



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:05 AM UTC

PDB ID : 9D1K / pdb\_00009d1k  
Title : The alpha-E7 carboxylesterase from *Anopheles gambiae*  
Authors : Frkic, R.L.; Esmaily, M.; Fraser, N.; Mabbitt, P.D.; Jackson, C.J.  
Deposited on : 2024-08-07  
Resolution : 1.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

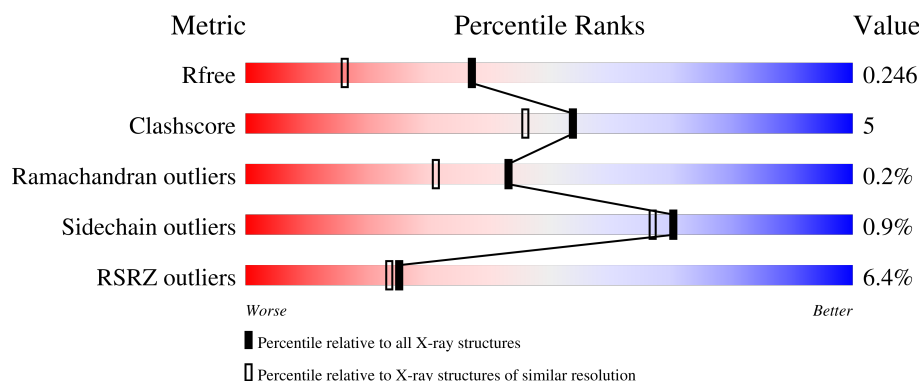
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	540	<div> <div>2%</div> <div>93%</div> <div>6%</div> </div>
2	B	540	<div> <div>4%</div> <div>89%</div> <div>9%</div> </div>
3	C	540	<div> <div>14%</div> <div>83%</div> <div>16%</div> </div>
4	D	540	<div> <div>6%</div> <div>86%</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 18024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	6	0
			4259	2726	712	800	21			

- Molecule 2 is a protein called Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	533	Total	C	N	O	S	0	4	0
			4220	2697	711	792	20			

- Molecule 3 is a protein called Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	534	Total	C	N	O	S	0	3	0
			4206	2693	702	791	20			

- Molecule 4 is a protein called Carboxylic ester hydrolase.

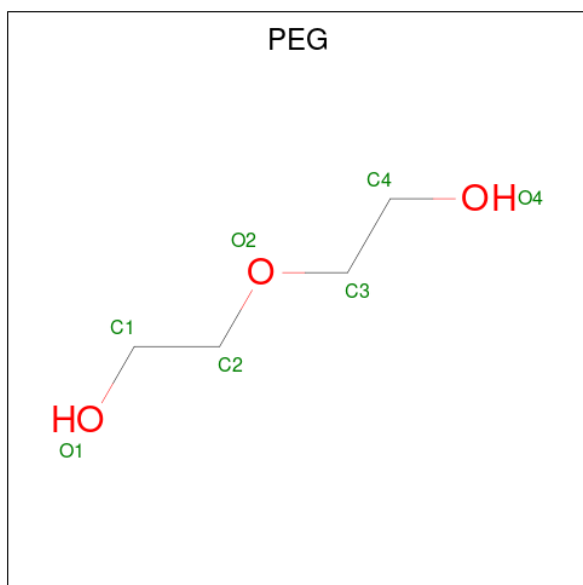
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	538	Total	C	N	O	S	0	0	0
			4230	2703	710	797	20			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



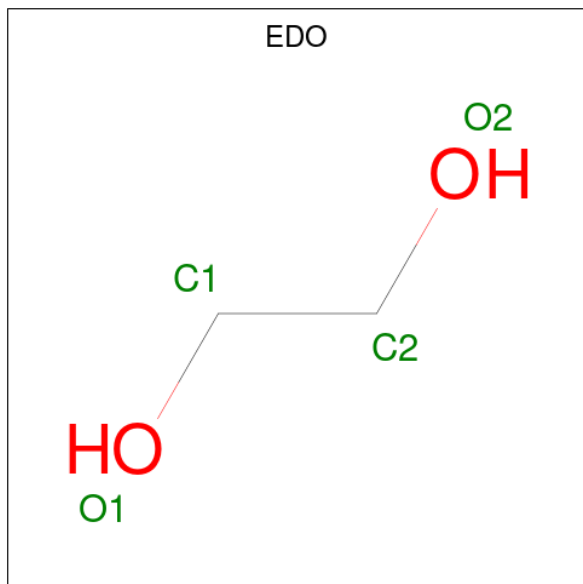
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



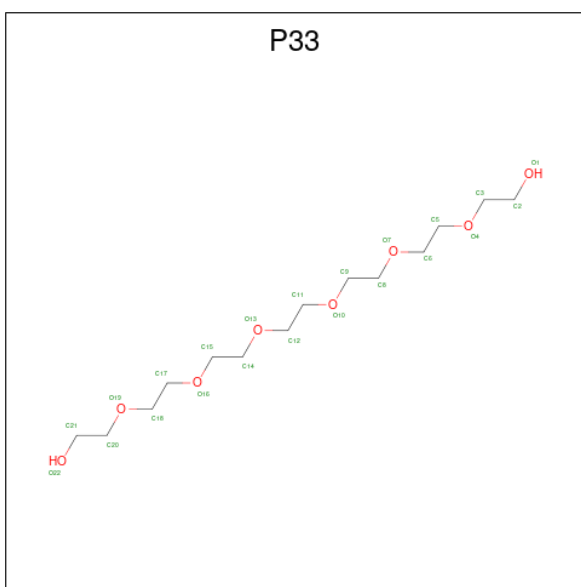
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



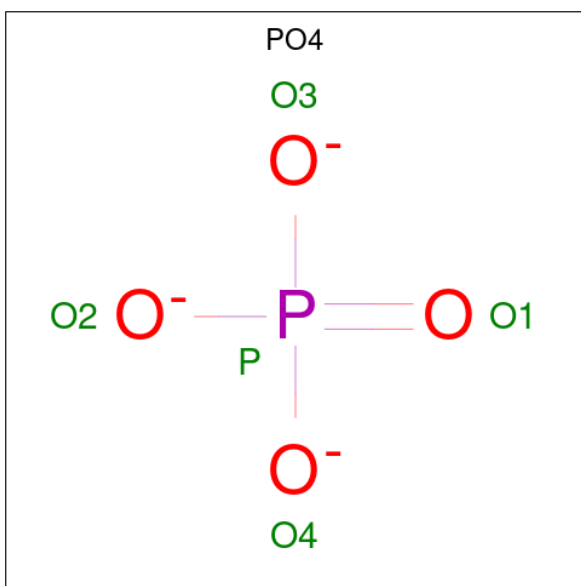
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 3,6,9,12,15,18-HEXA OXAICOSANE-1,20-DIOL (CCD ID: P33) (formula:  $C_{14}H_{30}O_8$ ).



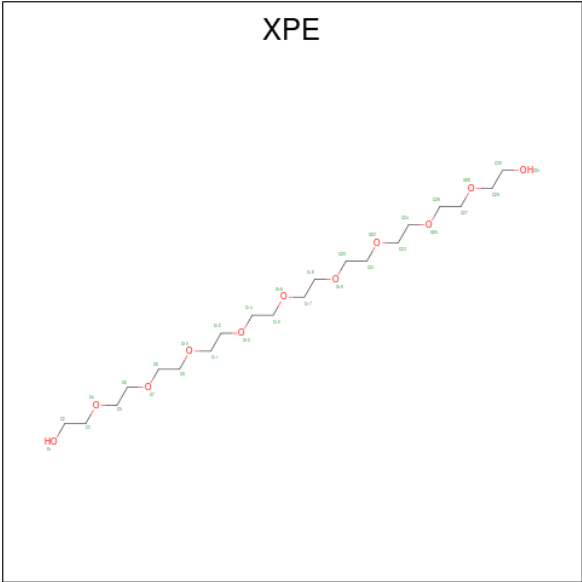
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C O	0	0
			22	14 8		

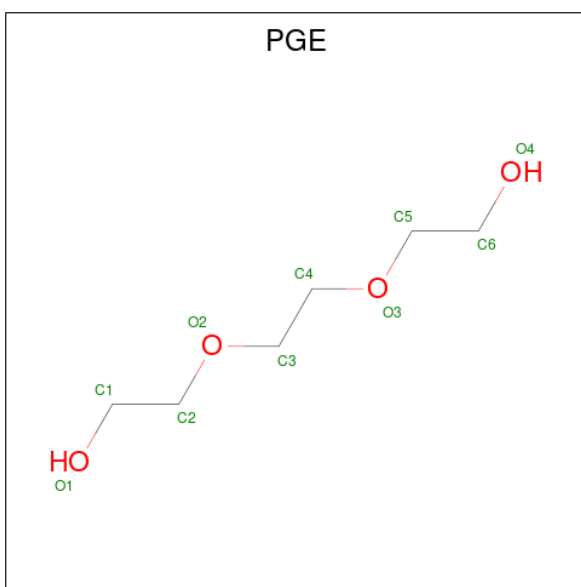
- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O P	0	0
			5	4 1		

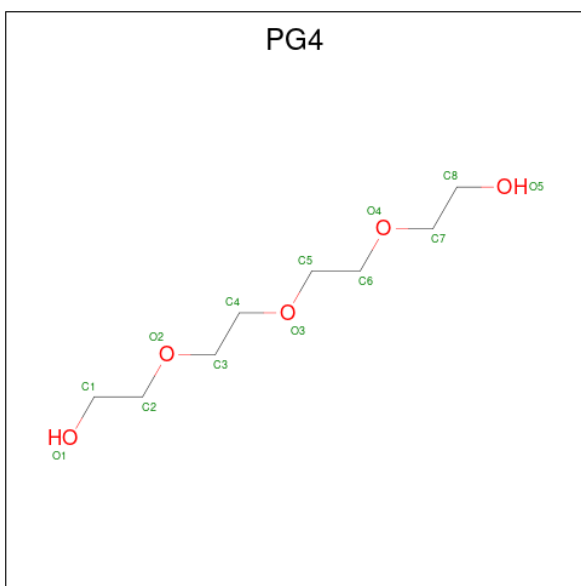
- Molecule 10 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (CCD ID: XPE) (formula:  $C_{20}H_{42}O_{11}$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 14 is water.

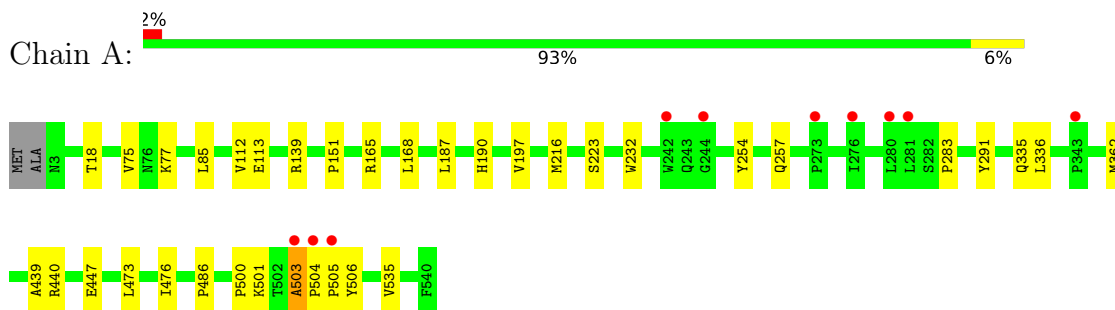


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	321	Total 321	O 321	0	0
14	B	251	Total 251	O 251	0	0
14	C	196	Total 196	O 196	0	0
14	D	188	Total 188	O 188	0	0

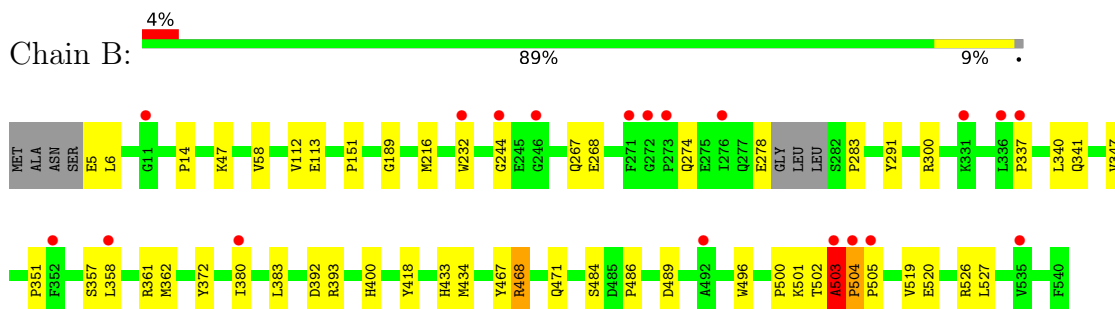
### 3 Residue-property plots [i](#)

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.

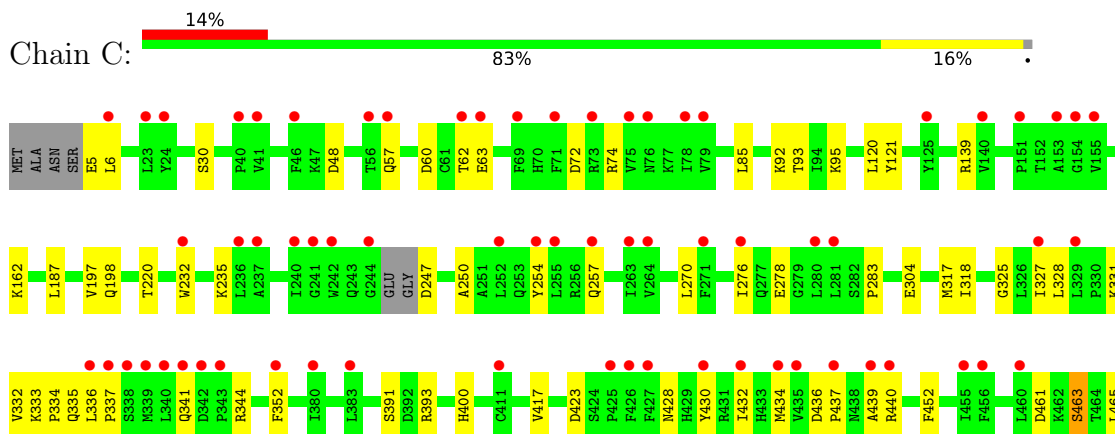
- Molecule 1: Carboxylic ester hydrolase



- Molecule 2: Carboxylic ester hydrolase

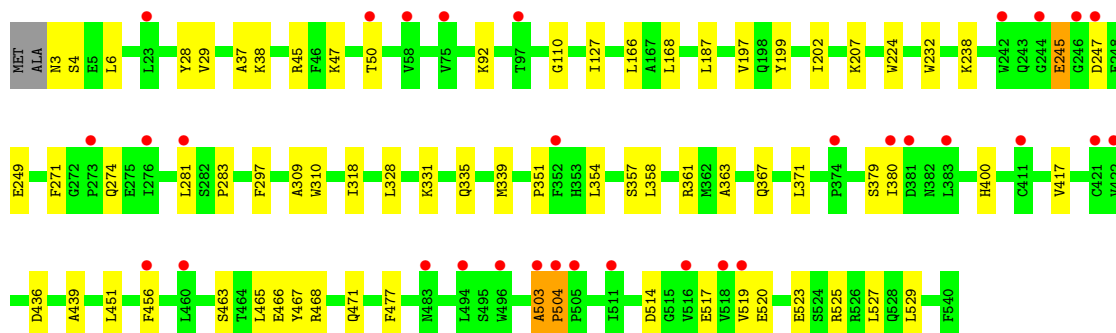
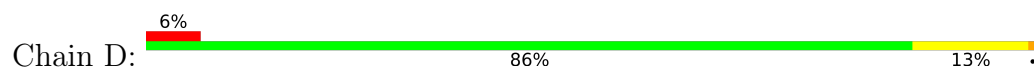


- Molecule 3: Carboxylic ester hydrolase





• Molecule 4: Carboxylic ester hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.52Å 108.12Å 115.62Å 90.00° 101.38° 90.00°	Depositor
Resolution (Å)	48.79 – 1.79 48.79 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.79-1.79) 99.5 (48.79-1.79)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.207 , 0.243 0.211 , 0.246	Depositor DCC
$R_{free}$ test set	9903 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MLZ, P33, PO4, PG4, EDO, GOL, P6G, XPE, MLY, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/4384	0.50	1/5968 (0.0%)
2	B	0.32	0/4315	0.55	3/5873 (0.1%)
3	C	0.27	0/4309	0.48	1/5869 (0.0%)
4	D	0.27	0/4314	0.47	1/5875 (0.0%)
All	All	0.29	0/17322	0.50	6/23585 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	PRO	N-CA-C	-8.05	100.88	110.70
1	A	503	ALA	N-CA-C	6.12	123.33	109.81
3	C	503	ALA	N-CA-C	5.82	122.68	109.81
2	B	504	PRO	CB-CA-C	5.76	117.95	110.92
2	B	503	ALA	N-CA-C	5.43	121.80	109.81
4	D	504	PRO	N-CA-C	5.23	117.09	110.70

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	4259	0	4156	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4220	0	4107	33	0
3	C	4206	0	4094	60	0
4	D	4230	0	4109	43	0
5	A	18	0	24	4	0
5	B	6	0	8	2	0
6	A	14	0	20	0	0
6	B	7	0	10	0	0
7	A	8	0	12	1	0
8	A	22	0	30	1	0
9	B	5	0	0	0	0
10	B	31	0	42	1	0
11	C	19	0	26	1	0
12	D	10	0	14	1	0
13	D	13	0	18	3	0
14	A	321	0	0	2	0
14	B	251	0	0	4	0
14	C	196	0	0	4	0
14	D	188	0	0	2	0
All	All	18024	0	16670	164	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 5.

All (164) 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)
2:B:351:PRO:HG3	5:B:603:GOL:H12	1.54	0.90
2:B:393:ARG:HG3	5:B:603:GOL:H11	1.54	0.89
4:D:503:ALA:HB1	4:D:504:PRO:HD2	1.58	0.84
3:C:93:THR:HG22	3:C:95:LYS:H	1.46	0.81
2:B:112:VAL:HG23	2:B:113:GLU:HG3	1.71	0.71
2:B:5:GLU:N	2:B:5:GLU:OE1	2.24	0.70
3:C:436:ASP:HB3	3:C:439:ALA:HB2	1.77	0.66
4:D:517:GLU:HG3	4:D:519:VAL:HG13	1.77	0.66
3:C:235:LYS:HD2	3:C:270:LEU:HB3	1.80	0.64
3:C:393:ARG:NH1	14:C:702:HOH:O	2.31	0.63
3:C:247:ASP:HB3	3:C:250:ALA:H	1.63	0.63
4:D:371:LEU:HD22	4:D:529:LEU:HD23	1.80	0.62
3:C:335:GLN:N	3:C:335:GLN:OE1	2.32	0.62
1:A:535:VAL:HG23	5:A:606:GOL:H31	1.81	0.61
1:A:335:GLN:N	1:A:335:GLN:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:GLY:O	2:B:216:MET:HB2	2.00	0.61
2:B:503:ALA:O	2:B:504:PRO:C	2.41	0.61
2:B:232:TRP:CD2	2:B:283:PRO:HB3	2.36	0.60
4:D:503:ALA:HB1	4:D:504:PRO:CD	2.31	0.59
2:B:347:VAL:HG21	2:B:362:MET:HE2	1.84	0.59
2:B:337:PRO:O	2:B:341:GLN:HG2	2.03	0.58
3:C:328:LEU:O	3:C:332:VAL:HG12	2.05	0.57
4:D:187:LEU:HG	4:D:197:VAL:HG22	1.86	0.57
2:B:340:LEU:HD11	2:B:383:LEU:HD21	1.86	0.56
1:A:165:ARG:HH12	5:A:607:GOL:H31	1.71	0.56
1:A:501[B]:LYS:HG3	14:A:942:HOH:O	2.07	0.55
3:C:500:PRO:O	3:C:503:ALA:HB2	2.07	0.55
2:B:151:PRO:HA	2:B:291:TYR:CZ	2.42	0.55
4:D:110:GLY:HA3	12:D:601:PGE:H2	1.89	0.53
4:D:224:TRP:HB3	4:D:281:LEU:HD23	1.89	0.53
8:A:605:P33:H181	14:A:884:HOH:O	2.07	0.53
1:A:112:VAL:HG13	1:A:113:GLU:HG2	1.89	0.53
3:C:333:LYS:HB3	3:C:334:PRO:HD3	1.91	0.53
3:C:93:THR:HG22	3:C:95:LYS:N	2.20	0.53
2:B:372:TYR:OH	2:B:392:ASP:OD2	2.22	0.53
4:D:525:ARG:NH1	14:D:707:HOH:O	2.42	0.53
3:C:428:ASN:O	3:C:432:ILE:HG13	2.09	0.52
4:D:247:ASP:OD2	4:D:249:GLU:HG2	2.09	0.52
3:C:60:ASP:OD1	3:C:62:THR:HG22	2.09	0.52
4:D:436:ASP:HB3	4:D:439:ALA:HB2	1.91	0.52
4:D:335:GLN:HG2	4:D:339:MET:HG3	1.91	0.52
3:C:472:HIS:ND1	3:C:490:SER:HB3	2.25	0.52
4:D:503:ALA:CB	4:D:504:PRO:HD2	2.34	0.52
3:C:57:GLN:H	3:C:57:GLN:CD	2.18	0.52
4:D:271:PHE:CE1	4:D:283:PRO:HG3	2.45	0.52
4:D:28:TYR:HB3	4:D:127:ILE:HD13	1.92	0.51
4:D:380:ILE:H	4:D:380:ILE:HD12	1.76	0.51
3:C:337:PRO:O	3:C:341:GLN:HG2	2.10	0.51
4:D:168:LEU:HD21	4:D:187:LEU:HD13	1.93	0.51
3:C:430:TYR:CE1	3:C:434:MET:HG3	2.46	0.50
4:D:6:LEU:HD13	4:D:29:VAL:HG13	1.94	0.49
10:B:602:XPE:H91	14:B:907:HOH:O	2.11	0.49
4:D:463:SER:O	4:D:468:ARG:NH2	2.46	0.49
3:C:5:GLU:OE1	3:C:6:LEU:N	2.32	0.49
2:B:357:SER:O	2:B:361:ARG:HG3	2.12	0.49
2:B:519:VAL:HG23	2:B:520:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:LYS:HB2	3:C:235:LYS:NZ	2.26	0.49
4:D:92:LYS:HG3	4:D:127:ILE:O	2.13	0.48
1:A:232:TRP:CD2	1:A:283:PRO:HB3	2.48	0.48
3:C:494:LEU:HD11	3:C:516:VAL:HG23	1.94	0.48
13:D:602:PG4:H71	14:D:811:HOH:O	2.12	0.48
1:A:439:ALA:O	1:A:440:ARG:HD2	2.13	0.48
3:C:333:LYS:HA	3:C:336:LEU:HD12	1.95	0.48
3:C:461:ASP:OD1	3:C:463:SER:HB2	2.13	0.48
4:D:232:TRP:CD2	4:D:283:PRO:HB3	2.49	0.48
1:A:75:VAL:HG23	1:A:77:LYS:HG2	1.96	0.48
4:D:456:PHE:CE2	13:D:602:PG4:H11	2.49	0.48
4:D:519:VAL:HG23	4:D:520:GLU:O	2.13	0.48
2:B:216:MET:HG2	2:B:418:TYR:OH	2.14	0.47
1:A:500:PRO:O	1:A:503:ALA:HB2	2.15	0.47
3:C:232:TRP:CD2	3:C:283:PRO:HB3	2.49	0.47
2:B:358:LEU:HD22	2:B:358:LEU:H	1.80	0.47
2:B:486:PRO:HB2	2:B:496:TRP:CZ3	2.50	0.47
3:C:334:PRO:HB2	3:C:335:GLN:OE1	2.14	0.47
2:B:467:TYR:O	2:B:471:GLN:HG2	2.15	0.47
2:B:500:PRO:O	2:B:503:ALA:HB2	2.14	0.47
3:C:434:MET:HE3	3:C:434:MET:HB3	1.76	0.47
2:B:503:ALA:C	2:B:505:PRO:N	2.74	0.46
1:A:254:TYR:O	1:A:257[B]:GLN:HG3	2.15	0.46
3:C:325:GLY:H	3:C:391:SER:HG	1.61	0.46
3:C:325:GLY:N	3:C:391:SER:OG	2.41	0.46
3:C:254:TYR:HA	3:C:257:GLN:HG2	1.97	0.46
4:D:238:LYS:HE3	4:D:245:GLU:HB2	1.98	0.46
4:D:328:LEU:HD12	4:D:331:LYS:HE3	1.97	0.45
1:A:165:ARG:HH22	5:A:607:GOL:H31	1.81	0.45
3:C:85:LEU:HD21	3:C:139:ARG:HG3	1.97	0.45
3:C:344:ARG:NH2	14:C:706:HOH:O	2.39	0.45
3:C:432:ILE:HG23	3:C:437:PRO:HA	1.98	0.45
3:C:400:HIS:HB2	3:C:527:LEU:HD13	1.97	0.45
3:C:48:ASP:CG	3:C:162:LYS:HD3	2.42	0.45
4:D:45:ARG:C	4:D:47:MLZ:H	2.25	0.45
4:D:207:MLY:HA	4:D:310:TRP:CE2	2.51	0.45
1:A:165:ARG:HH22	5:A:607:GOL:C3	2.30	0.45
2:B:526:ARG:HG3	14:B:784:HOH:O	2.17	0.45
4:D:351:PRO:HB2	4:D:354:LEU:HG	1.99	0.44
3:C:232:TRP:CE3	3:C:283:PRO:HB3	2.52	0.44
1:A:168:LEU:HD21	1:A:187:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362[A]:MET:HE3	1:A:362[A]:MET:HB3	1.85	0.44
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.79	0.44
2:B:267:GLN:HG3	2:B:268:GLU:HG3	1.99	0.44
3:C:317:MET:HE1	3:C:476:ILE:HG22	2.00	0.44
3:C:467:TYR:O	3:C:471:GLN:HG2	2.18	0.44
2:B:5:GLU:HG2	2:B:6:LEU:H	1.82	0.43
1:A:187:LEU:HG	1:A:197:VAL:HG22	2.01	0.43
3:C:62:THR:HG23	3:C:63:GLU:CD	2.43	0.43
3:C:120:LEU:HD22	11:C:601:P6G:H52	2.01	0.43
4:D:456:PHE:HE2	13:D:602:PG4:H11	1.84	0.43
1:A:447:GLU:OE1	1:A:447:GLU:N	2.49	0.43
3:C:121:TYR:HA	3:C:452:PHE:HB3	2.01	0.42
3:C:465:LEU:HA	3:C:468:ARG:CZ	2.49	0.42
3:C:503:ALA:O	3:C:506:TYR:HD2	2.02	0.42
4:D:357:SER:O	4:D:361:ARG:HG3	2.18	0.42
3:C:501:LYS:HA	3:C:501:LYS:HD3	1.89	0.42
2:B:434:MET:HE3	2:B:434:MET:HB3	1.90	0.42
2:B:468[A]:ARG:NH2	2:B:471:GLN:HG3	2.34	0.42
3:C:318:ILE:O	3:C:417:VAL:HA	2.20	0.42
3:C:503:ALA:O	3:C:504:PRO:C	2.61	0.42
3:C:503:ALA:N	3:C:504:PRO:HD2	2.34	0.42
3:C:517:GLU:HG2	3:C:519:VAL:HG13	2.01	0.42
2:B:300:ARG:NH2	14:B:708:HOH:O	2.41	0.42
3:C:502:THR:C	3:C:504:PRO:HD2	2.44	0.42
4:D:202:ILE:HA	4:D:309:ALA:HB1	2.01	0.42
4:D:380:ILE:HD12	4:D:380:ILE:N	2.35	0.42
2:B:502:THR:C	2:B:504:PRO:HD2	2.44	0.42
4:D:523:GLU:OE1	4:D:523:GLU:N	2.52	0.42
1:A:85:LEU:HD21	1:A:139:ARG:HG3	2.02	0.42
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.88	0.42
4:D:467:TYR:O	4:D:471:GLN:HG2	2.20	0.42
1:A:503:ALA:O	1:A:504:PRO:C	2.63	0.41
1:A:503:ALA:O	1:A:506:TYR:HD2	2.02	0.41
2:B:400:HIS:HB2	2:B:527:LEU:HD13	2.02	0.41
3:C:198:GLN:HB3	3:C:220:THR:HG23	2.03	0.41
3:C:254:TYR:CD1	3:C:254:TYR:C	2.98	0.41
1:A:223:SER:HA	7:A:608:EDO:H21	2.01	0.41
3:C:472:HIS:O	3:C:476:ILE:HD12	2.19	0.41
4:D:514:ASP:OD1	4:D:514:ASP:N	2.52	0.41
3:C:187:LEU:HG	3:C:197:VAL:HG22	2.03	0.41
3:C:327:ILE:O	3:C:331:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:451:LEU:HD11	4:D:477:PHE:CE2	2.55	0.41
2:B:433:HIS:ND1	2:B:433:HIS:N	2.68	0.41
3:C:333:LYS:HA	3:C:336:LEU:CD1	2.51	0.41
2:B:274:GLN:HE21	2:B:278:GLU:CD	2.29	0.41
3:C:332:VAL:O	3:C:335:GLN:N	2.52	0.41
3:C:423:ASP:OD2	3:C:440:ARG:HG3	2.21	0.41
4:D:318:ILE:O	4:D:417:VAL:HA	2.21	0.41
4:D:363:ALA:O	4:D:367:GLN:HG3	2.20	0.41
2:B:14:PRO:HG2	2:B:58:VAL:HA	2.02	0.41
3:C:486:PRO:HB2	3:C:496:TRP:CZ3	2.56	0.41
4:D:199:TYR:HB3	4:D:297:PHE:HE2	1.85	0.41
3:C:72:ASP:OD1	3:C:74:ARG:N	2.54	0.40
4:D:400:HIS:HB2	4:D:527:LEU:HD13	2.03	0.40
1:A:190:HIS:HA	1:A:216:MET:HB2	2.03	0.40
3:C:278:GLU:HG2	3:C:352:PHE:CE2	2.56	0.40
3:C:304:GLU:HG3	14:C:889:HOH:O	2.21	0.40
2:B:47:LYS:HE3	2:B:47:LYS:HB3	1.79	0.40
3:C:332:VAL:HG22	3:C:336:LEU:HG	2.04	0.40
3:C:497:THR:HG22	14:C:837:HOH:O	2.22	0.40
2:B:380:ILE:HG23	14:B:865:HOH:O	2.21	0.40
1:A:151:PRO:HA	1:A:291:TYR:CZ	2.56	0.40
1:A:476:ILE:HG23	1:A:486:PRO:HB2	2.04	0.40
4:D:37:ALA:HB2	4:D:166:LEU:HD23	2.04	0.40
4:D:38:LYS:HB2	4:D:38:LYS:HE2	1.95	0.40
4:D:465:LEU:HD12	4:D:466:GLU:N	2.37	0.40
4:D:503:ALA:O	4:D:504:PRO:C	2.63	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	541/540 (100%)	524 (97%)	16 (3%)	1 (0%)	43	31
2	B	530/540 (98%)	511 (96%)	17 (3%)	2 (0%)	30	19
3	C	531/540 (98%)	505 (95%)	26 (5%)	0	100	100
4	D	533/540 (99%)	513 (96%)	18 (3%)	2 (0%)	30	19
All	All	2135/2160 (99%)	2053 (96%)	77 (4%)	5 (0%)	43	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	503	ALA
4	D	245	GLU
2	B	503	ALA
1	A	505	PRO
2	B	244	GLY

### 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	468/463 (101%)	467 (100%)	1 (0%)	87	87
2	B	460/461 (100%)	455 (99%)	5 (1%)	65	60
3	C	460/462 (100%)	455 (99%)	5 (1%)	65	60
4	D	460/461 (100%)	454 (99%)	6 (1%)	61	54
All	All	1848/1847 (100%)	1831 (99%)	17 (1%)	70	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
2	B	468[A]	ARG
2	B	468[B]	ARG
2	B	484	SER
2	B	489	ASP
2	B	501	LYS

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Mol	Chain	Res	Type
3	C	30	SER
3	C	92	LYS
3	C	276	ILE
3	C	463	SER
3	C	484	SER
4	D	3	ASN
4	D	4	SER
4	D	50	THR
4	D	274	GLN
4	D	358	LEU
4	D	379	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	367	GLN
1	A	370	GLN
2	B	54	ASN
2	B	76	ASN
2	B	341	GLN
2	B	367	GLN
2	B	377	ASN
2	B	483	ASN
3	C	54	ASN
3	C	257	GLN
3	C	266	HIS
3	C	277	GLN
3	C	367	GLN
3	C	471	GLN
4	D	277	GLN
4	D	408	ASN
4	D	536	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	MLY	A	207	1	9,10,11	0.59	0	6,11,13	0.80	0
3	MLY	C	269	3	9,10,11	0.61	0	6,11,13	0.88	0
2	MLZ	B	77	2	8,9,10	0.73	0	4,9,11	0.85	0
2	MLZ	B	269	2	8,9,10	0.73	0	4,9,11	0.87	0
4	MLZ	D	47	4	8,9,10	0.77	0	4,9,11	0.78	0
4	MLY	D	207	4	9,10,11	0.62	0	6,11,13	0.55	0
4	MLZ	D	501	4	8,9,10	0.80	0	4,9,11	0.89	0
2	MLY	B	207	2	9,10,11	0.72	0	6,11,13	0.84	0
3	MLZ	C	207	3	8,9,10	0.79	0	4,9,11	0.68	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	MLY	A	207	1	-	1/8/9/11	-
3	MLY	C	269	3	-	1/8/9/11	-
2	MLZ	B	77	2	-	0/7/8/10	-
2	MLZ	B	269	2	-	1/7/8/10	-
4	MLZ	D	47	4	-	2/7/8/10	-
4	MLY	D	207	4	-	2/8/9/11	-
4	MLZ	D	501	4	-	3/7/8/10	-
2	MLY	B	207	2	-	1/8/9/11	-
3	MLZ	C	207	3	-	0/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	269	MLZ	CD-CE-NZ-CM
3	C	269	MLY	O-C-CA-CB
4	D	47	MLZ	CD-CE-NZ-CM
4	D	501	MLZ	CD-CE-NZ-CM
4	D	207	MLY	CD-CE-NZ-CH1
4	D	207	MLY	CD-CE-NZ-CH2
2	B	207	MLY	CD-CE-NZ-CH1
4	D	501	MLZ	CE-CD-CG-CB
4	D	501	MLZ	CA-CB-CG-CD
1	A	207	MLY	CD-CE-NZ-CH1
4	D	47	MLZ	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	47	MLZ	1	0
4	D	207	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	PEG	A	602	-	6,6,6	0.21	0	5,5,5	0.11	0
7	EDO	A	604	-	3,3,3	0.40	0	2,2,2	0.36	0
8	P33	A	605	-	21,21,21	0.32	0	20,20,20	0.21	0
9	PO4	B	601	-	4,4,4	0.88	0	6,6,6	0.45	0
11	P6G	C	601	-	18,18,18	0.15	0	17,17,17	0.12	0
6	PEG	B	604	-	6,6,6	0.28	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	606	-	5,5,5	0.91	0	5,5,5	0.98	0
13	PG4	D	602	-	12,12,12	0.19	0	11,11,11	0.59	0
12	PGE	D	601	-	9,9,9	0.40	0	8,8,8	0.31	0
10	XPE	B	602	-	30,30,30	0.55	0	29,29,29	0.46	0
7	EDO	A	608	-	3,3,3	0.41	0	2,2,2	0.44	0
6	PEG	A	603	-	6,6,6	0.19	0	5,5,5	0.05	0
5	GOL	B	603	-	5,5,5	0.98	0	5,5,5	1.10	0
5	GOL	A	601	-	5,5,5	0.91	0	5,5,5	1.01	0
5	GOL	A	607	-	5,5,5	1.16	1 (20%)	5,5,5	1.02	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
6	PEG	A	602	-	-	2/4/4/4	-
7	EDO	A	604	-	-	0/1/1/1	-
8	P33	A	605	-	-	10/19/19/19	-
11	P6G	C	601	-	-	7/16/16/16	-
6	PEG	B	604	-	-	4/4/4/4	-
5	GOL	A	606	-	-	4/4/4/4	-
13	PG4	D	602	-	-	7/10/10/10	-
12	PGE	D	601	-	-	4/7/7/7	-
10	XPE	B	602	-	-	14/28/28/28	-
7	EDO	A	608	-	-	1/1/1/1	-
6	PEG	A	603	-	-	3/4/4/4	-
5	GOL	B	603	-	-	2/4/4/4	-
5	GOL	A	601	-	-	2/4/4/4	-
5	GOL	A	607	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	607	GOL	C1-C2	2.11	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	GOL	C1-C2-C3-O3
5	A	606	GOL	C1-C2-C3-O3
10	B	602	XPE	C14-C15-O16-C17
8	A	605	P33	C12-C11-O10-C9
10	B	602	XPE	O10-C11-C12-O13
8	A	605	P33	O16-C17-C18-O19
10	B	602	XPE	O13-C14-C15-O16
6	A	603	PEG	O1-C1-C2-O2
12	D	601	PGE	O1-C1-C2-O2
11	C	601	P6G	O10-C11-C12-O13
13	D	602	PG4	O3-C5-C6-O4
10	B	602	XPE	O16-C17-C18-O19
10	B	602	XPE	O28-C29-C30-O31
13	D	602	PG4	O4-C7-C8-O5
5	A	606	GOL	O1-C1-C2-C3
5	A	607	GOL	C1-C2-C3-O3
5	B	603	GOL	C1-C2-C3-O3
11	C	601	P6G	O7-C8-C9-O10
5	A	601	GOL	O2-C2-C3-O3
5	A	606	GOL	O1-C1-C2-O2
5	A	606	GOL	O2-C2-C3-O3
5	B	603	GOL	O2-C2-C3-O3
6	B	604	PEG	O2-C3-C4-O4
11	C	601	P6G	O13-C14-C15-O16
5	A	607	GOL	O2-C2-C3-O3
11	C	601	P6G	O4-C5-C6-O7
10	B	602	XPE	O25-C26-C27-O28
6	B	604	PEG	C1-C2-O2-C3
6	B	604	PEG	O1-C1-C2-O2
10	B	602	XPE	C18-C17-O16-C15
12	D	601	PGE	C4-C3-O2-C2
13	D	602	PG4	C5-C6-O4-C7
8	A	605	P33	C18-C17-O16-C15
10	B	602	XPE	C15-C14-O13-C12
12	D	601	PGE	C3-C4-O3-C5
12	D	601	PGE	O2-C3-C4-O3
6	A	603	PEG	C1-C2-O2-C3
11	C	601	P6G	C9-C8-O7-C6
8	A	605	P33	O4-C5-C6-O7
13	D	602	PG4	C3-C4-O3-C5
8	A	605	P33	O19-C20-C21-O22
8	A	605	P33	C15-C14-O13-C12

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Mol	Chain	Res	Type	Atoms
13	D	602	PG4	C4-C3-O2-C2
10	B	602	XPE	C26-C27-O28-C29
11	C	601	P6G	O1-C2-C3-O4
10	B	602	XPE	C30-C29-O28-C27
10	B	602	XPE	O22-C23-C24-O25
10	B	602	XPE	C5-C6-O7-C8
6	A	602	PEG	C1-C2-O2-C3
13	D	602	PG4	C1-C2-O2-C3
8	A	605	P33	O10-C11-C12-O13
6	A	602	PEG	C4-C3-O2-C2
8	A	605	P33	C9-C8-O7-C6
10	B	602	XPE	O4-C5-C6-O7
13	D	602	PG4	O1-C1-C2-O2
8	A	605	P33	C17-C18-O19-C20
8	A	605	P33	O7-C8-C9-O10
6	B	604	PEG	C4-C3-O2-C2
11	C	601	P6G	C2-C3-O4-C5
6	A	603	PEG	C4-C3-O2-C2
10	B	602	XPE	O7-C8-C9-O10
7	A	608	EDO	O1-C1-C2-O2

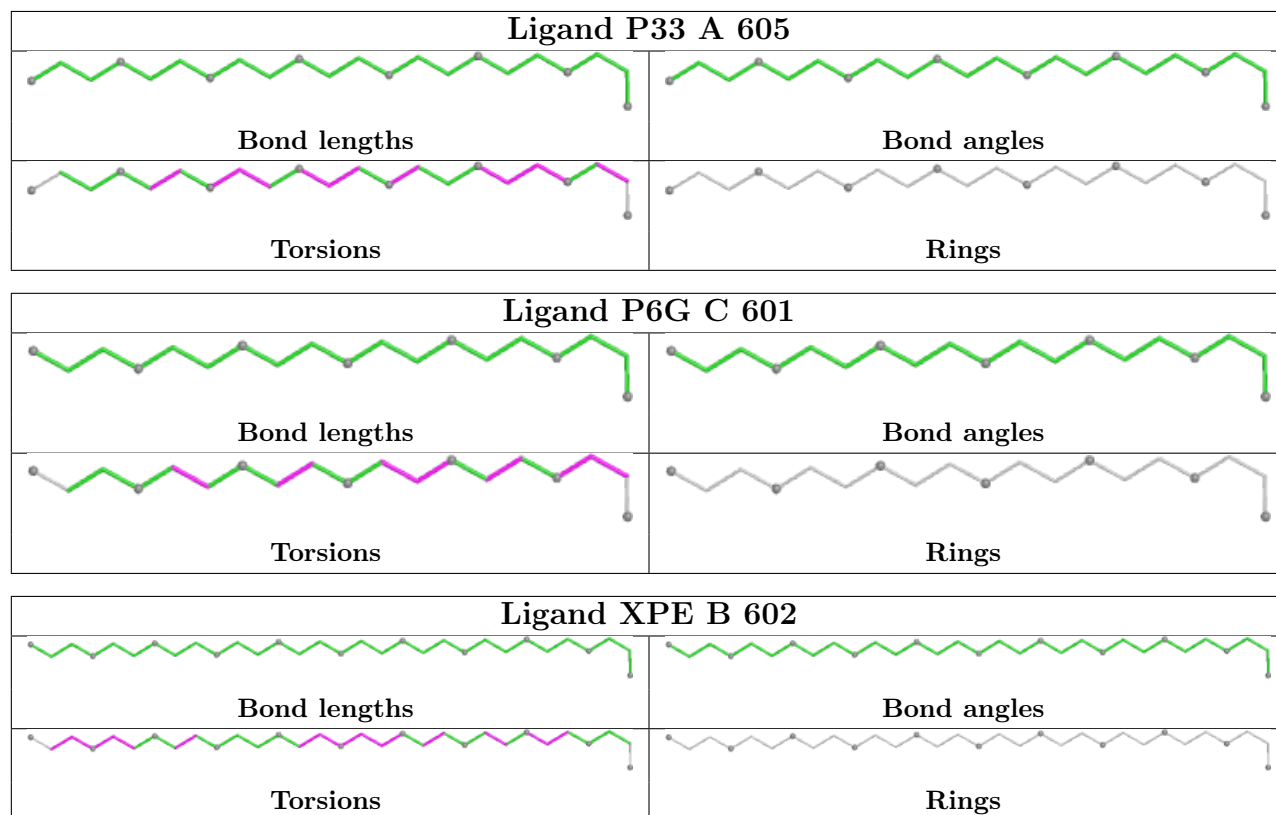
There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	605	P33	1	0
11	C	601	P6G	1	0
5	A	606	GOL	1	0
13	D	602	PG4	3	0
12	D	601	PGE	1	0
10	B	602	XPE	1	0
7	A	608	EDO	1	0
5	B	603	GOL	2	0
5	A	607	GOL	3	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 ⓘ

### 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	537/540 (99%)	0.14	10 (1%) 66 66	17, 31, 53, 76	6 (1%)
2	B	530/540 (98%)	0.44	19 (3%) 46 46	19, 35, 61, 78	4 (0%)
3	C	532/540 (98%)	0.95	75 (14%) 6 5	19, 42, 70, 88	3 (0%)
4	D	535/540 (99%)	0.79	32 (5%) 27 26	24, 42, 71, 86	0
All	All	2134/2160 (98%)	0.58	136 (6%) 25 24	17, 37, 67, 88	13 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	503	ALA	7.4
2	B	503	ALA	6.5
1	A	504	PRO	5.3
3	C	504	PRO	5.3
3	C	23	LEU	4.6
2	B	504	PRO	4.5
3	C	75	VAL	4.4
4	D	504	PRO	4.4
3	C	79[A]	VAL	4.3
4	D	281	LEU	4.3
1	A	244	GLY	4.2
1	A	503	ALA	4.2
2	B	246	GLY	4.2
3	C	244	GLY	4.0
3	C	242	TRP	4.0
3	C	271	PHE	3.7
4	D	518	VAL	3.7
2	B	336	LEU	3.7
3	C	71	PHE	3.6
1	A	273	PRO	3.6
2	B	505	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	69	PHE	3.5
1	A	505	PRO	3.5
4	D	242	TRP	3.4
3	C	505	PRO	3.4
3	C	280	LEU	3.4
3	C	427	PHE	3.3
3	C	153	ALA	3.3
3	C	340	LEU	3.3
3	C	254	TYR	3.2
3	C	240	ILE	3.2
3	C	276	ILE	3.2
3	C	281	LEU	3.2
3	C	252	LEU	3.2
3	C	336	LEU	3.1
2	B	244	GLY	3.1
4	D	276	ILE	3.1
4	D	374	PRO	3.0
2	B	352	PHE	3.0
3	C	343	PRO	3.0
3	C	426	PHE	3.0
4	D	352	PHE	3.0
2	B	358	LEU	2.9
3	C	237	ALA	2.9
3	C	460	LEU	2.9
3	C	327	ILE	2.9
3	C	24	TYR	2.9
4	D	503	ALA	2.8
3	C	437	PRO	2.8
4	D	97	THR	2.8
3	C	46	PHE	2.8
1	A	276	ILE	2.8
3	C	456	PHE	2.8
3	C	492	ALA	2.8
3	C	78	ILE	2.8
1	A	242	TRP	2.7
4	D	505	PRO	2.7
3	C	263	ILE	2.7
2	B	272	GLY	2.7
1	A	280	LEU	2.7
4	D	380	ILE	2.7
3	C	380	ILE	2.7
4	D	516	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	236	LEU	2.6
4	D	494	LEU	2.6
2	B	492	ALA	2.6
1	A	343	PRO	2.6
3	C	255	LEU	2.6
2	B	273	PRO	2.6
4	D	421	CYS	2.5
3	C	73	ARG	2.5
4	D	273	PRO	2.5
4	D	244	GLY	2.5
4	D	456	PHE	2.5
3	C	430	TYR	2.5
3	C	57	GLN	2.5
3	C	155	VAL	2.5
4	D	247	ASP	2.5
3	C	425	PRO	2.5
3	C	434	MET	2.4
3	C	455	ILE	2.4
3	C	411	CYS	2.4
4	D	383	LEU	2.4
4	D	496	TRP	2.4
3	C	439	ALA	2.4
2	B	380	ILE	2.4
4	D	511	ILE	2.4
1	A	281	LEU	2.4
3	C	432	ILE	2.3
2	B	535	VAL	2.3
4	D	58	VAL	2.3
4	D	75	VAL	2.3
3	C	41	VAL	2.3
3	C	264	VAL	2.3
4	D	422	VAL	2.3
4	D	50	THR	2.3
3	C	435	VAL	2.3
2	B	232	TRP	2.2
3	C	40	PRO	2.2
3	C	337	PRO	2.2
4	D	23	LEU	2.2
4	D	460	LEU	2.2
3	C	338	SER	2.2
3	C	467	TYR	2.2
2	B	276	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	56	THR	2.2
3	C	497	THR	2.2
3	C	494	LEU	2.2
3	C	154	GLY	2.2
3	C	125	TYR	2.2
3	C	470	ILE	2.2
2	B	337	PRO	2.2
4	D	381	ASP	2.2
3	C	257	GLN	2.2
3	C	329	LEU	2.2
3	C	62	THR	2.2
4	D	519	VAL	2.1
3	C	241	GLY	2.1
3	C	76	ASN	2.1
3	C	339	MET	2.1
3	C	352	PHE	2.1
3	C	140	VAL	2.1
3	C	383	LEU	2.1
3	C	341	GLN	2.1
3	C	342	ASP	2.1
2	B	271	PHE	2.1
2	B	11	GLY	2.1
2	B	331	LYS	2.1
4	D	246	GLY	2.1
4	D	411	CYS	2.1
3	C	440	ARG	2.1
3	C	232	TRP	2.1
3	C	63	GLU	2.0
3	C	6	LEU	2.0
3	C	151	PRO	2.0
4	D	483	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
3	MLY	C	269	11/12	0.78	0.13	50,53,57,60	0
4	MLZ	D	47	10/11	0.85	0.13	32,43,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLZ	B	269	10/11	0.87	0.11	37,40,47,52	0
4	MLZ	D	501	10/11	0.87	0.12	41,46,52,53	0
3	MLZ	C	207	10/11	0.93	0.08	24,26,35,35	0
4	MLY	D	207	11/12	0.93	0.09	22,29,42,43	0
2	MLZ	B	77	10/11	0.93	0.10	33,39,51,55	0
1	MLY	A	207	11/12	0.94	0.07	21,23,35,37	0
2	MLY	B	207	11/12	0.94	0.09	19,24,37,39	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

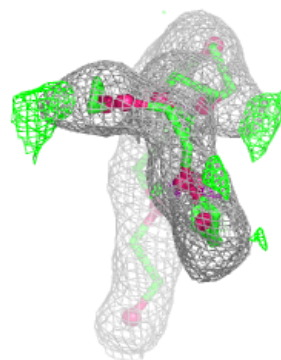
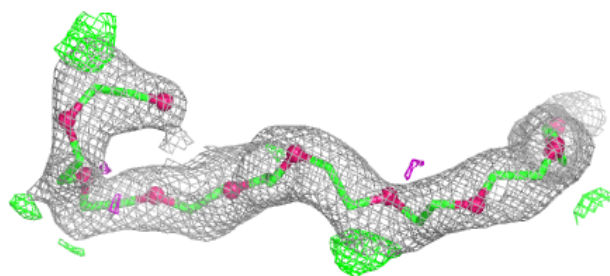
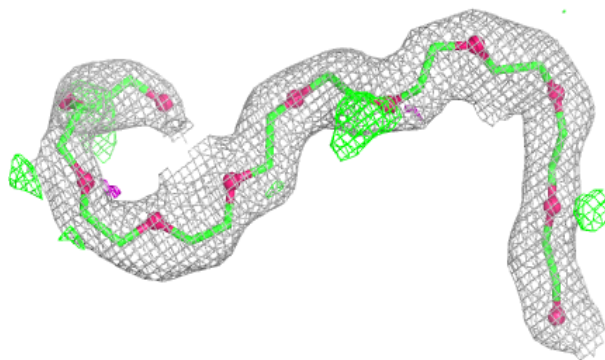
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PO4	B	601	5/5	0.67	0.13	50,52,61,77	5
6	PEG	B	604	7/7	0.71	0.19	42,49,59,62	0
6	PEG	A	602	7/7	0.71	0.17	35,37,44,44	7
7	EDO	A	604	4/4	0.74	0.15	38,40,44,48	4
12	PGE	D	601	10/10	0.76	0.16	45,52,55,60	0
6	PEG	A	603	7/7	0.77	0.19	33,43,46,51	7
7	EDO	A	608	4/4	0.78	0.15	39,40,45,55	0
5	GOL	B	603	6/6	0.79	0.14	38,46,51,59	0
5	GOL	A	606	6/6	0.82	0.12	37,50,53,57	0
10	XPE	B	602	31/31	0.84	0.14	31,45,52,56	0
5	GOL	A	607	6/6	0.85	0.13	38,46,50,51	0
13	PG4	D	602	13/13	0.85	0.13	38,45,58,58	0
11	P6G	C	601	19/19	0.86	0.13	44,52,60,64	0
5	GOL	A	601	6/6	0.87	0.15	40,48,52,52	0
8	P33	A	605	22/22	0.89	0.11	35,44,50,55	0

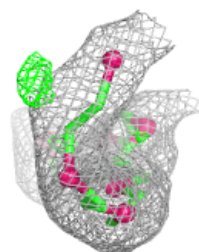
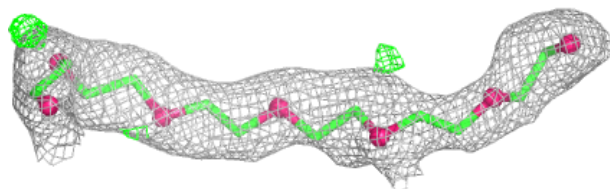
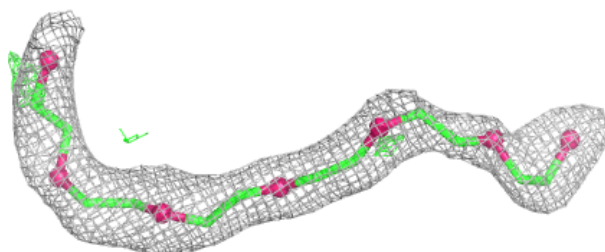
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XPE B 602:**

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

**Electron density around P6G C 601:**

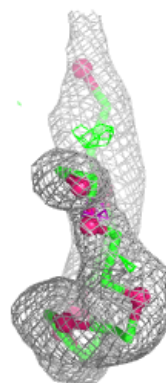
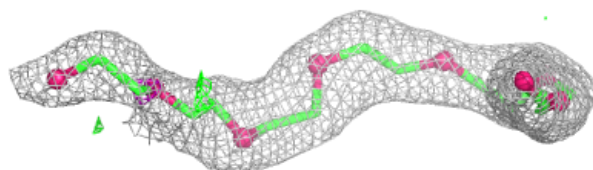
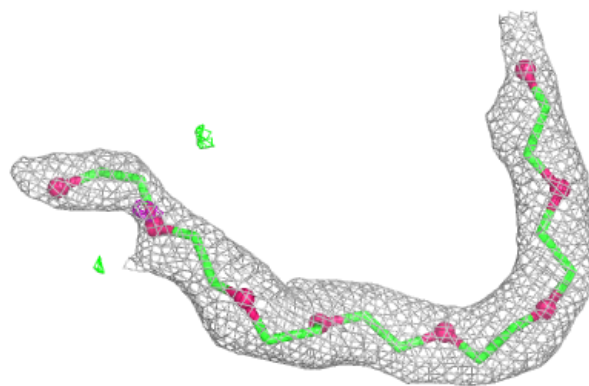
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around P33 A 605:**

$2mF_o-DF_c$  (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.