



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 02:38 AM EDT

PDB ID : 6YNF  
Title : GAPDH purified from the supernatant of HEK293F cells: crystal form 3 of 4.  
Authors : Roversi, P.; Lia, A.  
Deposited on : 2020-04-13  
Resolution : 2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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 : 2.37.1  
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) : 2.37.1

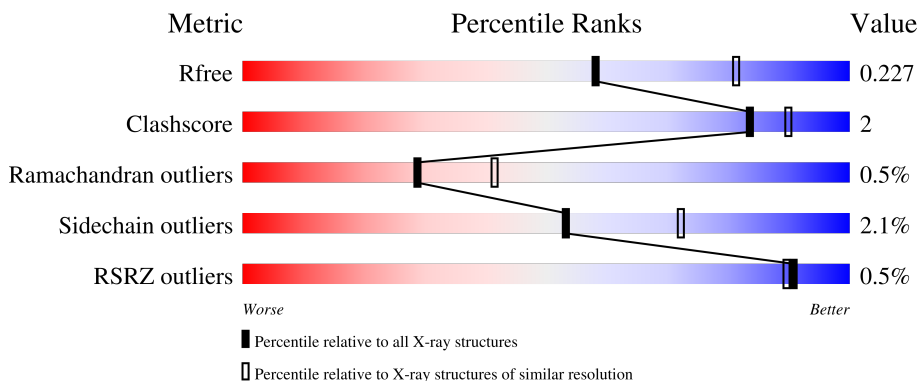
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

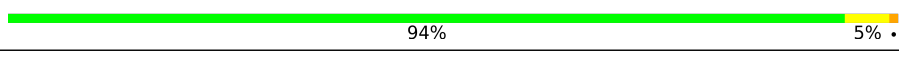
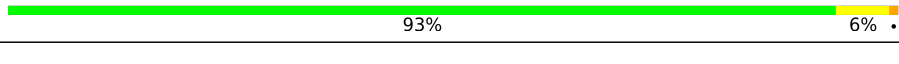
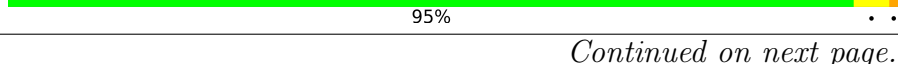
The reported resolution of this entry is 2.39 Å.

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.



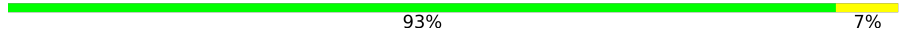
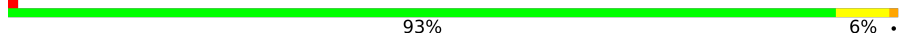

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	334	 93% 6% .
1	B	334	 95% . .
1	C	334	 94% 5% .
1	D	334	 93% 6% .
1	E	334	 95% . .

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	334	 93% 7%
1	G	334	 % 93% 6% •
1	H	334	 2% 93% 5% •

## 2 Entry composition

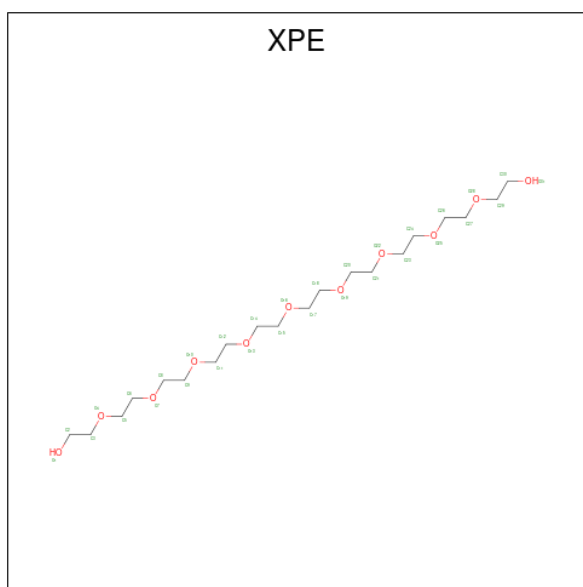
There are 3 unique types of molecules in this entry. The entry contains 41539 atoms, of which 20389 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	334	5081	1606	2537	442	482	14	0	3	0
1	B	334	5079	1606	2535	442	482	14	1	3	0
1	C	334	5069	1601	2532	440	482	14	0	2	0
1	D	333	5073	1604	2533	441	481	14	1	3	0
1	E	333	5061	1599	2528	439	481	14	0	2	0
1	F	334	5093	1610	2543	442	484	14	1	4	0
1	G	333	5072	1604	2532	441	481	14	1	3	0
1	H	333	5070	1603	2531	439	483	14	1	3	0

- Molecule 2 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (three-letter code: XPE) (formula: C<sub>20</sub>H<sub>42</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	H	O	0	0
			31	9	17	5		
2	B	1	Total	C	H	O	0	0
			31	9	17	5		
2	D	1	Total	C	H	O	0	0
			31	9	17	5		
2	E	1	Total	C	H	O	0	0
			31	9	17	5		
2	F	1	Total	C	H	O	0	0
			23	7	12	4		
2	F	1	Total	C	H	O	0	0
			37	10	21	6		
2	G	1	Total	C	H	O	0	0
			31	9	17	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	118	Total	O	0	0
			118	118		
3	C	79	Total	O	0	0
			79	79		
3	D	115	Total	O	0	0
			115	115		
3	E	77	Total	O	0	0
			77	77		

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	F	129	Total 129	O 129	0	0
3	G	79	Total 79	O 79	0	0
3	H	58	Total 58	O 58	0	0

### 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: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:  93% 6%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain B:  95%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain C:  94% 5%



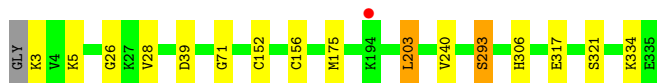
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain D:  93% 6%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain E:  95%

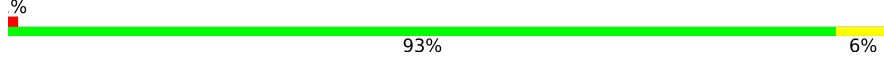


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain F:  93% 7%

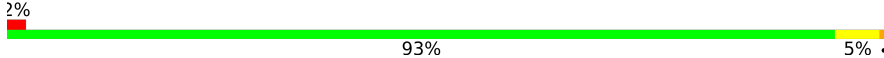


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain G:  93% 6%



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain H:  93% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.14Å 111.43Å 135.94Å 90.00° 96.02° 90.00°	Depositor
Resolution (Å)	135.18 – 2.39 135.19 – 2.39	Depositor EDS
% Data completeness (in resolution range)	58.2 (135.18-2.39) 58.2 (135.19-2.39)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.40Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, $R_{free}$	0.179 , 0.219 0.188 , 0.227	Depositor DCC
$R_{free}$ test set	2940 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	41539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: XPE, CSU

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	0.40	0/2588	0.60	0/3500
1	B	0.43	0/2588	0.62	0/3500
1	C	0.42	0/2577	0.63	1/3485 (0.0%)
1	D	0.44	0/2584	0.63	0/3495
1	E	0.43	0/2573	0.61	0/3480
1	F	0.46	0/2597	0.63	0/3512
1	G	0.41	0/2584	0.60	0/3495
1	H	0.41	0/2582	0.59	0/3492
All	All	0.43	0/20673	0.61	1/27959 (0.0%)

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	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	LEU	CB-CG-CD2	5.52	120.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	152[B]	CSU	Mainchain

## 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	2544	2537	2531	14	0
1	B	2544	2535	2531	13	0
1	C	2537	2532	2524	14	0
1	D	2540	2533	2527	17	0
1	E	2533	2528	2520	11	0
1	F	2550	2543	2536	17	0
1	G	2540	2532	2528	20	0
1	H	2539	2531	2527	16	0
2	A	14	17	17	0	0
2	B	14	17	17	0	0
2	D	14	17	17	0	0
2	E	14	17	17	0	0
2	F	27	33	33	0	0
2	G	14	17	17	0	0
3	A	71	0	0	3	0
3	B	118	0	0	2	0
3	C	79	0	0	0	0
3	D	115	0	0	3	0
3	E	77	0	0	2	0
3	F	129	0	0	4	0
3	G	79	0	0	7	0
3	H	58	0	0	2	0
All	All	21150	20389	20342	96	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 2.

All (96) 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:203:LEU:CD1	1:E:203:LEU:HD22	1.34	1.58
1:A:203:LEU:HD12	1:E:203:LEU:CD2	1.35	1.51
1:B:203:LEU:HD12	1:D:203:LEU:CD2	1.43	1.48
1:B:203:LEU:CD1	1:D:203:LEU:HD22	1.41	1.47
1:F:203:LEU:CD1	1:G:203:LEU:HD12	1.46	1.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HD22	1:H:203:LEU:CD1	1.46	1.45
1:F:203:LEU:HD12	1:G:203:LEU:CD1	1.45	1.44
1:C:203:LEU:CD2	1:H:203:LEU:HD12	1.49	1.42
1:A:203:LEU:HD11	1:E:203:LEU:HD22	1.30	1.08
1:B:203:LEU:HD11	1:D:203:LEU:HD22	1.36	1.05
1:C:203:LEU:HD22	1:H:203:LEU:HD11	1.38	1.05
1:A:203:LEU:HD12	1:E:203:LEU:HD21	1.42	1.01
1:C:203:LEU:HD22	1:H:203:LEU:HD12	1.03	0.97
1:F:203:LEU:HD12	1:G:203:LEU:HD11	1.47	0.94
1:A:203:LEU:CD1	1:E:203:LEU:CD2	2.13	0.94
1:F:203:LEU:HD11	1:G:203:LEU:HD12	1.49	0.90
1:B:203:LEU:HD12	1:D:203:LEU:HD21	1.54	0.88
1:B:203:LEU:CD1	1:D:203:LEU:CD2	2.22	0.87
1:F:203:LEU:CD1	1:G:203:LEU:CD1	2.24	0.87
1:F:203:LEU:HD12	1:G:203:LEU:HD12	0.95	0.85
1:C:203:LEU:HD21	1:H:203:LEU:HD12	1.56	0.83
1:C:203:LEU:CD2	1:H:203:LEU:CD1	2.26	0.83
1:G:289:ASP:O	3:G:3101:HOH:O	2.03	0.76
1:G:318:PHE:HB2	3:G:3101:HOH:O	1.85	0.76
1:G:318:PHE:CB	3:G:3101:HOH:O	2.33	0.75
1:H:255:TYR:O	1:H:258:ILE:HG12	1.88	0.72
1:F:219:LYS:NZ	3:F:3102:HOH:O	2.23	0.71
1:H:85:ILE:HG21	1:H:87:TRP:CE2	2.27	0.69
1:D:170:ILE:HG23	3:D:3101:HOH:O	1.93	0.68
1:F:254:LYS:NZ	3:F:3101:HOH:O	2.22	0.66
1:F:258:ILE:O	1:F:262:VAL:HG23	1.98	0.63
1:C:168:PHE:O	1:C:251:LYS:HG3	2.01	0.60
1:D:248:ARG:O	3:D:3101:HOH:O	2.16	0.59
1:G:315:ASP:HB3	3:G:3101:HOH:O	2.02	0.59
1:D:223:GLU:HG3	3:D:3185:HOH:O	2.03	0.58
1:C:239:ASN:OD1	1:C:317:GLU:HG3	2.04	0.58
1:F:85:ILE:HG21	1:F:87:TRP:CE2	2.40	0.57
1:D:44:VAL:HG21	1:D:62:ALA:HB2	1.85	0.57
1:D:9:ASN:ND2	1:D:97:GLU:OE1	2.36	0.56
1:G:156:CYS:SG	1:G:293:SER:HB2	2.47	0.54
1:H:168:PHE:CE2	1:H:258:ILE:HG22	2.44	0.53
1:H:255:TYR:CD1	1:H:258:ILE:HD11	2.44	0.53
1:A:85:ILE:HG21	1:A:87:TRP:CE2	2.44	0.52
1:H:260:LYS:NZ	3:H:402:HOH:O	2.42	0.52
1:G:318:PHE:HB3	3:G:3101:HOH:O	2.04	0.51
1:B:85:ILE:HG21	1:B:87:TRP:CE2	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:HD12	1:D:120:ILE:N	2.26	0.50
1:F:3:LYS:HD3	1:F:26:GLY:O	2.12	0.49
1:B:3:LYS:HD3	1:B:26:GLY:O	2.13	0.49
1:D:3:LYS:HD3	1:D:26:GLY:O	2.12	0.48
1:C:271:LYS:HD3	3:F:3151:HOH:O	2.13	0.48
1:E:71:GLY:HA3	1:F:89:ASP:OD2	2.14	0.48
1:E:3:LYS:HD3	1:E:26:GLY:O	2.13	0.47
1:D:248:ARG:NE	1:G:248:ARG:HD2	2.30	0.47
1:A:3:LYS:HD3	1:A:26:GLY:O	2.15	0.46
1:H:3:LYS:HD3	1:H:26:GLY:O	2.14	0.46
1:C:156:CYS:SG	1:C:293:SER:HB2	2.56	0.46
1:H:156:CYS:SG	1:H:293:SER:HB2	2.56	0.46
1:H:185:GLN:HB3	3:H:416:HOH:O	2.16	0.45
1:B:234:ARG:HG2	3:B:3119:HOH:O	2.17	0.45
1:B:156:CYS:SG	1:B:293:SER:HB2	2.57	0.45
1:E:156:CYS:SG	1:E:293:SER:HB2	2.57	0.45
1:G:155:ASN:O	1:G:292:SER:HB3	2.17	0.45
1:A:156:CYS:SG	1:A:293:SER:HB2	2.58	0.44
1:A:5:LYS:HG2	3:A:3101:HOH:O	2.18	0.44
1:G:164:ILE:HG22	3:G:3102:HOH:O	2.16	0.44
1:D:303:LEU:CD2	1:G:172:GLU:HB2	2.48	0.44
1:A:186:LYS:NZ	3:A:3105:HOH:O	2.36	0.43
1:D:156:CYS:SG	1:D:293:SER:HB2	2.59	0.42
1:G:249:LEU:HD22	3:G:3102:HOH:O	2.19	0.42
1:B:194:LYS:HG2	3:B:3205:HOH:O	2.18	0.42
1:E:5:LYS:NZ	3:E:3103:HOH:O	2.51	0.42
1:A:165:HIS:ND1	1:A:224:LEU:HD21	2.33	0.42
1:D:53:HIS:CG	1:D:318:PHE:CE1	3.07	0.42
1:C:132:VAL:HB	1:C:135:VAL:HG22	2.00	0.42
1:B:248:ARG:HA	1:B:306:HIS:O	2.20	0.42
1:C:248:ARG:HA	1:C:306:HIS:O	2.19	0.42
1:C:165:HIS:CG	1:C:224:LEU:HD21	2.55	0.42
1:E:334:LYS:HE2	3:E:3121:HOH:O	2.19	0.41
1:F:252:PRO:HB3	3:F:3148:HOH:O	2.20	0.41
1:D:248:ARG:HA	1:D:306:HIS:O	2.21	0.41
1:G:317:GLU:O	1:G:321:SER:OG	2.34	0.41
1:H:248:ARG:HA	1:H:306:HIS:O	2.20	0.41
1:A:334:LYS:O	1:A:335:GLU:OXT	2.38	0.41
1:B:248:ARG:HD2	1:F:248:ARG:HD2	2.01	0.41
1:F:248:ARG:HA	1:F:306:HIS:O	2.21	0.41
1:B:175:MET:HG2	1:B:176:THR:N	2.35	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:HB2	3:A:3137:HOH:O	2.19	0.41
1:A:248:ARG:HA	1:A:306:HIS:O	2.20	0.41
1:C:85:ILE:HG21	1:C:87:TRP:CE2	2.55	0.41
1:E:317:GLU:O	1:E:321:SER:OG	2.36	0.41
1:G:168:PHE:CD1	1:G:253:ALA:HB2	2.56	0.40
1:F:120:ILE:N	1:F:120:ILE:HD12	2.37	0.40
1:F:132:VAL:HG23	1:F:220:VAL:HG11	2.03	0.40
1:G:175:MET:HG2	1:G:176:THR:N	2.37	0.40
1:H:152[B]:CSU:HB2	1:H:320:TYR:HB2	2.04	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	333/334 (100%)	320 (96%)	11 (3%)	2 (1%)	25	36
1	B	333/334 (100%)	324 (97%)	7 (2%)	2 (1%)	25	36
1	C	332/334 (99%)	323 (97%)	8 (2%)	1 (0%)	41	55
1	D	332/334 (99%)	322 (97%)	8 (2%)	2 (1%)	25	36
1	E	331/334 (99%)	320 (97%)	10 (3%)	1 (0%)	41	55
1	F	334/334 (100%)	323 (97%)	9 (3%)	2 (1%)	25	36
1	G	332/334 (99%)	322 (97%)	8 (2%)	2 (1%)	25	36
1	H	332/334 (99%)	323 (97%)	7 (2%)	2 (1%)	25	36
All	All	2659/2672 (100%)	2577 (97%)	68 (3%)	14 (0%)	29	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	VAL

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	240	VAL
1	C	240	VAL
1	D	240	VAL
1	E	240	VAL
1	F	240	VAL
1	G	240	VAL
1	H	240	VAL
1	B	189	ASP
1	G	189	ASP
1	A	189	ASP
1	D	189	ASP
1	F	189	ASP
1	H	189	ASP

### 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	271/269 (101%)	264 (97%)	7 (3%)	46	66
1	B	271/269 (101%)	268 (99%)	3 (1%)	73	87
1	C	270/269 (100%)	265 (98%)	5 (2%)	57	75
1	D	271/269 (101%)	263 (97%)	8 (3%)	41	61
1	E	270/269 (100%)	264 (98%)	6 (2%)	52	71
1	F	272/269 (101%)	265 (97%)	7 (3%)	46	66
1	G	271/269 (101%)	266 (98%)	5 (2%)	59	76
1	H	271/269 (101%)	266 (98%)	5 (2%)	59	76
All	All	2167/2152 (101%)	2121 (98%)	46 (2%)	53	72

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	73	PRO

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	148	SER
1	A	175	MET
1	A	203	LEU
1	A	293	SER
1	A	321	SER
1	B	39	ASP
1	B	203	LEU
1	B	293	SER
1	C	39	ASP
1	C	61	LYS
1	C	203	LEU
1	C	293	SER
1	C	303	LEU
1	D	28	VAL
1	D	61	LYS
1	D	66	LYS
1	D	97	GLU
1	D	175	MET
1	D	203	LEU
1	D	248	ARG
1	D	293	SER
1	E	28	VAL
1	E	39	ASP
1	E	175	MET
1	E	203	LEU
1	E	293	SER
1	E	306	HIS
1	F	39	ASP
1	F	57[A]	HIS
1	F	57[B]	HIS
1	F	61	LYS
1	F	175	MET
1	F	203	LEU
1	F	293	SER
1	G	39	ASP
1	G	148	SER
1	G	203	LEU
1	G	293	SER
1	G	321	SER
1	H	39	ASP
1	H	73	PRO
1	H	175	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	H	203	LEU
1	H	293	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	264	GLN
1	F	48	GLN
1	H	78	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

16 non-standard protein/DNA/RNA residues 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
1	CSU	G	152[A]	1	4,5,10	0.88	0	1,5,14	0.47	0
1	CSU	A	152[B]	1	6,9,10	0.56	0	3,12,14	1.12	0
1	CSU	C	152[A]	1	4,5,10	0.66	0	1,5,14	0.25	0
1	CSU	E	152[B]	1	6,9,10	1.47	1 (16%)	3,12,14	1.98	1 (33%)
1	CSU	H	152[B]	1	6,9,10	1.09	0	3,12,14	0.80	0
1	CSU	D	152[A]	1	4,5,10	0.78	0	1,5,14	0.76	0
1	CSU	G	152[B]	1	6,9,10	0.71	0	3,12,14	1.17	0
1	CSU	C	152[B]	1	6,9,10	0.72	0	3,12,14	1.16	0
1	CSU	F	152[A]	1	4,5,10	0.74	0	1,5,14	0.26	0
1	CSU	H	152[A]	1	4,5,10	0.66	0	1,5,14	0.07	0
1	CSU	D	152[B]	1	6,9,10	1.28	1 (16%)	3,12,14	2.15	1 (33%)
1	CSU	B	152[A]	1	4,5,10	0.79	0	1,5,14	0.52	0
1	CSU	F	152[B]	1	6,9,10	1.44	1 (16%)	3,12,14	2.06	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSU	A	152[A]	1	4,5,10	0.76	0	1,5,14	0.48	0
1	CSU	E	152[A]	1	4,5,10	0.64	0	1,5,14	0.72	0
1	CSU	B	152[B]	1	6,9,10	0.90	0	3,12,14	1.27	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
1	CSU	G	152[A]	1	-	0/1/4/10	-
1	CSU	A	152[B]	1	-	3/4/8/10	-
1	CSU	C	152[A]	1	-	0/1/4/10	-
1	CSU	E	152[B]	1	-	3/4/8/10	-
1	CSU	H	152[B]	1	-	3/4/8/10	-
1	CSU	D	152[A]	1	-	0/1/4/10	-
1	CSU	G	152[B]	1	-	1/4/8/10	-
1	CSU	C	152[B]	1	-	3/4/8/10	-
1	CSU	F	152[A]	1	-	0/1/4/10	-
1	CSU	H	152[A]	1	-	0/1/4/10	-
1	CSU	D	152[B]	1	-	3/4/8/10	-
1	CSU	B	152[A]	1	-	0/1/4/10	-
1	CSU	F	152[B]	1	-	2/4/8/10	-
1	CSU	A	152[A]	1	-	0/1/4/10	-
1	CSU	E	152[A]	1	-	0/1/4/10	-
1	CSU	B	152[B]	1	-	2/4/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	152[B]	CSU	OD3-S	3.30	1.55	1.45
1	E	152[B]	CSU	OD1-S	3.25	1.55	1.45
1	D	152[B]	CSU	OD3-S	2.62	1.53	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	152[B]	CSU	OD2-S-OD1	3.43	125.20	112.78
1	D	152[B]	CSU	OD2-S-OD1	3.33	124.84	112.78
1	E	152[B]	CSU	OD2-S-OD3	3.02	123.72	112.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	152[B]	CSU	OD2-S-SG-CB
1	B	152[B]	CSU	N-CA-CB-SG
1	B	152[B]	CSU	OD3-S-SG-CB
1	C	152[B]	CSU	OD1-S-SG-CB
1	C	152[B]	CSU	OD2-S-SG-CB
1	D	152[B]	CSU	OD2-S-SG-CB
1	D	152[B]	CSU	OD3-S-SG-CB
1	E	152[B]	CSU	OD1-S-SG-CB
1	E	152[B]	CSU	OD2-S-SG-CB
1	E	152[B]	CSU	OD3-S-SG-CB
1	F	152[B]	CSU	OD2-S-SG-CB
1	H	152[B]	CSU	N-CA-CB-SG
1	H	152[B]	CSU	OD2-S-SG-CB
1	A	152[B]	CSU	N-CA-CB-SG
1	G	152[B]	CSU	N-CA-CB-SG
1	A	152[B]	CSU	OD3-S-SG-CB
1	C	152[B]	CSU	OD3-S-SG-CB
1	D	152[B]	CSU	OD1-S-SG-CB
1	F	152[B]	CSU	OD3-S-SG-CB
1	H	152[B]	CSU	OD1-S-SG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	152[B]	CSU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
2	XPE	B	3001	-	13,13,30	0.31	0	12,12,29	0.18	0
2	XPE	G	3001	-	13,13,30	0.23	0	12,12,29	0.12	0
2	XPE	D	3001	-	13,13,30	0.37	0	12,12,29	0.24	0
2	XPE	E	3001	-	13,13,30	0.24	0	12,12,29	0.17	0
2	XPE	F	3002	-	15,15,30	0.25	0	14,14,29	0.18	0
2	XPE	F	3001	-	10,10,30	0.18	0	9,9,29	0.25	0
2	XPE	A	3001	-	13,13,30	0.33	0	12,12,29	0.18	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	XPE	B	3001	-	-	5/11/11/28	-
2	XPE	G	3001	-	-	3/11/11/28	-
2	XPE	D	3001	-	-	4/11/11/28	-
2	XPE	E	3001	-	-	1/11/11/28	-
2	XPE	F	3002	-	-	6/13/13/28	-
2	XPE	F	3001	-	-	2/8/8/28	-
2	XPE	A	3001	-	-	3/11/11/28	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3002	XPE	O22-C23-C24-O25
2	A	3001	XPE	O25-C26-C27-O28
2	F	3002	XPE	O19-C20-C21-O22
2	B	3001	XPE	O25-C26-C27-O28
2	B	3001	XPE	O22-C23-C24-O25
2	A	3001	XPE	O28-C29-C30-O31
2	F	3002	XPE	O25-C26-C27-O28
2	F	3002	XPE	C23-C24-O25-C26

*Continued on next page...*

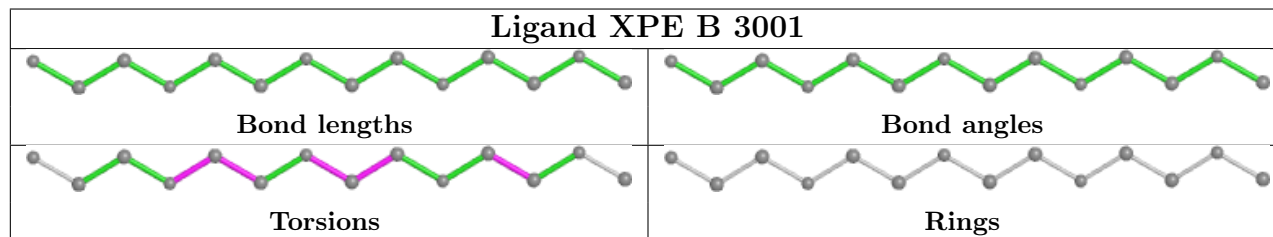
Continued from previous page...

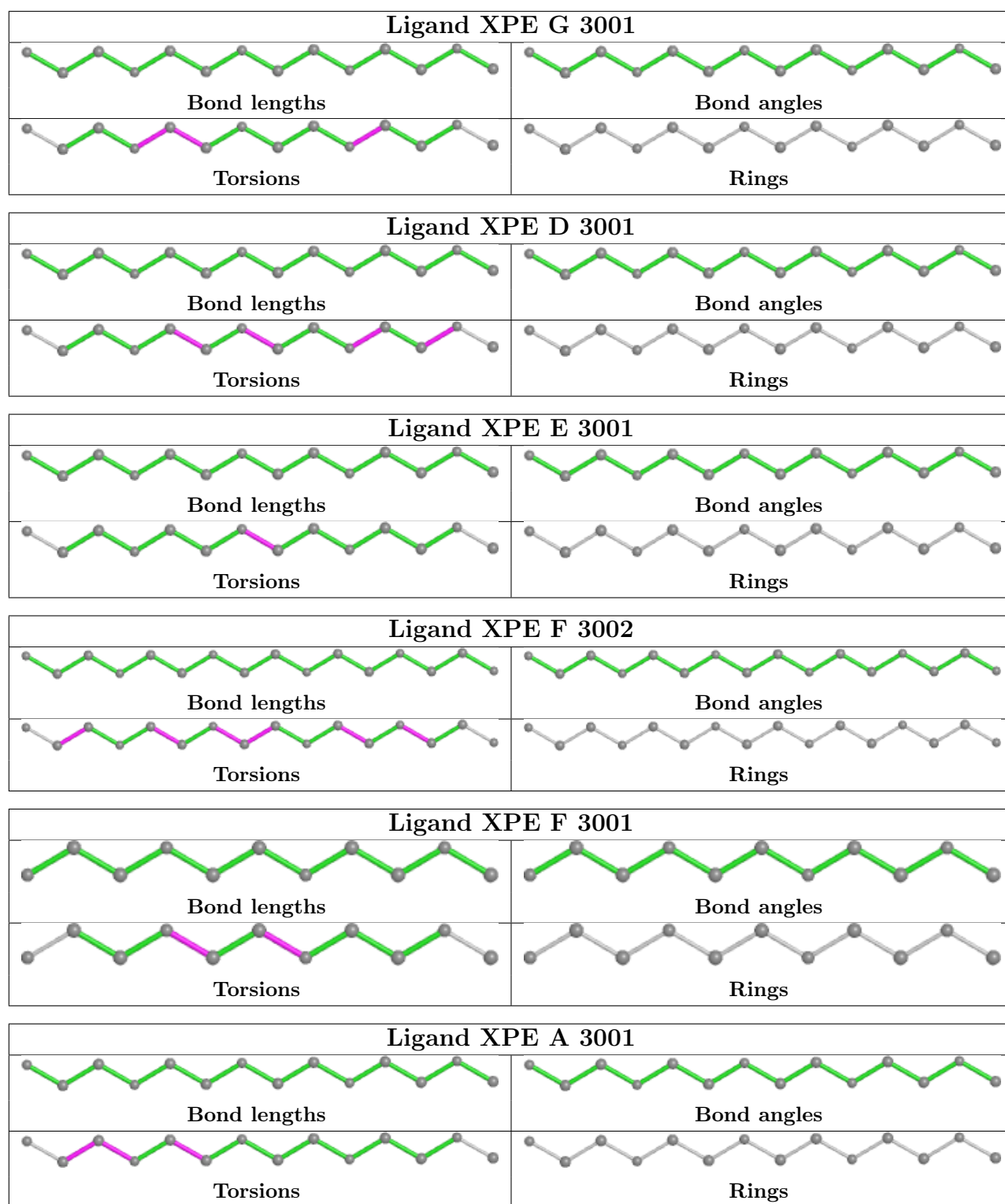
Mol	Chain	Res	Type	Atoms
2	G	3001	XPE	C26-C27-O28-C29
2	A	3001	XPE	C30-C29-O28-C27
2	G	3001	XPE	C20-C21-O22-C23
2	F	3002	XPE	O28-C29-C30-O31
2	D	3001	XPE	C20-C21-O22-C23
2	B	3001	XPE	O19-C20-C21-O22
2	E	3001	XPE	C23-C24-O25-C26
2	F	3001	XPE	C23-C24-O25-C26
2	D	3001	XPE	C23-C24-O25-C26
2	G	3001	XPE	O25-C26-C27-O28
2	F	3002	XPE	C17-C18-O19-C20
2	D	3001	XPE	O25-C26-C27-O28
2	B	3001	XPE	C23-C24-O25-C26
2	B	3001	XPE	C26-C27-O28-C29
2	D	3001	XPE	C21-C20-O19-C18
2	F	3001	XPE	C24-C23-O22-C21

There are no ring outliers.

No monomer is involved in short contacts.

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

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	333/334 (99%)	0.07	1 (0%) 94 93	22, 40, 58, 68	0
1	B	333/334 (99%)	-0.16	1 (0%) 94 93	17, 29, 43, 55	0
1	C	333/334 (99%)	0.03	1 (0%) 94 93	22, 39, 57, 70	0
1	D	332/334 (99%)	-0.18	0 100 100	15, 28, 44, 56	0
1	E	332/334 (99%)	-0.04	1 (0%) 94 93	20, 33, 53, 65	0
1	F	333/334 (99%)	-0.17	1 (0%) 94 93	10, 26, 39, 53	0
1	G	332/334 (99%)	0.05	2 (0%) 89 88	20, 35, 56, 72	0
1	H	332/334 (99%)	0.33	6 (1%) 68 66	25, 46, 71, 85	0
All	All	2660/2672 (99%)	-0.01	13 (0%) 91 89	10, 34, 57, 85	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLY	5.4
1	H	57	HIS	4.0
1	B	2	GLY	2.7
1	G	57[A]	HIS	2.6
1	F	2	GLY	2.5
1	H	116	ALA	2.4
1	C	2	GLY	2.3
1	H	87	TRP	2.2
1	H	90	ALA	2.1
1	H	194	LYS	2.1
1	H	14	ILE	2.0
1	E	194	LYS	2.0
1	G	24	ASN	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSU	H	152[A]	6/11	0.90	0.17	36,36,43,43	9
1	CSU	H	152[B]	10/11	0.90	0.17	19,37,44,88	14
1	CSU	A	152[A]	6/11	0.94	0.17	35,35,42,42	9
1	CSU	A	152[B]	10/11	0.94	0.17	36,41,46,46	14
1	CSU	G	152[A]	6/11	0.95	0.15	27,28,33,34	10
1	CSU	G	152[B]	10/11	0.95	0.15	28,31,36,36	13
1	CSU	D	152[A]	6/11	0.95	0.17	29,31,38,38	10
1	CSU	D	152[B]	10/11	0.95	0.17	29,33,38,38	14
1	CSU	E	152[A]	6/11	0.96	0.13	30,30,36,36	10
1	CSU	E	152[B]	10/11	0.96	0.13	30,32,38,38	14
1	CSU	C	152[A]	6/11	0.96	0.12	36,37,44,44	10
1	CSU	C	152[B]	10/11	0.96	0.12	36,40,46,46	14
1	CSU	B	152[A]	6/11	0.96	0.12	28,29,35,35	9
1	CSU	B	152[B]	10/11	0.96	0.12	29,32,37,37	14
1	CSU	F	152[A]	6/11	0.97	0.11	25,25,30,30	10
1	CSU	F	152[B]	10/11	0.97	0.11	25,30,33,33	14

## 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.

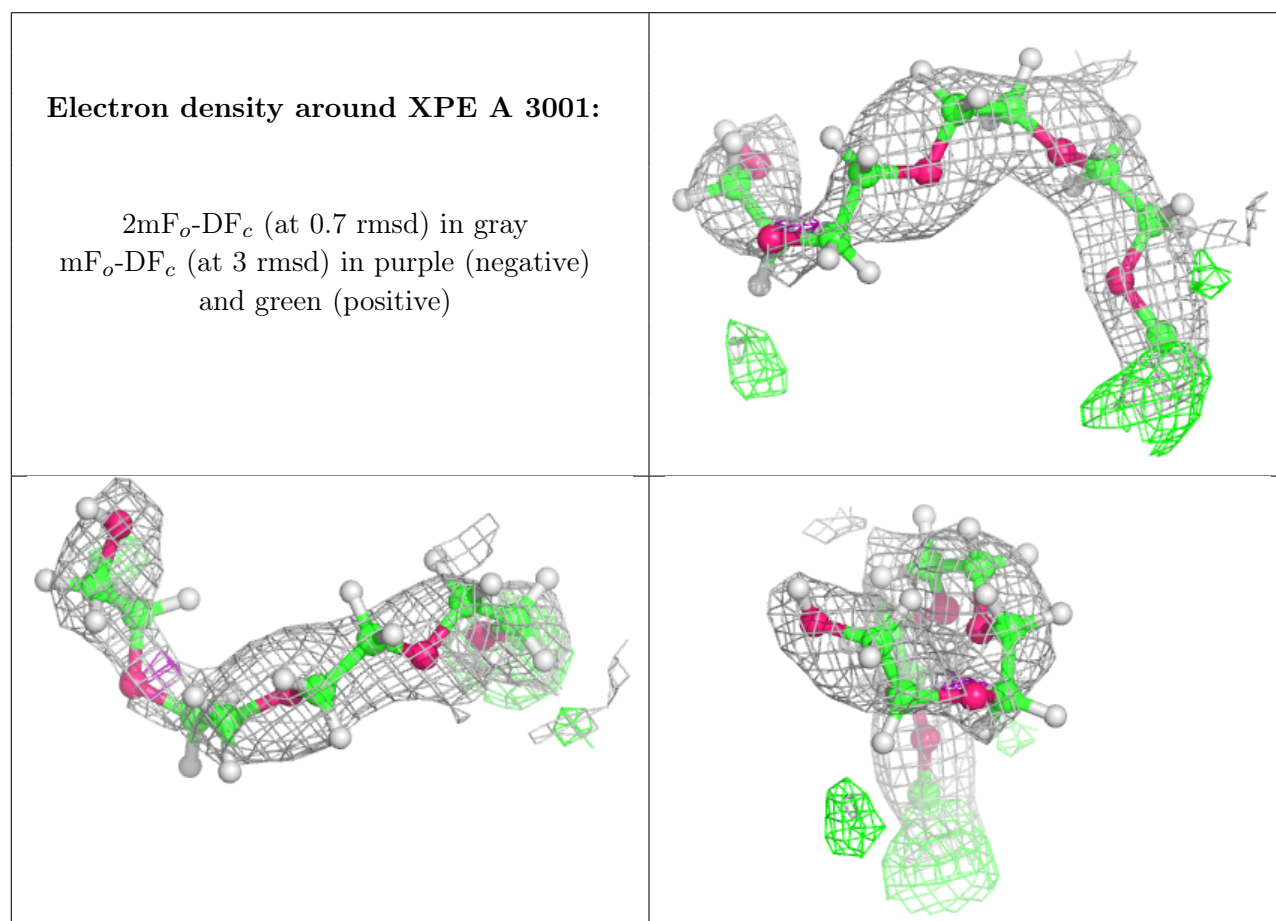
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	XPE	A	3001	14/31	0.79	0.22	51,62,63,63	0
2	XPE	F	3002	16/31	0.79	0.25	52,63,69,69	0
2	XPE	E	3001	14/31	0.86	0.19	52,63,66,66	0
2	XPE	D	3001	14/31	0.86	0.15	41,49,55,55	0
2	XPE	G	3001	14/31	0.86	0.18	57,69,73,73	0
2	XPE	B	3001	14/31	0.88	0.19	45,55,64,64	0

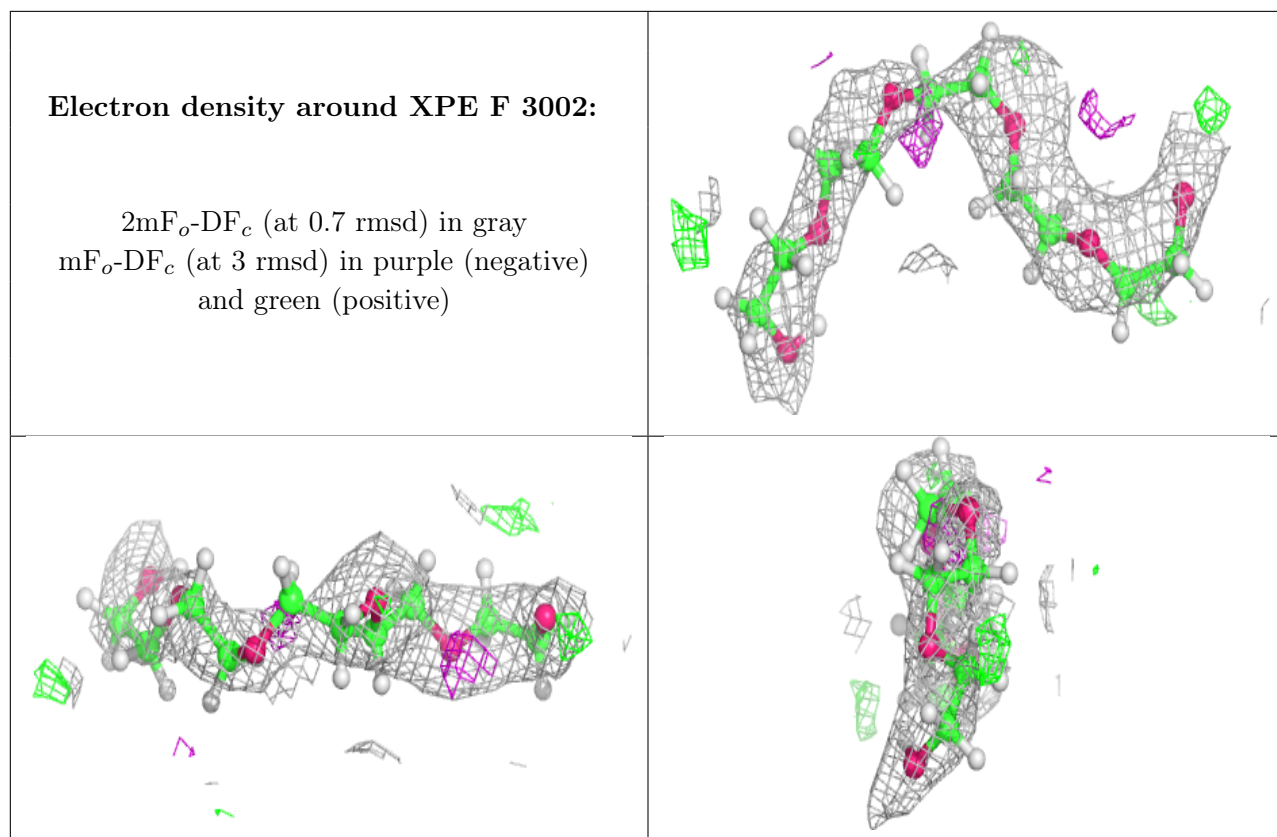
*Continued on next page...*

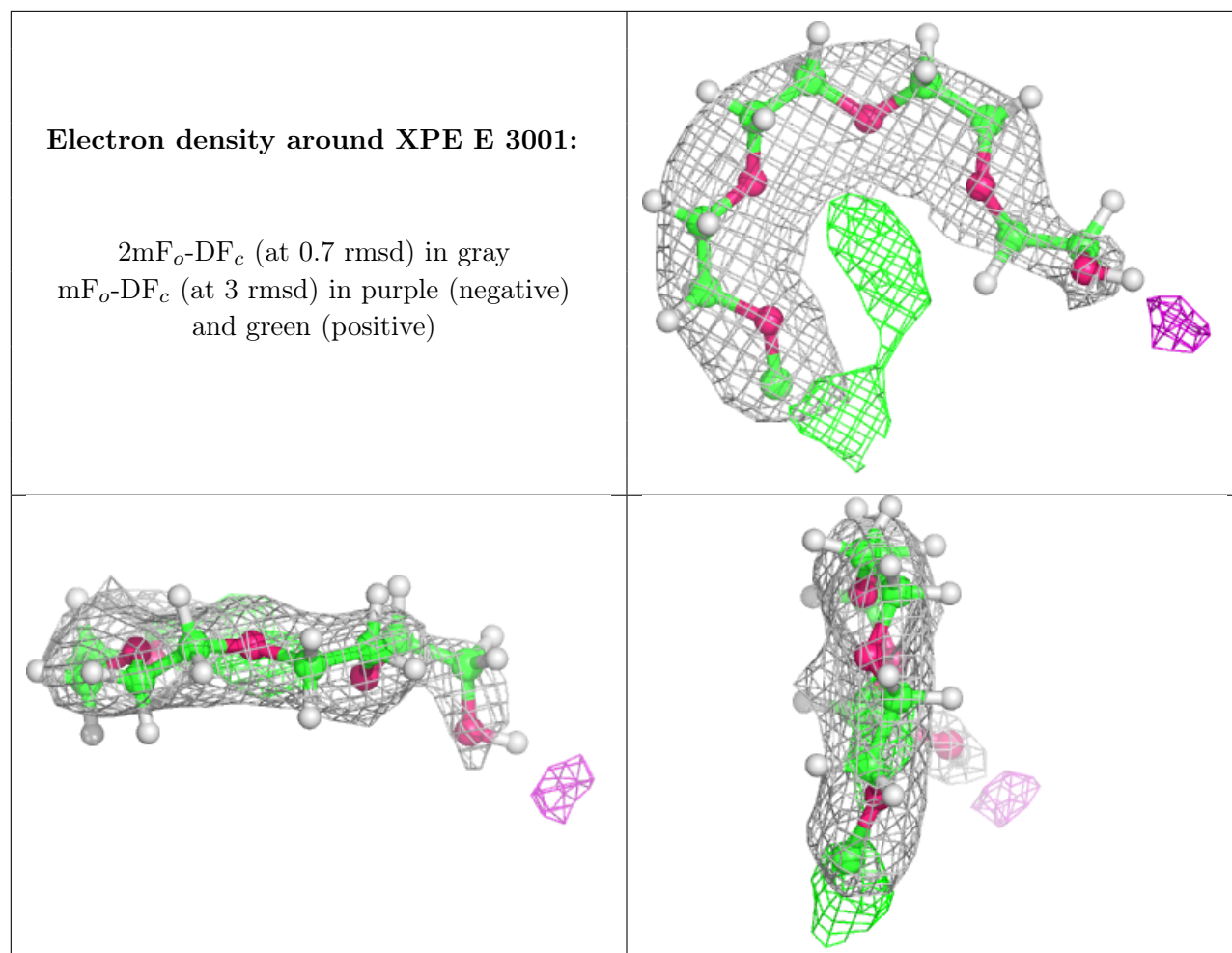
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XPE	F	3001	11/31	0.95	0.10	29,35,40,41	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.

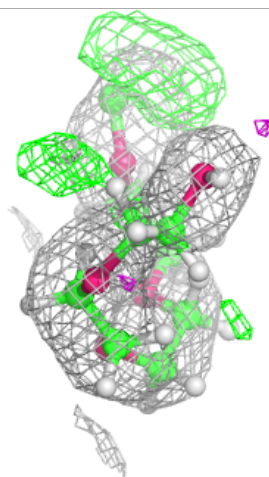
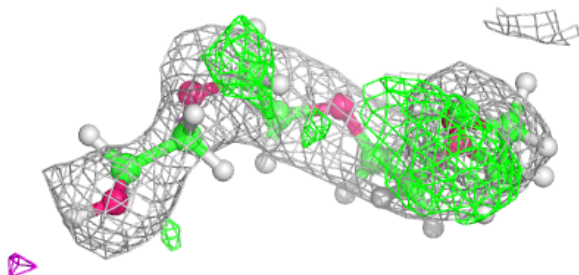
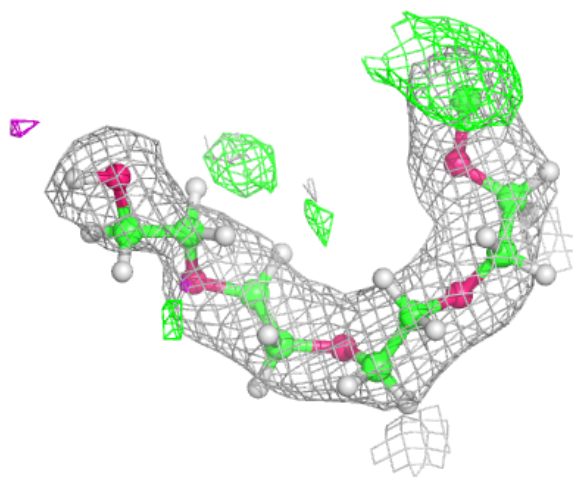






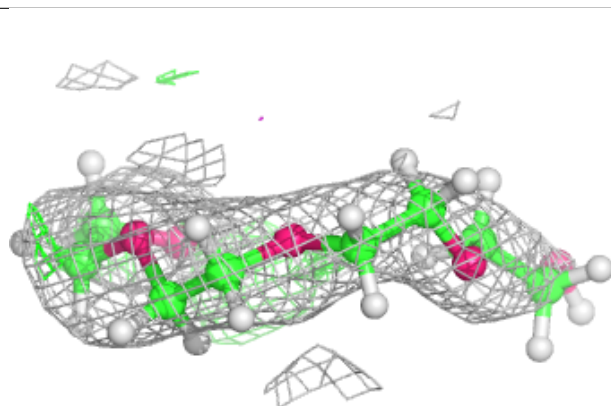
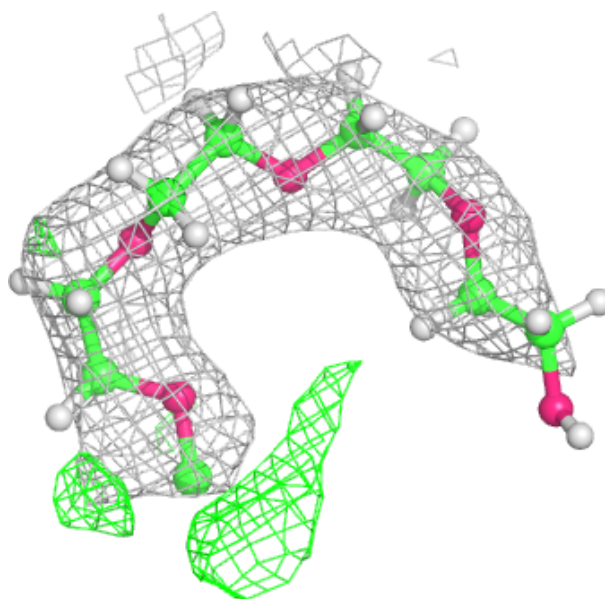
**Electron density around XPE D 3001:**

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



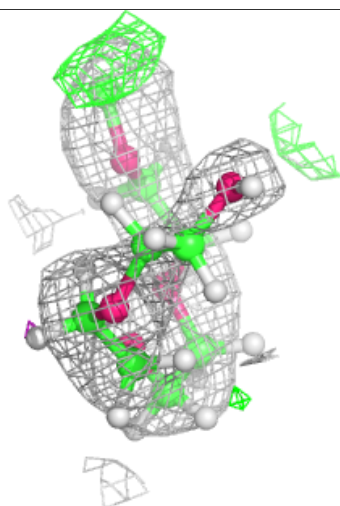
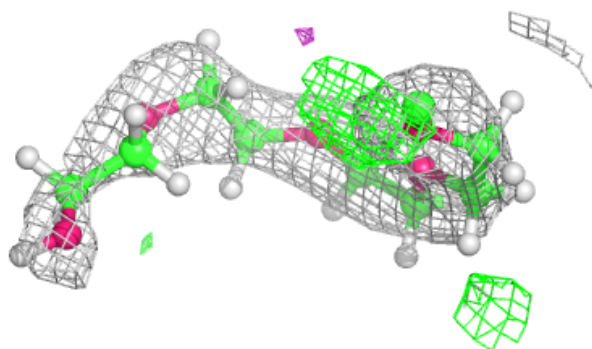
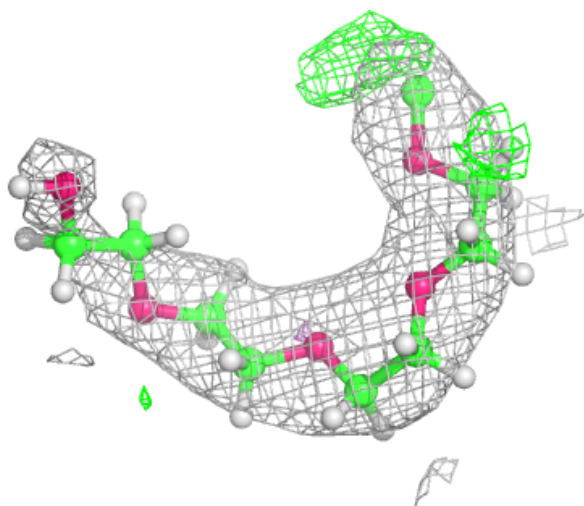
**Electron density around XPE G 3001:**

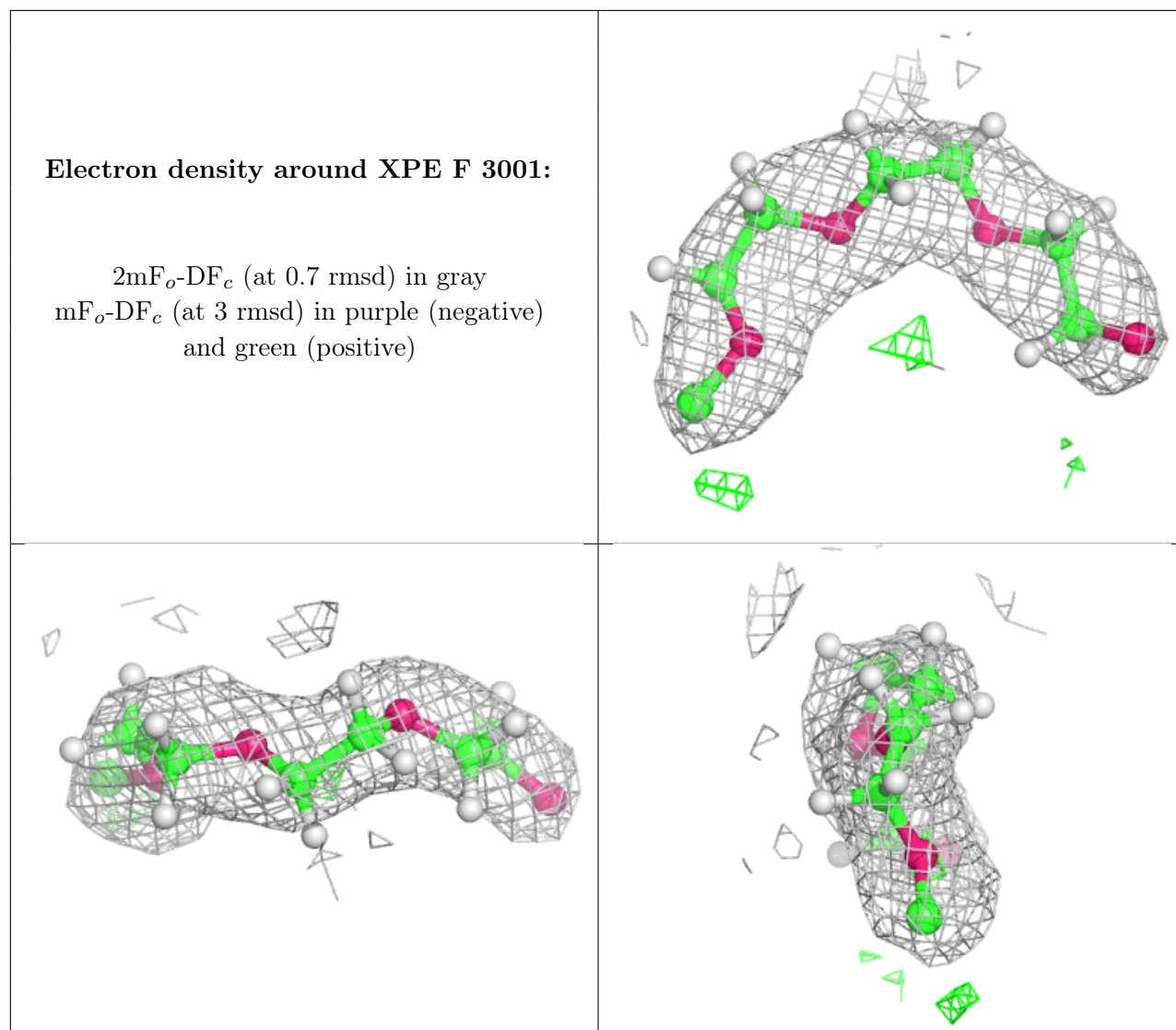
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around XPE B 3001:**

$2mF_o-DF_c$  (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.