



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:38 AM UTC

PDB ID : 4CZU / pdb_00004czu
Title : Crystal structure of the kinase domain of CIPK23 T190D mutant
Authors : Chaves-Sanjuan, A.; Sanchez-Barrena, M.J.; Albert, A.
Deposited on : 2014-04-22
Resolution : 1.90 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

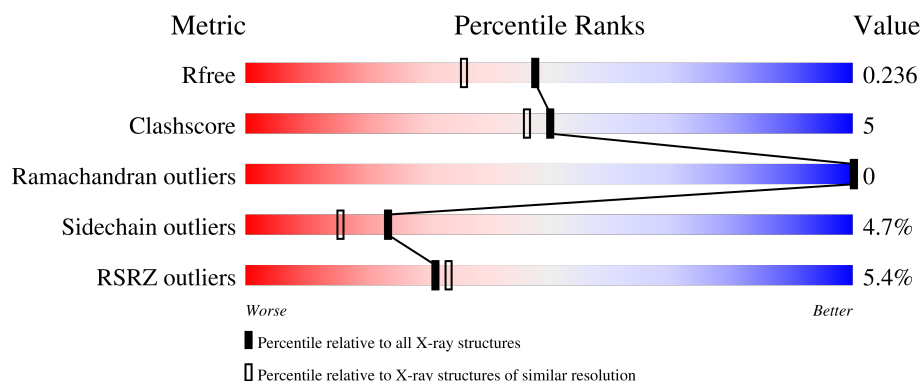
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	464	5% 52% 12% . 36%
1	B	464	2% 54% 7% 38%
1	C	464	2% 54% 6% 39%
1	D	464	4% 57% 6% . 35%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CPS	C	1314	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10595 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 CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	5	0
			2384	1532	405	438	9			
1	B	287	Total	C	N	O	S	0	6	0
			2317	1492	393	422	10			
1	C	281	Total	C	N	O	S	0	4	0
			2268	1462	385	412	9			
1	D	302	Total	C	N	O	S	0	3	0
			2425	1554	418	444	9			

There are 28 discrepancies between the modelled and reference sequences:

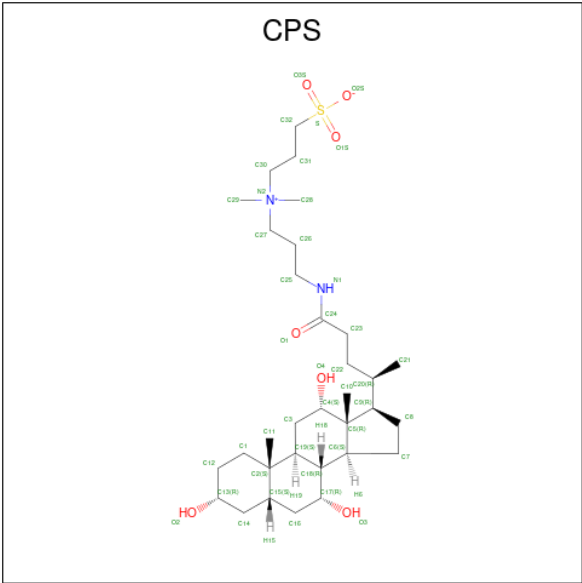
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	PRO	-	expression tag	UNP Q93VD3
A	20	GLY	-	expression tag	UNP Q93VD3
A	21	ILE	-	expression tag	UNP Q93VD3
A	22	HIS	-	expression tag	UNP Q93VD3
A	23	SER	-	expression tag	UNP Q93VD3
A	24	GLY	-	expression tag	UNP Q93VD3
A	190	ASP	THR	engineered mutation	UNP Q93VD3
B	19	PRO	-	expression tag	UNP Q93VD3
B	20	GLY	-	expression tag	UNP Q93VD3
B	21	ILE	-	expression tag	UNP Q93VD3
B	22	HIS	-	expression tag	UNP Q93VD3
B	23	SER	-	expression tag	UNP Q93VD3
B	24	GLY	-	expression tag	UNP Q93VD3
B	190	ASP	THR	engineered mutation	UNP Q93VD3
C	19	PRO	-	expression tag	UNP Q93VD3
C	20	GLY	-	expression tag	UNP Q93VD3
C	21	ILE	-	expression tag	UNP Q93VD3
C	22	HIS	-	expression tag	UNP Q93VD3
C	23	SER	-	expression tag	UNP Q93VD3
C	24	GLY	-	expression tag	UNP Q93VD3

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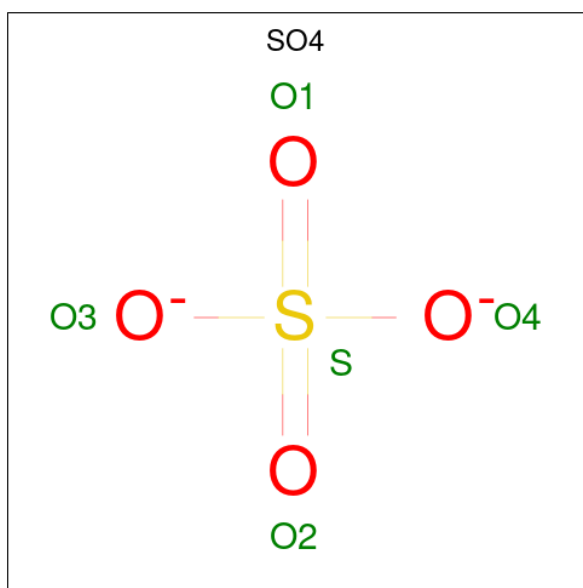
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Chain	Residue	Modelled	Actual	Comment	Reference
C	190	ASP	THR	engineered mutation	UNP Q93VD3
D	19	PRO	-	expression tag	UNP Q93VD3
D	20	GLY	-	expression tag	UNP Q93VD3
D	21	ILE	-	expression tag	UNP Q93VD3
D	22	HIS	-	expression tag	UNP Q93VD3
D	23	SER	-	expression tag	UNP Q93VD3
D	24	GLY	-	expression tag	UNP Q93VD3
D	190	ASP	THR	engineered mutation	UNP Q93VD3

- Molecule 2 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	234	Total	O	0	0
			234	234		
4	C	166	Total	O	0	0
			166	166		
4	D	176	Total	O	0	0
			176	176		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.70Å 91.73Å 207.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 1.90 49.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.97-1.90) 96.2 (49.97-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.192 , 0.233 0.194 , 0.236	Depositor DCC
R_{free} test set	5512 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10595	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/2447	0.79	0/3293
1	B	0.50	0/2382	0.77	1/3205 (0.0%)
1	C	0.47	0/2326	0.76	0/3131
1	D	0.48	0/2483	0.79	1/3344 (0.0%)
All	All	0.48	0/9638	0.78	2/12973 (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	D	21	ILE	N-CA-C	5.55	116.57	108.58
1	B	26	THR	N-CA-C	-5.08	107.13	113.38

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	2384	0	2426	38	0
1	B	2317	0	2361	25	0
1	C	2268	0	2310	15	0
1	D	2425	0	2456	24	0
2	A	42	0	58	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	84	0	116	2	0
2	C	84	0	116	7	0
2	D	84	0	116	7	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	C	25	0	0	0	0
3	D	20	0	0	1	0
4	A	246	0	0	5	0
4	B	234	0	0	6	0
4	C	166	0	0	2	0
4	D	176	0	0	4	0
All	All	10595	0	9959	105	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 5.

All (105) 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:A:27:ARG:NH1	1:A:29:GLY:O	2.01	0.94
1:A:123:ASN:O	1:C:35:ARG:NH2	2.22	0.73
1:B:246:LYS:NZ	1:B:248:GLU:OE1	2.22	0.72
1:A:312:SER:HB3	1:A:314:GLU:HG2	1.73	0.70
1:C:27:ARG:NH1	1:C:29:GLY:O	2.26	0.67
1:B:230:LEU:HD12	1:D:191:THR:HG21	1.76	0.66
1:D:246:LYS:HD3	2:D:1326:CPS:H30	1.81	0.62
1:A:140[A]:ASN:OD1	1:A:290:TYR:OH	2.17	0.62
1:B:165:ASN:OD1	1:B:165:ASN:N	2.34	0.60
1:B:119:LYS:NZ	4:B:2094:HOH:O	2.33	0.60
2:C:1314:CPS:H19	2:C:1314:CPS:H10B	1.84	0.60
1:D:126:LEU:HD13	1:D:130:GLU:HG2	1.85	0.58
2:C:1314:CPS:H10A	2:C:1314:CPS:H21A	1.83	0.58
1:C:84:LYS:HG3	1:C:94:MET:HE3	1.85	0.57
1:A:42:PHE:CD1	1:A:66:LYS:HG3	2.41	0.56
1:B:193:GLY:HA3	1:B:230:LEU:HD11	1.89	0.54
1:B:46:LYS:NZ	4:B:2023:HOH:O	2.40	0.54
1:A:127:LYS:HG2	4:A:2117:HOH:O	2.08	0.54
1:C:66:LYS:NZ	1:C:181:GLN:OE1	2.32	0.53
1:A:112:THR:HA	2:A:1321:CPS:H28B	1.91	0.52
1:B:62:ILE:HD12	1:B:106:PHE:CE2	2.44	0.52
1:D:246:LYS:HE3	2:D:1326:CPS:H32A	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:SER:CB	1:A:314:GLU:HG2	2.38	0.51
1:D:181:GLN:H	1:D:181:GLN:CD	2.19	0.51
3:D:1330:SO4:O1	4:D:2175:HOH:O	2.18	0.51
1:A:29:GLY:H	1:A:314:GLU:HB3	1.75	0.51
1:A:144:TYR:OH	1:A:148:ARG:NH1	2.43	0.51
1:C:206:LYS:HB2	2:C:1314:CPS:H30A	1.93	0.51
1:D:26:THR:HG22	1:D:322:ARG:HG3	1.92	0.51
1:D:204:ASN:ND2	4:D:2110:HOH:O	2.32	0.50
1:D:194:THR:HG23	1:D:198:VAL:HG21	1.93	0.50
1:C:237:LEU:HB3	2:C:1314:CPS:H11A	1.94	0.50
1:D:26:THR:HG22	1:D:322:ARG:HA	1.94	0.50
1:A:238:THR:OG1	2:C:1314:CPS:N1	2.45	0.50
1:D:172:ASP:OD1	2:D:1325:CPS:O2	2.27	0.50
1:A:37:LEU:HD21	4:A:2243:HOH:O	2.12	0.49
1:B:130:GLU:HG2	4:B:2105:HOH:O	2.11	0.49
1:A:69[C]:LYS:HD2	1:B:208:TYR:CD2	2.47	0.49
1:A:236:ASN:HD21	2:C:1314:CPS:H271	1.77	0.49
1:D:318:LEU:HD12	1:D:319:VAL:N	2.28	0.48
1:B:265:ARG:NH1	4:B:2212:HOH:O	2.41	0.48
1:A:65:GLU:HG2	4:A:2052:HOH:O	2.14	0.48
1:A:19:PRO:HB3	1:A:49:ARG:HH12	1.79	0.48
1:D:123:ASN:ND2	4:D:2066:HOH:O	2.46	0.48
1:D:246:LYS:HD3	2:D:1326:CPS:H271	1.96	0.47
1:A:69[A]:LYS:HG3	1:B:208:TYR:CE2	2.50	0.47
1:A:22:HIS:CG	1:A:25:ARG:HG3	2.50	0.47
1:C:311:ASP:OD1	1:C:312:SER:N	2.48	0.47
1:A:178:LEU:HB2	1:A:183:ARG:HG3	1.97	0.47
1:B:93:ARG:NE	3:B:1317:SO4:O3	2.47	0.47
1:A:111:VAL:HG11	1:A:169:LYS:HG3	1.96	0.47
1:B:238:THR:HG22	1:B:242:LYS:HE2	1.98	0.46
1:B:193:GLY:HA3	1:B:230:LEU:CD1	2.45	0.46
1:D:26:THR:CG2	1:D:322:ARG:HG3	2.45	0.46
2:C:1314:CPS:H28	2:C:1314:CPS:H31A	1.64	0.45
2:D:1326:CPS:C24	2:D:1326:CPS:H272	2.45	0.45
1:A:35:ARG:HH11	1:A:35:ARG:HG2	1.80	0.45
1:D:127:LYS:HA	1:D:127:LYS:HD3	1.76	0.45
1:A:60:LYS:HE3	1:A:185:ASP:HB3	1.99	0.45
2:B:1314:CPS:H29B	2:B:1314:CPS:H261	1.71	0.44
2:D:1326:CPS:H28	2:D:1326:CPS:H31	1.73	0.44
1:A:132:ARG:HG3	1:A:285:TRP:CH2	2.53	0.44
1:B:81:SER:OG	1:B:308:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	4:B:2103:HOH:O	2.21	0.44
1:A:27:ARG:HH12	1:A:30:LYS:HA	1.83	0.43
1:A:78:ARG:NH1	1:B:75:GLN:HG3	2.33	0.43
1:C:194:THR:HB	1:C:195:PRO:HD3	1.99	0.43
1:D:127:LYS:HE3	4:D:2023:HOH:O	2.18	0.43
1:A:148:ARG:HA	1:A:148:ARG:HD3	1.88	0.43
2:A:1321:CPS:H29A	2:A:1321:CPS:H32	2.00	0.43
1:B:239:SER:HA	1:B:242:LYS:HE3	2.00	0.43
1:C:144:TYR:OH	1:C:148:ARG:NH1	2.49	0.43
1:C:275:ILE:HG12	1:C:279:GLU:HB2	2.01	0.43
1:B:153:ARG:NH2	1:B:207:GLY:O	2.51	0.43
1:C:183[C]:ARG:NH2	4:C:2098:HOH:O	2.52	0.43
1:D:318:LEU:HD12	1:D:319:VAL:H	1.83	0.43
1:A:93:ARG:HG2	1:A:95:PHE:CE1	2.53	0.42
1:C:59:ILE:HD12	1:C:107:VAL:HG22	2.01	0.42
1:D:260:LYS:HE3	1:D:264:LYS:HE3	2.01	0.42
1:A:75:GLN:NE2	4:A:2065:HOH:O	2.47	0.42
1:A:146:HIS:CE1	1:A:211:ALA:HA	2.55	0.42
1:B:37[B]:LEU:HD21	1:B:47:PHE:CZ	2.55	0.42
1:C:156:LYS:HE3	4:C:2088:HOH:O	2.19	0.42
1:B:144:TYR:CZ	1:B:148:ARG:CZ	3.02	0.42
1:C:178:LEU:O	1:C:183[A]:ARG:NH1	2.52	0.42
1:A:31:TYR:OH	4:A:2009:HOH:O	2.21	0.42
1:A:206:LYS:HB3	1:A:206:LYS:HE2	1.87	0.42
2:B:1315:CPS:H271	2:B:1315:CPS:H31	1.65	0.41
1:D:292:ALA:HA	1:D:293:PRO:HD3	1.76	0.41
1:B:128:GLU:HB2	4:B:2104:HOH:O	2.20	0.41
1:A:33:LEU:HD23	1:A:48:ALA:HB2	2.03	0.41
1:A:112:THR:HG22	2:A:1321:CPS:H28	2.03	0.41
1:C:144:TYR:HH	1:C:148:ARG:NH1	2.18	0.41
1:D:27:ARG:HG2	1:D:31:TYR:O	2.21	0.41
1:D:230:LEU:HB2	1:D:233:GLU:HG2	2.03	0.41
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.96	0.41
1:B:212:LYS:HE2	1:B:274:ARG:HB3	2.03	0.41
1:D:21:ILE:HD11	1:D:47:PHE:HB2	2.03	0.41
1:A:69[C]:LYS:HD2	1:B:208:TYR:HD2	1.84	0.41
1:B:133:LYS:HB2	1:B:133:LYS:HE3	1.90	0.41
1:A:303:ASP:HA	1:A:304:ASP:HA	1.65	0.41
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.87	0.40
1:A:101:LYS:HB3	1:A:101:LYS:HE3	1.91	0.40
1:D:49:ARG:HE	1:D:54:GLY:HA2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LYS:CD	2:D:1326:CPS:H271	2.51	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	198/464 (43%)	192 (97%)	6 (3%)	0	100	100
1	B	289/464 (62%)	282 (98%)	7 (2%)	0	100	100
1	C	232/464 (50%)	220 (95%)	12 (5%)	0	100	100
1	D	301/464 (65%)	293 (97%)	8 (3%)	0	100	100
All	All	1020/1856 (55%)	987 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	260/393 (66%)	245 (94%)	15 (6%)	18	10
1	B	252/393 (64%)	244 (97%)	8 (3%)	34	27
1	C	245/393 (62%)	235 (96%)	10 (4%)	27	19
1	D	263/393 (67%)	249 (95%)	14 (5%)	20	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1020/1572 (65%)	973 (95%)	47 (5%)	23	16

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	23	SER
1	A	26	THR
1	A	35	ARG
1	A	66	LYS
1	A	72	MET
1	A	101	LYS
1	A	172	ASP
1	A	204	ASN
1	A	237	LEU
1	A	265	ARG
1	A	294	LYS
1	A	296	GLU
1	A	303	ASP
1	A	308	ILE
1	B	23	SER
1	B	84	LYS
1	B	96	GLU
1	B	110	PHE
1	B	130	GLU
1	B	165	ASN
1	B	205	ASN
1	B	291	LYS
1	C	27	ARG
1	C	30	LYS
1	C	67	VAL
1	C	69	LYS
1	C	71	LYS
1	C	72	MET
1	C	155	LEU
1	C	182	VAL
1	C	297	ASN
1	C	304	ASP
1	D	30	LYS
1	D	52	GLU
1	D	53	ASN
1	D	55	ASP

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Mol	Chain	Res	Type
1	D	101	LYS
1	D	172	ASP
1	D	175	LEU
1	D	194	THR
1	D	233	GLU
1	D	291	LYS
1	D	295	PHE
1	D	308	ILE
1	D	319	VAL
1	D	322	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	C	56	ASN
1	D	90	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	SO4	D	1330	-	4,4,4	0.24	0	6,6,6	0.08	0
2	CPS	D	1325	-	45,45,45	0.20	0	70,70,70	0.57	1 (1%)
3	SO4	A	1324	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	C	1316	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	A	1325	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	1318	-	4,4,4	0.29	0	6,6,6	0.05	0
3	SO4	C	1317	-	4,4,4	0.23	0	6,6,6	0.09	0
2	CPS	C	1314	-	45,45,45	0.48	0	70,70,70	1.19	6 (8%)
3	SO4	B	1316	-	4,4,4	0.23	0	6,6,6	0.11	0
2	CPS	A	1321	-	45,45,45	0.25	0	70,70,70	0.69	2 (2%)
3	SO4	D	1328	-	4,4,4	0.23	0	6,6,6	0.22	0
2	CPS	D	1326	-	45,45,45	0.22	0	70,70,70	0.51	1 (1%)
2	CPS	C	1313	-	45,45,45	0.18	0	70,70,70	0.57	1 (1%)
3	SO4	A	1322	-	4,4,4	0.24	0	6,6,6	0.13	0
2	CPS	B	1314	-	45,45,45	0.19	0	70,70,70	0.61	1 (1%)
3	SO4	C	1319	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	A	1323	-	4,4,4	0.22	0	6,6,6	0.14	0
2	CPS	B	1315	-	45,45,45	0.16	0	70,70,70	0.60	1 (1%)
3	SO4	D	1329	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	B	1317	-	4,4,4	0.21	0	6,6,6	0.19	0
3	SO4	C	1318	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	B	1319	-	4,4,4	0.22	0	6,6,6	0.05	0
3	SO4	D	1327	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	C	1315	-	4,4,4	0.28	0	6,6,6	0.11	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	CPS	D	1326	-	-	8/25/90/90	0/4/4/4
2	CPS	C	1313	-	-	13/25/90/90	0/4/4/4
2	CPS	D	1325	-	-	11/25/90/90	0/4/4/4
2	CPS	B	1314	-	-	8/25/90/90	0/4/4/4
2	CPS	B	1315	-	-	9/25/90/90	0/4/4/4
2	CPS	C	1314	-	1/1/14/15	13/25/90/90	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPS	A	1321	-	-	10/25/90/90	0/4/4/4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1314	CPS	C27-C26-C25	5.10	120.93	110.95
2	D	1325	CPS	C27-C26-C25	3.19	117.19	110.95
2	B	1314	CPS	C27-C26-C25	3.09	116.99	110.95
2	C	1314	CPS	C10-C5-C6	2.81	115.60	111.20
2	A	1321	CPS	C30-C31-C32	2.81	117.14	109.43
2	C	1314	CPS	C5-C9-C20	2.78	122.85	119.48
2	A	1321	CPS	C27-C26-C25	2.50	115.84	110.95
2	B	1315	CPS	C22-C23-C24	-2.43	107.66	113.06
2	C	1314	CPS	C30-C31-C32	2.31	115.78	109.43
2	C	1313	CPS	C30-C31-C32	2.22	115.52	109.43
2	D	1326	CPS	C27-C26-C25	2.17	115.19	110.95
2	C	1314	CPS	C3-C4-C5	2.09	113.39	111.26
2	C	1314	CPS	C22-C20-C9	-2.04	106.11	110.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1314	CPS	C5

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1321	CPS	C31-C30-N2-C27
2	A	1321	CPS	C31-C32-S-O2S
2	A	1321	CPS	C31-C32-S-O3S
2	B	1314	CPS	N2-C30-C31-C32
2	B	1315	CPS	N2-C30-C31-C32
2	B	1315	CPS	C31-C30-N2-C27
2	B	1315	CPS	C30-C31-C32-S
2	C	1314	CPS	C26-C27-N2-C30
2	C	1314	CPS	N2-C30-C31-C32
2	C	1314	CPS	C31-C32-S-O2S
2	C	1314	CPS	C31-C32-S-O1S
2	D	1325	CPS	C21-C20-C9-C5
2	D	1325	CPS	C22-C20-C9-C8

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Mol	Chain	Res	Type	Atoms
2	D	1325	CPS	N2-C30-C31-C32
2	D	1325	CPS	C31-C32-S-O1S
2	D	1326	CPS	N2-C30-C31-C32
2	D	1326	CPS	C31-C30-N2-C27
2	D	1325	CPS	C21-C20-C9-C8
2	D	1325	CPS	C22-C20-C9-C5
2	A	1321	CPS	C31-C30-N2-C28
2	A	1321	CPS	C31-C30-N2-C29
2	B	1314	CPS	C26-C27-N2-C28
2	B	1315	CPS	C31-C30-N2-C28
2	B	1315	CPS	C31-C30-N2-C29
2	C	1313	CPS	C31-C30-N2-C28
2	C	1314	CPS	C26-C27-N2-C28
2	C	1314	CPS	C26-C27-N2-C29
2	C	1314	CPS	C31-C30-N2-C28
2	C	1314	CPS	C31-C30-N2-C29
2	D	1326	CPS	C31-C30-N2-C28
2	D	1326	CPS	C31-C30-N2-C29
2	B	1314	CPS	C26-C27-N2-C29
2	C	1313	CPS	C31-C30-N2-C29
2	B	1314	CPS	C31-C32-S-O2S
2	B	1314	CPS	C26-C27-N2-C30
2	C	1314	CPS	C31-C30-N2-C27
2	B	1315	CPS	C9-C20-C22-C23
2	C	1314	CPS	N1-C25-C26-C27
2	D	1326	CPS	C9-C20-C22-C23
2	D	1325	CPS	C31-C32-S-O2S
2	D	1326	CPS	C21-C20-C22-C23
2	C	1313	CPS	C26-C25-N1-C24
2	C	1313	CPS	C22-C23-C24-N1
2	C	1313	CPS	C30-C31-C32-S
2	C	1313	CPS	C22-C23-C24-O1
2	D	1325	CPS	C20-C22-C23-C24
2	C	1313	CPS	C26-C27-N2-C28
2	D	1325	CPS	C22-C23-C24-O1
2	B	1314	CPS	C25-C26-C27-N2
2	D	1326	CPS	C25-C26-C27-N2
2	D	1325	CPS	C22-C23-C24-N1
2	A	1321	CPS	N1-C25-C26-C27
2	C	1313	CPS	C31-C30-N2-C27
2	C	1313	CPS	N1-C25-C26-C27
2	A	1321	CPS	C31-C32-S-O1S

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Mol	Chain	Res	Type	Atoms
2	B	1314	CPS	C31-C32-S-O3S
2	B	1314	CPS	C31-C32-S-O1S
2	C	1314	CPS	C31-C32-S-O3S
2	D	1325	CPS	C31-C32-S-O3S
2	C	1313	CPS	C26-C27-N2-C29
2	D	1326	CPS	C30-C31-C32-S
2	C	1313	CPS	C26-C27-N2-C30
2	A	1321	CPS	N2-C30-C31-C32
2	C	1313	CPS	N2-C30-C31-C32
2	C	1314	CPS	C26-C25-N1-C24
2	B	1315	CPS	N1-C25-C26-C27
2	B	1315	CPS	C25-C26-C27-N2
2	C	1314	CPS	C25-C26-C27-N2
2	A	1321	CPS	C22-C23-C24-O1
2	A	1321	CPS	C22-C23-C24-N1
2	B	1315	CPS	C21-C20-C22-C23
2	C	1313	CPS	C20-C22-C23-C24

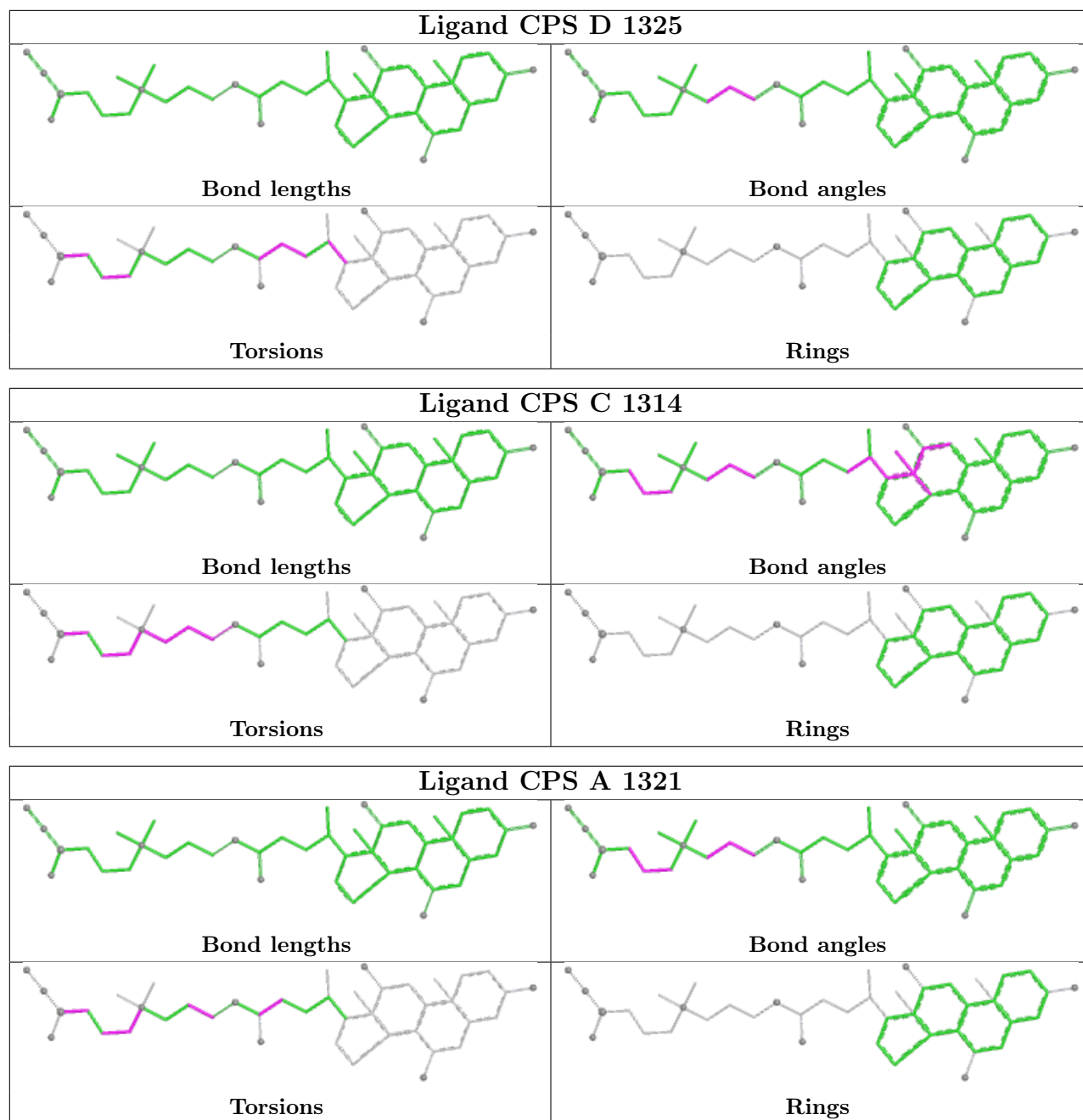
There are no ring outliers.

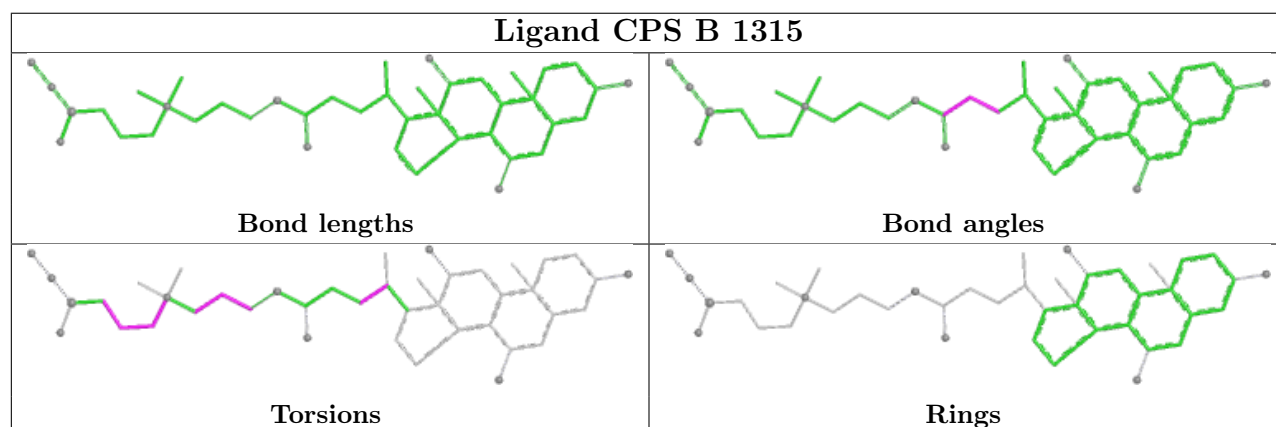
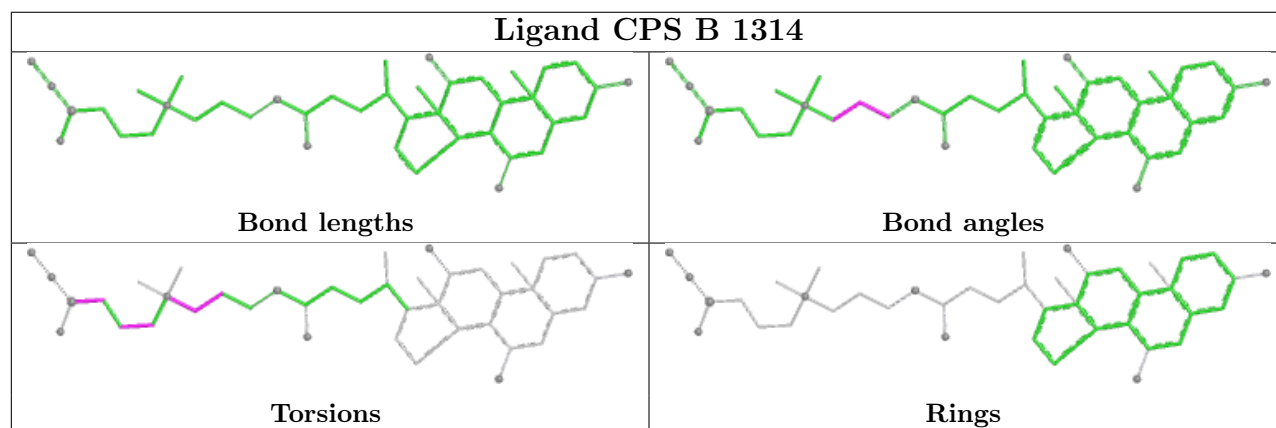
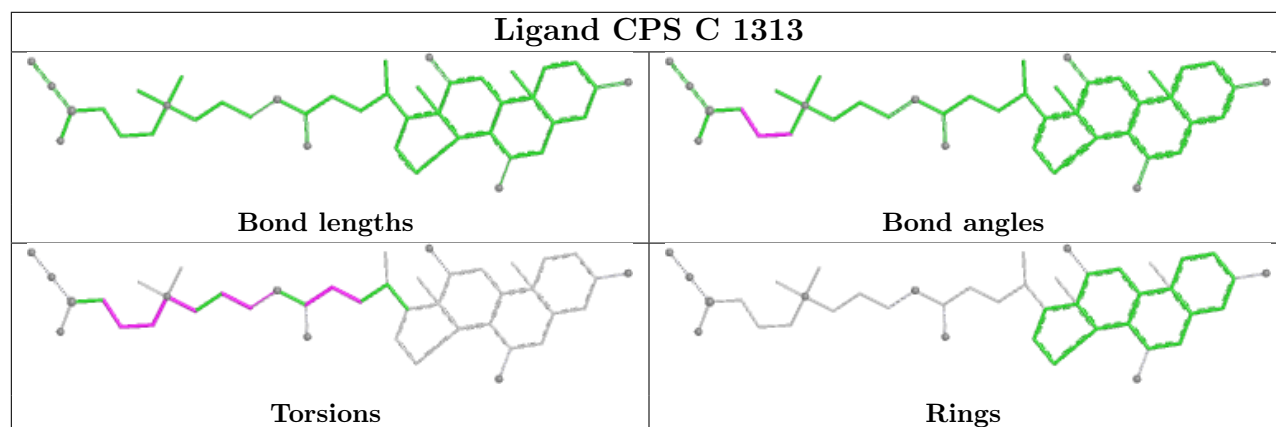
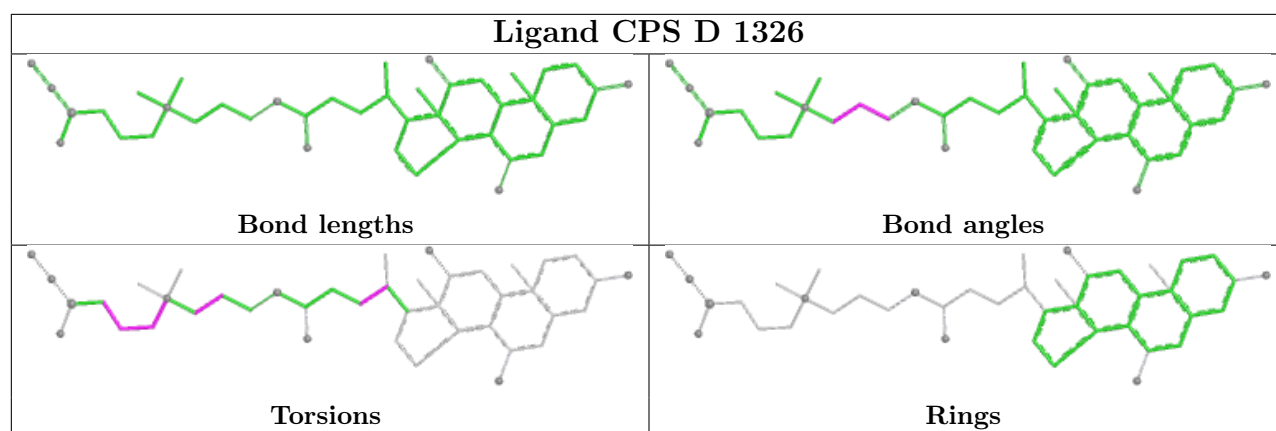
8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1330	SO4	1	0
2	D	1325	CPS	1	0
2	C	1314	CPS	7	0
2	A	1321	CPS	3	0
2	D	1326	CPS	6	0
2	B	1314	CPS	1	0
2	B	1315	CPS	1	0
3	B	1317	SO4	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	297/464 (64%)	0.25	24 (8%)	18 19	13, 24, 62, 92	5 (1%)
1	B	287/464 (61%)	-0.01	9 (3%)	51 55	9, 21, 47, 95	6 (2%)
1	C	281/464 (60%)	0.16	10 (3%)	46 49	11, 25, 55, 83	4 (1%)
1	D	302/464 (65%)	0.24	20 (6%)	24 26	8, 24, 57, 95	3 (0%)
All	All	1167/1856 (62%)	0.17	63 (5%)	31 33	8, 24, 59, 95	18 (1%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ILE	7.3
1	A	24	GLY	4.5
1	D	295	PHE	4.4
1	A	303	ASP	4.4
1	C	28	VAL	4.3
1	A	318	LEU	4.3
1	A	319	VAL	4.3
1	D	319	VAL	4.2
1	D	110	PHE	4.0
1	B	24	GLY	3.9
1	B	22	HIS	3.9
1	B	23	SER	3.9
1	A	19	PRO	3.9
1	A	110	PHE	3.7
1	C	29	GLY	3.6
1	A	21	ILE	3.6
1	C	298	ALA	3.5
1	A	317	ASN	3.4
1	D	19	PRO	3.3
1	B	165	ASN	3.3
1	D	20	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	315	SER	3.1
1	A	297	ASN	3.0
1	A	320	VAL	2.9
1	A	26	THR	2.9
1	C	35	ARG	2.9
1	C	312	SER	2.9
1	D	298	ALA	2.8
1	A	23	SER	2.7
1	D	193	GLY	2.6
1	A	295	PHE	2.6
1	D	55	ASP	2.6
1	C	101	LYS	2.6
1	D	294	LYS	2.6
1	A	22	HIS	2.5
1	B	110	PHE	2.4
1	A	314	GLU	2.4
1	D	317	ASN	2.4
1	C	293	PRO	2.3
1	D	51	VAL	2.3
1	A	123	ASN	2.3
1	D	56	ASN	2.3
1	C	164	ALA	2.3
1	C	310	ASP	2.3
1	A	316	LYS	2.3
1	D	123	ASN	2.2
1	B	303	ASP	2.2
1	B	295	PHE	2.2
1	D	22[A]	HIS	2.2
1	A	292	ALA	2.2
1	A	27	ARG	2.2
1	A	20	GLY	2.1
1	A	291	LYS	2.1
1	A	296	GLU	2.1
1	D	23	SER	2.1
1	B	164	ALA	2.1
1	D	322	ARG	2.1
1	D	302	LEU	2.1
1	A	25	ARG	2.1
1	D	305	VAL	2.0
1	D	192	CYS	2.0
1	C	292	ALA	2.0
1	D	320	VAL	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 oligosaccharides 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.

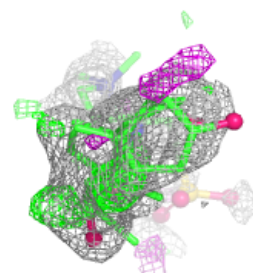
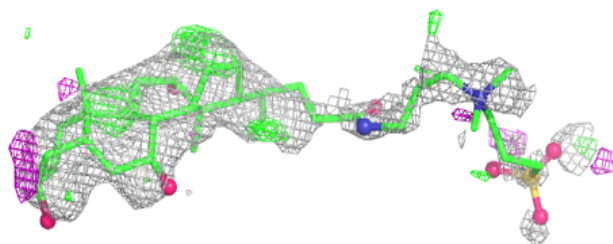
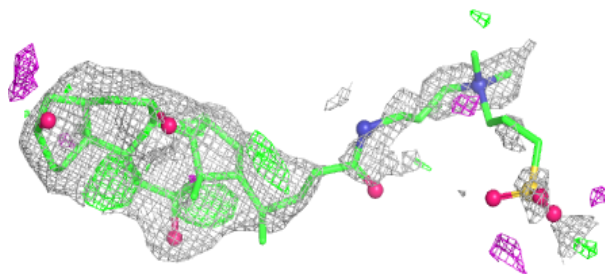
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1325	5/5	0.58	0.16	79,92,103,111	0
3	SO4	C	1317	5/5	0.59	0.14	75,83,98,110	0
3	SO4	C	1318	5/5	0.59	0.13	86,90,106,106	0
3	SO4	B	1318	5/5	0.64	0.13	62,64,83,93	0
3	SO4	D	1330	5/5	0.64	0.14	70,78,102,104	0
3	SO4	D	1329	5/5	0.66	0.13	80,90,103,117	0
2	CPS	C	1314	42/42	0.66	0.24	56,70,114,137	0
3	SO4	D	1328	5/5	0.67	0.15	82,93,106,111	0
3	SO4	C	1319	5/5	0.70	0.12	80,83,99,104	0
2	CPS	A	1321	42/42	0.70	0.20	33,45,76,89	0
2	CPS	D	1325	42/42	0.73	0.18	32,52,106,131	0
3	SO4	A	1324	5/5	0.73	0.15	61,70,76,86	0
2	CPS	B	1314	42/42	0.76	0.17	24,37,99,117	0
2	CPS	D	1326	42/42	0.76	0.16	31,42,83,105	0
3	SO4	A	1322	5/5	0.76	0.10	72,73,97,100	0
3	SO4	A	1323	5/5	0.78	0.16	70,77,79,82	0
3	SO4	D	1327	5/5	0.80	0.13	65,70,73,73	0
3	SO4	B	1317	5/5	0.81	0.12	75,78,86,101	0
3	SO4	B	1319	5/5	0.82	0.11	61,64,76,84	0
2	CPS	B	1315	42/42	0.87	0.13	25,35,81,113	0
3	SO4	B	1316	5/5	0.87	0.09	48,58,62,70	0
2	CPS	C	1313	42/42	0.88	0.13	21,31,128,140	0
3	SO4	C	1316	5/5	0.92	0.08	40,47,53,55	0
3	SO4	C	1315	5/5	0.92	0.07	40,43,56,56	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.

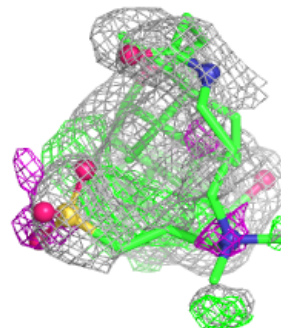
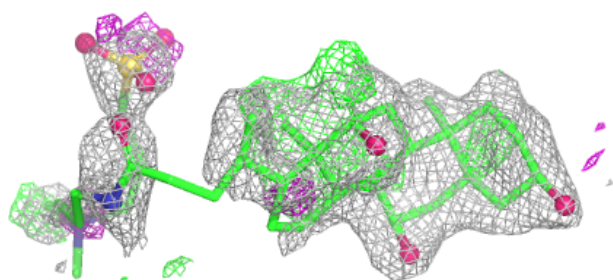
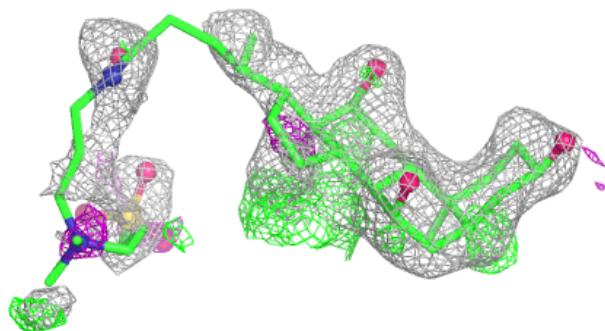
Electron density around CPS C 1314:

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



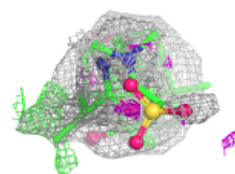
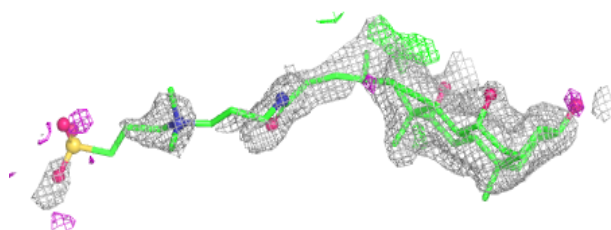
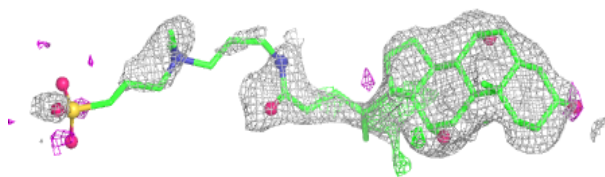
Electron density around CPS A 1321:

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

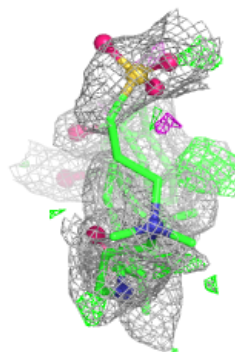
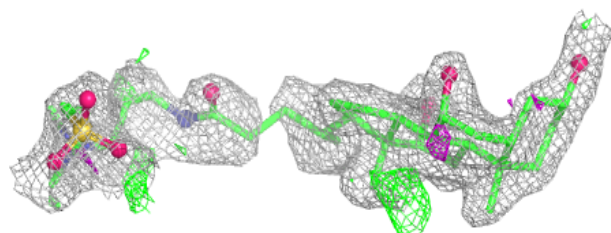
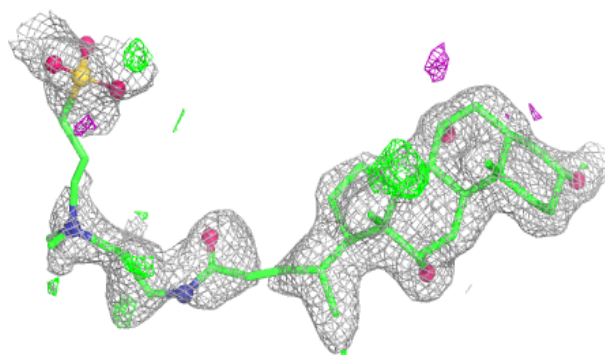


Electron density around CPS D 1325:

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

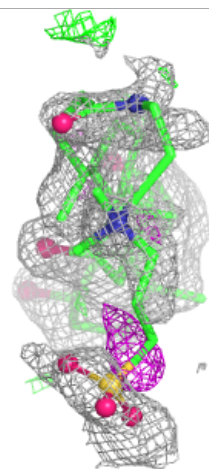
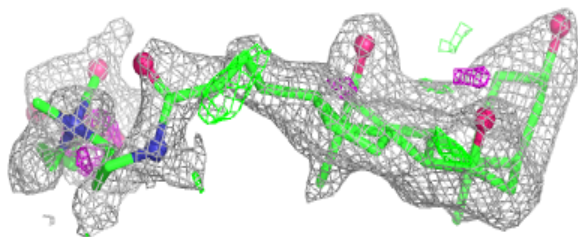
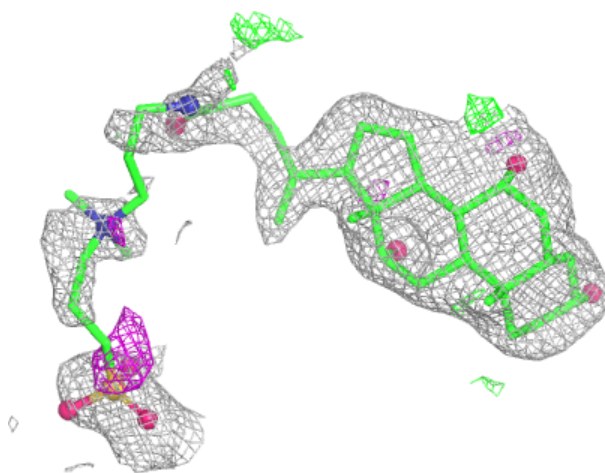
**Electron density around CPS B 1314:**

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



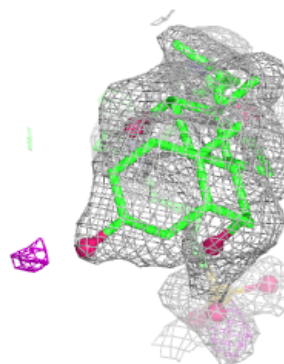
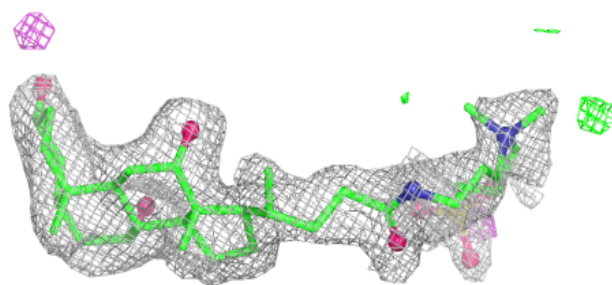
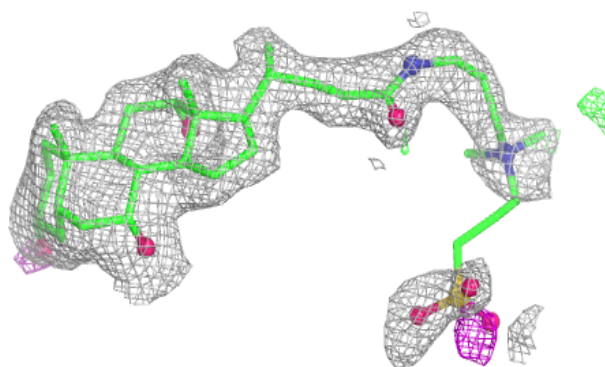
Electron density around CPS D 1326:

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

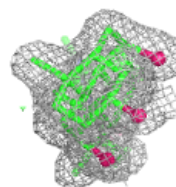
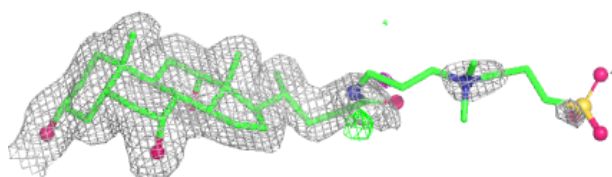
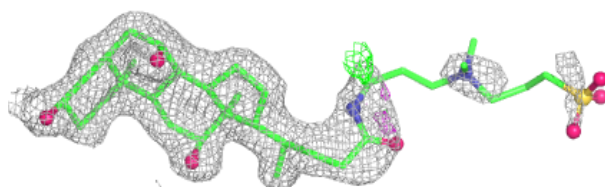


Electron density around CPS B 1315:

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

**Electron density around CPS C 1313:**

$2mF_o-DF_c$ (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.