:ALA:O	1:D:285:SER:N	2.52	0.43
1:A:137:PHE:CE2	1:A:195:PHE:CE2	3.07	0.43
1:D:224:ASP:O	1:D:229:ARG:NH1	2.50	0.43
1:D:249:LEU:HD21	1:D:293:HIS:CD2	2.54	0.42
1:D:258:LEU:O	1:D:261:SER:HB3	2.19	0.42
1:C:114:GLU:HG2	1:C:115:VAL:N	2.34	0.42
1:D:156:ASP:OD1	1:D:193:ARG:HG3	2.19	0.42
1:C:161:ILE:HG12	1:C:188:MET:HG2	2.01	0.42
1:D:218:ILE:CD1	1:D:232:LEU:HD11	2.50	0.42
1:C:119:LYS:HD3	1:C:123:GLY:O	2.19	0.42
1:D:295:ILE:CG2	1:D:296:PRO:HD2	2.46	0.42
1:C:294:THR:HG22	1:C:295:ILE:N	2.35	0.42
1:D:270:MET:CE	1:D:278:ILE:HD12	2.50	0.42
1:D:272:ALA:O	1:D:274:ILE:N	2.53	0.42
1:B:223:LYS:O	1:B:224:ASP:C	2.58	0.42
1:D:249:LEU:HD21	1:D:293:HIS:NE2	2.35	0.42
1:C:238:ILE:HG23	1:C:267:ILE:HG23	2.02	0.42
1:C:210:GLY:HA3	1:C:225:SER:HB2	2.01	0.41
1:D:142:GLN:HG2	1:D:143:ALA:O	2.20	0.41
1:D:203:LYS:HD2	1:D:263:THR:HA	2.02	0.41
1:D:204:ASP:N	1:D:208:HIS:O	2.52	0.41
1:D:244:GLN:NE2	1:D:295:ILE:HD11	2.35	0.41
1:C:251:ASP:HB3	1:D:206:THR:HG21	2.02	0.41
1:D:244:GLN:O	1:D:246:VAL:HG13	2.19	0.41
1:B:198:THR:HG23	1:B:266:THR:HG23	2.02	0.41
1:D:195:PHE:CD2	1:D:278:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197[A]:ARG:NH2	8:C:406:HOH:O	2.47	0.41
1:D:248:GLY:O	1:D:249:LEU:O	2.39	0.41
1:D:261:SER:HB3	1:D:265:VAL:HG22	2.01	0.41
1:B:253:GLN:NE2	8:B:406:HOH:O	2.51	0.41
1:C:294:THR:CG2	1:C:295:ILE:N	2.84	0.41
1:D:275:PHE:CZ	1:D:279:ILE:HG21	2.56	0.41
1:C:248:GLY:O	1:C:249:LEU:C	2.60	0.40
1:D:143:ALA:O	1:D:144:ASN:CB	2.68	0.40
1:D:215:ASN:HB2	8:D:403:HOH:O	2.21	0.40
1:D:222:VAL:O	1:D:225:SER:HB3	2.22	0.40
1:D:248:GLY:CA	1:D:287:MET:HE3	2.50	0.40
1:B:202:HIS:HA	1:B:263:THR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	190/195 (97%)	179 (94%)	9 (5%)	2 (1%)	14	11
1	B	192/195 (98%)	179 (93%)	10 (5%)	3 (2%)	9	6
1	C	194/195 (100%)	180 (93%)	13 (7%)	1 (0%)	29	28
1	D	190/195 (97%)	158 (83%)	29 (15%)	3 (2%)	9	6
All	All	766/780 (98%)	696 (91%)	61 (8%)	9 (1%)	13	9

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	LYS
1	D	249	LEU
1	B	120	ASP

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Mol	Chain	Res	Type
1	D	262	GLY
1	D	144	ASN
1	B	263	THR
1	A	193	ARG
1	A	279	ILE
1	C	210	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%)	159 (96%)	7 (4%)	30	35
1	B	167/168 (99%)	163 (98%)	4 (2%)	49	59
1	C	169/168 (101%)	164 (97%)	5 (3%)	41	49
1	D	166/168 (99%)	161 (97%)	5 (3%)	41	49
All	All	668/672 (99%)	647 (97%)	21 (3%)	39	48

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	CYS
1	A	140	LEU
1	A	148	SER
1	A	226	SER
1	A	252	SER
1	A	281	ARG
1	A	289	SER
1	B	122	ASP
1	B	202	HIS
1	B	220	SER
1	B	266	THR
1	C	110	GLN
1	C	117	LEU
1	C	122	ASP
1	C	209	VAL

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Mol	Chain	Res	Type
1	C	263	THR
1	D	184	GLU
1	D	190	ILE
1	D	266	THR
1	D	267	ILE
1	D	289	SER

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

Mol	Chain	Res	Type
1	A	180	GLN
1	B	134	ASN
1	B	139	GLN
1	B	230	ASN
1	C	110	GLN
1	C	134	ASN
1	D	142	GLN
1	D	144	ASN
1	D	162	ASN
1	D	180	GLN
1	D	237	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	302	-	3,3,3	0.12	0	2,2,2	0.23	0
3	EDO	B	302	-	3,3,3	0.47	0	2,2,2	0.85	0
6	SO4	D	303	-	4,4,4	0.31	0	6,6,6	0.07	0
2	O0J	A	301	-	14,17,17	<b>2.83</b>	<b>5 (35%)</b>	18,23,23	<b>2.12</b>	<b>5 (27%)</b>
3	EDO	D	301	-	3,3,3	0.17	0	2,2,2	0.10	0
5	GLY	C	304	-	4,4,4	0.94	0	3,4,4	1.09	0
7	ALA	D	305	-	5,5,5	0.85	0	6,6,6	0.84	0
6	SO4	D	304	-	4,4,4	0.35	0	6,6,6	0.12	0
3	EDO	C	303	-	3,3,3	0.91	0	2,2,2	1.07	0
3	EDO	C	301	-	3,3,3	0.30	0	2,2,2	0.40	0
3	EDO	D	302	-	3,3,3	0.13	0	2,2,2	0.17	0
4	DGL	B	303	-	8,9,9	0.90	0	10,11,11	1.17	<b>1 (10%)</b>
5	GLY	D	307	-	4,4,4	0.98	0	3,4,4	1.04	0
3	EDO	B	301	-	3,3,3	0.09	0	2,2,2	0.16	0
3	EDO	C	302	-	3,3,3	0.23	0	2,2,2	0.30	0
4	DGL	D	306	-	8,9,9	0.94	0	10,11,11	1.27	<b>1 (10%)</b>

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
2	O0J	A	301	-	-	0/8/8/8	0/2/2/2
3	EDO	D	301	-	-	0/1/1/1	-
5	GLY	C	304	-	-	<b>2/2/2/2</b>	-
7	ALA	D	305	-	-	<b>4/4/4/4</b>	-
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	C	301	-	-	1/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
4	DGL	B	303	-	-	<b>3/9/9/9</b>	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLY	D	307	-	-	2/2/2/2	-
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
4	DGL	D	306	-	-	5/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	O0J	C9-S	-6.23	1.60	1.70
2	A	301	O0J	C1-N	6.01	1.47	1.36
2	A	301	O0J	C8-N2	3.50	1.48	1.37
2	A	301	O0J	C10-N1	3.05	1.44	1.35
2	A	301	O0J	C2-N	2.68	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	O0J	C9-C8-C5	-5.38	121.96	129.44
2	A	301	O0J	C5-C8-N2	3.32	126.36	120.78
2	A	301	O0J	C6-C5-C8	-3.04	116.48	121.28
4	B	303	DGL	CB-CA-C	2.60	116.50	110.30
2	A	301	O0J	C8-C9-S	-2.46	108.77	111.79
2	A	301	O0J	N1-C10-N2	2.34	126.22	123.19
4	D	306	DGL	CB-CA-C	2.08	115.24	110.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	304	GLY	O-C-CA-N
5	C	304	GLY	OXT-C-CA-N
5	D	307	GLY	O-C-CA-N
5	D	307	GLY	OXT-C-CA-N
3	C	301	EDO	O1-C1-C2-O2
3	C	303	EDO	O1-C1-C2-O2
7	D	305	ALA	O-C-CA-CB
7	D	305	ALA	OXT-C-CA-CB
4	B	303	DGL	CA-CB-CG-CD
4	D	306	DGL	OXT-C-CA-CB
4	D	306	DGL	CA-CB-CG-CD
4	D	306	DGL	O-C-CA-CB

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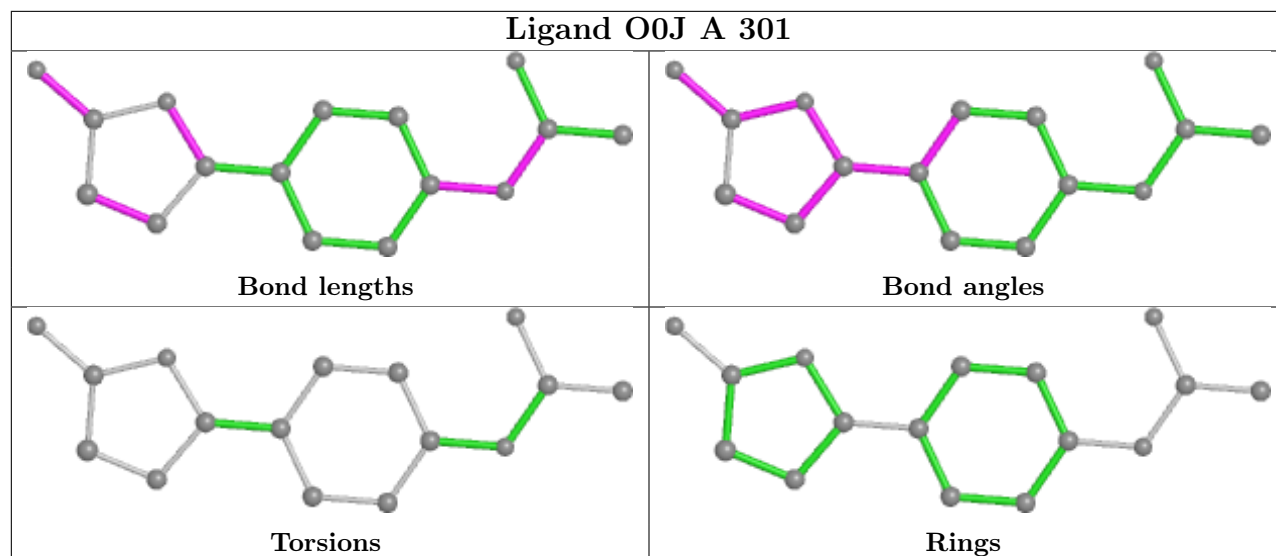
Mol	Chain	Res	Type	Atoms
7	D	305	ALA	OXT-C-CA-N
3	C	302	EDO	O1-C1-C2-O2
4	D	306	DGL	OE2-CD-CG-CB
4	B	303	DGL	OE1-CD-CG-CB
4	D	306	DGL	OE1-CD-CG-CB
4	B	303	DGL	OE2-CD-CG-CB
7	D	305	ALA	O-C-CA-N
3	A	302	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	303	SO4	1	0
2	A	301	O0J	4	0
6	D	304	SO4	1	0
4	B	303	DGL	1	0
3	B	301	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	191/195 (97%)	0.35	5 (2%) 56 56	20, 49, 82, 153	1 (0%)
1	B	193/195 (98%)	0.25	5 (2%) 56 56	17, 50, 77, 104	1 (0%)
1	C	193/195 (98%)	0.39	10 (5%) 27 28	21, 51, 82, 110	3 (1%)
1	D	191/195 (97%)	0.86	29 (15%) 2 2	26, 63, 89, 113	1 (0%)
All	All	768/780 (98%)	0.46	49 (6%) 19 20	17, 54, 84, 153	6 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ALA	11.3
1	C	273[A]	PHE	6.4
1	C	197[A]	ARG	6.4
1	D	273[A]	PHE	5.7
1	D	116	ILE	5.7
1	B	273[A]	PHE	5.6
1	A	273[A]	PHE	5.2
1	B	110	GLN	5.0
1	D	265	VAL	4.5
1	B	106	ALA	4.4
1	A	282	MET	4.2
1	D	258	LEU	4.0
1	D	125	ILE	3.7
1	D	163	GLY	3.6
1	A	110	GLN	3.5
1	D	298	VAL	3.4
1	C	110	GLN	3.4
1	D	213	PHE	3.4
1	C	106	ALA	3.3
1	D	178	LEU	3.3
1	D	184	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	184	GLU	3.2
1	D	254	ILE	3.2
1	D	110	GLN	3.1
1	C	144[A]	ASN	3.1
1	D	264	VAL	3.0
1	A	108	ILE	3.0
1	C	109	LYS	2.9
1	D	189	THR	2.9
1	C	108	ILE	2.9
1	B	125	ILE	2.8
1	D	182	PHE	2.7
1	D	112	ILE	2.6
1	D	280	LYS	2.6
1	D	207	GLY	2.5
1	C	107	GLU	2.5
1	D	249	LEU	2.5
1	D	187	THR	2.4
1	D	144	ASN	2.4
1	D	288	LYS	2.4
1	D	190	ILE	2.4
1	D	141	VAL	2.3
1	D	185	LYS	2.3
1	D	286	ILE	2.3
1	C	281	ARG	2.2
1	B	281	ARG	2.2
1	D	150	VAL	2.0
1	D	177	VAL	2.0
1	D	149	LEU	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.

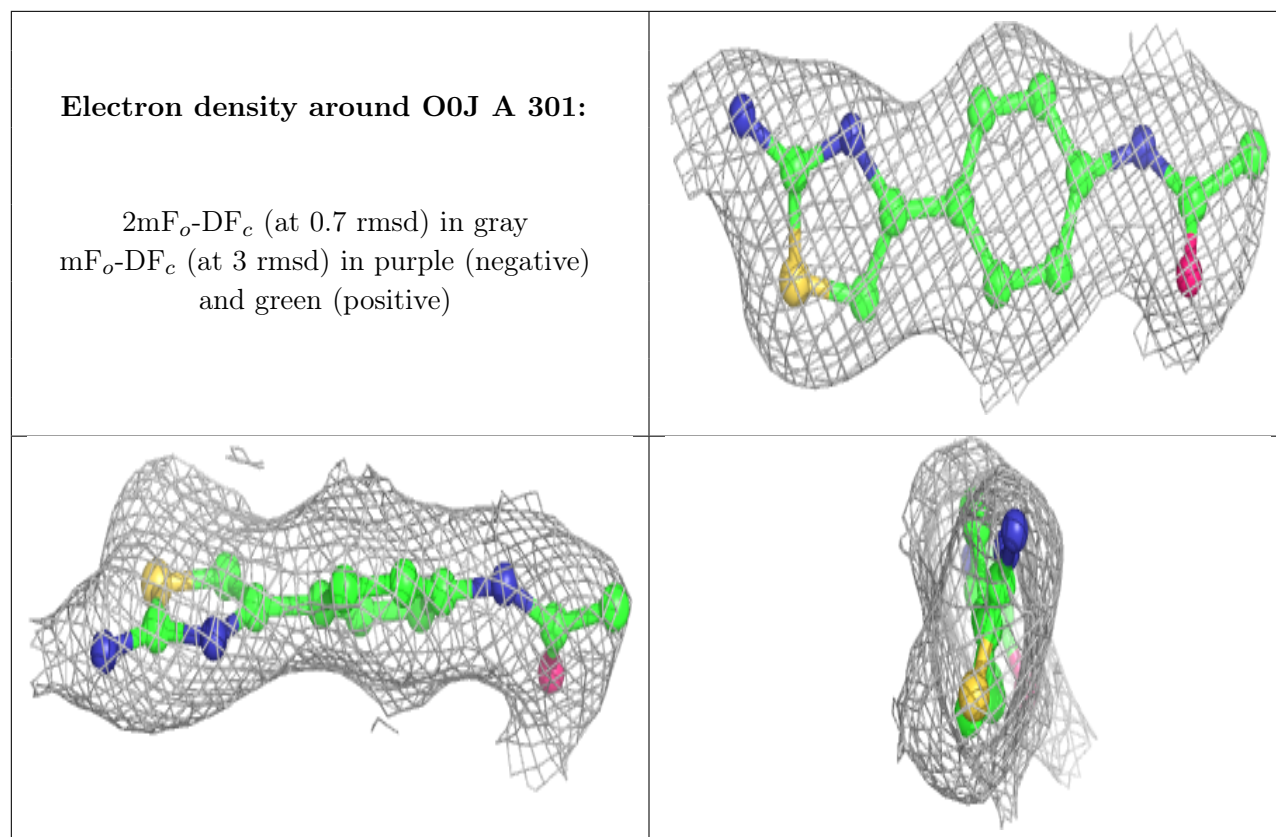
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	DGL	B	303	10/10	0.77	0.31	67,85,91,93	0
4	DGL	D	306	10/10	0.83	0.24	60,98,115,120	0
5	GLY	D	307	5/5	0.83	0.19	60,61,62,63	0
7	ALA	D	305	6/6	0.86	0.18	65,67,72,91	0
3	EDO	C	303	4/4	0.88	0.20	38,50,52,52	0
3	EDO	D	302	4/4	0.90	0.17	46,47,49,52	0
3	EDO	A	302	4/4	0.92	0.15	51,54,58,59	0
6	SO4	D	304	5/5	0.92	0.10	80,105,107,108	0
5	GLY	C	304	5/5	0.92	0.17	62,67,84,96	0
3	EDO	B	301	4/4	0.94	0.14	38,46,46,49	0
3	EDO	D	301	4/4	0.94	0.16	45,50,52,58	0
3	EDO	C	302	4/4	0.94	0.16	41,41,41,46	0
6	SO4	D	303	5/5	0.95	0.19	84,87,92,103	0
2	O0J	A	301	16/16	0.95	0.13	47,52,59,60	0
3	EDO	C	301	4/4	0.95	0.12	38,41,45,47	0
3	EDO	B	302	4/4	0.96	0.19	37,37,39,44	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.