



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:37 PM BST

PDB ID : 3GUH  
Title : Crystal Structure of Wild-type E.coli GS in complex with ADP and DGM  
Authors : Sheng, F.; Geiger, J.  
Deposited on : 2009-03-30  
Resolution : 2.79 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 : 2.13.1  
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) : 2.13.1

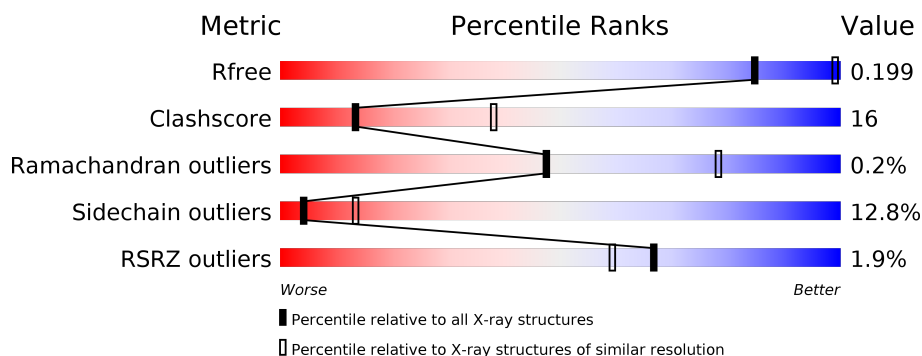
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	485	

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
4	ASO	A	488	-	-	X	-
6	ACT	A	493	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	494	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4055 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.

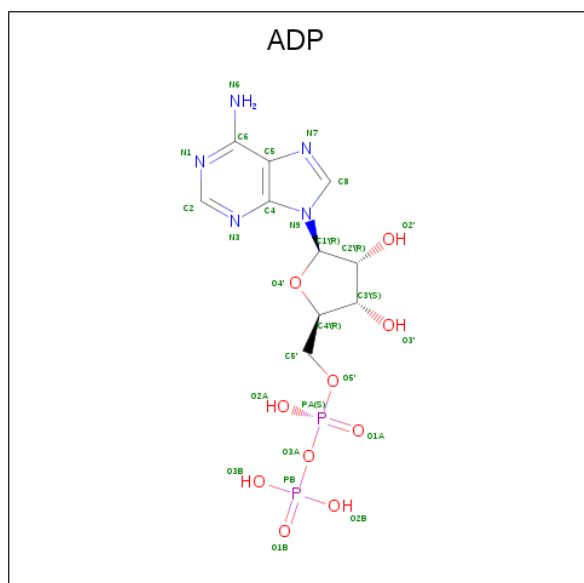
- Molecule 1 is a protein called Glycogen synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	477	3735	2401	652	669	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

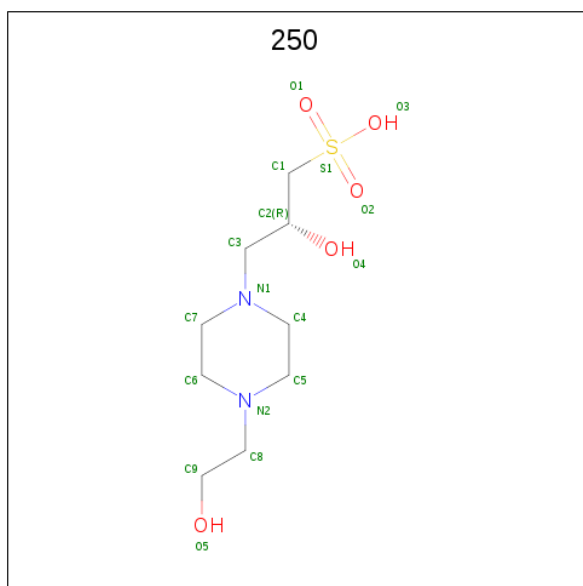
Chain	Residue	Modelled	Actual	Comment	Reference
A	478	LEU	-	expression tag	UNP P0A6U8
A	479	GLU	-	expression tag	UNP P0A6U8
A	480	HIS	-	expression tag	UNP P0A6U8
A	481	HIS	-	expression tag	UNP P0A6U8
A	482	HIS	-	expression tag	UNP P0A6U8
A	483	HIS	-	expression tag	UNP P0A6U8
A	484	HIS	-	expression tag	UNP P0A6U8
A	485	HIS	-	expression tag	UNP P0A6U8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



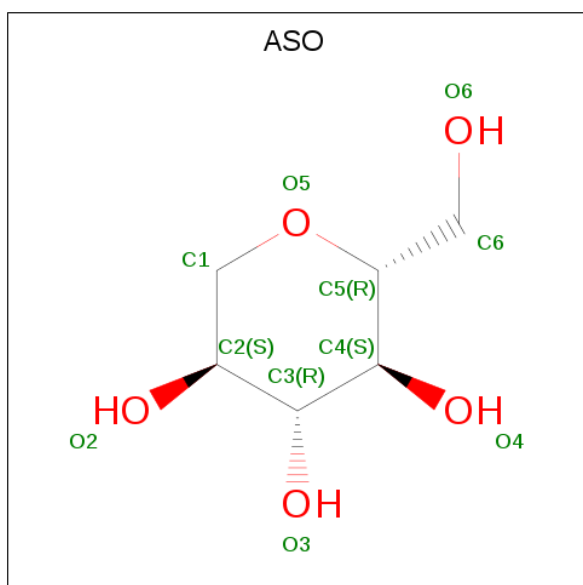
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is (2R)-2-hydroxy-3-[4-(2-hydroxyethyl)piperazin-1-yl]propane-1-sulfonic acid (three-letter code: 250) (formula:  $C_9H_{20}N_2O_5S$ ).



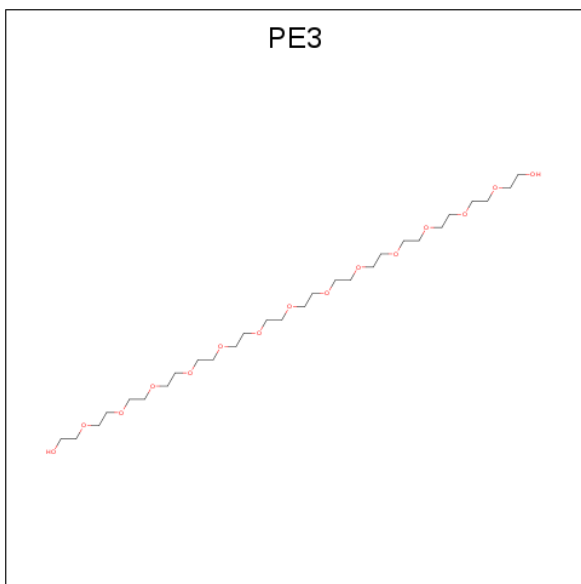
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			17	9	2	5	1		

- Molecule 4 is 1,5-anhydro-D-glucitol (three-letter code: ASO) (formula:  $C_6H_{12}O_5$ ).



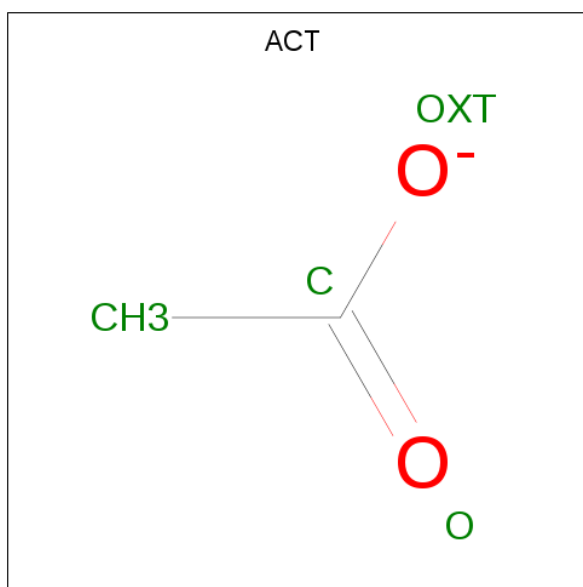
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 3,6,9,12,15,18,21,24,27,30,33,36,39-TRIDECAXAHENTETRACONTANE-1,41-DIOL (three-letter code: PE3) (formula:  $C_{28}H_{58}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			37	24	13		
5	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

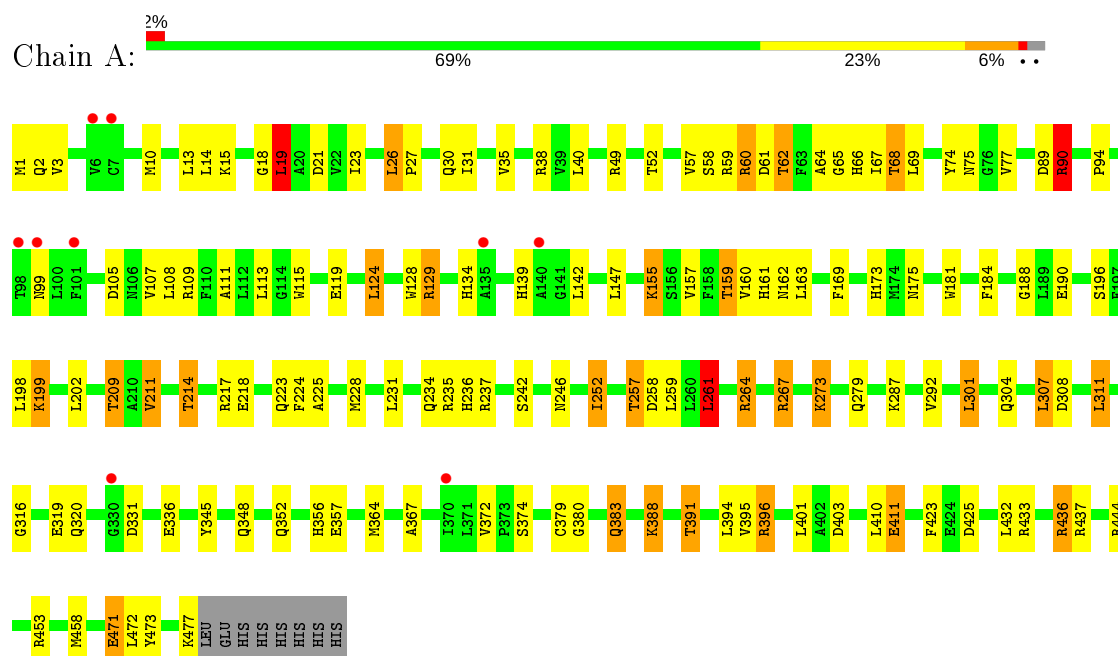
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		

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

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 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: Glycogen synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.84Å 125.84Å 153.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.79 29.93 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.79) 98.5 (29.93-2.79)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.169 , 0.200 0.166 , 0.199	Depositor DCC
$R_{free}$ test set	1478 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: 250, ACT, ASO, ADP, PE3

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	1.12	4/3834 (0.1%)	1.11	14/5213 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	GLU	CB-CG	6.68	1.64	1.52
1	A	411	GLU	CB-CG	-6.52	1.39	1.52
1	A	345	TYR	CE2-CZ	5.66	1.46	1.38
1	A	336	GLU	CB-CG	5.20	1.62	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	90	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	261	LEU	CA-CB-CG	6.66	130.62	115.30
1	A	437	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	19	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	A	267	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	129	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	425	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	237	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	307	LEU	CA-CB-CG	-5.20	103.34	115.30
1	A	21	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	264	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	410	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	89	ASP	CB-CG-OD1	5.12	122.91	118.30

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	3735	0	3679	118	0
2	A	27	0	12	1	0
3	A	17	0	20	4	0
4	A	11	0	12	6	0
5	A	48	0	61	7	0
6	A	8	0	6	0	0
7	A	209	0	0	24	0
All	All	4055	0	3790	123	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 16.

All (123) 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:331:ASP:HB2	7:A:557:HOH:O	1.38	1.22
3:A:487:250:H92	4:A:488:ASO:C1	1.71	1.18
1:A:234:GLN:HG3	7:A:526:HOH:O	1.47	1.12
1:A:217:ARG:HB3	5:A:489:PE3:H332	1.36	1.05
3:A:487:250:C9	4:A:488:ASO:H11	1.87	1.03
1:A:90:ARG:HD3	7:A:626:HOH:O	1.58	1.00
3:A:487:250:H92	4:A:488:ASO:H11	0.92	0.91
1:A:209:THR:CG2	7:A:512:HOH:O	2.18	0.91
1:A:258:ASP:HB3	1:A:261:LEU:HD22	1.50	0.90
1:A:383:GLN:H	1:A:383:GLN:HE21	1.19	0.89
1:A:273:LYS:NZ	1:A:391:THR:HG22	1.87	0.89
1:A:129:ARG:HD3	7:A:685:HOH:O	1.77	0.85
1:A:273:LYS:HZ3	1:A:391:THR:HG22	1.42	0.84
1:A:62:THR:HG22	1:A:64:ALA:H	1.41	0.84
1:A:62:THR:CG2	1:A:64:ALA:H	1.91	0.83
1:A:356:HIS:HB3	7:A:698:HOH:O	1.82	0.80
1:A:257:THR:HG21	7:A:525:HOH:O	1.81	0.79
1:A:10:MET:HG3	1:A:23:ILE:HG22	1.64	0.78
1:A:69:LEU:HD22	1:A:124:LEU:HD13	1.65	0.77
1:A:364:MET:O	1:A:391:THR:HG21	1.88	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:NE2	1:A:159:THR:CG2	2.51	0.72
1:A:159:THR:HB	1:A:209:THR:HG22	1.71	0.72
1:A:471:GLU:HB3	7:A:671:HOH:O	1.90	0.71
1:A:383:GLN:NE2	1:A:383:GLN:H	1.89	0.70
1:A:199:LYS:HG2	1:A:228:MET:CE	2.21	0.70
1:A:217:ARG:HE	5:A:489:PE3:H321	1.57	0.69
1:A:184:PHE:CZ	1:A:190:GLU:HG3	2.29	0.67
1:A:383:GLN:N	1:A:383:GLN:HE21	1.90	0.67
1:A:214:THR:HG23	1:A:403:ASP:CG	2.15	0.67
1:A:211:VAL:HG13	1:A:379:CYS:HB2	1.78	0.66
1:A:49:ARG:HD3	7:A:657:HOH:O	1.94	0.66
1:A:264:ARG:NE	7:A:680:HOH:O	2.09	0.66
1:A:59:ARG:HD2	1:A:68:THR:HB	1.79	0.64
1:A:3:VAL:HG21	1:A:473:TYR:CE2	2.34	0.63
1:A:209:THR:HG23	7:A:512:HOH:O	1.92	0.63
1:A:14:LEU:HD21	1:A:94:PRO:HG3	1.81	0.62
2:A:486:ADP:O1A	4:A:488:ASO:O4	2.08	0.62
1:A:252:ILE:O	1:A:252:ILE:HD12	2.00	0.61
1:A:236:HIS:CE1	5:A:489:PE3:H382	2.36	0.61
1:A:199:LYS:HG2	1:A:228:MET:HE1	1.83	0.61
1:A:134:HIS:NE2	1:A:159:THR:HG23	2.17	0.60
1:A:209:THR:HA	1:A:242:SER:O	2.01	0.60
1:A:273:LYS:HZ1	1:A:391:THR:HG22	1.67	0.59
1:A:161:HIS:O	4:A:488:ASO:H12	2.03	0.59
1:A:196:SER:HB3	1:A:199:LYS:HB2	1.85	0.59
1:A:436:ARG:HD2	7:A:583:HOH:O	2.03	0.59
1:A:62:THR:HB	1:A:65:GLY:O	2.02	0.59
1:A:62:THR:HG22	1:A:64:ALA:N	2.16	0.58
1:A:287:LYS:HE2	7:A:688:HOH:O	2.03	0.58
1:A:115:TRP:CH2	1:A:119:GLU:HG3	2.39	0.57
1:A:199:LYS:HG2	1:A:228:MET:HE3	1.85	0.57
1:A:134:HIS:NE2	1:A:159:THR:HG21	2.20	0.57
1:A:18:GLY:HA3	4:A:488:ASO:H5	1.88	0.56
5:A:491:PE3:C11	7:A:591:HOH:O	2.53	0.56
1:A:52:THR:N	7:A:568:HOH:O	2.38	0.56
1:A:111:ALA:HA	1:A:142:LEU:HD12	1.87	0.55
1:A:214:THR:HB	1:A:217:ARG:NH1	2.23	0.54
1:A:38:ARG:HD3	1:A:128:TRP:CZ2	2.43	0.54
1:A:458:MET:HE3	7:A:495:HOH:O	2.06	0.54
1:A:184:PHE:CE2	1:A:190:GLU:HG3	2.43	0.53
1:A:26:LEU:HD22	1:A:30:GLN:HG3	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TRP:HZ3	7:A:556:HOH:O	1.89	0.53
1:A:388:LYS:HB2	7:A:661:HOH:O	2.08	0.53
1:A:62:THR:HG23	1:A:64:ALA:H	1.72	0.52
1:A:214:THR:HG21	5:A:489:PE3:H241	1.90	0.52
1:A:380:GLY:O	1:A:383:GLN:NE2	2.36	0.52
1:A:436:ARG:CD	7:A:583:HOH:O	2.58	0.51
1:A:163:LEU:HD23	1:A:225:ALA:HA	1.93	0.50
1:A:62:THR:HG22	1:A:65:GLY:N	2.27	0.49
1:A:159:THR:HB	1:A:209:THR:CG2	2.40	0.49
1:A:223:GLN:HB3	7:A:587:HOH:O	2.13	0.49
1:A:19:LEU:HD23	1:A:161:HIS:CE1	2.47	0.49
1:A:383:GLN:NE2	1:A:383:GLN:N	2.57	0.48
1:A:27:PRO:O	1:A:31:ILE:HG12	2.13	0.48
1:A:155:LYS:HD3	7:A:575:HOH:O	2.12	0.48
1:A:109:ARG:NH2	7:A:604:HOH:O	2.46	0.48
1:A:74:TYR:O	1:A:75:ASN:HB2	2.13	0.48
1:A:2:GLN:HB3	1:A:128:TRP:CZ2	2.48	0.48
1:A:267:ARG:HD2	1:A:453:ARG:O	2.14	0.48
1:A:188:GLY:O	1:A:199:LYS:HD2	2.14	0.47
1:A:258:ASP:HB3	1:A:261:LEU:CD2	2.35	0.47
1:A:199:LYS:HA	1:A:228:MET:HE1	1.96	0.47
1:A:301:LEU:HD12	1:A:307:LEU:CD1	2.44	0.47
1:A:90:ARG:NH2	1:A:105:ASP:OD2	2.47	0.47
1:A:301:LEU:HD12	1:A:307:LEU:HD12	1.97	0.47
1:A:214:THR:CG2	1:A:403:ASP:OD1	2.63	0.47
1:A:217:ARG:HD2	5:A:489:PE3:H351	1.97	0.46
1:A:139:HIS:NE2	3:A:487:250:H2	2.30	0.46
1:A:15:LYS:HD3	1:A:357:GLU:OE2	2.16	0.46
1:A:367:ALA:O	1:A:391:THR:HB	2.15	0.46
1:A:161:HIS:O	1:A:162:ASN:HB2	2.16	0.46
1:A:38:ARG:HD3	1:A:128:TRP:CE2	2.51	0.46
1:A:252:ILE:C	1:A:252:ILE:HD12	2.37	0.45
1:A:308:ASP:OD1	1:A:308:ASP:N	2.48	0.45
1:A:217:ARG:HE	5:A:489:PE3:H302	1.82	0.45
1:A:38:ARG:HD2	7:A:492:HOH:O	2.16	0.45
1:A:214:THR:HG23	1:A:403:ASP:OD1	2.16	0.45
1:A:173:HIS:C	1:A:175:ASN:H	2.19	0.45
1:A:67:ILE:HG13	1:A:67:ILE:O	2.16	0.45
1:A:380:GLY:C	1:A:383:GLN:HE22	2.18	0.44
1:A:214:THR:HG23	1:A:403:ASP:OD2	2.17	0.44
1:A:388:LYS:O	1:A:388:LYS:HG3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:HB	1:A:169:PHE:CD2	2.53	0.43
1:A:211:VAL:HG22	1:A:246:ASN:ND2	2.33	0.43
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.71	0.43
1:A:57:VAL:O	1:A:58:SER:HB3	2.18	0.43
1:A:374:SER:O	1:A:396:ARG:HD3	2.18	0.43
1:A:202:LEU:HD12	1:A:228:MET:HE2	2.01	0.43
1:A:90:ARG:HH22	1:A:105:ASP:CG	2.22	0.43
1:A:173:HIS:C	1:A:175:ASN:N	2.72	0.43
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.65	0.42
1:A:396:ARG:HG3	1:A:423:PHE:CE1	2.53	0.42
1:A:211:VAL:HG22	1:A:246:ASN:HD21	1.84	0.42
1:A:26:LEU:N	1:A:27:PRO:CD	2.83	0.42
1:A:218:GLU:HB3	1:A:224:PHE:CD1	2.55	0.42
1:A:61:ASP:HA	1:A:66:HIS:HD2	1.85	0.41
1:A:202:LEU:HD12	1:A:228:MET:CE	2.50	0.41
1:A:372:VAL:HB	1:A:395:VAL:HG12	2.01	0.41
1:A:394:LEU:C	1:A:394:LEU:HD23	2.41	0.41
1:A:60:ARG:NH1	7:A:662:HOH:O	2.40	0.41
1:A:395:VAL:HB	1:A:401:LEU:HD13	2.03	0.41
1:A:316:GLY:O	1:A:320:GLN:HG3	2.21	0.41
1:A:31:ILE:HA	1:A:35:VAL:O	2.22	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	475/485 (98%)	451 (95%)	23 (5%)	1 (0%)	47 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLN

### 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	382/390 (98%)	333 (87%)	49 (13%)	4 13

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	LEU
1	A	19	LEU
1	A	26	LEU
1	A	40	LEU
1	A	60	ARG
1	A	62	THR
1	A	68	THR
1	A	77	VAL
1	A	90	ARG
1	A	99	ASN
1	A	108	LEU
1	A	113	LEU
1	A	124	LEU
1	A	147	LEU
1	A	155	LYS
1	A	157	VAL
1	A	159	THR
1	A	160	VAL
1	A	198	LEU
1	A	199	LYS
1	A	209	THR
1	A	211	VAL
1	A	214	THR
1	A	231	LEU
1	A	235	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	252	ILE
1	A	257	THR
1	A	259	LEU
1	A	261	LEU
1	A	273	LYS
1	A	279	GLN
1	A	292	VAL
1	A	301	LEU
1	A	311	LEU
1	A	319	GLU
1	A	348	GLN
1	A	352	GLN
1	A	383	GLN
1	A	388	LYS
1	A	391	THR
1	A	396	ARG
1	A	411	GLU
1	A	432	LEU
1	A	433	ARG
1	A	436	ARG
1	A	444	ARG
1	A	472	LEU
1	A	477	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	166	GLN
1	A	207	HIS
1	A	223	GLN
1	A	233	GLN
1	A	236	HIS
1	A	246	ASN
1	A	281	GLN
1	A	320	GLN
1	A	352	GLN
1	A	383	GLN
1	A	454	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

7 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	$\# Z  > 2$
6	ACT	A	493	-	1,3,3	2.84	1 (100%)	0,3,3	0.00	-
4	ASO	A	488	-	11,11,11	1.03	0	15,15,15	3.97	7 (46%)
6	ACT	A	494	-	1,3,3	2.60	1 (100%)	0,3,3	0.00	-
5	PE3	A	489	-	36,36,42	0.74	0	35,35,41	0.71	0
3	250	A	487	-	17,17,17	1.13	2 (11%)	21,23,23	2.97	10 (47%)
2	ADP	A	486	-	24,29,29	0.85	0	29,45,45	1.50	3 (10%)
5	PE3	A	491	-	10,10,42	0.83	0	9,9,41	0.92	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	ASO	A	488	-	-	2/2/19/19	0/1/1/1
5	PE3	A	489	-	-	19/34/34/40	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PE3	A	491	-	-	6/8/8/40	-
3	250	A	487	-	-	3/12/22/22	0/1/1/1
2	ADP	A	486	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	493	ACT	CH3-C	2.84	1.52	1.48
3	A	487	250	C1-C2	2.70	1.56	1.51
6	A	494	ACT	CH3-C	2.60	1.52	1.48
3	A	487	250	C1-S1	-2.27	1.69	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	488	ASO	O5-C1-C2	9.89	126.03	110.77
4	A	488	ASO	C1-O5-C5	8.71	123.99	112.19
3	A	487	250	C4-N1-C7	5.68	121.62	108.83
3	A	487	250	C5-N2-C6	5.36	120.89	108.83
4	A	488	ASO	C3-C4-C5	5.34	119.77	110.24
2	A	486	ADP	N3-C2-N1	-5.02	120.83	128.68
3	A	487	250	O1-S1-C1	4.97	112.85	106.94
3	A	487	250	C8-N2-C5	4.46	122.65	111.23
3	A	487	250	C4-N1-C3	4.27	123.59	111.20
3	A	487	250	C7-C6-N2	-4.20	102.03	110.64
4	A	488	ASO	O4-C4-C5	-3.53	100.53	109.30
2	A	486	ADP	O2B-PB-O1B	2.98	122.35	110.68
3	A	487	250	O2-S1-O1	-2.80	104.27	113.95
3	A	487	250	C2-C3-N1	-2.67	107.38	112.23
4	A	488	ASO	O4-C4-C3	-2.44	104.71	110.35
2	A	486	ADP	C1'-N9-C4	-2.42	122.39	126.64
3	A	487	250	O3-S1-C1	-2.40	101.91	105.74
4	A	488	ASO	C6-C5-C4	-2.15	107.98	113.00
4	A	488	ASO	O5-C5-C4	-2.07	105.80	110.83
3	A	487	250	C8-N2-C6	2.02	116.39	111.23

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	486	ADP	PB-O3A-PA-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	486	ADP	O4'-C4'-C5'-O5'
2	A	486	ADP	C3'-C4'-C5'-O5'
5	A	491	PE3	O4-C5-C6-O7
5	A	489	PE3	O31-C32-C33-O34
5	A	489	PE3	O16-C17-C18-O19
4	A	488	ASO	O5-C5-C6-O6
5	A	489	PE3	O19-C20-C21-O22
3	A	487	250	C2-C3-N1-C7
5	A	491	PE3	O7-C8-C9-O10
4	A	488	ASO	C4-C5-C6-O6
5	A	489	PE3	O22-C23-C24-O25
5	A	489	PE3	O28-C29-C30-O31
2	A	486	ADP	PA-O3A-PB-O1B
5	A	489	PE3	C23-C24-O25-C26
5	A	489	PE3	C11-C12-O13-C14
3	A	487	250	C9-C8-N2-C6
5	A	489	PE3	C29-C30-O31-C32
5	A	491	PE3	C2-C3-O4-C5
5	A	491	PE3	C6-C5-O4-C3
5	A	489	PE3	O4-C5-C6-O7
5	A	489	PE3	C36-C35-O34-C33
5	A	491	PE3	C8-C9-O10-C11
5	A	489	PE3	C33-C32-O31-C30
5	A	489	PE3	C21-C20-O19-C18
5	A	489	PE3	C9-C8-O7-C6
5	A	489	PE3	C14-C15-O16-C17
5	A	489	PE3	C17-C18-O19-C20
3	A	487	250	N2-C8-C9-O5
5	A	489	PE3	C26-C27-O28-C29
5	A	489	PE3	O10-C11-C12-O13
5	A	489	PE3	C24-C23-O22-C21
5	A	489	PE3	O25-C26-C27-O28
5	A	491	PE3	O1-C2-C3-O4

There are no ring outliers.

5 monomers are involved in 14 short contacts:

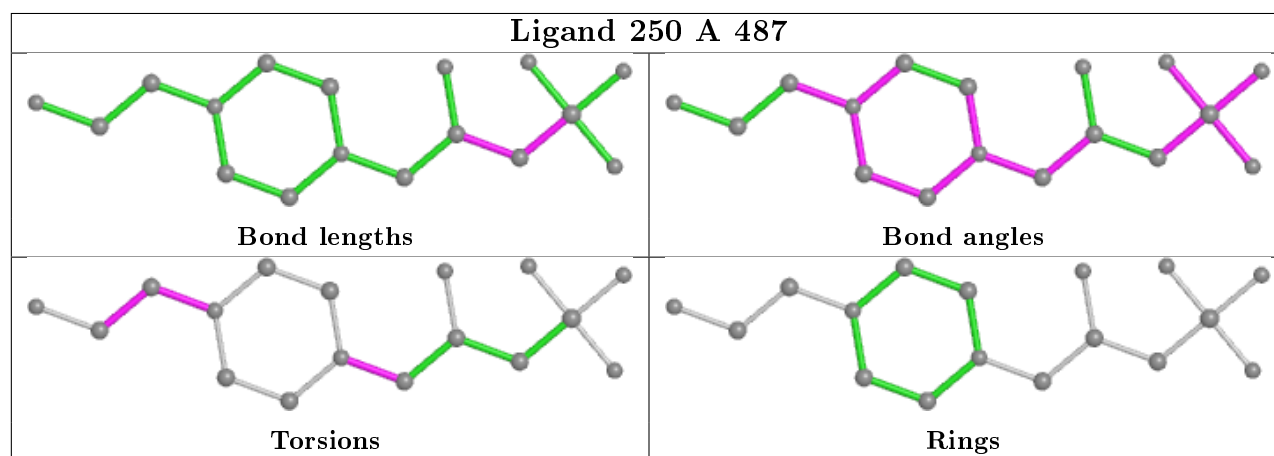
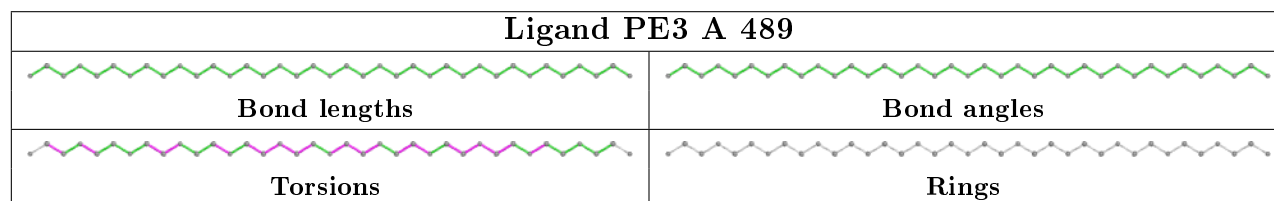
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	488	ASO	6	0
5	A	489	PE3	6	0
3	A	487	250	4	0
2	A	486	ADP	1	0

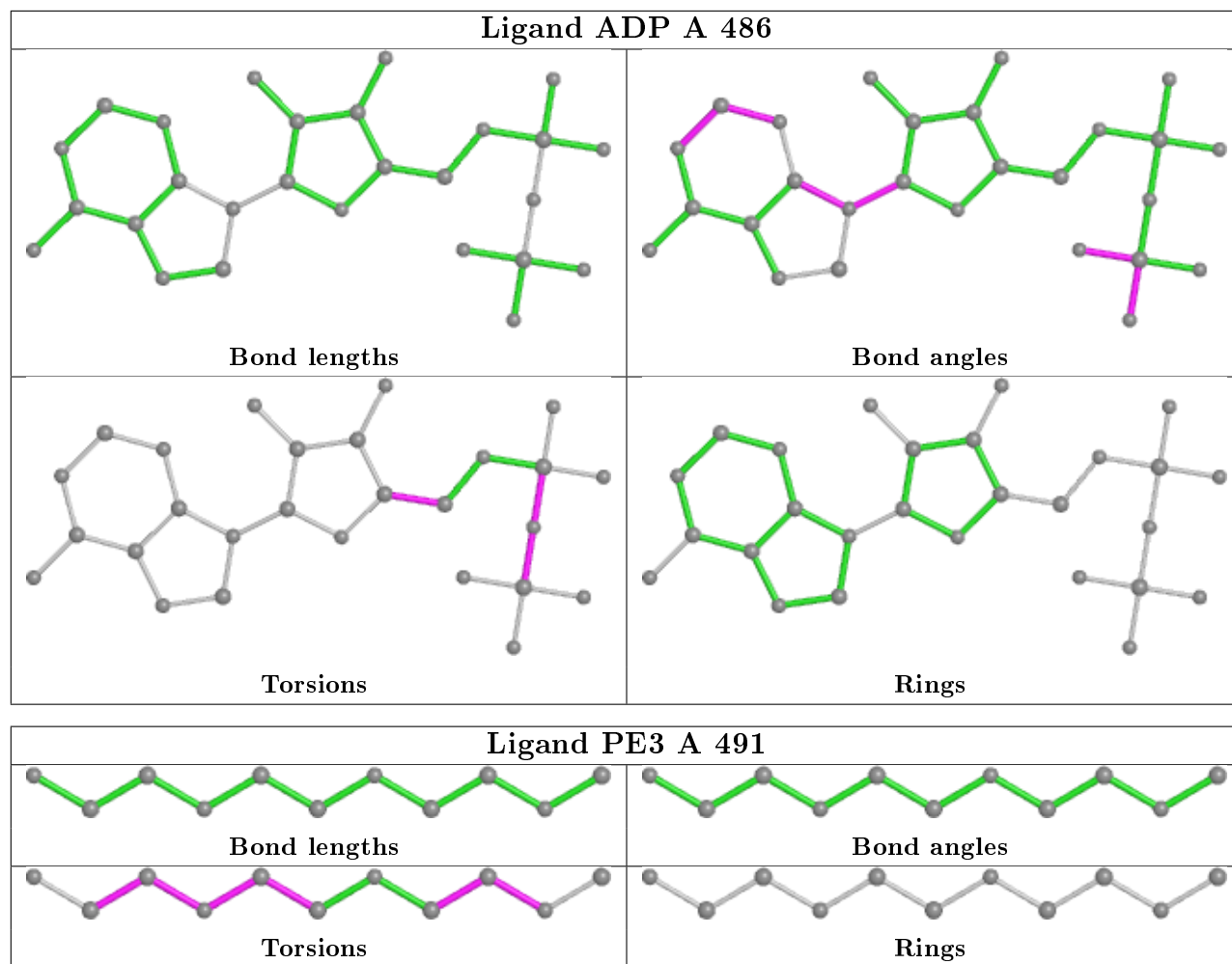
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	491	PE3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	477/485 (98%)	-0.51	9 (1%) 66 59	22, 37, 57, 75	28 (5%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	GLY	2.6
1	A	99	ASN	2.5
1	A	135	ALA	2.5
1	A	98	THR	2.3
1	A	101	PHE	2.3
1	A	140	ALA	2.2
1	A	6	VAL	2.1
1	A	370	ILE	2.1
1	A	7	CYS	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

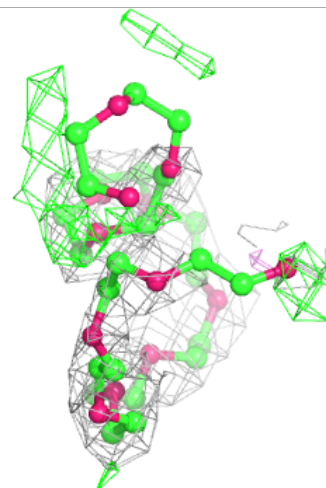
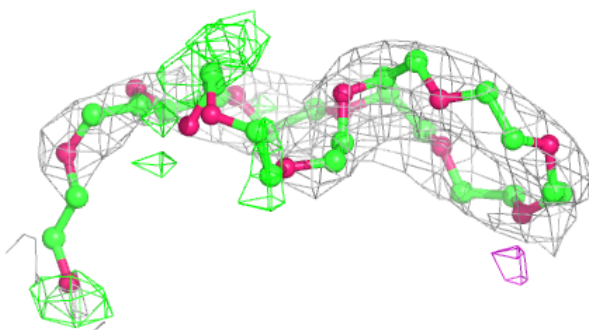
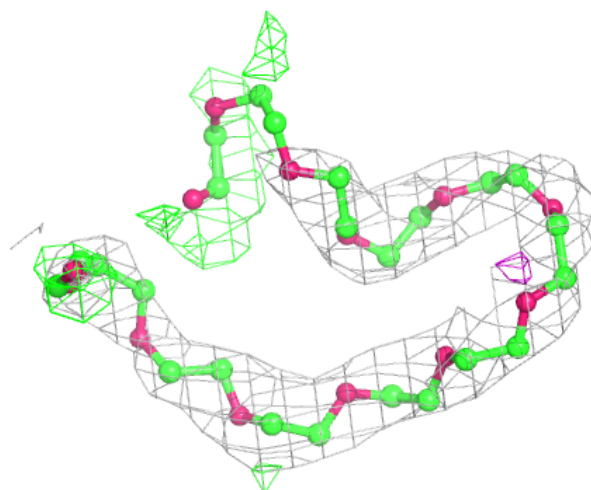
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ACT	A	494	4/4	0.58	0.47	122,122,122,122	0
6	ACT	A	493	4/4	0.69	0.46	111,112,112,112	0
5	PE3	A	489	37/43	0.89	0.36	65,77,90,91	9
5	PE3	A	491	11/43	0.89	0.18	67,76,80,80	0
3	250	A	487	17/17	0.93	0.21	54,63,70,71	0
4	ASO	A	488	11/11	0.95	0.33	2,19,22,27	11
2	ADP	A	486	27/27	0.98	0.10	34,41,45,48	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.

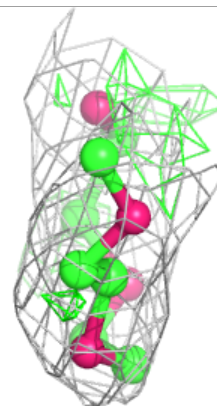
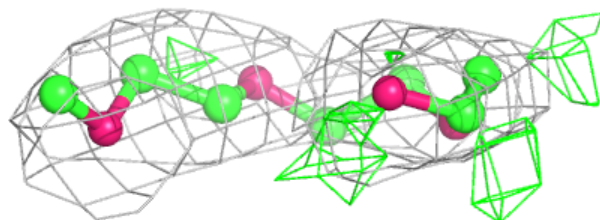
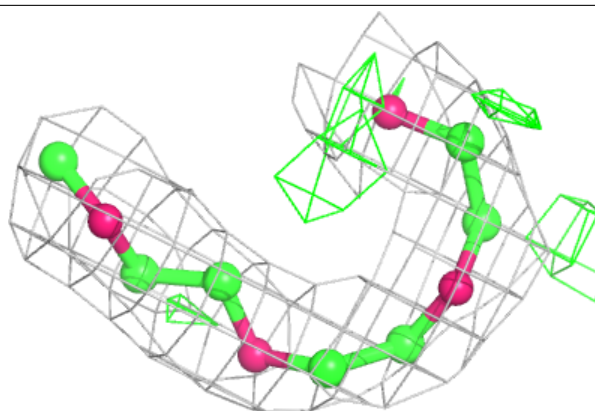
**Electron density around PE3 A 489:**

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)

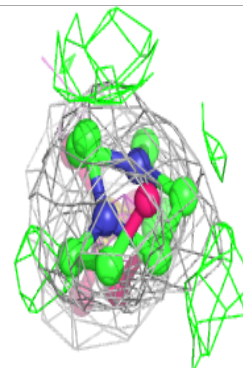
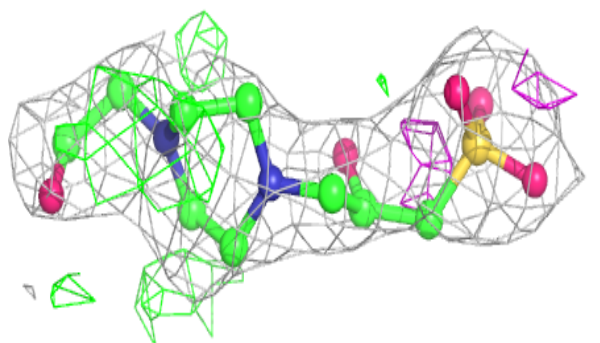
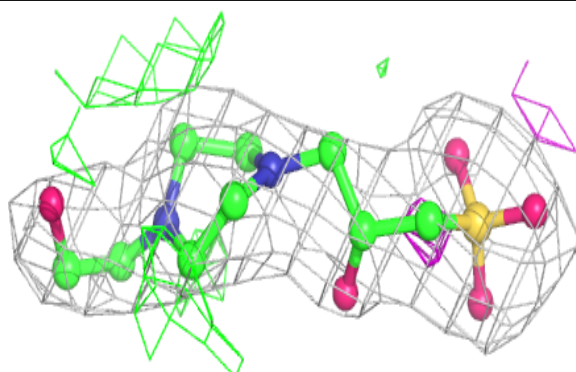


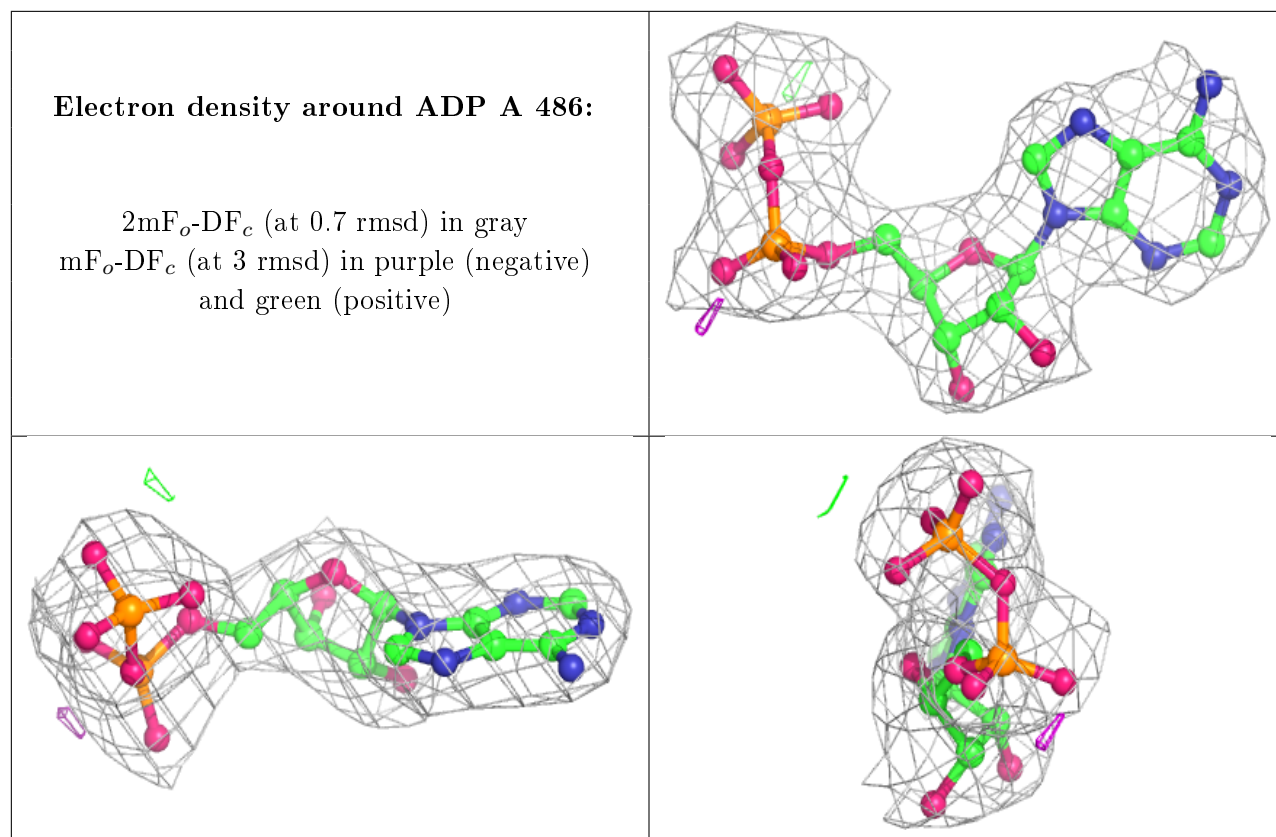
**Electron density around PE3 A 491:**

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

**Electron density around 250 A 487:**

$2mF_o-DF_c$  (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.