



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:33 pm BST

PDB ID : 2Y4N  
Title : PaaK1 in complex with phenylacetyl adenylate  
Authors : Law, A.; Boulanger, M.J.  
Deposited on : 2011-01-07  
Resolution : 1.92 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 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

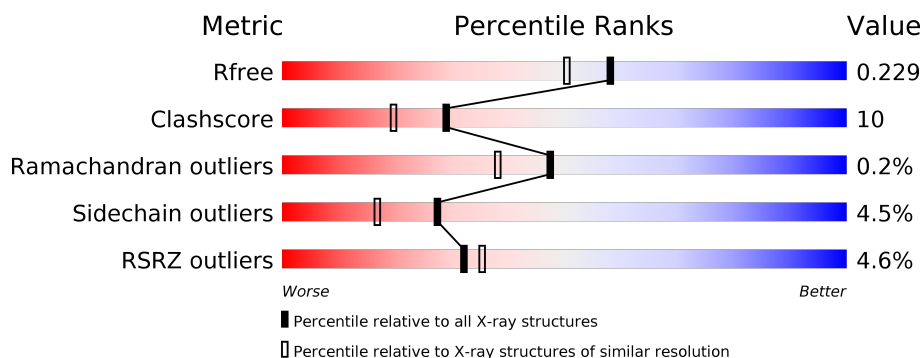
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	437	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	437	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>

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	503	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7400 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 PHENYLACETATE-COENZYME A LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	1	0
			3317	2097	582	626	12			
1	B	423	Total	C	N	O	S	0	3	0
			3312	2094	581	624	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP B4E7B5
A	-3	SER	-	expression tag	UNP B4E7B5
A	-2	HIS	-	expression tag	UNP B4E7B5
A	-1	MET	-	expression tag	UNP B4E7B5
A	0	ALA	-	expression tag	UNP B4E7B5
A	1	SER	-	expression tag	UNP B4E7B5
B	-4	GLY	-	expression tag	UNP B4E7B5
B	-3	SER	-	expression tag	UNP B4E7B5
B	-2	HIS	-	expression tag	UNP B4E7B5
B	-1	MET	-	expression tag	UNP B4E7B5
B	0	ALA	-	expression tag	UNP B4E7B5
B	1	SER	-	expression tag	UNP B4E7B5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

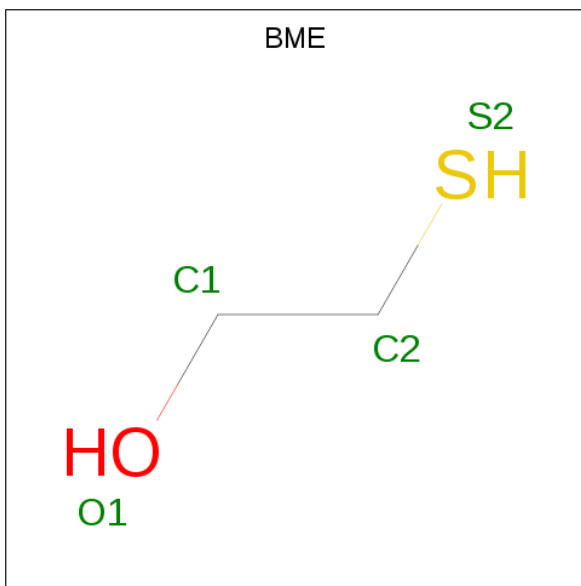
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



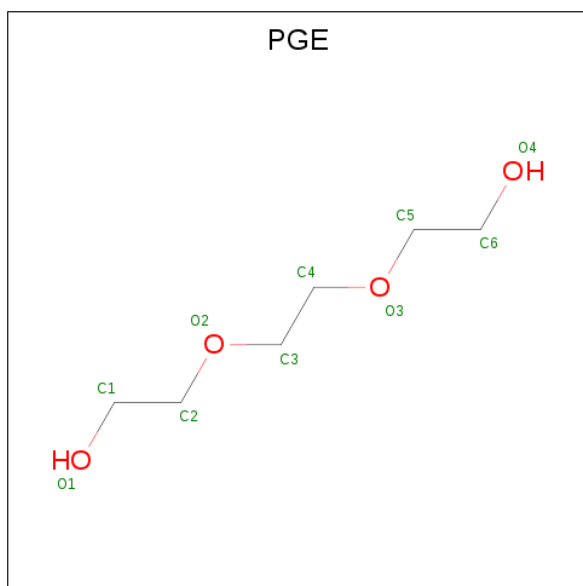
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 32	C 18	N 5	O 8	P 1	0	0
5	B	1	Total 32	C 18	N 5	O 8	P 1	0	0

- 
- Chemical structure of PAC (Phenylacetic acid) showing the phenyl ring and the acetic acid side chain. The atoms are labeled as follows:
- O1: Carbonyl oxygen
  - O2: Hydroxyl oxygen
  - C1: Carbonyl carbon
  - C2: Methylene carbon
  - C1': Aromatic carbon (ipso)
  - C2': Aromatic carbon (ortho)
  - C3': Aromatic carbon (meta)
  - C4': Aromatic carbon (para)
  - C5': Aromatic carbon (meta)
  - C6': Aromatic carbon (ortho)

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

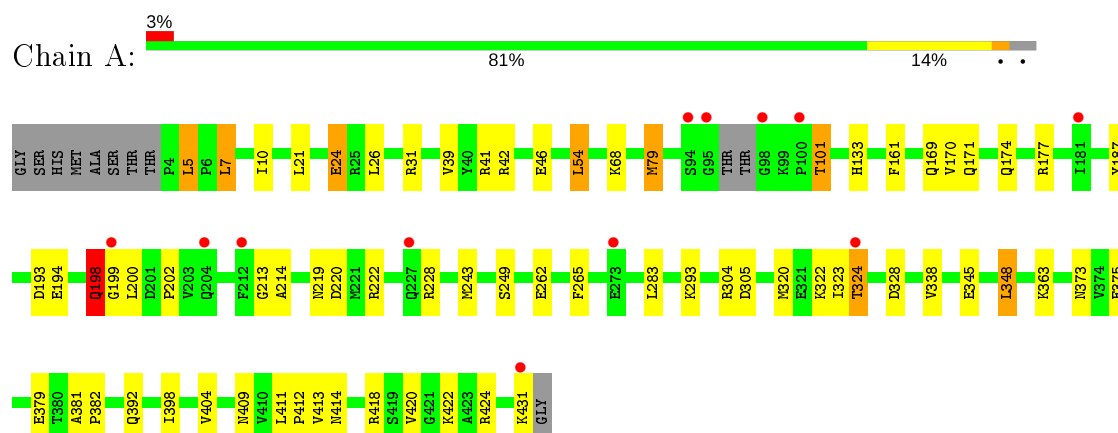
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	394	Total	O	0	0
			394	394		
8	B	270	Total	O	0	0
			270	270		

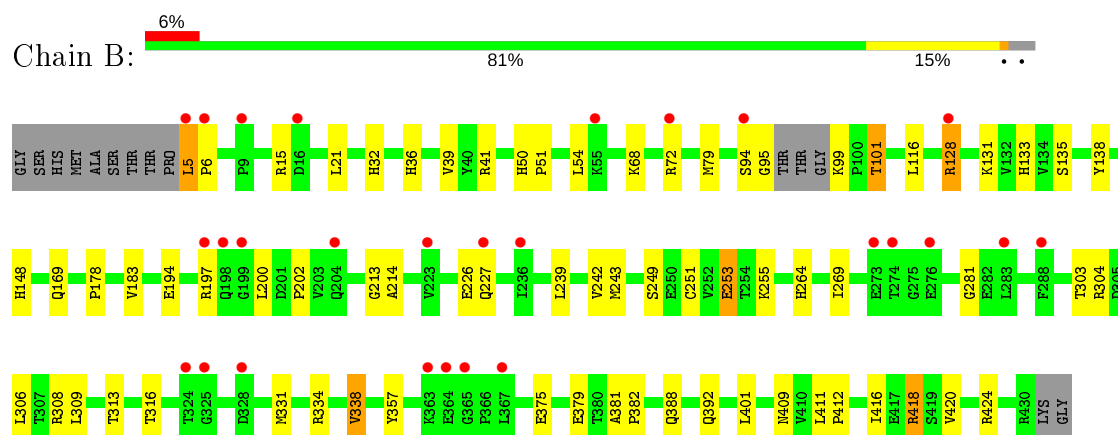
### 3 Residue-property plots [i](#)

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: PHENYLACETATE-COENZYME A LIGASE



#### • Molecule 1: PHENYLACETATE-COENZYME A LIGASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.26 Å 62.39 Å 76.59 Å 91.16° 108.33° 106.27°	Depositor
Resolution (Å)	27.01 – 1.92 27.01 – 1.92	Depositor EDS
% Data completeness (in resolution range)	93.8 (27.01-1.92) 93.8 (27.01-1.92)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 1.92 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.181 , 0.232 0.180 , 0.229	Depositor DCC
$R_{free}$ test set	3457 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: MG, PGE, BME, DLL, PAC, PEG

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	0.31	0/3386	0.45	0/4594
1	B	0.28	0/3388	0.43	0/4600
All	All	0.30	0/6774	0.44	0/9194

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	GLN	Peptide
1	A	7	LEU	Peptide

### 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	3317	0	3337	61	0
1	B	3312	0	3331	63	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	7	0	10	10	0
4	A	4	0	5	1	0
4	B	8	0	11	2	0
5	A	32	0	18	0	0
5	B	32	0	18	0	0
6	B	10	0	7	3	0
7	B	10	0	14	0	0
8	A	394	0	0	17	1
8	B	270	0	0	13	1
All	All	7400	0	6751	129	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 10.

All (129) 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:251:CYS:HB3	1:B:253:GLU:OE2	1.42	1.17
1:A:198:GLN:HG3	1:A:198:GLN:O	1.61	0.97
1:A:219:ASN:HD21	3:A:503:PEG:H42	1.30	0.96
1:A:379:GLU:HG2	8:A:977:HOH:O	1.65	0.95
1:A:424:ARG:HH11	1:A:424:ARG:HG3	1.29	0.93
1:A:219:ASN:ND2	3:A:503:PEG:H42	1.88	0.87
1:A:379:GLU:CG	8:A:977:HOH:O	2.19	0.86
1:A:305:ASP:HB3	1:A:323:ILE:HD13	1.60	0.84
1:B:251:CYS:CB	1:B:253:GLU:OE2	2.27	0.82
1:A:375:GLU:OE2	1:A:418:ARG:NH2	2.15	0.78
1:A:322:LYS:H	3:A:503:PEG:H22	1.50	0.77
1:A:322:LYS:H	3:A:503:PEG:C2	1.97	0.77
1:A:219:ASN:HD21	3:A:503:PEG:C4	1.98	0.76
1:B:388:GLN:O	1:B:392:GLN:HG2	1.85	0.76
1:B:304:ARG:NH1	8:B:603:HOH:O	2.19	0.75
4:B:505:BME:H12	8:B:801:HOH:O	1.87	0.74
1:A:68:LYS:HE3	1:A:101:THR:HG21	1.68	0.74
1:B:95:GLY:HA3	8:B:852:HOH:O	1.88	0.74
1:A:328:ASP:CB	8:A:826:HOH:O	2.37	0.71
8:A:628:HOH:O	1:B:94:SER:HA	1.89	0.71
1:A:375:GLU:CD	1:A:418:ARG:HH22	1.94	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:GLU:OE2	1:B:418:ARG:NH2	2.26	0.69
1:A:328:ASP:HB2	8:A:826:HOH:O	1.93	0.69
1:B:68:LYS:HE3	1:B:101:THR:HG21	1.74	0.69
1:B:253:GLU:H	1:B:253:GLU:CD	1.97	0.69
1:B:5:LEU:N	8:B:607:HOH:O	2.26	0.68
1:B:304:ARG:HG3	1:B:304:ARG:HH11	1.57	0.67
1:B:313:THR:O	8:B:602:HOH:O	2.13	0.66
1:A:219:ASN:OD1	3:A:503:PEG:H41	1.95	0.66
1:A:283:LEU:HD11	1:A:324:THR:HG21	1.76	0.66
1:B:128:ARG:CG	1:B:128:ARG:HH11	2.08	0.66
1:A:198:GLN:CG	1:A:198:GLN:O	2.42	0.65
1:A:220:ASP:OD2	1:A:345:GLU:HG3	1.97	0.65
1:A:392:GLN:NE2	8:A:603:HOH:O	2.28	0.65
1:B:331:MET:HE3	1:B:338:VAL:HG22	1.78	0.64
1:B:331:MET:CE	1:B:338:VAL:HG22	2.28	0.63
1:B:50[A]:HIS:CG	1:B:51:PRO:HD2	2.34	0.63
3:A:503:PEG:H32	8:A:765:HOH:O	1.99	0.62
1:B:133:HIS:HD2	8:B:808:HOH:O	1.81	0.62
1:B:375:GLU:CD	1:B:418:ARG:HH22	2.03	0.61
1:A:42:ARG:O	1:A:46:GLU:HG3	2.01	0.61
1:A:219:ASN:ND2	3:A:503:PEG:C4	2.58	0.61
1:B:128:ARG:HG2	1:B:128:ARG:HH11	1.66	0.61
1:B:226:GLU:OE2	1:B:255:LYS:NZ	2.31	0.60
1:B:128:ARG:HG2	1:B:128:ARG:NH1	2.17	0.60
1:B:200:LEU:O	1:B:202:PRO:HD3	2.03	0.59
6:B:503:PAC:O1	6:B:503:PAC:H2'	2.00	0.59
1:A:363:LYS:HE3	8:A:670:HOH:O	2.01	0.58
1:B:5:LEU:N	1:B:6:PRO:CD	2.67	0.58
1:A:324:THR:HG22	8:A:625:HOH:O	2.02	0.57
1:A:222:ARG:HH21	3:A:503:PEG:H41	1.69	0.57
1:A:328:ASP:HB3	8:A:826:HOH:O	2.00	0.57
1:A:373:ASN:ND2	1:A:409:ASN:HD22	2.04	0.56
1:B:68:LYS:HE2	1:B:72:ARG:NH2	2.20	0.56
1:B:213:GLY:O	1:B:214:ALA:HB3	2.06	0.55
1:B:304:ARG:NH1	1:B:304:ARG:HG3	2.22	0.55
1:A:424:ARG:HG3	1:A:424:ARG:NH1	2.07	0.54
1:A:293:LYS:HE2	8:A:731:HOH:O	2.08	0.54
1:B:5:LEU:N	1:B:6:PRO:HD2	2.22	0.54
1:A:424:ARG:HH11	1:A:424:ARG:CG	2.06	0.53
1:A:262:GLU:HA	1:A:265:PHE:O	2.08	0.53
1:A:133:HIS:HE1	1:A:169:GLN:OE1	1.92	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLY:O	1:A:214:ALA:HB3	2.09	0.53
1:A:177:ARG:NH1	8:A:612:HOH:O	2.40	0.53
1:A:193:ASP:OD1	1:A:228:ARG:NH2	2.26	0.52
1:A:373:ASN:HD22	1:A:409:ASN:HB3	1.73	0.52
1:B:39:VAL:HG21	1:B:79:MET:HG3	1.92	0.52
1:B:388:GLN:O	1:B:392:GLN:CG	2.54	0.52
1:B:409:ASN:ND2	1:B:411:LEU:HD21	2.26	0.51
1:B:281:GLY:O	1:B:308:ARG:HD3	2.12	0.50
1:B:99:LYS:N	8:B:614:HOH:O	2.43	0.50
1:B:135:SER:HB2	1:B:183:VAL:HG23	1.93	0.50
1:A:379:GLU:H	1:A:379:GLU:CD	2.15	0.50
1:B:131:LYS:HB2	1:B:178:PRO:HA	1.93	0.49
1:B:68:LYS:HE3	1:B:101:THR:CG2	2.41	0.49
1:B:32:HIS:ND1	1:B:36:HIS:HD2	2.09	0.49
1:B:401:LEU:N	1:B:401:LEU:HD12	2.28	0.49
6:B:503:PAC:H2'	4:B:505:BME:H11	1.94	0.49
1:A:133:HIS:HD2	8:A:846:HOH:O	1.95	0.49
1:B:138:TYR:OH	1:B:148:HIS:HD2	1.96	0.49
1:A:228:ARG:NH1	8:A:601:HOH:O	2.01	0.48
1:B:128:ARG:HB3	1:B:128:ARG:HH11	1.79	0.47
1:B:15:ARG:HD3	1:B:15:ARG:O	2.15	0.47
1:A:39:VAL:HG21	1:A:79:MET:HG3	1.96	0.47
8:A:628:HOH:O	1:B:94:SER:CA	2.57	0.47
1:A:10:ILE:HD11	1:A:21:LEU:HD21	1.97	0.47
1:A:21:LEU:HA	1:A:24:GLU:HG3	1.97	0.46
1:B:128:ARG:CB	1:B:128:ARG:HH11	2.28	0.46
1:A:5:LEU:HG	8:A:818:HOH:O	2.16	0.46
1:B:116:LEU:HD21	1:B:264:HIS:CD2	2.51	0.45
1:A:322:LYS:N	3:A:503:PEG:H22	2.26	0.45
1:B:411:LEU:HB3	1:B:412:PRO:HD2	1.97	0.45
1:A:424:ARG:NH1	1:A:424:ARG:CG	2.69	0.45
1:B:251:CYS:C	1:B:253:GLU:OE2	2.55	0.45
1:B:239:LEU:HD23	1:B:239:LEU:N	2.32	0.45
1:A:305:ASP:CB	1:A:323:ILE:HD13	2.40	0.45
1:B:41:ARG:NH1	8:B:601:HOH:O	2.11	0.45
1:B:303:THR:O	1:B:304:ARG:HB2	2.16	0.45
1:B:194:GLU:OE2	1:B:197:ARG:NH1	2.51	0.44
1:A:348:LEU:HA	1:A:348:LEU:HD12	1.86	0.43
1:B:313:THR:HG21	8:B:625:HOH:O	2.18	0.43
1:A:411:LEU:HB3	1:A:412:PRO:HD2	1.99	0.43
1:B:50[A]:HIS:CE1	1:B:51:PRO:HG2	2.53	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLU:HG2	8:B:736:HOH:O	2.19	0.43
6:B:503:PAC:C6'	8:B:771:HOH:O	2.66	0.43
1:A:187:TYR:CD1	1:A:420:VAL:HA	2.53	0.43
1:A:413:VAL:O	1:A:414:ASN:HB2	2.18	0.43
1:B:133:HIS:HE1	1:B:169:GLN:OE1	2.02	0.43
1:B:41:ARG:HD3	8:B:601:HOH:O	2.18	0.42
1:A:398:ILE:CG2	1:A:404:VAL:CG2	2.97	0.42
1:A:161:PHE:CZ	1:A:169:GLN:HG2	2.55	0.42
1:A:68:LYS:CE	1:A:101:THR:HG21	2.45	0.42
1:B:381:ALA:HB3	1:B:382:PRO:HD3	2.01	0.41
1:B:72:ARG:HD3	8:B:856:HOH:O	2.19	0.41
1:A:381:ALA:N	1:A:382:PRO:HD2	2.35	0.41
1:B:135:SER:HB2	1:B:183:VAL:CG2	2.50	0.41
4:A:504:BME:H11	8:A:805:HOH:O	2.19	0.41
1:B:357:TYR:HA	1:B:416:ILE:HD13	2.01	0.41
1:A:171:GLN:HE21	1:B:99:LYS:HE2	1.85	0.41
1:A:170:VAL:HG21	1:A:194:GLU:CG	2.50	0.41
1:A:161:PHE:CE1	1:A:169:GLN:HG2	2.56	0.41
1:A:214:ALA:O	1:A:422:LYS:HE2	2.21	0.41
1:B:68:LYS:CE	1:B:101:THR:HG21	2.46	0.41
1:B:401:LEU:N	1:B:401:LEU:CD1	2.84	0.41
1:A:26:LEU:HD23	1:A:54:LEU:HD21	2.03	0.40
1:B:269:ILE:CG1	1:B:309:LEU:HG	2.51	0.40
1:A:198:GLN:N	1:A:199:GLY:HA2	2.35	0.40
1:A:200:LEU:O	1:A:202:PRO:HD3	2.22	0.40
1:B:239:LEU:HD21	1:B:242:VAL:HG21	2.03	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)
8:A:876:HOH:O	8:B:697:HOH:O[1_565]	2.11	0.09

## 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	423/437 (97%)	413 (98%)	9 (2%)	1 (0%)	47	38
1	B	422/437 (97%)	406 (96%)	14 (3%)	2 (0%)	29	18
All	All	845/874 (97%)	819 (97%)	23 (3%)	3 (0%)	47	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243[A]	MET
1	B	243[B]	MET
1	A	243	MET

### 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	356/364 (98%)	339 (95%)	17 (5%)	25	15
1	B	357/364 (98%)	342 (96%)	15 (4%)	30	19
All	All	713/728 (98%)	681 (96%)	32 (4%)	27	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	LEU
1	A	24	GLU
1	A	31	ARG
1	A	41	ARG
1	A	54	LEU
1	A	79	MET
1	A	101	THR
1	A	174	GLN
1	A	198	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	249	SER
1	A	304	ARG
1	A	320	MET
1	A	324	THR
1	A	338	VAL
1	A	348	LEU
1	A	431	LYS
1	B	5	LEU
1	B	21	LEU
1	B	54	LEU
1	B	101	THR
1	B	128	ARG
1	B	227	GLN
1	B	249	SER
1	B	253	GLU
1	B	306	LEU
1	B	316	THR
1	B	334	ARG
1	B	338	VAL
1	B	418	ARG
1	B	420	VAL
1	B	424	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	148	HIS
1	A	171	GLN
1	A	373	ASN
1	B	36	HIS
1	B	84	GLN
1	B	133	HIS
1	B	148	HIS
1	B	165	GLN
1	B	174	GLN
1	B	198	GLN

### 5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
5	DLL	A	505	-	31,35,35	1.68	4 (12%)	35,51,51	1.42	5 (14%)
4	BME	A	504	1	3,3,3	0.34	0	1,2,2	0.41	0
3	PEG	A	503	-	6,6,6	0.49	0	5,5,5	0.26	0
6	PAC	B	503	-	7,10,10	0.44	0	8,12,12	0.40	0
4	BME	B	505	-	3,3,3	0.45	0	1,2,2	0.03	0
4	BME	B	506	1	3,3,3	0.35	0	1,2,2	0.40	0
5	DLL	B	507	-	31,35,35	1.65	4 (12%)	35,51,51	1.26	3 (8%)
7	PGE	B	504	-	9,9,9	0.44	0	8,8,8	0.34	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
5	DLL	A	505	-	-	1/13/35/35	0/4/4/4
4	BME	A	504	1	-	0/1/1/1	-
3	PEG	A	503	-	-	2/4/4/4	-
6	PAC	B	503	-	-	0/2/4/4	0/1/1/1
4	BME	B	505	-	-	1/1/1/1	-
4	BME	B	506	1	-	1/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DLL	B	507	-	-	1/13/35/35	0/4/4/4
7	PGE	B	504	-	-	6/7/7/7	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	507	DLL	C8-N7	7.21	1.47	1.34
5	A	505	DLL	C8-N7	6.99	1.47	1.34
5	A	505	DLL	O4'-C4'	-3.49	1.37	1.45
5	B	507	DLL	O4'-C4'	-3.04	1.38	1.45
5	A	505	DLL	O4'-C1'	2.45	1.44	1.41
5	B	507	DLL	O5'-C5'	-2.41	1.35	1.44
5	A	505	DLL	O5'-C5'	-2.17	1.36	1.44
5	B	507	DLL	O4'-C1'	2.01	1.43	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	DLL	N3-C2-N1	-4.96	120.92	128.68
5	B	507	DLL	N3-C2-N1	-4.60	121.48	128.68
5	A	505	DLL	O4'-C4'-C5'	3.40	120.55	109.37
5	A	505	DLL	O4'-C4'-C3'	2.98	111.02	105.11
5	B	507	DLL	O4'-C4'-C5'	2.96	119.10	109.37
5	B	507	DLL	O4'-C4'-C3'	2.42	109.90	105.11
5	A	505	DLL	C5'-C4'-C3'	2.27	123.68	115.18
5	A	505	DLL	O5'-C5'-C4'	2.25	116.74	108.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	DLL	O4'-C4'-C5'-O5'
4	B	505	BME	O1-C1-C2-S2
5	B	507	DLL	O4'-C4'-C5'-O5'
3	A	503	PEG	O2-C3-C4-O4
7	B	504	PGE	O2-C3-C4-O3
7	B	504	PGE	O1-C1-C2-O2
4	B	506	BME	O1-C1-C2-S2
3	A	503	PEG	C4-C3-O2-C2
7	B	504	PGE	C3-C4-O3-C5
7	B	504	PGE	C1-C2-O2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	B	504	PGE	C4-C3-O2-C2
7	B	504	PGE	O3-C5-C6-O4

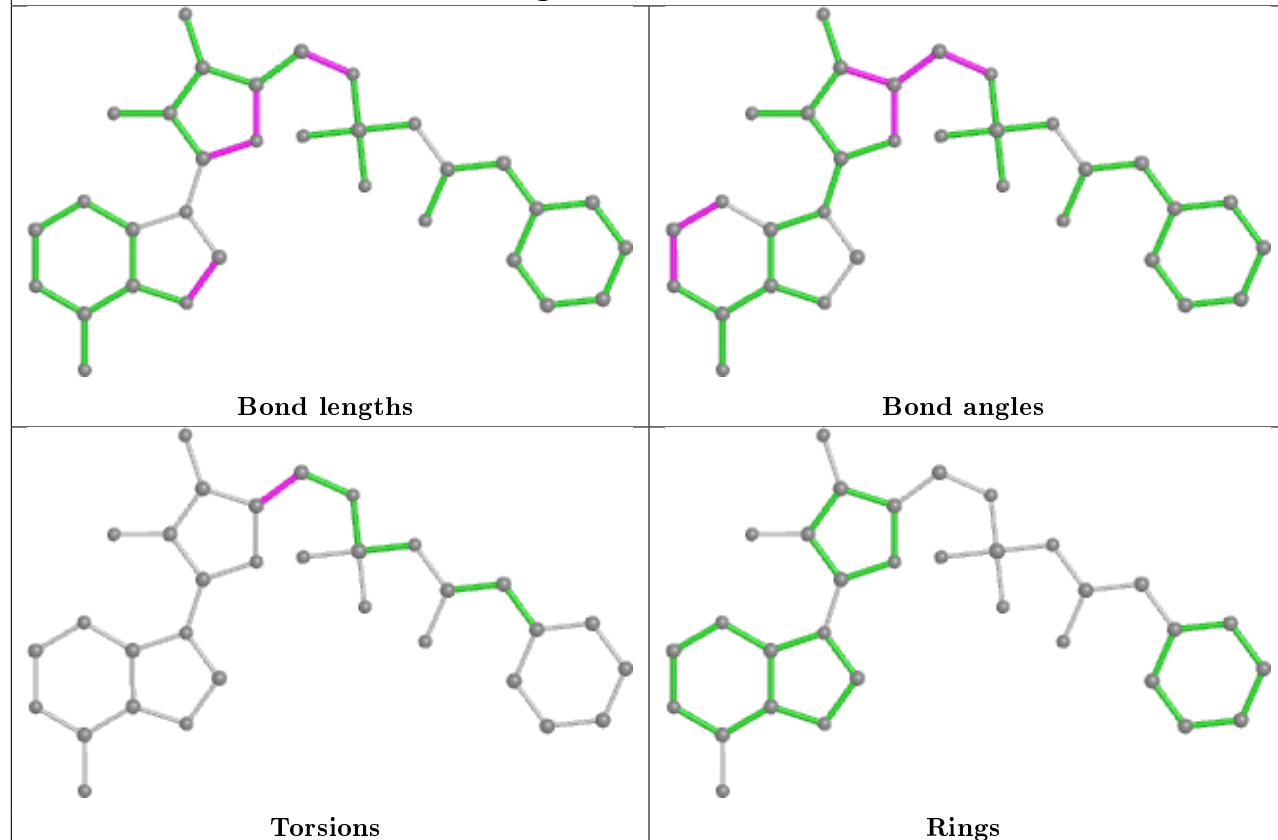
There are no ring outliers.

4 monomers are involved in 15 short contacts:

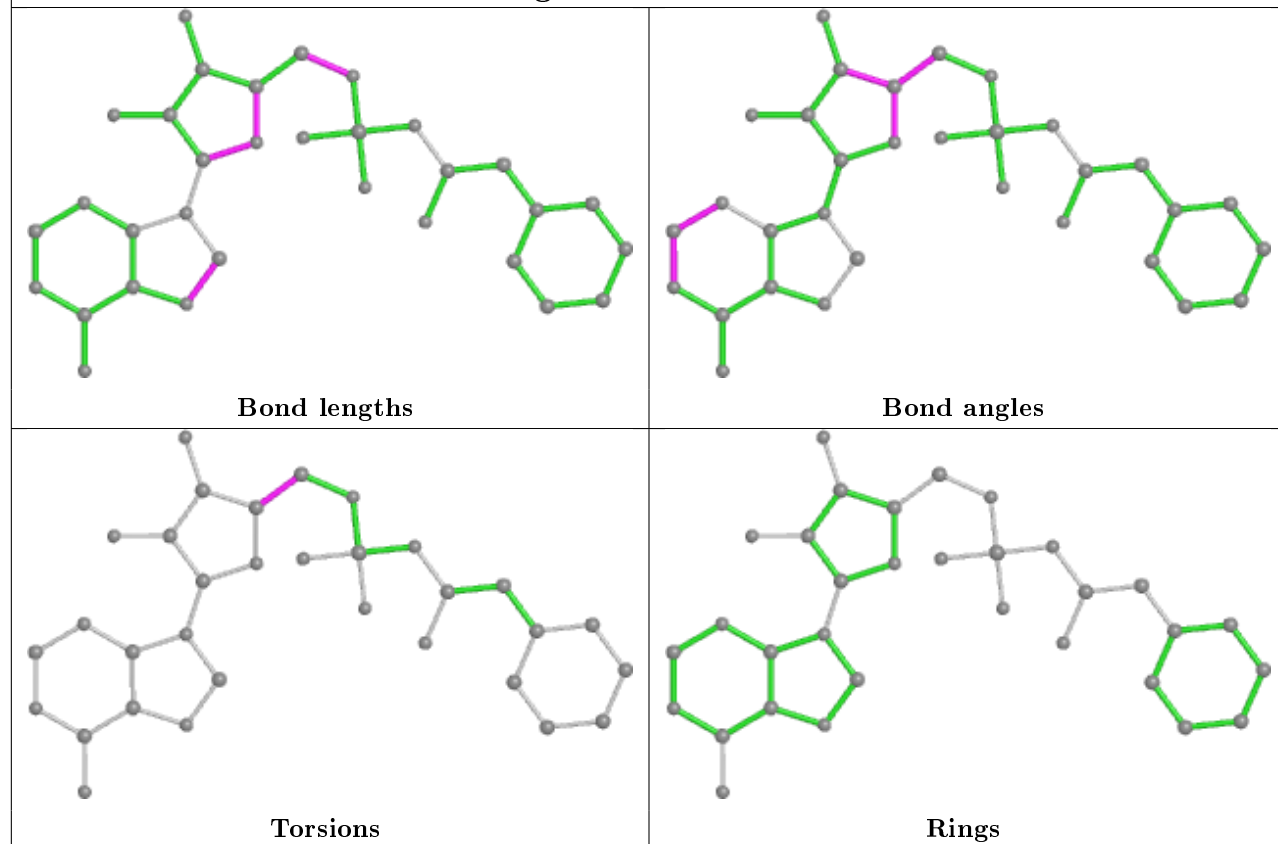
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	BME	1	0
3	A	503	PEG	10	0
6	B	503	PAC	3	0
4	B	505	BME	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 DLL A 505



## Ligand DLL B 507



## 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	426/437 (97%)	-0.07	12 (2%) 53 56	13, 25, 43, 57	1 (0%)
1	B	423/437 (96%)	0.20	27 (6%) 19 22	14, 31, 52, 65	0
All	All	849/874 (97%)	0.07	39 (4%) 32 35	13, 27, 49, 65	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	6.0
1	B	199	GLY	4.7
1	B	367	LEU	4.5
1	A	94	SER	4.3
1	A	431	LYS	4.2
1	B	273	GLU	3.6
1	A	324	THR	3.4
1	B	365	GLY	3.3
1	A	199	GLY	3.2
1	B	6	PRO	3.2
1	B	94	SER	3.1
1	A	95	GLY	3.1
1	B	5	LEU	3.1
1	B	364	GLU	3.0
1	B	227	GLN	3.0
1	B	55	LYS	3.0
1	B	324	THR	2.8
1	B	274	THR	2.7
1	B	204	GLN	2.7
1	B	223	VAL	2.7
1	B	325	GLY	2.7
1	B	328	ASP	2.7
1	A	181	ILE	2.7
1	B	9	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	72	ARG	2.5
1	B	197	ARG	2.5
1	B	128	ARG	2.5
1	A	273	GLU	2.5
1	A	212	PHE	2.4
1	A	100	PRO	2.3
1	B	288	PHE	2.3
1	B	363	LYS	2.2
1	B	283	LEU	2.2
1	B	198	GLN	2.2
1	A	227	GLN	2.2
1	B	16	ASP	2.2
1	A	204	GLN	2.2
1	B	276	GLU	2.1
1	B	236	ILE	2.1

## 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
6	PAC	B	503	10/10	0.64	0.21	56,61,70,74	0
7	PGE	B	504	10/10	0.82	0.16	53,61,66,67	0
3	PEG	A	503	7/7	0.84	0.28	28,38,39,41	0
4	BME	B	505	4/4	0.87	0.18	51,56,56,59	0
5	DLL	B	507	32/32	0.96	0.08	18,21,28,29	0
5	DLL	A	505	32/32	0.96	0.09	14,20,26,27	0
2	MG	A	502	1/1	0.97	0.06	43,43,43,43	0
2	MG	B	501	1/1	0.97	0.09	34,34,34,34	0

*Continued on next page...*

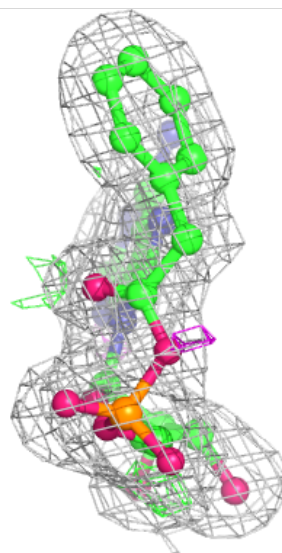
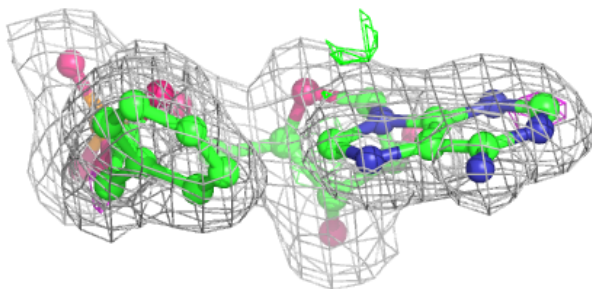
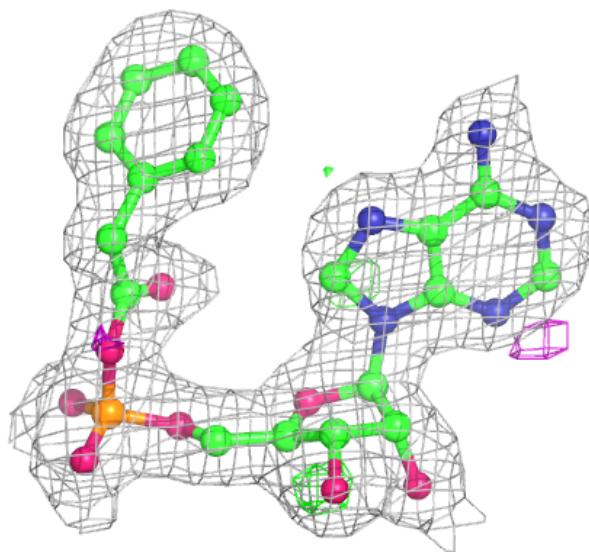
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	501	1/1	0.97	0.04	29,29,29,29	0
4	BME	A	504	4/4	0.97	0.14	35,38,39,43	2
4	BME	B	506	4/4	0.98	0.11	45,46,46,48	2
2	MG	B	502	1/1	0.98	0.17	45,45,45,45	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 DLL B 507:**

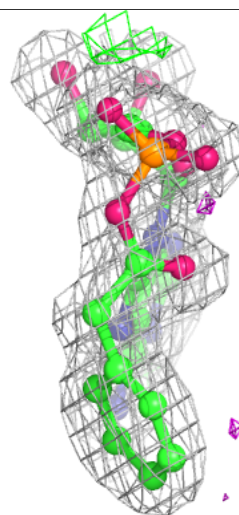
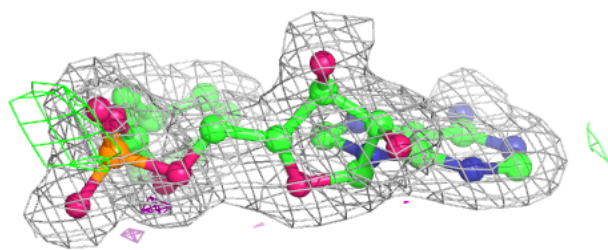
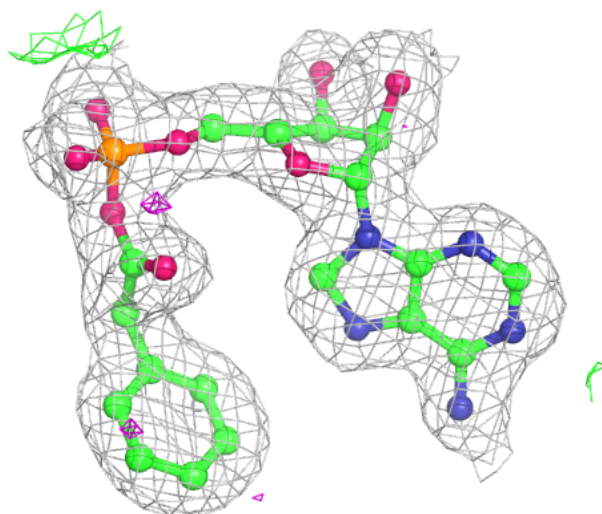
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around DLL A 505:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.