



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:22 PM UTC

PDB ID : 5GTD / pdb_00005gtd
Title : o-Succinylbenzoate CoA Synthetase (MenE) from Bacillus Subtilis in Complex with the Acyl-adenylate Intermediate OSB-AMP
Authors : Chen, Y.; Guo, Z.
Deposited on : 2016-08-20
Resolution : 2.69 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)	:	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

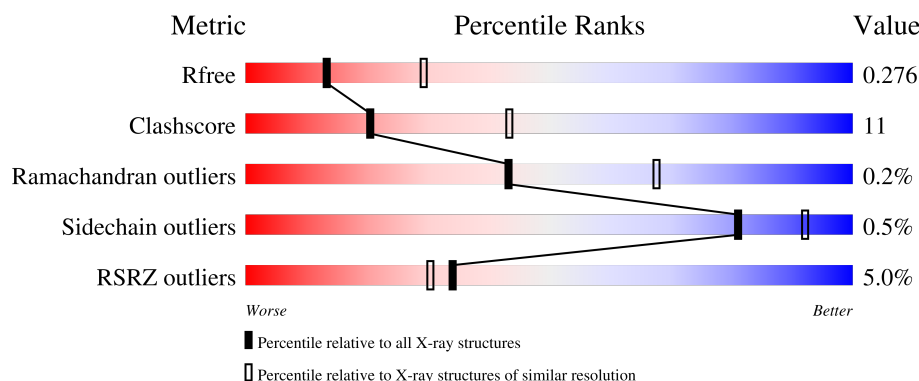
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	3% 81% 16% .
1	B	494	5% 63% 13% . 23%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	504	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6495 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 2-succinylbenzoate--CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3583	2286	598	678	21			
1	B	380	Total	C	N	O	S	0	2	0
			2780	1771	459	529	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P23971
A	0	GLY	-	expression tag	UNP P23971
A	487	HIS	-	expression tag	UNP P23971
A	488	HIS	-	expression tag	UNP P23971
A	489	HIS	-	expression tag	UNP P23971
A	490	HIS	-	expression tag	UNP P23971
A	491	HIS	-	expression tag	UNP P23971
A	492	HIS	-	expression tag	UNP P23971
B	-1	MET	-	initiating methionine	UNP P23971
B	0	GLY	-	expression tag	UNP P23971
B	487	HIS	-	expression tag	UNP P23971
B	488	HIS	-	expression tag	UNP P23971
B	489	HIS	-	expression tag	UNP P23971
B	490	HIS	-	expression tag	UNP P23971
B	491	HIS	-	expression tag	UNP P23971
B	492	HIS	-	expression tag	UNP P23971

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

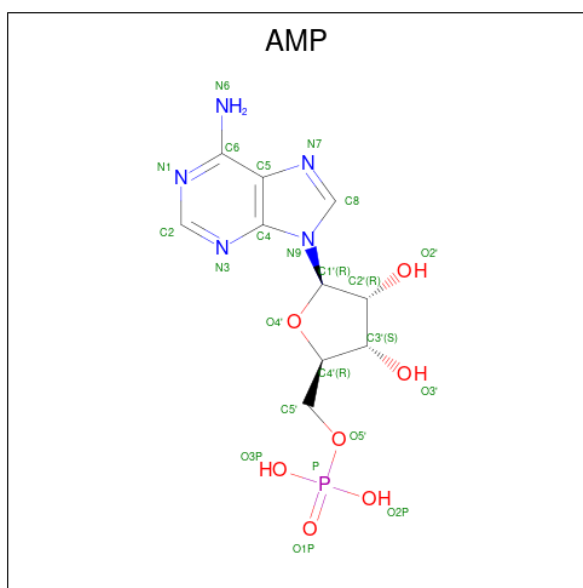
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



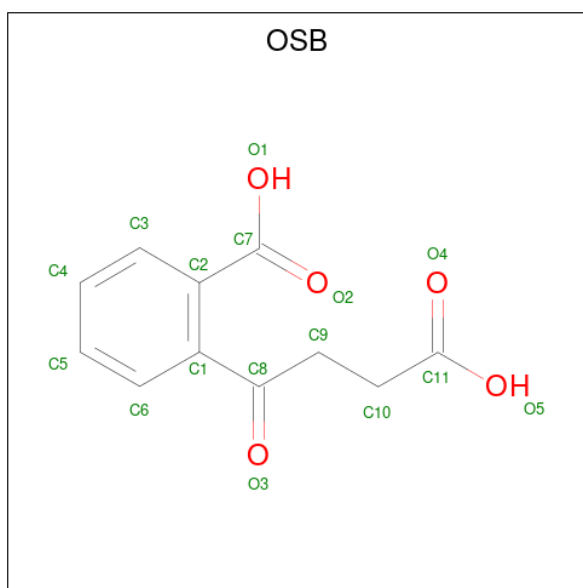
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is 2-SUCCINYLBENZOATE (CCD ID: OSB) (formula: $C_{11}H_{10}O_5$).

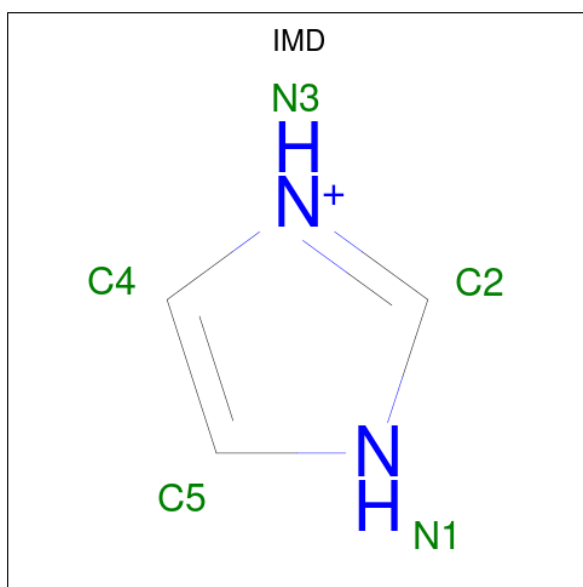


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	11	5		
5	B	1	Total	C	O	0	0
			16	11	5		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).

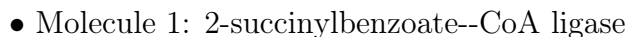


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	27	Total	O	0	0
			27	27		
8	B	12	Total	O	0	0
			12	12		

- Molecule 1: 2-succinylbenzoate--CoA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	121.81Å 121.81Å 98.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.96 – 2.69 31.96 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.96-2.69) 99.1 (31.96-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.200 , 0.237 (Not available) , 0.276	Depositor DCC
R_{free} test set	1996 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6495	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, OSB, AMP, PEG, MG, IMD

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	0.39	0/3658	0.74	1/4978 (0.0%)
1	B	0.36	0/2838	0.71	1/3862 (0.0%)
All	All	0.38	0/6496	0.73	2/8840 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ARG	N-CA-C	6.37	116.97	108.38
1	B	114	GLU	N-CA-C	-5.47	106.27	113.17

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	3583	0	3379	71	1
1	B	2780	0	2568	69	1
2	A	3	0	0	0	0
2	B	1	0	0	1	0
3	A	7	0	10	4	0
4	A	22	0	12	1	0
4	B	22	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	16	0	8	1	0
5	B	16	0	8	0	0
6	B	1	0	0	0	0
7	B	5	0	5	1	0
8	A	27	0	0	1	0
8	B	12	0	0	0	0
All	All	6495	0	6002	140	1

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 (140) 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:276:ARG:NH1	1:A:304:MET:CB	2.09	1.16
1:B:220:SER:OG	1:B:223:ASP:OD1	1.70	1.08
1:B:344:MET:HE1	1:B:347:TYR:CD1	1.96	1.00
1:B:308:GLY:C	1:B:378:TYR:HE1	1.69	1.00
1:B:306:LYS:O	1:B:378:TYR:CZ	2.16	0.99
1:A:410:ALA:HB2	1:A:433:HIS:CD2	1.97	0.97
1:A:303:SER:O	1:A:307:LEU:HA	1.64	0.96
1:B:309:SER:HB2	1:B:378:TYR:CZ	2.00	0.96
1:B:367:ASP:OD1	1:B:382:ARG:HD3	1.65	0.94
1:B:25:GLU:OE2	1:B:25:GLU:N	2.02	0.91
1:A:299:SER:OG	3:A:504:PEG:O2	1.88	0.90
1:A:410:ALA:HB2	1:A:433:HIS:NE2	1.86	0.90
1:A:429:TYR:CD1	1:A:477:LEU:HD23	2.07	0.89
1:B:344:MET:HE1	1:B:347:TYR:CE1	2.06	0.89
1:B:111:GLU:OE1	1:B:112:LYS:O	1.91	0.88
1:A:294:GLN:NE2	1:A:297:THR:HG21	1.90	0.87
1:B:308:GLY:C	1:B:378:TYR:CE1	2.53	0.85
1:B:309:SER:CA	1:B:378:TYR:CE1	2.61	0.83
1:A:477:LEU:O	1:A:479:ASP:HA	1.79	0.82
1:A:301:GLU:OE1	1:A:302:PHE:CE1	2.35	0.80
1:B:162:VAL:HG13	1:B:344:MET:SD	2.23	0.77
1:B:309:SER:N	1:B:378:TYR:CE1	2.53	0.77
1:B:220:SER:HG	1:B:223:ASP:CG	1.90	0.76
1:A:410:ALA:CB	1:A:433:HIS:NE2	2.48	0.76
1:A:301:GLU:OE1	1:A:302:PHE:HE1	1.70	0.74
1:B:309:SER:HA	1:B:378:TYR:CD1	2.22	0.74
1:A:276:ARG:HH11	1:A:304:MET:CB	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:CZ	1:A:304:MET:CB	2.67	0.73
1:B:309:SER:N	1:B:378:TYR:HE1	1.86	0.72
1:B:220:SER:OG	1:B:223:ASP:CG	2.32	0.71
1:B:366:GLY:O	1:B:382:ARG:HD2	1.90	0.71
1:B:309:SER:HA	1:B:378:TYR:CE1	2.25	0.71
1:B:309:SER:HB2	1:B:378:TYR:CE1	2.26	0.71
1:A:126:GLU:HA	1:A:129:LYS:HE2	1.72	0.70
1:B:288:MET:HG3	1:B:290:GLU:HB2	1.72	0.70
1:B:25:GLU:HB3	1:B:26:ASP:OD1	1.92	0.70
1:A:62:ASN:HB2	1:A:217:GLN:HA	1.74	0.69
1:A:294:GLN:HE21	1:A:297:THR:CG2	2.05	0.69
1:B:62:ASN:HB2	1:B:217:GLN:HA	1.75	0.68
1:A:292:CYS:O	1:A:293:SER:OG	2.10	0.67
1:B:313:PRO:HG3	1:B:319:ILE:HG12	1.77	0.66
1:B:367:ASP:OD1	1:B:382:ARG:CD	2.43	0.65
1:B:366:GLY:O	1:B:382:ARG:CD	2.45	0.64
1:B:293:SER:OG	1:B:294:GLN:N	2.24	0.63
1:B:123:ASP:HB3	1:B:126:GLU:HB2	1.79	0.63
1:A:303:SER:O	1:A:307:LEU:CA	2.42	0.63
1:B:63:ARG:NH1	1:B:107:ASP:OD2	2.32	0.62
1:A:25:GLU:OE1	1:A:25:GLU:HA	1.98	0.62
1:A:299:SER:HB2	1:A:302:PHE:CD1	2.35	0.62
1:B:187:ARG:HG2	1:B:212:THR:HB	1.82	0.62
1:A:294:GLN:NE2	1:A:297:THR:CG2	2.60	0.61
1:A:337:MET:HE2	1:A:364:LYS:HG2	1.83	0.61
1:A:82:LEU:HD13	1:A:150:MET:HE2	1.81	0.61
1:A:367:ASP:OD1	4:A:505:AMP:O2'	2.18	0.61
1:A:299:SER:OG	3:A:504:PEG:H12	2.01	0.60
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.84	0.60
1:B:20:ILE:HD12	1:B:187:ARG:NH2	2.17	0.59
1:B:96:LEU:HD22	1:B:119:VAL:HG11	1.83	0.59
1:A:63:ARG:NH2	1:A:125:ASP:OD1	2.35	0.59
1:A:220:SER:OG	1:A:223:ASP:HB2	2.03	0.59
1:B:309:SER:CB	1:B:378:TYR:CE1	2.85	0.59
1:A:474:ARG:HA	1:A:477:LEU:HD13	1.85	0.59
1:B:220:SER:OG	1:B:223:ASP:HB2	2.03	0.58
1:A:299:SER:OG	3:A:504:PEG:C1	2.52	0.58
1:B:294:GLN:OE1	1:B:297:THR:HG21	2.04	0.57
1:B:225:LEU:O	1:B:229:ASN:ND2	2.37	0.57
1:A:313:PRO:HG3	1:A:319:ILE:HG12	1.85	0.57
1:A:294:GLN:HE22	1:A:297:THR:HG21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:HB2	1:A:302:PHE:CE1	2.40	0.56
1:A:302:PHE:CD1	1:A:302:PHE:N	2.72	0.56
1:B:42:ALA:HB1	1:B:76:LEU:HD13	1.88	0.56
1:A:299:SER:HB2	1:A:302:PHE:CE1	2.41	0.55
1:B:308:GLY:O	1:B:378:TYR:CD1	2.61	0.54
1:B:189:LEU:HD21	1:B:224:VAL:HG13	1.89	0.53
1:B:220:SER:OG	1:B:223:ASP:CB	2.56	0.53
1:B:308:GLY:O	1:B:378:TYR:CE1	2.60	0.53
1:A:63:ARG:NH1	1:A:107:ASP:OD2	2.42	0.53
1:A:26:ASP:CB	1:A:230:ARG:HH12	2.22	0.53
1:A:410:ALA:CB	1:A:433:HIS:CD2	2.84	0.52
1:B:183:THR:HG22	1:B:185:GLN:H	1.75	0.52
1:B:219:PHE:CE1	1:B:224:VAL:HG21	2.45	0.52
1:B:189:LEU:HD11	1:B:216:HIS:CD2	2.44	0.52
1:A:24:TYR:O	1:A:25:GLU:HB2	2.11	0.51
1:A:301:GLU:HB2	1:A:302:PHE:CD1	2.46	0.50
1:A:84:ASN:HB3	1:A:87:LEU:HG	1.94	0.50
1:B:292:CYS:O	1:B:293:SER:HB3	2.12	0.49
1:A:75:LEU:HD22	1:A:137:ILE:HD12	1.94	0.49
1:A:187:ARG:HG2	1:A:212:THR:HB	1.95	0.49
1:B:219:PHE:CD1	1:B:224:VAL:HG21	2.48	0.49
1:A:81:VAL:HG22	1:A:149:LEU:HB3	1.95	0.49
1:A:299:SER:OG	3:A:504:PEG:C2	2.62	0.48
1:A:60:LEU:HD11	1:A:124:VAL:HG21	1.94	0.47
1:B:63:ARG:NH2	1:B:125:ASP:OD1	2.46	0.47
1:B:298:LEU:HD23	1:B:311:GLY:HA2	1.94	0.47
1:A:65:GLU:HB3	1:A:124:VAL:HG11	1.96	0.47
1:B:25:GLU:HA	1:B:26:ASP:HA	1.48	0.47
1:A:140:TYR:OH	1:B:318:GLU:OE1	2.26	0.47
1:B:92:ARG:NH1	1:B:115:TYR:OH	2.48	0.46
1:A:117:HIS:ND1	1:A:118:ILE:HG12	2.30	0.46
1:A:82:LEU:CD1	1:A:150:MET:HE2	2.46	0.46
1:A:189:LEU:HB2	1:A:233:VAL:HG11	1.98	0.46
1:B:372:ASP:OD1	1:B:376:PHE:N	2.45	0.45
1:A:219:PHE:CD1	1:A:242:MET:HE3	2.51	0.45
1:A:399:VAL:HB	1:A:414:VAL:HG21	1.98	0.45
1:B:84:ASN:HB3	1:B:87:LEU:HG	1.97	0.45
1:B:20:ILE:HD12	1:B:187:ARG:HH21	1.82	0.45
1:B:221:VAL:CG2	1:B:246:LEU:HD23	2.47	0.45
5:A:506:OSB:H91	8:A:614:HOH:O	2.16	0.45
1:B:172:SER:OG	2:B:501:CL:CL	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLY:HA2	1:A:380:LEU:HG	1.98	0.44
1:A:298:LEU:HD13	1:A:311:GLY:HA2	1.99	0.44
1:B:319:ILE:HG22	1:B:338:VAL:HG12	1.99	0.44
1:B:366:GLY:O	1:B:382:ARG:HD3	2.17	0.44
1:A:306:LYS:NZ	1:A:374:GLU:OE2	2.43	0.44
1:A:125:ASP:HA	1:A:128:MET:HE2	2.01	0.43
1:A:299:SER:C	1:A:301:GLU:N	2.76	0.43
1:A:328:CYS:HB3	1:A:332:GLU:HB3	2.01	0.43
1:A:269:LEU:O	1:A:273:GLU:HG3	2.19	0.43
1:B:19:ARG:HH12	7:B:503:IMD:C2	2.31	0.43
1:B:168:ASN:HB3	1:B:292:CYS:SG	2.59	0.43
1:B:287:GLY:HA3	1:B:294:GLN:HA	2.00	0.43
1:B:112:LYS:C	1:B:114:GLU:H	2.26	0.42
1:A:299:SER:O	1:A:301:GLU:N	2.53	0.42
1:B:290:GLU:HG3	1:B:344:MET:SD	2.59	0.42
1:A:354:ASN:O	1:A:358:PHE:HD2	2.03	0.42
1:A:177:ALA:HB1	1:A:182:ILE:HD11	2.01	0.41
1:A:82:LEU:HD22	1:A:195:PHE:HA	2.01	0.41
1:B:221:VAL:HG13	1:B:222:SER:N	2.34	0.41
1:A:42:ALA:HB1	1:A:76:LEU:HG	2.02	0.41
1:B:294:GLN:OE1	1:B:297:THR:CG2	2.68	0.41
1:A:299:SER:O	1:A:300:PRO:C	2.63	0.41
1:B:219:PHE:CG	1:B:242:MET:HG2	2.55	0.41
1:A:288:MET:HG3	1:A:290:GLU:HB2	2.02	0.41
1:A:400:GLU:HG3	1:A:414:VAL:HG23	2.02	0.41
1:B:301:GLU:CD	1:B:301:GLU:H	2.29	0.41
1:B:292:CYS:O	1:B:293:SER:CB	2.69	0.41
1:B:87:LEU:O	1:B:92:ARG:NH2	2.53	0.40
1:A:150:MET:HE3	1:A:150:MET:HB2	1.91	0.40
1:A:276:ARG:CZ	1:A:304:MET:CA	2.99	0.40
1:A:292:CYS:O	1:A:293:SER:CB	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TYR:OH	1:B:97:GLU:OE1[2_634]	1.98	0.22

5.3 Torsion angles

5.3.1 Protein backbone

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	482/494 (98%)	467 (97%)	14 (3%)	1 (0%)	43	68
1	B	378/494 (76%)	361 (96%)	16 (4%)	1 (0%)	36	60
All	All	860/988 (87%)	828 (96%)	30 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	SER
1	B	293	SER

5.3.2 Protein sidechains

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	354/421 (84%)	352 (99%)	2 (1%)	78	91
1	B	271/421 (64%)	270 (100%)	1 (0%)	84	93
All	All	625/842 (74%)	622 (100%)	3 (0%)	81	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	GLU
1	A	457	LYS
1	B	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	163	GLN
1	A	294	GLN
1	A	360	ASN
1	B	179	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	AMP	B	504	5	21,24,25	2.62	11 (52%)	30,35,38	3.17	12 (40%)
5	OSB	A	506	4	16,16,16	1.53	3 (18%)	21,21,21	1.11	1 (4%)
7	IMD	B	503	-	5,5,5	0.66	0	5,5,5	0.43	0
5	OSB	B	505	4	16,16,16	2.11	4 (25%)	21,21,21	1.12	1 (4%)
4	AMP	A	505	5	21,24,25	2.62	11 (52%)	30,35,38	3.16	11 (36%)
3	PEG	A	504	-	6,6,6	0.56	0	5,5,5	0.28	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	AMP	B	504	5	-	0/7/25/26	0/3/3/3
5	OSB	A	506	4	-	6/13/13/13	0/1/1/1
7	IMD	B	503	-	-	-	0/1/1/1
5	OSB	B	505	4	-	7/13/13/13	0/1/1/1
4	AMP	A	505	5	-	0/7/25/26	0/3/3/3
3	PEG	A	504	-	-	1/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	OSB	O4-C11	6.22	1.42	1.22
4	B	504	AMP	C8-N7	4.63	1.40	1.31
4	A	505	AMP	C8-N7	4.58	1.40	1.31
4	B	504	AMP	C5-C4	3.84	1.45	1.39
4	A	505	AMP	C5-C4	3.83	1.45	1.39
4	A	505	AMP	O4'-C1'	3.83	1.50	1.42
4	B	504	AMP	O4'-C1'	3.82	1.50	1.42
4	A	505	AMP	C4-N3	3.72	1.41	1.34
4	B	504	AMP	C4-N3	3.69	1.41	1.34
4	B	504	AMP	C8-N9	3.64	1.43	1.37
4	A	505	AMP	C8-N9	3.64	1.43	1.37
5	A	506	OSB	O5-C11	3.50	1.42	1.30
4	A	505	AMP	C2-N1	-3.33	1.28	1.33
4	A	505	AMP	C6-N6	3.32	1.42	1.34
4	B	504	AMP	C2-N1	-3.31	1.28	1.33
4	B	504	AMP	C6-N6	3.29	1.42	1.34
4	A	505	AMP	O4'-C4'	2.90	1.51	1.45
4	B	504	AMP	O4'-C4'	2.88	1.51	1.45
5	A	506	OSB	C9-C8	2.75	1.55	1.51
5	B	505	OSB	C9-C8	2.71	1.55	1.51
5	B	505	OSB	O5-C11	-2.67	1.22	1.30
4	A	505	AMP	C2'-C3'	-2.66	1.46	1.53
4	B	504	AMP	C2'-C3'	-2.66	1.46	1.53
5	A	506	OSB	C1-C8	2.60	1.53	1.48
5	B	505	OSB	C1-C8	2.57	1.53	1.48
4	A	505	AMP	C2-N3	2.48	1.38	1.33
4	B	504	AMP	C2-N3	2.48	1.38	1.33
4	A	505	AMP	C1'-N9	-2.20	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	AMP	C1'-N9	-2.17	1.40	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	AMP	C5-C4-N3	-7.91	115.83	126.72
4	A	505	AMP	C5-C4-N3	-7.91	115.83	126.72
4	B	504	AMP	N3-C4-N9	6.40	138.06	127.17
4	A	505	AMP	N3-C4-N9	6.39	138.03	127.17
4	A	505	AMP	N3-C2-N1	-6.17	119.24	128.58
4	B	504	AMP	N3-C2-N1	-6.16	119.26	128.58
4	B	504	AMP	N9-C8-N7	-5.82	105.67	113.94
4	A	505	AMP	N9-C8-N7	-5.77	105.75	113.94
4	B	504	AMP	C4-N9-C8	5.14	111.14	105.74
4	A	505	AMP	C4-N9-C8	5.06	111.05	105.74
4	A	505	AMP	C2-N1-C6	4.56	126.21	118.73
4	B	504	AMP	C2-N1-C6	4.55	126.20	118.73
4	B	504	AMP	C5-N7-C8	3.81	109.44	103.45
4	A	505	AMP	C5-N7-C8	3.81	109.44	103.45
4	A	505	AMP	C3'-C2'-C1'	3.74	108.53	101.46
4	B	504	AMP	C3'-C2'-C1'	3.69	108.45	101.46
4	B	504	AMP	C2-N3-C4	3.53	120.45	111.83
4	A	505	AMP	C2-N3-C4	3.53	120.45	111.83
4	B	504	AMP	C2'-C3'-C4'	3.00	108.41	102.61
4	A	505	AMP	C2'-C3'-C4'	3.00	108.40	102.61
5	B	505	OSB	C10-C9-C8	-2.60	109.42	112.60
4	A	505	AMP	C4-C5-N7	-2.59	107.62	110.58
4	B	504	AMP	C4-C5-N7	-2.58	107.63	110.58
5	A	506	OSB	C10-C9-C8	-2.50	109.55	112.60
4	B	504	AMP	C4'-O4'-C1'	-2.02	105.01	109.47

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	OSB	C11-C10-C9-C8
5	B	505	OSB	C11-C10-C9-C8
3	A	504	PEG	O2-C3-C4-O4
5	A	506	OSB	C3-C2-C7-O1
5	B	505	OSB	C3-C2-C7-O1
5	A	506	OSB	C3-C2-C7-O2
5	B	505	OSB	C3-C2-C7-O2

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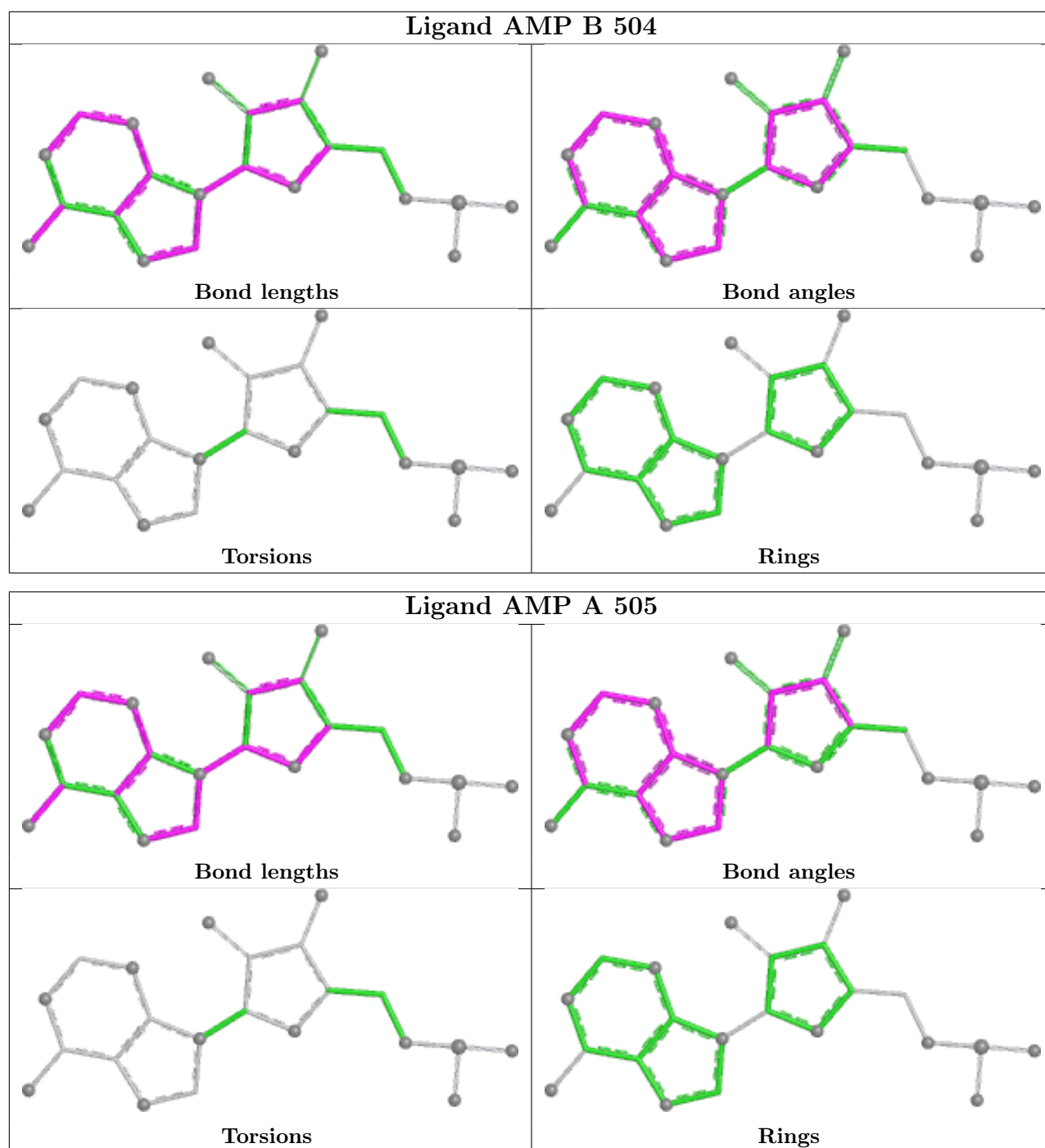
Mol	Chain	Res	Type	Atoms
5	B	505	OSB	C6-C1-C8-C9
5	A	506	OSB	C1-C2-C7-O1
5	B	505	OSB	C9-C10-C11-O4
5	A	506	OSB	C1-C2-C7-O2
5	B	505	OSB	C1-C8-C9-C10
5	A	506	OSB	C6-C1-C8-O3
5	B	505	OSB	C9-C10-C11-O5

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	OSB	1	0
7	B	503	IMD	1	0
4	A	505	AMP	1	0
3	A	504	PEG	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/494 (97%)	0.22	16 (3%) 49 45	47, 80, 122, 155	0
1	B	380/494 (76%)	0.43	27 (7%) 22 19	44, 89, 152, 182	2 (0%)
All	All	864/988 (87%)	0.31	43 (4%) 34 30	44, 84, 138, 182	2 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	LEU	6.1
1	B	153	SER	6.1
1	B	383	ARG	5.4
1	B	382	ARG	5.2
1	B	264	GLY	3.8
1	B	266	PRO	3.6
1	A	303	SER	3.6
1	B	324	ASP	3.5
1	B	311	GLY	3.3
1	A	135	ILE	3.2
1	B	126	GLU	3.2
1	B	97	GLU	3.1
1	A	447	GLU	3.0
1	B	304	MET	3.0
1	A	485	LEU	2.7
1	A	481	ARG	2.7
1	B	113	LYS	2.7
1	B	344	MET	2.6
1	B	298	LEU	2.6
1	A	126	GLU	2.5
1	B	305	GLU	2.5
1	B	252	ARG	2.5
1	A	251	ASN	2.5
1	B	274	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	302	PHE	2.5
1	A	184	GLU	2.4
1	A	475	ASN	2.3
1	A	480	ALA	2.3
1	B	268	PRO	2.2
1	B	280	PHE	2.2
1	B	117	HIS	2.2
1	B	248	GLU	2.2
1	B	359	GLN	2.2
1	A	155	THR	2.1
1	A	252	ARG	2.1
1	B	108	SER	2.1
1	A	478	LYS	2.1
1	B	380	LEU	2.1
1	B	265	GLY	2.1
1	B	3	THR	2.1
1	A	304	MET	2.0
1	A	477	LEU	2.0
1	B	308	GLY	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 [i](#)

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

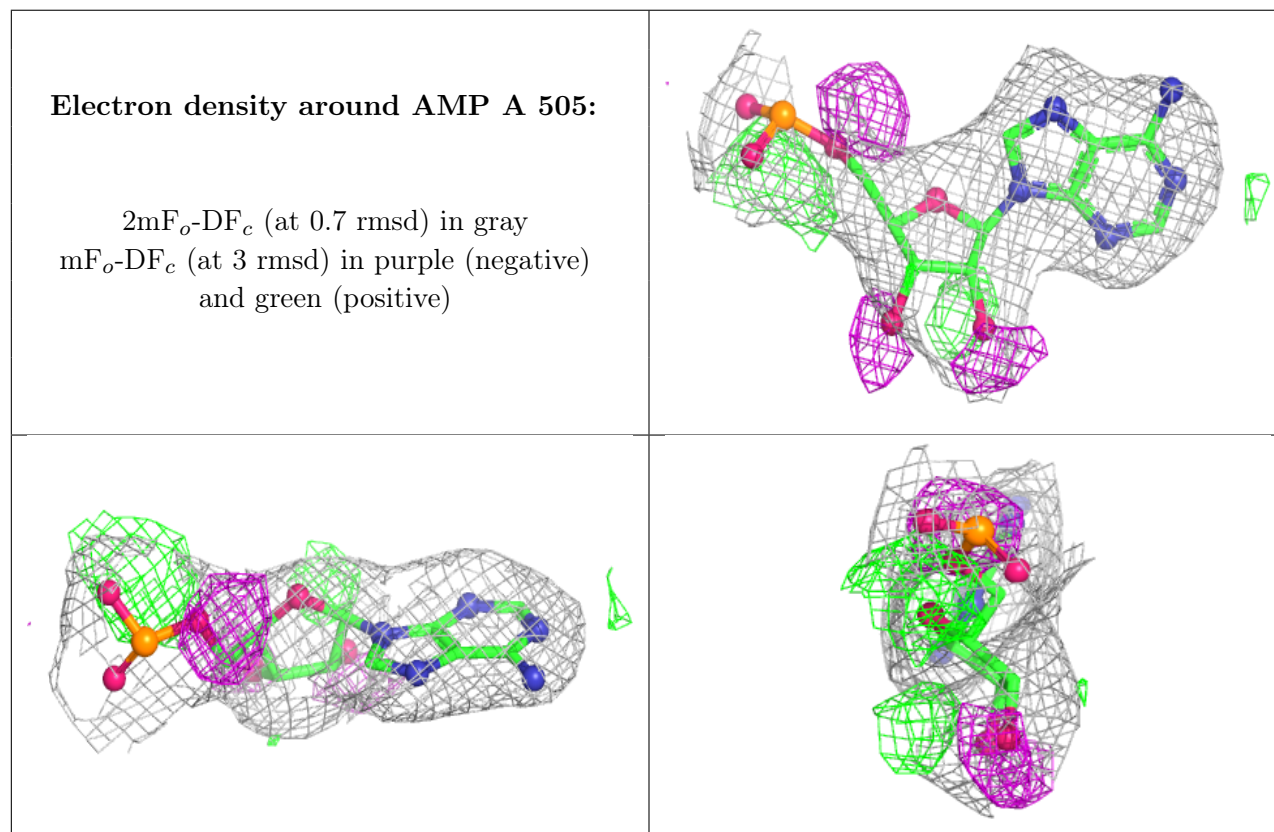
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	504	7/7	0.75	0.27	99,106,112,115	0
2	CL	A	501	1/1	0.77	0.31	120,120,120,120	0
7	IMD	B	503	5/5	0.84	0.23	103,104,105,106	0
6	MG	B	502	1/1	0.86	0.15	78,78,78,78	0

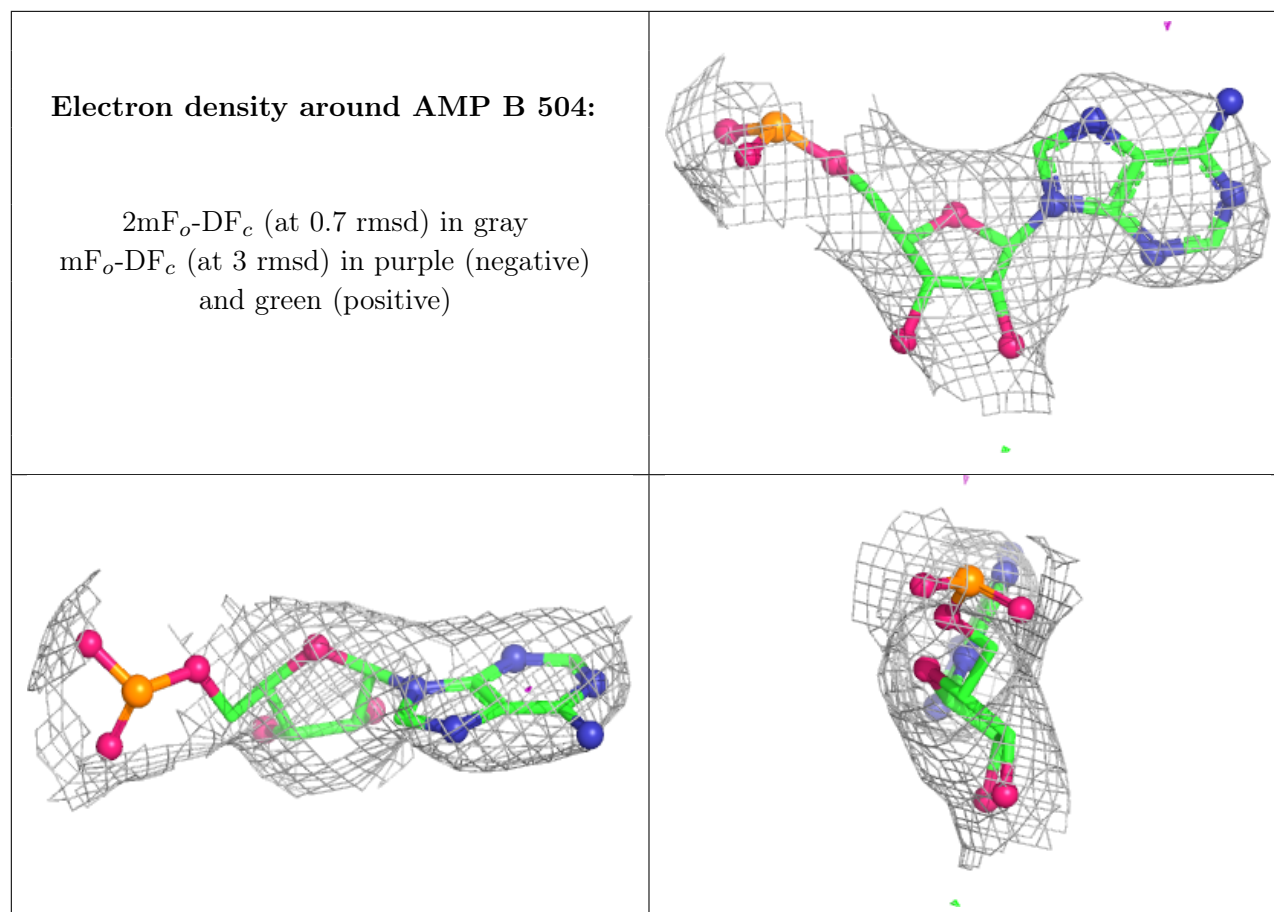
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	501	1/1	0.86	0.21	96,96,96,96	0
4	AMP	A	505	22/23	0.90	0.10	48,52,62,66	0
5	OSB	A	506	16/16	0.90	0.15	63,80,101,105	0
5	OSB	B	505	16/16	0.91	0.14	104,112,120,122	0
2	CL	A	503	1/1	0.92	0.35	30,30,30,30	0
2	CL	A	502	1/1	0.92	0.27	125,125,125,125	0
4	AMP	B	504	22/23	0.93	0.10	97,112,121,121	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.