



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:05 PM UTC

PDB ID : 6YND / pdb_00006ynd
Title : GAPDH purified from the supernatant of HEK293F cells: crystal form 1 of 4.
Authors : Roversi, P.; Lia, A.
Deposited on : 2020-04-13
Resolution : 1.52 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

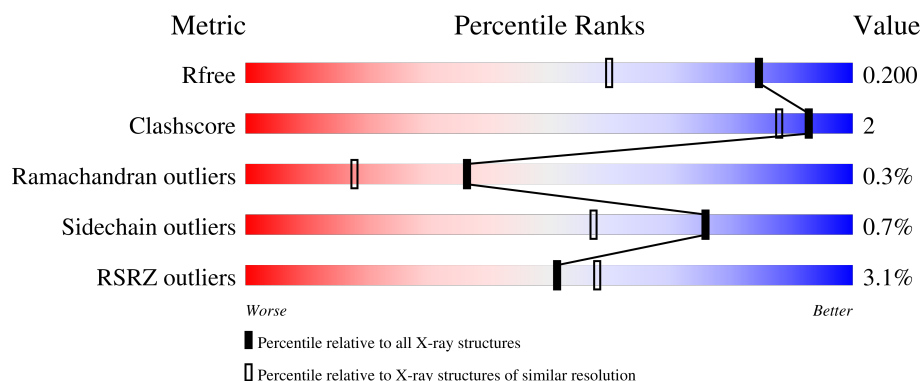
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	335	 3% 98%
1	B	335	 % 97%
1	C	335	 2% 95%
1	D	335	 4% 97%
1	E	335	 4% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	335	% 98%
1	G	335	2% 94% 5%
1	H	335	7% 97%

2 Entry composition

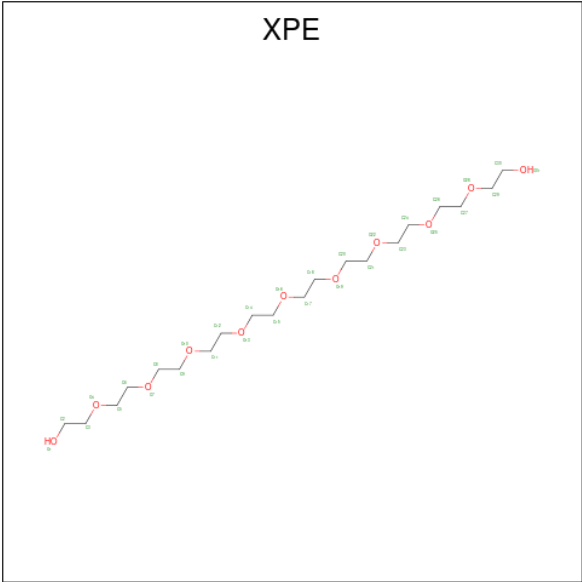
There are 3 unique types of molecules in this entry. The entry contains 43512 atoms, of which 21008 are hydrogens and 0 are deuteriums.

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
1	A	334	Total	C	H	N	O	S	0	13	0
			5204	1637	2613	451	489	14			
1	B	334	Total	C	H	N	O	S	0	12	0
			5186	1633	2600	450	489	14			
1	C	334	Total	C	H	N	O	S	0	9	0
			5161	1626	2586	446	489	14			
1	D	333	Total	C	H	N	O	S	1	13	0
			5205	1639	2611	450	491	14			
1	E	334	Total	C	H	N	O	S	1	11	0
			5193	1639	2600	446	493	15			
1	F	334	Total	C	H	N	O	S	0	7	0
			5164	1628	2583	449	489	15			
1	G	333	Total	C	H	N	O	S	0	12	0
			5203	1639	2610	448	492	14			
1	H	333	Total	C	H	N	O	S	0	5	0
			5121	1617	2561	443	486	14			

- Molecule 2 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula: C₂₀H₄₂O₁₁).



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
			30	8	17	5		
2	B	1	Total	C	H	O	0	0
			37	10	21	6		
2	C	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	D	1	Total	C	H	O	0	0
			37	10	21	6		
2	E	1	Total	C	H	O	0	0
			31	9	17	5		
2	F	1	Total	C	H	O	0	0
			30	8	17	5		
2	F	1	Total	C	H	O	0	0
			13	5	6	2		
2	G	1	Total	C	H	O	0	0
			73	20	42	11		
2	G	1	Total	C	H	O	0	1
			26	7	15	4		
2	H	1	Total	C	H	O	0	0
			37	10	21	6		
2	H	1	Total	C	H	O	0	0
			29	8	16	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total 232	O 232	0	0
3	B	224	Total 224	O 224	0	0
3	C	192	Total 192	O 192	0	0
3	D	171	Total 171	O 171	0	0
3	E	197	Total 197	O 197	0	0
3	F	199	Total 199	O 199	0	0
3	G	247	Total 247	O 247	0	0
3	H	177	Total 177	O 177	0	0

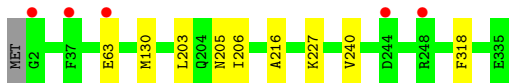
3 Residue-property plots [i](#)

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



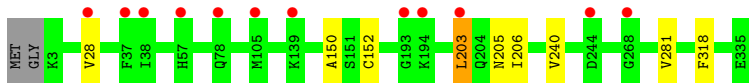
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



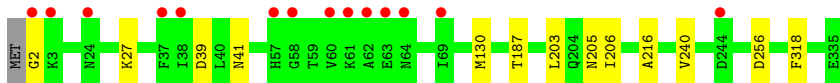
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



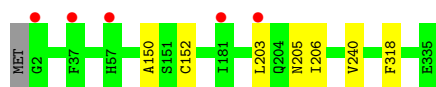
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



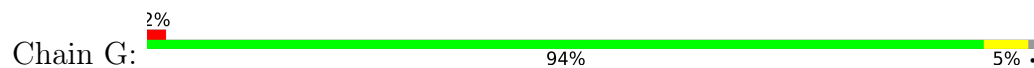
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



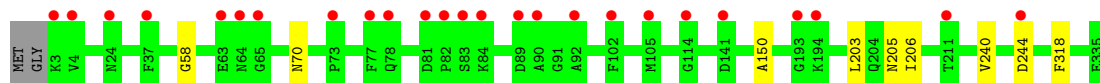
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.89Å 124.45Å 141.99Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	140.09 – 1.52 140.08 – 1.52	Depositor EDS
% Data completeness (in resolution range)	69.4 (140.09-1.52) 69.4 (140.08-1.52)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.52Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.182 , 0.200 (Not available) , 0.200	Depositor DCC
R_{free} test set	14686 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	43512	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.71	0/2667	0.94	2/3606 (0.1%)
1	B	0.69	0/2661	0.93	2/3598 (0.1%)
1	C	0.70	1/2630 (0.0%)	0.92	3/3556 (0.1%)
1	D	0.68	1/2664 (0.0%)	0.93	3/3601 (0.1%)
1	E	0.69	0/2647	0.93	2/3578 (0.1%)
1	F	0.68	1/2620 (0.0%)	0.93	2/3541 (0.1%)
1	G	0.70	1/2653 (0.0%)	0.92	2/3588 (0.1%)
1	H	0.70	1/2596 (0.0%)	0.94	3/3511 (0.1%)
All	All	0.69	5/21138 (0.0%)	0.93	19/28579 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	150	ALA	CA-C	5.74	1.60	1.52
1	G	150	ALA	CA-C	5.61	1.60	1.52
1	D	150	ALA	CA-C	5.46	1.60	1.52
1	H	150	ALA	CA-C	5.41	1.60	1.52
1	C	150	ALA	CA-C	5.36	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ILE	N-CA-C	-6.09	99.82	108.58
1	B	206	ILE	N-CA-C	-6.03	99.90	108.58
1	A	206	ILE	N-CA-C	-5.99	99.95	108.58
1	D	206	ILE	N-CA-C	-5.95	100.01	108.58
1	H	205	ASN	N-CA-C	5.92	118.86	109.50
1	H	206	ILE	N-CA-C	-5.90	100.08	108.58
1	A	205	ASN	N-CA-C	5.84	118.72	109.50
1	F	206	ILE	N-CA-C	-5.83	100.19	108.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	205	ASN	N-CA-C	5.78	118.64	109.50
1	C	205	ASN	N-CA-C	5.74	118.56	109.50
1	F	205	ASN	N-CA-C	5.73	118.55	109.50
1	D	205	ASN	N-CA-C	5.64	118.41	109.50
1	G	205	ASN	N-CA-C	5.63	118.40	109.50
1	E	206	ILE	N-CA-C	-5.62	100.49	108.58
1	G	206	ILE	N-CA-C	-5.58	100.54	108.58
1	B	205	ASN	N-CA-C	5.52	118.23	109.50
1	H	244	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	281	VAL	N-CA-C	5.27	115.79	110.05
1	D	281	VAL	N-CA-C	5.05	115.55	110.05

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	2591	2613	2582	4	0
1	B	2586	2600	2558	5	0
1	C	2575	2586	2576	23	0
1	D	2594	2611	2594	4	0
1	E	2593	2600	2598	22	0
1	F	2581	2583	2578	17	0
1	G	2593	2610	2607	27	0
1	H	2560	2561	2557	5	0
2	A	14	17	17	0	0
2	B	29	38	38	0	0
2	C	14	17	17	0	0
2	D	30	38	38	0	0
2	E	14	17	17	0	0
2	F	20	23	23	0	0
2	G	42	57	42	0	0
2	H	29	37	37	0	0
3	A	232	0	0	0	0
3	B	224	0	0	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	192	0	0	1	0
3	D	171	0	0	0	0
3	E	197	0	0	0	0
3	F	199	0	0	0	0
3	G	247	0	0	3	1
3	H	177	0	0	0	0
All	All	22504	21008	20879	64	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (64) 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:C:203[B]:LEU:CD1	1:E:203[B]:LEU:HD11	1.48	1.42
1:F:203[B]:LEU:HD11	1:G:203[B]:LEU:CD1	1.49	1.41
1:F:203[B]:LEU:CD1	1:G:203[B]:LEU:HD11	1.50	1.39
1:C:203[B]:LEU:HD11	1:E:203[B]:LEU:CD1	1.49	1.39
1:F:203[B]:LEU:HG	1:G:203[B]:LEU:HD21	1.27	1.11
1:F:203[B]:LEU:HG	1:G:203[B]:LEU:CD2	1.81	1.10
1:F:203[B]:LEU:HD21	1:G:203[B]:LEU:HG	1.28	1.09
1:F:203[B]:LEU:CD2	1:G:203[B]:LEU:HG	1.83	1.09
1:C:203[B]:LEU:HD21	1:E:203[B]:LEU:HG	1.34	1.08
1:C:203[B]:LEU:HG	1:E:203[B]:LEU:CD2	1.82	1.07
1:C:203[B]:LEU:CD2	1:E:203[B]:LEU:HG	1.84	1.07
1:C:203[B]:LEU:HG	1:E:203[B]:LEU:HD21	1.32	1.06
1:F:203[B]:LEU:HD11	1:G:203[B]:LEU:HD11	1.01	0.99
1:C:203[B]:LEU:HD12	1:E:203[B]:LEU:HD11	1.47	0.96
1:C:203[B]:LEU:HD11	1:E:203[B]:LEU:HD12	1.47	0.93
1:C:203[B]:LEU:HG	1:E:203[B]:LEU:CG	2.01	0.91
1:F:203[B]:LEU:HD12	1:G:203[B]:LEU:HD11	1.52	0.89
1:F:203[B]:LEU:HD11	1:G:203[B]:LEU:HD12	1.53	0.89
1:C:203[B]:LEU:CG	1:E:203[B]:LEU:HG	2.02	0.89
1:F:203[B]:LEU:CD1	1:G:203[B]:LEU:CD1	2.27	0.88
1:C:203[B]:LEU:CD1	1:E:203[B]:LEU:CD1	2.23	0.87
1:F:203[B]:LEU:CG	1:G:203[B]:LEU:HG	2.06	0.86
1:F:203[B]:LEU:HG	1:G:203[B]:LEU:CG	2.07	0.84
1:C:203[B]:LEU:CG	1:E:203[B]:LEU:CG	2.56	0.84
1:A:203[A]:LEU:HD21	1:H:203[A]:LEU:HB2	1.60	0.83
1:F:203[B]:LEU:CG	1:G:203[B]:LEU:CG	2.59	0.79
1:C:203[B]:LEU:HD11	1:E:203[B]:LEU:HD11	1.06	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203[B]:LEU:HB2	1:H:203[B]:LEU:HD21	1.67	0.77
1:B:227:LYS:NZ	3:B:3101:HOH:O	2.14	0.74
1:G:185:GLN:OE1	1:G:234[B]:ARG:HG2	1.86	0.74
1:A:203[A]:LEU:HD22	1:H:203[A]:LEU:HD13	1.72	0.72
1:G:24[A]:ASN:ND2	3:G:3102:HOH:O	2.29	0.65
1:B:203[B]:LEU:HD21	1:D:203[B]:LEU:HB2	1.78	0.64
1:C:203[B]:LEU:HG	1:E:203[B]:LEU:HG	1.73	0.64
1:G:47:PHE:CD2	1:G:60:VAL:HG11	2.34	0.63
1:G:185:GLN:OE1	1:G:234[B]:ARG:CG	2.50	0.59
1:G:47:PHE:HD2	1:G:60:VAL:HG11	1.67	0.59
1:E:2:GLY:HA2	1:E:27:LYS:O	2.07	0.54
1:C:203[B]:LEU:CD1	1:E:203[B]:LEU:CG	2.83	0.53
1:G:185:GLN:CD	1:G:234[B]:ARG:HG2	2.34	0.53
1:C:260:LYS:O	1:C:264:GLN:HG2	2.09	0.53
1:F:203[B]:LEU:CG	1:G:203[B]:LEU:CD1	2.87	0.51
1:B:203[A]:LEU:HB2	1:D:203[A]:LEU:HD21	1.93	0.50
1:C:203[B]:LEU:CG	1:E:203[B]:LEU:HD11	2.33	0.50
1:F:203[B]:LEU:CD1	1:G:203[B]:LEU:CG	2.84	0.50
1:C:203[B]:LEU:CG	1:E:203[B]:LEU:CD1	2.82	0.50
1:G:287:ASN:HB3	3:G:3130:HOH:O	2.14	0.48
1:F:203[B]:LEU:HD11	1:G:203[B]:LEU:CG	2.33	0.47
1:C:203[A]:LEU:HD13	1:E:203[A]:LEU:HD13	1.99	0.45
1:G:237[B]:THR:HG21	3:G:3194:HOH:O	2.15	0.45
1:G:60:VAL:HG12	1:G:69:ILE:HG12	1.98	0.45
1:H:58:GLY:HA3	1:H:70:ASN:OD1	2.17	0.45
1:F:203[A]:LEU:HD13	1:G:203[A]:LEU:HD13	1.98	0.45
1:B:203[B]:LEU:HD22	1:D:203[B]:LEU:HD13	1.99	0.44
1:C:85:ILE:HG21	1:C:87:TRP:CE2	2.52	0.44
1:D:203[A]:LEU:N	1:D:203[A]:LEU:HD23	2.31	0.44
1:G:39:ASP:OD1	1:G:41[B]:ASN:OD1	2.38	0.42
1:C:37:PHE:HE1	1:C:80:ARG:NH2	2.17	0.42
1:C:181:ILE:HD12	1:E:187:THR:HB	2.02	0.42
1:E:39:ASP:OD1	1:E:41[B]:ASN:OD1	2.38	0.42
1:E:130[B]:MET:HE1	1:E:216:ALA:HB1	2.02	0.42
1:B:130:MET:HE1	1:B:216:ALA:HB1	2.01	0.41
1:A:203[B]:LEU:HD13	1:H:203[B]:LEU:HD22	2.03	0.41
1:C:237[B]:THR:HG21	3:C:3128:HOH:O	2.20	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3301:HOH:O	3:G:3346:HOH:O[1_455]	2.01	0.19

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	343/335 (102%)	333 (97%)	9 (3%)	1 (0%)	36	18
1	B	342/335 (102%)	333 (97%)	8 (2%)	1 (0%)	36	18
1	C	339/335 (101%)	331 (98%)	7 (2%)	1 (0%)	36	18
1	D	342/335 (102%)	334 (98%)	7 (2%)	1 (0%)	36	18
1	E	341/335 (102%)	332 (97%)	8 (2%)	1 (0%)	36	18
1	F	337/335 (101%)	328 (97%)	8 (2%)	1 (0%)	36	18
1	G	341/335 (102%)	332 (97%)	8 (2%)	1 (0%)	36	18
1	H	334/335 (100%)	325 (97%)	8 (2%)	1 (0%)	36	18
All	All	2719/2680 (102%)	2648 (97%)	63 (2%)	8 (0%)	36	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	VAL
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

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	281/270 (104%)	276 (98%)	5 (2%)	51	23
1	B	280/270 (104%)	278 (99%)	2 (1%)	76	57
1	C	277/270 (103%)	276 (100%)	1 (0%)	84	71
1	D	281/270 (104%)	277 (99%)	4 (1%)	59	31
1	E	278/270 (103%)	276 (99%)	2 (1%)	76	57
1	F	275/270 (102%)	274 (100%)	1 (0%)	84	71
1	G	280/270 (104%)	278 (99%)	2 (1%)	76	57
1	H	273/270 (101%)	272 (100%)	1 (0%)	84	71
All	All	2225/2160 (103%)	2207 (99%)	18 (1%)	76	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203[A]	LEU
1	A	203[B]	LEU
1	A	261[A]	VAL
1	A	261[B]	VAL
1	A	318	PHE
1	B	63	GLU
1	B	318	PHE
1	C	318	PHE
1	D	28	VAL
1	D	203[A]	LEU
1	D	203[B]	LEU
1	D	318	PHE
1	E	256	ASP
1	E	318	PHE
1	F	318	PHE
1	G	63	GLU
1	G	318	PHE
1	H	318	PHE

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

Mol	Chain	Res	Type
1	A	72	ASN
1	A	167	ASN
1	B	72	ASN
1	C	24	ASN
1	C	322	ASN
1	D	142	ASN
1	E	239	ASN
1	F	72	ASN
1	F	239	ASN
1	G	142	ASN
1	H	72	ASN
1	H	330	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	152[B]	1	7,9,10	0.92	0	4,12,14	1.23	1 (25%)
1	CSU	C	152[B]	1	7,9,10	0.94	0	4,12,14	1.15	0
1	CSU	F	152[A]	1	4,5,10	0.79	0	1,5,14	0.23	0
1	CSU	H	152[B]	1	7,9,10	0.98	0	4,12,14	1.19	0
1	CSU	E	152[A]	1	4,5,10	0.85	0	1,5,14	0.06	0
1	CSU	A	152[B]	1	7,9,10	0.97	0	4,12,14	1.26	0
1	CSU	B	152[A]	1	4,5,10	0.76	0	1,5,14	0.52	0
1	CSU	F	152[B]	1	7,9,10	0.97	0	4,12,14	1.24	1 (25%)
1	CSU	G	152[A]	1	4,5,10	0.76	0	1,5,14	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSU	H	152[A]	1	4,5,10	0.73	0	1,5,14	0.77	0
1	CSU	D	152[A]	1	4,5,10	0.68	0	1,5,14	0.64	0
1	CSU	C	152[A]	1	4,5,10	0.77	0	1,5,14	0.40	0
1	CSU	E	152[B]	1	7,9,10	0.98	0	4,12,14	1.19	0
1	CSU	G	152[B]	1	7,9,10	1.09	1 (14%)	4,12,14	1.36	1 (25%)
1	CSU	B	152[B]	1	7,9,10	1.01	0	4,12,14	1.19	0
1	CSU	A	152[A]	1	4,5,10	0.69	0	1,5,14	0.30	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	D	152[B]	1	-	3/4/8/10	-
1	CSU	C	152[B]	1	-	3/4/8/10	-
1	CSU	F	152[A]	1	-	0/1/4/10	-
1	CSU	H	152[B]	1	-	0/4/8/10	-
1	CSU	E	152[A]	1	-	0/1/4/10	-
1	CSU	A	152[B]	1	-	2/4/8/10	-
1	CSU	B	152[A]	1	-	0/1/4/10	-
1	CSU	F	152[B]	1	-	1/4/8/10	-
1	CSU	G	152[A]	1	-	0/1/4/10	-
1	CSU	H	152[A]	1	-	0/1/4/10	-
1	CSU	D	152[A]	1	-	0/1/4/10	-
1	CSU	C	152[A]	1	-	0/1/4/10	-
1	CSU	E	152[B]	1	-	3/4/8/10	-
1	CSU	G	152[B]	1	-	4/4/8/10	-
1	CSU	B	152[B]	1	-	2/4/8/10	-
1	CSU	A	152[A]	1	-	0/1/4/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	152[B]	CSU	OD1-S	-2.10	1.39	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	152[B]	CSU	OD2-S-OD1	-2.12	105.67	112.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152[B]	CSU	OD2-S-OD1	-2.05	105.91	112.74
1	F	152[B]	CSU	OD2-S-OD1	-2.01	106.06	112.74

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

14 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	D	3001	-	13,13,30	0.20	0	12,12,29	0.12	0
2	XPE	A	3001	-	13,13,30	0.14	0	12,12,29	0.22	0
2	XPE	F	3002	-	6,6,30	0.26	0	5,5,29	0.15	0
2	XPE	E	3001	-	13,13,30	0.13	0	12,12,29	0.11	0
2	XPE	H	402	-	12,12,30	0.12	0	11,11,29	0.19	0
2	XPE	B	3001	-	12,12,30	0.13	0	11,11,29	0.19	0
2	XPE	C	3001	-	13,13,30	0.19	0	12,12,29	0.12	0
2	XPE	H	401	-	15,15,30	0.17	0	14,14,29	0.12	0
2	XPE	B	3002	-	15,15,30	0.15	0	14,14,29	0.14	0
2	XPE	F	3001	-	12,12,30	0.16	0	11,11,29	0.12	0
2	XPE	D	3002	-	15,15,30	0.16	0	14,14,29	0.13	0
2	XPE	G	3001	-	30,30,30	0.22	0	29,29,29	0.13	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	D	3001	-	-	1/11/11/28	-
2	XPE	A	3001	-	-	3/11/11/28	-
2	XPE	F	3002	-	-	1/4/4/28	-
2	XPE	E	3001	-	-	3/11/11/28	-
2	XPE	H	402	-	-	1/10/10/28	-
2	XPE	B	3001	-	-	1/10/10/28	-
2	XPE	C	3001	-	-	1/11/11/28	-
2	XPE	H	401	-	-	4/13/13/28	-
2	XPE	B	3002	-	-	4/13/13/28	-
2	XPE	F	3001	-	-	1/10/10/28	-
2	XPE	D	3002	-	-	4/13/13/28	-
2	XPE	G	3001	-	-	7/28/28/28	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

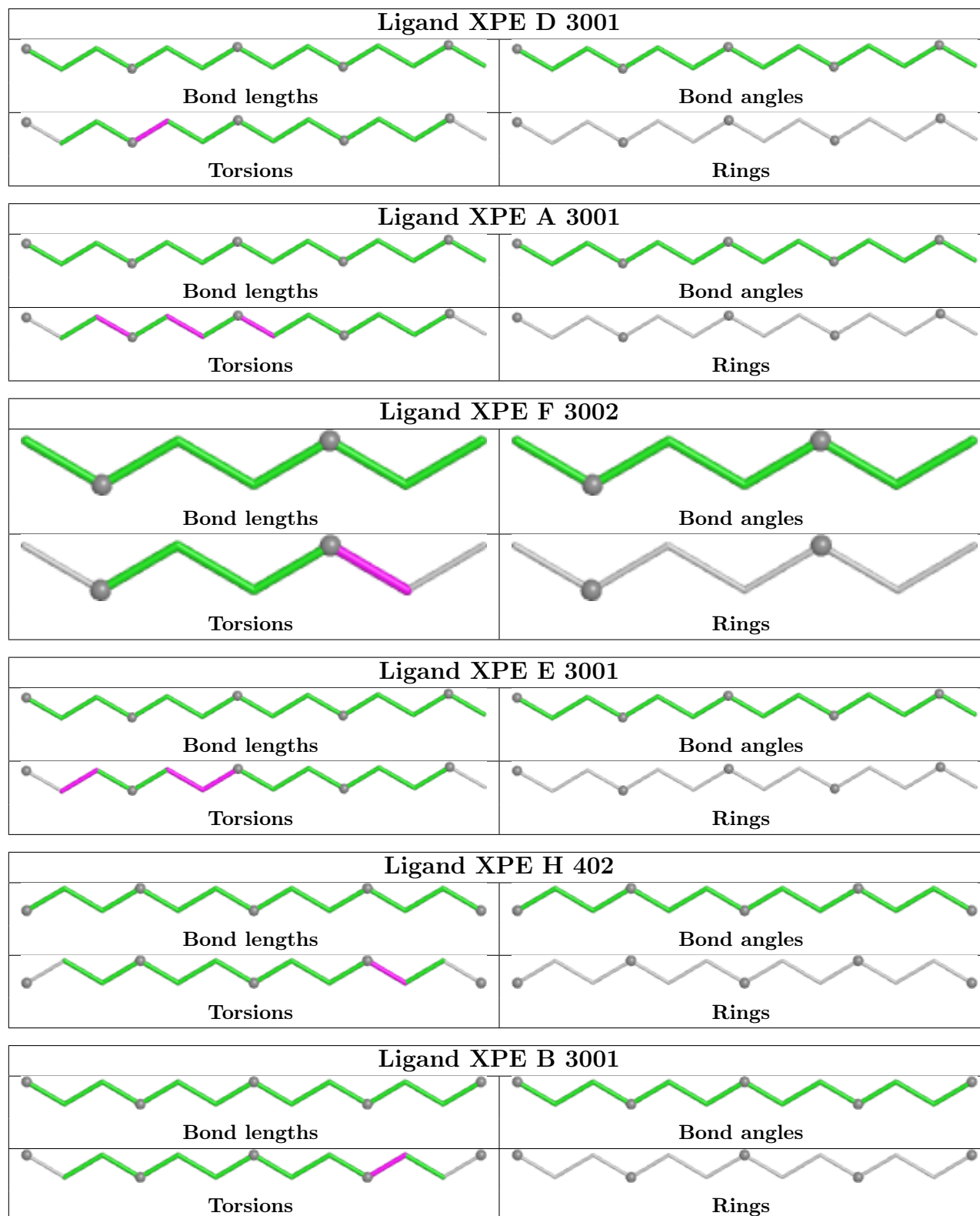
Mol	Chain	Res	Type	Atoms
2	A	3001	XPE	O25-C26-C27-O28
2	E	3001	XPE	O25-C26-C27-O28
2	H	401	XPE	O22-C23-C24-O25
2	D	3002	XPE	O22-C23-C24-O25
2	B	3002	XPE	O22-C23-C24-O25
2	G	3001	XPE	O13-C14-C15-O16
2	B	3002	XPE	O28-C29-C30-O31
2	D	3002	XPE	O28-C29-C30-O31
2	H	401	XPE	O28-C29-C30-O31
2	G	3001	XPE	C15-C14-O13-C12
2	B	3001	XPE	C20-C21-O22-C23
2	F	3001	XPE	C30-C29-O28-C27
2	A	3001	XPE	C30-C29-O28-C27
2	C	3001	XPE	C26-C27-O28-C29
2	F	3002	XPE	C23-C24-O25-C26
2	D	3001	XPE	C26-C27-O28-C29
2	A	3001	XPE	C23-C24-O25-C26
2	E	3001	XPE	O28-C29-C30-O31
2	G	3001	XPE	C26-C27-O28-C29
2	G	3001	XPE	C6-C5-O4-C3
2	G	3001	XPE	C14-C15-O16-C17
2	B	3002	XPE	C23-C24-O25-C26
2	H	401	XPE	C23-C24-O25-C26
2	D	3002	XPE	C23-C24-O25-C26
2	G	3001	XPE	O10-C11-C12-O13
2	H	401	XPE	C24-C23-O22-C21
2	D	3002	XPE	C24-C23-O22-C21
2	B	3002	XPE	C24-C23-O22-C21
2	H	402	XPE	C17-C18-O19-C20
2	G	3001	XPE	C12-C11-O10-C9
2	E	3001	XPE	C27-C26-O25-C24

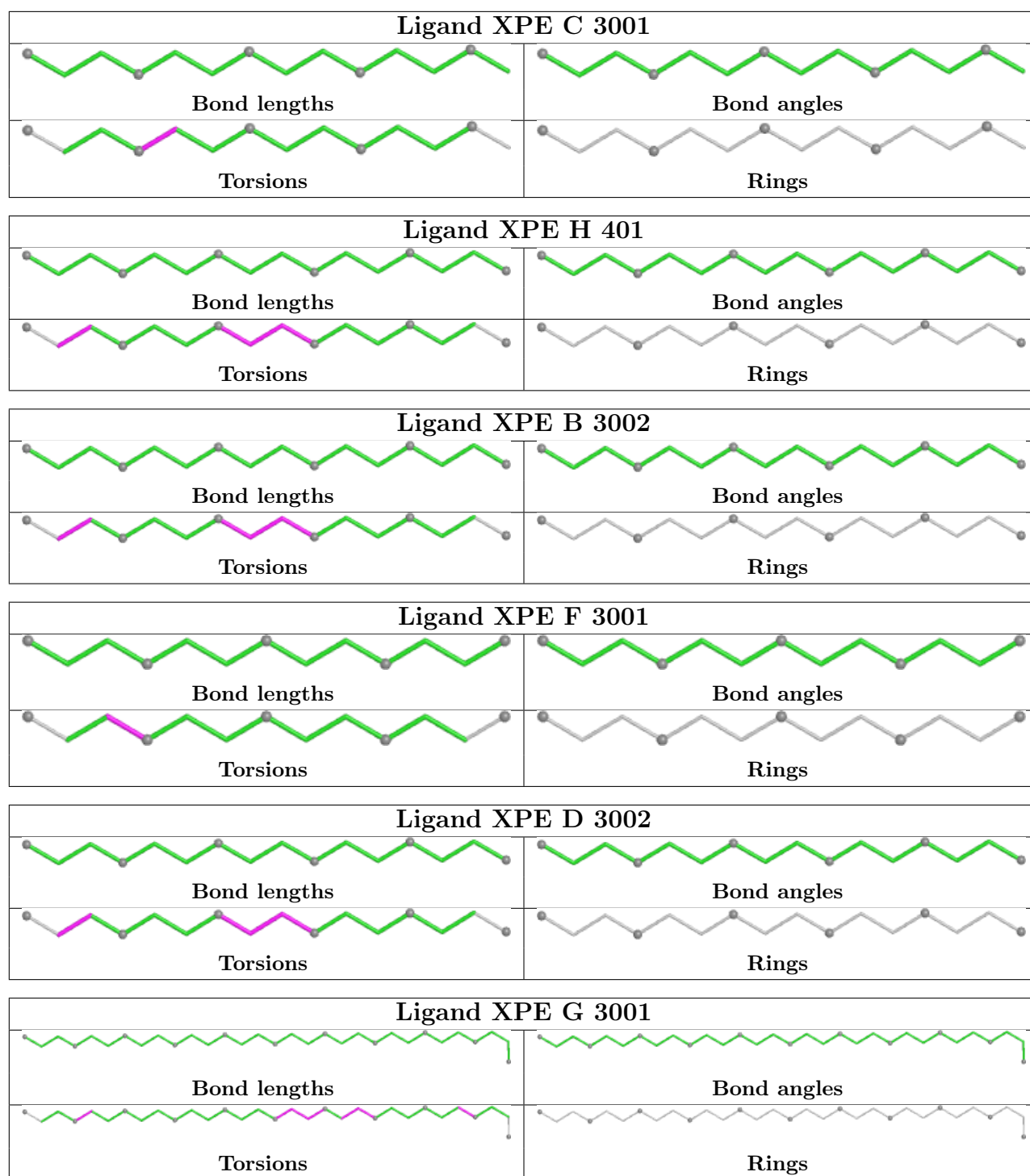
There are no ring outliers.

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	333/335 (99%)	0.10	10 (3%)	52	59	9, 23, 38, 50	9 (2%)
1	B	333/335 (99%)	0.04	5 (1%)	72	77	10, 24, 39, 50	7 (2%)
1	C	333/335 (99%)	0.23	6 (1%)	67	73	10, 25, 41, 52	7 (2%)
1	D	332/335 (99%)	0.42	12 (3%)	46	53	10, 28, 44, 54	10 (3%)
1	E	333/335 (99%)	0.36	14 (4%)	40	47	10, 25, 42, 53	10 (3%)
1	F	333/335 (99%)	0.15	5 (1%)	72	77	10, 25, 40, 49	6 (1%)
1	G	332/335 (99%)	-0.05	6 (1%)	67	73	9, 21, 37, 48	11 (3%)
1	H	332/335 (99%)	0.46	25 (7%)	20	24	9, 27, 49, 58	4 (1%)
All	All	2661/2680 (99%)	0.21	83 (3%)	51	58	9, 25, 42, 58	64 (2%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	GLY	6.8
1	B	37	PHE	5.5
1	E	57	HIS	3.9
1	E	37	PHE	3.7
1	H	37	PHE	3.6
1	C	2	GLY	3.4
1	A	37	PHE	3.3
1	C	194	LYS	3.2
1	H	3	LYS	3.2
1	B	2	GLY	3.2
1	D	37	PHE	3.2
1	H	90	ALA	3.2
1	F	181	ILE	3.1
1	E	60	VAL	3.0
1	H	193	GLY	3.0
1	H	194	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	37	PHE	2.9
1	G	37	PHE	2.9
1	H	77	PHE	2.8
1	C	244	ASP	2.8
1	B	244	ASP	2.8
1	D	28	VAL	2.7
1	G	60	VAL	2.7
1	H	244	ASP	2.7
1	F	37	PHE	2.7
1	H	82	PRO	2.7
1	A	57	HIS	2.7
1	D	57	HIS	2.7
1	A	244	ASP	2.6
1	H	73	PRO	2.6
1	E	38	ILE	2.6
1	F	57	HIS	2.6
1	H	64	ASN	2.6
1	E	64	ASN	2.6
1	D	38	ILE	2.5
1	H	114	GLY	2.5
1	H	81	ASP	2.5
1	G	194	LYS	2.5
1	D	193	GLY	2.4
1	D	194	LYS	2.4
1	F	2	GLY	2.4
1	G	24[A]	ASN	2.4
1	D	244	ASP	2.4
1	A	203[A]	LEU	2.4
1	H	63	GLU	2.4
1	H	92	ALA	2.4
1	E	63	GLU	2.4
1	D	203[A]	LEU	2.4
1	E	244	ASP	2.3
1	H	65	GLY	2.3
1	D	139	LYS	2.3
1	E	61	LYS	2.3
1	E	24	ASN	2.3
1	E	69	ILE	2.3
1	E	62	ALA	2.3
1	H	141	ASP	2.3
1	C	38	ILE	2.3
1	H	102	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	57	HIS	2.2
1	E	58	GLY	2.2
1	H	4	VAL	2.2
1	H	84	LYS	2.2
1	H	24	ASN	2.2
1	A	194	LYS	2.2
1	G	26	GLY	2.1
1	H	78	GLN	2.1
1	A	63	GLU	2.1
1	A	248[A]	ARG	2.1
1	D	268	GLY	2.1
1	F	203[A]	LEU	2.1
1	H	105	MET	2.1
1	C	251	LYS	2.1
1	E	3	LYS	2.1
1	H	211	THR	2.1
1	B	63	GLU	2.1
1	H	83	SER	2.1
1	D	105	MET	2.1
1	A	24[A]	ASN	2.1
1	D	78[A]	GLN	2.0
1	A	64	ASN	2.0
1	B	248[A]	ARG	2.0
1	A	142	ASN	2.0
1	H	89	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSU	F	152[A]	6/11	0.91	0.18	19,23,28,28	10
1	CSU	F	152[B]	10/11	0.91	0.18	20,23,26,27	15
1	CSU	D	152[A]	6/11	0.94	0.16	18,22,26,26	10
1	CSU	D	152[B]	10/11	0.94	0.16	19,23,26,28	15
1	CSU	E	152[A]	6/11	0.95	0.14	16,21,25,25	10
1	CSU	E	152[B]	10/11	0.95	0.14	17,19,23,24	15
1	CSU	B	152[A]	6/11	0.95	0.13	15,20,24,24	10
1	CSU	B	152[B]	10/11	0.95	0.13	16,19,21,23	15

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSU	C	152[A]	6/11	0.96	0.15	18,21,26,26	0
1	CSU	C	152[B]	10/11	0.96	0.15	18,20,23,24	15
1	CSU	A	152[A]	6/11	0.96	0.13	16,20,25,25	10
1	CSU	A	152[B]	10/11	0.96	0.13	16,19,22,23	15
1	CSU	H	152[A]	6/11	0.96	0.14	18,23,27,27	0
1	CSU	H	152[B]	10/11	0.96	0.14	18,20,23,24	15
1	CSU	G	152[A]	6/11	0.97	0.11	14,17,21,21	10
1	CSU	G	152[B]	10/11	0.97	0.11	15,18,20,22	15

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

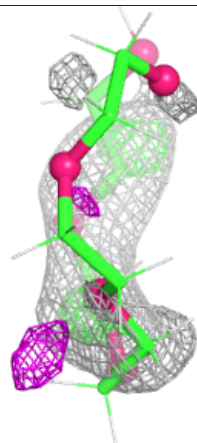
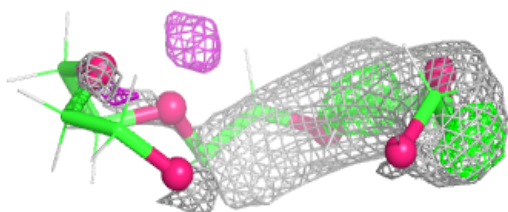
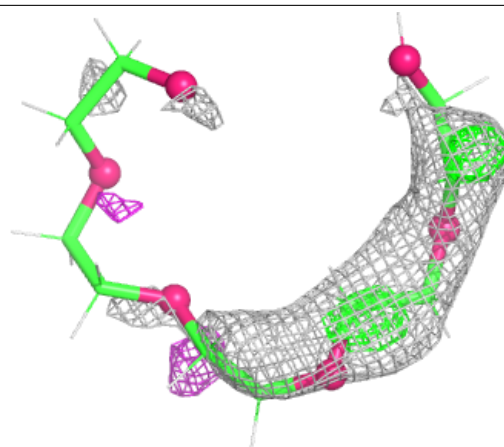
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XPE	D	3002	16/31	0.67	0.27	92,111,114,114	0
2	XPE	F	3002	7/31	0.68	0.33	54,55,66,66	0
2	XPE	D	3001	14/31	0.70	0.21	41,51,62,62	0
2	XPE	H	401	16/31	0.70	0.26	82,98,100,100	0
2	XPE	B	3002	16/31	0.73	0.23	69,83,88,88	0
2	XPE	C	3001	14/31	0.73	0.19	43,52,63,64	0
2	XPE	G	3001	31/31	0.76	0.19	30,50,79,79	0
2	XPE	F	3001	13/31	0.78	0.18	42,51,61,61	0
2	XPE	E	3001	14/31	0.80	0.16	36,45,57,58	0
2	XPE	G	3002[B]	11/31	0.81	0.19	48,57,60,60	1
2	XPE	G	3002[A]	11/31	0.81	0.19	48,57,60,60	1
2	XPE	A	3001	14/31	0.84	0.16	36,44,55,56	0
2	XPE	B	3001	13/31	0.85	0.14	40,49,53,54	0
2	XPE	H	402	13/31	0.86	0.14	46,55,57,58	0

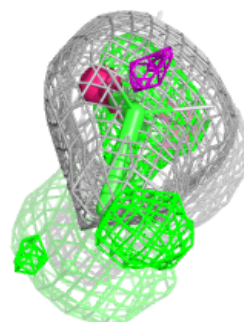
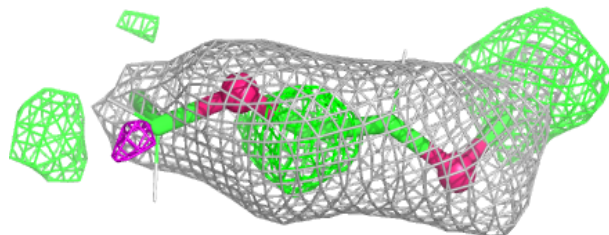
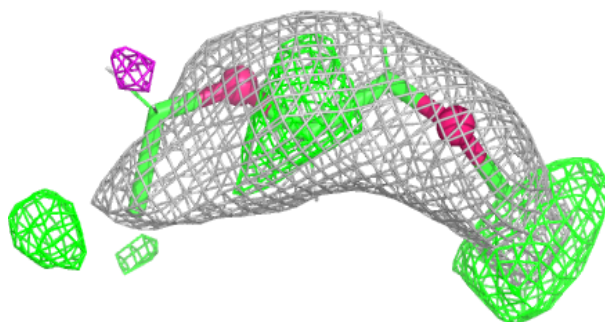
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XPE D 3002:

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

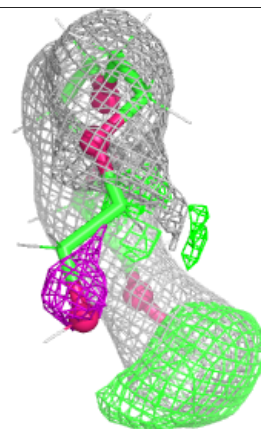
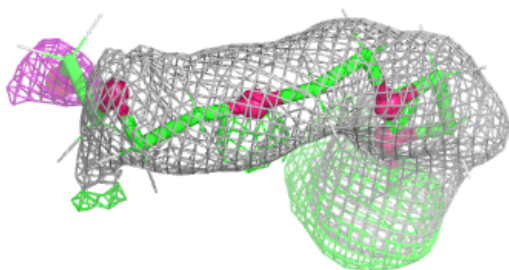
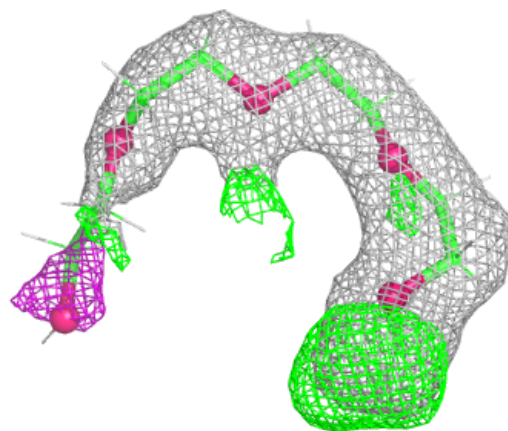
**Electron density around XPE F 3002:**

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



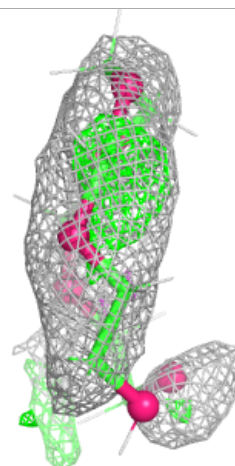
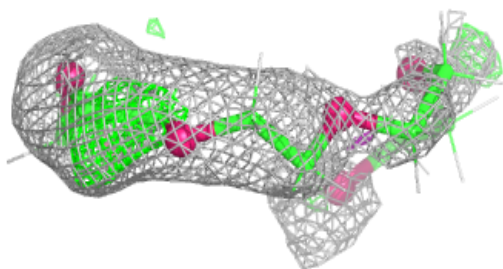
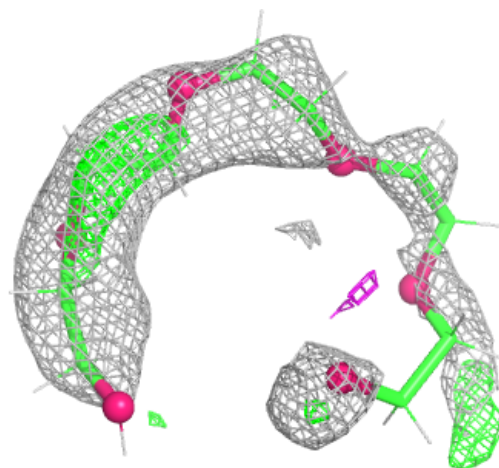
Electron density around XPE D 3001:

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



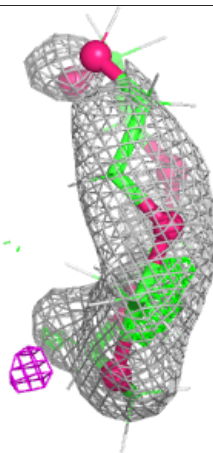
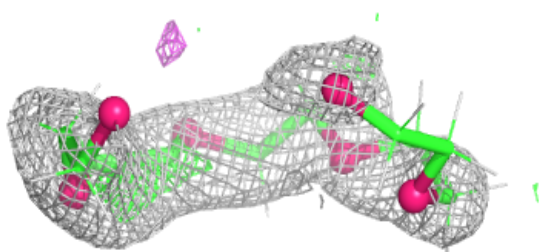
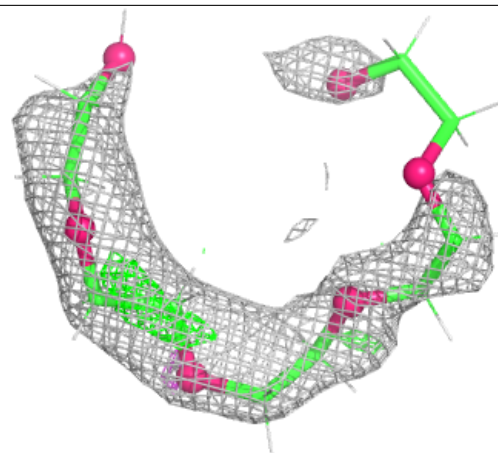
Electron density around XPE H 401:

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



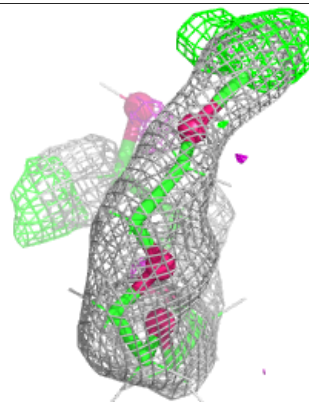
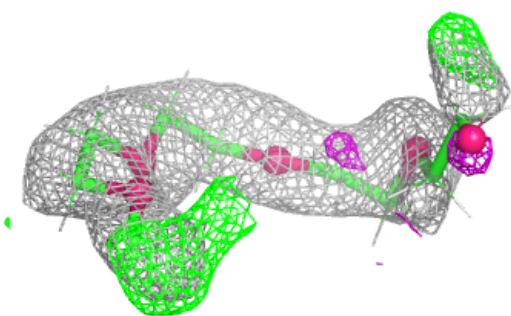
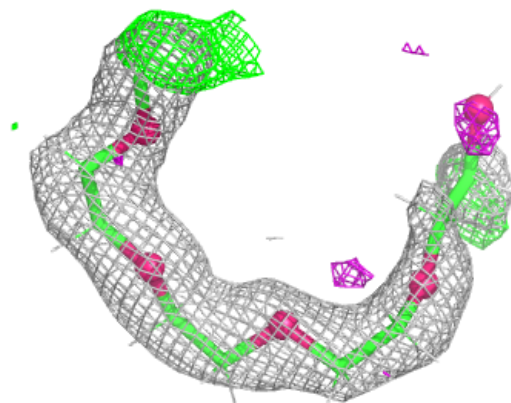
Electron density around XPE B 3002:

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

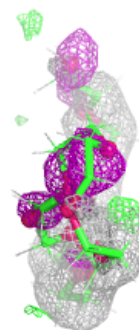
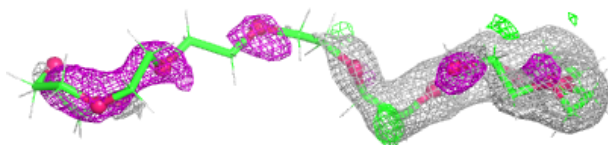
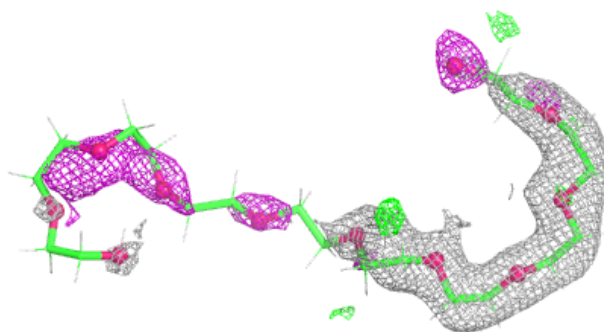


Electron density around XPE C 3001:

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

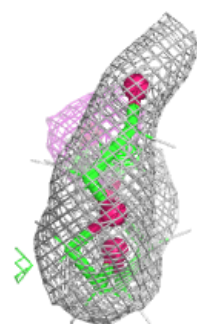
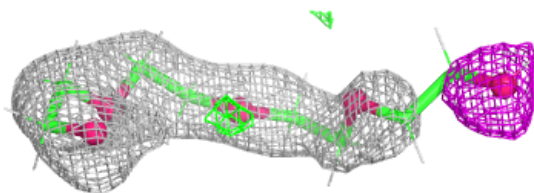
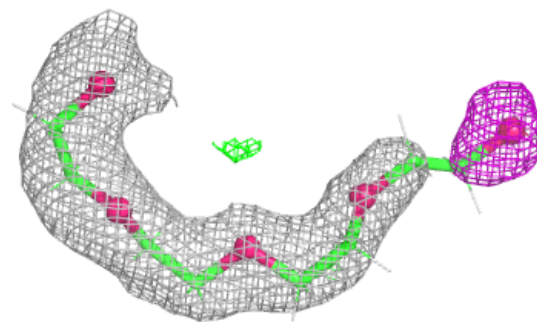
**Electron density around XPE G 3001:**

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



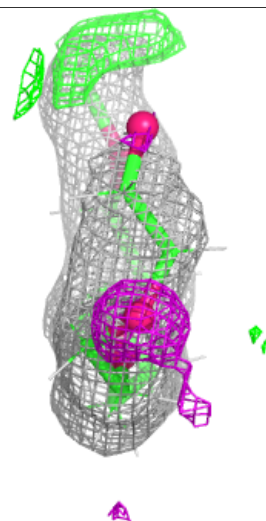
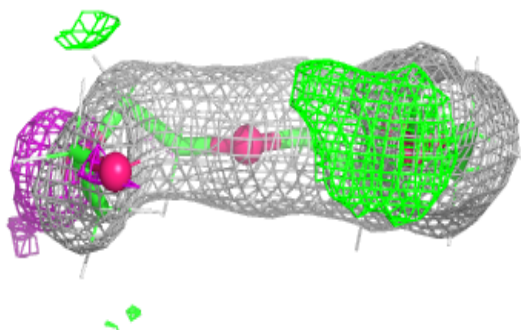
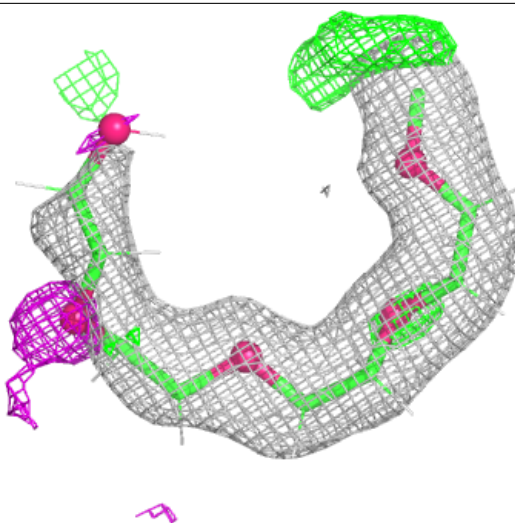
Electron density around XPE F 3001:

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



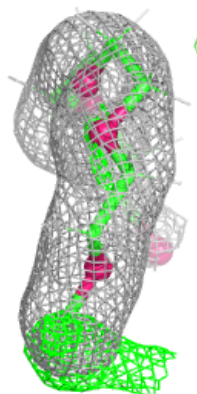
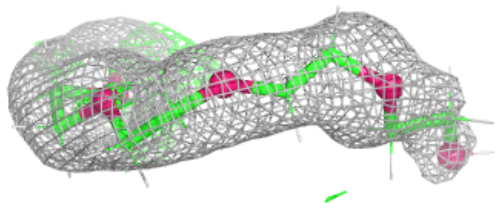
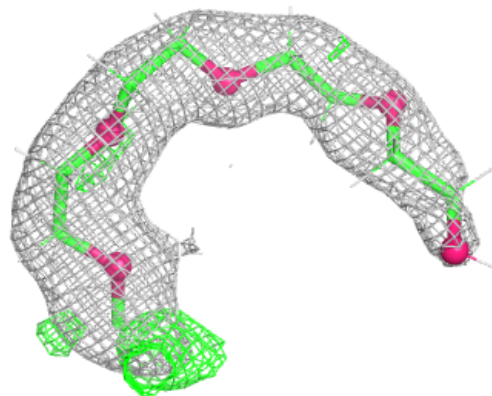
Electron density around XPE E 3001:

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

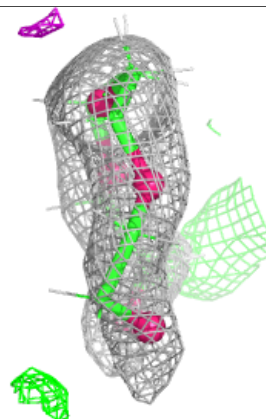
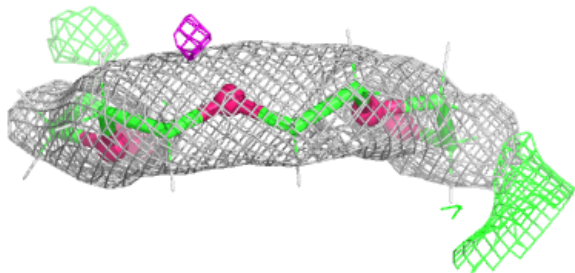
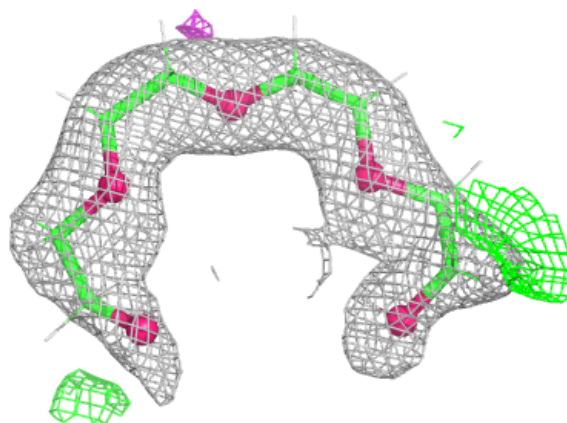


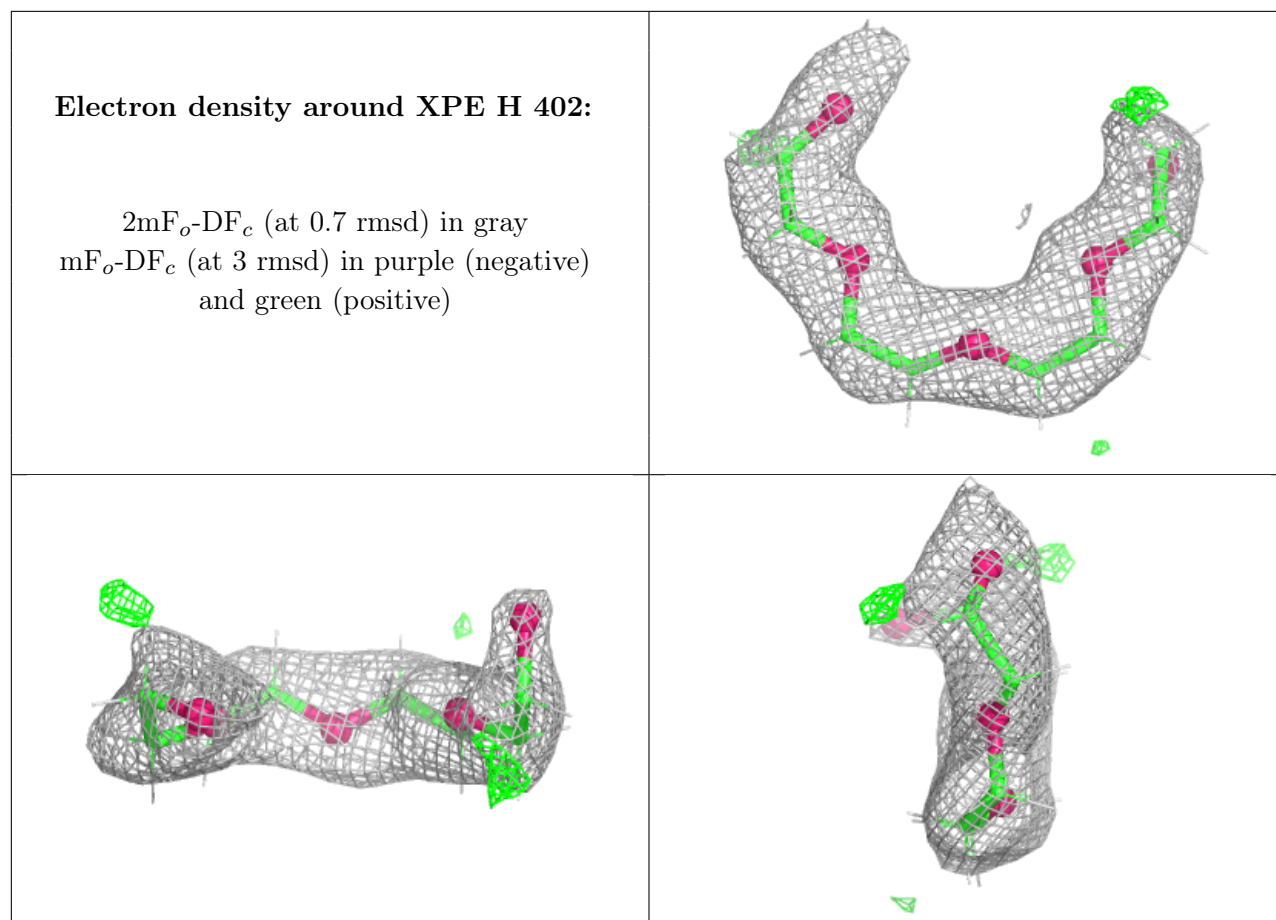
Electron density around XPE A 3001:

$2mF_o-DF_c$ (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.