Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:57 am BST

PDB ID	:	2UZL
Title	:	Crystal structure of human CDK2 complexed with a thiazolidinone inhibitor
Authors	:	Richardson, C.M.; Dokurno, P.; Murray, J.B.; Surgenor, A.E.
Deposited on	:	2007-04-30
Resolution	:	2.40 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:

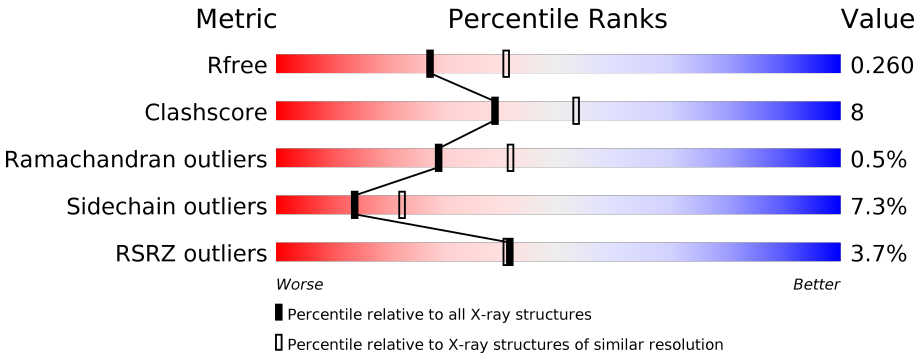
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	298	6% 77% 19%
1	C	298	6% 77% 19%
2	B	258	2% 84% 14%
2	D	258	% 77% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	160	X	-	-	-
1	TPO	C	160	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9387 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.

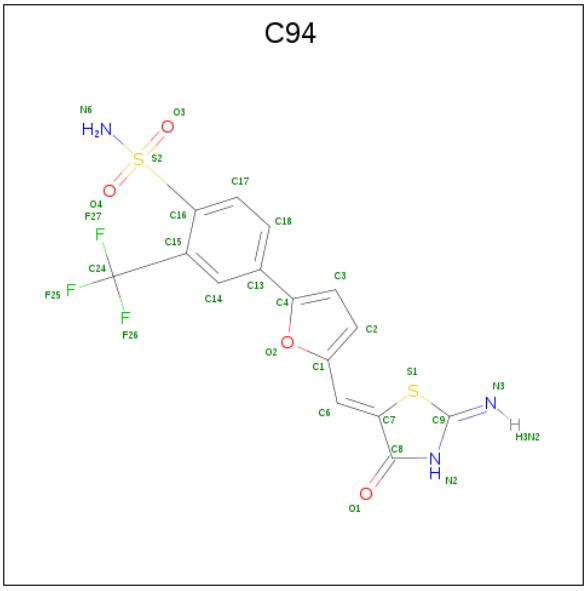
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	1
			2383	1547	404	423	1	8			
1	C	297	Total	C	N	O	P	S	0	0	1
			2383	1547	404	423	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2077	1345	338	383	11			
2	D	257	Total	C	N	O	S	0	0	0
			2077	1345	338	383	11			

- Molecule 3 is 4-{5-[(Z)-(2-IMINO-4-OXO-1,3-THIAZOLIDIN-5-YLIDENE)METHYL]FURAN-2-YL}-2-(TRIFLUOROMETHYL)BENZENESULFONAMIDE (three-letter code: C94) (formula: $C_{15}H_{10}F_3N_3O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			27	15	3	3	4	2		
3	C	1	Total	C	F	N	O	S	0	0
			27	15	3	3	4	2		

- Molecule 4 is water.

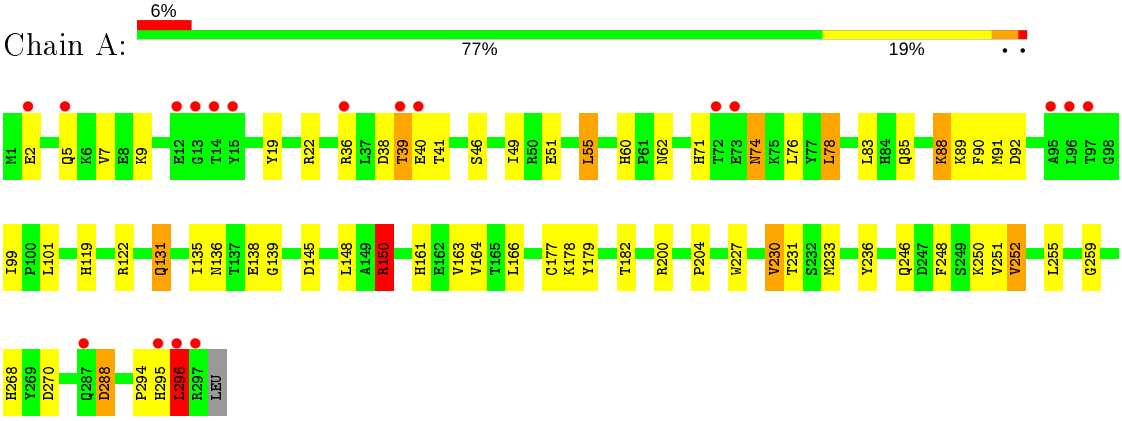
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	123	Total	O	0	0
			123	123		
4	C	90	Total	O	0	0
			90	90		
4	D	105	Total	O	0	0
			105	105		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

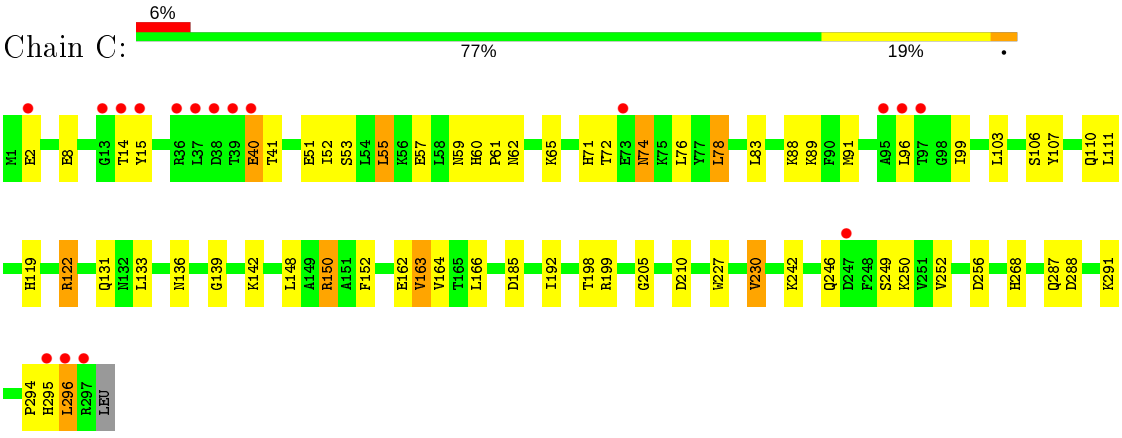
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



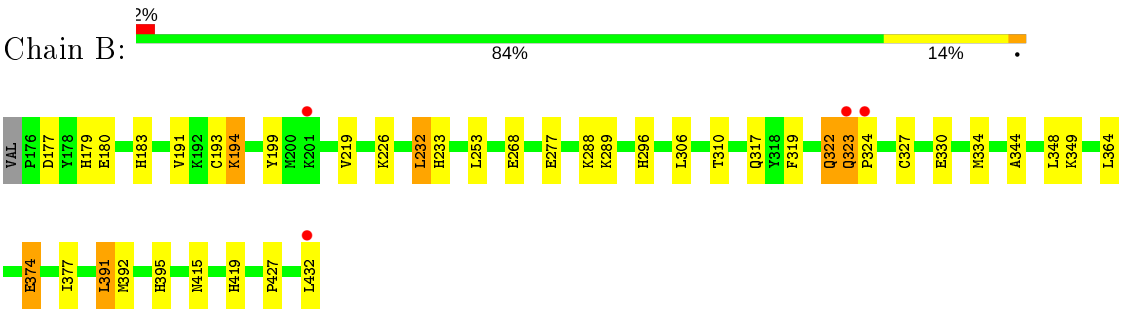
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C:



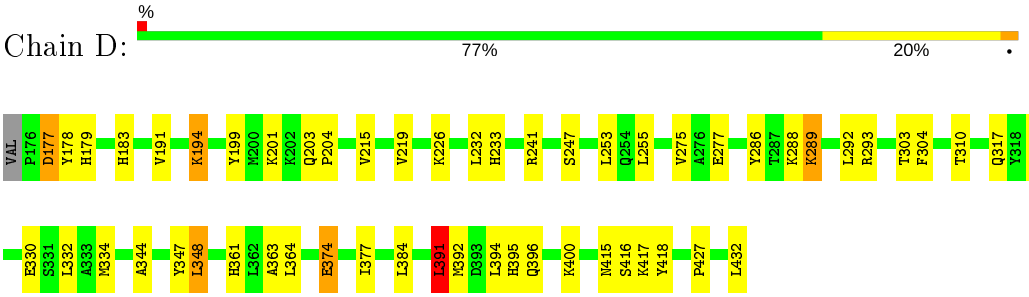
- Molecule 2: CYCLIN A2

Chain B:



• Molecule 2: CYCLIN A2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.60Å 73.28Å 152.37Å 90.00° 129.33° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.9 (15.00-2.40) 87.9 (15.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.263 0.202 , 0.260	Depositor DCC
R_{free} test set	3132 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.2	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	0.93	EDS
Total number of atoms	9387	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: TPO, C94

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	0.66	0/2433	1.01	5/3302 (0.2%)
1	C	0.64	0/2433	1.00	4/3302 (0.1%)
2	B	0.65	0/2127	0.80	2/2886 (0.1%)
2	D	0.65	0/2127	0.84	5/2886 (0.2%)
All	All	0.65	0/9120	0.92	16/12376 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	C	1	0
All	All	2	0

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	296	LEU	O-C-N	-28.05	77.82	122.70
1	A	296	LEU	O-C-N	-27.82	78.19	122.70
2	D	432	LEU	CA-C-O	20.59	163.33	120.10
1	A	296	LEU	CA-C-O	19.68	161.43	120.10
1	C	296	LEU	CA-C-O	19.15	160.31	120.10
2	B	432	LEU	CA-C-O	-17.33	83.71	120.10
1	C	296	LEU	CA-C-N	-15.76	82.52	117.20
1	A	296	LEU	CA-C-N	-15.38	83.37	117.20
1	A	78	LEU	CA-CB-CG	6.68	130.67	115.30
2	B	391	LEU	CA-CB-CG	6.49	130.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	391	LEU	CA-CB-CG	6.29	129.75	115.30
1	A	150	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	150	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	D	241	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	D	364	LEU	CA-CB-CG	5.66	128.31	115.30
2	D	241	ARG	NE-CZ-NH1	5.13	122.86	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	160	TPO	CB
1	C	160	TPO	CB

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	2383	0	2425	42	0
1	C	2383	0	2425	39	0
2	B	2077	0	2099	25	0
2	D	2077	0	2099	32	0
3	A	27	0	9	2	0
3	C	27	0	9	1	0
4	A	95	0	0	6	0
4	B	123	0	0	8	0
4	C	90	0	0	8	0
4	D	105	0	0	7	0
All	All	9387	0	9066	136	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 8.

All (136) 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:85:GLN:NE2	1:A:89:LYS:HD3	1.84	0.91
2:B:374:GLU:HG3	4:B:2099:HOH:O	1.74	0.87
1:A:101:LEU:O	1:A:101:LEU:HG	1.75	0.86
1:A:177:CYS:HB2	4:A:2058:HOH:O	1.77	0.84
1:C:60:HIS:HD2	1:C:62:ASN:H	1.27	0.82
1:C:227:TRP:O	1:C:230:VAL:HG22	1.81	0.80
1:C:60:HIS:CD2	1:C:62:ASN:H	2.00	0.80
1:C:15:TYR:CE2	4:C:2003:HOH:O	2.36	0.79
1:C:59:ASN:HD21	1:C:65:LYS:HD2	1.47	0.79
1:C:15:TYR:CZ	4:C:2003:HOH:O	2.33	0.79
1:C:74:ASN:HD22	1:C:74:ASN:H	1.32	0.77
2:B:330:GLU:O	2:B:334:MET:HG3	1.85	0.76
1:A:60:HIS:HD2	1:A:62:ASN:H	1.37	0.72
1:C:74:ASN:ND2	1:C:74:ASN:H	1.89	0.71
2:B:415:ASN:HB3	4:B:2120:HOH:O	1.91	0.71
1:C:163:VAL:HG23	4:C:2042:HOH:O	1.90	0.71
1:A:60:HIS:CD2	1:A:62:ASN:H	2.10	0.68
1:A:92:ASP:HB3	4:A:2027:HOH:O	1.92	0.68
2:D:395:HIS:HE1	2:D:427:PRO:O	1.78	0.67
2:D:415:ASN:HB3	4:D:2104:HOH:O	1.95	0.67
1:A:295:HIS:O	1:A:296:LEU:C	2.33	0.67
4:C:2084:HOH:O	2:D:177:ASP:HB3	1.95	0.66
1:A:227:TRP:O	1:A:230:VAL:HG22	1.95	0.66
2:B:395:HIS:HE1	2:B:427:PRO:O	1.79	0.66
1:C:131:GLN:HB2	4:C:2036:HOH:O	1.95	0.66
1:C:61:PRO:O	1:C:142:LYS:HE2	1.97	0.64
1:A:233:MET:SD	4:A:2058:HOH:O	2.55	0.64
2:B:183:HIS:HD2	4:B:2017:HOH:O	1.80	0.64
2:B:319:PHE:O	2:B:322:GLN:HG3	1.98	0.64
2:D:191:VAL:O	2:D:194:LYS:HD3	1.97	0.63
1:C:252:VAL:HG13	1:C:252:VAL:O	1.98	0.63
2:D:319:PHE:O	2:D:322:GLN:HG3	1.99	0.63
2:D:330:GLU:O	2:D:334:MET:HG3	1.99	0.62
2:D:183:HIS:HD2	4:D:2010:HOH:O	1.83	0.62
1:A:85:GLN:HE21	1:A:89:LYS:HD3	1.61	0.61
4:A:2089:HOH:O	2:B:177:ASP:HB3	1.98	0.61
1:A:252:VAL:O	1:A:252:VAL:HG13	1.99	0.61
2:D:178:TYR:HB2	4:D:2008:HOH:O	2.00	0.61
1:C:246:GLN:NE2	1:C:250:LYS:HE3	2.17	0.60
2:B:191:VAL:O	2:B:194:LYS:HD2	2.02	0.60
2:B:233:HIS:HE1	4:B:2089:HOH:O	1.84	0.60
1:C:268:HIS:CD2	4:C:2074:HOH:O	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:O	1:A:55:LEU:HB2	2.03	0.59
2:D:395:HIS:CE1	2:D:427:PRO:O	2.56	0.59
2:D:415:ASN:CB	4:D:2104:HOH:O	2.51	0.58
1:C:198:THR:O	1:C:199:ARG:HB2	2.03	0.57
1:C:163:VAL:CG2	4:C:2042:HOH:O	2.49	0.57
2:D:289:LYS:HE3	2:D:293:ARG:HE	1.68	0.57
1:A:246:GLN:HE21	1:A:250:LYS:HG2	1.71	0.55
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.88	0.55
2:D:233:HIS:HE1	4:D:2067:HOH:O	1.90	0.54
1:A:178:LYS:HD3	1:A:179:TYR:CE2	2.44	0.53
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.91	0.53
1:A:7:VAL:CG2	1:A:22:ARG:HG3	2.37	0.53
2:B:296:HIS:HB2	4:B:2010:HOH:O	2.09	0.52
1:C:52:ILE:HD11	1:C:78:LEU:HD22	1.91	0.52
2:D:233:HIS:HD2	4:D:2061:HOH:O	1.92	0.52
3:A:1297:C94:O2	3:A:1297:C94:S1	2.66	0.52
1:A:39:THR:O	1:A:40:GLU:C	2.48	0.52
3:C:1297:C94:O2	3:C:1297:C94:S1	2.68	0.52
1:A:161:HIS:HD2	4:A:2057:HOH:O	1.93	0.52
1:A:90:PHE:HB2	1:A:135:ILE:HD11	1.92	0.52
1:C:119:HIS:HD2	4:D:2009:HOH:O	1.93	0.51
1:A:38:ASP:HB2	1:A:41:THR:OG1	2.11	0.50
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.93	0.50
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.93	0.50
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.94	0.50
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.94	0.49
2:D:417:LYS:HD2	2:D:418:TYR:CE2	2.47	0.49
1:A:131:GLN:HB3	4:A:2031:HOH:O	2.13	0.49
1:A:9:LYS:HE2	1:A:19:TYR:CE2	2.48	0.49
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.47	0.49
1:A:150:ARG:NH2	2:B:268:GLU:O	2.35	0.49
2:B:191:VAL:O	2:B:194:LYS:CD	2.60	0.48
1:C:60:HIS:HD2	1:C:62:ASN:N	2.05	0.48
1:A:248:PHE:HA	1:A:251:VAL:HB	1.95	0.48
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.49	0.48
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.96	0.48
1:A:246:GLN:NE2	1:A:250:LYS:HG2	2.29	0.48
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.50	0.47
1:C:106:SER:O	1:C:110:GLN:HG3	2.14	0.47
2:D:347:TYR:OH	2:D:394:LEU:HA	2.15	0.47
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LYS:HG2	4:C:2072:HOH:O	2.15	0.47
1:A:119:HIS:HD2	4:B:2015:HOH:O	1.96	0.47
2:B:322:GLN:NE2	2:B:330:GLU:OE2	2.48	0.47
2:B:349:LYS:NZ	4:B:2095:HOH:O	2.36	0.47
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.96	0.46
2:D:275:VAL:HG21	2:D:292:LEU:HD21	1.98	0.46
1:A:252:VAL:CG1	1:A:252:VAL:O	2.64	0.46
1:C:295:HIS:O	1:C:296:LEU:HB2	2.15	0.45
1:A:9:LYS:HE2	1:A:19:TYR:HE2	1.80	0.45
2:D:323:GLN:HA	2:D:324:PRO:HA	1.80	0.45
3:A:1297:C94:F26	3:A:1297:C94:O4	2.24	0.45
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.52	0.45
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.45
1:A:231:THR:HA	1:A:236:TYR:CD1	2.51	0.45
2:D:233:HIS:HB3	2:D:310:THR:HB	1.97	0.45
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.51	0.45
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.97	0.45
2:D:396:GLN:O	2:D:400:LYS:HG2	2.17	0.45
1:C:107:TYR:O	1:C:111:LEU:HG	2.17	0.44
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.99	0.44
1:A:200:ARG:HH21	1:A:204:PRO:HG3	1.83	0.44
1:C:88:LYS:HA	1:C:91:MET:HE2	1.99	0.44
1:A:74:ASN:ND2	1:A:74:ASN:H	2.16	0.44
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.53	0.43
1:A:88:LYS:HA	1:A:91:MET:HE2	2.00	0.43
1:A:288:ASP:OD2	1:A:288:ASP:N	2.50	0.43
1:A:40:GLU:HG2	2:B:288:LYS:HD3	1.99	0.43
1:C:74:ASN:HD22	1:C:74:ASN:N	2.09	0.43
2:D:303:THR:O	2:D:304:PHE:HB2	2.17	0.43
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.00	0.43
1:C:198:THR:O	1:C:199:ARG:CB	2.66	0.43
1:C:205:GLY:HA2	1:C:210:ASP:OD2	2.19	0.43
1:C:252:VAL:CG1	1:C:252:VAL:O	2.66	0.43
2:D:199:TYR:C	2:D:199:TYR:CD1	2.93	0.42
1:A:119:HIS:CD2	1:A:182:THR:HB	2.53	0.42
2:B:323:GLN:HA	2:B:324:PRO:HA	1.93	0.42
2:D:361:HIS:HD2	2:D:391:LEU:HD11	1.84	0.42
2:B:233:HIS:HB3	2:B:310:THR:HB	2.01	0.42
2:D:203:GLN:HA	2:D:204:PRO:HD3	1.91	0.42
1:C:83:LEU:HD23	1:C:136:ASN:HB3	2.02	0.41
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:LYS:HE3	2:D:293:ARG:NE	2.34	0.41
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.86	0.41
2:D:215:VAL:O	2:D:219:VAL:HG23	2.21	0.41
2:B:193:CYS:SG	4:B:2047:HOH:O	2.23	0.41
1:C:40:GLU:HG2	2:D:288:LYS:HE2	2.02	0.41
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.03	0.41
1:C:99:ILE:HG23	1:C:103:LEU:HD23	2.03	0.41
2:B:374:GLU:HA	2:B:377:ILE:HD12	2.04	0.40
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.04	0.40
2:D:255:LEU:HD13	2:D:286:TYR:CG	2.56	0.40
1:A:268:HIS:HD2	1:A:270:ASP:H	1.70	0.40
1:C:53:SER:HB3	2:D:304:PHE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/298 (99%)	275 (94%)	16 (5%)	3 (1%)	15 23
1	C	294/298 (99%)	278 (95%)	13 (4%)	3 (1%)	15 23
2	B	255/258 (99%)	251 (98%)	4 (2%)	0	100 100
2	D	255/258 (99%)	248 (97%)	7 (3%)	0	100 100
All	All	1098/1112 (99%)	1052 (96%)	40 (4%)	6 (0%)	29 41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LEU
1	C	8	GLU
1	C	14	THR

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Mol	Chain	Res	Type
1	C	164	VAL
1	A	145	ASP
1	A	164	VAL

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	260/262 (99%)	241 (93%)	19 (7%)	14	22
1	C	260/262 (99%)	238 (92%)	22 (8%)	10	16
2	B	231/232 (100%)	217 (94%)	14 (6%)	18	30
2	D	231/232 (100%)	214 (93%)	17 (7%)	13	22
All	All	982/988 (99%)	910 (93%)	72 (7%)	14	22

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	5	GLN
1	A	36	ARG
1	A	39	THR
1	A	46	SER
1	A	55	LEU
1	A	74	ASN
1	A	78	LEU
1	A	88	LYS
1	A	122	ARG
1	A	131	GLN
1	A	138	GLU
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	166	LEU
1	A	230	VAL
1	A	252	VAL

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Mol	Chain	Res	Type
1	A	288	ASP
2	B	179	HIS
2	B	180	GLU
2	B	194	LYS
2	B	226	LYS
2	B	232	LEU
2	B	253	LEU
2	B	277	GLU
2	B	289	LYS
2	B	322	GLN
2	B	323	GLN
2	B	364	LEU
2	B	374	GLU
2	B	391	LEU
2	B	392	MET
1	C	2	GLU
1	C	40	GLU
1	C	41	THR
1	C	55	LEU
1	C	57	GLU
1	C	72	THR
1	C	74	ASN
1	C	78	LEU
1	C	89	LYS
1	C	96	LEU
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	162	GLU
1	C	163	VAL
1	C	166	LEU
1	C	230	VAL
1	C	249	SER
1	C	256	ASP
1	C	287	GLN
1	C	288	ASP
1	C	291	LYS
2	D	177	ASP
2	D	179	HIS
2	D	194	LYS
2	D	201	LYS
2	D	226	LYS

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Mol	Chain	Res	Type
2	D	232	LEU
2	D	247	SER
2	D	253	LEU
2	D	277	GLU
2	D	289	LYS
2	D	322	GLN
2	D	348	LEU
2	D	374	GLU
2	D	384	LEU
2	D	391	LEU
2	D	392	MET
2	D	416	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	84	HIS
1	A	85	GLN
1	A	119	HIS
1	A	161	HIS
1	A	246	GLN
1	A	268	HIS
1	A	272	ASN
1	A	287	GLN
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	317	GLN
2	B	395	HIS
1	C	59	ASN
1	C	60	HIS
1	C	71	HIS
1	C	74	ASN
1	C	84	HIS
1	C	119	HIS
1	C	246	GLN
1	C	268	HIS
2	D	179	HIS

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Mol	Chain	Res	Type
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	395	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	C	160	1	8,10,11	1.05	1 (12%)	10,14,16	2.18	2 (20%)
1	TPO	A	160	1	8,10,11	1.27	1 (12%)	10,14,16	1.54	2 (20%)

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
1	TPO	C	160	1	1/1/3/4	5/9/11/13	-
1	TPO	A	160	1	1/1/3/4	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	2.95	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O1P	2.34	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	P-OG1-CB	5.56	140.01	123.21
1	C	160	TPO	CG2-CB-CA	3.56	120.18	113.16
1	A	160	TPO	P-OG1-CB	3.41	133.51	123.21
1	A	160	TPO	CG2-CB-CA	2.80	118.69	113.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	160	TPO	CB
1	A	160	TPO	CB

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	N-CA-CB-CG2
1	C	160	TPO	N-CA-CB-OG1
1	C	160	TPO	C-CA-CB-CG2
1	C	160	TPO	O-C-CA-CB
1	C	160	TPO	CA-CB-OG1-P
1	A	160	TPO	N-CA-CB-CG2
1	A	160	TPO	N-CA-CB-OG1
1	A	160	TPO	C-CA-CB-CG2
1	A	160	TPO	O-C-CA-CB
1	A	160	TPO	CG2-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	C94	C	1297	-	24,29,29	1.90	4 (16%)	33,45,45	1.92	3 (9%)
3	C94	A	1297	-	24,29,29	1.94	4 (16%)	33,45,45	1.90	7 (21%)

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	C94	C	1297	-	-	5/16/32/32	0/3/3/3
3	C94	A	1297	-	-	7/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1297	C94	C9-S1	-6.18	1.66	1.74
3	C	1297	C94	C9-S1	-6.06	1.66	1.74
3	A	1297	C94	C8-C7	-5.28	1.39	1.48
3	C	1297	C94	C8-C7	-5.24	1.39	1.48
3	A	1297	C94	C7-S1	-3.40	1.66	1.73
3	C	1297	C94	C7-S1	-3.28	1.67	1.73
3	C	1297	C94	C13-C4	2.25	1.50	1.46
3	A	1297	C94	C13-C4	2.24	1.50	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1297	C94	O3-S2-O4	-5.53	109.66	118.76
3	A	1297	C94	C6-C7-C8	5.52	124.84	120.47
3	C	1297	C94	C6-C7-C8	5.47	124.79	120.47
3	A	1297	C94	O3-S2-O4	-4.01	112.16	118.76
3	C	1297	C94	C6-C7-S1	-3.69	124.50	129.22
3	A	1297	C94	C6-C7-S1	-3.64	124.56	129.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1297	C94	O3-S2-N6	3.06	111.90	107.36
3	A	1297	C94	O4-S2-N6	2.89	111.64	107.36
3	A	1297	C94	F27-C24-C15	-2.07	109.09	112.70
3	A	1297	C94	C7-C8-N2	2.04	111.92	110.22

There are no chirality outliers.

All (12) torsion outliers are listed below:

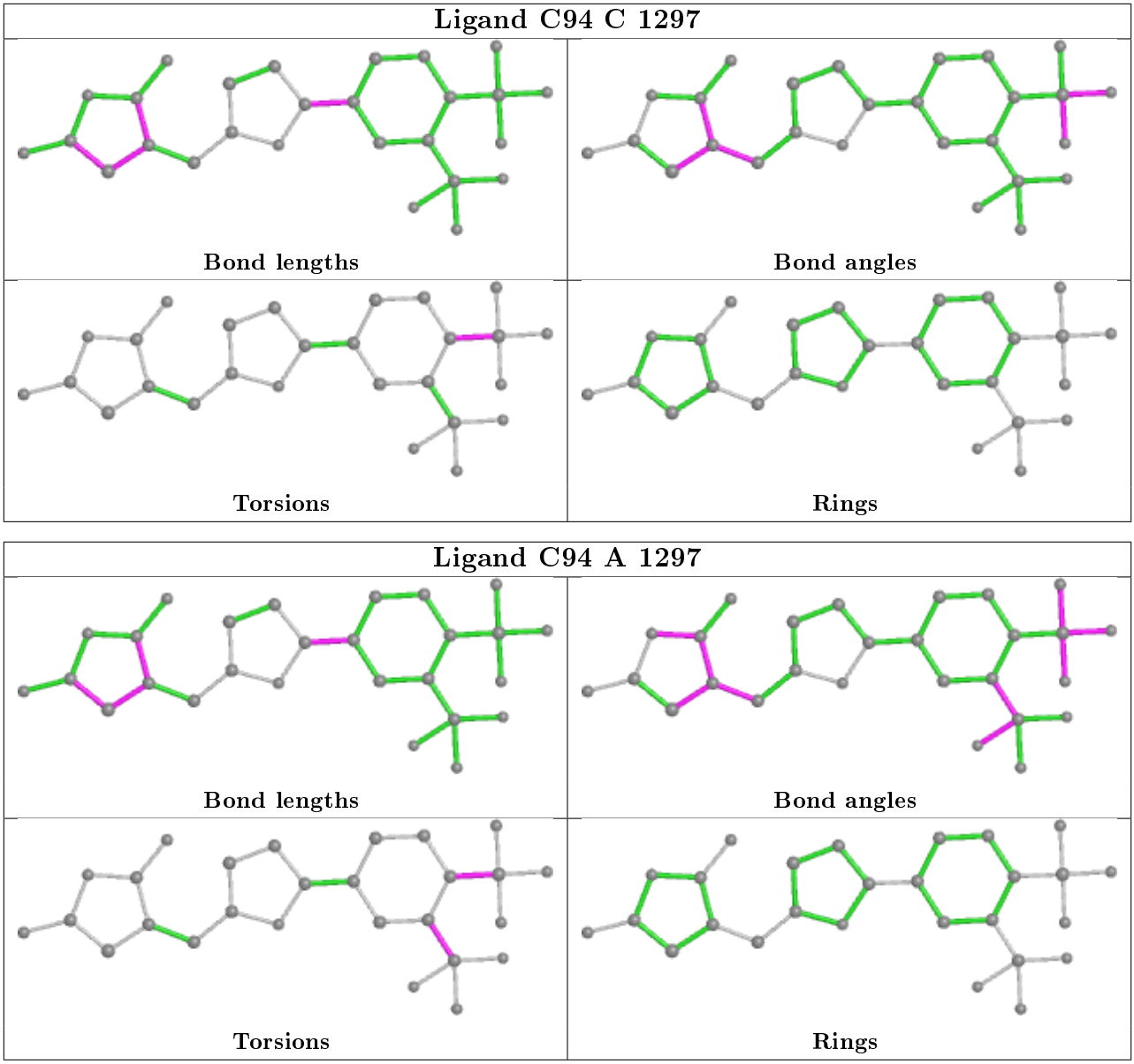
Mol	Chain	Res	Type	Atoms
3	C	1297	C94	C15-C16-S2-O4
3	C	1297	C94	C15-C16-S2-N6
3	A	1297	C94	C15-C16-S2-O3
3	A	1297	C94	C15-C16-S2-N6
3	C	1297	C94	C17-C16-S2-N6
3	A	1297	C94	C17-C16-S2-N6
3	C	1297	C94	C17-C16-S2-O4
3	A	1297	C94	C17-C16-S2-O3
3	C	1297	C94	C17-C16-S2-O3
3	A	1297	C94	C17-C16-S2-O4
3	A	1297	C94	C15-C16-S2-O4
3	A	1297	C94	C16-C15-C24-F26

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	C94	1	0
3	A	1297	C94	2	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.



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, 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	296/298 (99%)	-0.26	18 (6%)	21	20	7, 21, 49, 60	11 (3%)
1	C	296/298 (99%)	-0.19	17 (5%)	23	22	9, 22, 50, 61	10 (3%)
2	B	257/258 (99%)	-0.52	4 (1%)	72	70	8, 19, 38, 52	0
2	D	257/258 (99%)	-0.55	2 (0%)	86	84	8, 20, 38, 52	0
All	All	1106/1112 (99%)	-0.37	41 (3%)	41	41	7, 21, 46, 61	21 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	11.2
1	C	296	LEU	9.7
1	C	39	THR	8.9
1	C	295	HIS	6.8
1	A	295	HIS	6.2
1	A	296	LEU	6.0
1	C	14	THR	5.3
1	C	297	ARG	4.7
1	C	15	TYR	4.5
2	B	324	PRO	3.9
1	A	96	LEU	3.9
1	C	13	GLY	3.8
1	A	73	GLU	3.8
1	C	96	LEU	3.4
1	A	14	THR	3.4
2	B	323	GLN	3.2
1	C	37	LEU	3.2
1	A	297	ARG	3.1
1	A	97	THR	3.0
2	D	323	GLN	2.9
1	C	73	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	2.7
1	C	38	ASP	2.6
1	C	40	GLU	2.6
1	C	2	GLU	2.6
1	A	12	GLU	2.5
1	A	72	THR	2.4
1	C	97	THR	2.4
1	A	95	ALA	2.4
1	A	40	GLU	2.4
1	A	36	ARG	2.3
1	C	36	ARG	2.3
2	B	432	LEU	2.3
1	A	13	GLY	2.2
1	C	247	ASP	2.2
2	B	201	LYS	2.1
1	A	287	GLN	2.1
1	A	2	GLU	2.1
1	C	95	ALA	2.0
1	A	5	GLN	2.0
2	D	324	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	TPO	C	160	11/12	0.98	0.11	17,19,21,21	0
1	TPO	A	160	11/12	0.98	0.11	18,19,21,21	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

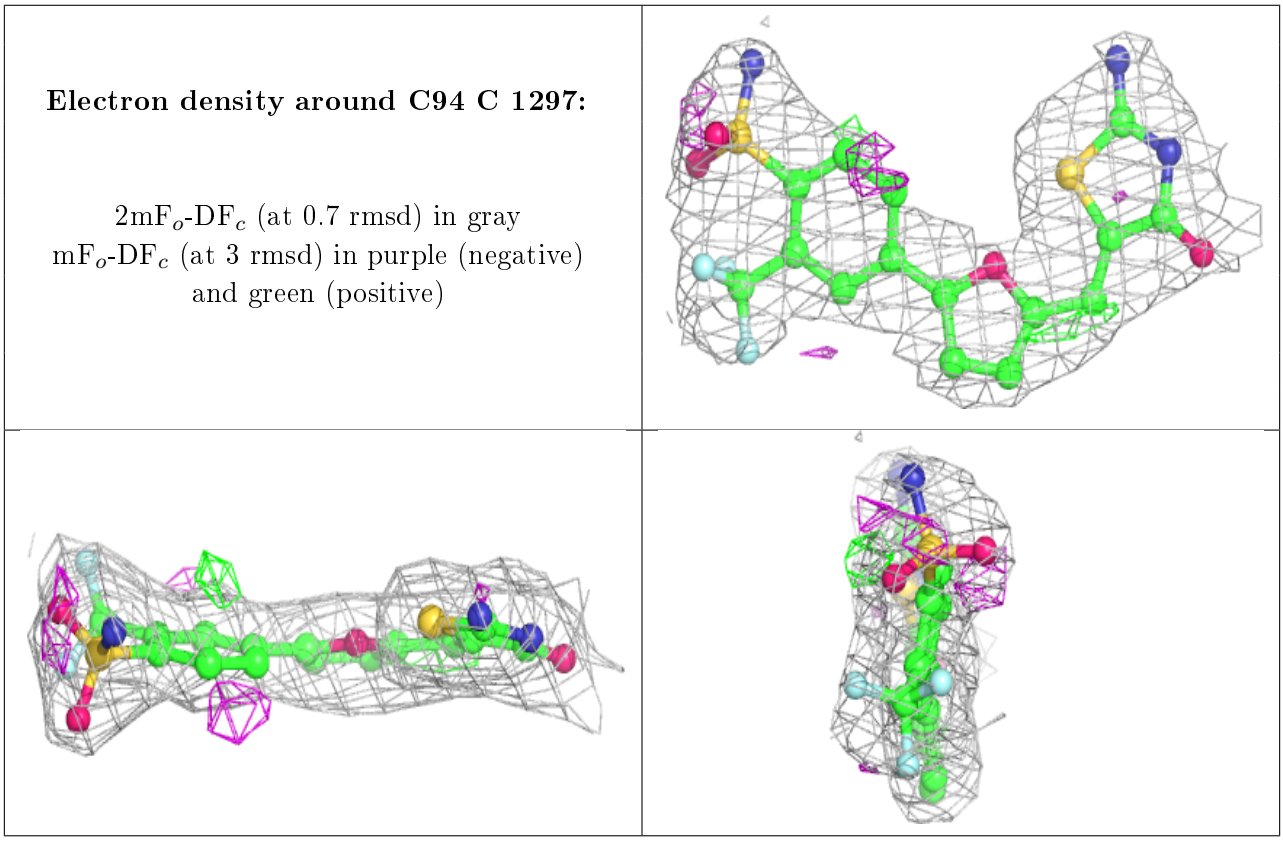
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C94	C	1297	27/27	0.85	0.20	41,47,53,55	0
3	C94	A	1297	27/27	0.88	0.18	44,49,51,51	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.

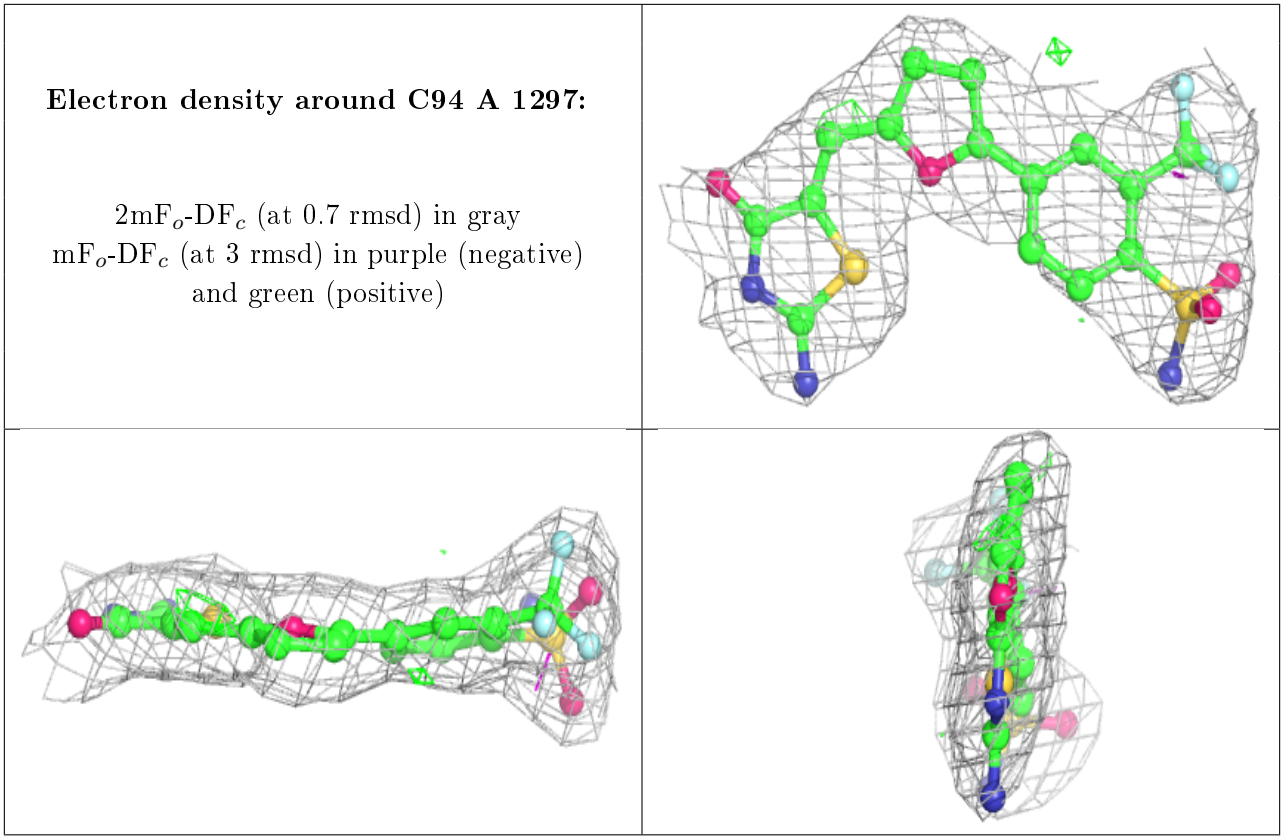
Electron density around C94 C 1297:

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



Electron density around C94 A 1297:

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



6.5 Other polymers (i)

There are no such residues in this entry.