WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 12:11 PM JST

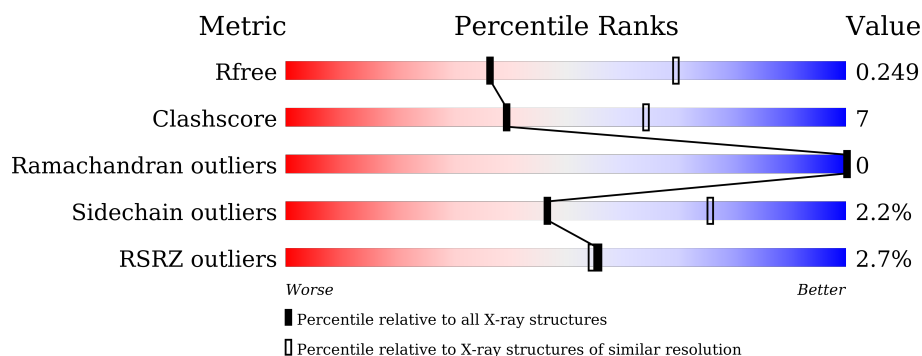|		
PDB ID	:	9KNJ / pdb_00009knj
Title	:	Crystal structure of glycerol-bound full-length PHA synthase (PhaC) from Aeromonas caviae
Authors	:	Chek, M.F.; Kim, S.Y.; Mori, T.; Hakoshima, T.
Deposited on	:	2024-11-19
Resolution	:	2.70 Å(reported)

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 2.70 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		2.7%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 <=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	596	.% 81% 10% 8%
1	B	596	.% 73% 17% • 10%
1	C	596	5% 72% 17% 11%

2 Entity composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12874 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 PHA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4309	2750	748	798	13			
1	B	538	Total	C	N	O	S	0	0	0
			4254	2720	738	783	13			
1	C	533	Total	C	N	O	S	0	0	0
			4218	2697	735	773	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O32471
A	0	PRO	-	expression tag	UNP O32471
B	-1	GLY	-	expression tag	UNP O32471
B	0	PRO	-	expression tag	UNP O32471
C	-1	GLY	-	expression tag	UNP O32471
C	0	PRO	-	expression tag	UNP O32471

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

GOL

C3

OH O3

C1 C2

HO

O1

OH

O2

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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 r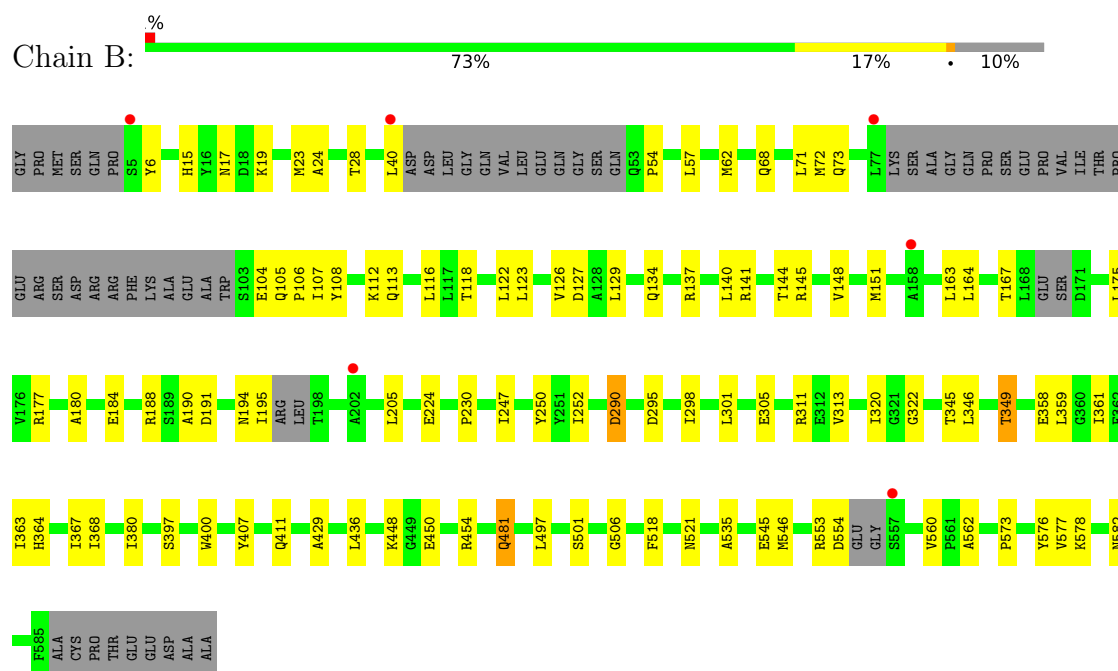ed = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
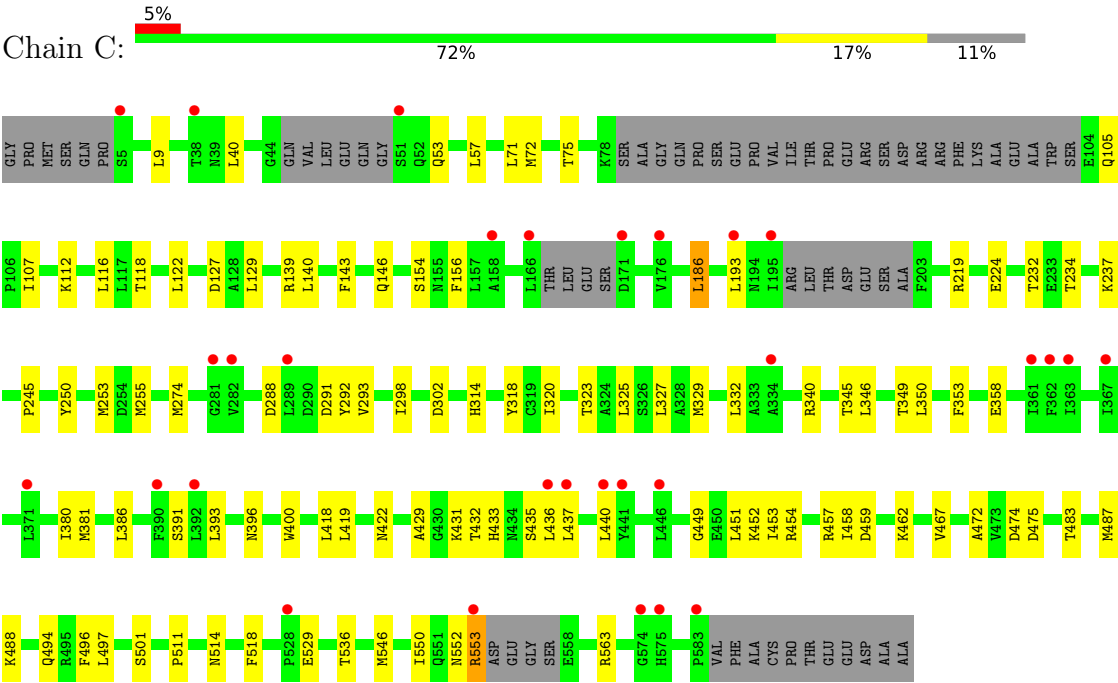
• Molecule 1: PHA synthase

• Molecule 1: PHA synthase

• Molecule 1: PHA synthase

Chain C:

5%

72%　　　　17%　　11%
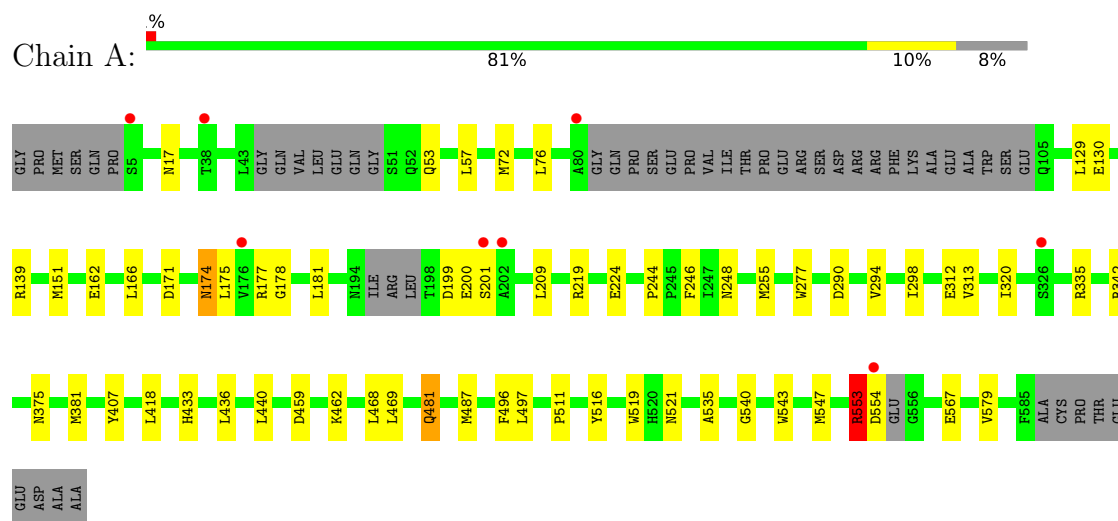
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.03Å 96.07Å 143.30Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	48.04 – 2.70 48.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.04-2.70) 90.1 (48.04-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.249 0.210 , 0.249	Depositor DCC
R_{free} test set	56799 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.008 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.016 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.016 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12874	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: GOL

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	0.27	0/4407	0.44	0/5990
1	B	0.30	0/4351	0.50	0/5914
1	C	0.30	0/4314	0.49	0/5861
All	All	0.29	0/13072	0.48	0/17765

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	553	ARG	Sidechain

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4309	0	4267	40	1
1	B	4254	0	4219	69	0
1	C	4218	0	4190	74	0
2	A	30	0	40	0	0
2	B	24	0	32	0	0
2	C	12	0	16	1	0
3	A	19	0	0	2	0
3	B	8	0	0	0	0
All	All	12874	0	12764	169	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 7.

All (169) 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:375:ASN:HD21	1:A:381:MET:HE2	1.38	0.87
1:B:107:ILE:HG13	1:C:72:MET:HE1	1.59	0.82
1:B:364:HIS:HB2	1:B:367:ILE:HD12	1.62	0.80
1:B:122:LEU:HD13	1:C:122:LEU:HG	1.71	0.71
1:A:151:MET:CE	3:A:704:HOH:O	2.38	0.71
1:C:451:LEU:HB3	1:C:458:ILE:HD11	1.73	0.70
1:A:151:MET:HE3	3:A:704:HOH:O	1.91	0.69
1:C:380:ILE:HG22	1:C:429:ALA:HA	1.75	0.69
1:C:291:ASP:OD1	1:C:454:ARG:NH2	2.25	0.68
1:B:167:THR:HA	1:B:175:LEU:HD11	1.78	0.66
1:C:250:TYR:HD1	1:C:274:MET:HE2	1.61	0.66
1:B:305:GLU:OE2	1:B:311:ARG:NH1	2.29	0.65
1:C:288:ASP:HB2	1:C:431:LYS:HE2	1.77	0.65
1:B:195:ILE:HD12	1:B:582:ASN:HB3	1.81	0.63
1:C:53:GLN:HE21	1:C:140:LEU:HD23	1.65	0.62
1:C:288:ASP:HB2	1:C:431:LYS:CE	2.30	0.61
1:B:151:MET:HE2	1:C:112:LYS:HE2	1.84	0.60
1:B:298:ILE:HA	1:B:301:LEU:HD12	1.84	0.58
1:C:250:TYR:CD1	1:C:274:MET:HE2	2.37	0.58
1:A:166:LEU:HB3	1:A:175:LEU:HD13	1.86	0.58
1:B:205:LEU:O	1:B:578:LYS:NZ	2.36	0.58
1:C:219:ARG:NH1	1:C:224:GLU:OE2	2.31	0.58
1:B:108:TYR:HH	1:C:400:TRP:CD1	2.22	0.57
1:B:134:GLN:HG3	1:B:137:ARG:HH21	1.69	0.57
1:A:57:LEU:HD22	1:A:129:LEU:HD21	1.86	0.57
1:C:237:LYS:O	1:C:563:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:O	1:B:72:MET:HG3	2.05	0.57
1:B:144:THR:O	1:B:148:VAL:HG23	2.05	0.57
1:B:553:ARG:O	1:B:554:ASP:C	2.49	0.56
1:A:335:ARG:HH22	1:B:195:ILE:HG12	1.71	0.56
1:B:184:GLU:O	1:B:188:ARG:HG3	2.05	0.56
1:C:156:PHE:CE2	1:C:391:SER:HB3	2.41	0.55
1:C:57:LEU:HD22	1:C:129:LEU:HD21	1.89	0.55
1:C:253:MET:HE3	1:C:274:MET:HE1	1.89	0.55
1:C:487:MET:SD	1:C:494:GLN:HB3	2.47	0.55
1:A:139:ARG:HG3	1:A:201:SER:HB2	1.89	0.55
1:C:293:VAL:O	1:C:298:ILE:HG12	2.06	0.54
1:A:436:LEU:HD23	1:A:440:LEU:HD12	1.90	0.54
1:C:345:THR:HG21	1:C:546:MET:HG3	1.89	0.54
1:B:145:ARG:NH1	1:C:127:ASP:OD2	2.41	0.53
1:C:459:ASP:HB3	1:C:462:LYS:HG2	1.90	0.52
1:C:472:ALA:HB3	1:C:475:ASP:HB2	1.90	0.52
1:B:54:PRO:HG2	1:B:57:LEU:HB2	1.91	0.52
1:B:518:PHE:CZ	1:B:545:GLU:HG3	2.45	0.52
1:B:230:PRO:HB3	1:B:562:ALA:HB1	1.93	0.51
1:A:53:GLN:HG3	1:A:407:TYR:CE1	2.45	0.51
1:B:448:LYS:HB2	1:B:450:GLU:HG3	1.91	0.51
1:C:302:ASP:OD1	1:C:340:ARG:NH1	2.39	0.51
1:C:346:LEU:HD23	1:C:467:VAL:HG13	1.92	0.51
1:A:459:ASP:HB3	1:A:462:LYS:HD2	1.92	0.51
1:B:104:GLU:HG3	1:C:9:LEU:HD21	1.92	0.51
1:B:501:SER:HB3	1:B:506:GLY:N	2.26	0.51
1:B:363:ILE:O	1:B:364:HIS:ND1	2.43	0.50
1:A:375:ASN:ND2	1:A:381:MET:HE2	2.18	0.50
1:C:472:ALA:HB1	1:C:501:SER:O	2.11	0.50
1:C:325:LEU:O	1:C:329:MET:HG3	2.12	0.50
1:A:166:LEU:HD21	1:A:178:GLY:HA3	1.94	0.49
1:B:57:LEU:HD22	1:B:129:LEU:HD21	1.94	0.49
1:C:298:ILE:HD12	1:C:332:LEU:HD21	1.94	0.49
1:C:487:MET:HE1	1:C:496:PHE:HB2	1.94	0.49
1:C:436:LEU:HD12	1:C:440:LEU:HD12	1.95	0.49
1:A:468:LEU:HD11	1:A:497:LEU:HG	1.94	0.49
1:B:180:ALA:O	1:B:184:GLU:HG2	2.13	0.49
1:C:71:LEU:O	1:C:75:THR:HG23	2.12	0.48
1:C:381:MET:HE2	1:C:433:HIS:CE1	2.48	0.48
1:B:15:HIS:CE1	1:B:19:LYS:HZ1	2.31	0.48
1:B:290:ASP:N	1:B:290:ASP:OD1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:HG21	1:B:546:MET:HG3	1.93	0.48
1:C:245:PRO:HD3	1:C:318:TYR:HB3	1.94	0.48
1:C:292:TYR:CE2	1:C:432:THR:HG21	2.48	0.48
1:B:363:ILE:HA	1:B:368:ILE:HD11	1.94	0.48
1:C:458:ILE:O	1:C:458:ILE:HD12	2.14	0.48
1:B:521:ASN:HB2	1:B:535:ALA:HA	1.94	0.48
1:C:433:HIS:O	1:C:437:LEU:HG	2.13	0.48
1:C:393:LEU:HD23	1:C:422:ASN:HB2	1.96	0.47
1:A:199:ASP:OD1	1:A:199:ASP:N	2.47	0.47
1:C:146:GLN:HB2	1:C:419:LEU:HD13	1.96	0.47
1:B:23:MET:HE1	1:B:407:TYR:CE1	2.50	0.47
1:C:358:GLU:H	1:C:358:GLU:CD	2.23	0.47
1:A:335:ARG:HH12	1:B:195:ILE:HG12	1.80	0.47
1:C:497:LEU:HD12	1:C:518:PHE:HD2	1.79	0.47
1:A:219:ARG:NH1	1:A:224:GLU:OE2	2.44	0.47
1:C:529:GLU:H	1:C:529:GLU:CD	2.22	0.47
1:A:553:ARG:O	1:A:554:ASP:C	2.58	0.46
1:C:232:THR:OG1	1:C:234:THR:O	2.32	0.46
1:B:6:TYR:HE2	1:B:73:GLN:HA	1.81	0.46
1:C:346:LEU:HB3	1:C:349:THR:OG1	2.16	0.46
1:B:118:THR:HG23	1:C:118:THR:HG23	1.98	0.46
1:B:346:LEU:HB3	1:B:349:THR:HG21	1.97	0.46
1:A:312:GLU:OE2	1:A:342:ARG:HD2	2.16	0.46
1:A:521:ASN:HB2	1:A:535:ALA:HA	1.97	0.46
1:B:17:ASN:HD22	1:B:17:ASN:C	2.21	0.46
1:B:71:LEU:HD11	1:B:113:GLN:HB3	1.97	0.46
1:C:327:LEU:HD22	1:C:453:ILE:HD11	1.98	0.46
1:B:177:ARG:HA	1:B:177:ARG:HD2	1.63	0.46
1:B:380:ILE:HD13	1:B:429:ALA:HA	1.98	0.46
1:B:573:PRO:HB2	1:B:577:VAL:HG11	1.98	0.46
1:C:488:LYS:HA	1:C:488:LYS:HD2	1.68	0.46
1:C:255:MET:HE3	1:C:255:MET:HB3	1.84	0.45
1:B:112:LYS:O	1:B:116:LEU:HD22	2.17	0.45
1:B:191:ASP:O	1:B:195:ILE:HG22	2.17	0.45
1:A:171:ASP:CG	1:A:174:ASN:HD21	2.25	0.45
1:A:496:PHE:O	1:A:497:LEU:HD23	2.17	0.45
1:B:134:GLN:N	1:B:134:GLN:OE1	2.50	0.45
1:B:104:GLU:O	1:B:104:GLU:HG2	2.16	0.45
1:B:322:GLY:HA3	1:B:349:THR:HG21	1.99	0.45
1:C:323:THR:O	1:C:327:LEU:HD12	2.16	0.45
1:B:122:LEU:HD23	2:C:602:GOL:H11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD13	1:A:487:MET:HG3	1.99	0.45
1:B:190:ALA:O	1:B:194:ASN:HB2	2.16	0.44
1:B:122:LEU:O	1:B:126:VAL:HG23	2.18	0.44
1:A:209:LEU:HA	1:A:255:MET:O	2.18	0.44
1:C:452:LYS:HB2	1:C:452:LYS:HE3	1.87	0.44
1:C:143:PHE:HA	1:C:146:GLN:HG3	1.99	0.44
1:A:547:MET:HA	1:A:547:MET:HE2	1.99	0.44
1:A:481:GLN:HE21	1:A:481:GLN:HB2	1.57	0.44
1:C:449:GLY:O	1:C:457:ARG:NH1	2.51	0.44
1:C:497:LEU:HD12	1:C:518:PHE:CD2	2.52	0.44
1:C:386:LEU:HD12	1:C:386:LEU:HA	1.86	0.43
1:A:177:ARG:O	1:A:181:LEU:HG	2.19	0.43
1:A:381:MET:HE3	1:A:433:HIS:CE1	2.53	0.43
1:A:290:ASP:OD1	1:A:290:ASP:N	2.51	0.43
1:A:516:TYR:O	1:A:540:GLY:N	2.38	0.43
1:B:320:ILE:HD11	1:B:436:LEU:HD11	2.01	0.43
1:C:245:PRO:HA	1:C:320:ILE:HG22	2.01	0.43
1:C:552:ASN:HB2	1:C:553:ARG:HH21	1.84	0.43
1:C:139:ARG:HB3	1:C:143:PHE:CE2	2.54	0.43
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.85	0.43
1:A:579:VAL:HG11	1:C:40:LEU:HD21	2.01	0.43
1:B:250:TYR:C	1:B:252:ILE:N	2.77	0.43
1:C:105:GLN:HG2	1:C:107:ILE:HG22	2.00	0.43
1:C:314:HIS:CE1	1:C:550:ILE:HG23	2.54	0.43
1:A:244:PRO:HG2	1:A:277:TRP:CD1	2.54	0.42
1:B:15:HIS:CE1	1:B:19:LYS:NZ	2.87	0.42
1:B:24:ALA:O	1:B:28:THR:HG23	2.19	0.42
1:B:163:LEU:HG	1:B:361:ILE:HD11	2.01	0.42
1:A:255:MET:HE2	1:A:418:LEU:HD23	2.01	0.42
1:C:298:ILE:HG12	1:C:298:ILE:H	1.72	0.42
1:B:72:MET:HE2	1:C:107:ILE:HD11	2.00	0.42
1:B:546:MET:HE2	1:B:546:MET:HB3	1.90	0.42
1:B:224:GLU:HG3	1:B:576:TYR:CD2	2.55	0.42
1:C:288:ASP:HB2	1:C:431:LYS:NZ	2.35	0.41
1:C:436:LEU:HD12	1:C:436:LEU:HA	1.94	0.41
1:A:72:MET:HE2	1:A:72:MET:HB2	1.94	0.41
1:C:393:LEU:HD11	1:C:418:LEU:HB3	2.02	0.41
1:C:511:PRO:O	1:C:514:ASN:ND2	2.53	0.41
1:B:358:GLU:O	1:B:361:ILE:HG22	2.21	0.41
1:C:186:LEU:HD12	1:C:186:LEU:HA	1.79	0.41
1:A:320:ILE:HD12	1:A:320:ILE:HA	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:TYR:O	1:B:252:ILE:N	2.54	0.41
1:A:294:VAL:O	1:A:298:ILE:HB	2.20	0.41
1:C:353:PHE:CE2	1:C:440:LEU:HD22	2.56	0.41
1:A:553:ARG:HA	1:A:553:ARG:HD3	1.84	0.41
1:B:6:TYR:CE1	1:C:107:ILE:HD13	2.56	0.41
1:B:295:ASP:OD2	1:B:454:ARG:NH2	2.53	0.41
1:C:396:ASN:ND2	1:C:474:ASP:OD2	2.53	0.41
1:A:162:GLU:O	1:A:166:LEU:HD12	2.21	0.40
1:B:481:GLN:HE21	1:B:481:GLN:HB2	1.57	0.40
1:C:452:LYS:HG2	1:C:457:ARG:HA	2.02	0.40
1:B:105:GLN:N	1:B:106:PRO:HD2	2.37	0.40
1:C:350:LEU:HD23	1:C:483:THR:HG22	2.04	0.40
1:B:380:ILE:HD13	1:B:380:ILE:HA	2.00	0.40
1:B:397:SER:HB2	1:B:400:TRP:HB2	2.02	0.40
1:A:335:ARG:HH22	1:B:195:ILE:HG23	1.86	0.40
1:A:511:PRO:HD3	1:A:543:TRP:CE3	2.56	0.40
1:C:292:TYR:HE2	1:C:432:THR:HG21	1.85	0.40
1:B:62:MET:HE2	1:B:62:MET:HA	2.03	0.40
1:B:148:VAL:HG13	1:C:116:LEU:HD12	2.04	0.40
1:B:359:LEU:HD23	1:B:359:LEU:HA	1.83	0.40

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)
1:A:519:TRP:NE1	1:A:567:GLU:OE2[4_446]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	536/596 (90%)	525 (98%)	11 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	526/596 (88%)	507 (96%)	19 (4%)	0	100	100
1	C	521/596 (87%)	511 (98%)	10 (2%)	0	100	100
All	All	1583/1788 (88%)	1543 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	453/494 (92%)	444 (98%)	9 (2%)	50	78
1	B	447/494 (90%)	433 (97%)	14 (3%)	35	64
1	C	442/494 (90%)	436 (99%)	6 (1%)	62	84
All	All	1342/1482 (91%)	1313 (98%)	29 (2%)	47	76

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	130	GLU
1	A	174	ASN
1	A	200	GLU
1	A	246	PHE
1	A	248	ASN
1	A	313	VAL
1	A	481	GLN
1	A	553	ARG
1	B	40	LEU
1	B	123	LEU
1	B	127	ASP
1	B	140	LEU
1	B	141	ARG
1	B	164	LEU
1	B	247	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	290	ASP
1	B	313	VAL
1	B	349	THR
1	B	411	GLN
1	B	481	GLN
1	B	497	LEU
1	B	560	VAL
1	C	154	SER
1	C	186	LEU
1	C	193	LEU
1	C	435	SER
1	C	536	THR
1	C	553	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	52	GLN
1	A	59	GLN
1	A	146	GLN
1	A	248	ASN
1	A	355	GLN
1	A	375	ASN
1	A	420	HIS
1	A	434	ASN
1	A	481	GLN
1	A	509	ASN
1	A	520	HIS
1	A	552	ASN
1	B	149	ASN
1	B	160	ASN
1	B	227	GLN
1	B	248	ASN
1	B	375	ASN
1	B	422	ASN
1	B	434	ASN
1	B	481	GLN
1	B	509	ASN
1	B	520	HIS
1	B	575	HIS
1	C	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	146	GLN
1	C	149	ASN
1	C	270	GLN
1	C	422	ASN
1	C	485	GLN
1	C	514	ASN
1	C	520	HIS
1	C	551	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	GOL	B	602	-	5,5,5	0.54	0	5,5,5	0.36	0
2	GOL	A	601	-	5,5,5	0.55	0	5,5,5	0.28	0
2	GOL	B	603	-	5,5,5	0.54	0	5,5,5	0.21	0
2	GOL	C	601	-	5,5,5	0.54	0	5,5,5	0.23	0
2	GOL	A	604	-	5,5,5	0.57	0	5,5,5	0.33	0
2	GOL	A	603	-	5,5,5	0.56	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	C	602	-	5,5,5	0.56	0	5,5,5	0.32	0
2	GOL	B	601	-	5,5,5	0.55	0	5,5,5	0.34	0
2	GOL	B	604	-	5,5,5	0.57	0	5,5,5	0.27	0
2	GOL	A	605	-	5,5,5	0.09	0	5,5,5	0.35	0
2	GOL	A	602	-	5,5,5	0.58	0	5,5,5	0.28	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	GOL	B	602	-	-	0/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	B	603	-	-	0/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	A	604	-	-	0/4/4/4	-
2	GOL	A	603	-	-	0/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	B	604	-	-	0/4/4/4	-
2	GOL	A	605	-	-	0/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-C3
2	C	601	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand GOL B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 603

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 604

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 604

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 605

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 602

Bond lengths

Bond angles

Torsions

Rings

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(Å²)	Q<0.9
1	A	546/596 (91%)	-0.14	8 (1%)	71	71	39, 64, 110, 155	0
1	B	538/596 (90%)	0.05	6 (1%)	77	77	52, 77, 123, 142	0
1	C	533/596 (89%)	0.53	30 (5%)	31	29	65, 104, 141, 162	0
All	All	1617/1788 (90%)	0.14	44 (2%)	56	54	39, 81, 132, 162	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	436	LEU	4.1
1	C	195	ILE	3.9
1	B	40	LEU	3.6
1	A	201	SER	3.6
1	C	367	ILE	3.5
1	A	202	ALA	3.4
1	C	362	PHE	3.4
1	C	574	GLY	3.3
1	C	281	GLY	3.1
1	C	441	TYR	3.1
1	C	176	VAL	3.0
1	C	193	LEU	3.0
1	C	363	ILE	2.9
1	C	371	LEU	2.9
1	C	392	LEU	2.7
1	C	282	VAL	2.7
1	C	583	PRO	2.6
1	C	440	LEU	2.5
1	B	158	ALA	2.5
1	B	202	ALA	2.5
1	B	557	SER	2.5
1	B	77	LEU	2.5
1	C	158	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	166	LEU	2.5
1	A	554	ASP	2.5
1	C	289	LEU	2.4
1	C	437	LEU	2.4
1	C	390	PHE	2.4
1	C	51	SER	2.4
1	C	171	ASP	2.3
1	C	446	LEU	2.3
1	C	361	ILE	2.3
1	C	528	PRO	2.2
1	A	326	SER	2.2
1	C	5	SER	2.2
1	C	575	HIS	2.2
1	C	553	ARG	2.2
1	A	38	THR	2.1
1	B	5	SER	2.1
1	A	80	ALA	2.1
1	A	5	SER	2.0
1	C	334	ALA	2.0
1	C	38	THR	2.0
1	A	176	VAL	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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
2	GOL	A	601	6/6	0.84	0.22	86,89,92,99	0
2	GOL	C	602	6/6	0.85	0.24	84,94,108,117	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	601	6/6	0.86	0.21	89,95,99,102	0
2	GOL	B	603	6/6	0.87	0.16	89,101,106,118	0
2	GOL	B	604	6/6	0.87	0.15	87,96,101,105	0
2	GOL	C	601	6/6	0.87	0.20	72,98,103,106	0
2	GOL	A	603	6/6	0.87	0.15	81,85,94,105	0
2	GOL	A	605	6/6	0.88	0.18	83,83,83,83	0
2	GOL	A	602	6/6	0.89	0.40	75,88,89,108	0
2	GOL	A	604	6/6	0.93	0.21	67,78,80,82	0
2	GOL	B	602	6/6	0.93	0.22	81,83,88,106	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 GOL A 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
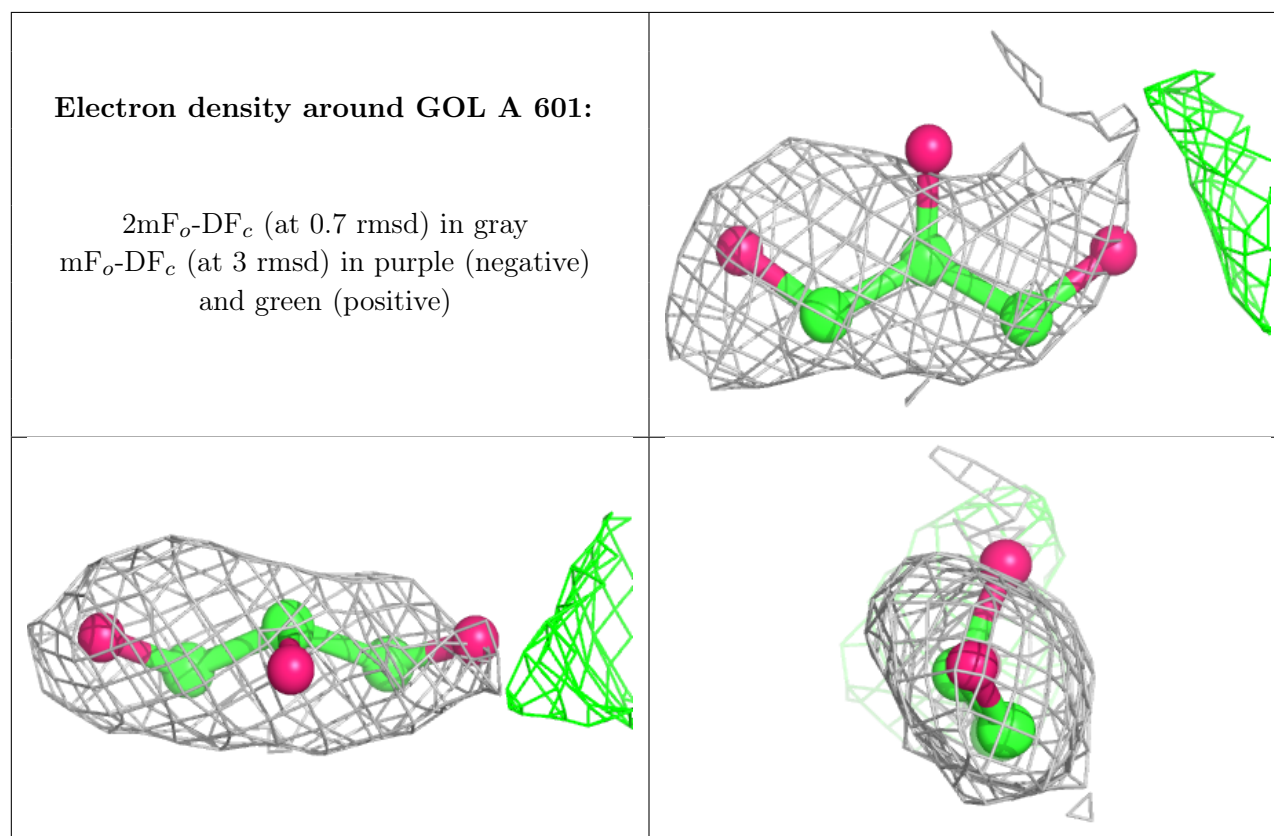
Electron density around GOL C 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
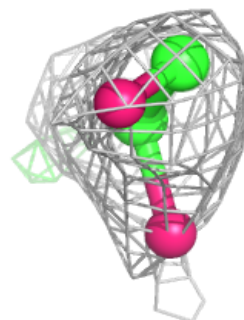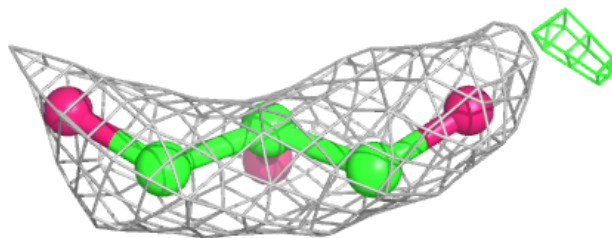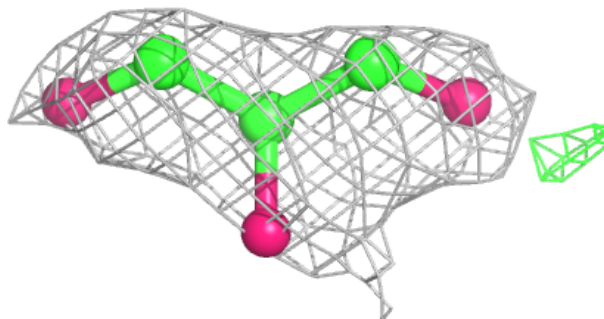and green (positive)
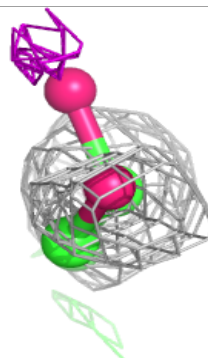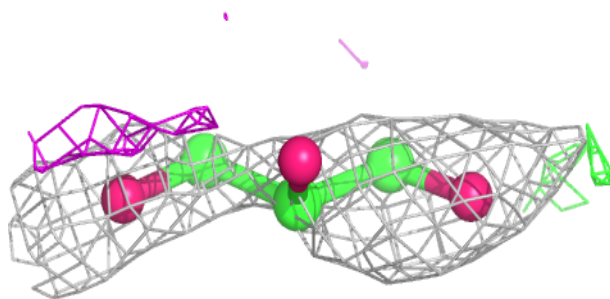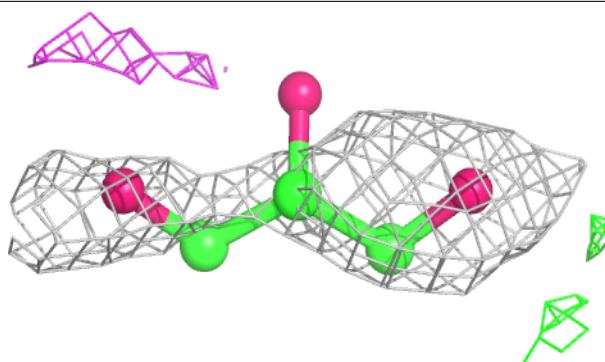
Electron density around GOL B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
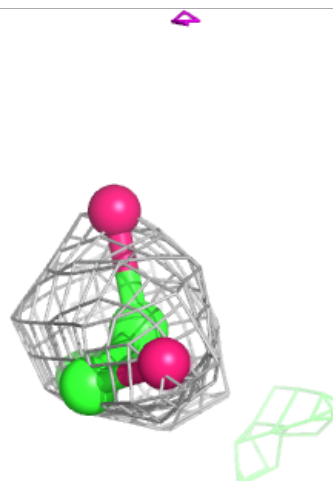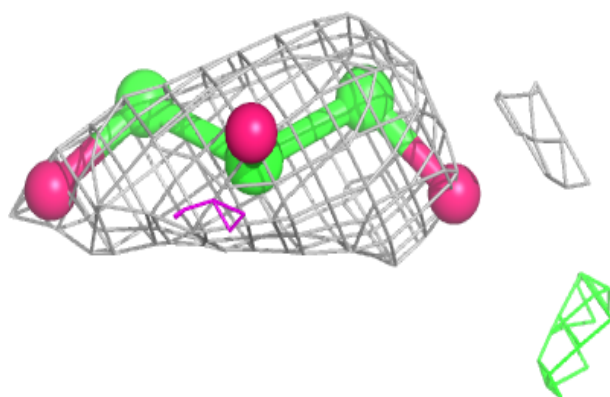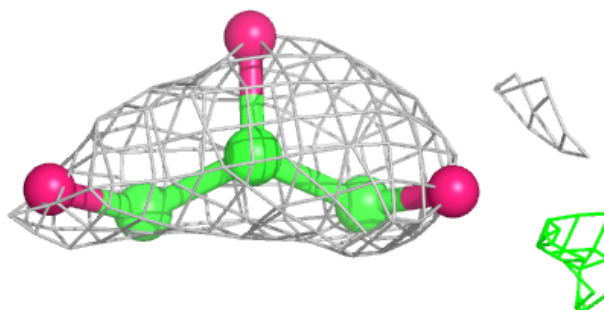
Electron density around GOL B 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
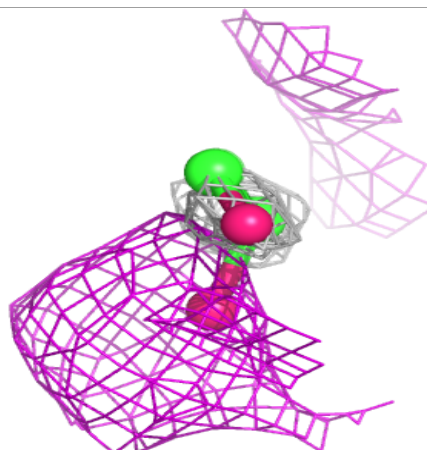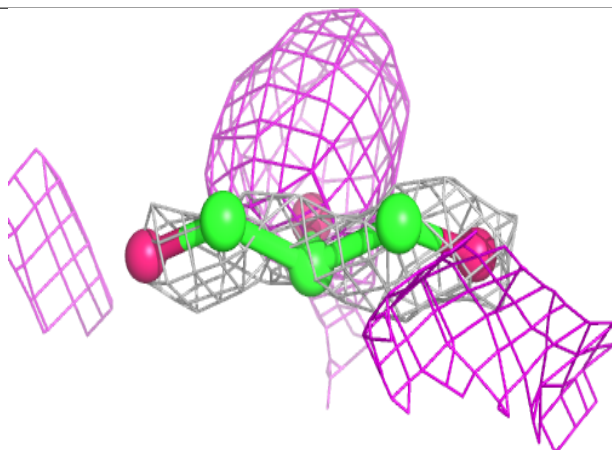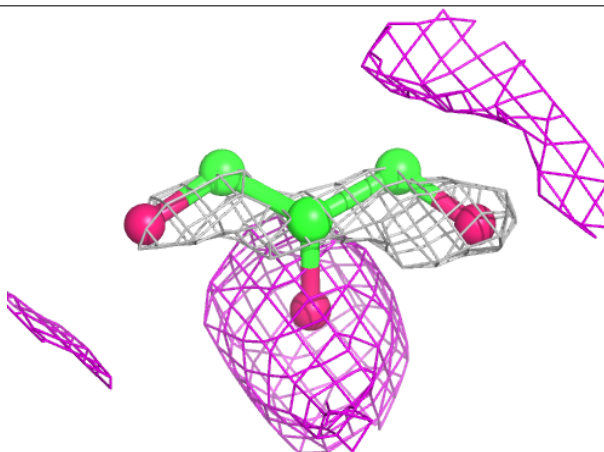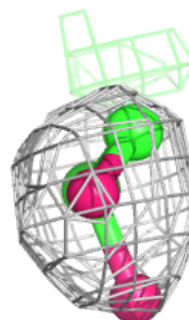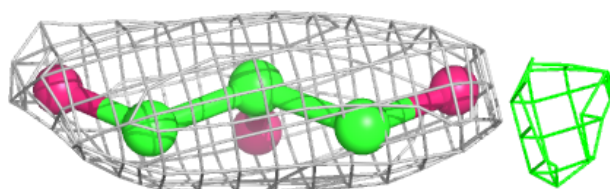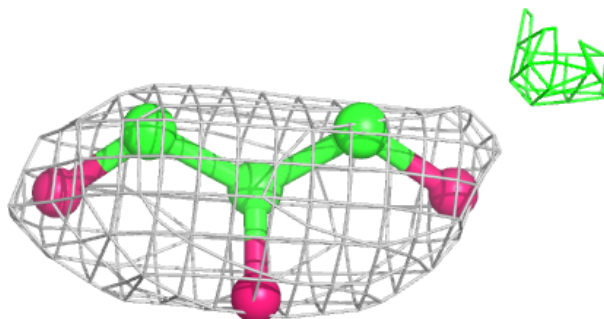mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
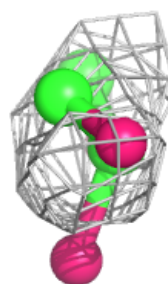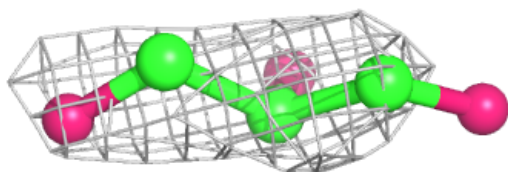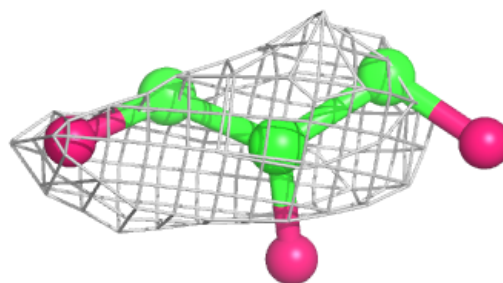
Electron density around GOL B 604:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
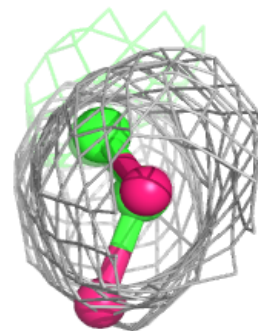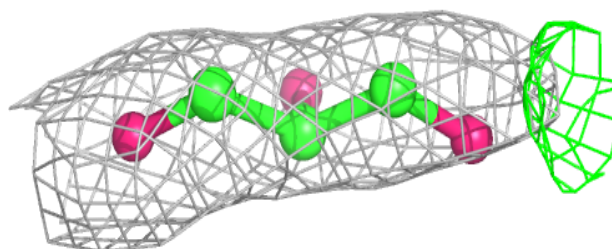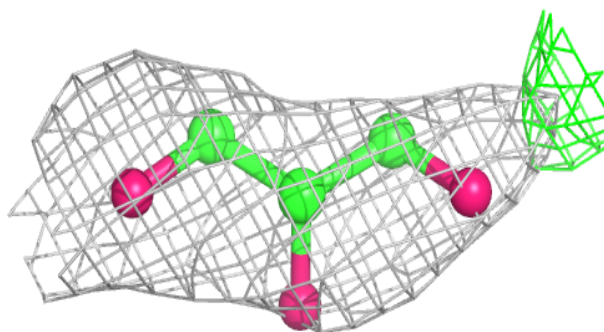
Electron density around GOL C 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
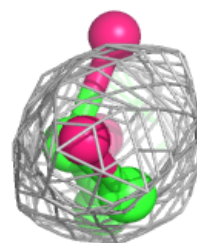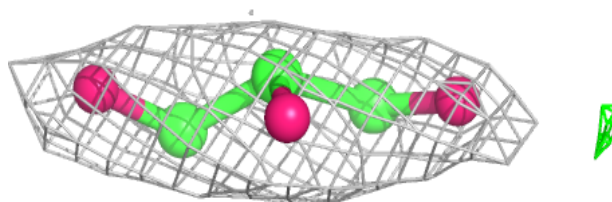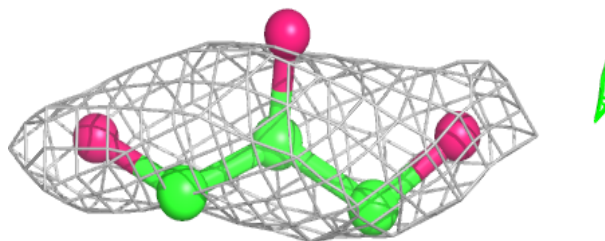
Electron density around GOL A 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
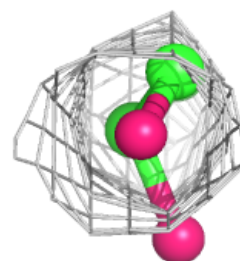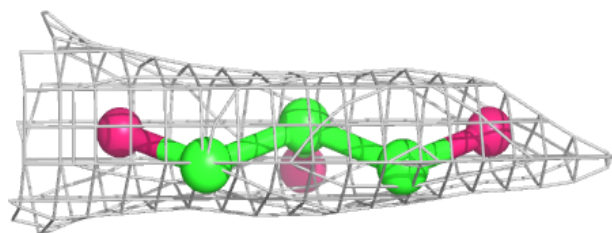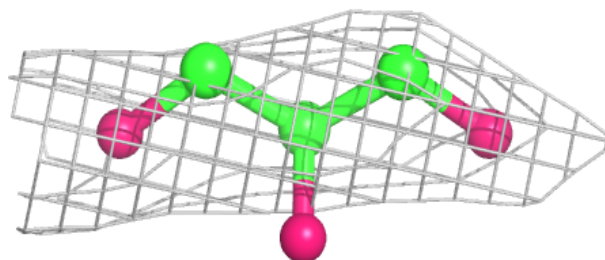
Electron density around GOL A 605:

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

Electron density around GOL A 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 GOL A 604:

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

Electron density around GOL B 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
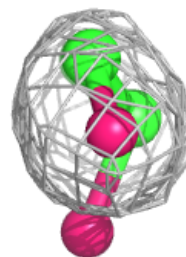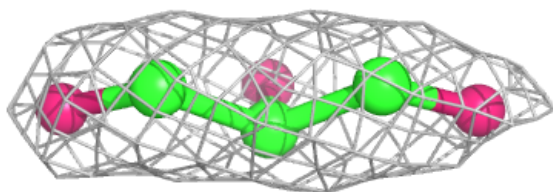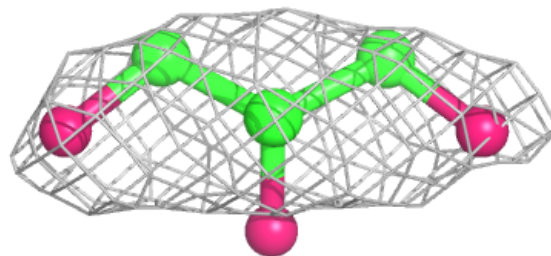
6.5 Other polymers (i)

There are no such residues in this entry.