



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:07 AM UTC

PDB ID : 6FD2 / pdb\_00006fd2  
Title : Radical SAM 1,2-diol dehydratase AprD4 in complex with its substrate paromamine  
Authors : Liu, W.Q.; Amara, P.; Mouesca, J.M.; Ji, X.; Renoux, O.; Martin, L.; Zhang, C.; Zhang, Q.; Nicolet, Y.  
Deposited on : 2017-12-21  
Resolution : 2.55 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.

The types of validation reports are described at

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

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

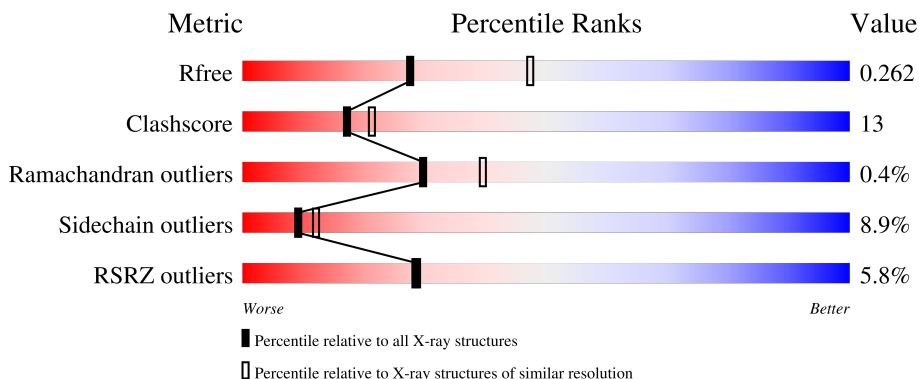
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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	457	
1	B	457	

## 2 Entry composition [i](#)

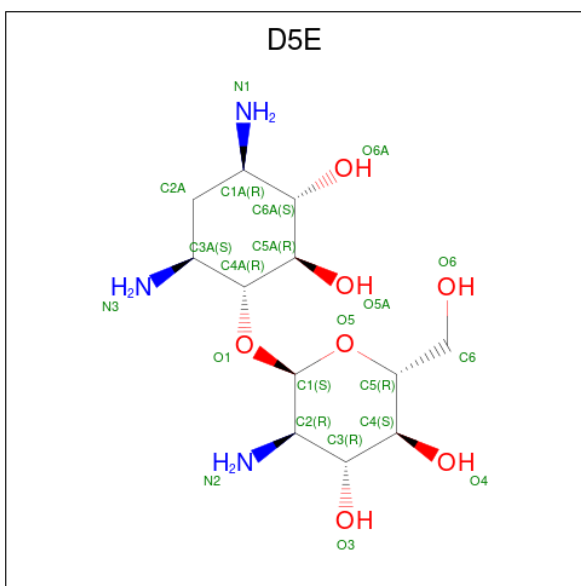
There are 6 unique types of molecules in this entry. The entry contains 7161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative apramycin biosynthetic oxidoreductase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	453	Total	C	N	O	S	0	0	0
			3502	2213	618	654	17			
1	A	454	Total	C	N	O	S	0	0	0
			3508	2218	619	653	18			

- Molecule 2 is paromamine (CCD ID: D5E) (formula:  $C_{12}H_{25}N_3O_7$ ).



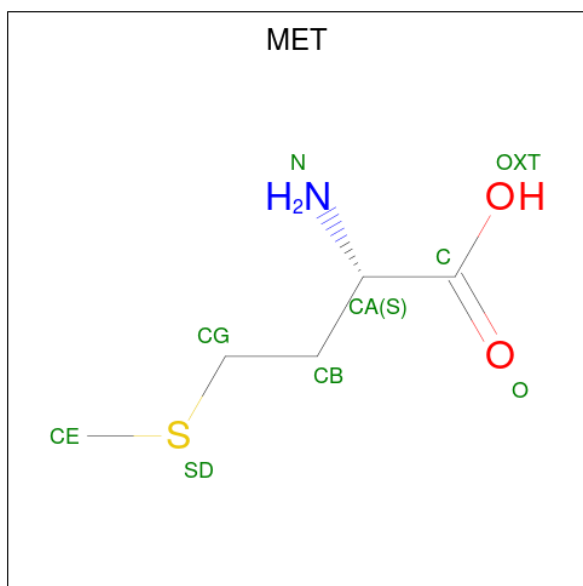
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	Total	C	N	O	0	0
			22	12	3	7		
2	A	1	Total	C	N	O	0	0
			22	12	3	7		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



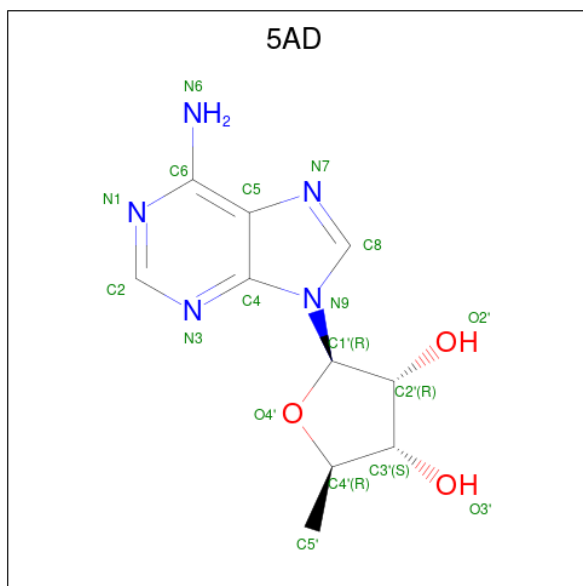
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is METHIONINE (CCD ID: MET) (formula:  $C_5H_{11}NO_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			6	3	1	2		
4	A	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 5 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	A	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	24	Total	O	0	0
			24	24		
6	A	19	Total	O	0	0
			19	19		



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.82Å 121.82Å 233.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 – 2.55 48.08 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.08-2.55) 99.2 (48.08-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (1.11rc3_2542: ???)	Depositor
R, $R_{free}$	0.228 , 0.263 0.231 , 0.262	Depositor DCC
$R_{free}$ test set	3207 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7161	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 5AD, D5E

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	0.25	0/3589	0.58	0/4883
1	B	0.24	0/3583	0.54	0/4876
All	All	0.24	0/7172	0.56	0/9759

There are no bond length outliers.

There are no bond angle outliers.

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	3508	0	3462	114	0
1	B	3502	0	3453	65	0
2	A	22	0	0	0	0
2	B	22	0	0	1	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
4	A	6	0	1	0	0
4	B	6	0	1	0	0
5	A	18	0	13	1	0
5	B	18	0	13	0	0
6	A	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	24	0	0	0	0
All	All	7161	0	6943	177	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 13.

All (177) 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:444:GLU:OE2	1:A:448:ARG:NH2	2.06	0.87
1:B:354:ARG:HH21	1:B:456:ASP:HA	1.41	0.84
1:A:23:GLN:HE22	1:A:41:LEU:H	1.26	0.83
1:A:312:ASP:OD1	1:A:351:ARG:NH1	2.17	0.78
1:A:23:GLN:NE2	1:A:39:PHE:O	2.18	0.77
1:B:280:GLU:HG3	1:B:303:GLU:HB2	1.70	0.74
1:B:405:THR:HG22	1:B:407:HIS:H	1.51	0.74
1:A:394:LYS:NZ	1:A:414:ASP:OD1	2.21	0.74
1:A:113:ARG:HH22	1:A:166:PRO:HB3	1.56	0.70
1:A:76:PRO:HB3	1:A:103:GLY:HA3	1.75	0.69
1:A:227:TYR:O	1:A:260:ARG:NH2	2.24	0.68
1:B:25:THR:OG1	1:B:250:ARG:NH2	2.27	0.68
1:A:207:PRO:HD3	1:A:224:ILE:HD12	1.76	0.67
1:B:354:ARG:NH1	1:B:420:ASP:OD1	2.27	0.67
1:A:456:ASP:OD2	1:A:456:ASP:N	2.28	0.66
1:B:387:LEU:HD11	1:B:411:MET:HE1	1.76	0.66
1:A:115:PRO:HB3	1:A:158:LEU:HD21	1.78	0.65
1:B:94:GLU:HG2	1:B:124:ARG:HH21	1.63	0.64
1:B:149:VAL:O	1:B:162:ARG:NH2	2.31	0.63
1:B:312:ASP:OD2	1:B:351:ARG:NH1	2.28	0.63
1:A:113:ARG:NH1	1:A:218:LEU:O	2.32	0.63
1:B:52:VAL:HG12	1:B:175:PRO:HD2	1.81	0.62
1:B:227:TYR:O	1:B:260:ARG:NH2	2.28	0.61
1:A:225:ARG:HA	1:A:225:ARG:HH11	1.65	0.61
1:A:160:ASP:C	1:A:162:ARG:H	2.10	0.59
1:A:350:PRO:O	1:A:351:ARG:HB2	2.01	0.59
1:A:79:THR:HG21	1:A:143:LEU:HD21	1.83	0.59
1:A:84:VAL:HG11	1:A:89:LEU:HD13	1.84	0.59
1:A:365:LEU:HD13	1:A:442:ARG:HD3	1.84	0.59
1:A:402:ASN:OD1	1:A:402:ASN:N	2.30	0.58
1:B:113:ARG:HH22	1:B:134:GLU:CD	2.11	0.58
1:A:117:GLN:OE1	1:A:401:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:HA	1:A:124:ARG:HH21	1.69	0.57
1:A:382:TYR:OH	1:A:406:SER:OG	2.20	0.57
1:A:416:LEU:HD23	1:A:421:LEU:HG	1.85	0.57
1:A:427:PHE:CE2	1:A:449:VAL:HG22	2.39	0.57
1:A:14:PRO:O	1:A:24:ARG:NH2	2.38	0.57
1:A:9:VAL:HB	1:A:60:ILE:HD13	1.87	0.57
1:B:441:GLU:OE1	1:B:441:GLU:N	2.36	0.57
1:A:18:PHE:CD1	1:A:33:VAL:HG11	2.40	0.57
1:A:160:ASP:HB3	1:A:162:ARG:HD2	1.87	0.57
1:B:335:ARG:NH1	1:B:373:GLU:OE1	2.38	0.56
1:A:365:LEU:HD21	1:A:431:LEU:HD11	1.86	0.56
1:A:225:ARG:HA	1:A:225:ARG:NH1	2.20	0.56
1:A:225:ARG:NH1	1:A:226:THR:H	2.03	0.56
1:A:423:ARG:O	1:A:427:PHE:HD1	1.88	0.56
1:B:403:ALA:C	1:B:405:THR:H	2.13	0.56
1:A:108:ALA:O	1:A:131:LEU:N	2.32	0.55
1:B:181:LEU:HD22	1:A:223:LYS:HE2	1.87	0.55
1:B:418:ILE:O	1:B:422:GLU:HB2	2.07	0.55
1:A:423:ARG:HG3	1:A:427:PHE:HE1	1.71	0.55
1:A:434:VAL:HG11	1:A:442:ARG:HA	1.89	0.55
1:A:86:LEU:HA	1:A:112:ILE:HD11	1.88	0.55
1:A:399:GLY:HA3	1:A:410:VAL:HG13	1.87	0.55
1:B:50:ALA:O	1:B:54:ARG:HB2	2.07	0.55
1:A:138:PHE:CD2	1:A:150:PRO:HD2	2.41	0.55
1:A:445:PHE:O	1:A:449:VAL:HG23	2.07	0.55
1:B:425:SER:O	1:B:428:VAL:HG22	2.07	0.54
1:B:20:ARG:NH2	1:B:186:PRO:O	2.37	0.54
1:B:369:LEU:HD23	1:B:374:PHE:HB3	1.90	0.54
1:A:305:GLY:HA2	1:A:344:LEU:HB2	1.90	0.54
1:B:328:ARG:NH2	1:B:366:GLU:OE1	2.41	0.54
1:B:174:GLU:O	1:B:231:ARG:NH1	2.40	0.54
1:A:22:LEU:HA	1:A:33:VAL:HG13	1.91	0.53
1:A:442:ARG:HB3	1:A:442:ARG:HH11	1.73	0.53
1:B:412:HIS:HB2	1:B:416:LEU:O	2.07	0.53
1:A:34:CYS:SG	1:A:35:LYS:N	2.82	0.53
1:A:255:SER:OG	1:A:285:ARG:O	2.25	0.53
1:A:113:ARG:NH2	1:A:166:PRO:HB3	2.24	0.53
1:B:334:ALA:HB3	1:B:341:LEU:HD11	1.90	0.53
1:A:23:GLN:HE22	1:A:41:LEU:N	2.02	0.52
1:B:348:GLY:O	1:B:379:ILE:HG21	2.10	0.52
1:B:33:VAL:HB	1:B:405:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLU:HG2	1:B:124:ARG:NH2	2.25	0.52
1:A:119:ARG:HA	1:A:122:PHE:HD1	1.73	0.52
1:B:189:PHE:CE1	1:B:191:PRO:HG2	2.46	0.51
1:A:146:ASP:OD1	1:A:147:HIS:N	2.44	0.51
1:B:335:ARG:HH12	1:B:373:GLU:CD	2.18	0.50
1:A:403:ALA:HB1	1:A:408:ASN:HD22	1.76	0.50
1:B:9:VAL:O	1:B:60:ILE:HA	2.11	0.50
1:B:416:LEU:HD23	1:B:421:LEU:HG	1.94	0.50
1:A:291:VAL:HG13	1:A:339:LEU:HD22	1.93	0.50
1:A:423:ARG:HG3	1:A:427:PHE:CE1	2.46	0.49
1:A:44:LEU:O	1:A:48:ARG:HG3	2.12	0.49
1:A:6:LEU:HB2	1:A:56:ASP:O	2.12	0.49
1:B:434:VAL:HG12	1:B:442:ARG:HG2	1.93	0.49
1:A:248:VAL:HG13	1:A:278:TRP:HB3	1.94	0.49
1:B:444:GLU:O	1:B:448:ARG:HG3	2.12	0.49
1:A:399:GLY:CA	1:A:410:VAL:HG13	2.42	0.49
1:B:48:ARG:NH1	1:B:227:TYR:OH	2.46	0.49
1:B:378:VAL:O	1:B:380:THR:HG23	2.13	0.49
1:B:405:THR:C	1:B:407:HIS:H	2.20	0.49
1:A:23:GLN:NE2	1:A:40:LEU:HA	2.28	0.49
1:A:154:THR:OG1	1:A:156:ASP:N	2.32	0.48
1:A:24:ARG:NH1	1:A:83:HIS:O	2.46	0.48
1:B:184:HIS:O	1:B:196:GLY:HA2	2.14	0.48
1:A:5:ARG:O	1:A:5:ARG:NH2	2.43	0.48
1:A:207:PRO:HD3	1:A:224:ILE:CD1	2.43	0.48
1:A:256:PHE:HA	1:A:285:ARG:HD3	1.95	0.48
1:A:94:GLU:OE2	1:A:124:ARG:NH2	2.47	0.48
1:A:162:ARG:HD3	1:A:163:HIS:CE1	2.49	0.47
1:A:427:PHE:CD2	1:A:449:VAL:HG22	2.49	0.47
1:B:86:LEU:HB3	1:B:87:PRO:HD3	1.97	0.47
1:B:236:PHE:HB3	1:B:273:THR:HG21	1.95	0.47
1:A:119:ARG:HA	1:A:122:PHE:CD1	2.49	0.47
1:A:190:PRO:HB3	1:A:194:ARG:NH2	2.29	0.47
1:A:309:GLY:HA3	1:A:360:THR:HA	1.97	0.47
1:A:412:HIS:HB2	1:A:416:LEU:O	2.15	0.47
1:A:105:ARG:HD3	1:A:107:TYR:HE1	1.79	0.47
1:A:425:SER:O	1:A:428:VAL:HG22	2.15	0.47
1:B:119:ARG:O	1:B:123:GLU:HG2	2.16	0.47
1:A:14:PRO:HB3	1:A:95:ARG:HG2	1.97	0.47
1:A:440:ALA:O	1:A:444:GLU:HB2	2.15	0.46
1:A:176:LEU:HD22	1:A:235:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HG22	1:A:175:PRO:HD2	1.96	0.46
1:B:48:ARG:NH1	1:B:174:GLU:OE2	2.48	0.46
1:B:320:LYS:NZ	3:B:502:SF4:S2	2.89	0.46
1:A:354:ARG:NH1	1:A:457:ALA:HB2	2.31	0.46
1:A:381:PRO:HG3	1:A:411:MET:SD	2.56	0.46
1:A:405:THR:O	1:A:406:SER:HB2	2.16	0.45
1:B:23:GLN:OE1	1:B:40:LEU:HA	2.17	0.45
1:A:5:ARG:O	1:A:5:ARG:HD3	2.17	0.45
1:A:154:THR:HG1	1:A:156:ASP:H	1.57	0.45
1:A:160:ASP:O	1:A:162:ARG:N	2.50	0.45
1:A:21:ASP:O	1:A:33:VAL:HA	2.16	0.45
1:A:84:VAL:CG1	1:A:89:LEU:HD13	2.47	0.45
1:A:97:ALA:O	1:A:100:ARG:HB3	2.17	0.45
1:A:206:CYS:O	1:A:222:ARG:HA	2.16	0.45
1:B:128:GLU:N	1:B:128:GLU:OE1	2.50	0.45
1:A:354:ARG:HH12	1:A:457:ALA:HB2	1.82	0.45
1:A:378:VAL:HG21	1:A:408:ASN:C	2.41	0.45
1:B:153:VAL:HG22	1:B:163:HIS:CD2	2.52	0.45
1:A:20:ARG:NH2	1:A:186:PRO:O	2.50	0.44
1:A:135:SER:HB3	1:A:151:GLY:HA3	1.99	0.44
1:A:160:ASP:C	1:A:162:ARG:N	2.74	0.44
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.87	0.44
1:B:58:ASP:O	1:A:225:ARG:NH2	2.51	0.44
1:B:405:THR:C	1:B:407:HIS:N	2.76	0.43
1:B:403:ALA:C	1:B:405:THR:N	2.76	0.43
1:A:354:ARG:NH1	1:A:452:TRP:O	2.44	0.43
1:B:189:PHE:HB2	1:B:197:ILE:HG13	2.00	0.43
1:B:33:VAL:O	1:B:405:THR:HG23	2.18	0.43
1:A:307:GLU:OE1	5:A:504:5AD:O2'	2.33	0.43
1:B:279:CYS:SG	1:B:302:VAL:HG12	2.58	0.43
1:A:188:MET:HG3	1:A:194:ARG:HA	2.00	0.43
1:A:370:ALA:HB3	1:A:373:GLU:HG3	2.01	0.42
1:B:11:LEU:HB3	1:B:46:LEU:HD22	2.01	0.42
1:B:22:LEU:HD13	1:B:24:ARG:HG2	2.02	0.42
1:A:118:TRP:CZ3	1:A:153:VAL:HG11	2.55	0.42
1:A:132:LEU:O	1:A:135:SER:OG	2.30	0.42
1:A:433:ALA:HA	1:A:436:LYS:HD3	2.00	0.42
1:B:169:GLY:O	1:B:225:ARG:NH2	2.53	0.42
1:A:48:ARG:O	1:A:52:VAL:HG23	2.19	0.42
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.84	0.42
1:A:182:VAL:HG22	1:A:184:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD21	1:A:290:VAL:HG22	2.01	0.41
1:B:278:TRP:HE1	1:B:303:GLU:HG3	1.85	0.41
1:B:288:GLU:HG2	1:B:333:VAL:CG1	2.50	0.41
1:B:288:GLU:HG2	1:B:333:VAL:HG11	2.02	0.41
1:A:365:LEU:HB3	1:A:442:ARG:HE	1.86	0.41
1:A:109:TYR:HA	1:A:131:LEU:O	2.21	0.41
1:A:154:THR:OG1	1:A:156:ASP:HB2	2.21	0.41
1:A:309:GLY:HA2	1:A:324:LEU:HD21	2.03	0.41
1:B:283:ILE:HG13	1:B:304:VAL:HB	2.03	0.41
1:A:89:LEU:O	1:A:89:LEU:HD12	2.21	0.41
1:B:256:PHE:HA	1:B:285:ARG:HD3	2.03	0.41
1:A:119:ARG:O	1:A:123:GLU:HG2	2.20	0.41
1:A:138:PHE:HB2	1:A:149:VAL:HG23	2.03	0.41
1:B:153:VAL:HG22	1:B:163:HIS:NE2	2.37	0.40
1:A:4:MET:SD	1:A:5:ARG:HG3	2.62	0.40
1:A:412:HIS:HB3	1:A:418:ILE:HG22	2.02	0.40
1:B:197:ILE:HB	1:B:246:ALA:HB3	2.03	0.40
1:B:280:GLU:OE1	2:B:501:D5E:N2	2.54	0.40
1:B:427:PHE:CE2	1:B:449:VAL:HG22	2.56	0.40
1:A:168:PHE:HD1	1:A:168:PHE:HA	1.75	0.40
1:A:434:VAL:CG1	1:A:442:ARG:HA	2.50	0.40
1:A:40:LEU:HD13	1:A:188:MET:HE3	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	452/457 (99%)	423 (94%)	26 (6%)	3 (1%)	18	25
1	B	451/457 (99%)	420 (93%)	30 (7%)	1 (0%)	43	56
All	All	903/914 (99%)	843 (93%)	56 (6%)	4 (0%)	30	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	ARG
1	B	455	GLY
1	A	350	PRO
1	A	161	PRO

### 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	372/376 (99%)	327 (88%)	45 (12%)	<b>5</b> <b>5</b>
1	B	372/376 (99%)	351 (94%)	21 (6%)	19 29
All	All	744/752 (99%)	678 (91%)	66 (9%)	<b>9</b> <b>12</b>

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	ARG
1	B	11	LEU
1	B	12	VAL
1	B	22	LEU
1	B	30	LEU
1	B	54	ARG
1	B	132	LEU
1	B	137	SER
1	B	159	LEU
1	B	197	ILE
1	B	210	CYS
1	B	229	VAL
1	B	230	GLU
1	B	250	ARG
1	B	280	GLU
1	B	354	ARG
1	B	369	LEU
1	B	373	GLU
1	B	401	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	405	THR
1	B	418	ILE
1	A	4	MET
1	A	5	ARG
1	A	6	LEU
1	A	12	VAL
1	A	33	VAL
1	A	34	CYS
1	A	71	VAL
1	A	82	CYS
1	A	96	LEU
1	A	127	CYS
1	A	132	LEU
1	A	137	SER
1	A	140	ARG
1	A	143	LEU
1	A	149	VAL
1	A	153	VAL
1	A	154	THR
1	A	156	ASP
1	A	159	LEU
1	A	162	ARG
1	A	168	PHE
1	A	182	VAL
1	A	194	ARG
1	A	210	CYS
1	A	224	ILE
1	A	225	ARG
1	A	245	THR
1	A	259	ASP
1	A	269	LYS
1	A	344	LEU
1	A	347	ILE
1	A	352	GLU
1	A	392	VAL
1	A	394	LYS
1	A	402	ASN
1	A	416	LEU
1	A	418	ILE
1	A	422	GLU
1	A	425	SER
1	A	436	LYS

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Mol	Chain	Res	Type
1	A	441	GLU
1	A	442	ARG
1	A	444	GLU
1	A	448	ARG
1	A	456	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	HIS
1	B	389	GLN
1	A	23	GLN
1	A	102	GLN
1	A	408	ASN
1	A	446	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](#)

8 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
5	5AD	B	504	-	20,20,20	1.18	2 (10%)	28,30,30	2.30	10 (35%)
2	D5E	B	501	-	23,23,23	0.82	0	32,34,34	0.88	1 (3%)
4	MET	A	503	3	5,5,8	1.38	2 (40%)	6,6,9	1.36	1 (16%)
2	D5E	A	501	-	23,23,23	0.77	0	32,34,34	0.87	0
5	5AD	A	504	-	20,20,20	1.12	2 (10%)	28,30,30	2.26	10 (35%)
3	SF4	B	502	4,1	0,12,12	-	-	-	-	-
3	SF4	A	502	4,1	0,12,12	-	-	-	-	-
4	MET	B	503	3	5,5,8	1.40	2 (40%)	6,6,9	1.31	1 (16%)

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
5	5AD	B	504	-	-	0/4/20/20	0/3/3/3
2	D5E	B	501	-	-	2/6/46/46	0/2/2/2
4	MET	A	503	3	-	0/4/4/8	-
2	D5E	A	501	-	-	1/6/46/46	0/2/2/2
5	5AD	A	504	-	-	0/4/20/20	0/3/3/3
3	SF4	B	502	4,1	-	-	0/6/5/5
3	SF4	A	502	4,1	-	-	0/6/5/5
4	MET	B	503	3	-	0/4/4/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	504	5AD	C2-N3	2.79	1.38	1.33
5	B	504	5AD	C2-N1	2.53	1.38	1.33
5	A	504	5AD	C2-N3	2.49	1.38	1.33
5	A	504	5AD	C2-N1	2.41	1.38	1.33
4	A	503	MET	OXT-C	-2.17	1.23	1.30
4	B	503	MET	OXT-C	-2.15	1.23	1.30
4	A	503	MET	CA-C	-2.10	1.52	1.54
4	B	503	MET	CA-C	-2.09	1.52	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	5AD	N3-C2-N1	-5.59	120.12	128.58
5	B	504	5AD	C5-C4-N3	-4.96	119.88	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	5AD	N3-C2-N1	-4.89	121.18	128.58
5	A	504	5AD	C5-C4-N3	-4.84	120.06	126.72
5	B	504	5AD	C5'-C4'-C3'	-3.93	111.57	115.70
5	A	504	5AD	N9-C8-N7	-3.77	108.58	113.94
5	B	504	5AD	N3-C4-N9	3.68	133.43	127.17
5	B	504	5AD	N9-C8-N7	-3.57	108.86	113.94
5	A	504	5AD	N3-C4-N9	3.46	133.06	127.17
5	A	504	5AD	C2-N3-C4	3.44	120.24	111.83
5	A	504	5AD	C5-N7-C8	3.37	108.75	103.45
5	B	504	5AD	C2-N3-C4	3.24	119.74	111.83
5	B	504	5AD	C5-N7-C8	3.18	108.45	103.45
5	A	504	5AD	C5'-C4'-C3'	-3.05	112.49	115.70
2	B	501	D5E	O5-C5-C6	2.62	112.92	106.44
5	B	504	5AD	C2'-C1'-N9	-2.43	107.27	113.30
5	B	504	5AD	C3'-C2'-C1'	2.41	106.03	101.46
5	B	504	5AD	C6-C5-C4	2.35	120.38	117.18
4	A	503	MET	OXT-C-CA	2.32	121.78	113.79
4	B	503	MET	OXT-C-CA	2.28	121.64	113.79
5	A	504	5AD	C4-C5-N7	-2.22	108.05	110.58
5	A	504	5AD	C3'-C2'-C1'	2.14	105.51	101.46
5	A	504	5AD	C6-C5-C4	2.12	120.08	117.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	D5E	C5A-C4A-O1-C1
2	A	501	D5E	C5A-C4A-O1-C1
2	B	501	D5E	O5-C1-O1-C4A

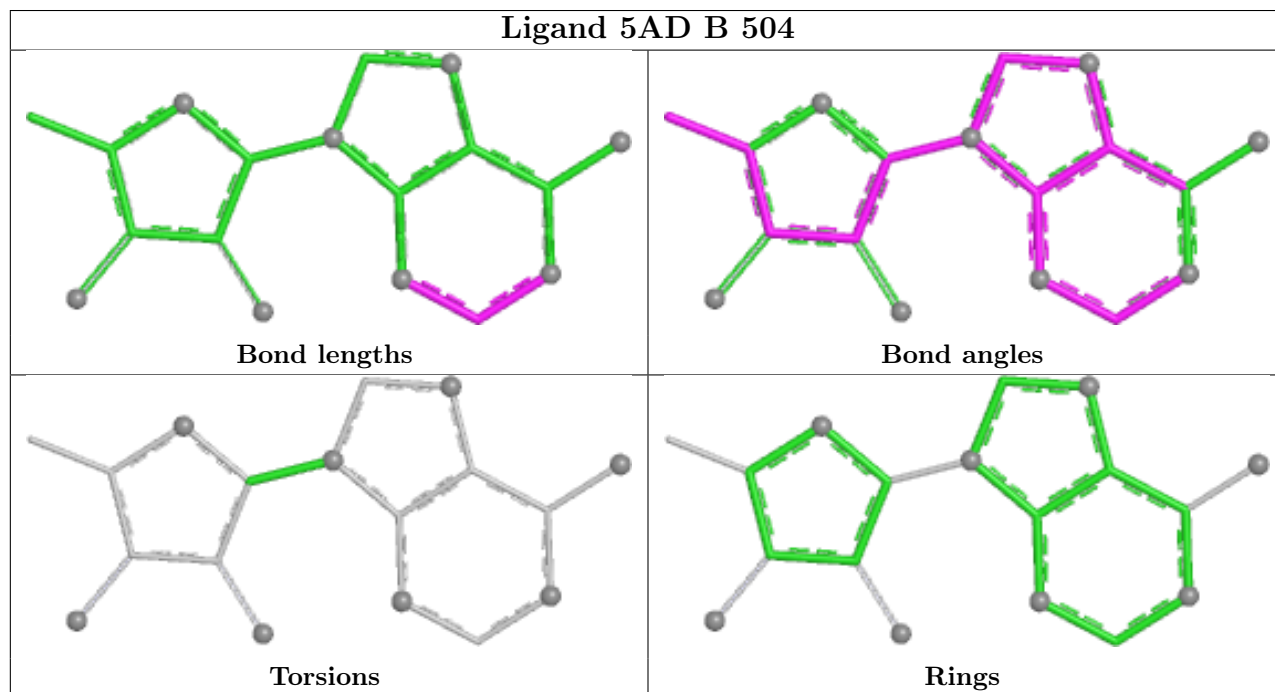
There are no ring outliers.

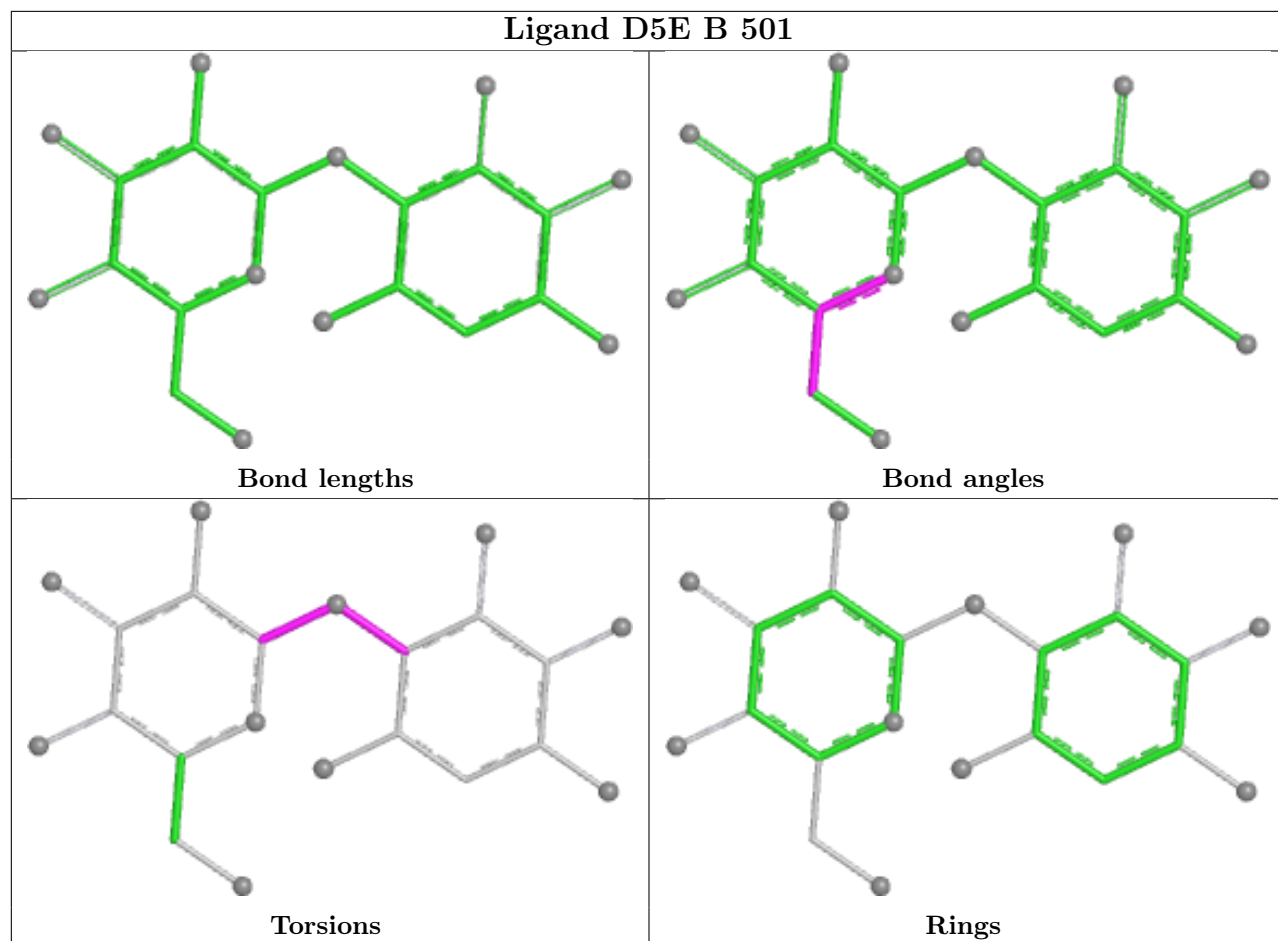
3 monomers are involved in 3 short contacts:

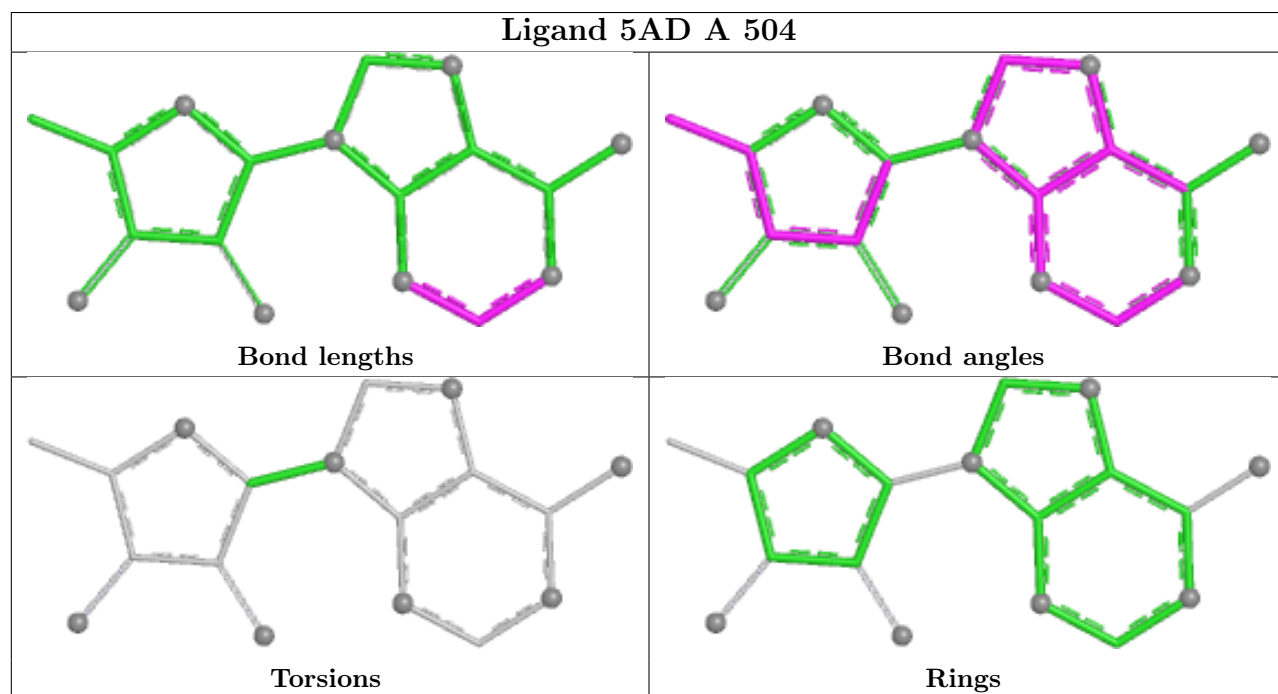
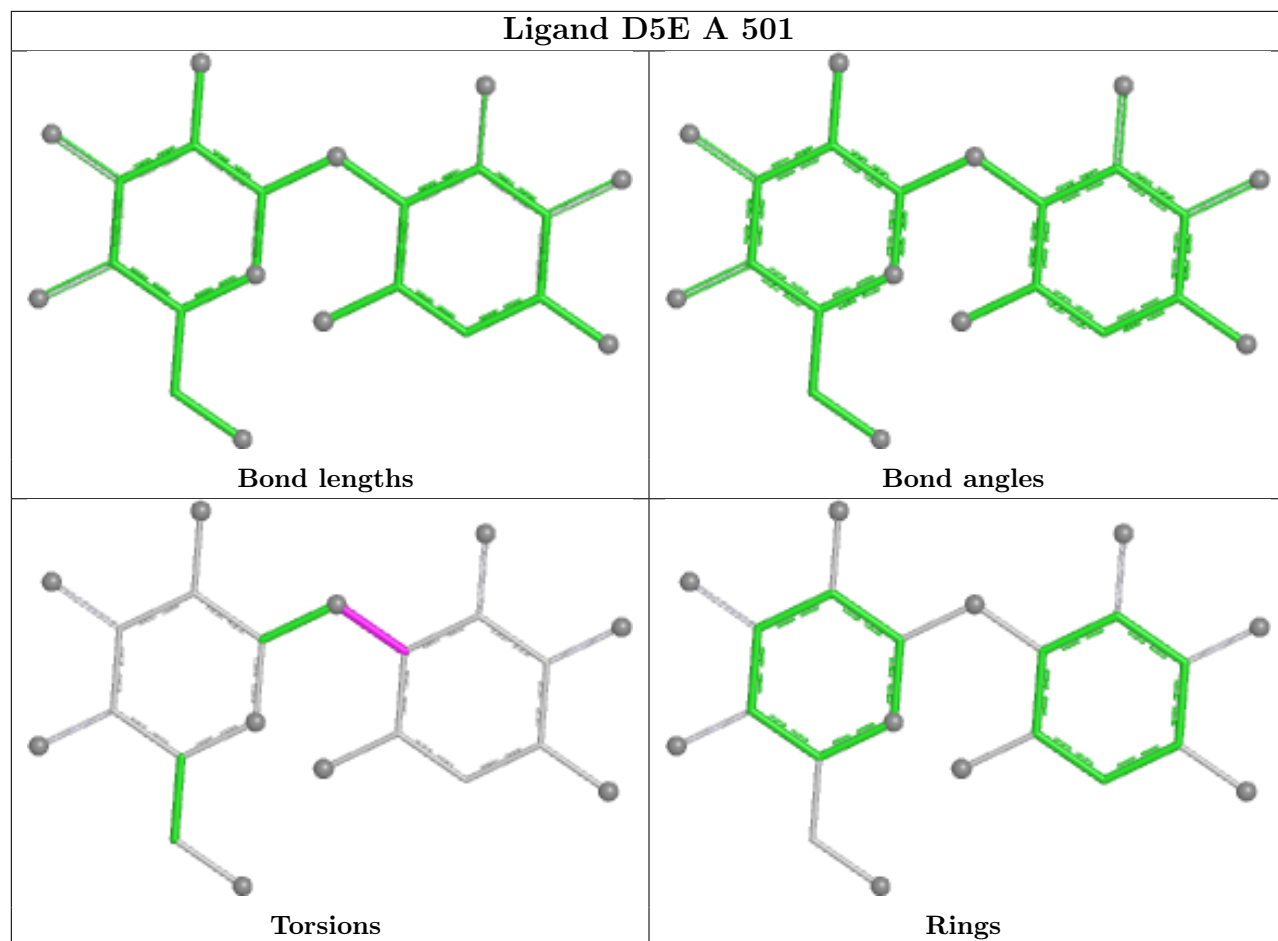
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	D5E	1	0
5	A	504	5AD	1	0
3	B	502	SF4	1	0

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, 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	454/457 (99%)	0.51	46 (10%) <span style="border: 1px solid red; padding: 2px;">12</span> <span style="border: 1px solid red; padding: 2px;">11</span>	55, 95, 161, 195	0
1	B	453/457 (99%)	0.09	7 (1%) <span style="border: 1px solid blue; padding: 2px;">72</span> <span style="border: 1px solid blue; padding: 2px;">73</span>	53, 85, 130, 173	0
All	All	907/914 (99%)	0.30	53 (5%) <span style="border: 1px solid red; padding: 2px;">29</span> <span style="border: 1px solid red; padding: 2px;">28</span>	53, 88, 151, 195	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	ASP	7.3
1	A	142	ALA	4.9
1	A	125	GLY	4.2
1	B	159	LEU	3.8
1	A	158	LEU	3.8
1	A	4	MET	3.7
1	A	457	ALA	3.6
1	A	137	SER	3.5
1	A	80	VAL	3.3
1	A	115	PRO	3.3
1	B	457	ALA	3.1
1	A	35	LYS	3.1
1	A	150	PRO	3.1
1	A	116	ALA	3.0
1	A	157	SER	3.0
1	B	167	ALA	2.9
1	A	153	VAL	2.8
1	A	139	ALA	2.8
1	A	90	LEU	2.7
1	A	167	ALA	2.7
1	A	159	LEU	2.6
1	A	440	ALA	2.6
1	A	144	ALA	2.5
1	A	96	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	THR	2.4
1	A	78	THR	2.4
1	A	72	PRO	2.4
1	B	5	ARG	2.4
1	A	55	GLU	2.4
1	A	87	PRO	2.3
1	B	383	PRO	2.3
1	A	400	SER	2.3
1	A	58	ASP	2.3
1	B	280	GLU	2.3
1	A	141	ALA	2.3
1	B	405	THR	2.3
1	A	406	SER	2.3
1	A	6	LEU	2.3
1	A	149	VAL	2.2
1	A	225	ARG	2.2
1	A	107	TYR	2.2
1	A	75	GLU	2.2
1	A	305	GLY	2.2
1	A	93	ALA	2.2
1	A	121	LEU	2.2
1	A	455	GLY	2.1
1	A	418	ILE	2.1
1	A	164	HIS	2.1
1	A	407	HIS	2.1
1	A	120	THR	2.0
1	A	154	THR	2.0
1	A	436	LYS	2.0
1	A	38	ASP	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 oligosaccharides in this entry.

## 6.4 Ligands

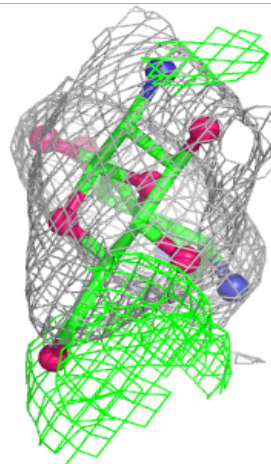
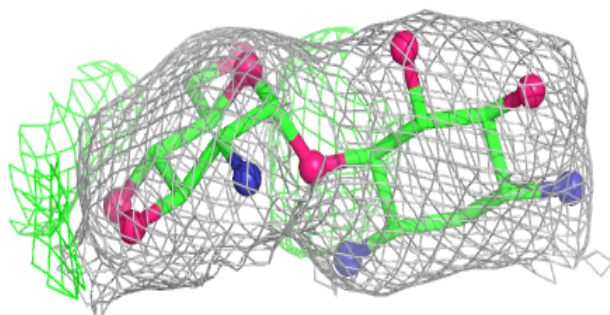
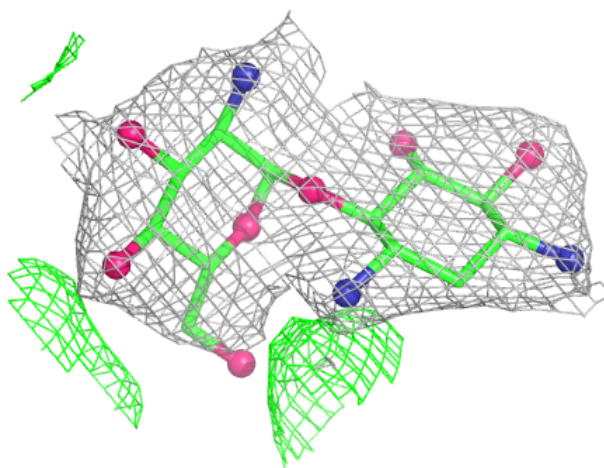
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	D5E	A	501	22/22	0.93	0.10	63,77,95,114	0
2	D5E	B	501	22/22	0.94	0.09	65,75,83,88	0
4	MET	B	503	6/9	0.94	0.14	63,76,89,96	0
4	MET	A	503	6/9	0.95	0.10	49,55,59,62	0
5	5AD	B	504	18/18	0.95	0.11	52,86,99,103	0
5	5AD	A	504	18/18	0.95	0.12	74,86,98,99	0
3	SF4	B	502	8/8	0.99	0.06	58,67,89,95	0
3	SF4	A	502	8/8	0.99	0.04	58,65,79,90	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.

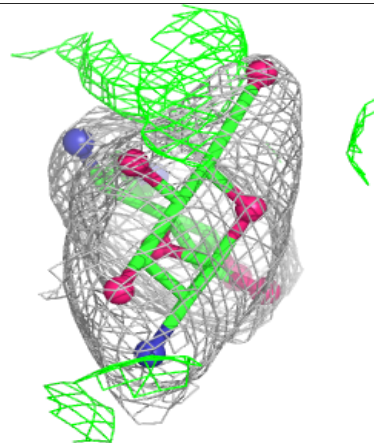
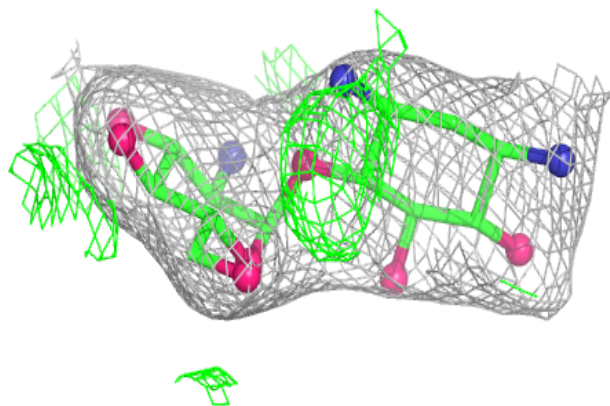
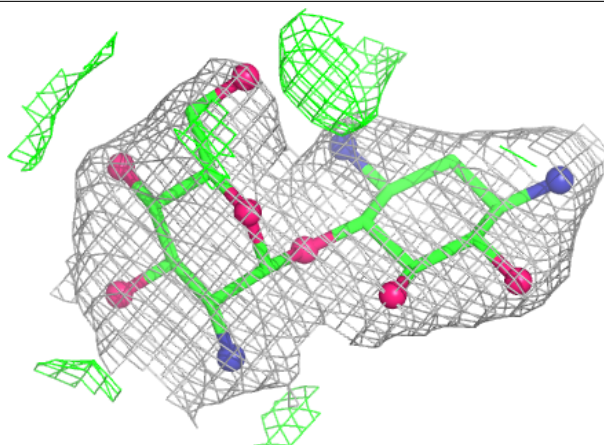
**Electron density around D5E A 501:**

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



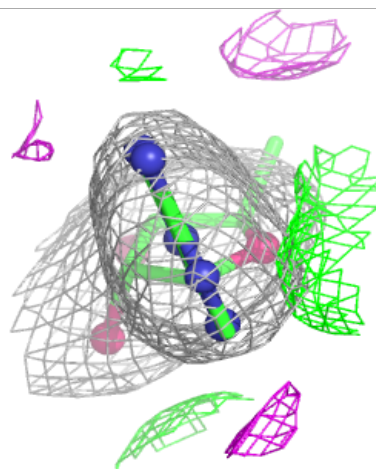
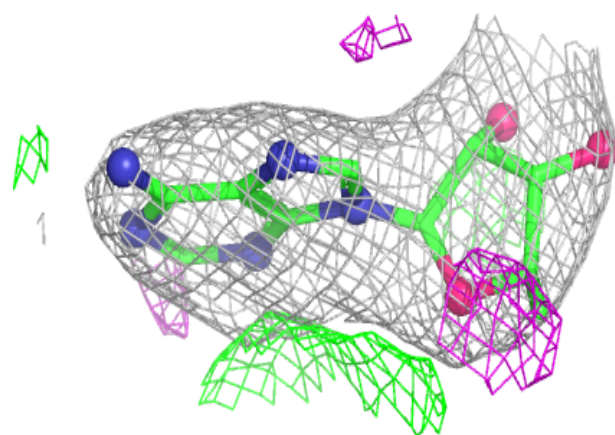
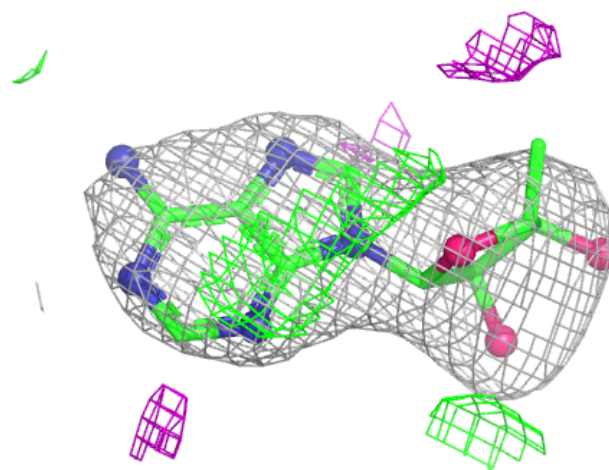
**Electron density around D5E B 501:**

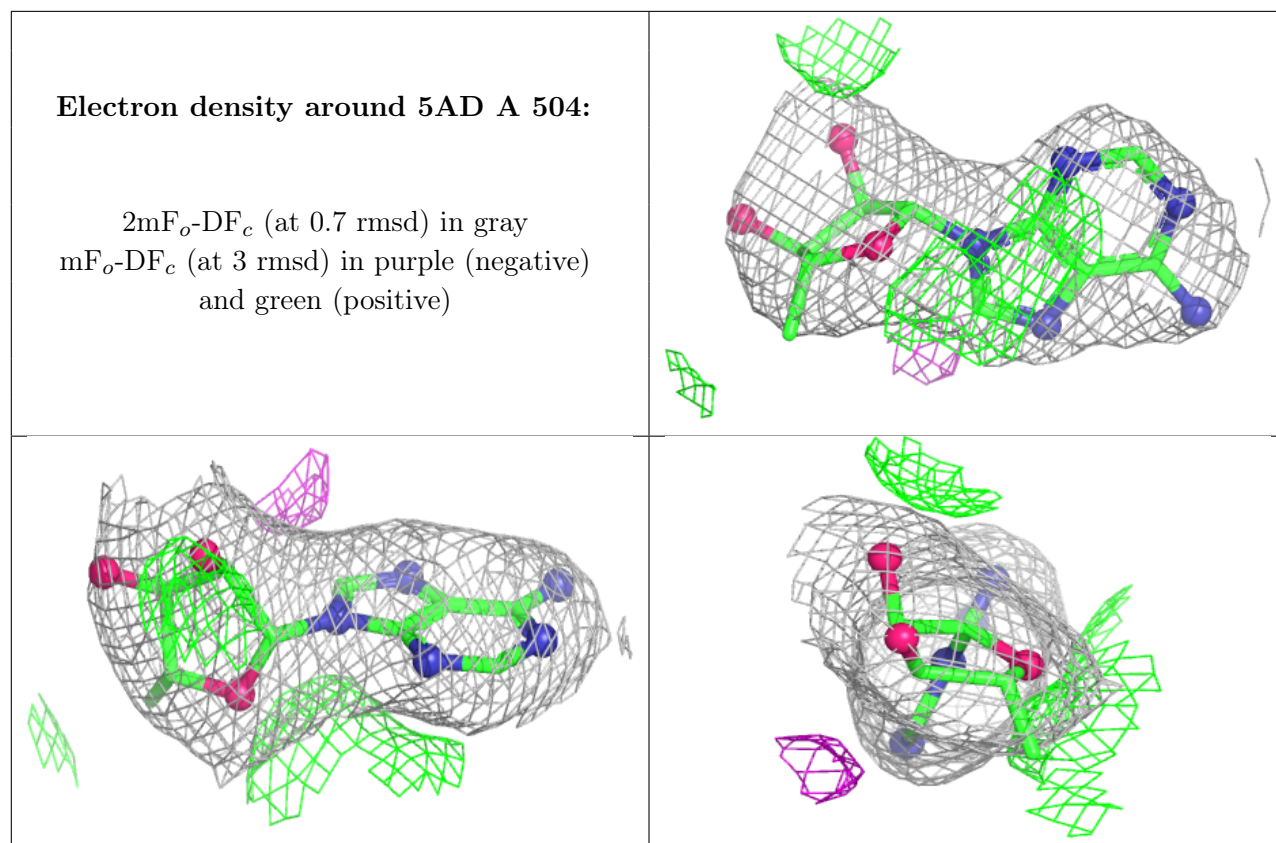
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 5AD B 504:**

$2mF_o-DF_c$  (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.