



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:35 am BST

PDB ID : 6Q5F
Title : OXA-48_P68A-CAZ. Evolutionary trade-offs of OXA-48 mediated ceftazidim
e-avibactam resistance
Authors : Frohlich, C.; Sorum, V.; Thomassen, A.M.; Johnsen, P.J.; Leiros, H.-K.S.;
Samuelsen, O.
Deposited on : 2018-12-08
Resolution : 2.50 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 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 : 2.11
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) : 2.11

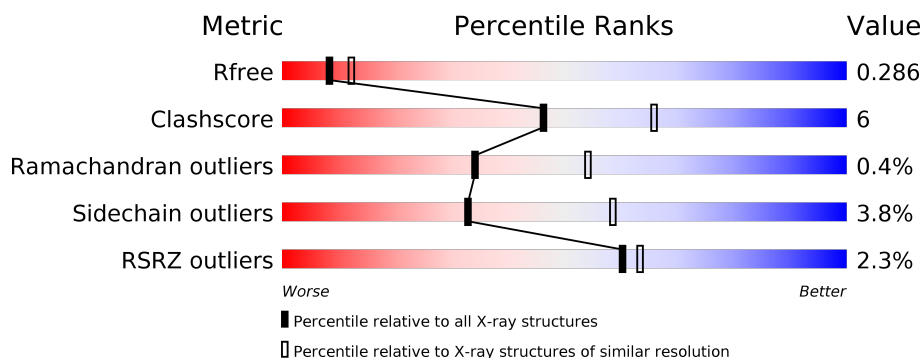
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


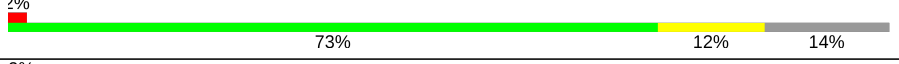


The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	265	 <p>2% 68% 17% 14%</p>
1	C	265	 <p>2% 73% 12% 14%</p>
2	B	265	 <p>3% 79% 12% 9%</p>
2	D	265	 <p>2% 74% 16% 9%</p>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PGE	B	303	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15947 atoms, of which 7662 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	229	Total	C	H	N	O	S	0	0	0
			3729	1198	1847	334	343	7			
1	C	229	Total	C	H	N	O	S	1	2	0
			3730	1199	1846	335	343	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	PRO	engineered mutation	UNP Q6XEC0
C	68	ALA	PRO	engineered mutation	UNP Q6XEC0

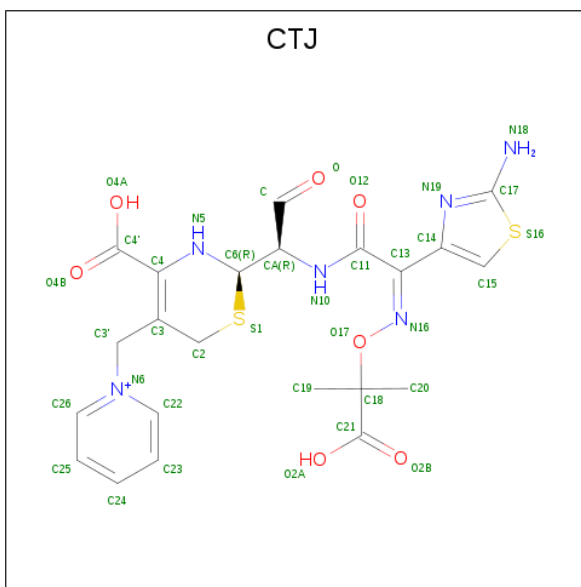
- Molecule 2 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	242	Total	C	H	N	O	S	0	0	0
			3911	1260	1930	349	365	7			
2	D	242	Total	C	H	N	O	S	0	4	0
			3935	1267	1941	350	370	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	68	ALA	PRO	engineered mutation	UNP Q6XEC0
D	68	ALA	PRO	engineered mutation	UNP Q6XEC0

- Molecule 3 is 1-({(2R)-2-[(1R)-1-[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-[(2-carboxypropan-2-yl)oxy]imino}acetyl]amino}-2-oxoethyl]-4-carboxy-3,6-dihydro-2H-1,3-thiazin-5-yl)methyl)pyridinium (three-letter code: CTJ) (formula: C₂₂H₂₅N₆O₇S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			60	22	23	6	7	2		
3	C	1	Total	C	H	N	O	S	0	0
			60	22	23	6	7	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

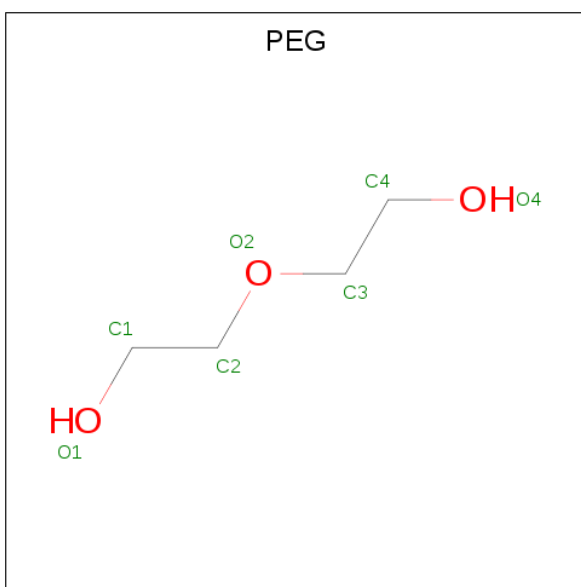
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



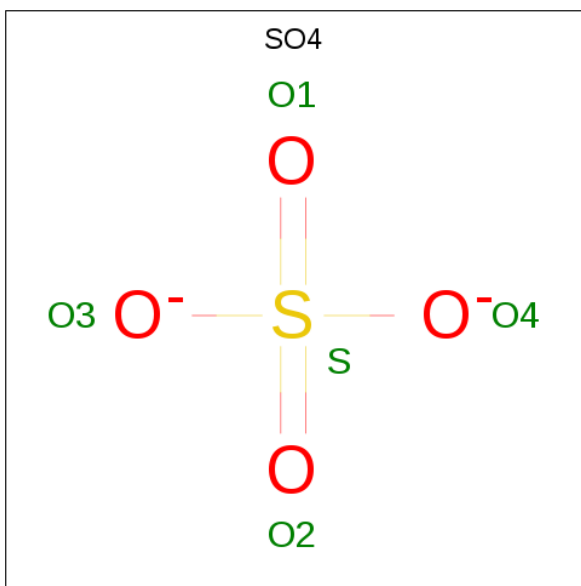
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	14	4		
5	B	1	Total	C	H	O	0	0
			24	6	14	4		
5	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

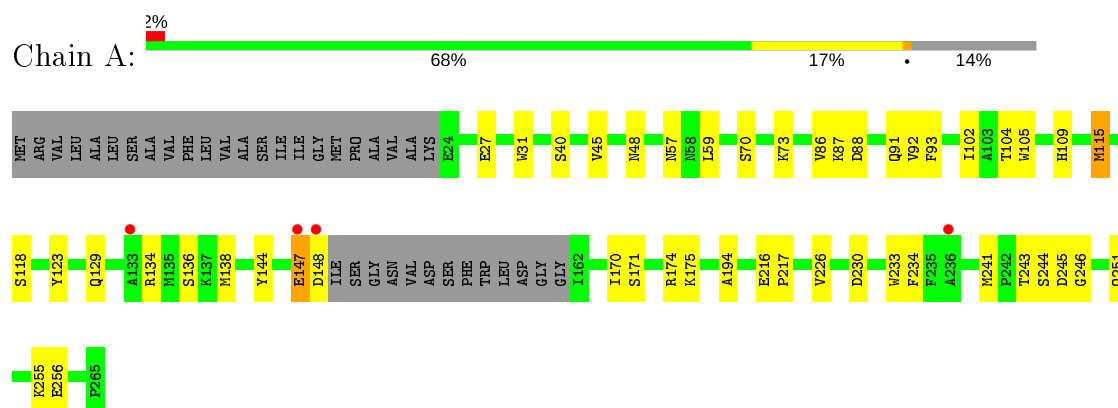
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	111	Total	O	0	0
			111	111		
8	B	106	Total	O	0	0
			106	106		
8	C	94	Total	O	0	0
			94	94		
8	D	111	Total	O	0	0
			111	111		

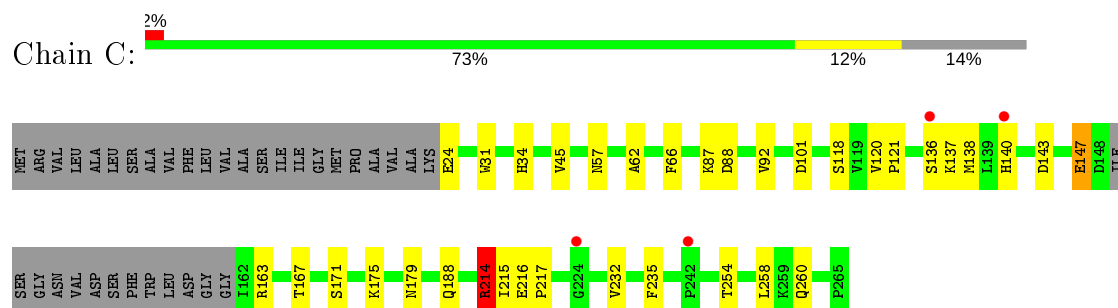
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

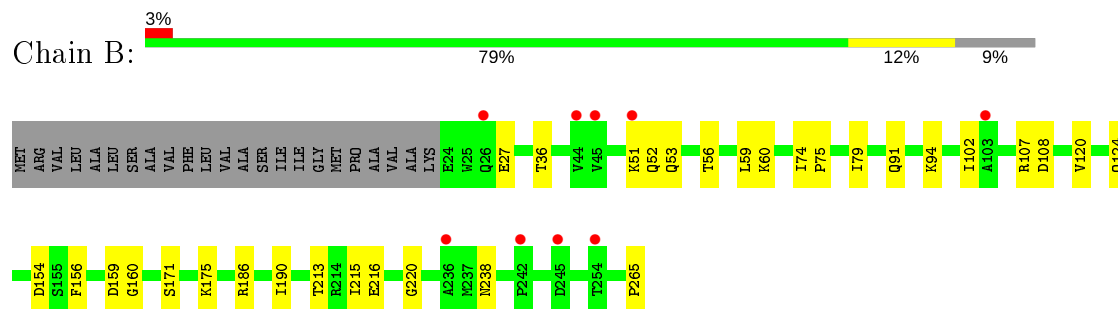
• Molecule 1: Beta-lactamase



• Molecule 1: Beta-lactamase

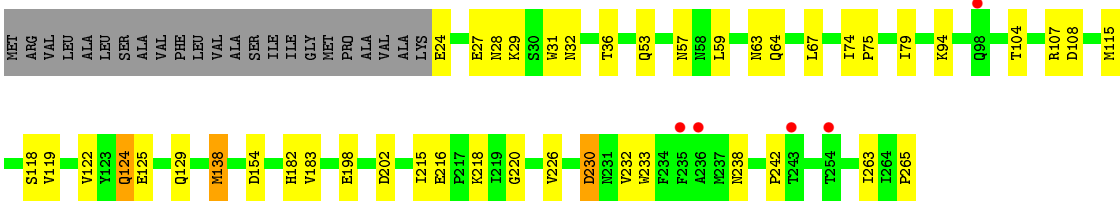


• Molecule 2: Beta-lactamase



• Molecule 2: Beta-lactamase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.99Å 105.37Å 125.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 2.50 24.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.97-2.50) 97.8 (24.97-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.50Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.224 , 0.286 0.224 , 0.286	Depositor DCC
R_{free} test set	2024 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15947	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 53.32 % 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 4.2853e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: PGE, CL, SO4, PEG, KCX, CTJ

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	0.68	0/1926	0.73	0/2601
1	C	0.65	0/1937	0.73	1/2616 (0.0%)
2	B	0.67	0/2016	0.70	1/2725 (0.0%)
2	D	0.68	0/2040	0.71	0/2757
All	All	0.67	0/7919	0.72	2/10699 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	154	ASP	CB-CG-OD1	-5.21	113.62	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1882	1847	1847	28	0
1	C	1884	1846	1829	19	1
2	B	1981	1930	1930	17	1
2	D	1994	1941	1929	30	0
3	A	37	23	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	37	23	22	5	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	10	14	14	1	0
5	B	10	14	14	0	0
5	C	10	14	14	0	0
6	C	7	10	10	3	0
7	D	5	0	0	0	0
8	A	111	0	0	4	0
8	B	106	0	0	3	0
8	C	94	0	0	1	0
8	D	111	0	0	7	0
All	All	8285	7662	7631	98	1

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 6.

All (98) 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)
2:D:230[A]:ASP:OD2	8:D:401:HOH:O	1.92	0.87
1:A:243:THR:O	8:A:401:HOH:O	2.00	0.78
5:A:304:PGE:O4	8:A:402:HOH:O	2.04	0.74
2:D:67:LEU:HD11	2:D:215:ILE:HD12	1.67	0.74
3:C:301:CTJ:H20	6:C:304:PEG:H42	1.71	0.73
2:D:94:LYS:NZ	8:D:402:HOH:O	2.23	0.72
2:D:215:ILE:HG22	2:D:216:GLU:O	1.93	0.68
1:C:140:HIS:ND1	1:C:147:GLU:OE1	2.29	0.66
1:A:147:GLU:HG3	1:A:147:GLU:O	1.99	0.63
2:D:216:GLU:OE1	2:D:218:LYS:NZ	2.29	0.63
2:D:119:VAL:HG12	2:D:122:VAL:HG23	1.82	0.61
1:C:214:ARG:HG2	3:C:301:CTJ:H19	1.84	0.60
1:C:31:TRP:HB2	1:C:57:ASN:HB3	1.85	0.59
2:B:265:PRO:OXT	8:B:401:HOH:O	2.17	0.59
2:B:159:ASP:OD2	8:B:402:HOH:O	2.18	0.57
1:C:62:ALA:O	1:C:167:THR:HG23	2.05	0.56
1:A:230:ASP:N	1:A:230:ASP:OD1	2.39	0.55
1:A:31:TRP:HB2	1:A:57:ASN:HB3	1.89	0.55
3:C:301:CTJ:C20	6:C:304:PEG:H42	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:VAL:CG1	2:D:122:VAL:HG23	2.36	0.55
2:D:75:PRO:O	2:D:79:ILE:HG13	2.07	0.55
1:C:216:GLU:OE2	1:C:217:PRO:HA	2.07	0.55
2:D:79:ILE:HG12	2:D:138:MET:HG2	1.90	0.54
1:A:104:THR:O	1:A:109:HIS:NE2	2.35	0.53
2:B:107:ARG:HG3	2:B:108:ASP:O	2.08	0.53
2:D:233:TRP:CD2	2:D:263:ILE:HD11	2.44	0.52
1:A:102:ILE:HD12	1:A:105:TRP:CZ2	2.45	0.51
1:A:245:ASP:OD1	8:A:403:HOH:O	2.19	0.51
1:A:73:LYS:HB3	1:A:115:MET:CE	2.40	0.51
2:D:28:ASN:ND2	8:D:407:HOH:O	2.39	0.51
1:A:73:LYS:HB3	1:A:115:MET:HE2	1.93	0.50
2:D:124:GLN:HB3	2:D:154:ASP:HB2	1.93	0.50
3:C:301:CTJ:H20	6:C:304:PEG:C4	2.40	0.49
2:B:27:GLU:HB2	2:B:59:LEU:HD11	1.94	0.48
2:D:216:GLU:OE1	2:D:218:LYS:HG3	2.13	0.48
1:A:241:MET:HE1	1:A:246:GLY:O	2.13	0.48
1:A:27:GLU:HB2	1:A:59:LEU:HD11	1.96	0.48
2:D:182:HIS:O	2:D:183:VAL:HG13	2.14	0.48
2:D:28:ASN:HB3	8:D:410:HOH:O	2.14	0.47
1:A:171:SER:O	1:A:175:LYS:HG3	2.15	0.47
1:C:214:ARG:CG	3:C:301:CTJ:H19	2.45	0.46
1:C:101:ASP:OD1	1:C:101:ASP:N	2.49	0.46
2:B:159:ASP:HA	2:B:215:ILE:HD12	1.97	0.46
1:C:66:PHE:O	1:C:163:ARG:HA	2.16	0.46
2:B:56:THR:CG2	2:B:59:LEU:HD23	2.46	0.46
2:D:27:GLU:OE2	2:D:29:LYS:HE3	2.16	0.45
1:A:102:ILE:CD1	1:A:105:TRP:CZ2	3.00	0.45
1:A:70:SER:N	3:A:301:CTJ:O	2.49	0.45
1:C:34:HIS:NE2	1:C:260:GLN:OE1	2.45	0.45
1:A:86:VAL:HG22	1:A:93:PHE:CZ	2.52	0.45
2:B:74:ILE:HB	2:B:75:PRO:HD3	1.98	0.45
2:D:104:THR:HG22	2:D:107:ARG:NH2	2.32	0.45
2:B:74:ILE:HB	2:B:75:PRO:CD	2.46	0.44
1:A:45:VAL:HG12	1:A:170:ILE:CD1	2.47	0.44
2:D:242:PRO:HA	8:D:414:HOH:O	2.17	0.44
2:D:32:ASN:O	2:D:36:THR:HG23	2.18	0.44
2:B:213:THR:HG22	8:B:438:HOH:O	2.17	0.44
2:D:107:ARG:HG3	2:D:108:ASP:O	2.17	0.44
2:D:24:GLU:N	8:D:416:HOH:O	2.49	0.44
2:B:220:GLY:O	2:B:238:ASN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HD3	1:C:215:ILE:HD12	2.00	0.43
1:A:216:GLU:OE2	1:A:217:PRO:HA	2.18	0.43
1:A:174:ARG:HA	1:A:234:PHE:CE2	2.53	0.43
1:A:48:ASN:HB2	1:A:233:TRP:CH2	2.54	0.43
2:B:215:ILE:HG22	2:B:216:GLU:O	2.19	0.43
1:C:45:VAL:O	1:C:235:PHE:HA	2.19	0.43
2:D:220:GLY:O	2:D:238:ASN:HA	2.19	0.43
2:D:31:TRP:HB2	2:D:57:ASN:HB3	2.00	0.43
2:D:74:ILE:HB	2:D:75:PRO:HD3	2.00	0.42
1:C:120:VAL:N	1:C:121:PRO:HD2	2.34	0.42
2:D:74:ILE:HB	2:D:75:PRO:CD	2.49	0.42
1:A:27:GLU:HB2	1:A:59:LEU:CD1	2.49	0.42
1:A:91:GLN:O	4:A:303:CL:CL	2.75	0.42
1:A:115:MET:HG2	1:A:194:ALA:O	2.20	0.42
1:C:214:ARG:CD	1:C:215:ILE:HD12	2.50	0.42
2:D:233:TRP:CD2	2:D:263:ILE:CD1	3.03	0.42
2:B:186:ARG:O	2:B:190:ILE:HG13	2.20	0.42
1:A:170:ILE:O	1:A:174:ARG:HG3	2.20	0.41
1:A:256:GLU:OE2	1:C:137:LYS:NZ	2.43	0.41
1:C:140:HIS:HB2	1:C:147:GLU:OE1	2.20	0.41
3:A:301:CTJ:H20	8:A:435:HOH:O	2.20	0.41
2:B:51:LYS:O	2:B:53:GLN:HG3	2.21	0.41
1:C:171:SER:O	1:C:175:LYS:HG3	2.20	0.41
1:C:24:GLU:N	8:C:410:HOH:O	2.53	0.41
2:D:125:GLU:O	2:D:129:GLN:HG3	2.19	0.41
2:D:59:LEU:O	2:D:63:ASN:ND2	2.54	0.41
1:A:87:LYS:HG2	1:A:88:ASP:OD2	2.20	0.41
2:B:156:PHE:HA	2:B:160:GLY:HA3	2.03	0.41
1:C:179:ASN:HA	1:C:188:GLN:OE1	2.20	0.41
2:D:202:ASP:OD2	2:D:265:PRO:HG2	2.20	0.41
1:A:115:MET:HE3	1:A:123:TYR:OH	2.21	0.41
1:A:251:GLN:O	1:A:255:LYS:HG3	2.21	0.41
2:B:171:SER:O	2:B:175:LYS:HG3	2.21	0.41
1:A:129:GLN:O	1:A:134:ARG:NH1	2.54	0.41
2:D:28:ASN:CB	8:D:410:HOH:O	2.68	0.41
1:C:254:THR:O	1:C:258:LEU:HG	2.21	0.40
2:B:120:VAL:O	2:B:124:GLN:HG3	2.22	0.40
2:B:75:PRO:O	2:B:79:ILE:HG13	2.21	0.40

All (1) 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)
2:B:60:LYS:NZ	1:C:143:ASP:OD1[2_554]	2.10	0.10

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	225/265 (85%)	212 (94%)	11 (5%)	2 (1%)	17	31
1	C	227/265 (86%)	214 (94%)	12 (5%)	1 (0%)	34	54
2	B	239/265 (90%)	227 (95%)	11 (5%)	1 (0%)	34	54
2	D	243/265 (92%)	235 (97%)	8 (3%)	0	100	100
All	All	934/1060 (88%)	888 (95%)	42 (4%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TYR
1	A	244	SER
2	B	52	GLN
1	C	147	GLU

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	200/227 (88%)	191 (96%)	9 (4%)	27	51
1	C	200/227 (88%)	192 (96%)	8 (4%)	31	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	209/226 (92%)	205 (98%)	4 (2%)	57	80
2	D	211/226 (93%)	200 (95%)	11 (5%)	23	44
All	All	820/906 (90%)	788 (96%)	32 (4%)	33	57

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	92	VAL
1	A	115	MET
1	A	118	SER
1	A	136	SER
1	A	138	MET
1	A	147	GLU
1	A	148	ASP
1	A	226	VAL
2	B	36	THR
2	B	91	GLN
2	B	94	LYS
2	B	102	ILE
1	C	87	LYS
1	C	88	ASP
1	C	92	VAL
1	C	118	SER
1	C	136	SER
1	C	138	MET
1	C	214	ARG
1	C	232	VAL
2	D	53	GLN
2	D	64	GLN
2	D	115	MET
2	D	118	SER
2	D	124	GLN
2	D	138	MET
2	D	198	GLU
2	D	226	VAL
2	D	230[A]	ASP
2	D	230[B]	ASP
2	D	232	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	KCX	D	73	2	7,11,12	0.81	0	4,12,14	0.44	0
2	KCX	B	73	2	7,11,12	0.81	0	4,12,14	1.06	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	KCX	D	73	2	-	0/7/10/12	-
2	KCX	B	73	2	-	0/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

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
5	PGE	B	303	-	9,9,9	0.82	0	8,8,8	1.07	1 (12%)
6	PEG	C	304	-	6,6,6	0.55	0	5,5,5	0.51	0
7	SO4	D	302	2	4,4,4	0.36	0	6,6,6	0.51	0
5	PGE	A	304	-	9,9,9	0.44	0	8,8,8	0.36	0
3	CTJ	A	301	1	27,39,39	4.49	14 (51%)	27,55,55	2.47	8 (29%)
3	CTJ	C	301	1	27,39,39	4.66	10 (37%)	27,55,55	2.36	5 (18%)
5	PGE	C	303	-	9,9,9	0.53	0	8,8,8	0.64	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
5	PGE	B	303	-	-	4/7/7/7	-
6	PEG	C	304	-	-	3/4/4/4	-
5	PGE	A	304	-	-	4/7/7/7	-
3	CTJ	A	301	1	-	6/16/51/51	0/2/3/3
3	CTJ	C	301	1	-	5/16/51/51	0/2/3/3
5	PGE	C	303	-	-	4/7/7/7	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	CTJ	C3-C4	16.17	1.72	1.34
3	A	301	CTJ	C3-C4	16.03	1.71	1.34
3	C	301	CTJ	C15-S16	-12.56	1.50	1.70
3	A	301	CTJ	C15-S16	-10.56	1.54	1.70
3	A	301	CTJ	C11-N10	6.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	CTJ	C11-N10	6.11	1.46	1.34
3	A	301	CTJ	C14-N19	6.10	1.56	1.37
3	C	301	CTJ	C14-N19	5.77	1.55	1.37
3	C	301	CTJ	C4-N5	5.76	1.52	1.33
3	A	301	CTJ	C4-N5	4.50	1.48	1.33
3	A	301	CTJ	C17-N18	4.16	1.47	1.35
3	C	301	CTJ	C13-N16	-3.65	1.23	1.29
3	C	301	CTJ	C2-S1	-3.42	1.74	1.82
3	A	301	CTJ	C13-N16	-3.27	1.23	1.29
3	C	301	CTJ	C17-N18	3.15	1.44	1.35
3	A	301	CTJ	O12-C11	-2.88	1.18	1.23
3	C	301	CTJ	C2-C3	-2.82	1.39	1.50
3	A	301	CTJ	O17-C18	-2.66	1.41	1.46
3	A	301	CTJ	C2-S1	-2.61	1.76	1.82
3	A	301	CTJ	C2-C3	-2.48	1.41	1.50
3	C	301	CTJ	O17-C18	-2.24	1.42	1.46
3	A	301	CTJ	C19-C18	2.23	1.57	1.53
3	A	301	CTJ	CA-N10	-2.23	1.43	1.46
3	A	301	CTJ	C3'-N6	-2.17	1.44	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	CTJ	C2-S1-C6	8.66	111.45	94.47
3	A	301	CTJ	C2-S1-C6	7.24	108.68	94.47
3	A	301	CTJ	O17-N16-C13	5.20	119.94	111.87
3	C	301	CTJ	C20-C18-C19	-4.36	103.21	110.14
3	C	301	CTJ	O17-N16-C13	4.24	118.46	111.87
3	A	301	CTJ	C6-N5-C4	-4.18	108.48	118.32
3	A	301	CTJ	C13-C11-N10	3.75	120.62	114.38
3	A	301	CTJ	C14-C15-S16	-3.68	107.27	111.79
3	C	301	CTJ	C14-C15-S16	-3.54	107.44	111.79
3	A	301	CTJ	O12-C11-C13	-3.52	116.30	120.35
3	A	301	CTJ	C20-C18-C19	-2.85	105.61	110.14
3	A	301	CTJ	C18-O17-N16	-2.60	108.02	110.33
3	C	301	CTJ	N18-C17-N19	2.60	126.55	123.19
5	B	303	PGE	C5-O3-C4	2.31	123.28	113.29

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	CTJ	C19-C18-O17-N16
3	A	301	CTJ	C20-C18-O17-N16
3	C	301	CTJ	C19-C18-O17-N16
3	C	301	CTJ	C20-C18-O17-N16
6	C	304	PEG	O1-C1-C2-O2
6	C	304	PEG	O2-C3-C4-O4
5	A	304	PGE	O1-C1-C2-O2
5	C	303	PGE	O1-C1-C2-O2
5	C	303	PGE	O3-C5-C6-O4
5	B	303	PGE	O3-C5-C6-O4
5	A	304	PGE	C1-C2-O2-C3
5	B	303	PGE	C6-C5-O3-C4
5	C	303	PGE	C1-C2-O2-C3
5	A	304	PGE	C3-C4-O3-C5
5	B	303	PGE	C3-C4-O3-C5
3	A	301	CTJ	C-CA-N10-C11
5	B	303	PGE	C1-C2-O2-C3
5	C	303	PGE	C4-C3-O2-C2
3	C	301	CTJ	O12-C11-C13-N16
3	A	301	CTJ	O12-C11-C13-N16
3	A	301	CTJ	N10-C11-C13-N16
3	C	301	CTJ	N10-C11-C13-N16
6	C	304	PEG	C1-C2-O2-C3
3	A	301	CTJ	O12-C11-C13-C14
3	C	301	CTJ	O12-C11-C13-C14
5	A	304	PGE	C4-C3-O2-C2

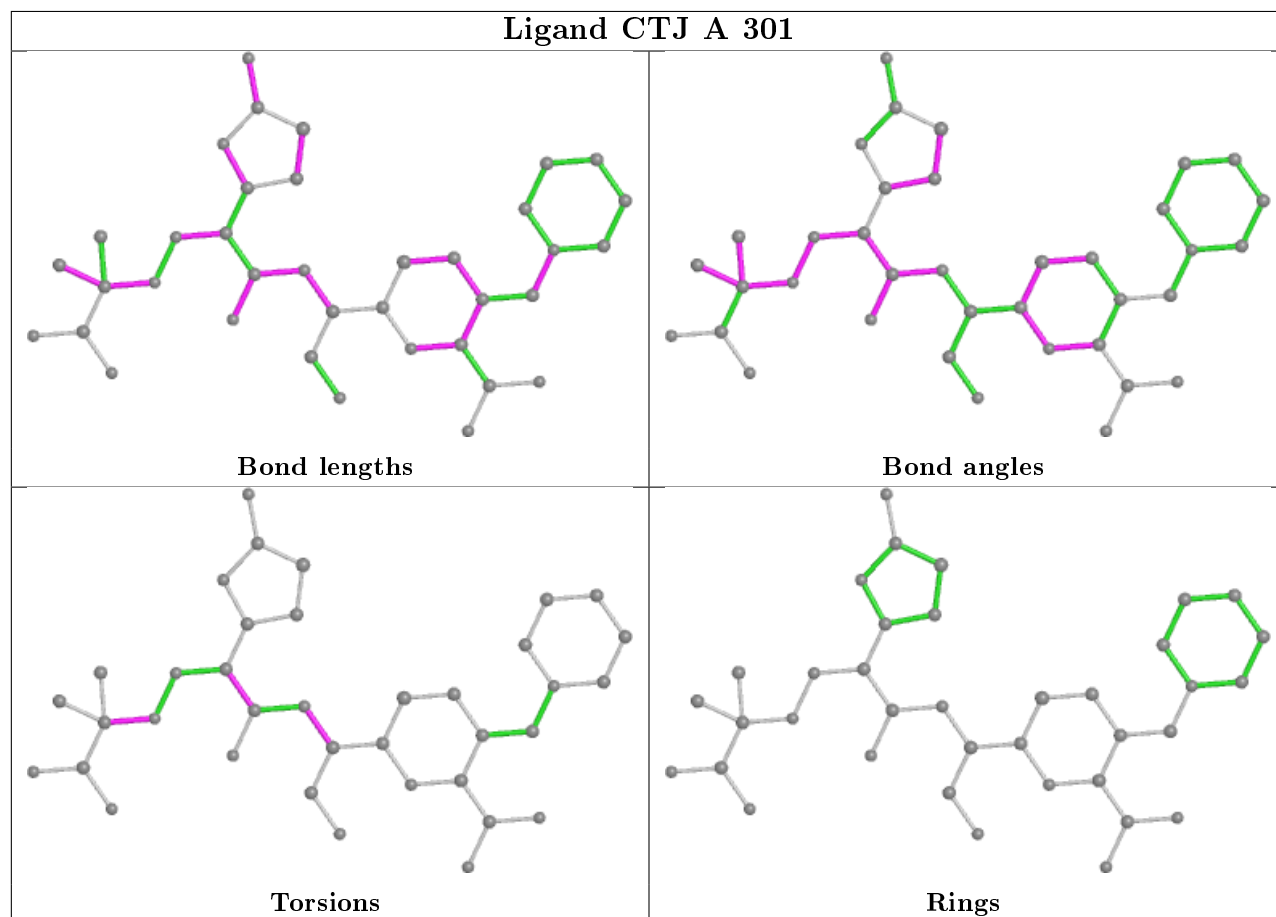
There are no ring outliers.

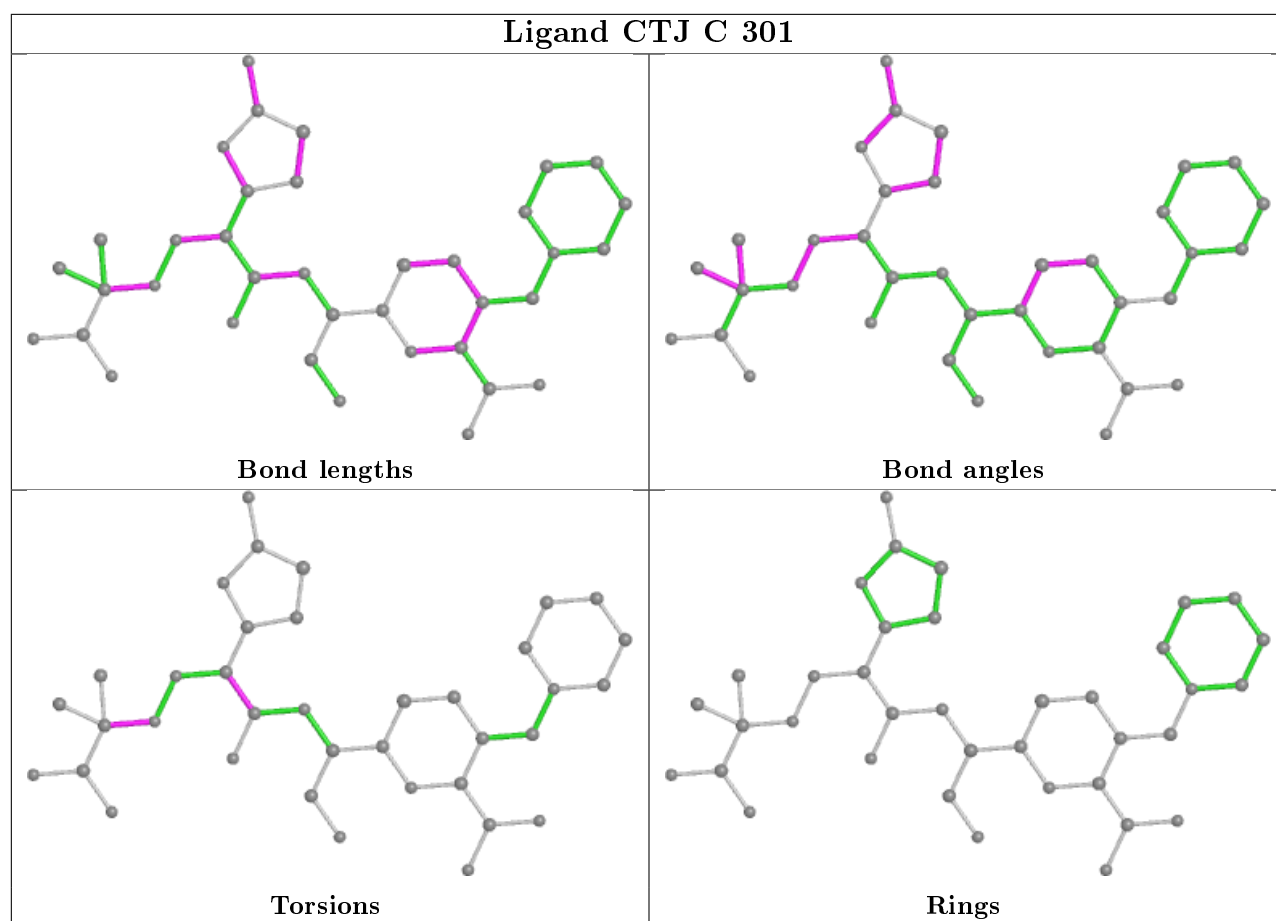
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	304	PEG	3	0
5	A	304	PGE	1	0
3	A	301	CTJ	2	0
3	C	301	CTJ	5	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	229/265 (86%)	0.03	4 (1%)	70	72	23, 29, 39, 57	1 (0%)
1	C	229/265 (86%)	0.04	4 (1%)	70	72	25, 30, 39, 48	3 (1%)
2	B	241/265 (90%)	0.04	9 (3%)	41	45	24, 28, 40, 47	3 (1%)
2	D	241/265 (90%)	0.02	5 (2%)	63	66	24, 29, 36, 40	0
All	All	940/1060 (88%)	0.03	22 (2%)	60	63	23, 29, 39, 57	7 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	236	ALA	3.1
2	B	254	THR	3.0
2	D	243	THR	2.9
2	B	44	VAL	2.8
2	D	254	THR	2.7
2	B	45	VAL	2.6
2	D	236	ALA	2.4
1	A	133	ALA	2.4
2	B	245	ASP	2.3
1	A	147	GLU	2.3
1	C	140	HIS	2.3
1	A	148	ASP	2.3
2	D	98	GLN	2.2
1	C	136	SER	2.2
2	B	103	ALA	2.2
2	B	242	PRO	2.1
2	D	235	PHE	2.1
1	C	224	GLY	2.1
1	A	236	ALA	2.1
1	C	242	PRO	2.1
2	B	26	GLN	2.1
2	B	51	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KCX	D	73	12/13	0.95	0.20	26,28,34,35	0
2	KCX	B	73	12/13	0.96	0.17	24,26,32,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

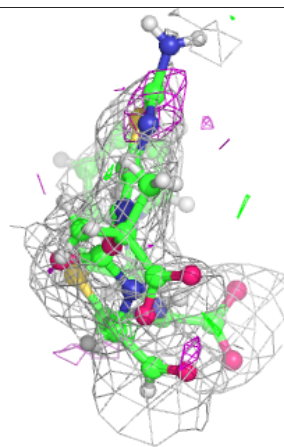
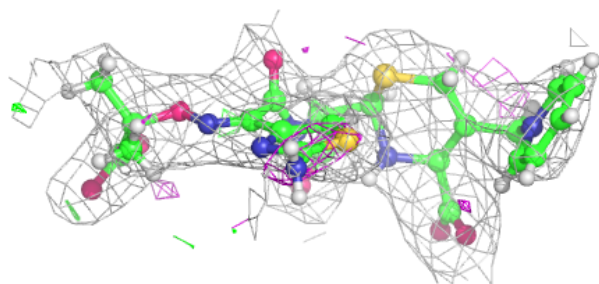
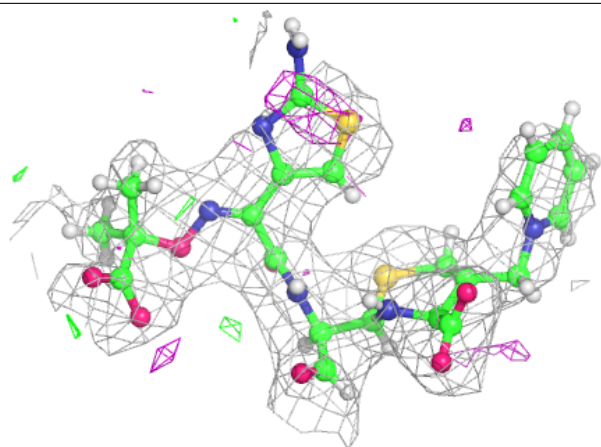
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGE	A	304	10/10	0.72	0.21	51,63,69,71	0
5	PGE	B	303	10/10	0.79	0.41	29,35,38,39	0
5	PGE	C	303	10/10	0.85	0.23	43,52,57,57	0
6	PEG	C	304	7/7	0.86	0.14	39,47,51,51	0
3	CTJ	A	301	37/37	0.87	0.18	28,34,45,47	8
3	CTJ	C	301	37/37	0.91	0.19	30,37,48,55	4
7	SO4	D	302	5/5	0.92	0.23	27,27,28,28	5
4	CL	A	303	1/1	0.95	0.12	29,29,29,29	0
4	CL	D	301	1/1	0.96	0.23	33,33,33,33	0
4	CL	B	301	1/1	0.96	0.23	31,31,31,31	0
4	CL	B	302	1/1	0.97	0.08	31,31,31,31	0
4	CL	C	302	1/1	0.99	0.07	24,24,24,24	0
4	CL	A	302	1/1	0.99	0.05	24,24,24,24	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.

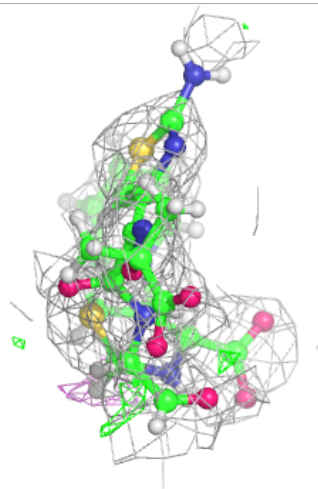
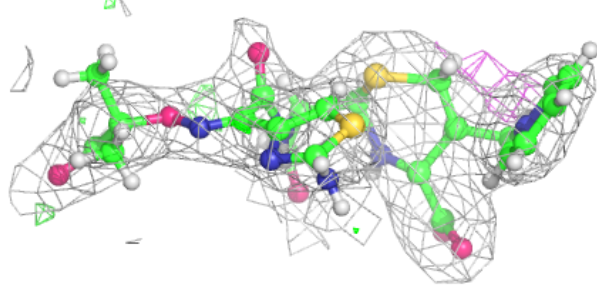
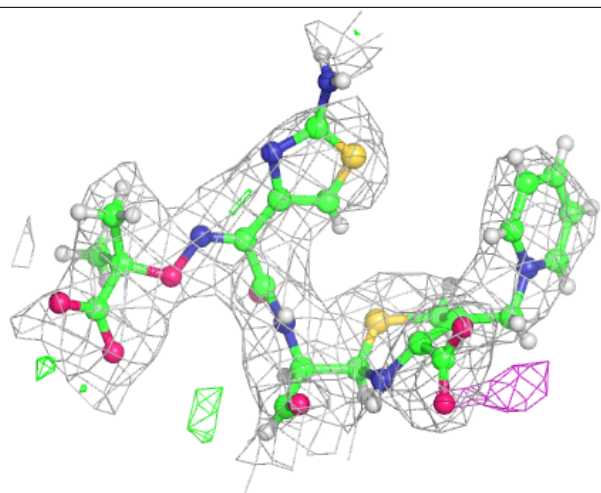
Electron density around CTJ A 301:

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



Electron density around CTJ C 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.