



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 11:20 PM EDT

PDB ID : 2D3U
Title : X-ray crystal structure of hepatitis C virus RNA dependent RNA polymerase in complex with non-nucleoside analogue inhibitor
Authors : Biswal, B.K.; Wang, M.; Cherney, M.M.; Chan, L.; Yannopoulos, C.G.; Bilimoria, D.; Bedard, J.; James, M.N.G.
Deposited on : 2005-10-02
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

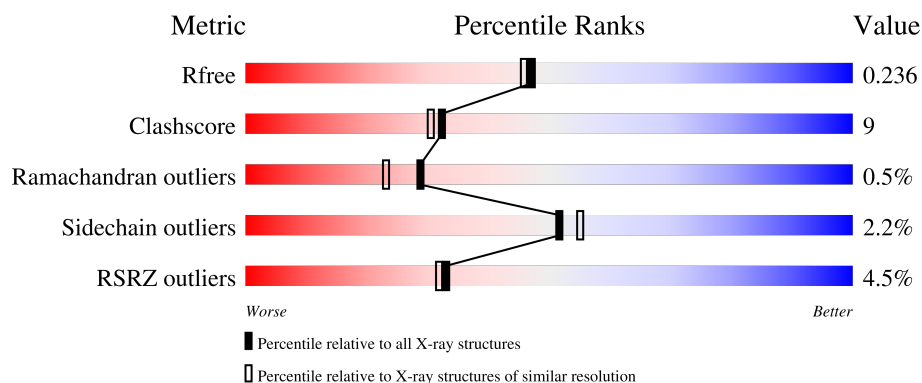
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	570	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	570	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

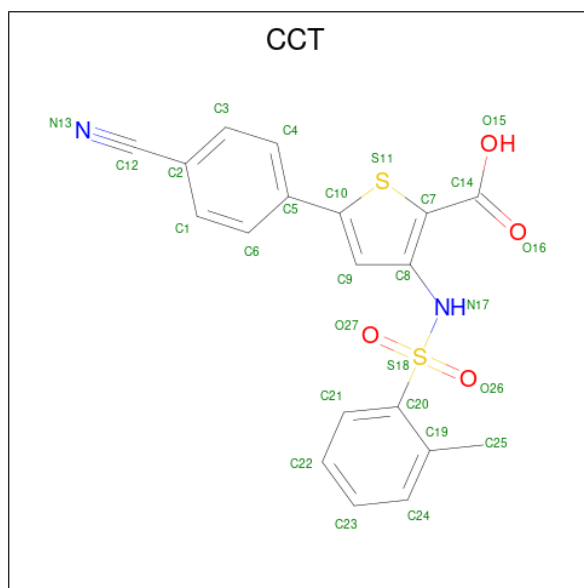
There are 3 unique types of molecules in this entry. The entry contains 9496 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4340	2738	765	806	31			
1	B	559	Total	C	N	O	S	0	0	0
			4348	2744	766	807	31			

- Molecule 2 is 5-(4-CYANOPHENYL)-3-[(2-METHYLPHENYL)SULFONYL]AMINO}THIOPHENE-2-CARBOXYLIC ACID (three-letter code: CCT) (formula: C₁₉H₁₄N₂O₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	19	2	4	2		
2	B	1	Total	C	N	O	S	0	0
			27	19	2	4	2		

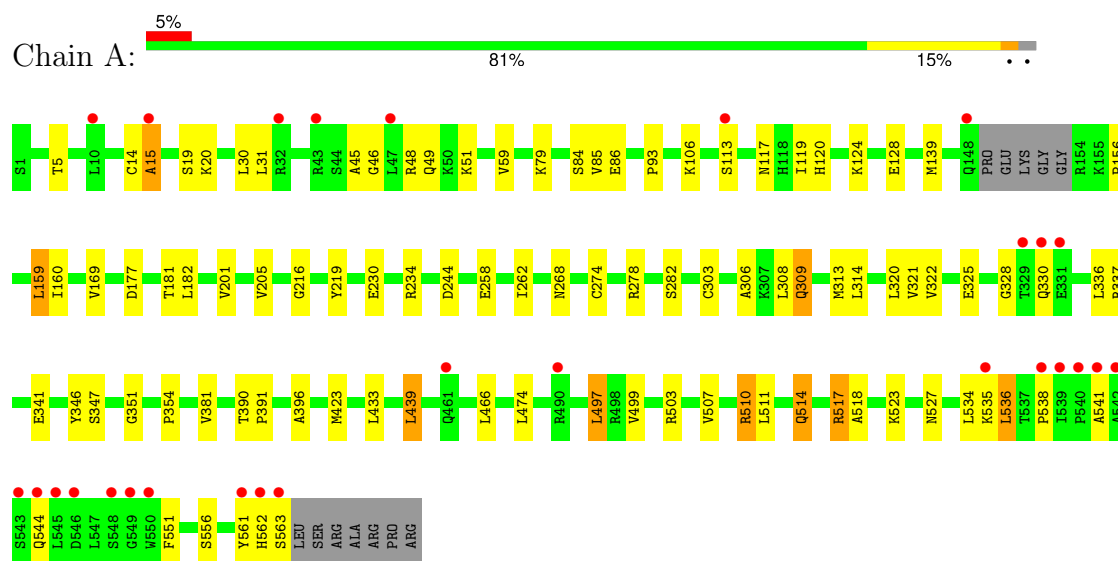
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	365	Total 365	O 365	0	0
3	B	389	Total 389	O 389	0	0

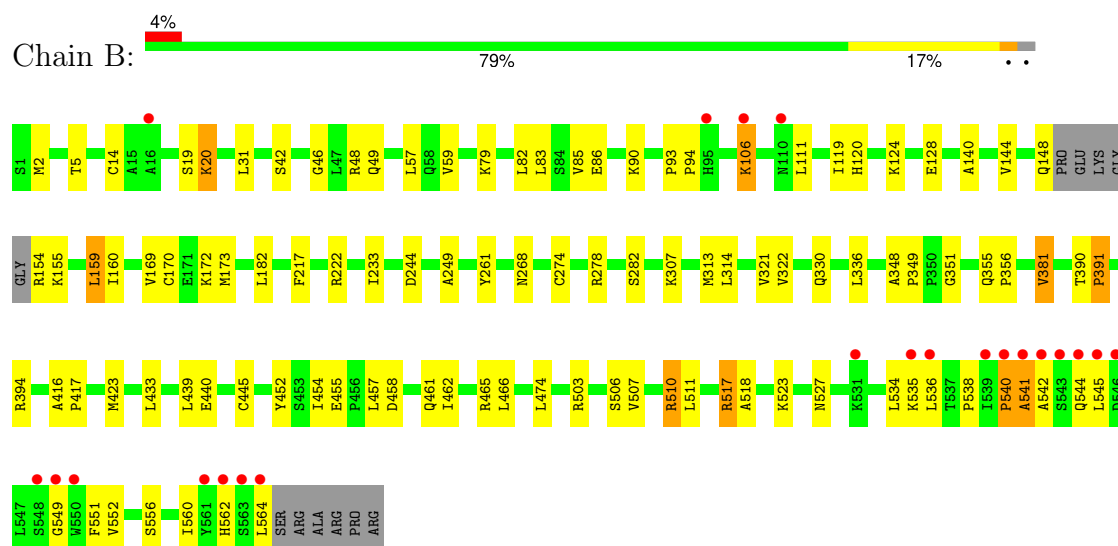
3 Residue-property plots [i](#)

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: polypeptide



- Molecule 1: polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.92Å 104.31Å 127.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.57 – 2.00 37.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (37.57-2.00) 98.9 (37.57-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.245 0.201 , 0.236	Depositor DCC
R_{free} test set	3865 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9496	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 50.36 % 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 6.5373e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/4434	0.63	1/6017 (0.0%)
1	B	0.41	0/4442	0.64	1/6028 (0.0%)
All	All	0.40	0/8876	0.64	2/12045 (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	B	351	GLY	N-CA-C	-5.34	99.75	113.10
1	A	351	GLY	N-CA-C	-5.07	100.44	113.10

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	4340	0	4357	70	0
1	B	4348	0	4368	85	0
2	A	27	0	13	1	0
2	B	27	0	13	1	0
3	A	365	0	0	2	0
3	B	389	0	0	11	0
All	All	9496	0	8751	154	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 9.

All (154) 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:B:5:THR:HG23	1:B:278:ARG:HH22	1.16	1.03
1:A:5:THR:HG23	1:A:278:ARG:HH22	1.39	0.88
1:A:336:LEU:HD21	1:A:354:PRO:HG2	1.56	0.88
1:B:5:THR:CG2	1:B:278:ARG:HH22	1.88	0.85
1:B:5:THR:HG23	1:B:278:ARG:NH2	1.91	0.84
1:A:5:THR:HG21	1:A:278:ARG:HH12	1.41	0.83
1:B:106:LYS:NZ	1:B:106:LYS:HA	1.93	0.82
1:B:462:ILE:HG13	3:B:2234:HOH:O	1.79	0.82
1:B:527:ASN:HD21	1:B:534:LEU:H	1.27	0.82
1:B:458:ASP:HB3	3:B:2234:HOH:O	1.80	0.80
1:A:527:ASN:HD21	1:A:534:LEU:H	1.27	0.79
1:B:222:ARG:HD3	3:B:2384:HOH:O	1.83	0.77
1:A:313:MET:HG2	1:A:322:VAL:HG22	1.67	0.76
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.67	0.76
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.69	0.75
1:B:148:GLN:HG3	3:B:2287:HOH:O	1.88	0.73
1:B:106:LYS:HA	1:B:106:LYS:HZ3	1.53	0.72
1:A:5:THR:CG2	1:A:278:ARG:HH12	2.01	0.72
1:B:541:ALA:O	1:B:544:GLN:HG2	1.91	0.70
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.22	0.70
1:A:337:ARG:O	1:A:341:GLU:HG3	1.90	0.70
1:B:433:LEU:HB3	1:B:439:LEU:HD12	1.72	0.70
1:A:510:ARG:HH11	1:A:510:ARG:HG2	1.57	0.68
1:B:455:GLU:HB3	3:B:2218:HOH:O	1.94	0.67
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.78	0.65
1:B:523:LYS:HE2	1:B:534:LEU:HD23	1.79	0.65
1:B:182:LEU:C	1:B:182:LEU:HD23	2.18	0.65
1:B:2:MET:HB2	1:B:278:ARG:HH21	1.62	0.64
1:B:86:GLU:O	1:B:90:LYS:HG2	1.97	0.64
1:A:336:LEU:CD2	1:A:354:PRO:HG2	2.28	0.64
1:B:154:ARG:N	3:B:2284:HOH:O	2.31	0.63
1:B:510:ARG:HG2	1:B:510:ARG:HH21	1.64	0.63
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.28	0.63
1:A:182:LEU:HD23	1:A:182:LEU:C	2.20	0.62
1:B:452:TYR:HA	1:B:562:HIS:O	1.99	0.62
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.80	0.62
1:B:170:CYS:HA	1:B:173:MET:CE	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:CYS:HA	1:B:173:MET:HE3	1.81	0.61
1:B:461:GLN:HG3	3:B:2217:HOH:O	2.00	0.60
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.32	0.59
1:A:423:MET:HB2	2:A:1001:CCT:H22	1.86	0.58
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.34	0.58
1:A:309:GLN:HB3	1:A:325:GLU:HB3	1.86	0.57
1:A:5:THR:HG23	1:A:278:ARG:NH2	2.15	0.57
1:A:510:ARG:HG2	1:A:510:ARG:NH1	2.20	0.57
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.85	0.57
1:A:19:SER:OG	1:A:20:LYS:HD2	2.06	0.56
1:B:314:LEU:HB3	1:B:321:VAL:HG12	1.87	0.55
1:B:564:LEU:HD23	3:B:2219:HOH:O	2.06	0.55
1:B:79:LYS:HA	1:B:244:ASP:HB3	1.89	0.55
1:A:556:SER:HB3	3:A:1349:HOH:O	2.06	0.54
1:B:510:ARG:HG2	1:B:510:ARG:NH2	2.22	0.54
1:B:124:LYS:O	1:B:128:GLU:HG3	2.07	0.54
1:B:527:ASN:ND2	1:B:534:LEU:H	2.01	0.54
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.89	0.54
1:B:461:GLN:HE21	1:B:541:ALA:C	2.10	0.54
1:B:511:LEU:HB3	1:B:518:ALA:O	2.09	0.53
1:A:14:CYS:HB2	1:A:139:MET:CE	2.38	0.53
1:B:86:GLU:HG2	1:B:111:LEU:HD13	1.89	0.53
1:B:423:MET:HB2	2:B:2001:CCT:H22	1.91	0.53
1:B:390:THR:HB	1:B:391:PRO:HD3	1.91	0.53
1:A:177:ASP:O	1:A:181:THR:HG23	2.10	0.52
1:A:314:LEU:HB3	1:A:321:VAL:HG12	1.89	0.52
1:A:541:ALA:O	1:A:544:GLN:HB2	2.11	0.51
1:B:556:SER:HB3	3:B:2341:HOH:O	2.10	0.51
1:B:83:LEU:HB2	1:B:173:MET:HA	1.92	0.51
1:A:390:THR:HB	1:A:391:PRO:HD3	1.93	0.51
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.50	0.51
1:B:461:GLN:HB3	1:B:545:LEU:HD11	1.93	0.51
1:A:20:LYS:HD2	1:A:20:LYS:N	2.26	0.50
1:B:506:SER:O	1:B:510:ARG:HD3	2.11	0.50
1:B:517:ARG:HG2	1:B:517:ARG:HH11	1.77	0.50
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.77	0.50
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.52	0.50
1:B:457:LEU:HB2	3:B:2218:HOH:O	2.11	0.50
1:A:46:GLY:HA2	1:A:49:GLN:HE21	1.77	0.49
1:A:160:ILE:HA	1:A:282:SER:OG	2.12	0.49
1:A:328:GLY:HA2	3:A:1286:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HB3	1:A:439:LEU:HD12	1.95	0.49
1:A:51:LYS:HE3	1:A:156:PRO:HG3	1.95	0.48
1:B:540:PRO:O	1:B:542:ALA:N	2.46	0.48
1:A:14:CYS:HB2	1:A:139:MET:HE2	1.96	0.48
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.95	0.48
1:A:113:SER:O	1:A:117:ASN:ND2	2.47	0.48
1:A:433:LEU:HB3	1:A:439:LEU:CD1	2.44	0.48
1:B:106:LYS:HA	1:B:106:LYS:HZ2	1.76	0.47
1:A:497:LEU:HD22	1:A:497:LEU:O	2.15	0.47
1:A:84:SER:OG	1:A:86:GLU:HG2	2.14	0.47
1:B:527:ASN:HD21	1:B:534:LEU:N	2.04	0.47
1:B:2:MET:HB2	1:B:278:ARG:NH2	2.29	0.47
1:A:14:CYS:O	1:A:15:ALA:HB2	2.14	0.47
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.54	0.47
1:B:182:LEU:HD23	1:B:182:LEU:O	2.15	0.46
1:B:313:MET:CE	3:B:2347:HOH:O	2.62	0.46
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.97	0.46
1:A:31:LEU:HD12	1:A:31:LEU:C	2.36	0.46
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.97	0.46
1:A:30:LEU:HD23	1:A:396:ALA:HA	1.97	0.46
1:A:527:ASN:ND2	1:A:534:LEU:H	2.04	0.46
1:A:46:GLY:HA2	1:A:49:GLN:NE2	2.31	0.45
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.82	0.45
1:A:511:LEU:HB3	1:A:518:ALA:O	2.16	0.45
1:B:86:GLU:HG3	1:B:111:LEU:HD22	1.98	0.45
1:A:499:VAL:O	1:A:503:ARG:HG3	2.16	0.45
1:A:79:LYS:HA	1:A:244:ASP:HB3	1.99	0.44
1:A:346:TYR:O	1:A:347:SER:HB3	2.17	0.44
1:B:19:SER:H	1:B:20:LYS:NZ	2.15	0.44
1:B:523:LYS:HG3	1:B:534:LEU:HD22	1.99	0.44
1:A:201:VAL:O	1:A:205:VAL:HG23	2.18	0.44
1:A:336:LEU:C	1:A:336:LEU:HD23	2.38	0.44
1:A:45:ALA:O	1:A:49:GLN:HG3	2.17	0.44
1:B:217:PHE:CE2	1:B:336:LEU:HD21	2.53	0.44
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.86	0.44
1:A:503:ARG:O	1:A:507:VAL:HG23	2.18	0.43
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.85	0.43
1:A:5:THR:HG21	1:A:278:ARG:NH1	2.22	0.43
1:B:416:ALA:HB3	1:B:417:PRO:HD3	2.01	0.43
1:A:514:GLN:HB3	1:A:518:ALA:HB3	2.00	0.43
1:A:124:LYS:HE2	1:A:128:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LYS:HG3	1:B:534:LEU:CD2	2.49	0.43
1:A:381:VAL:HG11	1:A:474:LEU:HD22	2.00	0.43
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.88	0.43
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.01	0.42
1:A:535:LYS:O	1:A:536:LEU:HB2	2.17	0.42
1:A:85:VAL:HG21	1:A:120:HIS:NE2	2.35	0.42
1:B:348:ALA:N	1:B:349:PRO:CD	2.82	0.42
1:A:59:VAL:CG1	1:B:59:VAL:HG13	2.49	0.42
1:B:160:ILE:HA	1:B:282:SER:OG	2.19	0.42
1:B:503:ARG:O	1:B:507:VAL:HG23	2.19	0.42
1:B:517:ARG:HG2	1:B:517:ARG:NH1	2.34	0.42
1:A:93:PRO:HG3	1:A:561:TYR:HB2	2.00	0.42
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.39	0.42
1:A:523:LYS:HE2	1:A:534:LEU:HD23	2.00	0.42
1:B:42:SER:HA	1:B:140:ALA:CB	2.50	0.42
1:B:535:LYS:HG3	1:B:536:LEU:N	2.35	0.42
1:B:46:GLY:HA2	1:B:49:GLN:HE21	1.84	0.42
1:B:85:VAL:HG21	1:B:120:HIS:CE1	2.54	0.42
1:B:355:GLN:O	1:B:355:GLN:HG3	2.19	0.41
1:A:230:GLU:HG3	1:A:262:ILE:HG23	2.01	0.41
1:B:465:ARG:HH11	1:B:465:ARG:HG3	1.85	0.41
1:A:313:MET:HE2	1:A:313:MET:HB2	1.80	0.41
1:B:170:CYS:HA	1:B:173:MET:HE2	2.03	0.41
1:B:461:GLN:CB	1:B:545:LEU:HD11	2.51	0.41
1:B:307:LYS:HE3	1:B:307:LYS:HB2	1.89	0.41
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.84	0.41
1:B:233:ILE:HD13	1:B:261:TYR:O	2.20	0.41
1:A:216:GLY:HA2	1:A:322:VAL:O	2.20	0.41
1:A:535:LYS:HG3	1:A:536:LEU:H	1.86	0.41
1:A:306:ALA:HB3	1:A:308:LEU:HD13	2.03	0.40
1:A:330:GLN:HA	1:A:330:GLN:OE1	2.21	0.40
1:B:182:LEU:C	1:B:182:LEU:CD2	2.89	0.40
1:B:549:GLY:HA2	1:B:552:VAL:CG2	2.52	0.40
1:A:562:HIS:O	1:A:563:SER:C	2.59	0.40
1:B:535:LYS:CG	1:B:536:LEU:N	2.85	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	554/570 (97%)	540 (98%)	11 (2%)	3 (0%)	29	23
1	B	555/570 (97%)	542 (98%)	10 (2%)	3 (0%)	29	23
All	All	1109/1140 (97%)	1082 (98%)	21 (2%)	6 (0%)	29	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	540	PRO
1	B	541	ALA
1	A	538	PRO
1	A	15	ALA
1	B	538	PRO
1	A	536	LEU

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	476/485 (98%)	467 (98%)	9 (2%)	57	61
1	B	477/485 (98%)	465 (98%)	12 (2%)	47	49
All	All	953/970 (98%)	932 (98%)	21 (2%)	52	55

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

Mol	Chain	Res	Type
1	A	106	LYS
1	A	159	LEU
1	A	303	CYS
1	A	309	GLN
1	A	439	LEU
1	A	497	LEU
1	A	510	ARG
1	A	514	GLN
1	A	517	ARG
1	B	14	CYS
1	B	20	LYS
1	B	31	LEU
1	B	57	LEU
1	B	106	LYS
1	B	159	LEU
1	B	330	GLN
1	B	381	VAL
1	B	391	PRO
1	B	440	GLU
1	B	510	ARG
1	B	517	ARG

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

Mol	Chain	Res	Type
1	A	34	HIS
1	A	49	GLN
1	A	273	ASN
1	A	374	HIS
1	A	514	GLN
1	A	527	ASN
1	A	544	GLN
1	B	49	GLN
1	B	120	HIS
1	B	273	ASN
1	B	330	GLN
1	B	461	GLN
1	B	527	ASN
1	B	544	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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$
2	CCT	B	2001	-	25,29,29	2.34	10 (40%)	28,42,42	1.86	3 (10%)
2	CCT	A	1001	-	25,29,29	2.18	9 (36%)	28,42,42	1.75	3 (10%)

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	CCT	B	2001	-	-	0/11/21/21	0/3/3/3
2	CCT	A	1001	-	-	0/11/21/21	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	CCT	C9-C8	5.50	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CCT	C9-C8	5.46	1.44	1.39
2	B	2001	CCT	S18-N17	4.25	1.70	1.63
2	B	2001	CCT	C21-C20	4.00	1.43	1.39
2	A	1001	CCT	S18-N17	3.94	1.69	1.63
2	A	1001	CCT	C21-C20	3.48	1.43	1.39
2	B	2001	CCT	C19-C20	3.09	1.44	1.40
2	B	2001	CCT	C6-C1	2.79	1.42	1.36
2	A	1001	CCT	C6-C1	2.61	1.42	1.36
2	A	1001	CCT	C19-C20	2.51	1.43	1.40
2	B	2001	CCT	C23-C24	2.48	1.43	1.38
2	B	2001	CCT	C4-C3	2.40	1.41	1.36
2	A	1001	CCT	C4-C3	2.38	1.41	1.36
2	A	1001	CCT	O26-S18	2.18	1.46	1.43
2	A	1001	CCT	C23-C24	2.17	1.42	1.38
2	B	2001	CCT	C1-C2	2.10	1.43	1.39
2	B	2001	CCT	C24-C19	2.05	1.43	1.39
2	B	2001	CCT	O27-S18	2.04	1.45	1.43
2	A	1001	CCT	C8-N17	2.00	1.46	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	CCT	C20-S18-N17	6.33	114.75	107.30
2	B	2001	CCT	O27-S18-O26	-5.87	112.39	119.52
2	A	1001	CCT	C20-S18-N17	5.84	114.18	107.30
2	A	1001	CCT	O27-S18-O26	-5.74	112.56	119.52
2	A	1001	CCT	C24-C19-C20	2.21	118.60	116.27
2	B	2001	CCT	C24-C19-C20	2.20	118.59	116.27

There are no chirality outliers.

There are no torsion outliers.

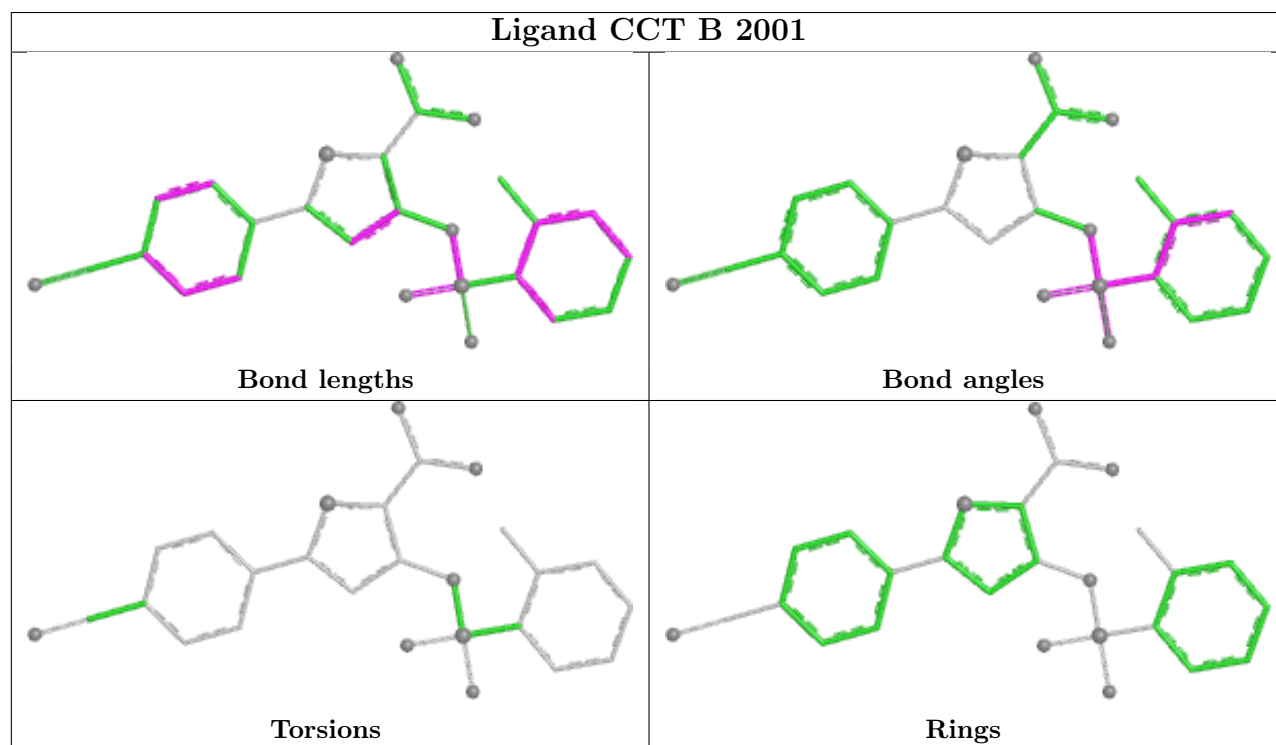
There are no ring outliers.

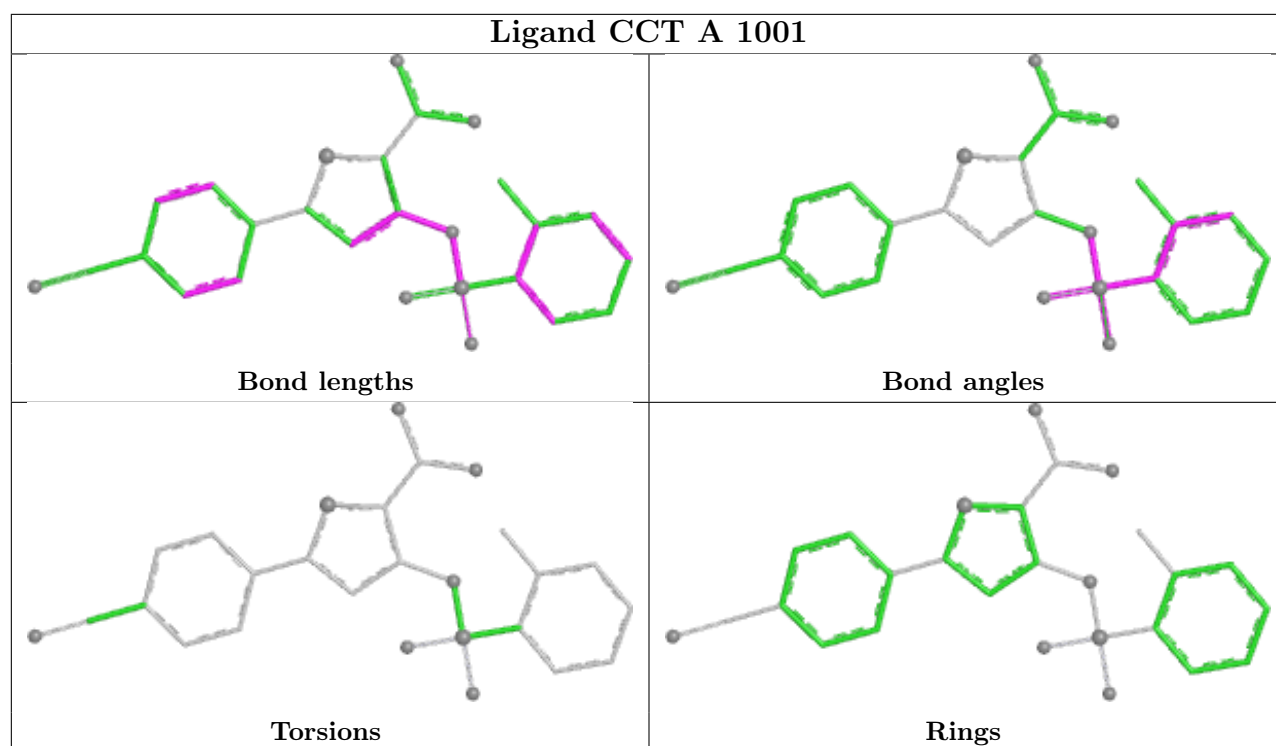
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	CCT	1	0
2	A	1001	CCT	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	558/570 (97%)	0.06	28 (5%)	28 28	14, 27, 50, 81	0
1	B	559/570 (98%)	0.00	22 (3%)	39 38	12, 25, 50, 79	0
All	All	1117/1140 (97%)	0.03	50 (4%)	33 32	12, 26, 50, 81	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	LEU	9.4
1	A	563	SER	8.9
1	A	541	ALA	7.8
1	B	563	SER	7.3
1	A	542	ALA	6.7
1	B	542	ALA	6.2
1	B	549	GLY	5.8
1	A	543	SER	5.7
1	A	544	GLN	5.7
1	B	544	GLN	5.3
1	B	562	HIS	4.6
1	A	539	ILE	4.6
1	B	543	SER	4.4
1	A	545	LEU	4.3
1	B	541	ALA	4.3
1	A	535	LYS	4.1
1	B	545	LEU	3.8
1	B	539	ILE	3.8
1	A	329	THR	3.7
1	B	546	ASP	3.5
1	A	549	GLY	3.5
1	A	548	SER	3.3
1	A	540	PRO	3.2
1	B	548	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	535	LYS	3.0
1	B	561	TYR	3.0
1	B	550	TRP	2.7
1	B	531	LYS	2.6
1	A	550	TRP	2.6
1	A	32	ARG	2.5
1	A	10	LEU	2.4
1	A	148	GLN	2.4
1	A	561	TYR	2.4
1	A	546	ASP	2.4
1	B	540	PRO	2.4
1	A	331	GLU	2.3
1	B	536	LEU	2.3
1	A	47	LEU	2.3
1	A	15	ALA	2.3
1	B	95	HIS	2.3
1	A	330	GLN	2.3
1	A	490	ARG	2.2
1	A	538	PRO	2.2
1	A	43	ARG	2.2
1	A	562	HIS	2.1
1	A	461	GLN	2.1
1	B	16	ALA	2.1
1	B	106	LYS	2.1
1	B	110	ASN	2.1
1	A	113	SER	2.0

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

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

6.3 Carbohydrates [i](#)

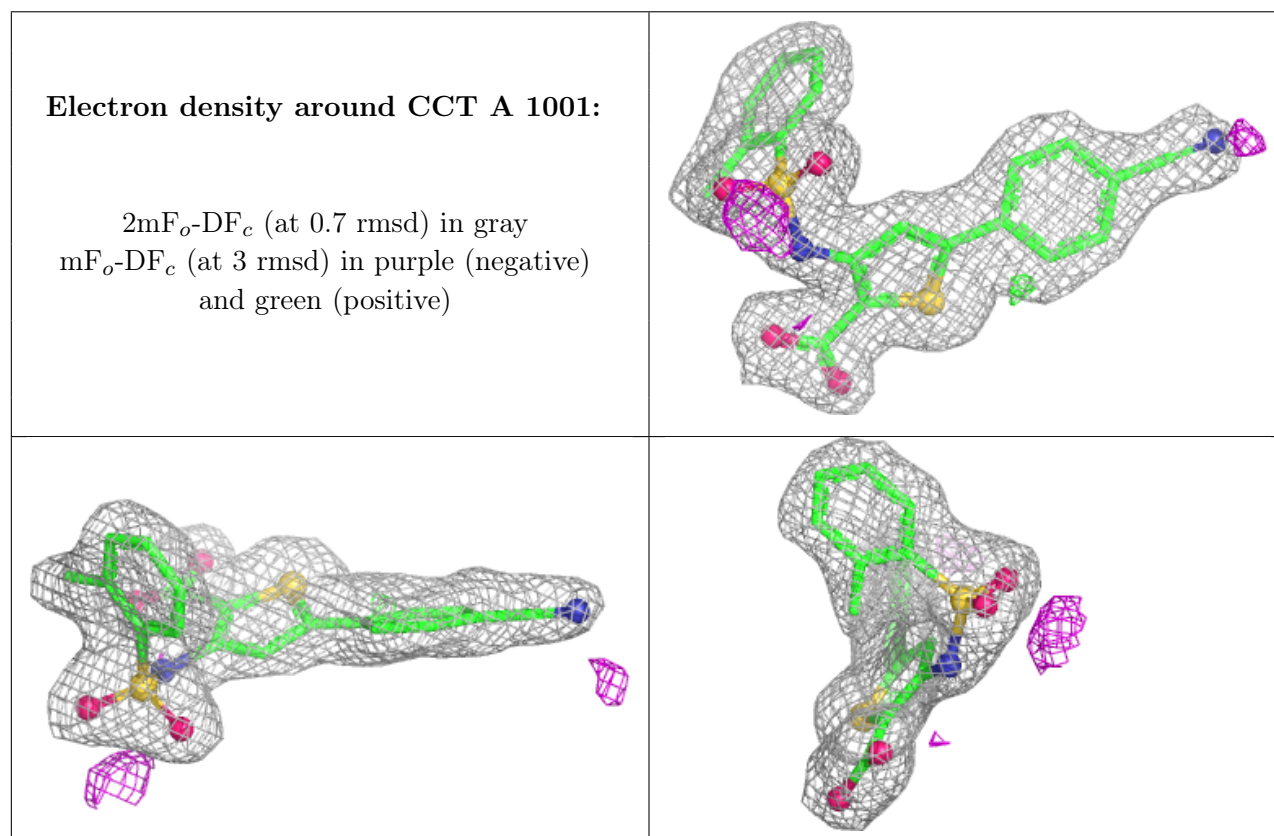
There are no monosaccharides in this entry.

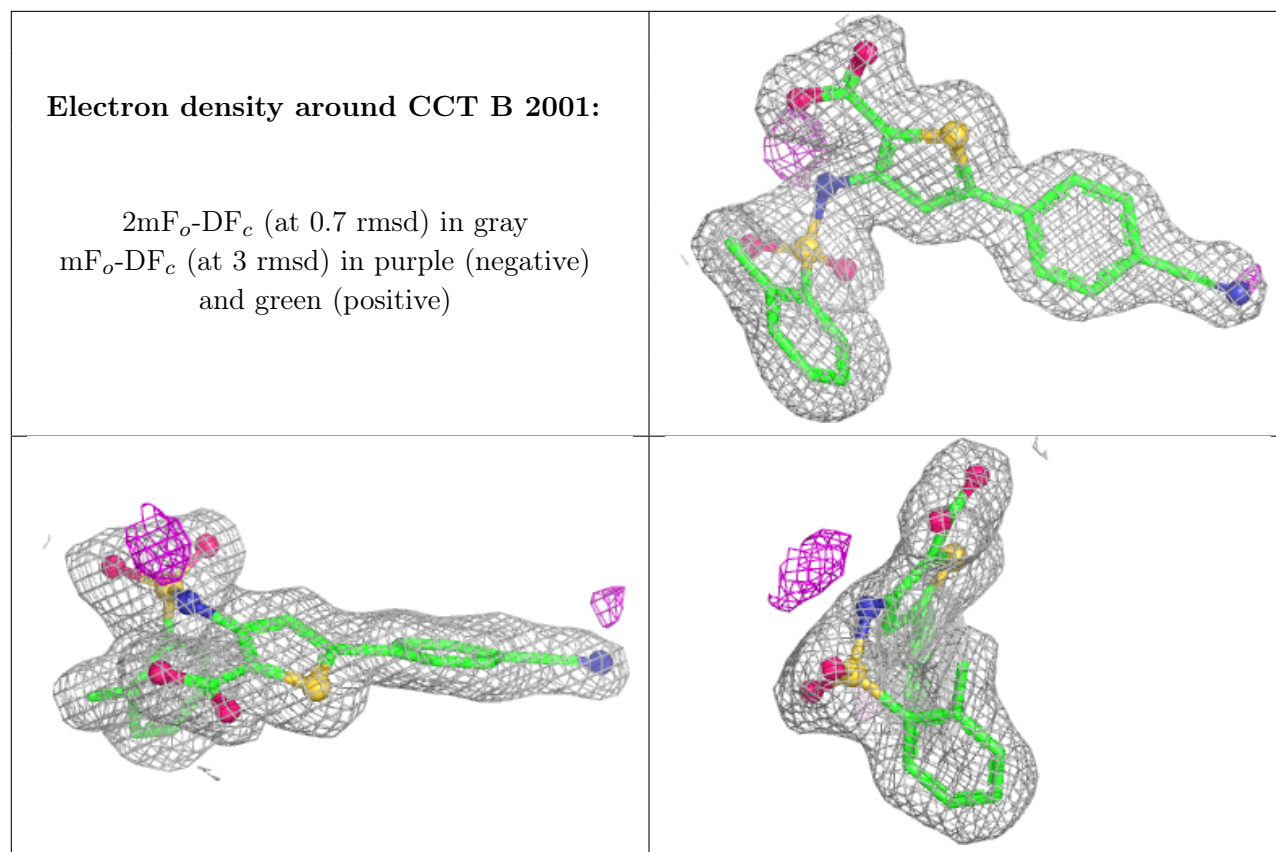
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	CCT	A	1001	27/27	0.96	0.12	26,31,35,36	0
2	CCT	B	2001	27/27	0.97	0.14	21,27,30,32	0

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





6.5 Other polymers ⓘ

There are no such residues in this entry.