



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:29 am BST

PDB ID : 1Q8J  
Title : Cobalamin-dependent methionine synthase (1-566) from *Thermotoga maritima* (Cd<sup>2+</sup>, Hcy, methyltetrahydrofolate complex)  
Authors : Evans, J.C.; Huddler, D.P.; Hilgers, M.T.; Romanchuk, G.; Matthews, R.G.; Ludwig, M.L.  
Deposited on : 2003-08-21  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

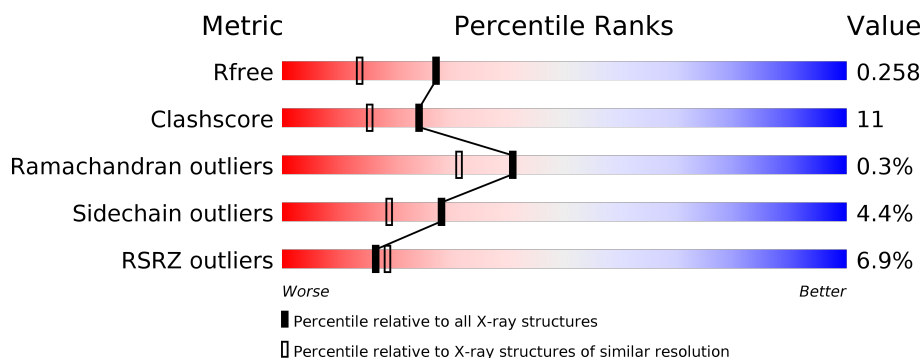
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	566	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>••</div> </div> </div>
1	B	566	<div> <div>9%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9128 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.

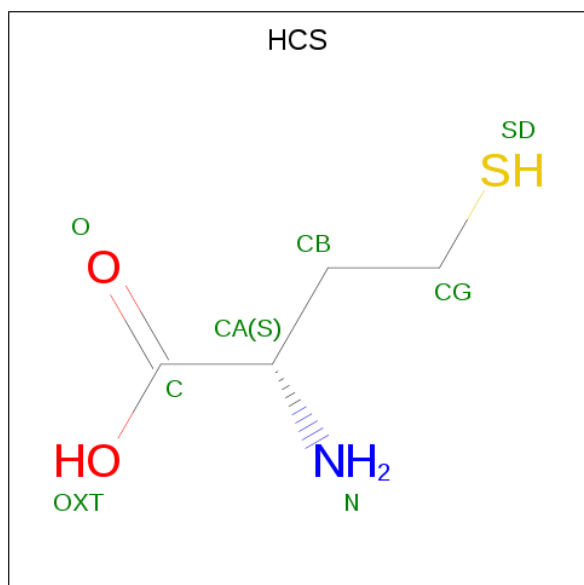
- Molecule 1 is a protein called 5-methyltetrahydrofolate S-homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4423	2839	738	833	13			
1	B	538	Total	C	N	O	S	0	0	0
			4264	2736	712	804	12			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

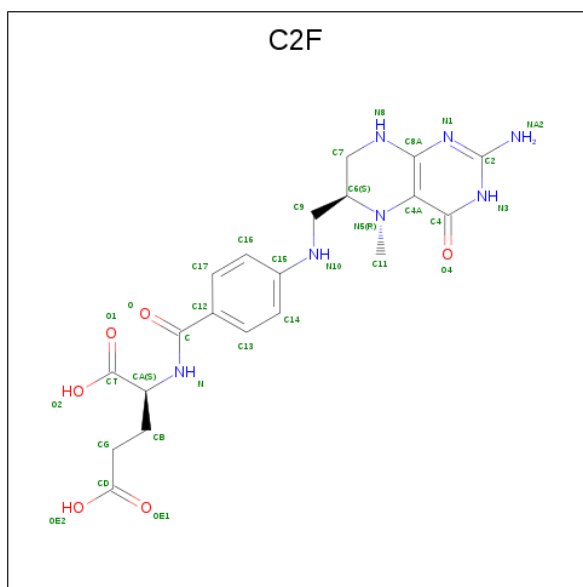
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cd	0	0
			1	1		
2	A	1	Total	Cd	0	0
			1	1		

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula:  $C_4H_9NO_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	
			8	4	1	2	1	
3	B	1	Total	C	N	O	S	
			8	4	1	2	1	

- Molecule 4 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (three-letter code: C2F) (formula: C<sub>20</sub>H<sub>25</sub>N<sub>7</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O		
			33	20	7	6		
4	B	1	Total	C	N	O		
			33	20	7	6		

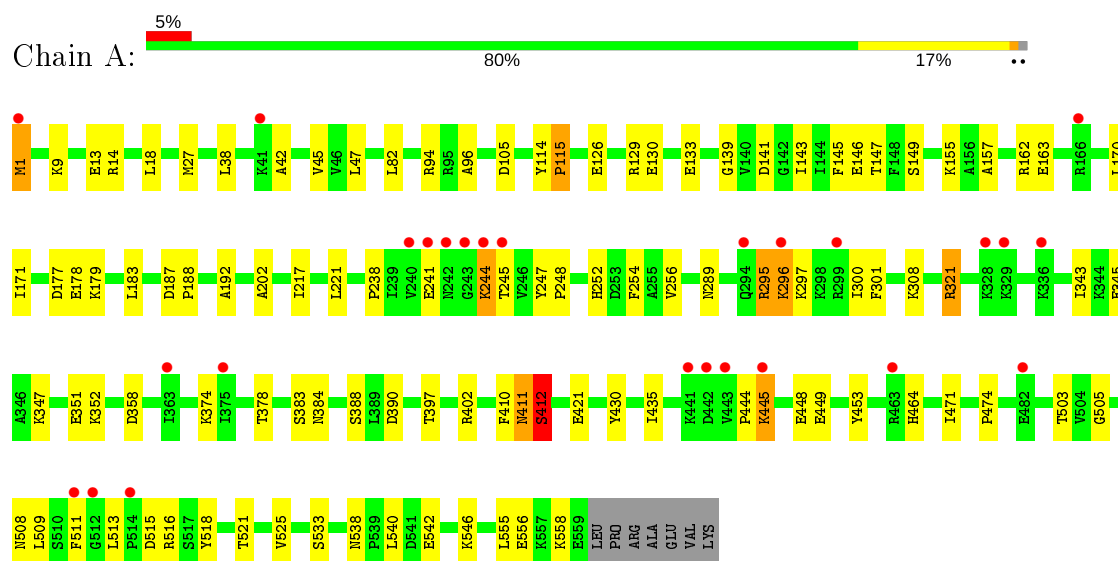
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total	O		
			240	240	0	0
5	B	117	Total	O		
			117	117	0	0

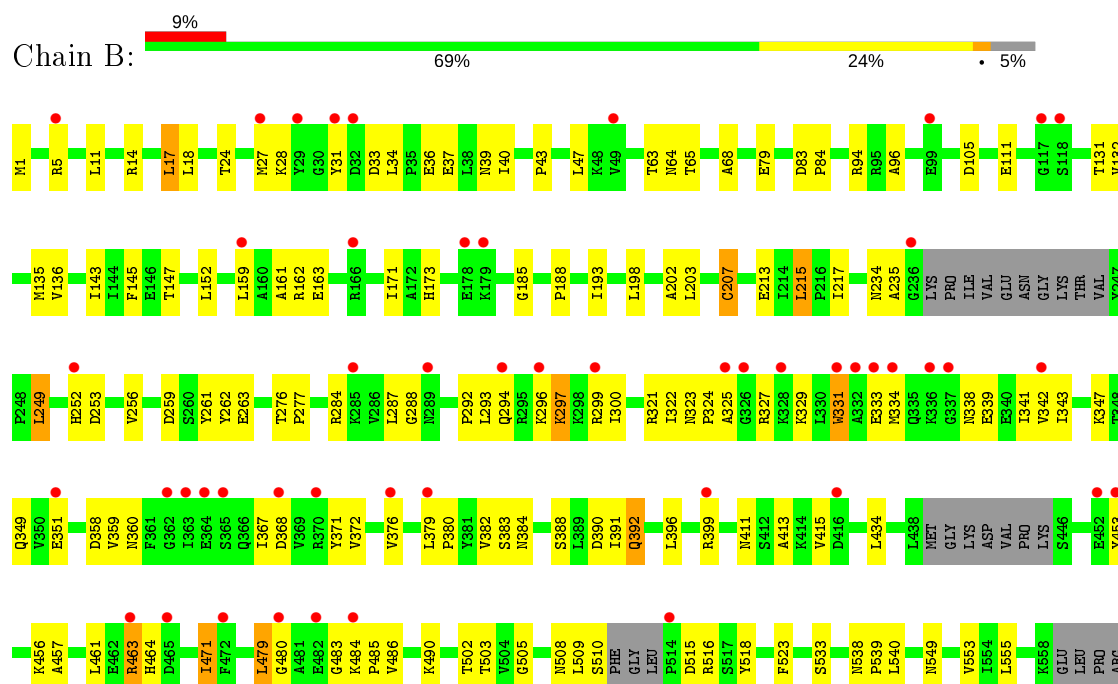
### 3 Residue-property plots [i](#)

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: 5-methyltetrahydrofolate S-homocysteine methyltransferase



- Molecule 1: 5-methyltetrahydrofolate S-homocysteine methyltransferase



ALA  
GLU  
VAL  
LYS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.98 Å   86.07 Å   125.82 Å 90.00°   100.30°   90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 98.4 (19.99-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 1.90 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.231   ,   0.267 0.220   ,   0.258	Depositor DCC
$R_{free}$ test set	3679 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 72.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HCS, C2F, CD

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	0.59	0/4505	0.76	5/6083 (0.1%)
1	B	0.45	0/4340	0.66	2/5856 (0.0%)
All	All	0.53	0/8845	0.71	7/11939 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	SER	N-CA-C	8.20	133.14	111.00
1	B	505	GLY	N-CA-C	-6.18	97.65	113.10
1	A	505	GLY	N-CA-C	-5.68	98.91	113.10
1	B	185	GLY	N-CA-C	5.50	126.86	113.10
1	A	177	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	321	ARG	N-CA-C	5.18	124.99	111.00
1	A	411	ASN	CA-C-N	-5.01	106.17	117.20

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	4423	0	4510	68	0
1	B	4264	0	4337	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	7	0	0
3	B	8	0	7	0	0
4	A	33	0	23	8	0
4	B	33	0	23	5	0
5	A	240	0	0	4	0
5	B	117	0	0	19	0
All	All	9128	0	8907	194	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 11.

All (194) 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:135:MET:SD	5:B:899:HOH:O	2.21	0.98
1:B:131:THR:HG22	5:B:899:HOH:O	1.65	0.95
1:B:105:ASP:HB3	5:B:890:HOH:O	1.69	0.92
1:A:508:ASN:HD21	4:A:801:C2F:C11	1.83	0.91
1:B:43:PRO:HD3	5:B:888:HOH:O	1.70	0.90
1:A:155:LYS:HD3	5:A:992:HOH:O	1.72	0.87
1:B:391:ILE:HG21	1:B:396:LEU:HD12	1.63	0.81
1:A:347:LYS:O	1:A:351:GLU:HG3	1.86	0.76
1:A:515:ASP:HB3	1:A:518:TYR:HD1	1.51	0.76
1:B:36:GLU:HA	5:B:887:HOH:O	1.85	0.75
1:B:34:LEU:HB2	1:B:37:GLU:HG3	1.68	0.74
1:B:471:ILE:HD11	1:B:502:THR:C	2.07	0.74
1:B:508:ASN:HD21	4:B:802:C2F:C11	2.01	0.73
1:B:64:ASN:ND2	5:B:887:HOH:O	2.21	0.73
1:B:259:ASP:O	1:B:263:GLU:HG2	1.90	0.71
1:B:479:LEU:HD22	1:B:509:LEU:O	1.91	0.70
1:A:508:ASN:ND2	4:A:801:C2F:C11	2.55	0.70
1:B:333:GLU:HB3	1:B:338:ASN:HB3	1.73	0.69
1:B:347:LYS:O	1:B:351:GLU:HG3	1.93	0.68
1:B:372:VAL:HG11	1:B:396:LEU:HD11	1.74	0.68
1:A:9:LYS:HE2	1:A:13:GLU:OE1	1.94	0.67
1:A:321:ARG:NE	1:A:540:LEU:HD22	2.09	0.67
1:B:360:ASN:HB2	1:B:390:ASP:HB3	1.76	0.67
1:A:114:TYR:CZ	1:A:374:LYS:HE2	2.31	0.66
1:A:143:ILE:HB	1:A:170:LEU:HD23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LYS:O	1:B:297:LYS:HB3	1.95	0.66
1:B:413:ALA:HB2	1:B:434:LEU:HD11	1.77	0.66
1:B:152:LEU:C	1:B:152:LEU:HD13	2.17	0.65
1:A:402:ARG:HG2	1:A:430:TYR:CE1	2.31	0.65
1:A:252:HIS:O	1:A:256:VAL:HG13	1.97	0.65
1:B:65:THR:OG1	5:B:890:HOH:O	2.14	0.65
1:B:484:LYS:N	1:B:485:PRO:HD3	2.12	0.64
1:B:508:ASN:HD21	4:B:802:C2F:H111	1.64	0.62
1:B:17:LEU:HD13	1:B:287:LEU:CD2	2.30	0.62
1:A:295:ARG:O	1:A:296:LYS:HB2	1.99	0.62
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.65	0.62
1:A:390:ASP:HA	1:A:411:ASN:HB3	1.83	0.60
1:B:379:LEU:HB2	1:B:380:PRO:HD3	1.81	0.60
1:B:510:SER:OG	1:B:516:ARG:HB2	2.01	0.60
1:A:38:LEU:HD13	1:A:45:VAL:HG11	1.83	0.60
1:A:14:ARG:NH1	1:A:289:ASN:OD1	2.35	0.59
1:A:412:SER:HA	1:A:435:ILE:O	2.01	0.59
1:B:94:ARG:HD2	5:B:900:HOH:O	2.01	0.59
1:A:171:ILE:HG12	1:A:202:ALA:HB3	1.85	0.58
1:B:14:ARG:HD3	5:B:870:HOH:O	2.03	0.58
1:B:391:ILE:CG2	1:B:396:LEU:HD12	2.32	0.58
1:B:11:LEU:O	1:B:292:PRO:HG2	2.03	0.57
1:B:463:ARG:NH2	1:B:463:ARG:HG3	2.20	0.57
1:B:39:ASN:ND2	5:B:887:HOH:O	2.37	0.57
1:B:486:VAL:HG12	5:B:803:HOH:O	2.04	0.57
1:B:17:LEU:HD13	1:B:287:LEU:HD23	1.87	0.57
1:B:396:LEU:O	1:B:396:LEU:HD13	2.05	0.57
1:A:155:LYS:HZ3	1:A:155:LYS:HB2	1.69	0.56
1:B:339:GLU:O	1:B:343:ILE:HG13	2.04	0.56
1:B:508:ASN:ND2	4:B:802:C2F:C11	2.68	0.56
1:A:188:PRO:HG3	1:A:217:ILE:HG23	1.87	0.56
1:B:27:MET:HA	1:B:31:TYR:O	2.05	0.56
1:B:390:ASP:HA	1:B:411:ASN:HB3	1.88	0.56
4:B:802:C2F:O4	4:B:802:C2F:H112	2.06	0.56
1:B:188:PRO:CG	1:B:217:ILE:HG23	2.36	0.55
1:B:43:PRO:CD	5:B:888:HOH:O	2.42	0.55
1:B:253:ASP:O	1:B:256:VAL:HG22	2.07	0.55
1:B:1:MET:HE1	1:B:136:VAL:O	2.06	0.55
1:B:479:LEU:HD23	1:B:480:GLY:N	2.21	0.55
1:B:479:LEU:HA	1:B:483:GLY:HA2	1.89	0.55
1:A:542:GLU:HG2	1:A:546:LYS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:NZ	1:A:155:LYS:HB2	2.21	0.54
1:B:358:ASP:HA	1:B:388:SER:HB3	1.90	0.54
1:B:463:ARG:HH21	1:B:463:ARG:HG3	1.73	0.53
1:B:299:ARG:HG3	1:B:299:ARG:HH11	1.74	0.53
1:B:331:TRP:CE3	1:B:331:TRP:HA	2.43	0.53
1:A:508:ASN:HD21	4:A:801:C2F:H111	1.70	0.53
1:B:331:TRP:HE3	1:B:331:TRP:HA	1.74	0.53
1:A:321:ARG:HE	1:A:540:LEU:HD22	1.73	0.52
1:A:516:ARG:HH12	4:A:801:C2F:HB2	1.73	0.52
1:A:129:ARG:NH1	1:A:133:GLU:OE1	2.41	0.52
1:B:485:PRO:HG3	1:B:509:LEU:HD11	1.92	0.52
1:B:372:VAL:O	1:B:376:VAL:HG23	2.10	0.52
1:B:83:ASP:HB3	1:B:84:PRO:CD	2.40	0.52
1:A:244:LYS:H	1:A:244:LYS:HD3	1.75	0.52
1:A:556:GLU:OE2	1:B:486:VAL:HG11	2.10	0.51
1:B:111:GLU:HB3	5:B:896:HOH:O	2.09	0.51
1:B:479:LEU:HA	1:B:483:GLY:CA	2.40	0.51
1:B:27:MET:HG3	1:B:28:LYS:N	2.26	0.51
1:B:188:PRO:HG2	1:B:217:ILE:HG23	1.92	0.51
1:B:321:ARG:CD	1:B:540:LEU:HD22	2.40	0.51
1:A:115:PRO:HG3	1:A:378:THR:HG23	1.93	0.51
1:A:358:ASP:HA	1:A:388:SER:HB3	1.92	0.51
1:A:515:ASP:HB3	1:A:518:TYR:CD1	2.41	0.50
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.76	0.50
1:A:508:ASN:ND2	4:A:801:C2F:H112	2.26	0.50
1:B:152:LEU:O	1:B:152:LEU:HD13	2.10	0.50
1:B:65:THR:N	5:B:890:HOH:O	2.29	0.50
1:A:445:LYS:HE3	1:A:449:GLU:OE2	2.11	0.50
1:A:321:ARG:HD2	1:A:538:ASN:OD1	2.12	0.50
1:A:444:PRO:HG3	1:A:453:TYR:CE1	2.47	0.50
1:B:47:LEU:HD12	1:B:96:ALA:HB2	1.94	0.50
1:B:325:ALA:O	1:B:327:ARG:HG3	2.12	0.49
1:B:40:ILE:C	5:B:888:HOH:O	2.50	0.49
1:B:471:ILE:HD11	1:B:503:THR:N	2.27	0.49
1:B:508:ASN:ND2	4:B:802:C2F:H111	2.27	0.49
1:A:383:SER:O	1:A:384:ASN:HB2	2.12	0.49
1:A:343:ILE:O	1:A:347:LYS:HG3	2.12	0.49
1:B:349:GLN:HB3	1:B:539:PRO:HG3	1.94	0.48
1:A:448:GLU:CD	1:A:448:GLU:H	2.16	0.48
1:B:132:VAL:HG13	1:B:143:ILE:CD1	2.43	0.48
1:B:215:LEU:HD13	1:B:261:TYR:CZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:OD1	1:A:146:GLU:OE1	2.31	0.48
1:A:42:ALA:O	1:A:45:VAL:HG12	2.14	0.48
1:B:202:ALA:C	1:B:203:LEU:HD12	2.33	0.48
1:A:143:ILE:HB	1:A:170:LEU:CD2	2.43	0.48
1:A:27:MET:SD	1:A:27:MET:C	2.92	0.48
1:A:1:MET:HB2	1:A:141:ASP:OD1	2.14	0.48
1:B:479:LEU:HD23	1:B:480:GLY:H	1.78	0.47
1:A:188:PRO:CG	1:A:217:ILE:HG23	2.44	0.47
1:B:79:GLU:HB3	5:B:893:HOH:O	2.13	0.47
1:A:145:PHE:CE2	1:A:157:ALA:HB1	2.50	0.47
1:A:1:MET:SD	1:A:139:GLY:O	2.73	0.47
1:A:521:THR:O	1:A:525:VAL:HG23	2.14	0.47
1:B:338:ASN:ND2	1:B:341:ILE:HB	2.29	0.47
1:B:359:VAL:HG23	1:B:359:VAL:O	2.15	0.47
1:B:372:VAL:HG11	1:B:396:LEU:HD21	1.96	0.47
1:A:192:ALA:HB2	1:A:221:LEU:HD12	1.98	0.46
1:B:368:ASP:O	1:B:371:TYR:N	2.47	0.46
1:A:301:PHE:CZ	1:A:471:ILE:HG13	2.49	0.46
1:B:171:ILE:HG12	1:B:202:ALA:HB3	1.97	0.46
1:B:413:ALA:CB	1:B:434:LEU:HD11	2.44	0.46
1:B:276:THR:HB	1:B:277:PRO:CD	2.46	0.46
1:B:63:THR:O	5:B:890:HOH:O	2.21	0.46
1:B:188:PRO:HG3	1:B:217:ILE:HG23	1.97	0.46
1:B:538:ASN:OD1	1:B:540:LEU:HB2	2.16	0.46
1:B:284:ARG:NH1	1:B:288:GLY:O	2.48	0.45
1:B:471:ILE:C	1:B:471:ILE:HD13	2.36	0.45
1:B:485:PRO:CG	1:B:509:LEU:HD11	2.46	0.45
1:B:65:THR:HB	1:B:68:ALA:HB3	1.97	0.45
1:B:17:LEU:HD13	1:B:287:LEU:HD22	1.99	0.45
1:B:252:HIS:O	1:B:256:VAL:HG13	2.16	0.45
1:B:415:VAL:HG12	1:B:456:LYS:HD3	1.98	0.45
1:A:244:LYS:H	1:A:244:LYS:CD	2.30	0.45
4:A:801:C2F:H112	4:A:801:C2F:O4	2.17	0.45
1:A:162:ARG:HA	1:A:162:ARG:HD3	1.65	0.45
1:B:235:ALA:O	1:B:249:LEU:HB2	2.17	0.45
1:A:513:LEU:HG	5:A:1013:HOH:O	2.16	0.44
1:B:207:CYS:HA	1:B:234:ASN:OD1	2.17	0.44
1:B:262:TYR:CZ	1:B:293:LEU:HD13	2.53	0.44
1:B:486:VAL:O	1:B:490:LYS:HG3	2.17	0.44
1:B:131:THR:C	5:B:899:HOH:O	2.55	0.44
1:B:24:THR:HB	1:B:27:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HG23	1:A:410:PHE:CE1	2.53	0.44
1:A:555:LEU:O	1:A:556:GLU:HB2	2.16	0.44
1:B:152:LEU:C	1:B:152:LEU:CD1	2.84	0.44
1:B:162:ARG:HD3	1:B:162:ARG:HA	1.67	0.44
1:A:474:PRO:HD2	1:A:503:THR:O	2.19	0.43
1:B:193:ILE:CD1	1:B:300:ILE:HD11	2.48	0.43
1:B:213:GLU:H	1:B:213:GLU:CD	2.21	0.43
1:B:213:GLU:CD	1:B:213:GLU:N	2.72	0.43
1:B:379:LEU:HA	1:B:382:VAL:CG2	2.49	0.43
1:A:94:ARG:HD2	5:A:985:HOH:O	2.19	0.43
1:B:323:ASN:O	1:B:327:ARG:HD3	2.19	0.43
1:B:484:LYS:N	1:B:485:PRO:CD	2.80	0.43
1:A:308:LYS:HB3	1:A:308:LYS:HE2	1.76	0.43
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.31	0.42
1:B:549:ASN:O	1:B:553:VAL:HG23	2.19	0.42
1:A:241:GLU:HB2	1:A:244:LYS:CE	2.49	0.42
1:B:132:VAL:HG11	1:B:161:ALA:HA	2.00	0.42
1:A:508:ASN:ND2	4:A:801:C2F:H111	2.29	0.42
1:B:276:THR:HB	1:B:277:PRO:HD2	2.02	0.42
1:B:341:ILE:HG23	1:B:342:VAL:N	2.34	0.42
1:B:463:ARG:HH21	1:B:463:ARG:CG	2.31	0.42
1:A:421:GLU:HG2	1:A:464:HIS:NE2	2.35	0.42
1:B:321:ARG:HG2	1:B:321:ARG:NH1	2.33	0.42
1:B:392:GLN:H	1:B:392:GLN:HG2	1.61	0.42
1:B:509:LEU:HD22	1:B:523:PHE:HB2	2.01	0.42
1:A:238:PRO:HB3	1:A:247:TYR:CE1	2.55	0.42
1:B:383:SER:O	1:B:384:ASN:HB2	2.20	0.42
1:A:126:GLU:OE1	1:A:130:GLU:OE2	2.38	0.42
1:A:187:ASP:HB2	1:A:188:PRO:CD	2.50	0.42
1:B:457:ALA:O	1:B:461:LEU:HG	2.20	0.42
1:A:296:LYS:O	1:A:297:LYS:HB3	2.20	0.41
1:B:380:PRO:O	1:B:384:ASN:HA	2.20	0.41
1:B:94:ARG:HG3	5:B:900:HOH:O	2.19	0.41
1:B:145:PHE:O	1:B:173:HIS:HB2	2.20	0.41
1:A:178:GLU:HG3	5:A:994:HOH:O	2.19	0.41
1:B:322:ILE:HG22	1:B:322:ILE:O	2.21	0.41
1:B:324:PRO:HG3	1:B:334:MET:SD	2.60	0.41
1:B:331:TRP:CZ3	1:B:367:ILE:HD11	2.55	0.41
1:A:47:LEU:HD12	1:A:96:ALA:HB2	2.01	0.41
1:B:368:ASP:O	1:B:371:TYR:HB3	2.21	0.41
1:B:390:ASP:C	1:B:391:ILE:HG13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:HB3	1:A:183:LEU:HB3	2.02	0.41
4:A:801:C2F:HB2	4:A:801:C2F:O	2.20	0.40
1:B:329:LYS:O	1:B:329:LYS:HD2	2.21	0.40
1:B:193:ILE:HD13	1:B:300:ILE:HD11	2.03	0.40
1:B:515:ASP:HB3	1:B:518:TYR:HD1	1.87	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	557/566 (98%)	531 (95%)	24 (4%)	2 (0%)	34	24
1	B	530/566 (94%)	496 (94%)	33 (6%)	1 (0%)	47	38
All	All	1087/1132 (96%)	1027 (94%)	57 (5%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	LYS
1	A	412	SER
1	A	296	LYS

### 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	488/494 (99%)	468 (96%)	20 (4%)	30	21
1	B	470/494 (95%)	448 (95%)	22 (5%)	26	16
All	All	958/988 (97%)	916 (96%)	42 (4%)	28	19

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	LEU
1	A	82	LEU
1	A	115	PRO
1	A	147	THR
1	A	163	GLU
1	A	179	LYS
1	A	244	LYS
1	A	245	THR
1	A	248	PRO
1	A	254	PHE
1	A	295	ARG
1	A	300	ILE
1	A	345	GLU
1	A	352	LYS
1	A	445	LYS
1	A	509	LEU
1	A	511	PHE
1	A	533	SER
1	A	558	LYS
1	B	5	ARG
1	B	17	LEU
1	B	18	LEU
1	B	33	ASP
1	B	147	THR
1	B	159	LEU
1	B	163	GLU
1	B	198	LEU
1	B	207	CYS
1	B	215	LEU
1	B	249	LEU
1	B	294	GLN
1	B	331	TRP
1	B	392	GLN
1	B	399	ARG

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Mol	Chain	Res	Type
1	B	453	TYR
1	B	463	ARG
1	B	464	HIS
1	B	471	ILE
1	B	479	LEU
1	B	533	SER
1	B	555	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	ASN
1	B	508	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	C2F	A	801	-	27,35,35	1.23	1 (3%)	27,49,49	1.61	7 (25%)
4	C2F	B	802	-	27,35,35	1.22	1 (3%)	27,49,49	1.46	6 (22%)
3	HCS	B	702	-	3,7,7	1.72	1 (33%)	2,8,8	0.63	0
3	HCS	A	701	-	3,7,7	0.95	0	2,8,8	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C2F	A	801	-	-	1/16/35/35	0/3/3/3
4	C2F	B	802	-	-	1/16/35/35	0/3/3/3
3	HCS	B	702	-	-	0/3/7/7	-
3	HCS	A	701	-	-	0/3/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	802	C2F	O4-C4	4.75	1.36	1.24
4	A	801	C2F	O4-C4	4.73	1.36	1.24
3	B	702	HCS	CB-CG	2.50	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	C2F	N3-C2-N1	-3.63	119.73	125.42
4	B	802	C2F	N3-C2-N1	-3.57	119.81	125.42
4	B	802	C2F	C4-N3-C2	3.39	121.31	115.93
4	A	801	C2F	C4-N3-C2	3.32	121.20	115.93
4	A	801	C2F	C2-N1-C8A	2.82	120.86	114.54
4	B	802	C2F	C2-N1-C8A	2.72	120.64	114.54
4	A	801	C2F	CA-N-C	2.69	125.81	122.34
4	A	801	C2F	CB-CA-N	2.52	113.87	110.19
4	A	801	C2F	C4-C4A-C8A	2.26	116.21	114.44
4	B	802	C2F	CA-N-C	2.15	125.11	122.34
4	B	802	C2F	C4-C4A-C8A	2.11	116.09	114.44
4	B	802	C2F	NA2-C2-N1	2.06	120.46	117.25
4	A	801	C2F	NA2-C2-N3	2.00	120.37	117.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	C2F	CB-CA-N-C
4	B	802	C2F	CB-CA-N-C

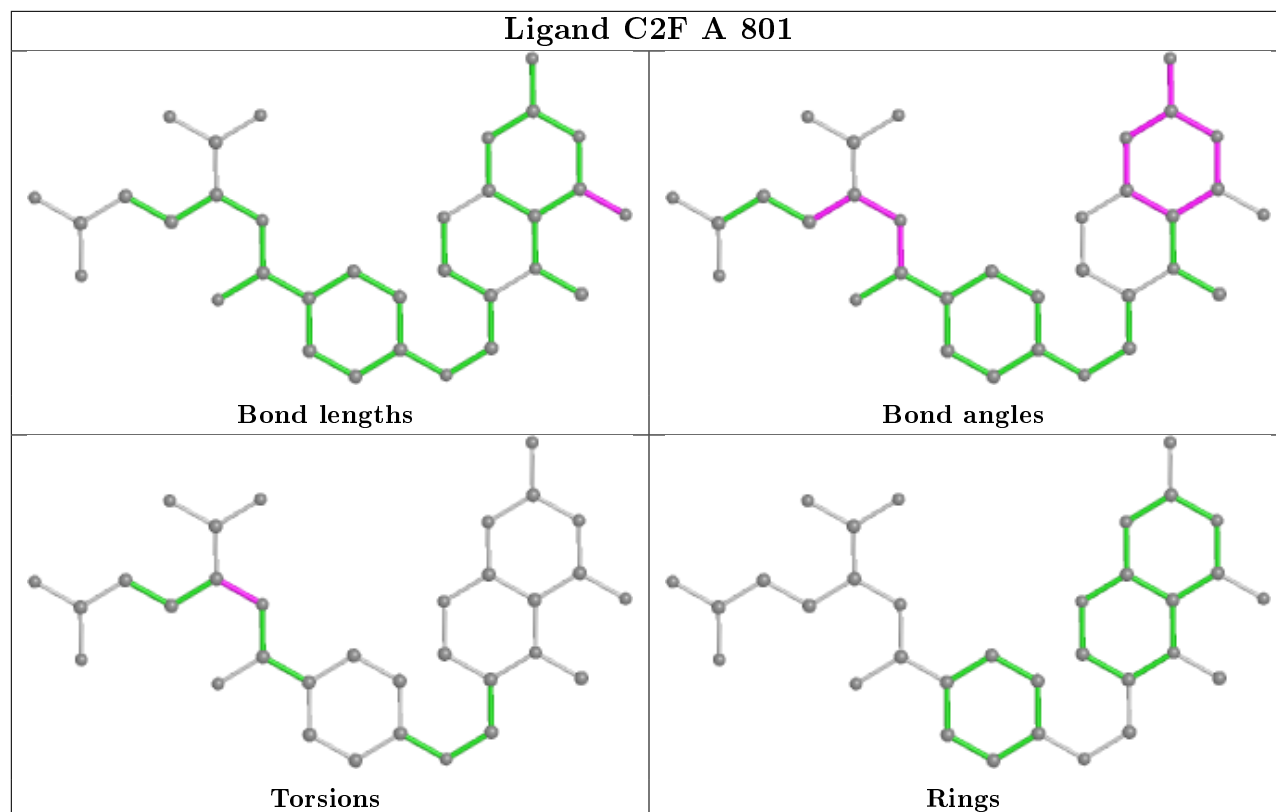
There are no ring outliers.

2 monomers are involved in 13 short contacts:

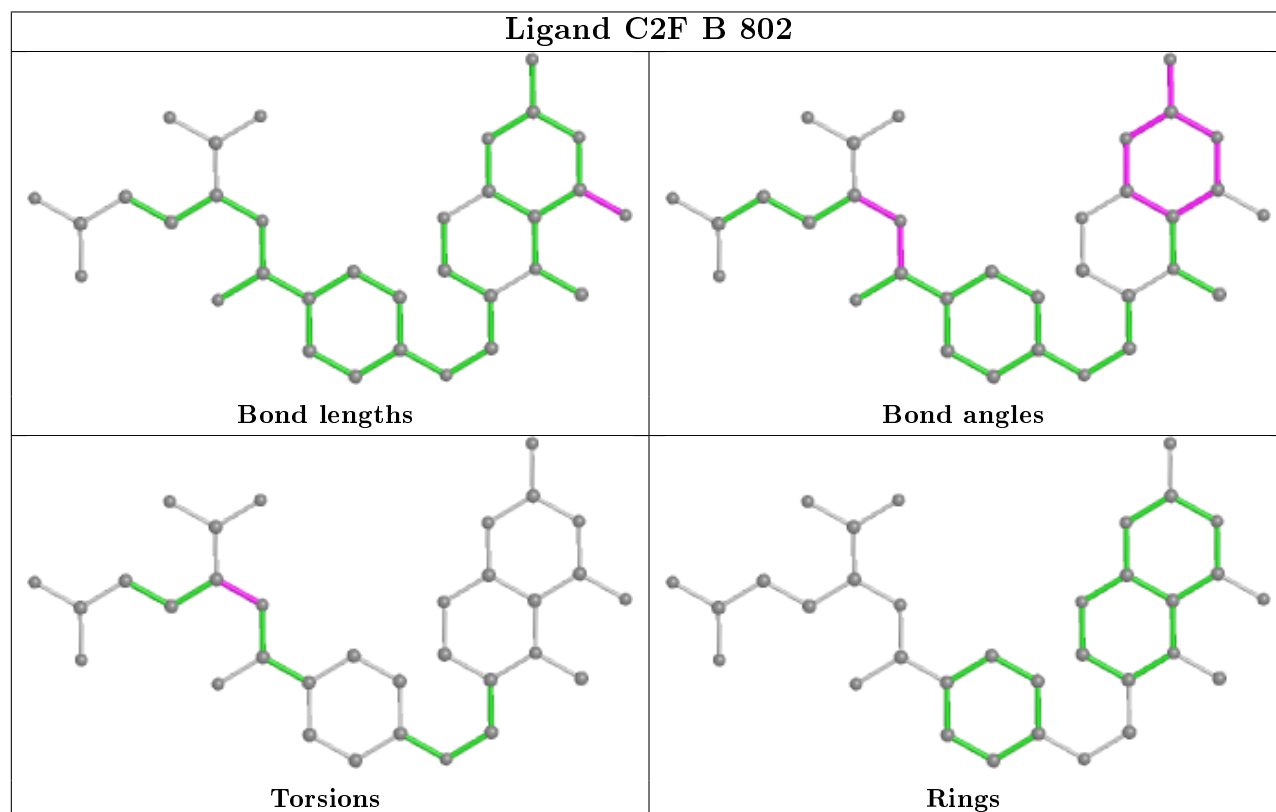
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	C2F	8	0
4	B	802	C2F	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand C2F A 801



## Ligand C2F B 802



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	559/566 (98%)	0.17	26 (4%) 31 34	15, 29, 51, 71	0
1	B	538/566 (95%)	0.66	50 (9%) 8 10	26, 43, 65, 76	0
All	All	1097/1132 (96%)	0.41	76 (6%) 16 19	15, 36, 63, 76	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	GLY	7.2
1	A	296	LYS	5.6
1	B	296	LYS	5.5
1	A	242	ASN	5.0
1	B	29	TYR	4.9
1	A	442	ASP	4.6
1	B	326	GLY	4.5
1	B	336	LYS	4.4
1	A	511	PHE	4.4
1	B	328	LYS	4.3
1	B	482	GLU	4.2
1	B	370	ARG	4.2
1	A	1	MET	4.2
1	B	362	GLY	4.1
1	A	244	LYS	3.9
1	B	32	ASP	3.8
1	B	363	ILE	3.7
1	B	236	GLY	3.7
1	A	441	LYS	3.6
1	A	241	GLU	3.6
1	B	299	ARG	3.5
1	A	512	GLY	3.3
1	A	245	THR	3.3
1	B	453	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	178	GLU	3.2
1	B	376	VAL	3.1
1	B	334	MET	3.1
1	B	332	ALA	3.1
1	B	179	LYS	3.0
1	B	472	PHE	3.0
1	B	31	TYR	3.0
1	B	365	SER	2.9
1	B	465	ASP	2.9
1	A	328	LYS	2.9
1	A	363	ILE	2.9
1	B	480	GLY	2.9
1	B	325	ALA	2.9
1	B	5	ARG	2.9
1	B	331	TRP	2.9
1	A	443	VAL	2.9
1	A	445	LYS	2.8
1	B	166	ARG	2.8
1	B	252	HIS	2.8
1	B	289	ASN	2.8
1	B	27	MET	2.7
1	B	333	GLU	2.7
1	A	514	PRO	2.7
1	A	294	GLN	2.7
1	B	285	LYS	2.7
1	B	159	LEU	2.7
1	B	368	ASP	2.5
1	A	240	VAL	2.5
1	B	117	GLY	2.5
1	B	118	SER	2.5
1	B	99	GLU	2.4
1	B	364	GLU	2.4
1	B	416	ASP	2.4
1	B	294	GLN	2.4
1	B	463	ARG	2.4
1	B	337	GLY	2.4
1	A	336	LYS	2.3
1	B	399	ARG	2.2
1	B	351	GLU	2.2
1	B	514	PRO	2.2
1	A	299	ARG	2.2
1	A	375	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	482	GLU	2.2
1	A	41	LYS	2.2
1	A	329	LYS	2.2
1	B	342	VAL	2.2
1	A	166	ARG	2.1
1	A	463	ARG	2.1
1	B	379	LEU	2.1
1	B	452	GLU	2.0
1	B	49	VAL	2.0
1	B	484	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

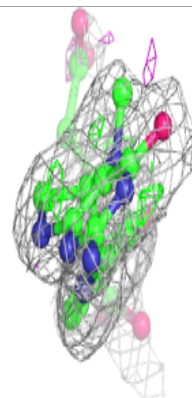
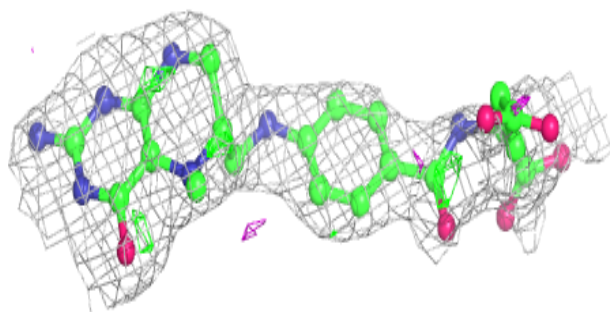
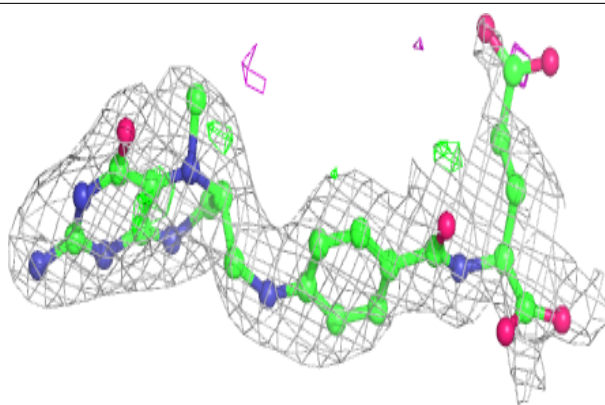
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	C2F	B	802	33/33	0.74	0.21	45,49,72,72	0
4	C2F	A	801	33/33	0.85	0.14	22,30,61,63	0
3	HCS	A	701	8/8	0.95	0.09	24,27,32,32	0
3	HCS	B	702	8/8	0.96	0.09	29,31,32,32	0
2	CD	A	601	1/1	0.97	0.04	29,29,29,29	0
2	CD	B	602	1/1	0.99	0.02	34,34,34,34	0

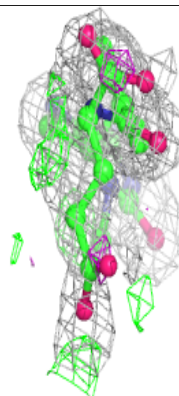
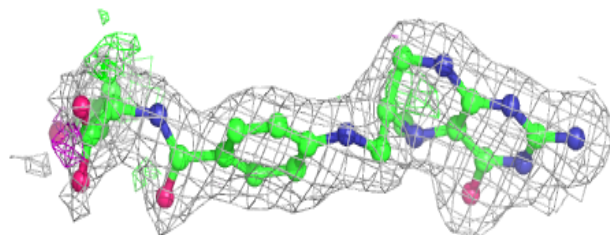
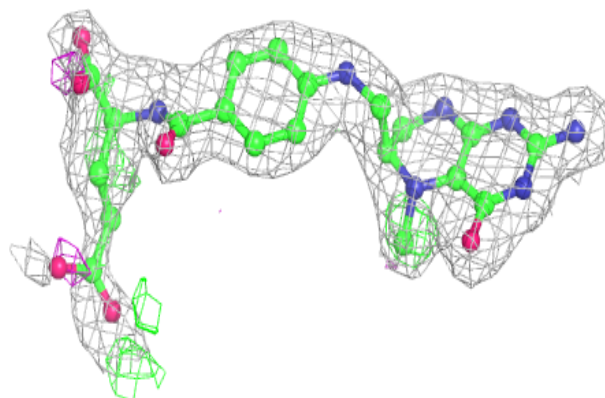
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around C2F B 802:**

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

**Electron density around C2F A 801:**

$2mF_o-DF_c$  (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.