Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2022 – 06:25 pm GMT

PDB ID	:	7PUV
Title	:	Crystal structure of carbonic anhydrase XII with methyl 2-(benzenesulfonyl)-4-chloro-5-sulfamoylbenzoate
Authors	:	Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on	:	2021-09-30
Resolution	:	1.40 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:

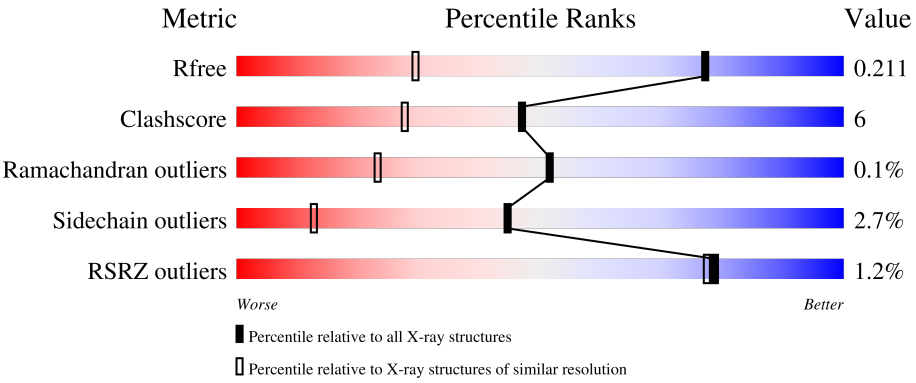
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 <=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	263	94% 5%
1	B	263	% 92% 7%
1	C	263	2% 87% 10%
1	D	263	% 90% 9%

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
3	EDO	A	303	-	-	X	-
5	PEG	B	303	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9817 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	3	0
			2105	1338	362	398	7			
1	B	261	Total	C	N	O	S	0	11	0
			2170	1374	369	420	7			
1	C	260	Total	C	N	O	S	0	6	0
			2117	1348	357	405	7			
1	D	261	Total	C	N	O	S	0	6	0
			2147	1362	365	411	9			

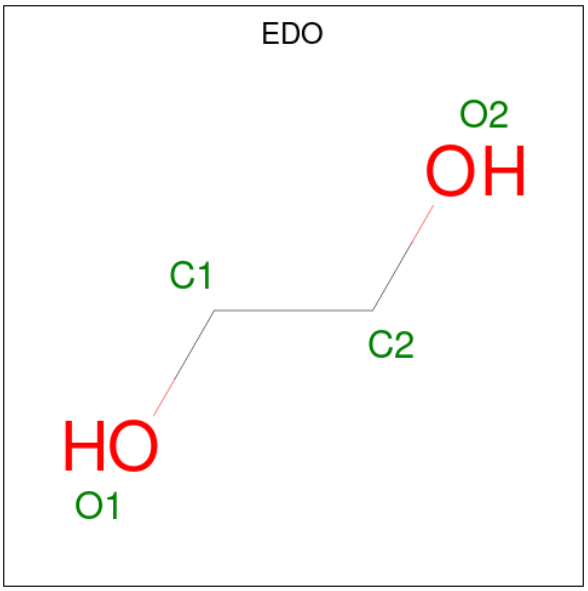
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

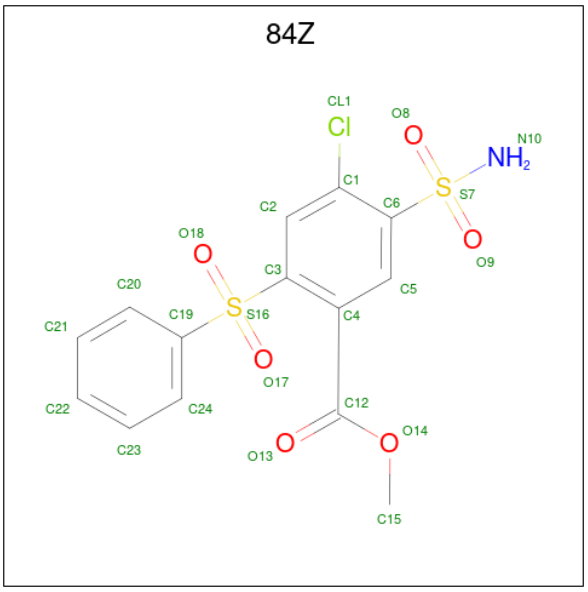
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



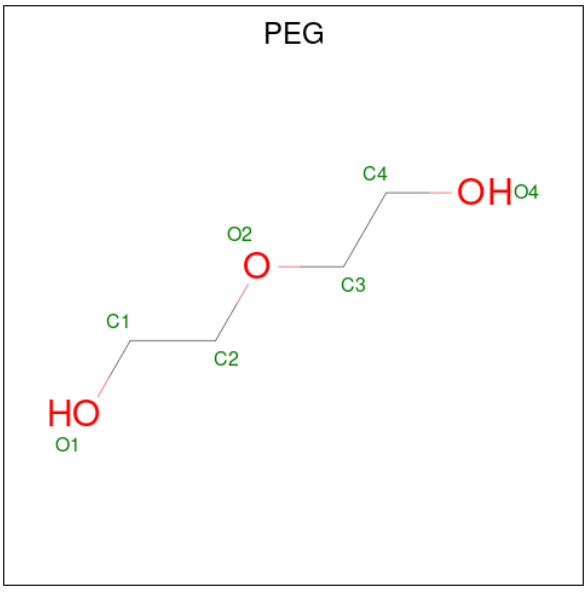
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is methyl 4-chloranyl-2-(phenylsulfonyl)-5-sulfamoyl-benzoate (three-letter code: 84Z) (formula: $C_{14}H_{12}ClNO_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			24	14	1	1	6	2		
4	B	1	Total	C	Cl	N	O	S	0	0
			24	14	1	1	6	2		
4	C	1	Total	C	Cl	N	O	S	0	0
			24	14	1	1	6	2		
4	D	1	Total	C	Cl	N	O	S	0	0
			24	14	1	1	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

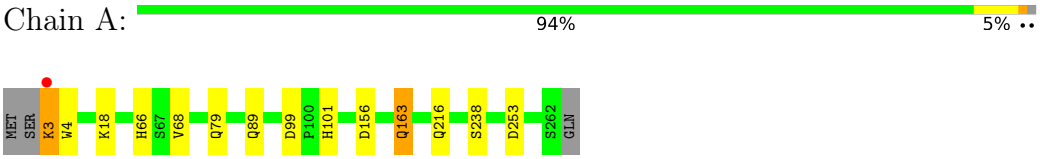
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	280	Total O 280 280	0	0
6	B	313	Total O 313 313	0	0
6	C	221	Total O 221 221	0	0
6	D	329	Total O 329 329	0	0

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.

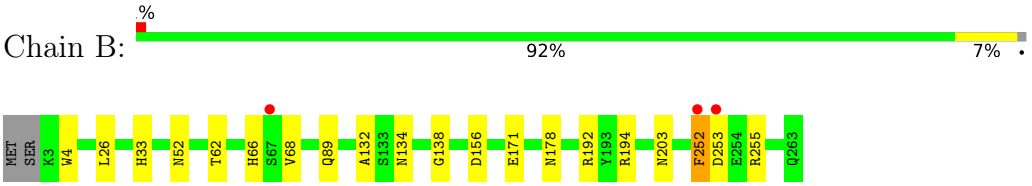
• Molecule 1: Carbonic anhydrase 12

Chain A:



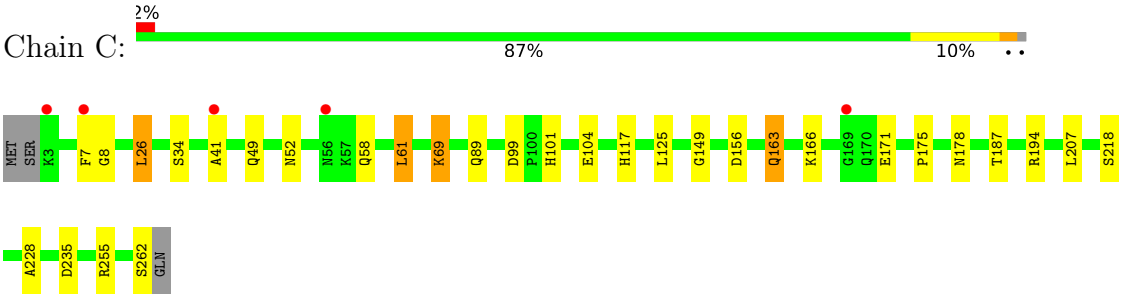
• Molecule 1: Carbonic anhydrase 12

Chain B:



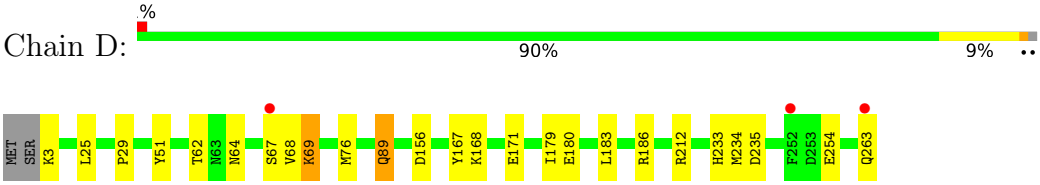
• Molecule 1: Carbonic anhydrase 12

Chain C:



• Molecule 1: Carbonic anhydrase 12

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.43Å 74.46Å 91.91Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	73.24 – 1.40 73.24 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (73.24-1.40) 97.6 (73.24-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.159 , 0.217 0.158 , 0.211	Depositor DCC
R_{free} test set	18914 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9817	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 75.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1817e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, PEG, 84Z

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	0.61	0/2168	0.94	0/2951
1	B	0.74	0/2234	1.03	1/3045 (0.0%)
1	C	0.57	0/2180	0.93	0/2971
1	D	0.74	0/2211	1.04	0/3009
All	All	0.67	0/8793	0.99	1/11976 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	252	PHE	CB-CA-C	10.40	131.21	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2105	0	1998	17	0
1	B	2170	0	2031	29	0
1	C	2117	0	1990	22	0
1	D	2147	0	2024	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	12	4	0
3	B	4	0	6	2	0
3	C	12	0	18	2	0
3	D	4	0	6	0	0
4	A	24	0	0	0	0
4	B	24	0	0	3	0
4	C	24	0	0	0	0
4	D	24	0	0	0	0
5	B	7	0	10	8	0
6	A	280	0	0	11	0
6	B	313	0	0	7	0
6	C	221	0	0	4	0
6	D	329	0	0	8	0
All	All	9817	0	8095	104	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 6.

All (104) 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)
4:B:304:84Z:N10	4:B:304:84Z:S7	1.96	1.38
1:D:67:SER:HB3	6:D:622:HOH:O	1.31	1.24
1:D:62:THR:HG22	1:D:171:GLU:HG2	1.34	1.06
6:A:453:HOH:O	3:B:302:EDO:H22	1.54	1.04
3:A:303:EDO:H21	3:B:302:EDO:O1	1.65	0.97
1:C:194:ARG:NH1	1:C:207:LEU:HD13	1.78	0.97
1:C:194:ARG:HH12	1:C:207:LEU:HD13	1.31	0.95
1:B:194:ARG:HG3	1:B:194:ARG:HH11	1.32	0.92
1:A:18[A]:LYS:HE2	6:A:630:HOH:O	1.72	0.89
1:A:18[A]:LYS:HG2	6:A:630:HOH:O	1.73	0.88
1:C:194:ARG:HH11	1:C:194:ARG:HG2	1.39	0.87
1:A:3:LYS:HA	6:A:578:HOH:O	1.78	0.83
1:D:64:ASN:HB3	6:D:436:HOH:O	1.78	0.81
1:D:51:TYR:HA	1:D:76[B]:MET:HE2	1.62	0.81
3:A:303:EDO:H12	1:B:33:HIS:CD2	2.20	0.77
1:D:180[B]:GLU:OE2	6:D:401:HOH:O	2.03	0.77
1:D:69:LYS:HE2	1:D:89:GLN:NE2	2.01	0.76
1:D:186:ARG:HA	6:D:648:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:TYR:HA	1:D:76[B]:MET:CE	2.16	0.75
1:D:233[B]:HIS:ND1	1:D:235:ASP:OD1	2.24	0.71
1:C:187:THR:OG1	3:C:304:EDO:H12	1.91	0.70
1:C:194:ARG:NH1	1:C:194:ARG:HG2	2.04	0.68
1:D:212:ARG:HH12	1:D:263:GLN:HB3	1.58	0.68
1:B:192:ARG:HH22	5:B:303:PEG:C1	2.07	0.67
1:B:62[A]:THR:HG23	6:B:570:HOH:O	1.95	0.67
1:D:76[B]:MET:HE1	1:D:179:ILE:CB	2.24	0.67
1:A:163:GLN:HE21	1:A:163:GLN:H	1.43	0.67
1:D:76[B]:MET:HE1	1:D:179:ILE:HB	1.78	0.66
1:D:76[B]:MET:HE1	1:D:179:ILE:CG1	2.27	0.65
1:D:76[B]:MET:HE1	1:D:179:ILE:HG13	1.79	0.64
1:D:76[B]:MET:CE	1:D:179:ILE:HB	2.27	0.64
1:B:192:ARG:HH12	5:B:303:PEG:H31	1.63	0.64
1:B:194:ARG:HG3	1:B:194:ARG:NH1	2.06	0.62
1:B:252:PHE:CZ	1:B:255:ARG:HB3	2.35	0.62
1:A:18[A]:LYS:CG	6:A:630:HOH:O	2.41	0.62
1:B:252:PHE:CZ	1:B:255:ARG:CB	2.83	0.61
1:B:255:ARG:HD2	6:B:459:HOH:O	1.99	0.61
1:A:18[A]:LYS:CE	6:A:630:HOH:O	2.40	0.60
1:B:255:ARG:CD	6:B:459:HOH:O	2.49	0.60
3:C:303:EDO:H11	6:C:525:HOH:O	2.01	0.60
1:B:62[B]:THR:HG22	1:B:171:GLU:HG2	1.82	0.60
1:D:51:TYR:CG	1:D:76[B]:MET:HE2	2.37	0.60
1:D:212:ARG:HH12	1:D:263:GLN:CB	2.13	0.60
5:B:303:PEG:H32	6:B:624:HOH:O	2.03	0.59
1:D:168:LYS:HE2	1:D:233[A]:HIS:NE2	2.17	0.59
1:C:69:LYS:HE3	6:C:521:HOH:O	2.03	0.58
1:C:166:LYS:HG2	1:C:228:ALA:O	2.05	0.57
1:A:99:ASP:OD1	1:A:101:HIS:HD2	1.90	0.55
1:C:8:GLY:HA2	1:D:25:LEU:HD21	1.88	0.54
1:D:68:VAL:CG1	6:D:402:HOH:O	2.56	0.54
1:B:252:PHE:CE1	1:B:255:ARG:HB2	2.43	0.54
1:D:76[B]:MET:CE	1:D:179:ILE:CG1	2.85	0.54
1:B:194:ARG:HH11	1:B:194:ARG:CG	2.14	0.53
1:A:18[A]:LYS:CD	6:A:630:HOH:O	2.56	0.53
1:B:252:PHE:CZ	1:B:255:ARG:HB2	2.43	0.53
1:C:194:ARG:NH1	1:C:194:ARG:CG	2.73	0.50
1:B:192:ARG:HH12	5:B:303:PEG:C1	2.24	0.50
1:C:149:GLY:O	1:C:218:SER:HA	2.12	0.50
1:A:3:LYS:HG2	1:A:4:TRP:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASN:HA	1:B:178:ASN:HA	1.95	0.48
4:B:304:84Z:N10	4:B:304:84Z:C5	2.76	0.48
1:B:194:ARG:NH1	1:B:194:ARG:CG	2.74	0.48
1:D:68:VAL:HG12	6:D:402:HOH:O	2.13	0.48
1:C:104:GLU:OE1	1:C:117:HIS:HE1	1.96	0.48
1:D:180[A]:GLU:HG3	1:D:183:LEU:HD12	1.94	0.48
1:A:163:GLN:HE21	1:A:163:GLN:N	2.10	0.47
1:B:192:ARG:HH12	5:B:303:PEG:H12	1.80	0.47
1:D:51:TYR:CA	1:D:76[B]:MET:HE2	2.37	0.47
1:B:192:ARG:HH22	5:B:303:PEG:H12	1.77	0.47
1:D:76[B]:MET:CE	1:D:179:ILE:HG13	2.43	0.47
1:C:58:GLN:HG2	1:C:175:PRO:HA	1.97	0.47
5:B:303:PEG:H31	5:B:303:PEG:O1	2.15	0.46
1:C:52:ASN:HA	1:C:178:ASN:HA	1.97	0.46
1:B:192:ARG:NH1	5:B:303:PEG:O1	2.48	0.46
1:C:166:LYS:CG	1:C:228:ALA:O	2.63	0.46
1:A:3:LYS:HD2	1:A:3:LYS:N	2.31	0.46
1:C:99:ASP:OD1	1:C:101:HIS:HD2	1.98	0.46
1:B:62[A]:THR:O	1:B:68:VAL:HA	2.17	0.45
1:D:64:ASN:ND2	6:D:412:HOH:O	2.49	0.45
1:B:252:PHE:CE1	1:B:255:ARG:CB	3.00	0.45
1:D:167:TYR:CE2	1:D:234[B]:MET:HG3	2.52	0.44
1:A:253:ASP:HB2	6:A:629:HOH:O	2.16	0.44
1:D:69:LYS:HB3	1:D:69:LYS:HE3	1.68	0.44
1:C:7:PHE:CD2	1:C:8:GLY:N	2.86	0.44
4:B:304:84Z:N10	4:B:304:84Z:C6	2.77	0.43
1:C:194:ARG:NH1	1:C:207:LEU:CD1	2.67	0.43
1:B:203[A]:ASN:ND2	6:B:401:HOH:O	2.21	0.43
1:A:101:HIS:CD2	3:A:303:EDO:H11	2.54	0.43
1:A:3:LYS:HG2	1:A:4:TRP:CD1	2.55	0.42
1:A:216:GLN:HG3	6:A:631:HOH:O	2.19	0.42
1:B:132:ALA:O	1:B:138:GLY:HA3	2.19	0.42
1:A:66:HIS:HA	6:A:569:HOH:O	2.19	0.42
1:B:4:TRP:O	1:B:66:HIS:HE1	2.01	0.42
1:B:134:ASN:HB3	6:B:643:HOH:O	2.20	0.42
1:C:26:LEU:HD22	1:C:255:ARG:NH1	2.34	0.42
1:C:61:LEU:O	1:C:171:GLU:HA	2.20	0.41
1:B:4:TRP:N	6:B:413:HOH:O	2.54	0.41
1:B:26:LEU:HD23	1:B:255:ARG:HD3	2.03	0.41
1:D:3:LYS:N	6:D:417:HOH:O	2.53	0.41
1:C:163:GLN:H	1:C:163:GLN:HG2	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:OE1	6:A:401:HOH:O	2.22	0.41
1:C:69:LYS:HE2	6:C:479:HOH:O	2.19	0.41
3:A:303:EDO:H12	1:B:33:HIS:NE2	2.37	0.40
1:C:69:LYS:CE	6:C:479:HOH:O	2.68	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	261/263 (99%)	258 (99%)	3 (1%)	0	100 100
1	B	270/263 (103%)	265 (98%)	5 (2%)	0	100 100
1	C	264/263 (100%)	253 (96%)	9 (3%)	2 (1%)	19 4
1	D	265/263 (101%)	258 (97%)	7 (3%)	0	100 100
All	All	1060/1052 (101%)	1034 (98%)	24 (2%)	2 (0%)	51 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41[A]	ALA
1	C	41[B]	ALA

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	231/235 (98%)	225 (97%)	6 (3%)	46 13
1	B	241/235 (103%)	238 (99%)	3 (1%)	71 47
1	C	231/235 (98%)	220 (95%)	11 (5%)	25 4
1	D	239/235 (102%)	234 (98%)	5 (2%)	53 21
All	All	942/940 (100%)	917 (97%)	25 (3%)	44 13

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	68	VAL
1	A	89	GLN
1	A	156	ASP
1	A	163	GLN
1	A	238	SER
1	B	89	GLN
1	B	156	ASP
1	B	253	ASP
1	C	26	LEU
1	C	34	SER
1	C	49	GLN
1	C	61	LEU
1	C	69	LYS
1	C	89	GLN
1	C	125	LEU
1	C	156	ASP
1	C	163	GLN
1	C	235	ASP
1	C	262	SER
1	D	29	PRO
1	D	69	LYS
1	D	89	GLN
1	D	156	ASP
1	D	254	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	163	GLN
1	B	66	HIS
1	B	101	HIS
1	C	49	GLN
1	C	58	GLN
1	C	111	HIS
1	C	233	HIS
1	D	98	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)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	EDO	B	302	-	3,3,3	0.58	0	2,2,2	0.34	0
3	EDO	C	304	-	3,3,3	0.35	0	2,2,2	0.76	0
4	84Z	B	304	2	25,25,25	4.29	11 (44%)	38,38,38	3.52	20 (52%)
3	EDO	C	303	-	3,3,3	1.57	0	2,2,2	1.57	0
3	EDO	D	302	-	3,3,3	0.83	0	2,2,2	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	84Z	A	304	2	25,25,25	2.77	10 (40%)	38,38,38	3.54	24 (63%)
3	EDO	A	303	-	3,3,3	0.44	0	2,2,2	0.70	0
3	EDO	A	302	-	3,3,3	0.16	0	2,2,2	0.53	0
4	84Z	D	303	2	25,25,25	2.25	11 (44%)	38,38,38	2.11	14 (36%)
3	EDO	C	302	-	3,3,3	0.30	0	2,2,2	0.58	0
4	84Z	C	305	2	25,25,25	2.30	10 (40%)	38,38,38	2.53	18 (47%)
5	PEG	B	303	-	6,6,6	0.33	0	5,5,5	0.44	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
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	C	304	-	-	1/1/1/1	-
4	84Z	B	304	2	-	2/24/24/24	0/2/2/2
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	D	302	-	-	0/1/1/1	-
4	84Z	A	304	2	-	0/24/24/24	0/2/2/2
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
4	84Z	D	303	2	-	2/24/24/24	0/2/2/2
3	EDO	C	302	-	-	0/1/1/1	-
4	84Z	C	305	2	-	2/24/24/24	0/2/2/2
5	PEG	B	303	-	-	3/4/4/4	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	84Z	S7-N10	18.22	1.96	1.60
4	A	304	84Z	S7-N10	8.41	1.77	1.60
4	A	304	84Z	O9-S7	5.66	1.54	1.43
4	A	304	84Z	O8-S7	5.65	1.54	1.43
4	B	304	84Z	C24-C19	-4.57	1.31	1.38
4	C	305	84Z	S7-N10	4.45	1.69	1.60
4	D	303	84Z	C6-S7	4.22	1.82	1.77
4	C	305	84Z	O17-S16	4.09	1.51	1.44
4	B	304	84Z	O14-C12	3.98	1.42	1.33
4	C	305	84Z	C4-C3	3.90	1.44	1.40
4	B	304	84Z	C19-S16	-3.90	1.70	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	84Z	O14-C15	-3.85	1.36	1.45
4	C	305	84Z	O14-C12	3.81	1.41	1.33
4	D	303	84Z	C3-S16	-3.66	1.73	1.78
4	B	304	84Z	C20-C19	3.59	1.44	1.38
4	C	305	84Z	C3-S16	-3.52	1.73	1.78
4	C	305	84Z	C19-S16	3.42	1.82	1.77
4	B	304	84Z	C2-C1	3.25	1.43	1.38
4	D	303	84Z	O18-S16	3.24	1.50	1.44
4	D	303	84Z	O8-S7	3.14	1.49	1.43
4	B	304	84Z	O14-C15	-3.10	1.38	1.45
4	D	303	84Z	C5-C4	2.97	1.44	1.39
4	A	304	84Z	O14-C15	-2.94	1.38	1.45
4	B	304	84Z	C21-C20	2.93	1.45	1.38
4	A	304	84Z	C19-S16	-2.84	1.72	1.77
4	C	305	84Z	O9-S7	-2.73	1.38	1.43
4	D	303	84Z	C4-C3	2.67	1.43	1.40
4	D	303	84Z	C4-C12	-2.60	1.44	1.50
4	D	303	84Z	C19-S16	-2.47	1.73	1.77
4	B	304	84Z	O18-S16	2.46	1.48	1.44
4	B	304	84Z	O13-C12	-2.41	1.16	1.22
4	A	304	84Z	C2-C1	2.37	1.42	1.38
4	A	304	84Z	C5-C6	2.35	1.42	1.39
4	A	304	84Z	O13-C12	-2.34	1.16	1.22
4	C	305	84Z	C21-C20	2.31	1.43	1.38
4	C	305	84Z	O18-S16	2.28	1.48	1.44
4	A	304	84Z	O18-S16	2.27	1.48	1.44
4	D	303	84Z	O14-C12	2.26	1.38	1.33
4	B	304	84Z	C6-S7	-2.17	1.74	1.77
4	A	304	84Z	C6-S7	-2.15	1.74	1.77
4	C	305	84Z	C1-C6	2.03	1.43	1.40
4	D	303	84Z	C23-C24	2.02	1.43	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	304	84Z	O9-S7-N10	12.63	126.08	107.36
4	A	304	84Z	O9-S7-O8	-9.89	102.51	118.76
4	B	304	84Z	C19-S16-C3	7.50	115.88	105.28
4	A	304	84Z	C19-S16-C3	6.96	115.12	105.28
4	C	305	84Z	O17-S16-C19	6.58	115.39	107.97
4	B	304	84Z	C1-C2-C3	-6.34	114.86	120.60
4	B	304	84Z	C6-S7-N10	-6.33	96.61	108.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	304	84Z	C1-C2-C3	-5.73	115.40	120.60
4	A	304	84Z	C5-C6-C1	-4.99	112.96	118.27
4	C	305	84Z	C19-S16-C3	4.84	112.11	105.28
4	A	304	84Z	C6-S7-N10	4.75	117.05	108.28
4	C	305	84Z	O17-S16-O18	-4.67	110.31	119.23
4	A	304	84Z	C2-C3-C4	4.60	124.63	120.24
4	D	303	84Z	C19-S16-C3	4.36	111.43	105.28
4	A	304	84Z	C24-C19-S16	4.35	125.06	119.52
4	A	304	84Z	C15-O14-C12	4.33	124.18	115.83
4	A	304	84Z	C2-C1-C6	4.26	125.68	121.38
4	A	304	84Z	C3-C4-C12	4.16	130.00	124.25
4	B	304	84Z	C21-C20-C19	3.97	123.08	118.95
4	A	304	84Z	O18-S16-C19	-3.94	103.53	107.97
4	A	304	84Z	O9-S7-C6	3.94	113.06	107.29
4	D	303	84Z	C20-C19-S16	3.94	124.53	119.52
4	A	304	84Z	O8-S7-C6	3.93	113.05	107.29
4	D	303	84Z	C1-C2-C3	-3.92	117.05	120.60
4	D	303	84Z	O17-S16-O18	-3.84	111.89	119.23
4	A	304	84Z	C23-C24-C19	3.83	122.93	118.95
4	B	304	84Z	C24-C19-S16	3.77	124.32	119.52
4	A	304	84Z	C20-C19-S16	-3.75	114.74	119.52
4	C	305	84Z	C15-O14-C12	3.73	123.03	115.83
4	D	303	84Z	C24-C19-S16	-3.55	114.99	119.52
4	C	305	84Z	C1-C2-C3	-3.55	117.38	120.60
4	C	305	84Z	C5-C4-C3	3.53	121.18	117.62
4	D	303	84Z	C15-O14-C12	3.51	122.60	115.83
4	B	304	84Z	C22-C21-C20	-3.49	114.87	120.19
4	B	304	84Z	C2-C3-C4	3.46	123.54	120.24
4	B	304	84Z	O13-C12-C4	3.45	133.17	121.57
4	C	305	84Z	C23-C24-C19	3.44	122.53	118.95
4	C	305	84Z	O17-S16-C3	-3.41	102.27	107.96
4	B	304	84Z	C23-C24-C19	3.38	122.46	118.95
4	D	303	84Z	O18-S16-C19	3.26	111.65	107.97
4	D	303	84Z	C2-C3-C4	3.26	123.34	120.24
4	C	305	84Z	C1-C6-S7	-3.23	119.39	123.49
4	A	304	84Z	C2-C1-CL1	-3.22	113.30	118.49
4	C	305	84Z	C24-C19-S16	-3.15	115.50	119.52
4	B	304	84Z	C15-O14-C12	3.15	121.90	115.83
4	B	304	84Z	O14-C12-O13	-3.10	117.39	123.45
4	B	304	84Z	O18-S16-C19	-3.07	104.51	107.97
4	C	305	84Z	C5-C4-C12	-3.06	112.33	118.41
4	C	305	84Z	C22-C23-C24	-2.97	115.67	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	304	84Z	C5-C6-C1	-2.96	115.12	118.27
4	A	304	84Z	C5-C4-C3	-2.77	114.83	117.62
4	C	305	84Z	C21-C20-C19	-2.74	116.11	118.95
4	C	305	84Z	C4-C5-C6	-2.69	118.35	122.02
4	A	304	84Z	O13-C12-C4	2.68	130.57	121.57
4	D	303	84Z	C6-C1-CL1	-2.64	119.56	121.49
4	C	305	84Z	C20-C19-S16	2.63	122.87	119.52
4	D	303	84Z	C4-C5-C6	-2.63	118.43	122.02
4	B	304	84Z	C20-C19-C24	-2.57	116.86	120.44
4	B	304	84Z	C2-C1-C6	2.56	123.96	121.38
4	A	304	84Z	O14-C12-O13	-2.53	118.49	123.45
4	C	305	84Z	C5-C6-C1	2.53	120.96	118.27
4	B	304	84Z	O9-S7-C6	-2.51	103.61	107.29
4	A	304	84Z	C22-C23-C24	-2.51	116.37	120.19
4	B	304	84Z	C2-C1-CL1	-2.49	114.47	118.49
4	B	304	84Z	O9-S7-O8	-2.47	114.70	118.76
4	A	304	84Z	C21-C20-C19	-2.45	116.42	118.95
4	A	304	84Z	C22-C21-C20	2.41	123.87	120.19
4	A	304	84Z	C4-C5-C6	2.41	125.31	122.02
4	A	304	84Z	C5-C6-S7	2.37	121.18	118.34
4	C	305	84Z	C2-C1-CL1	-2.33	114.73	118.49
4	D	303	84Z	C5-C6-C1	2.29	120.70	118.27
4	D	303	84Z	C3-C4-C12	2.28	127.40	124.25
4	D	303	84Z	O9-S7-N10	2.22	110.65	107.36
4	B	304	84Z	O14-C12-C4	-2.12	108.77	112.30
4	D	303	84Z	C21-C20-C19	2.11	121.15	118.95
4	C	305	84Z	O9-S7-C6	2.00	110.22	107.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	303	PEG	C1-C2-O2-C3
3	B	302	EDO	O1-C1-C2-O2
3	C	304	EDO	O1-C1-C2-O2
5	B	303	PEG	O2-C3-C4-O4
3	C	303	EDO	O1-C1-C2-O2
4	B	304	84Z	C1-C6-S7-N10
5	B	303	PEG	O1-C1-C2-O2
4	C	305	84Z	C4-C3-S16-O17
4	C	305	84Z	O13-C12-C4-C3
4	D	303	84Z	C5-C6-S7-N10

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Mol	Chain	Res	Type	Atoms
4	B	304	84Z	C20-C19-S16-O17
4	D	303	84Z	C24-C19-S16-O17

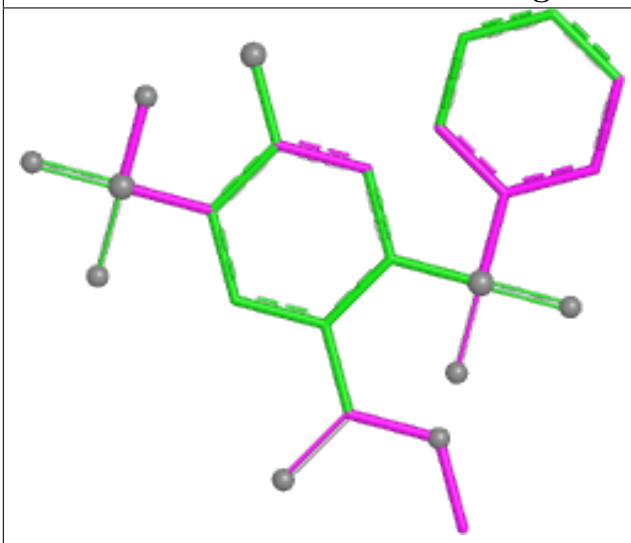
There are no ring outliers.

6 monomers are involved in 18 short contacts:

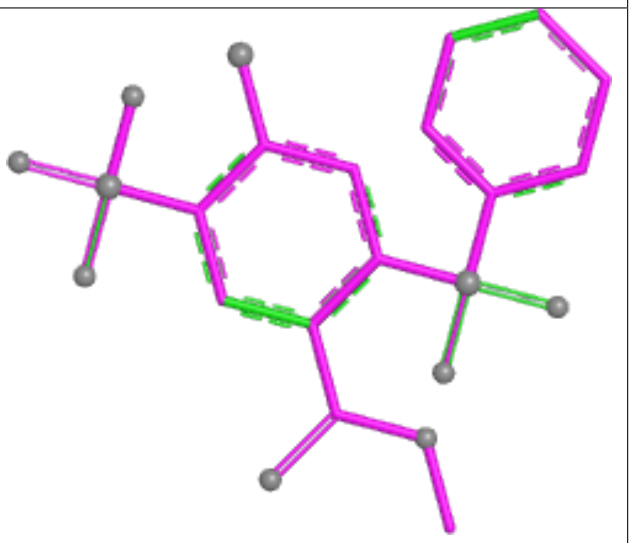
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	EDO	2	0
3	C	304	EDO	1	0
4	B	304	84Z	3	0
3	C	303	EDO	1	0
3	A	303	EDO	4	0
5	B	303	PEG	8	0

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 then 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.

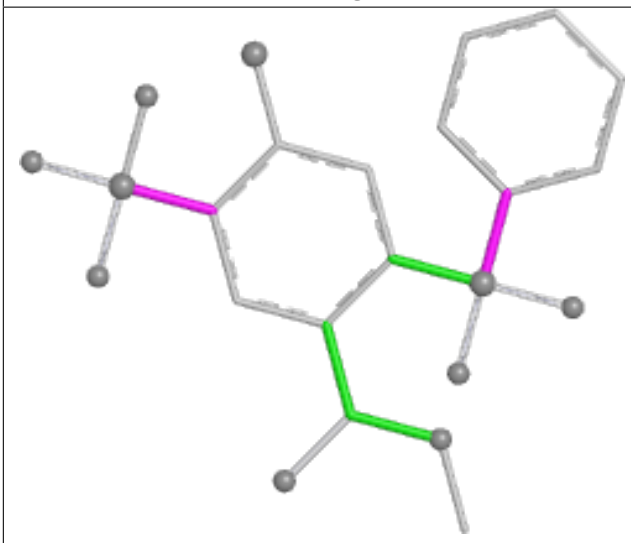
Ligand 84Z B 304



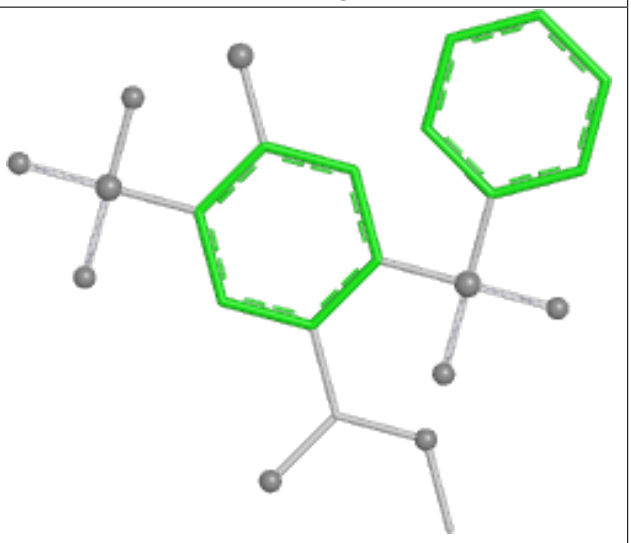
Bond lengths



Bond angles

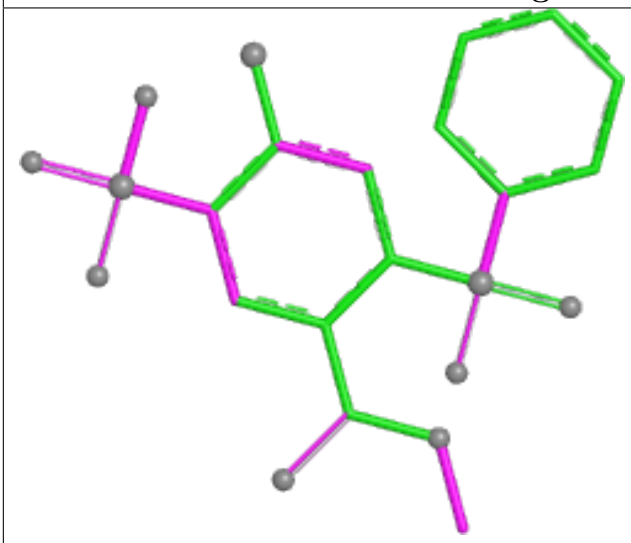


Torsions

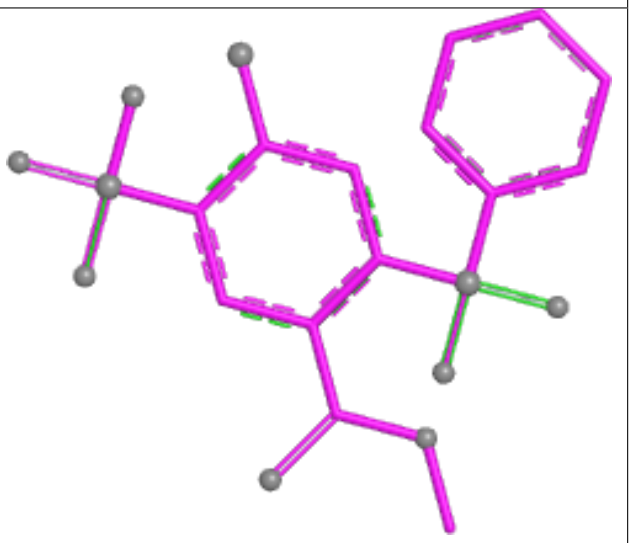


Rings

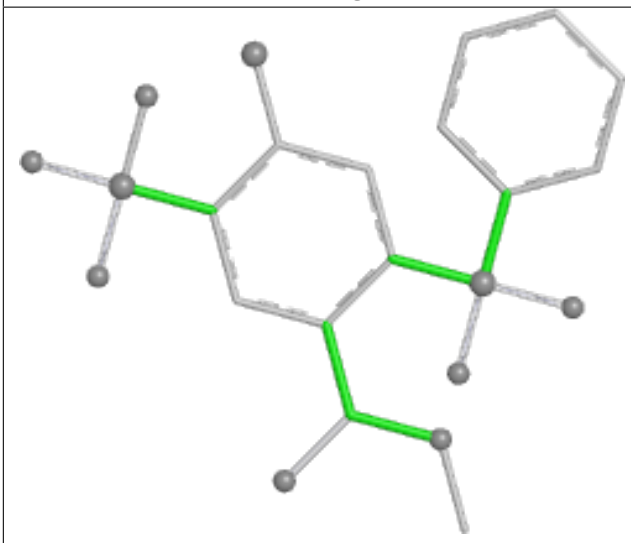
Ligand 84Z A 304



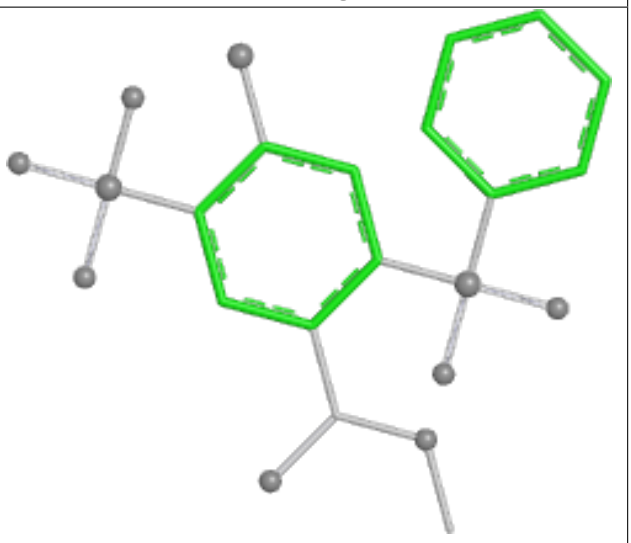
Bond lengths



Bond angles

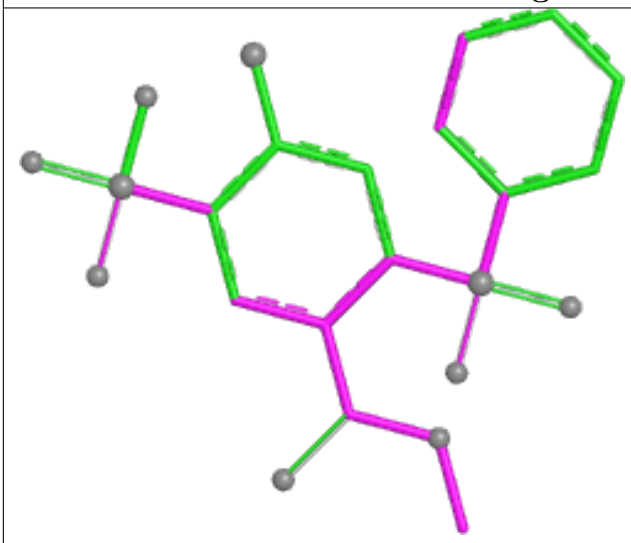


Torsions

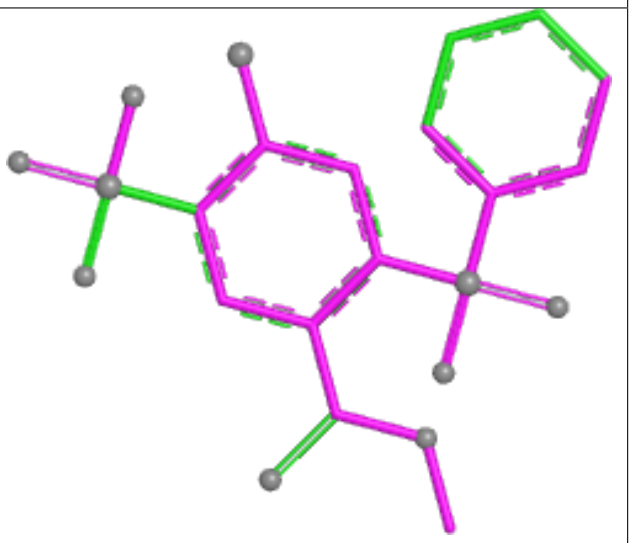


Rings

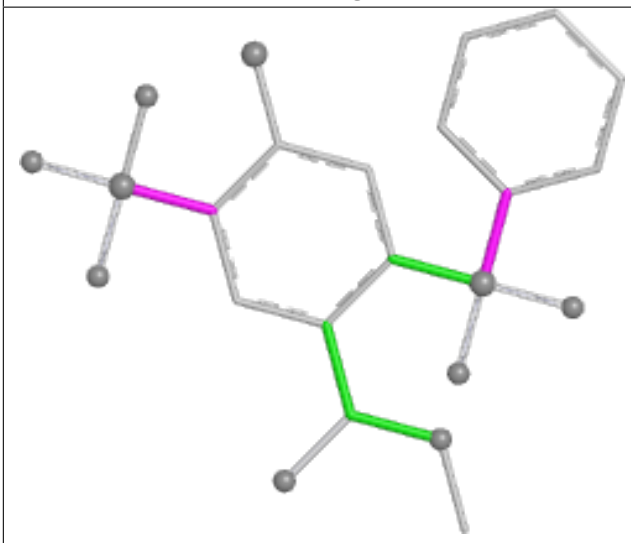
Ligand 84Z D 303



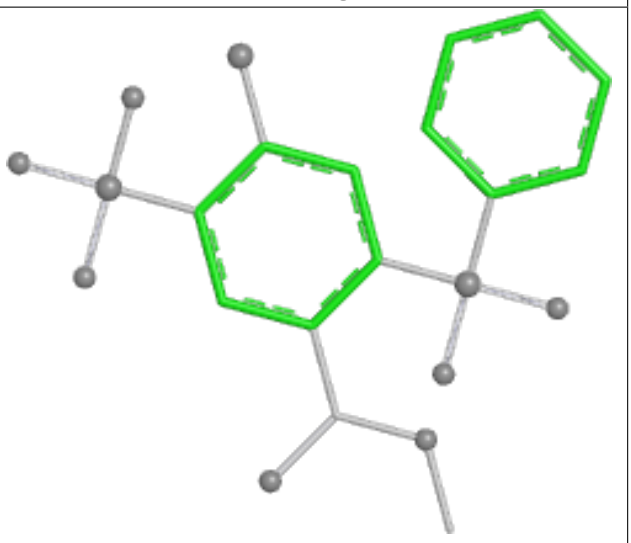
Bond lengths



Bond angles

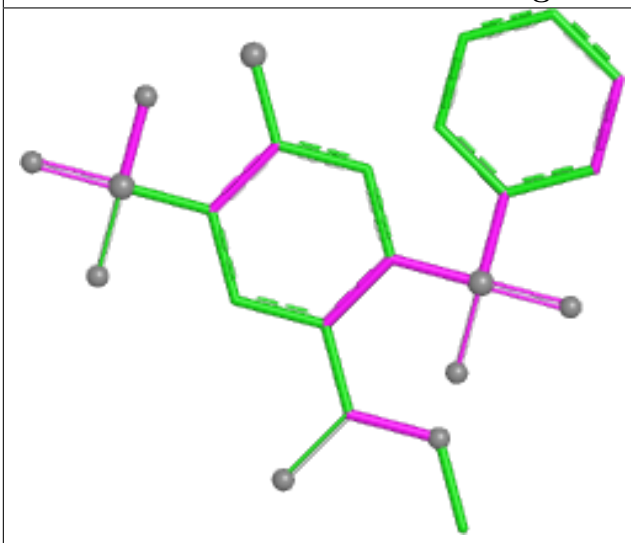


Torsions

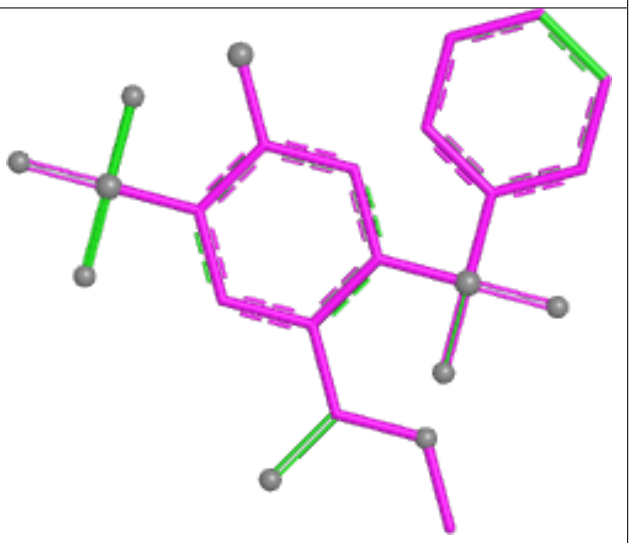


Rings

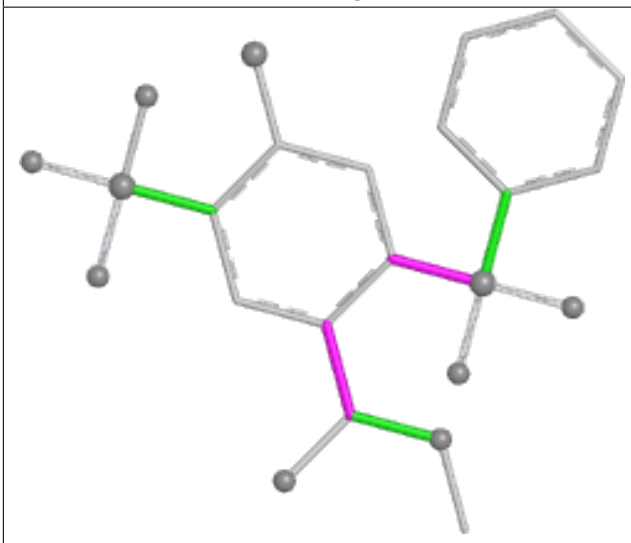
Ligand 84Z C 305



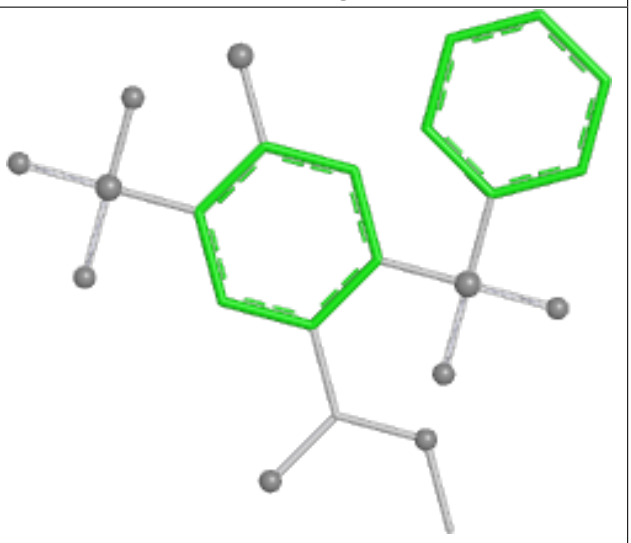
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	260/263 (98%)	-0.08	1 (0%)	92	91	8, 16, 36, 62	0
1	B	261/263 (99%)	0.08	3 (1%)	80	79	7, 12, 24, 44	0
1	C	260/263 (98%)	0.08	5 (1%)	66	67	8, 20, 41, 82	0
1	D	261/263 (99%)	0.05	3 (1%)	80	79	7, 13, 25, 58	0
All	All	1042/1052 (99%)	0.03	12 (1%)	79	77	7, 14, 34, 82	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	PHE	6.5
1	B	252	PHE	5.9
1	C	41[A]	ALA	3.5
1	B	253	ASP	3.3
1	C	169	GLY	3.1
1	A	3	LYS	2.9
1	D	67	SER	2.7
1	D	263	GLN	2.6
1	B	67	SER	2.4
1	D	252	PHE	2.4
1	C	3	LYS	2.3
1	C	56	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

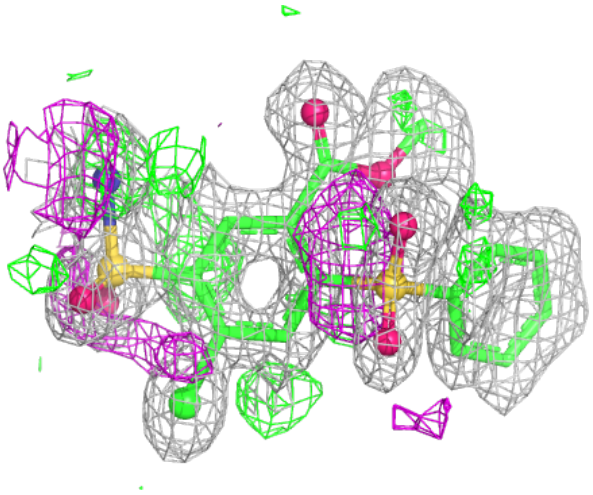
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

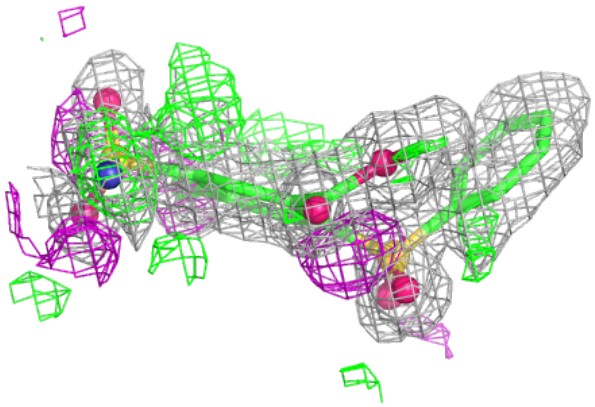
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	303	4/4	0.86	0.19	17,20,22,28	0
5	PEG	B	303	7/7	0.88	0.18	12,31,39,42	0
3	EDO	D	302	4/4	0.90	0.12	16,20,20,23	0
3	EDO	C	302	4/4	0.90	0.10	23,26,36,44	0
3	EDO	A	302	4/4	0.93	0.11	15,19,25,31	0
3	EDO	A	303	4/4	0.94	0.22	18,28,36,40	0
3	EDO	B	302	4/4	0.94	0.31	18,23,26,31	0
4	84Z	B	304	24/24	0.95	0.11	8,12,15,18	0
3	EDO	C	304	4/4	0.96	0.32	27,31,36,37	0
4	84Z	A	304	24/24	0.96	0.10	8,14,21,23	0
4	84Z	C	305	24/24	0.98	0.08	9,14,29,29	0
4	84Z	D	303	24/24	0.99	0.08	8,12,17,18	0
2	ZN	C	301	1/1	0.99	0.05	10,10,10,10	0
2	ZN	B	301	1/1	1.00	0.05	8,8,8,8	0
2	ZN	A	301	1/1	1.00	0.06	8,8,8,8	0
2	ZN	D	301	1/1	1.00	0.06	8,8,8,8	0

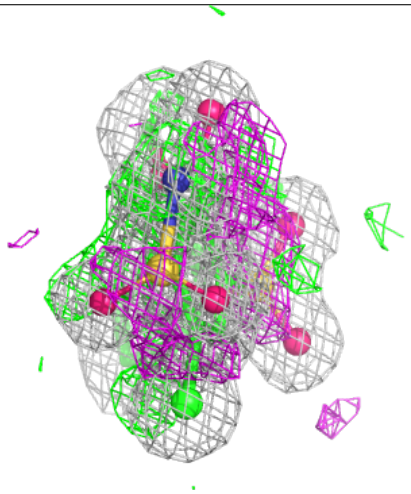
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 84Z B 304:

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

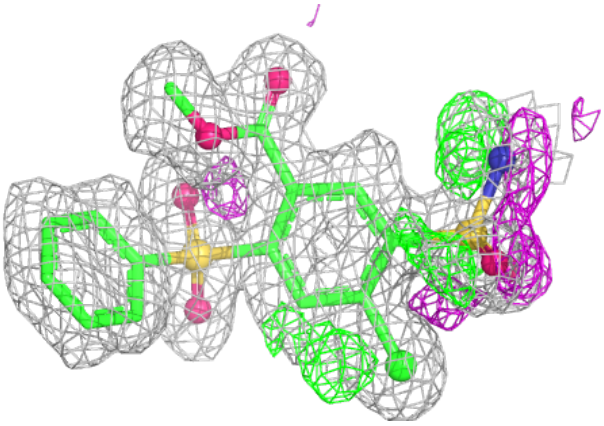


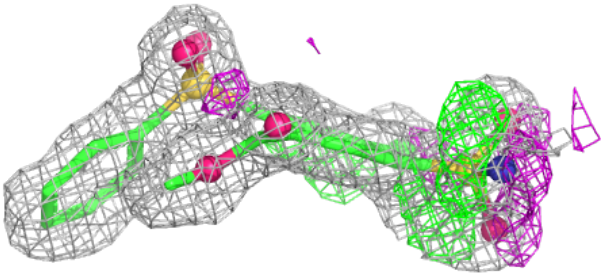


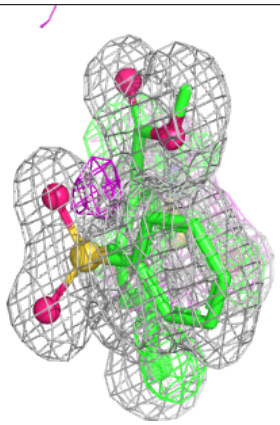


Electron density around 84Z A 304:

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

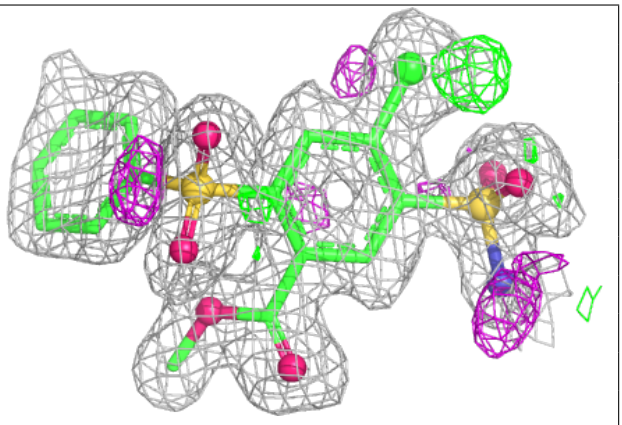


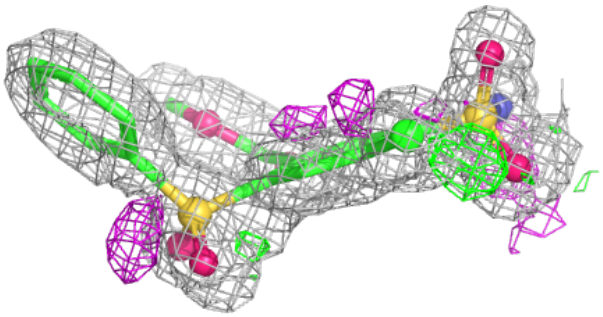


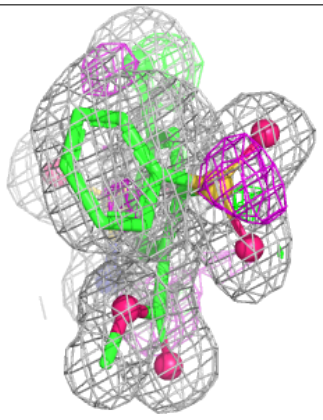


Electron density around 84Z C 305:

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

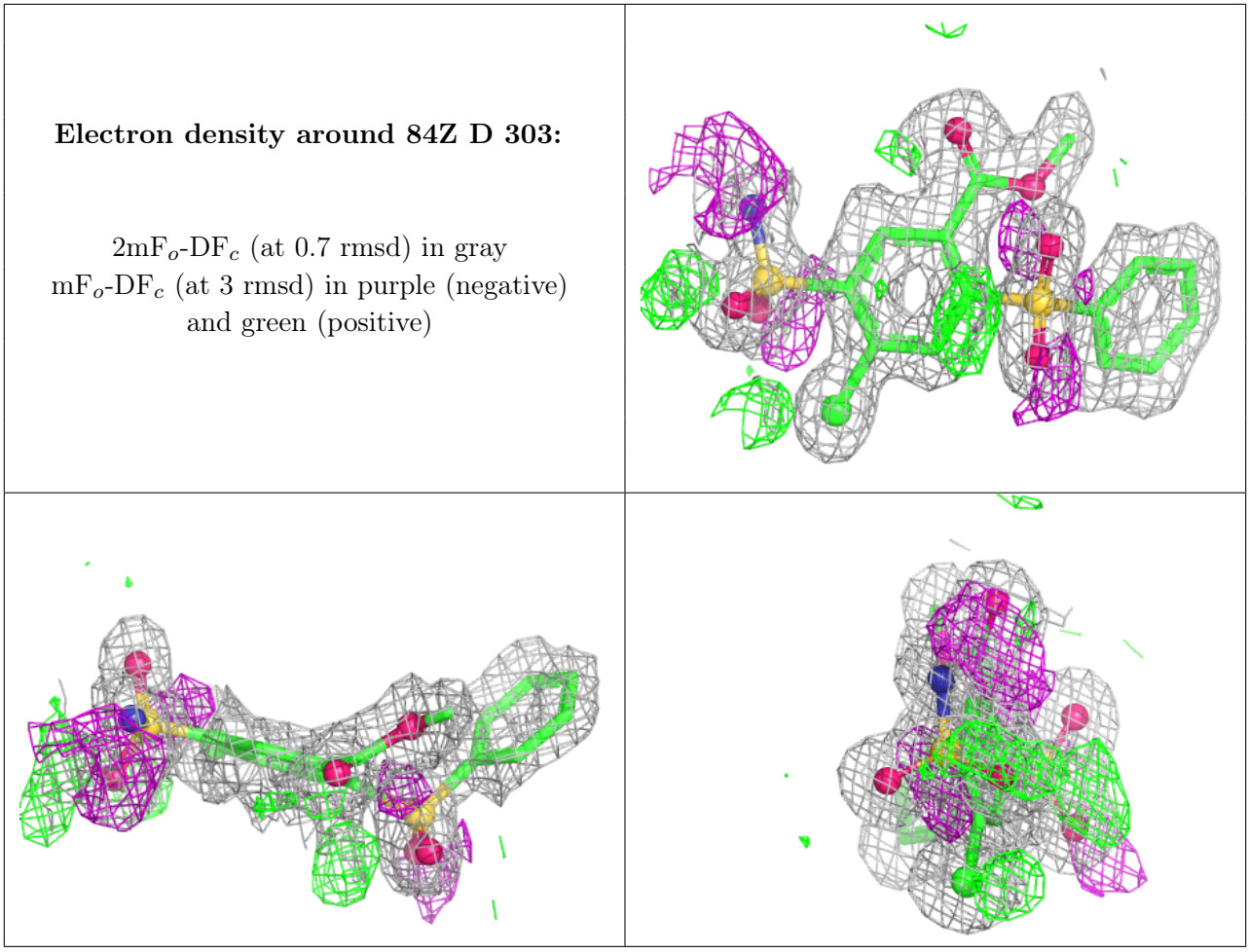






Electron density around 84Z D 303:

$2mF_o$-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.