



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:17 am BST

PDB ID : 5OE3  
Title : Crystal structure of the N-terminal domain of PqsA in complex with anthraniloyl-AMP (crystal form 1)  
Authors : Witzgall, F.; Ewert, W.; Blankenfeldt, W.  
Deposited on : 2017-07-07  
Resolution : 1.43 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.

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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

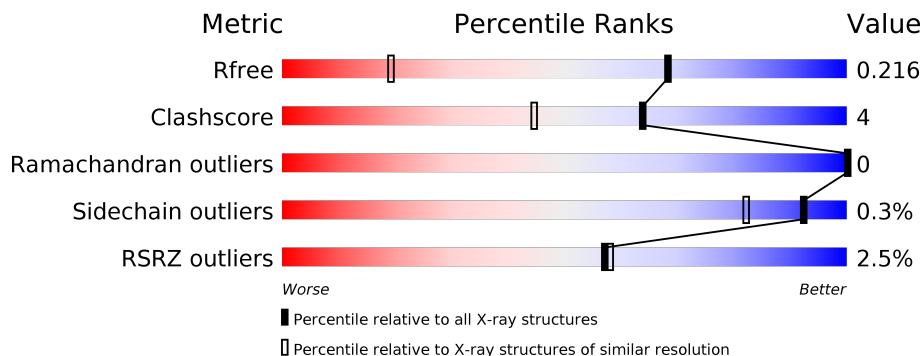
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	407	 2% 90% 7% •
1	B	407	 2% 88% 8% •
1	C	407	 3% 89% 7% •
1	D	407	 2% 92% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	503	-	-	X	-
5	ACT	B	905	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 28424 atoms, of which 13033 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 Anthranilate–CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	394	6310	2018	3154	561	564	13	0	22	0
1	B	393	6299	2012	3147	562	564	14	0	25	0
1	C	394	6448	2050	3233	579	572	14	0	32	0
1	D	393	6440	2048	3234	576	568	14	0	34	0

There are 32 discrepancies between the modelled and reference sequences:

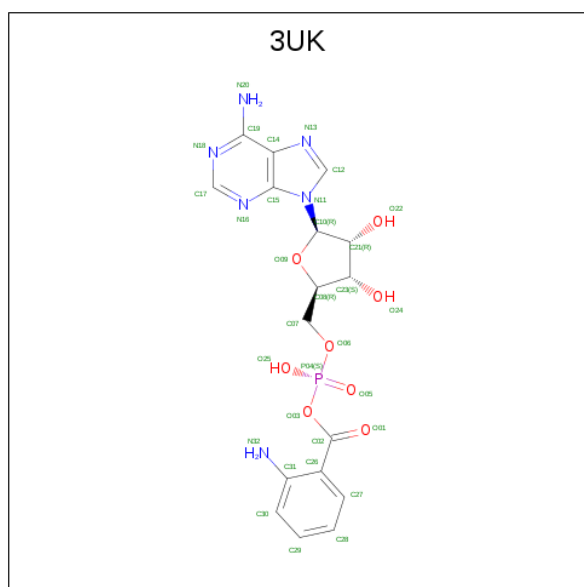
Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LEU	-	expression tag	UNP Q9I4X3
A	401	GLU	-	expression tag	UNP Q9I4X3
A	402	HIS	-	expression tag	UNP Q9I4X3
A	403	HIS	-	expression tag	UNP Q9I4X3
A	404	HIS	-	expression tag	UNP Q9I4X3
A	405	HIS	-	expression tag	UNP Q9I4X3
A	406	HIS	-	expression tag	UNP Q9I4X3
A	407	HIS	-	expression tag	UNP Q9I4X3
B	400	LEU	-	expression tag	UNP Q9I4X3
B	401	GLU	-	expression tag	UNP Q9I4X3
B	402	HIS	-	expression tag	UNP Q9I4X3
B	403	HIS	-	expression tag	UNP Q9I4X3
B	404	HIS	-	expression tag	UNP Q9I4X3
B	405	HIS	-	expression tag	UNP Q9I4X3
B	406	HIS	-	expression tag	UNP Q9I4X3
B	407	HIS	-	expression tag	UNP Q9I4X3
C	400	LEU	-	expression tag	UNP Q9I4X3
C	401	GLU	-	expression tag	UNP Q9I4X3
C	402	HIS	-	expression tag	UNP Q9I4X3
C	403	HIS	-	expression tag	UNP Q9I4X3
C	404	HIS	-	expression tag	UNP Q9I4X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	HIS	-	expression tag	UNP Q9I4X3
C	406	HIS	-	expression tag	UNP Q9I4X3
C	407	HIS	-	expression tag	UNP Q9I4X3
D	400	LEU	-	expression tag	UNP Q9I4X3
D	401	GLU	-	expression tag	UNP Q9I4X3
D	402	HIS	-	expression tag	UNP Q9I4X3
D	403	HIS	-	expression tag	UNP Q9I4X3
D	404	HIS	-	expression tag	UNP Q9I4X3
D	405	HIS	-	expression tag	UNP Q9I4X3
D	406	HIS	-	expression tag	UNP Q9I4X3
D	407	HIS	-	expression tag	UNP Q9I4X3

- Molecule 2 is 5'-O-[(S)-[(2-aminobenzoyl)oxy](hydroxy)phosphoryl]adenosine (three-letter code: 3UK) (formula: C<sub>17</sub>H<sub>19</sub>N<sub>6</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	H	N	O			P	
2	A	1	Total	51	17	19	6	8	1	0	0
2	B	1	Total	51	17	19	6	8	1	0	0
2	C	1	Total	51	17	19	6	8	1	0	0
2	D	1	Total	51	17	19	6	8	1	0	0

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



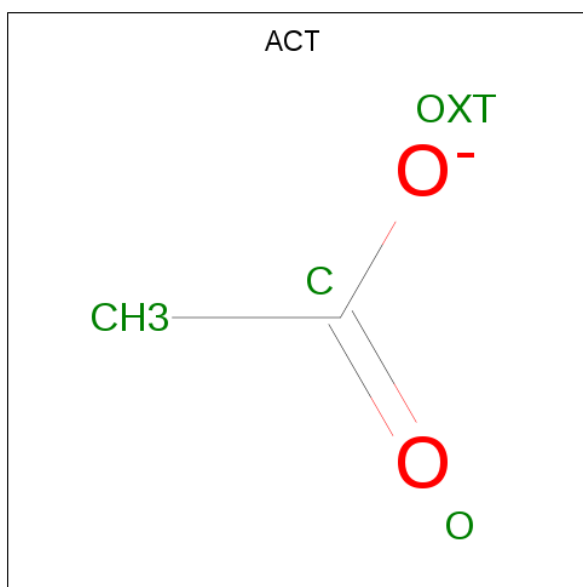
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	1
			34	8	20	6		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



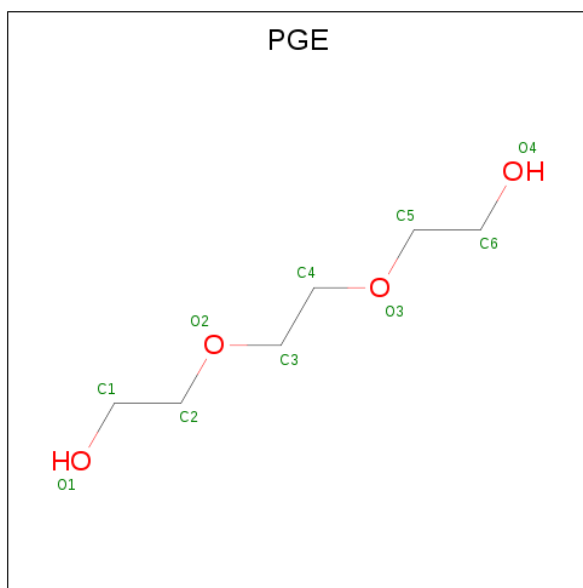
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	D	1	10	2	6	2	0	0
4	D	1	10	2	6	2	0	0
4	D	1	10	2	6	2	0	0
4	D	1	10	2	6	2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	D	1	24	6	14	4	0	0

- Molecule 7 is water.

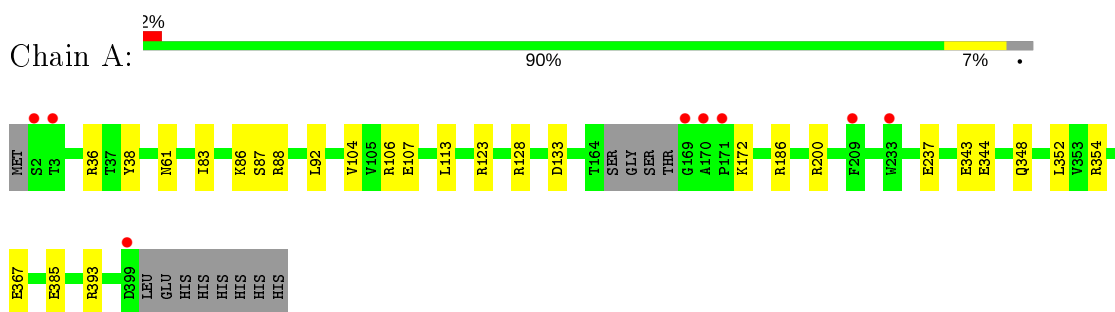


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	627	Total 628	O 628	0	6
7	B	615	Total 615	O 615	0	5
7	C	601	Total 602	O 602	0	4
7	D	557	Total 557	O 557	0	7

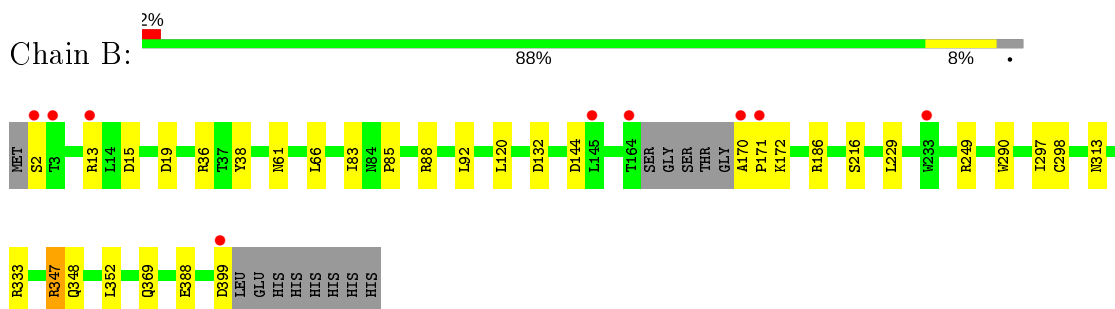
### 3 Residue-property plots [i](#)

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.

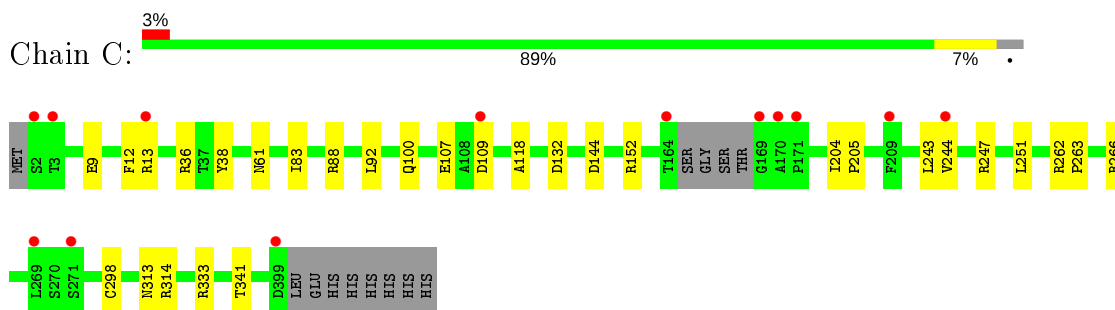
- Molecule 1: Anthranilate–CoA ligase



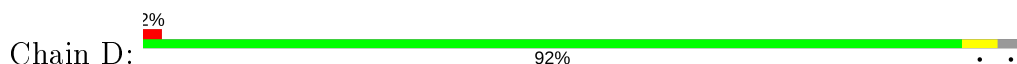
- Molecule 1: Anthranilate–CoA ligase

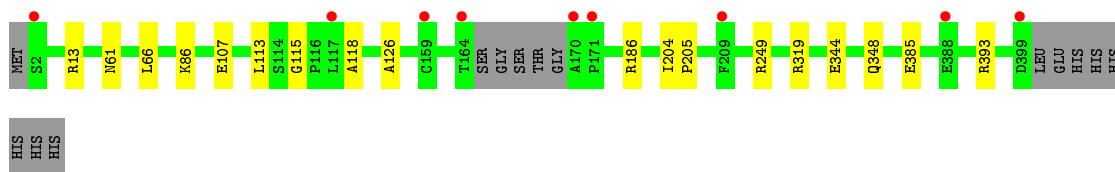


- Molecule 1: Anthranilate–CoA ligase



- Molecule 1: Anthranilate–CoA ligase





HIS  
HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.53Å 84.45Å 139.01Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	48.71 – 1.43 48.71 – 1.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.71-1.43) 100.0 (48.71-1.43)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 1.43Å)	Xtrriage
Refinement program	PHENIX 1.12rc2_2821	Depositor
R, $R_{free}$	0.190 , 0.216 0.190 , 0.216	Depositor DCC
$R_{free}$ test set	14966 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	28424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7624e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PEG, PGE, 3UK, EDO, ACT

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	0.28	0/3308	0.54	0/4496
1	B	0.27	0/3300	0.52	0/4482
1	C	0.27	0/3384	0.50	0/4593
1	D	0.28	0/3380	0.52	0/4589
All	All	0.28	0/13372	0.52	0/18160

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 [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	3156	3154	3145	24	0
1	B	3152	3147	3132	29	0
1	C	3215	3233	3204	27	0
1	D	3206	3234	3174	21	0
2	A	32	19	18	1	0
2	B	32	19	18	0	0
2	C	32	19	18	0	0
2	D	32	19	18	1	0
3	A	21	30	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	42	60	60	3	0
3	D	7	10	10	0	0
4	A	16	24	24	2	0
4	B	16	24	24	0	0
4	D	16	24	24	1	0
5	B	4	3	3	4	0
6	D	10	14	14	0	0
7	A	628	0	0	15	10
7	B	615	0	0	21	4
7	C	602	0	0	15	9
7	D	557	0	0	18	4
All	All	15391	13033	12916	109	15

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (109) 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:172[B]:LYS:NZ	7:B:1002:HOH:O	1.93	1.00
1:D:115:GLY:O	7:D:1001:HOH:O	1.81	0.97
1:B:144:ASP:OD1	7:B:1001:HOH:O	1.88	0.92
1:D:113:LEU:O	7:D:1002:HOH:O	1.93	0.86
1:D:393[B]:ARG:NH2	7:D:1003:HOH:O	2.10	0.84
1:B:347:ARG:NH1	7:B:1007:HOH:O	2.10	0.83
1:B:399:ASP:OD1	7:B:1003:HOH:O	1.96	0.82
1:B:186[B]:ARG:NH1	7:B:1011:HOH:O	2.15	0.80
1:C:152[A]:ARG:NH1	7:C:604:HOH:O	2.14	0.79
1:D:61:ASN:N	1:D:107[B]:GLU:OE1	2.16	0.78
1:A:38[B]:TYR:OH	7:A:602:HOH:O	2.03	0.76
1:B:88[A]:ARG:NH2	7:B:1012:HOH:O	2.17	0.76
1:B:13:ARG:NH1	7:B:1013:HOH:O	2.18	0.76
1:D:61:ASN:ND2	1:D:107[A]:GLU:OE2	2.19	0.75
1:B:348:GLN:OE1	7:B:1004:HOH:O	2.03	0.75
1:B:19[B]:ASP:OD1	7:B:1005:HOH:O	2.05	0.73
1:A:123:ARG:NE	7:A:611:HOH:O	2.21	0.73
1:B:172[B]:LYS:O	7:B:1006:HOH:O	2.07	0.73
1:C:144:ASP:OD1	7:C:601:HOH:O	2.07	0.72
1:C:314[A]:ARG:NH1	7:C:606:HOH:O	2.23	0.71
1:D:186[A]:ARG:NH2	7:D:1013:HOH:O	2.25	0.69
1:C:109:ASP:OD2	7:C:603:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249[B]:ARG:NH1	7:D:1014:HOH:O	2.26	0.69
1:A:348[A]:GLN:OE1	7:A:603:HOH:O	2.10	0.68
1:B:388:GLU:OE1	7:B:1009:HOH:O	2.12	0.68
1:C:244:VAL:O	1:C:247[B]:ARG:NE	2.26	0.68
1:B:249[A]:ARG:NH2	7:B:1014:HOH:O	2.26	0.68
1:A:128:ARG:NH2	7:A:610:HOH:O	2.19	0.67
1:A:133:ASP:OD1	7:A:604:HOH:O	2.13	0.66
1:B:15:ASP:OD1	7:B:1010:HOH:O	2.12	0.66
1:C:12:PHE:O	1:C:36[B]:ARG:NH2	2.30	0.65
1:A:237:GLU:OE2	7:A:605:HOH:O	2.14	0.65
1:D:186[B]:ARG:NH1	7:D:1017:HOH:O	2.30	0.65
1:A:88[B]:ARG:NH2	7:A:617:HOH:O	2.29	0.64
1:C:262:ARG:HB2	3:C:503:PEG:H12	1.79	0.64
1:A:172:LYS:O	7:A:606:HOH:O	2.15	0.63
1:A:86:LYS:HA	3:A:503:PEG:H22	1.81	0.63
1:C:118:ALA:N	7:C:612:HOH:O	2.32	0.62
1:C:266[A]:ARG:NH1	7:C:611:HOH:O	2.31	0.62
1:B:88[B]:ARG:NH1	7:B:1021:HOH:O	2.32	0.61
1:B:333[B]:ARG:NH1	7:B:1015:HOH:O	2.27	0.60
1:C:100[A]:GLN:OE1	3:C:504[A]:PEG:O4	2.14	0.60
1:B:172[A]:LYS:O	7:B:1006:HOH:O	2.15	0.60
1:C:88[C]:ARG:NH1	7:C:614:HOH:O	2.35	0.59
1:A:354[A]:ARG:NH2	7:A:625:HOH:O	2.37	0.57
1:A:385:GLU:OE2	1:A:393:ARG:NH2	2.37	0.57
1:C:38[A]:TYR:OH	1:C:132:ASP:O	2.17	0.57
1:D:344:GLU:OE1	7:D:1006:HOH:O	2.17	0.57
1:D:186[A]:ARG:NH1	7:D:1023:HOH:O	2.37	0.56
1:A:200[B]:ARG:NH1	7:A:627:HOH:O	2.38	0.55
1:B:36:ARG:NH2	7:B:1019:HOH:O	2.30	0.55
1:D:348:GLN:OE1	7:D:1007:HOH:O	2.18	0.55
1:A:106:ARG:NH2	3:A:503:PEG:H12	2.22	0.55
1:D:13[B]:ARG:NH1	7:D:1027:HOH:O	2.40	0.54
1:A:343:GLU:O	7:A:608:HOH:O	2.18	0.54
1:A:367:GLU:OE1	7:A:609:HOH:O	2.18	0.54
1:B:186[B]:ARG:NH2	7:B:1023:HOH:O	2.34	0.54
1:C:333[B]:ARG:NE	1:C:341:THR:OG1	2.38	0.53
4:A:506:EDO:O2	7:A:607:HOH:O	2.15	0.53
1:D:107[B]:GLU:OE2	7:D:1004:HOH:O	2.17	0.53
1:C:13[A]:ARG:NH1	7:C:623:HOH:O	2.42	0.52
1:C:100[B]:GLN:NE2	7:C:626:HOH:O	2.43	0.51
1:C:266[B]:ARG:NH2	7:C:608:HOH:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:905:ACT:H1	7:B:1111:HOH:O	2.11	0.51
1:B:38[A]:TYR:OH	1:B:132:ASP:O	2.25	0.50
1:D:204:ILE:HB	1:D:205:PRO:HD3	1.92	0.49
5:B:905:ACT:H3	7:B:1306:HOH:O	2.12	0.49
1:A:88[A]:ARG:NH1	7:A:623:HOH:O	2.34	0.49
1:A:83:ILE:HD11	1:A:92:LEU:HD13	1.95	0.48
4:D:904:EDO:O1	7:D:1008:HOH:O	2.20	0.47
1:D:118:ALA:N	7:D:1034:HOH:O	2.46	0.47
1:A:106:ARG:HH21	3:A:503:PEG:C1	2.28	0.47
1:B:120:LEU:N	5:B:905:ACT:OXT	2.43	0.46
1:C:152[A]:ARG:NH1	7:C:616:HOH:O	2.35	0.46
1:B:83:ILE:HD11	1:B:92:LEU:HD13	1.97	0.46
1:A:186:ARG:HE	4:A:506:EDO:C2	2.29	0.46
1:A:104[B]:VAL:HG11	1:A:113:LEU:HD13	1.98	0.46
1:C:107[B]:GLU:OE2	7:C:605:HOH:O	2.20	0.46
1:C:204:ILE:HB	1:C:205:PRO:HD3	1.98	0.45
1:B:170[B]:ALA:N	1:B:171[B]:PRO:HD2	2.32	0.45
1:C:88[A]:ARG:NH1	7:C:635:HOH:O	2.49	0.45
1:D:126:ALA:O	7:D:1011:HOH:O	2.21	0.45
1:C:88[A]:ARG:NH2	7:C:640:HOH:O	2.50	0.44
1:C:298[B]:CYS:SG	1:C:313:ASN:O	2.75	0.44
2:D:900:3UK:N32	2:D:900:3UK:O03	2.51	0.44
1:B:298[B]:CYS:SG	1:B:313:ASN:O	2.76	0.44
5:B:905:ACT:H2	7:B:1479:HOH:O	2.18	0.44
1:C:83:ILE:HD11	1:C:92:LEU:HD13	2.00	0.43
1:C:243:LEU:HD21	1:C:251:LEU:HD13	2.00	0.43
1:A:344:GLU:HG3	1:B:2:SER:HA	2.00	0.43
1:B:290:TRP:CD1	1:B:297:ILE:HD11	2.54	0.43
1:A:87:SER:O	3:A:503:PEG:H21	2.19	0.43
2:A:501:3UK:N32	2:A:501:3UK:O03	2.52	0.43
1:A:36[A]:ARG:NH1	7:A:631:HOH:O	2.42	0.43
1:C:61:ASN:N	1:C:107[B]:GLU:OE2	2.40	0.42
1:A:61:ASN:ND2	1:A:107:GLU:OE2	2.53	0.42
1:D:319:ARG:NH1	7:D:1054:HOH:O	2.53	0.41
1:C:9:GLU:O	1:C:13[A]:ARG:HG2	2.20	0.41
1:C:263:PRO:HD3	3:C:503:PEG:C1	2.50	0.41
1:B:61[A]:ASN:OD1	1:B:85:PRO:HG3	2.21	0.41
1:D:319:ARG:NH2	7:D:1033:HOH:O	2.45	0.41
1:D:385:GLU:OE2	1:D:393[B]:ARG:NH1	2.46	0.41
1:B:216[B]:SER:OG	1:B:229:LEU:CD2	2.69	0.40
1:B:172[B]:LYS:HE2	1:B:369:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ALA:HB2	7:D:1034:HOH:O	2.20	0.40

All (15) 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)
7:A:844:HOH:O	7:C:1126:HOH:O[2_545]	1.90	0.30
7:B:1381:HOH:O	7:D:1274:HOH:O[1_545]	1.98	0.22
7:B:1479:HOH:O	7:D:1498:HOH:O[2_746]	2.04	0.16
7:A:897:HOH:O	7:C:1047:HOH:O[1_545]	2.06	0.14
7:A:808:HOH:O	7:C:656:HOH:O[2_645]	2.08	0.12
7:C:611:HOH:O	7:C:848:HOH:O[2_545]	2.10	0.10
7:B:1089:HOH:O	7:D:1432:HOH:O[1_545]	2.12	0.08
7:A:615:HOH:O	7:C:966:HOH:O[2_545]	2.13	0.07
7:A:1046:HOH:O	7:C:822:HOH:O[2_545]	2.14	0.06
7:A:1041:HOH:O	7:C:1017:HOH:O[2_545]	2.14	0.06
7:B:1233:HOH:O	7:D:1512:HOH:O[1_545]	2.15	0.05
7:A:1149:HOH:O	7:A:1173:HOH:O[2_655]	2.17	0.03
7:A:1179:HOH:O	7:C:1140:HOH:O[2_645]	2.18	0.02
7:A:1036:HOH:O	7:A:1214:HOH:O[2_645]	2.18	0.02
7:A:780:HOH:O	7:C:745:HOH:O[2_645]	2.19	0.01

## 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	413/407 (102%)	406 (98%)	7 (2%)	0	100	100
1	B	413/407 (102%)	407 (98%)	6 (2%)	0	100	100
1	C	422/407 (104%)	417 (99%)	5 (1%)	0	100	100
1	D	422/407 (104%)	417 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1670/1628 (103%)	1647 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	330/320 (103%)	329 (100%)	1 (0%)	92	82
1	B	329/320 (103%)	327 (99%)	2 (1%)	86	68
1	C	338/320 (106%)	338 (100%)	0	100	100
1	D	338/320 (106%)	336 (99%)	2 (1%)	86	68
All	All	1335/1280 (104%)	1330 (100%)	5 (0%)	92	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	LEU
1	B	347	ARG
1	B	352	LEU
1	D	86[A]	LYS
1	D	86[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3UK	B	900	-	32,35,35	0.69	1 (3%)	39,52,52	0.93	3 (7%)
4	EDO	A	506	-	3,3,3	0.47	0	2,2,2	0.21	0
3	PEG	C	504[A]	-	6,6,6	0.48	0	5,5,5	0.28	0
4	EDO	B	902	-	3,3,3	0.48	0	2,2,2	0.18	0
4	EDO	D	904	-	3,3,3	0.45	0	2,2,2	0.30	0
2	3UK	C	502	-	32,35,35	0.65	0	39,52,52	0.85	3 (7%)
3	PEG	C	504[B]	-	6,6,6	0.49	0	5,5,5	0.43	0
4	EDO	B	901	-	3,3,3	0.44	0	2,2,2	0.31	0
3	PEG	C	505	-	6,6,6	0.48	0	5,5,5	0.35	0
3	PEG	C	501	-	6,6,6	0.50	0	5,5,5	0.39	0
2	3UK	A	501	-	32,35,35	0.68	0	39,52,52	0.79	2 (5%)
4	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.28	0
3	PEG	C	503	-	6,6,6	0.45	0	5,5,5	0.72	0
3	PEG	A	502	-	6,6,6	0.45	0	5,5,5	0.40	0
3	PEG	A	503	-	6,6,6	0.47	0	5,5,5	0.35	0
4	EDO	D	905	-	3,3,3	0.44	0	2,2,2	0.26	0
5	ACT	B	905	-	1,3,3	6.23	1 (100%)	0,3,3	0.00	-
4	EDO	A	505	-	3,3,3	0.46	0	2,2,2	0.29	0
4	EDO	B	903	-	3,3,3	0.40	0	2,2,2	0.27	0
4	EDO	D	903	-	3,3,3	0.38	0	2,2,2	0.35	0
3	PEG	D	901	-	6,6,6	0.47	0	5,5,5	0.28	0
4	EDO	A	507	-	3,3,3	0.43	0	2,2,2	0.26	0
6	PGE	D	906	-	9,9,9	0.28	0	8,8,8	0.33	0
2	3UK	D	900	-	32,35,35	0.64	0	39,52,52	0.83	2 (5%)
3	PEG	C	506	-	6,6,6	0.48	0	5,5,5	0.29	0
4	EDO	D	902	-	3,3,3	0.44	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	504	-	6,6,6	0.48	0	5,5,5	0.27	0
4	EDO	B	904	-	3,3,3	0.44	0	2,2,2	0.32	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
2	3UK	B	900	-	-	1/15/35/35	0/4/4/4
4	EDO	A	506	-	-	0/1/1/1	-
3	PEG	C	504[A]	-	-	2/4/4/4	-
4	EDO	B	902	-	-	1/1/1/1	-
4	EDO	D	904	-	-	1/1/1/1	-
2	3UK	C	502	-	-	1/15/35/35	0/4/4/4
3	PEG	C	504[B]	-	-	2/4/4/4	-
4	EDO	B	901	-	-	0/1/1/1	-
3	PEG	C	505	-	-	1/4/4/4	-
3	PEG	C	501	-	-	2/4/4/4	-
2	3UK	A	501	-	-	1/15/35/35	0/4/4/4
4	EDO	A	508	-	-	0/1/1/1	-
3	PEG	C	503	-	-	2/4/4/4	-
3	PEG	A	502	-	-	2/4/4/4	-
3	PEG	A	503	-	-	4/4/4/4	-
4	EDO	D	905	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	B	903	-	-	1/1/1/1	-
4	EDO	D	903	-	-	1/1/1/1	-
3	PEG	D	901	-	-	3/4/4/4	-
4	EDO	A	507	-	-	0/1/1/1	-
6	PGE	D	906	-	-	4/7/7/7	-
2	3UK	D	900	-	-	1/15/35/35	0/4/4/4
3	PEG	C	506	-	-	1/4/4/4	-
4	EDO	D	902	-	-	1/1/1/1	-
3	PEG	A	504	-	-	0/4/4/4	-
4	EDO	B	904	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	905	ACT	CH3-C	6.23	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	3UK	P04-O03	2.22	1.65	1.60

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	3UK	P04-O03-C02	3.11	129.89	123.04
2	D	900	3UK	P04-O03-C02	2.83	129.27	123.04
2	C	502	3UK	P04-O03-C02	2.78	129.16	123.04
2	A	501	3UK	P04-O03-C02	2.72	129.03	123.04
2	B	900	3UK	C14-C19-N20	2.31	123.86	120.35
2	C	502	3UK	C14-C19-N20	2.26	123.78	120.35
2	D	900	3UK	C14-C19-N20	2.24	123.76	120.35
2	C	502	3UK	O03-C02-O01	2.21	123.90	122.13
2	A	501	3UK	C14-C19-N20	2.19	123.68	120.35
2	B	900	3UK	O03-C02-C26	2.15	114.69	112.39

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	PEG	C4-C3-O2-C2
6	D	906	PGE	O2-C3-C4-O3
3	C	501	PEG	C1-C2-O2-C3
3	A	503	PEG	C4-C3-O2-C2
3	C	504[A]	PEG	O2-C3-C4-O4
3	C	506	PEG	O2-C3-C4-O4
4	D	904	EDO	O1-C1-C2-O2
3	C	501	PEG	O2-C3-C4-O4
3	C	503	PEG	O1-C1-C2-O2
3	D	901	PEG	O2-C3-C4-O4
4	B	903	EDO	O1-C1-C2-O2
4	D	902	EDO	O1-C1-C2-O2
3	A	503	PEG	O1-C1-C2-O2
3	A	502	PEG	O1-C1-C2-O2
3	C	504[B]	PEG	O2-C3-C4-O4
4	B	902	EDO	O1-C1-C2-O2
4	D	903	EDO	O1-C1-C2-O2
3	C	504[B]	PEG	C1-C2-O2-C3
3	D	901	PEG	C1-C2-O2-C3
3	C	504[A]	PEG	C1-C2-O2-C3
2	B	900	3UK	C02-O03-P04-O06
2	C	502	3UK	C02-O03-P04-O06

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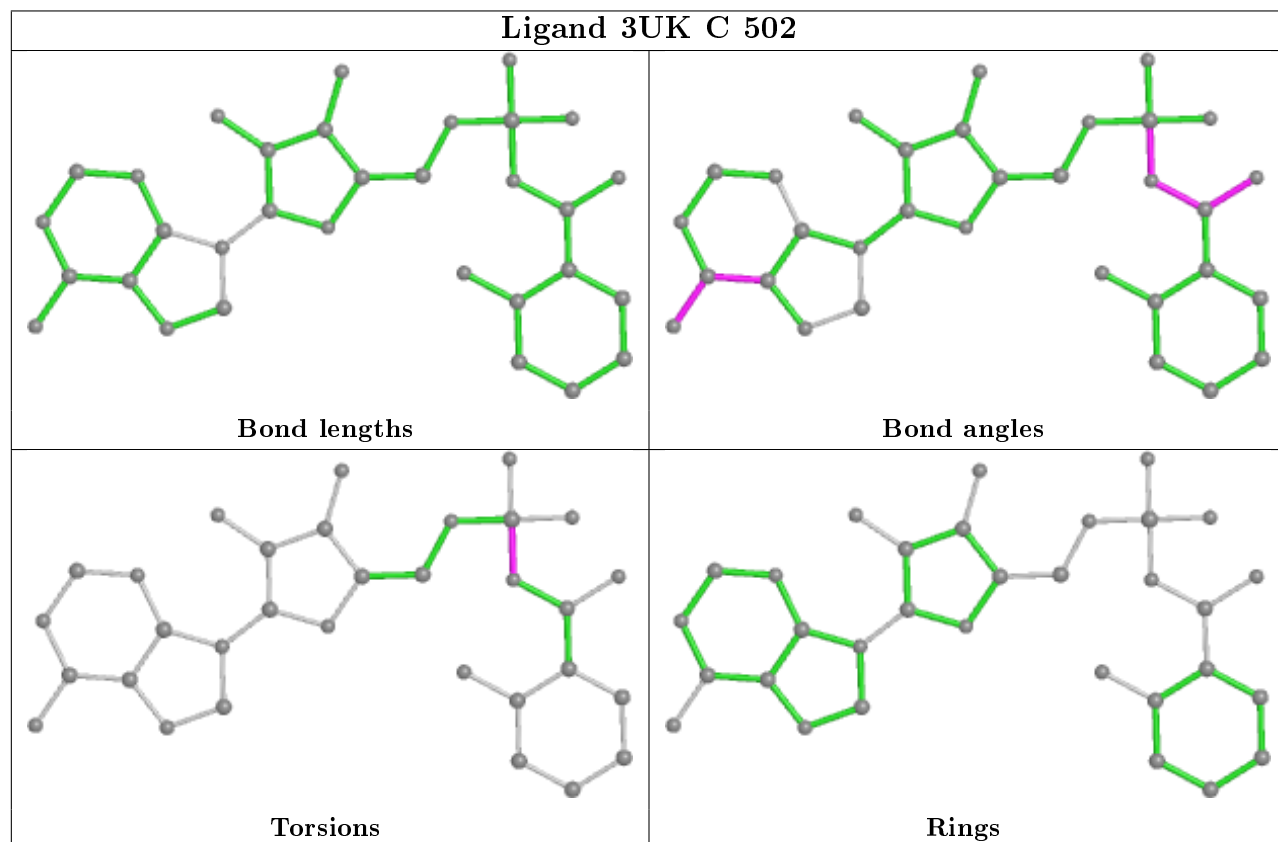
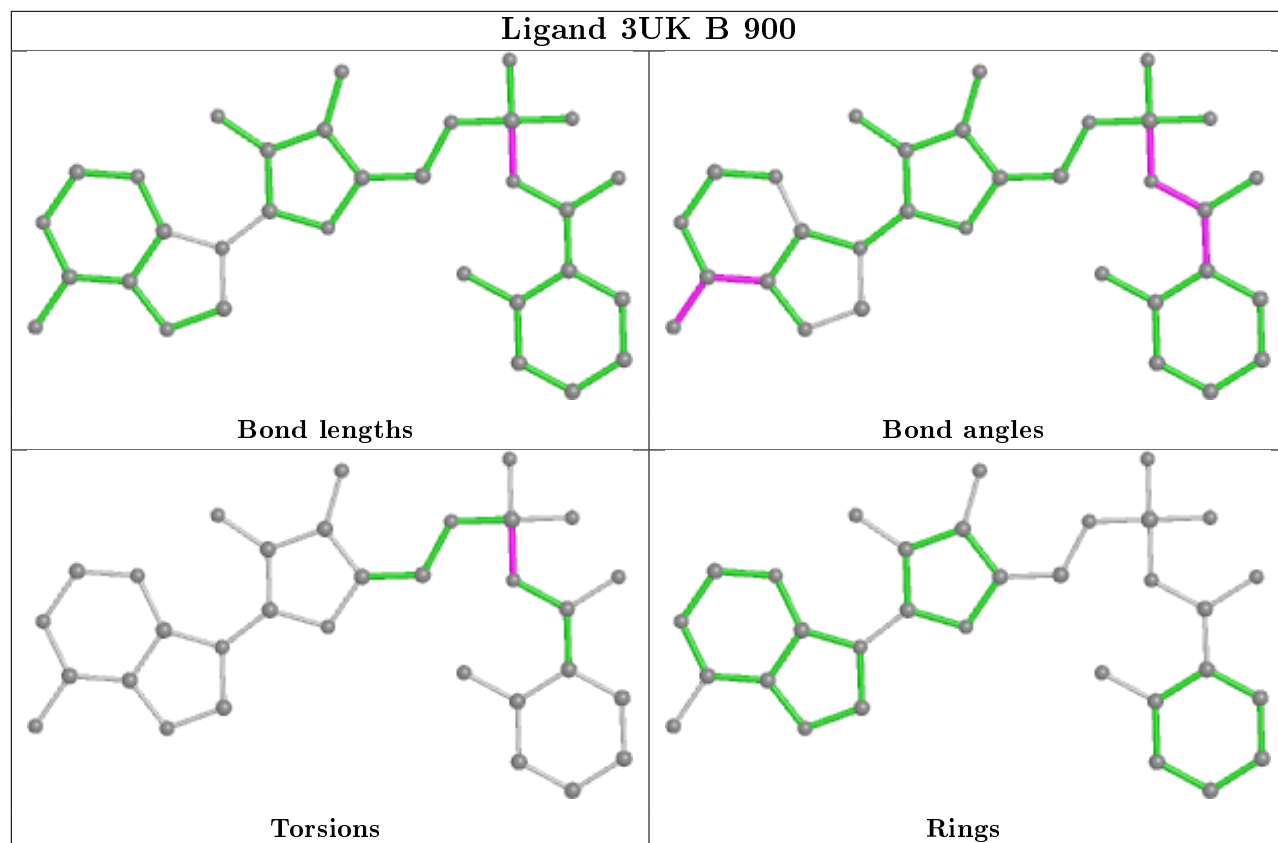
Mol	Chain	Res	Type	Atoms
2	A	501	3UK	C02-O03-P04-O06
2	D	900	3UK	C02-O03-P04-O06
3	A	502	PEG	C4-C3-O2-C2
6	D	906	PGE	O1-C1-C2-O2
3	A	503	PEG	C1-C2-O2-C3
6	D	906	PGE	C4-C3-O2-C2
6	D	906	PGE	C3-C4-O3-C5
4	B	904	EDO	O1-C1-C2-O2
3	C	505	PEG	O2-C3-C4-O4
3	D	901	PEG	C4-C3-O2-C2
3	A	503	PEG	O2-C3-C4-O4

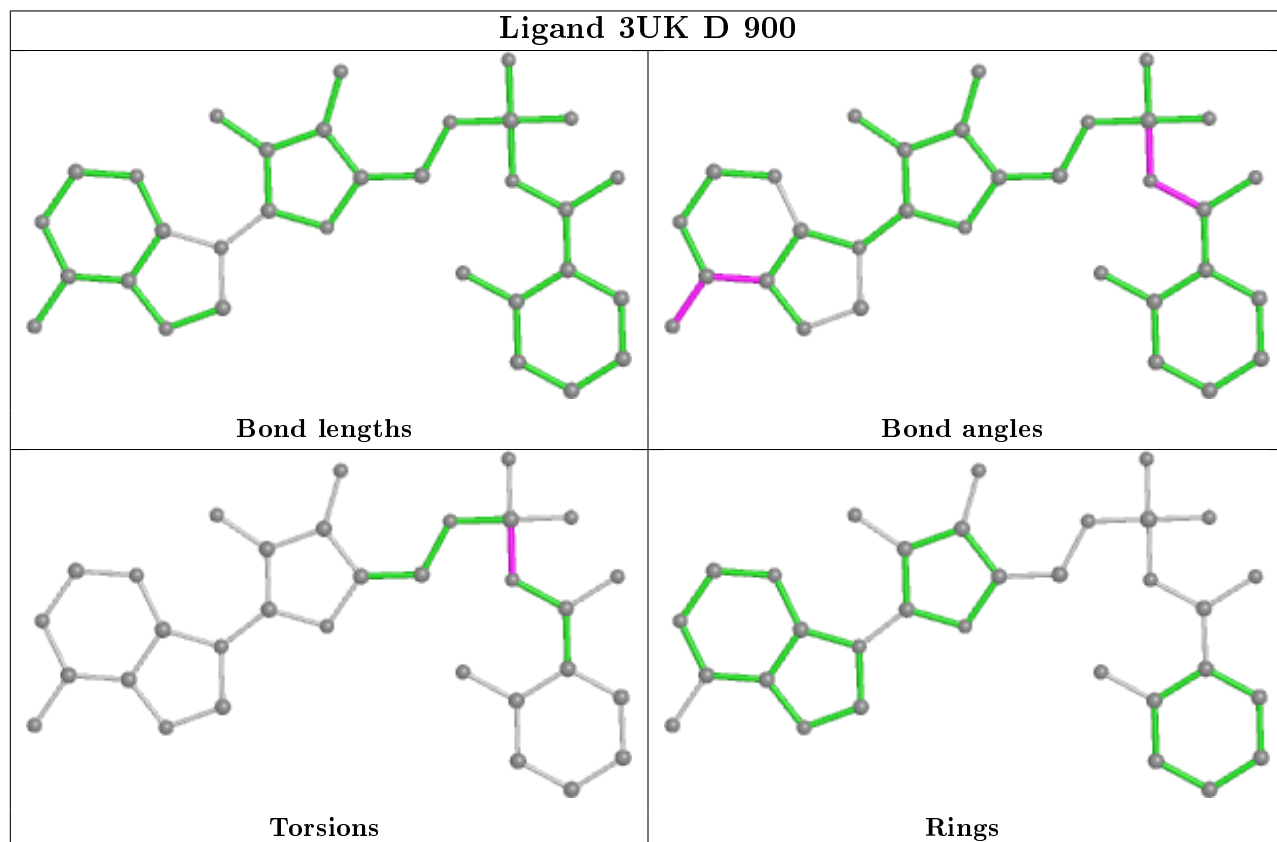
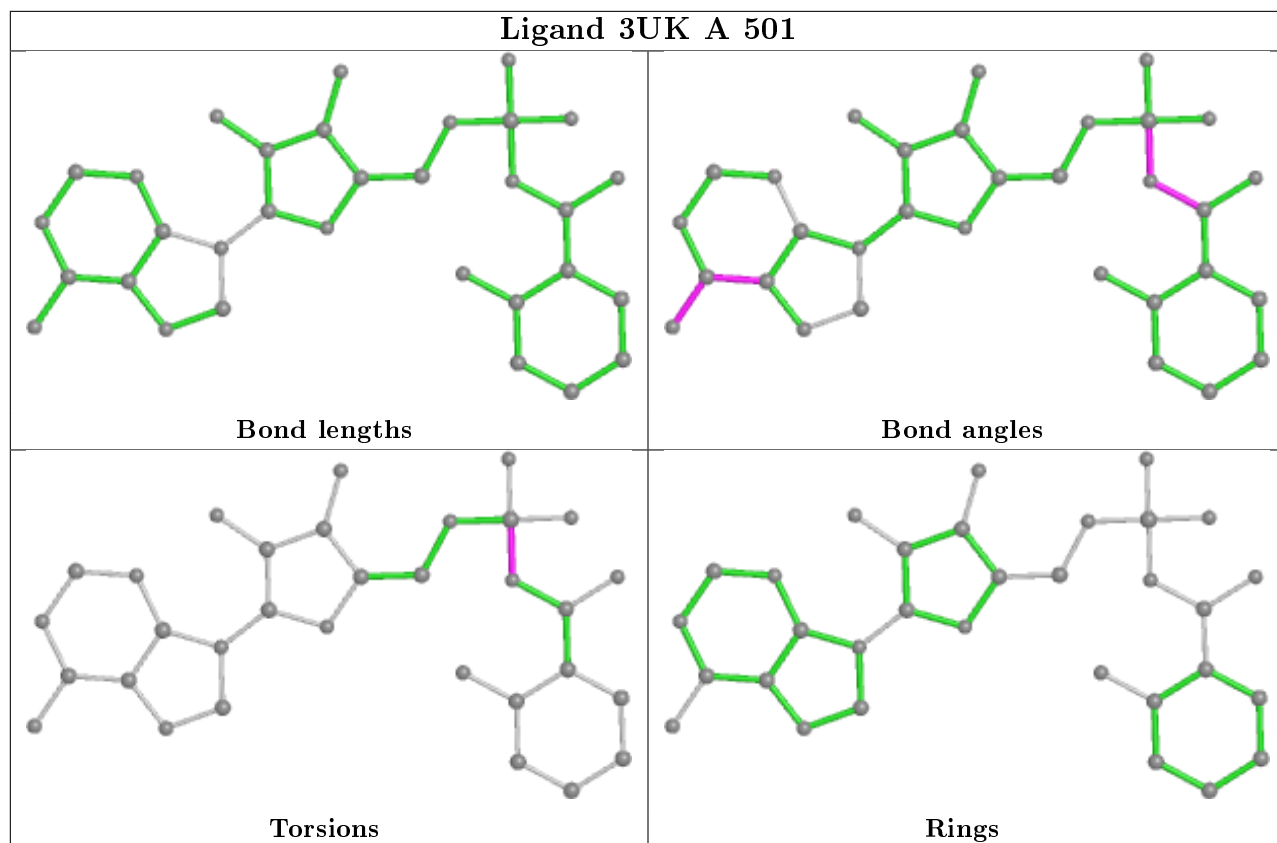
There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	EDO	2	0
3	C	504[A]	PEG	1	0
4	D	904	EDO	1	0
2	A	501	3UK	1	0
3	C	503	PEG	2	0
3	A	503	PEG	4	0
5	B	905	ACT	4	0
2	D	900	3UK	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	394/407 (96%)	-0.05	8 (2%) 65 65	6, 12, 25, 82	0
1	B	393/407 (96%)	-0.07	9 (2%) 60 61	6, 12, 27, 74	0
1	C	394/407 (96%)	0.05	13 (3%) 46 47	7, 14, 29, 58	0
1	D	393/407 (96%)	-0.00	9 (2%) 60 61	6, 13, 28, 69	0
All	All	1574/1628 (96%)	-0.02	39 (2%) 57 58	6, 13, 27, 82	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170[A]	ALA	8.9
1	C	170[A]	ALA	6.0
1	C	169[A]	GLY	5.7
1	B	399	ASP	5.7
1	A	169	GLY	4.8
1	B	170[A]	ALA	4.6
1	C	399	ASP	4.3
1	B	2	SER	4.3
1	A	399	ASP	4.2
1	C	171[A]	PRO	4.0
1	D	399	ASP	4.0
1	A	233[A]	TRP	3.9
1	C	269	LEU	3.8
1	C	3	THR	3.5
1	B	3	THR	3.3
1	B	233	TRP	3.2
1	A	2	SER	3.2
1	D	2	SER	3.0
1	C	244	VAL	2.9
1	B	171[A]	PRO	2.8
1	C	2	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	159[A]	CYS	2.7
1	C	164	THR	2.7
1	A	170	ALA	2.7
1	C	209[A]	PHE	2.7
1	A	171	PRO	2.6
1	D	171[A]	PRO	2.4
1	A	3	THR	2.4
1	C	271	SER	2.4
1	B	145	LEU	2.3
1	D	164	THR	2.3
1	C	13[A]	ARG	2.2
1	D	209[A]	PHE	2.1
1	C	109	ASP	2.1
1	D	388	GLU	2.1
1	A	209[A]	PHE	2.1
1	B	13	ARG	2.0
1	D	117[A]	LEU	2.0
1	B	164	THR	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 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
4	EDO	A	506	4/4	0.59	0.34	22,27,28,32	10
3	PEG	A	503	7/7	0.60	0.24	16,22,27,32	17
3	PEG	A	502	7/7	0.61	0.27	38,46,48,48	0
3	PEG	D	901	7/7	0.62	0.28	27,32,35,35	17
3	PEG	C	501	7/7	0.66	0.24	22,34,42,42	17

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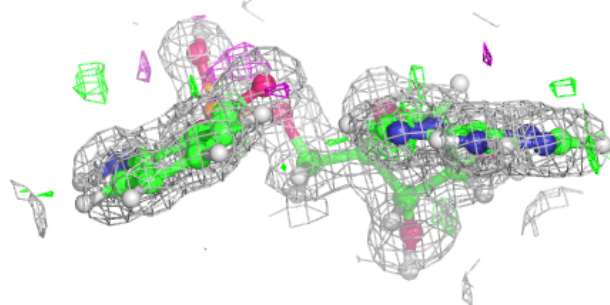
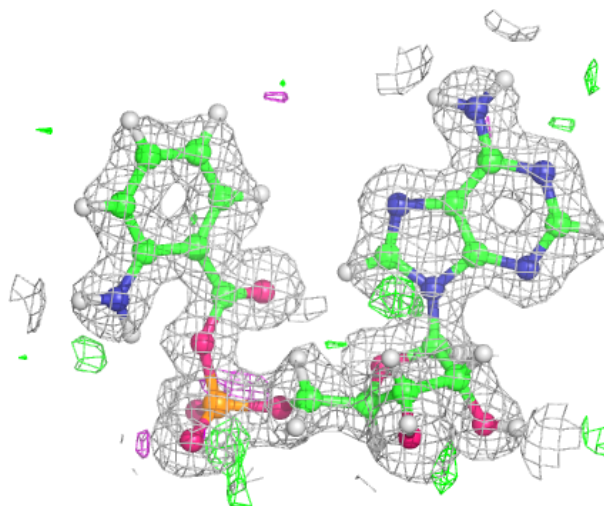
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	902	4/4	0.68	0.27	24,29,34,34	10
4	EDO	B	904	4/4	0.71	0.23	13,16,20,22	10
3	PEG	A	504	7/7	0.74	0.28	18,26,28,34	17
4	EDO	A	505	4/4	0.74	0.22	33,40,44,49	0
3	PEG	C	505	7/7	0.75	0.19	22,29,34,34	17
3	PEG	C	504[A]	7/7	0.76	0.24	19,27,34,35	17
3	PEG	C	504[B]	7/7	0.76	0.24	20,27,34,36	17
4	EDO	B	901	4/4	0.81	0.17	25,30,35,35	0
4	EDO	A	508	4/4	0.83	0.17	21,25,28,33	10
6	PGE	D	906	10/10	0.84	0.19	22,28,30,30	24
3	PEG	C	506	7/7	0.85	0.26	14,20,24,24	17
3	PEG	C	503	7/7	0.86	0.24	13,21,27,28	17
4	EDO	D	902	4/4	0.88	0.16	9,13,17,21	10
5	ACT	B	905	4/4	0.90	0.24	27,30,36,36	0
4	EDO	B	903	4/4	0.91	0.18	13,21,25,25	10
4	EDO	D	903	4/4	0.91	0.18	16,20,29,29	10
4	EDO	A	507	4/4	0.92	0.16	14,24,28,34	0
4	EDO	D	904	4/4	0.92	0.30	29,35,38,43	0
4	EDO	D	905	4/4	0.93	0.17	21,25,29,29	0
2	3UK	C	502	32/32	0.96	0.08	6,9,12,14	0
2	3UK	A	501	32/32	0.97	0.07	3,8,12,14	0
2	3UK	D	900	32/32	0.97	0.07	5,8,12,15	0
2	3UK	B	900	32/32	0.97	0.07	4,7,11,14	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.

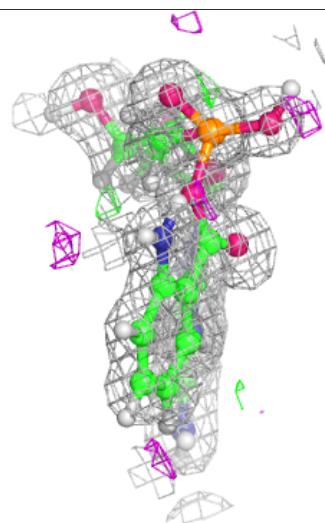
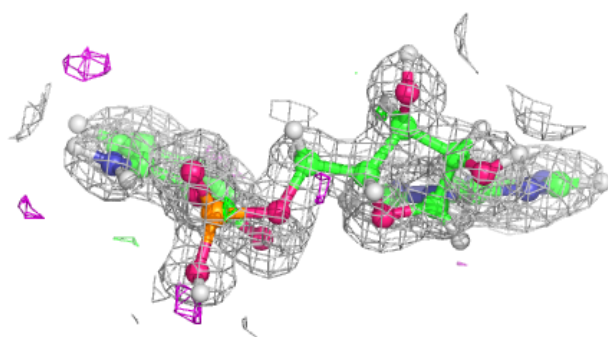
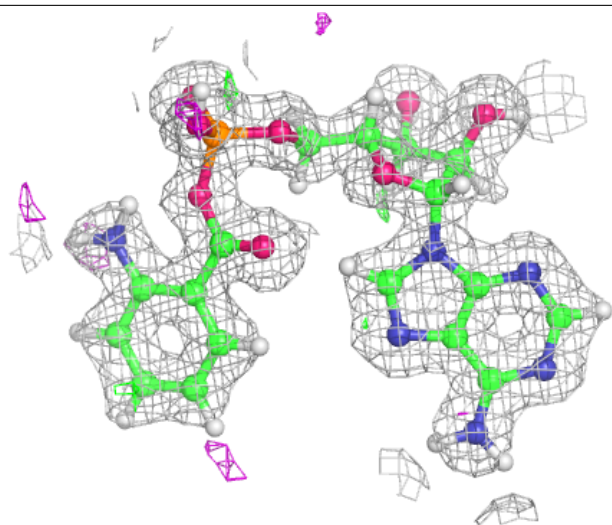
**Electron density around 3UK C 502:**

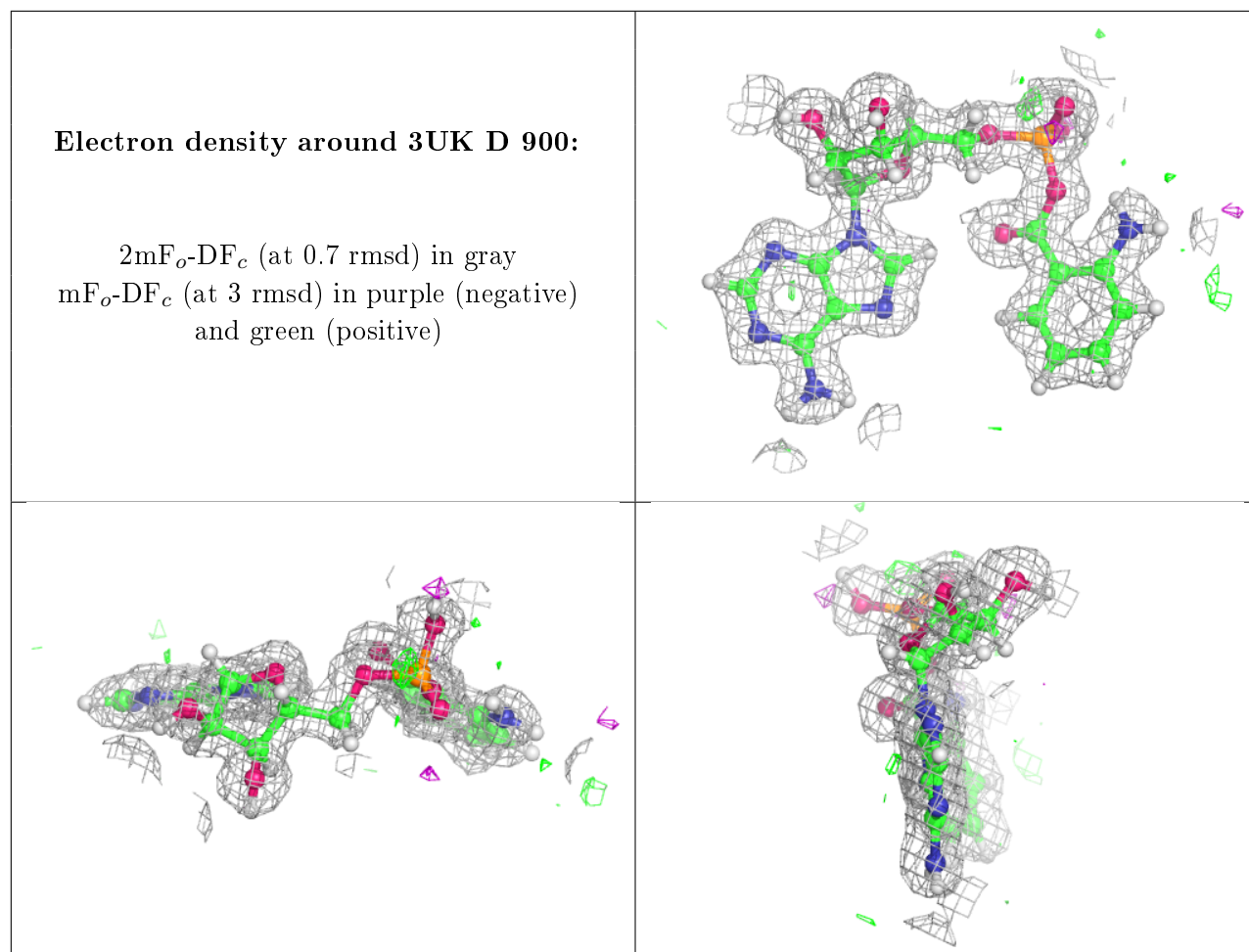
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

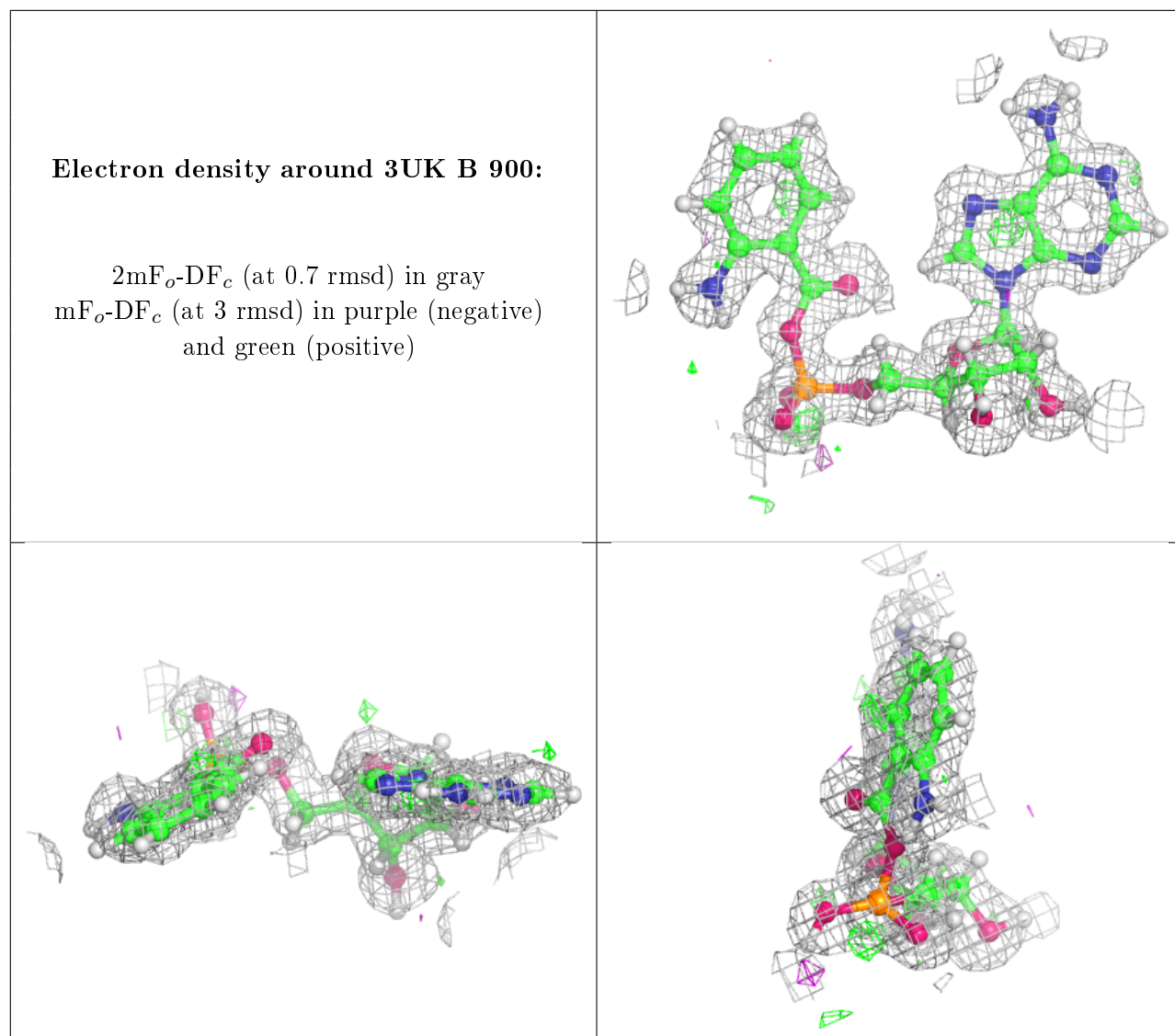


**Electron density around 3UK A 501:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.