WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 10:37 PM JST

PDB ID	:	7XFY
Title	:	Crystal structure of the ternary complex of Peptidoglycan recognition protein, PGRP-S with hexanoic and tartaric acids at 2.67 A resolution.
Authors	:	Maurya, A.; Singh, P.K.; Viswanathan, V.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2022-04-02
Resolution	:	2.67 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.67 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		0.267
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		7.8%
RSRZ outliers		0.3%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
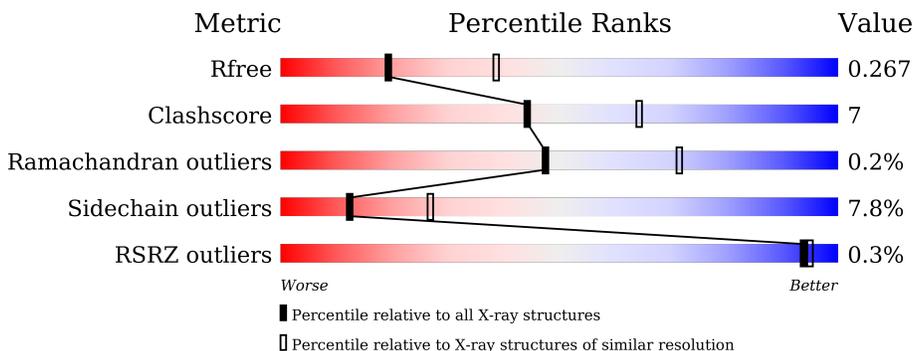
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	171	81% 13% ···
1	B	171	% 75% 18% ··
1	C	171	% 85% 11% ··
1	D	171	80% 16% ··

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 5625 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 Peptidoglycan recognition protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1301	812	249	232	8			
1	B	166	Total	C	N	O	S	0	0	0
			1301	812	249	232	8			
1	C	166	Total	C	N	O	S	0	0	0
			1301	812	249	232	8			
1	D	166	Total	C	N	O	S	0	0	0
			1300	812	249	231	8			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).
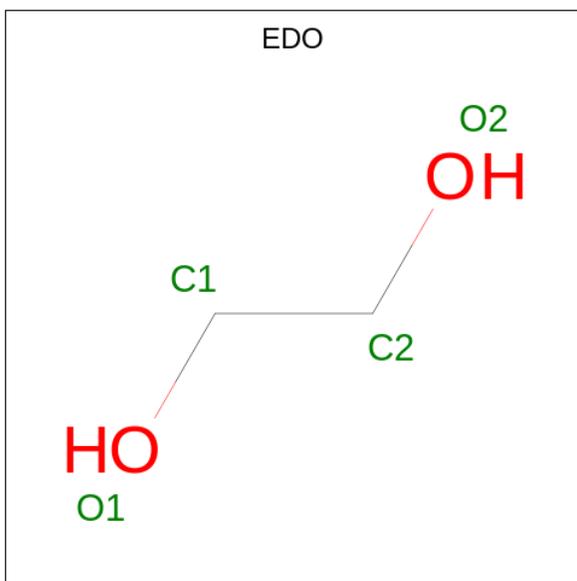

EDO

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$) (labeled as "Ligand of Interest" by depositor).
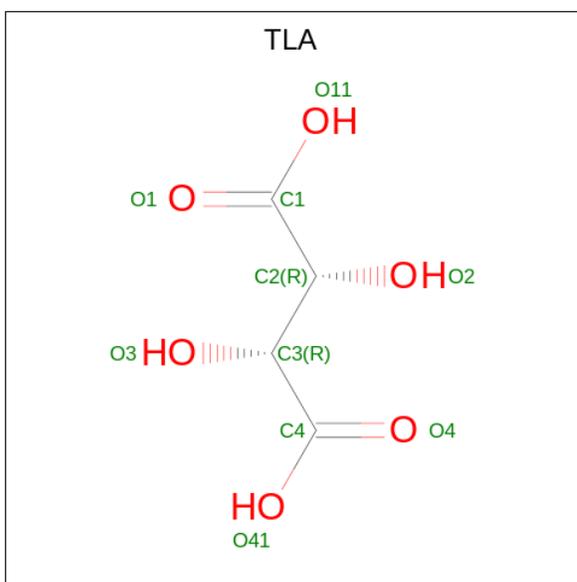

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 10	C 4	O 6	0	0
3	C	1	Total 10	C 4	O 6	0	0
3	D	1	Total 10	C 4	O 6	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).
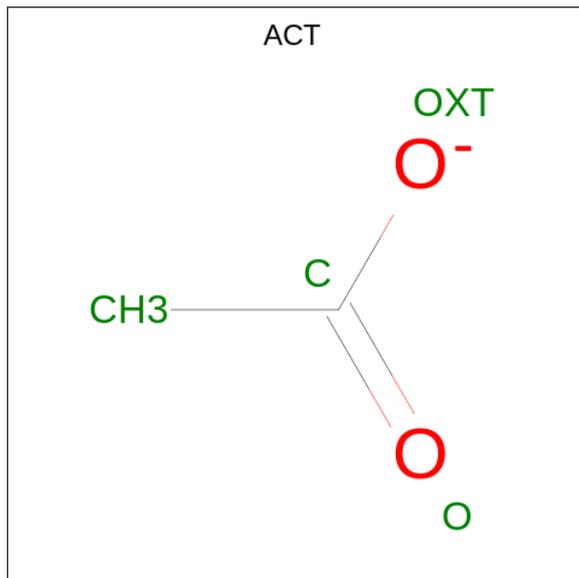
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0

- Molecule 6 is HEXANOIC ACID (three-letter code: 6NA) (formula: $C_6H_{12}O_2$) (labeled as "Ligand of Interest" by depositor).
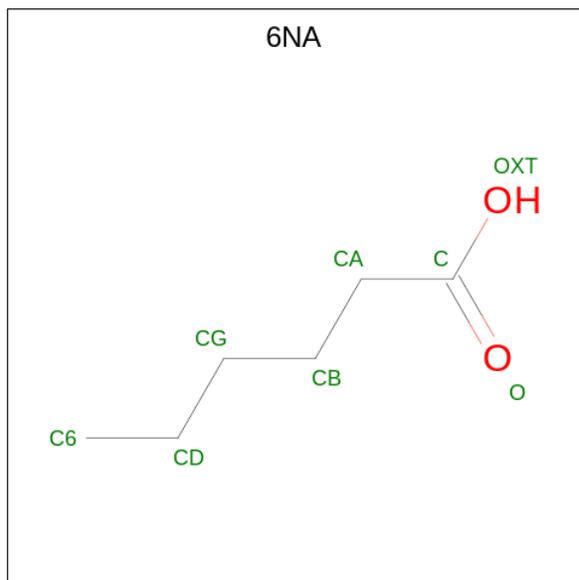
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 8	C 6	O 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).
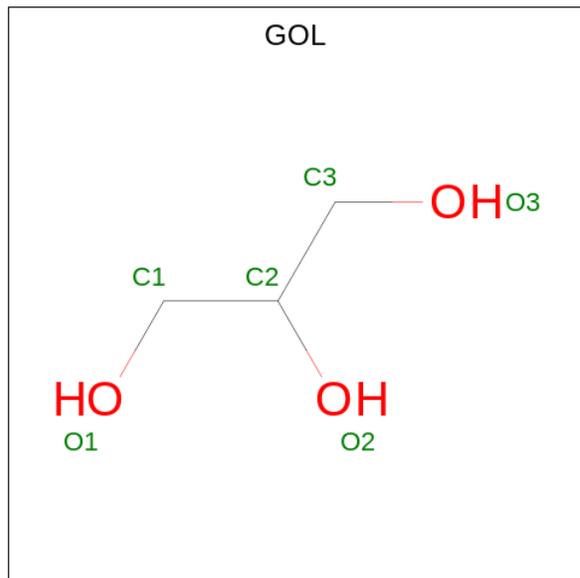
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 6	C 3	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	95	Total 95	O 95	0	0
8	B	79	Total 79	O 79	0	0
8	C	87	Total 87	O 87	0	0
8	D	88	Total 88	O 88	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 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: Peptidoglycan recognition protein 1
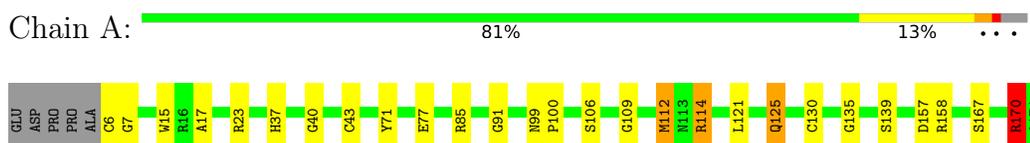
Chain A:

- Molecule 1: Peptidoglycan recognition protein 1

Chain B:

- Molecule 1: Peptidoglycan recognition protein 1

Chain C:

- Molecule 1: Peptidoglycan recognition protein 1

Chain D:
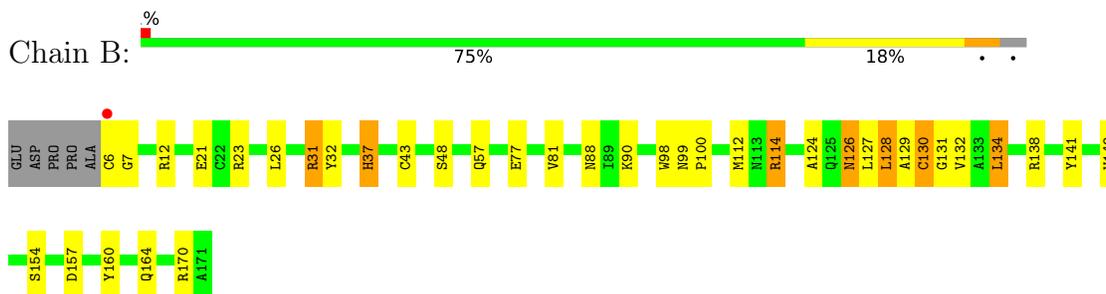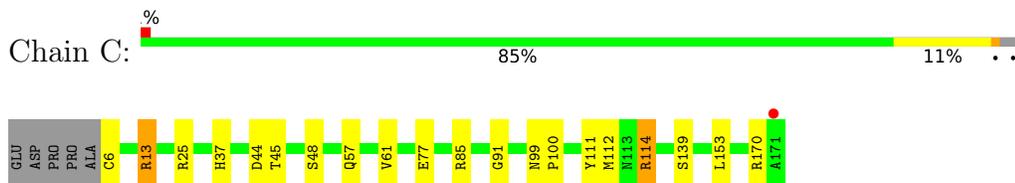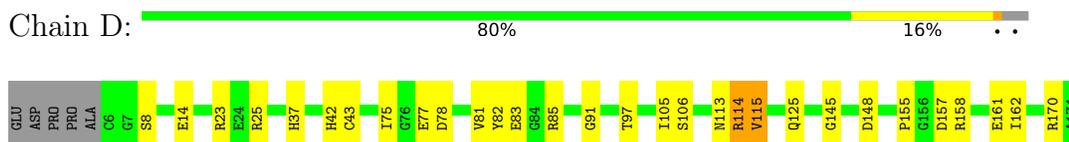
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	89.58Å 101.03Å 163.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.93 – 2.67 85.93 – 2.67	Depositor EDS
% Data completeness (in resolution range)	91.5 (85.93-2.67) 91.5 (85.93-2.67)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.175 , 0.266 0.184 , 0.267	Depositor DCC
R_{free} test set	961 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5625	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, CL, TLA, 6NA, EDO

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	0.75	0/1336	0.89	1/1817 (0.1%)
1	B	0.78	0/1336	0.93	0/1817
1	C	0.75	0/1336	0.91	0/1817
1	D	0.77	1/1335 (0.1%)	0.93	0/1817
All	All	0.76	1/5343 (0.0%)	0.91	1/7268 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLU	CD-OE1	5.48	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	170	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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	1301	0	1256	15	0
1	B	1301	0	1256	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1301	0	1256	10	0
1	D	1300	0	1256	16	0
2	A	4	0	6	0	0
2	B	8	0	12	2	0
2	C	4	0	6	0	0
2	D	8	0	12	0	0
3	A	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	B	1	0	0	0	0
5	C	4	0	3	0	0
6	D	8	0	11	0	0
7	D	6	0	8	0	0
8	A	95	0	0	1	0
8	B	79	0	0	6	0
8	C	87	0	0	1	0
8	D	88	0	0	2	0
All	All	5625	0	5094	68	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 7.

All (68) 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:D:78:ASP:OD2	1:D:82:TYR:OH	1.99	0.79
1:B:7:GLY:HA3	8:B:304:HOH:O	1.83	0.79
1:B:57:GLN:HB3	8:B:301:HOH:O	1.94	0.68
1:A:77:GLU:OE2	1:A:114:ARG:NH1	2.30	0.64
1:B:132:VAL:HB	8:B:312:HOH:O	2.01	0.59
1:B:126:ASN:C	1:B:126:ASN:HD22	2.09	0.56
1:D:42:HIS:CD2	1:D:114:ARG:HH12	2.24	0.56
1:D:42:HIS:CG	1:D:114:ARG:HH12	2.24	0.55
1:C:85:ARG:HD2	1:C:91:GLY:HA2	1.88	0.54
1:B:31:ARG:HG2	1:B:32:TYR:CE2	2.42	0.54
1:B:37:HIS:O	2:B:201:EDO:H11	2.08	0.53
1:B:77:GLU:OE2	1:B:114:ARG:NH1	2.42	0.52
1:C:112:MET:CE	1:C:153:LEU:HB3	2.38	0.52
1:B:37:HIS:O	2:B:201:EDO:C1	2.58	0.52
1:D:42:HIS:CG	1:D:114:ARG:NH1	2.78	0.51
1:A:7:GLY:N	1:B:126:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLY:O	1:A:109:GLY:HA2	2.11	0.51
1:C:57:GLN:O	1:C:61:VAL:HG23	2.11	0.51
1:D:105:ILE:O	1:D:105:ILE:HG13	2.10	0.50
1:A:121:LEU:O	1:A:125:GLN:HG3	2.11	0.50
1:B:134:LEU:HD23	1:B:134:LEU:N	2.26	0.50
1:A:43:CYS:O	1:A:77:GLU:HB2	2.12	0.50
1:D:145:GLY:O	1:D:148:ASP:HB2	2.12	0.50
1:D:157:ASP:O	1:D:161:GLU:HG3	2.12	0.49
1:D:43:CYS:O	1:D:77:GLU:HB2	2.12	0.49
1:D:42:HIS:CE1	1:D:114:ARG:NH1	2.81	0.49
1:C:77:GLU:OE2	1:C:114:ARG:NH1	2.46	0.49
1:D:158:ARG:HA	1:D:158:ARG:HD3	1.71	0.48
1:D:85:ARG:HD2	1:D:91:GLY:HA2	1.95	0.48
1:B:7:GLY:CA	8:B:304:HOH:O	2.53	0.48
1:A:112:MET:HE1	1:A:157:ASP:OD2	2.14	0.47
1:A:85:ARG:HD2	1:A:91:GLY:HA2	1.96	0.47
1:B:129:ALA:C	1:B:131:GLY:H	2.17	0.47
1:A:112:MET:HE3	1:A:157:ASP:H	1.78	0.47
1:B:99:ASN:N	1:B:100:PRO:HD2	2.30	0.47
1:C:44:ASP:OD1	1:C:44:ASP:N	2.48	0.47
1:B:160:TYR:O	1:B:164:GLN:HG3	2.15	0.46
1:C:112:MET:HE3	1:C:153:LEU:HB3	1.96	0.46
1:D:42:HIS:ND1	1:D:114:ARG:NH1	2.64	0.46
1:A:135:GLY:HA2	8:A:331:HOH:O	2.15	0.46
1:C:13:ARG:HB3	8:C:377:HOH:O	2.16	0.46
1:D:115:VAL:HG12	1:D:162:ILE:HD11	1.98	0.45
1:B:81:VAL:HG11	1:B:127:LEU:HD13	1.98	0.45
1:D:14:GLU:OE2	8:D:301:HOH:O	2.21	0.45
1:B:98:TRP:CD1	1:B:149:VAL:HB	2.52	0.45
1:B:112:MET:HA	1:B:157:ASP:H	1.83	0.44
1:B:43:CYS:O	1:B:77:GLU:HB2	2.18	0.44
1:C:45:THR:HG22	1:C:48:SER:H	1.83	0.44
1:A:112:MET:CE	1:A:157:ASP:OD2	2.66	0.43
1:A:77:GLU:CD	1:A:114:ARG:HH12	2.21	0.43
1:D:75:ILE:HD12	1:D:81:VAL:HG22	2.01	0.43
1:D:97:THR:HB	8:D:321:HOH:O	2.18	0.42
1:B:126:ASN:ND2	8:B:304:HOH:O	2.50	0.42
1:B:26:LEU:HG	1:B:90:LYS:HA	2.02	0.42
1:A:170:ARG:HA	1:A:170:ARG:HD3	1.94	0.42
1:B:31:ARG:HH11	1:B:138:ARG:NH2	2.18	0.41
1:B:90:LYS:HG3	1:B:100:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ASN:N	1:C:100:PRO:HD2	2.36	0.41
1:B:26:LEU:N	1:B:88:ASN:O	2.43	0.41
1:A:71:TYR:CD1	1:A:106:SER:HB2	2.55	0.41
1:A:99:ASN:N	1:A:100:PRO:HD2	2.35	0.41
1:C:77:GLU:OE2	1:C:111:TYR:OH	2.26	0.41
1:B:124:ALA:O	1:B:127:LEU:HB3	2.21	0.41
1:B:138:ARG:HD3	8:B:320:HOH:O	2.21	0.41
1:B:43:CYS:HB2	1:B:48:SER:OG	2.21	0.40
1:B:128:LEU:HD13	1:B:141:TYR:CE1	2.57	0.40
1:A:15:TRP:CH2	1:A:17:ALA:HB2	2.56	0.40
1:B:81:VAL:HG21	1:B:127:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

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	164/171 (96%)	154 (94%)	10 (6%)	0	100	100
1	B	164/171 (96%)	153 (93%)	10 (6%)	1 (1%)	25	47
1	C	164/171 (96%)	151 (92%)	13 (8%)	0	100	100
1	D	164/171 (96%)	154 (94%)	10 (6%)	0	100	100
All	All	656/684 (96%)	612 (93%)	43 (7%)	1 (0%)	47	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	130	CYS

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	135/139 (97%)	124 (92%)	11 (8%)	11	25
1	B	135/139 (97%)	122 (90%)	13 (10%)	8	18
1	C	135/139 (97%)	128 (95%)	7 (5%)	23	46
1	D	135/139 (97%)	124 (92%)	11 (8%)	11	25
All	All	540/556 (97%)	498 (92%)	42 (8%)	12	27

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	23	ARG
1	A	37	HIS
1	A	112	MET
1	A	114	ARG
1	A	125	GLN
1	A	130	CYS
1	A	139	SER
1	A	158	ARG
1	A	167	SER
1	A	170	ARG
1	B	6	CYS
1	B	12	ARG
1	B	21	GLU
1	B	23	ARG
1	B	31	ARG
1	B	37	HIS
1	B	114	ARG
1	B	126	ASN
1	B	128	LEU
1	B	130	CYS
1	B	134	LEU
1	B	154	SER
1	B	170	ARG

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Mol	Chain	Res	Type
1	C	6	CYS
1	C	13	ARG
1	C	25	ARG
1	C	37	HIS
1	C	114	ARG
1	C	139	SER
1	C	170	ARG
1	D	8	SER
1	D	23	ARG
1	D	25	ARG
1	D	37	HIS
1	D	106	SER
1	D	113	ASN
1	D	114	ARG
1	D	115	VAL
1	D	125	GLN
1	D	155	PRO
1	D	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	168	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	#$|Z| > 2$
3	TLA	A	202	-	9,9,9	1.23	0	12,12,12	1.31	2 (16%)
3	TLA	C	202	-	9,9,9	1.49	1 (11%)	12,12,12	1.18	0
2	EDO	D	205	-	3,3,3	0.21	0	2,2,2	0.28	0
6	6NA	D	202	-	7,7,7	0.73	0	7,7,7	0.92	0
2	EDO	B	201	-	3,3,3	0.34	0	2,2,2	0.47	0
3	TLA	D	204	-	9,9,9	1.17	0	12,12,12	0.90	0
5	ACT	C	201	-	3,3,3	1.21	0	3,3,3	0.55	0
7	GOL	D	203	-	5,5,5	0.14	0	5,5,5	0.51	0
2	EDO	C	203	-	3,3,3	0.23	0	2,2,2	0.21	0
2	EDO	A	201	-	3,3,3	0.28	0	2,2,2	0.53	0
2	EDO	D	201	-	3,3,3	0.45	0	2,2,2	0.46	0
2	EDO	B	202	-	3,3,3	0.23	0	2,2,2	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TLA	A	202	-	-	0/12/12/12	-
3	TLA	C	202	-	-	0/12/12/12	-
2	EDO	D	205	-	-	1/1/1/1	-
6	6NA	D	202	-	-	4/5/5/5	-
2	EDO	B	201	-	-	1/1/1/1	-
3	TLA	D	204	-	-	5/12/12/12	-
7	GOL	D	203	-	-	1/4/4/4	-
2	EDO	C	203	-	-	1/1/1/1	-
2	EDO	A	201	-	-	0/1/1/1	-
2	EDO	D	201	-	-	1/1/1/1	-
2	EDO	B	202	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	TLA	O2-C2	2.61	1.47	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	202	TLA	O3-C3-C2	2.99	116.17	110.23
3	A	202	TLA	O2-C2-C3	2.71	115.62	110.23

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	204	TLA	O1-C1-C2-O2
3	D	204	TLA	O11-C1-C2-O2
3	D	204	TLA	O1-C1-C2-C3
3	D	204	TLA	O11-C1-C2-C3
6	D	202	6NA	C-CA-CB-CG
6	D	202	6NA	CA-CB-CG-CD
2	B	202	EDO	O1-C1-C2-O2
2	D	201	EDO	O1-C1-C2-O2
2	C	203	EDO	O1-C1-C2-O2
7	D	203	GOL	C1-C2-C3-O3
2	B	201	EDO	O1-C1-C2-O2
6	D	202	6NA	O-C-CA-CB
2	D	205	EDO	O1-C1-C2-O2
6	D	202	6NA	OXT-C-CA-CB
3	D	204	TLA	O2-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	EDO	2	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 TLA A 202

Bond lengths

Bond angles

Torsions

Rings

Ligand TLA C 202

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 205

Bond lengths

Bond angles

Torsions

Rings

Ligand 6NA D 202

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand TLA D 204

Bond lengths

Bond angles

Torsions

Rings

Ligand ACT C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL D 203

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO C 203

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 202

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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, 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	166/171 (97%)	-0.36	0	100	100	20, 37, 59, 87	0
1	B	166/171 (97%)	-0.17	1 (0%)	89	90	21, 35, 63, 106	0
1	C	166/171 (97%)	-0.32	1 (0%)	89	90	18, 29, 55, 79	0
1	D	166/171 (97%)	-0.26	0	100	100	13, 31, 58, 73	0
All	All	664/684 (97%)	-0.28	2 (0%)	94	95	13, 33, 60, 106	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	ALA	3.1
1	B	6	CYS	2.4

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	EDO	A	201	4/4	0.88	0.19	46,50,51,53	0
2	EDO	B	202	4/4	0.88	0.15	36,37,39,40	0
6	6NA	D	202	8/8	0.89	0.24	60,61,63,65	0
2	EDO	D	201	4/4	0.90	0.16	41,48,49,53	0
3	TLA	D	204	10/10	0.91	0.28	54,68,74,76	0
3	TLA	A	202	10/10	0.91	0.25	44,55,60,66	0
2	EDO	B	201	4/4	0.93	0.23	47,50,51,51	0
5	ACT	C	201	4/4	0.94	0.24	46,50,50,51	0
2	EDO	C	203	4/4	0.94	0.23	27,29,31,33	4
2	EDO	D	205	4/4	0.95	0.14	36,39,39,40	4
7	GOL	D	203	6/6	0.96	0.22	38,39,41,42	0
3	TLA	C	202	10/10	0.97	0.21	24,25,39,40	0
4	CL	B	203	1/1	0.98	0.07	45,45,45,45	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 EDO A 201:

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

Electron density around EDO B 202:

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

Electron density around 6NA D 202:

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

Electron density around EDO D 201:

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

Electron density around TLA D 204:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
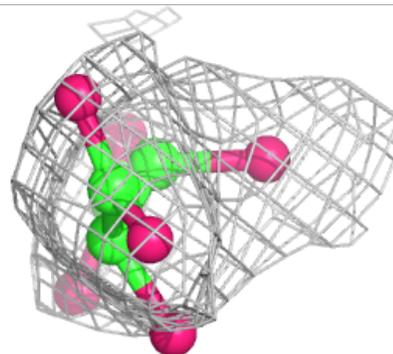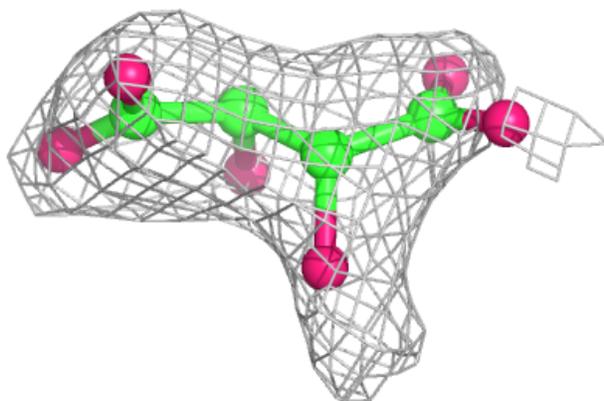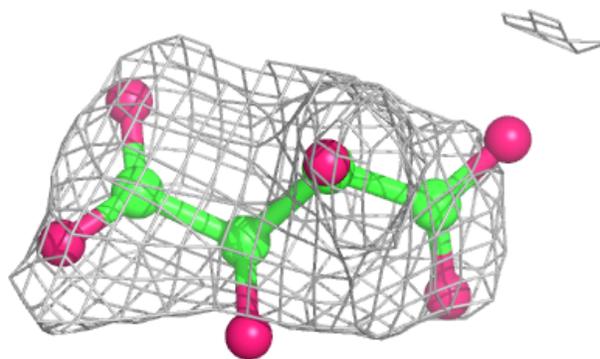
Electron density around TLA A 202:

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

**Electron density around EDO B 201:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
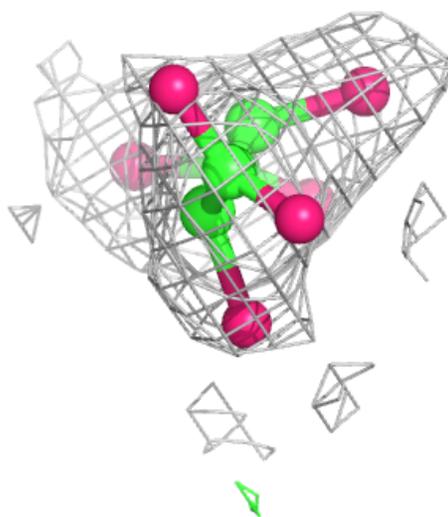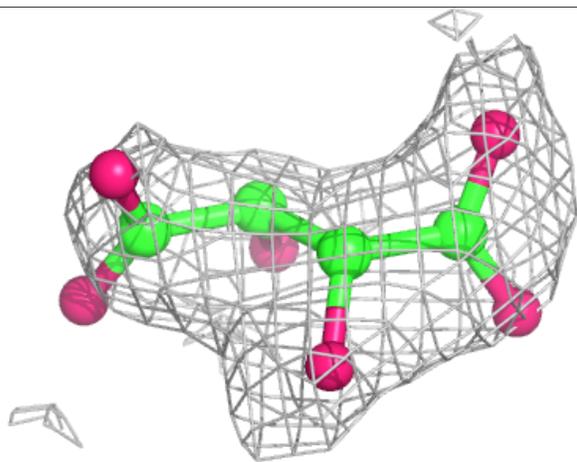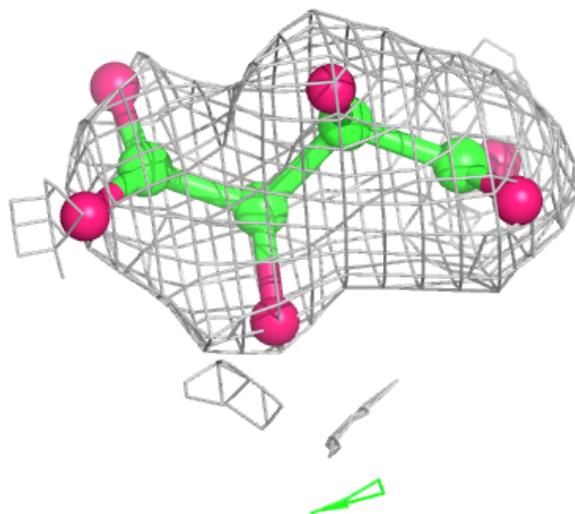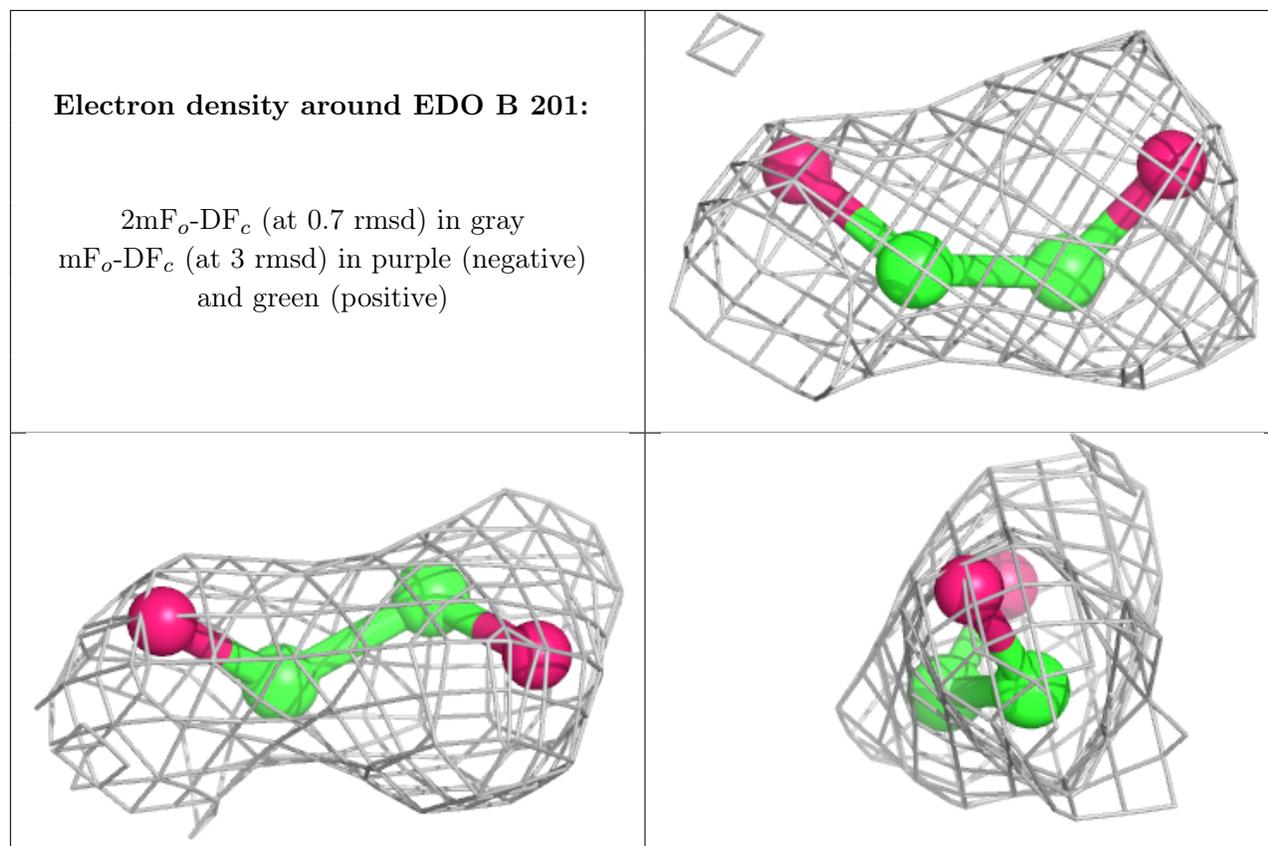
Electron density around ACT C 201:

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 EDO C 203:

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 EDO D 205:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
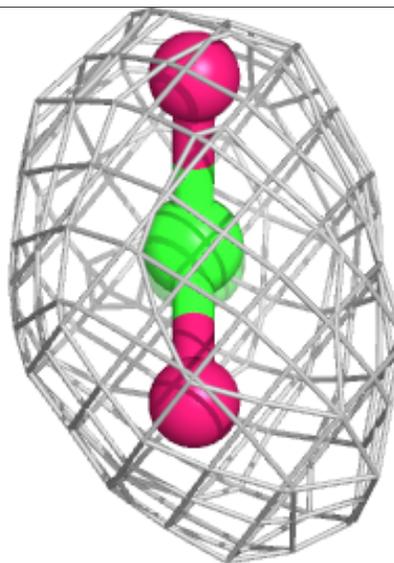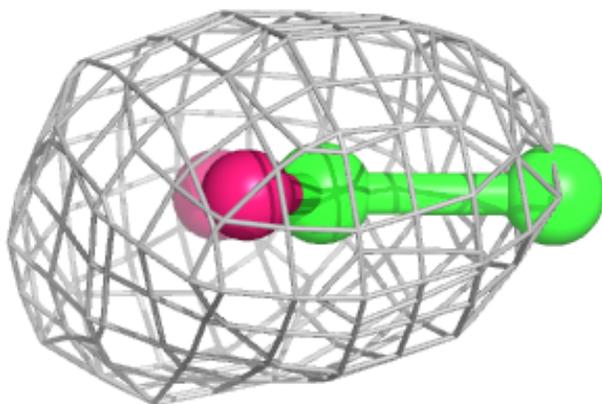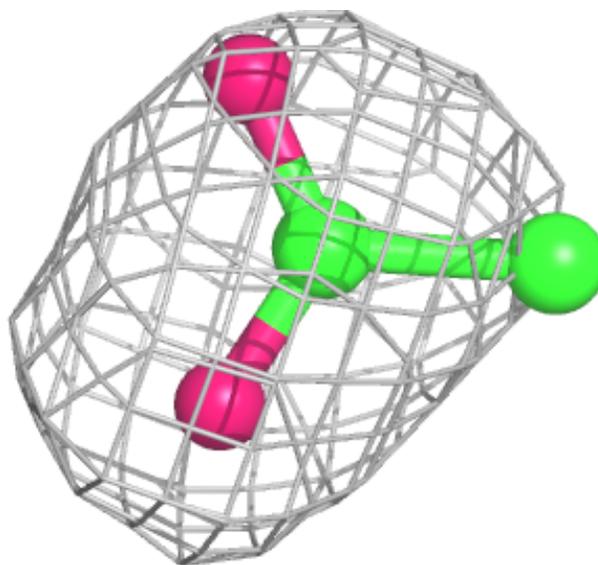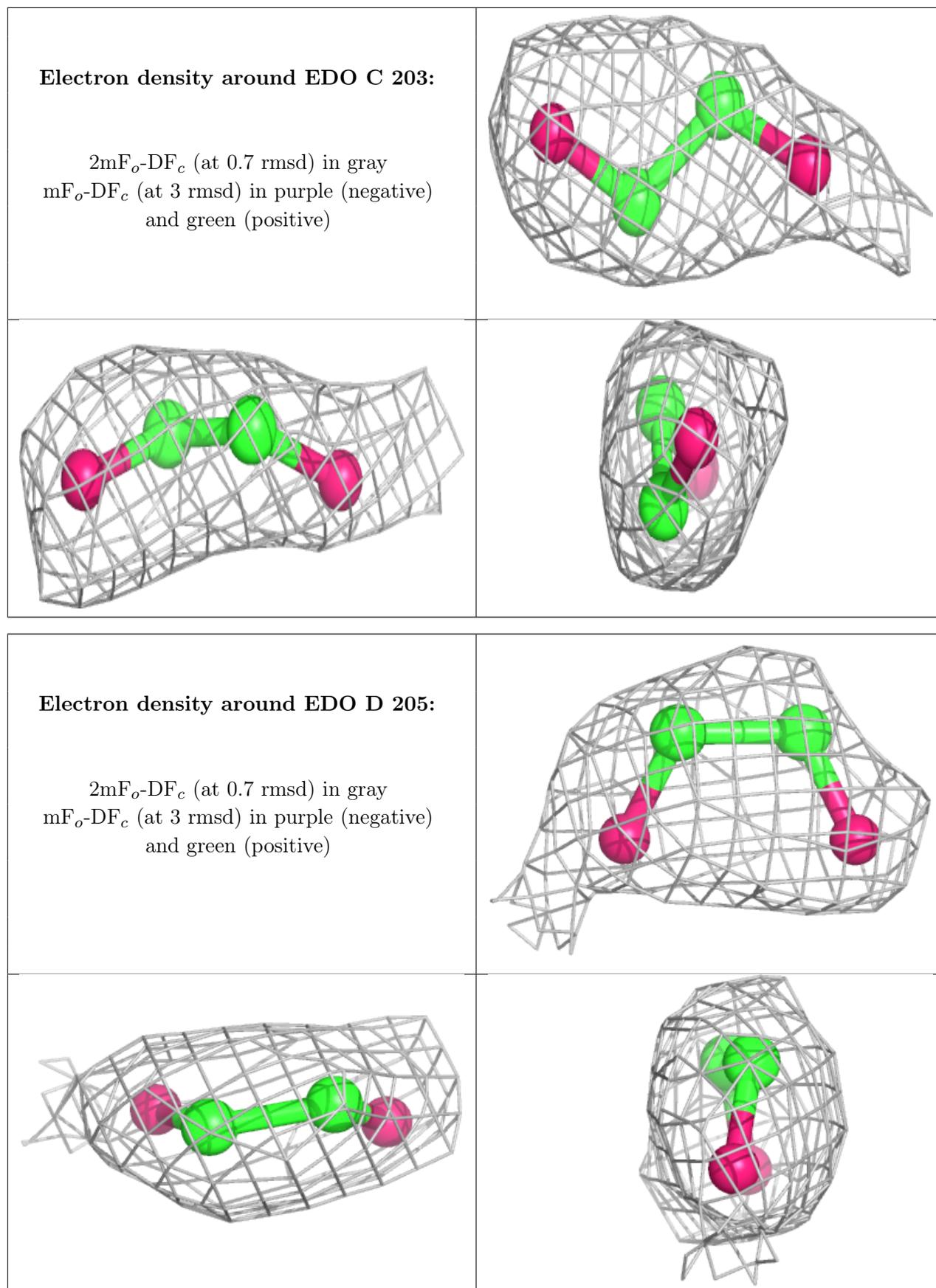
Electron density around GOL D 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
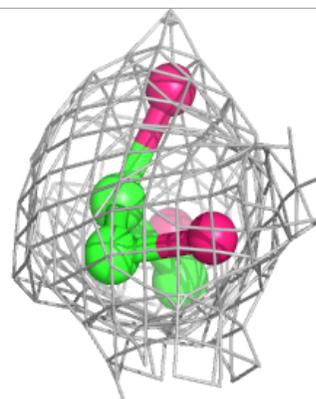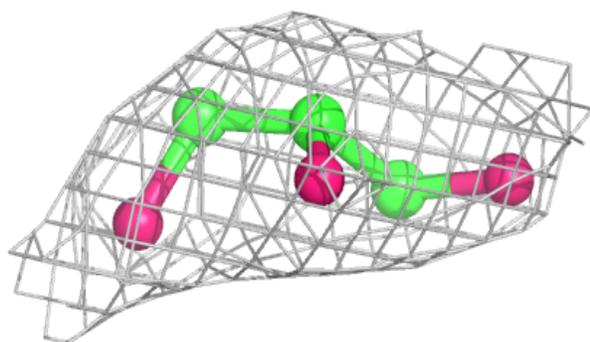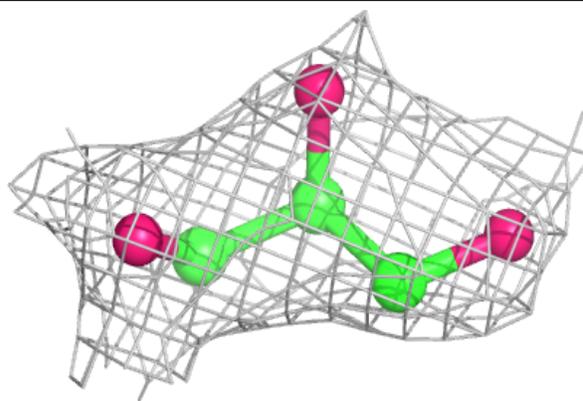
Electron density around TLA C 202:

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

Electron density around CL B 203:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.