



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:22 AM UTC

PDB ID : 2KCE / pdb_00002kce
Title : BINDING OF THE ANTICANCER DRUG ZD1694 TO E. COLI THYMIDYLATE SYNTHASE: ASSESSING SPECIFICITY AND AFFINITY
Authors : Rutenber, E.E.; Stroud, R.M.
Deposited on : 1997-06-09
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

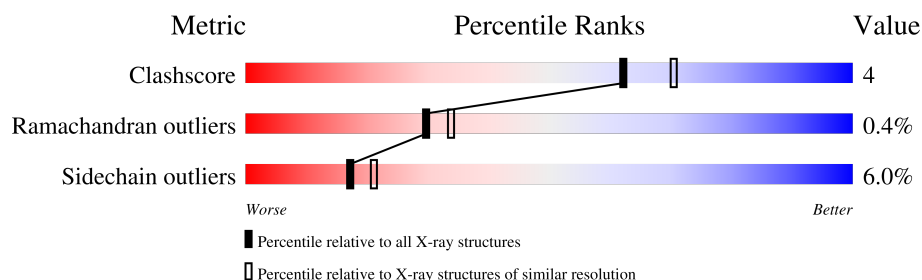
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	 74% 23% •
1	B	264	 77% 19% •

2 Entry composition [i](#)

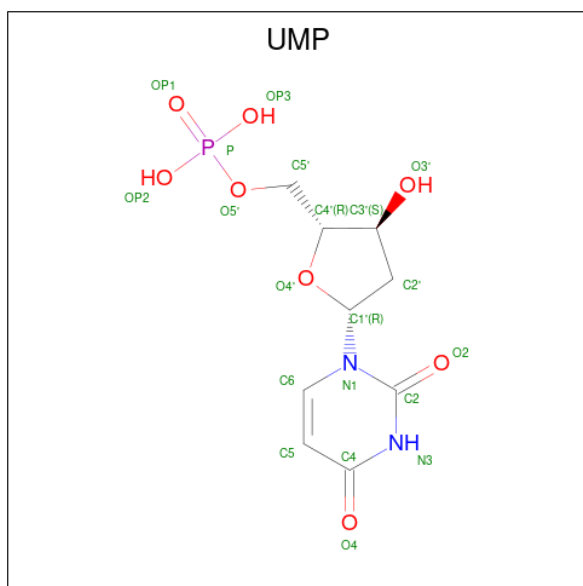
There are 4 unique types of molecules in this entry. The entry contains 6081 atoms, of which 1432 are hydrogens and 0 are deuteriums.

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 THYMIDYLATE SYNTHASE.

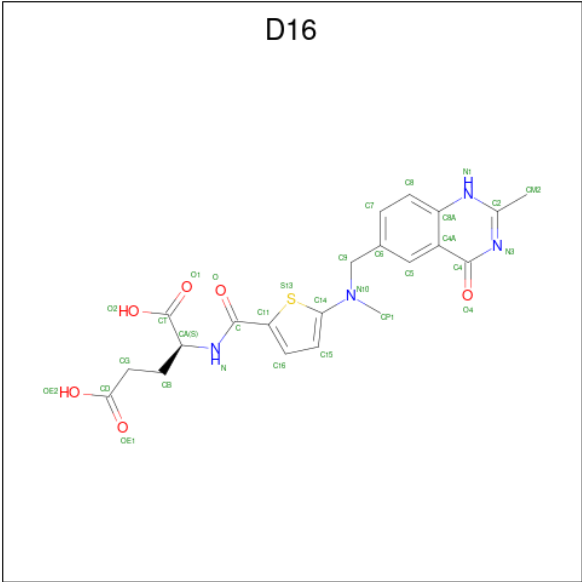
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	H	N	O	S	0	0	0
			2619	1374	469	371	393	12			
1	B	264	Total	C	H	N	O	S	0	0	0
			2619	1374	469	371	393	12			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			21	9	1	2	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			21	9	1	2	8	1		

- Molecule 3 is TOMUDEX (CCD ID: D16) (formula: $C_{21}H_{22}N_4O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			33	21	1	4	6	1		
3	B	1	Total	C	H	N	O	S	0	0
			33	21	1	4	6	1		

- Molecule 4 is water.

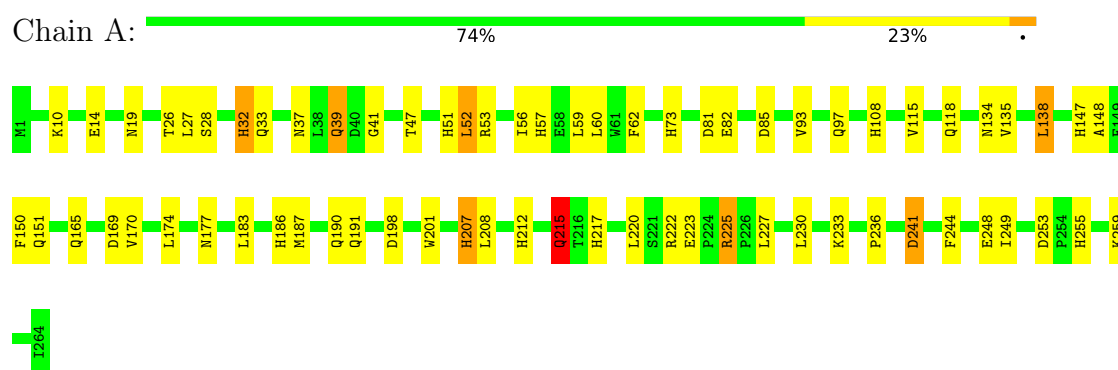
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	142	Total	H	O	0	0
			426	284	142		
4	B	103	Total	H	O	0	0
			309	206	103		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE



• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	126.80Å 126.80Å 67.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.0 (7.00-2.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6081	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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: D16, UMP

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	0.99	11/2210 (0.5%)	1.64	31/3000 (1.0%)
1	B	1.00	11/2210 (0.5%)	1.71	44/3000 (1.5%)
All	All	0.99	22/4420 (0.5%)	1.68	75/6000 (1.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIS	CD2-NE2	-7.58	1.29	1.37
1	B	207	HIS	CD2-NE2	-7.22	1.29	1.37
1	B	57	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	217	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	108	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.76	1.30	1.37
1	B	217	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	255	HIS	CD2-NE2	-6.58	1.30	1.37
1	B	32	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	108	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	186	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	32	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	51	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	255	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	51	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	207	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	147	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	57	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	212	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	147	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	186	HIS	CD2-NE2	-5.28	1.32	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CA-CB-CG	10.18	122.78	112.60
1	B	177	ASN	OD1-CG-ND2	-8.95	113.65	122.60
1	A	150	PHE	CA-CB-CG	8.44	122.24	113.80
1	A	147	HIS	CA-CB-CG	7.99	121.79	113.80
1	A	190	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	B	134	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	B	76	ASN	CA-CB-CG	-7.49	105.11	112.60
1	B	78	THR	N-CA-CB	-7.49	99.30	110.61
1	B	22	THR	N-CA-C	-7.34	98.60	110.20
1	A	57	HIS	CA-CB-CG	-7.17	106.63	113.80
1	B	22	THR	O-C-N	-7.10	114.63	123.01
1	A	148	ALA	N-CA-C	6.96	121.90	113.41
1	B	97	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	B	66	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	79	ILE	N-CA-C	6.88	119.65	111.05
1	B	78	THR	CA-CB-OG1	-6.80	99.40	109.60
1	B	150	PHE	CA-CB-CG	6.78	120.58	113.80
1	B	148	ALA	N-CA-C	6.61	121.47	113.41
1	B	19	ASN	N-CA-C	-6.59	99.28	109.76
1	B	117	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	A	28	SER	N-CA-C	6.43	119.97	109.24
1	B	57	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	134	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	B	233	LYS	N-CA-C	6.25	119.07	111.82
1	A	217	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	B	64	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	190	GLN	CG-CD-NE2	6.18	125.67	116.40
1	A	37	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	108	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	B	215	GLN	CA-CB-CG	6.12	126.34	114.10
1	B	147	HIS	CA-CB-CG	5.99	119.79	113.80
1	B	169	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	32	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	B	108	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	207	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	97	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	B	73	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	A	19	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	B	64	GLN	CB-CG-CD	5.66	122.23	112.60
1	A	169	ASP	CA-CB-CG	5.64	118.25	112.60
1	B	51	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	B	191	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	215	GLN	CA-CB-CG	5.58	125.26	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	85	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	73	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	151	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	198	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	80	TRP	CG-CD2-CE3	5.47	139.37	133.90
1	B	207	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	147	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	B	217	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	62	PHE	CA-CB-CG	5.42	119.22	113.80
1	B	255	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	A	27	LEU	N-CA-C	-5.32	100.06	108.73
1	B	22	THR	CA-C-O	-5.31	115.00	121.05
1	A	81	ASP	N-CA-C	5.28	117.03	111.28
1	B	249	ILE	N-CA-C	-5.28	100.88	108.53
1	B	201	TRP	CG-CD2-CE3	5.25	139.15	133.90
1	A	174	LEU	CA-C-O	-5.24	113.25	118.34
1	B	147	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	A	39	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	241	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	32	HIS	CA-CB-CG	-5.17	108.63	113.80
1	B	68	ASN	CA-CB-CG	-5.16	107.44	112.60
1	B	177	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	108	HIS	CB-CG-ND1	5.13	130.40	122.70
1	B	80	TRP	CE2-CD2-CG	-5.11	101.06	107.20
1	B	235	LYS	CA-C-N	5.08	125.36	119.92
1	B	235	LYS	C-N-CA	5.08	125.36	119.92
1	B	133	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	A	41	GLY	N-CA-C	-5.08	104.92	110.96
1	A	191	GLN	CG-CD-NE2	5.05	123.98	116.40
1	B	201	TRP	CB-CG-CD1	-5.05	119.33	126.90
1	B	19	ASN	OD1-CG-ND2	-5.01	117.59	122.60

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	2150	469	2081	22	0
1	B	2150	469	2081	12	0
2	A	20	1	10	1	0
2	B	20	1	10	0	0
3	A	32	1	20	0	0
3	B	32	1	20	1	0
4	A	142	284	0	1	0
4	B	103	206	0	1	0
All	All	4649	1432	4222	35	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 4.

All (35) 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:233:LYS:HE3	1:A:248:GLU:HB2	1.82	0.61
1:A:10:LYS:NZ	1:A:32:HIS:HD2	1.98	0.60
1:B:22:THR:HG21	1:B:263:ALA:HB1	1.86	0.58
1:A:177:ASN:HD21	2:A:565:UMP:HN3	1.51	0.57
1:A:225:ARG:HD3	1:A:253:ASP:O	2.04	0.56
1:A:59:LEU:HD23	1:A:187:MET:HE1	1.88	0.56
1:A:215:GLN:H	1:A:215:GLN:NE2	2.04	0.55
1:B:28:SER:HB3	1:B:207:HIS:HB3	1.88	0.54
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.89	0.53
1:B:234:ARG:O	1:B:236:PRO:HD3	2.10	0.52
1:A:10:LYS:HZ3	1:A:32:HIS:HD2	1.58	0.52
1:A:82:GLU:HG2	4:A:811:HOH:O	2.10	0.52
1:A:135:VAL:HA	1:A:138:LEU:HD22	1.93	0.51
1:A:165:GLN:HE22	1:A:177:ASN:ND2	2.10	0.49
1:A:52:LEU:HD11	1:A:249:ILE:HG13	1.96	0.47
1:A:165:GLN:HE22	1:A:177:ASN:HD22	1.63	0.46
1:A:215:GLN:H	1:A:215:GLN:HE21	1.61	0.46
1:A:183:LEU:HG	1:A:187:MET:CE	2.45	0.46
1:B:1:MET:N	4:B:792:HOH:O	2.44	0.46
1:B:170:VAL:HB	1:B:208:LEU:HD13	1.98	0.46
1:A:56:ILE:HG12	1:A:183:LEU:HD21	1.99	0.45
1:A:236:PRO:HB3	1:A:241:ASP:HB3	1.99	0.45
1:B:147:HIS:HB2	1:B:163:LEU:HD11	1.98	0.44
1:A:26:THR:HB	1:A:207:HIS:HB2	2.00	0.44
1:B:181:TYR:O	1:B:185:VAL:HG23	2.18	0.44
3:B:568:D16:H15	3:B:568:D16:HP11	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TRP:O	1:B:108:HIS:HA	2.19	0.43
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.84	0.42
1:B:59:LEU:HD23	1:B:183:LEU:HD12	2.02	0.42
1:A:59:LEU:CD2	1:A:187:MET:HE1	2.50	0.42
1:B:233:LYS:HD2	1:B:248:GLU:HG2	2.01	0.41
1:B:239:ILE:HA	1:B:242:TYR:HE1	1.86	0.41
1:A:33:GLN:HA	1:A:201:TRP:O	2.21	0.41
1:A:53:ARG:HA	1:A:244:PHE:HE1	1.86	0.41
1:B:236:PRO:HB3	1:B:241:ASP:HB2	2.02	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	262/264 (99%)	258 (98%)	3 (1%)	1 (0%)	30	34
1	B	262/264 (99%)	255 (97%)	6 (2%)	1 (0%)	30	34
All	All	524/528 (99%)	513 (98%)	9 (2%)	2 (0%)	30	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	TYR
1	A	93	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	233/233 (100%)	218 (94%)	15 (6%)	16	19
1	B	233/233 (100%)	220 (94%)	13 (6%)	19	24
All	All	466/466 (100%)	438 (94%)	28 (6%)	17	21

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	39	GLN
1	A	47	THR
1	A	52	LEU
1	A	60	LEU
1	A	138	LEU
1	A	215	GLN
1	A	220	LEU
1	A	222	ARG
1	A	223	GLU
1	A	225	ARG
1	A	227	LEU
1	A	230	LEU
1	A	241	ASP
1	A	259	LYS
1	B	14	GLU
1	B	38	LEU
1	B	39	GLN
1	B	74	GLU
1	B	76	ASN
1	B	78	THR
1	B	86	GLU
1	B	140	LYS
1	B	183	LEU
1	B	208	LEU
1	B	215	GLN
1	B	223	GLU
1	B	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	33	GLN
1	A	39	GLN
1	A	75	ASN
1	A	117	ASN
1	A	118	GLN
1	A	151	GLN
1	A	177	ASN
1	A	190	GLN
1	A	215	GLN
1	A	217	HIS
1	B	32	HIS
1	B	39	GLN
1	B	75	ASN
1	B	117	ASN
1	B	118	GLN
1	B	134	ASN
1	B	190	GLN
1	B	191	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	UMP	B	567	1	21,21,21	2.37	4 (19%)	30,31,31	2.33	9 (30%)
2	UMP	A	565	1	21,21,21	2.48	5 (23%)	30,31,31	1.80	7 (23%)
3	D16	A	566	-	33,34,34	2.00	6 (18%)	46,48,48	1.82	9 (19%)
3	D16	B	568	-	33,34,34	2.08	5 (15%)	46,48,48	2.31	14 (30%)

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	UMP	B	567	1	-	0/10/22/22	0/2/2/2
2	UMP	A	565	1	-	1/10/22/22	0/2/2/2
3	D16	A	566	-	-	3/25/25/25	0/3/3/3
3	D16	B	568	-	-	6/25/25/25	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	565	UMP	C6-C5	8.62	1.55	1.35
3	B	568	D16	O4-C4	8.45	1.37	1.23
2	B	567	UMP	C6-C5	8.30	1.54	1.35
3	A	566	D16	O4-C4	8.24	1.37	1.23
2	A	565	UMP	C6-N1	4.91	1.49	1.38
3	A	566	D16	C4A-C4	-4.67	1.40	1.48
3	B	568	D16	C4A-C4	-4.50	1.40	1.48
2	B	567	UMP	C5-C4	3.97	1.52	1.43
2	A	565	UMP	C5-C4	3.91	1.52	1.43
2	B	567	UMP	C6-N1	3.85	1.47	1.38
3	B	568	D16	C8A-N1	-2.54	1.35	1.39
3	A	566	D16	C8A-N1	-2.51	1.35	1.39
2	B	567	UMP	O4'-C1'	2.37	1.47	1.42
3	A	566	D16	O2-CT	-2.29	1.23	1.30
3	B	568	D16	O2-CT	-2.24	1.23	1.30
2	A	565	UMP	P-OP3	-2.23	1.46	1.54
3	A	566	D16	OE2-CD	-2.16	1.23	1.30
3	B	568	D16	C4-N3	-2.08	1.34	1.38
3	A	566	D16	C4-N3	-2.07	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	565	UMP	P-OP2	-2.04	1.47	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	567	UMP	C5-C6-N1	-8.48	108.05	121.84
3	B	568	D16	S13-C14-N10	7.41	127.94	120.99
3	B	568	D16	C15-C14-N10	-6.24	121.41	127.84
3	B	568	D16	CG-CB-CA	5.82	123.90	113.16
2	A	565	UMP	C5-C6-N1	-5.54	112.84	121.84
3	A	566	D16	CG-CB-CA	5.21	122.77	113.16
3	A	566	D16	S13-C14-N10	4.63	125.33	120.99
2	B	567	UMP	C1'-N1-C6	-4.46	112.75	121.53
3	B	568	D16	CA-N-C	4.24	129.13	122.00
3	B	568	D16	C-C11-S13	4.18	128.11	117.18
3	A	566	D16	C15-C14-N10	-3.88	123.84	127.84
3	B	568	D16	C15-C14-S13	-3.57	107.94	111.97
2	A	565	UMP	O4'-C1'-N1	3.41	113.91	107.86
2	B	567	UMP	O4-C4-C5	-3.30	119.48	125.16
2	B	567	UMP	C6-N1-C2	3.28	124.99	121.00
3	A	566	D16	C8A-C4A-C4	-3.27	116.58	120.11
2	B	567	UMP	C6-C5-C4	-3.18	115.47	119.53
2	A	565	UMP	C1'-N1-C6	-3.11	115.42	121.53
2	B	567	UMP	O4'-C1'-N1	3.08	113.34	107.86
3	B	568	D16	C8A-C4A-C4	-2.91	116.97	120.11
2	A	565	UMP	C6-C5-C4	-2.86	115.88	119.53
3	A	566	D16	C-C11-S13	2.77	124.42	117.18
3	A	566	D16	CT-CA-N	-2.76	104.16	110.57
2	A	565	UMP	O4-C4-C5	-2.57	120.72	125.16
3	B	568	D16	CB-CG-CD	2.53	119.24	112.49
3	A	566	D16	CM2-C2-N1	2.47	121.18	116.41
3	B	568	D16	CM2-C2-N1	2.45	121.13	116.41
2	B	567	UMP	O4-C4-N3	2.40	122.75	119.27
2	A	565	UMP	C5-C4-N3	2.35	118.08	114.80
2	B	567	UMP	C1'-N1-C2	2.34	122.24	117.66
3	A	566	D16	CB-CA-CT	-2.30	104.90	110.35
3	B	568	D16	N1-C2-N3	-2.24	120.06	122.96
2	A	565	UMP	C6-N1-C2	2.18	123.65	121.00
3	B	568	D16	C11-S13-C14	2.18	93.61	91.43
2	B	567	UMP	C5-C4-N3	2.12	117.77	114.80
3	A	566	D16	C6-C9-N10	2.11	117.00	113.02
3	B	568	D16	C16-C11-C	-2.10	121.49	129.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	568	D16	C16-C15-C14	2.06	115.02	112.01
3	B	568	D16	OE2-CD-CG	2.00	120.33	114.00

There are no chirality outliers.

All (10) torsion outliers are listed below:

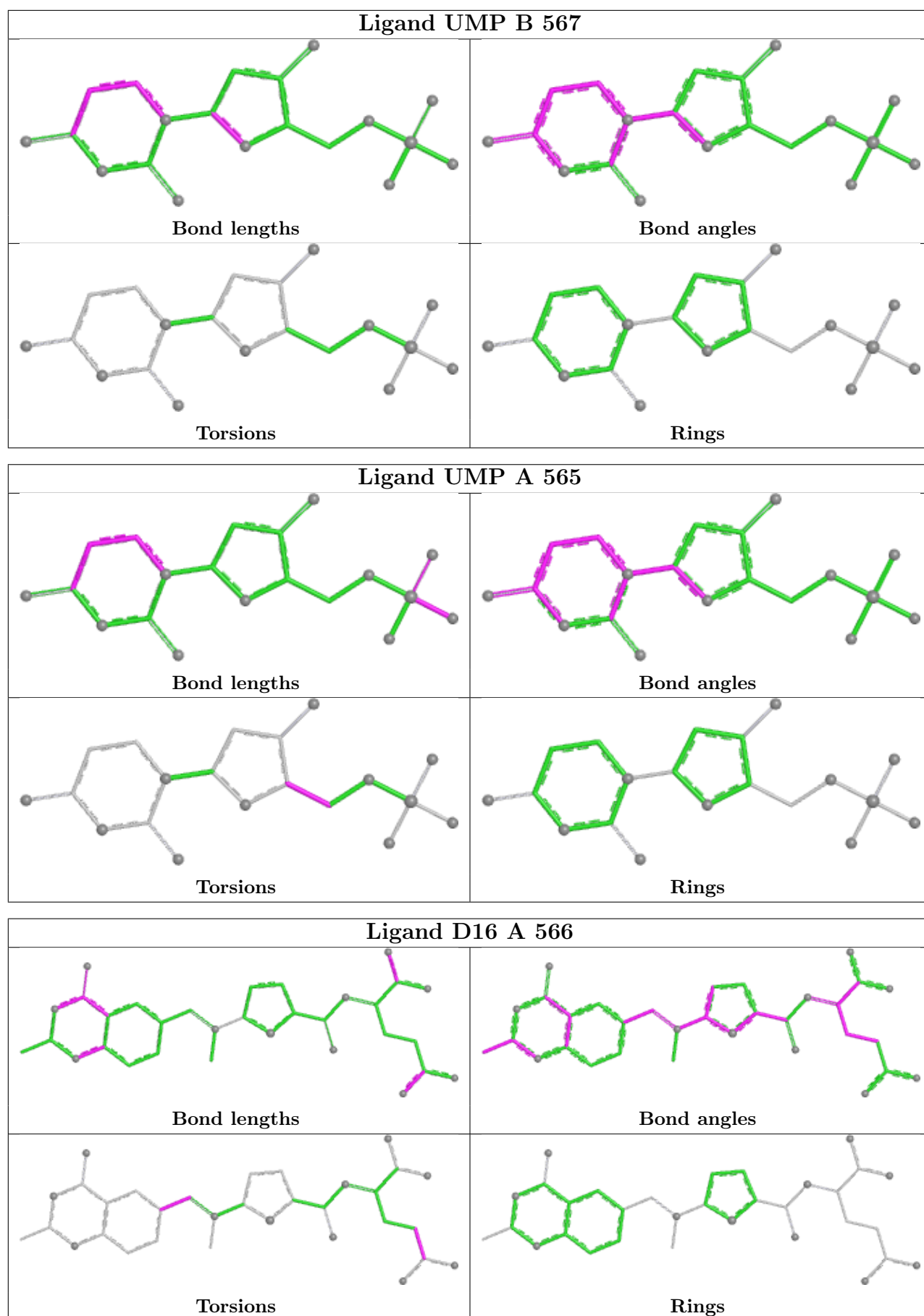
Mol	Chain	Res	Type	Atoms
3	B	568	D16	N-CA-CB-CG
3	B	568	D16	CT-CA-CB-CG
3	A	566	D16	OE1-CD-CG-CB
3	A	566	D16	OE2-CD-CG-CB
3	B	568	D16	C5-C6-C9-N10
3	B	568	D16	OE1-CD-CG-CB
3	A	566	D16	C5-C6-C9-N10
3	B	568	D16	OE2-CD-CG-CB
2	A	565	UMP	O4'-C4'-C5'-O5'
3	B	568	D16	CA-CB-CG-CD

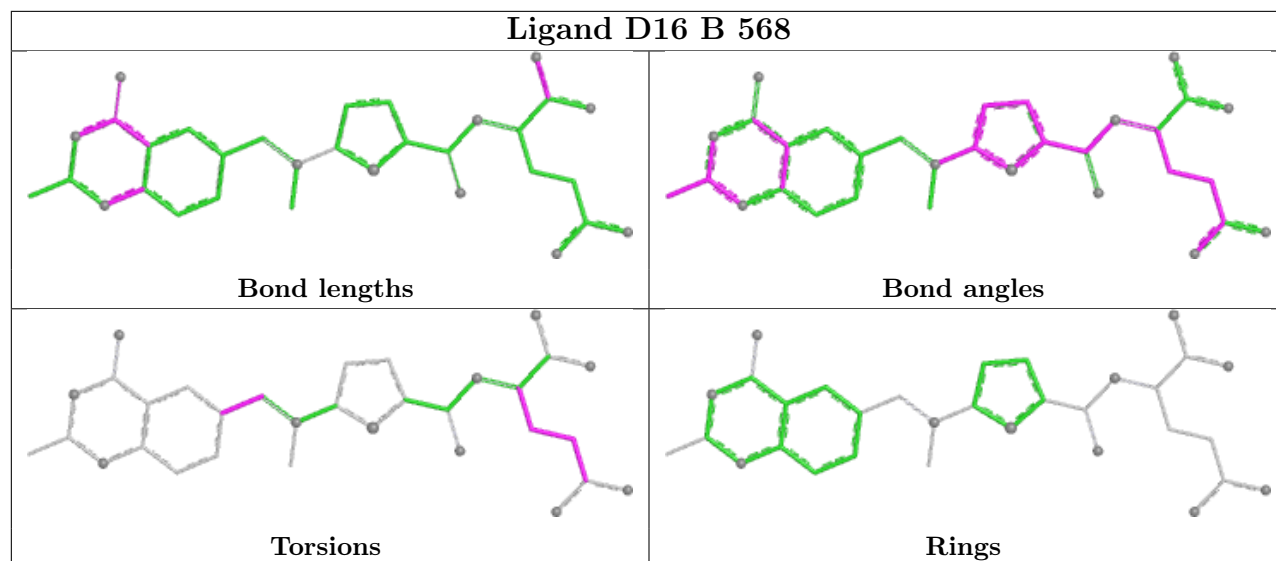
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	565	UMP	1	0
3	B	568	D16	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.