



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:17 PM EDT

PDB ID : 9J1H / pdb_00009j1h
Title : The binary complex structure of F2Y224-FtmOx1 mutant with alpha-ketoglutarate
Authors : Wang, X.Y.; Wang, J.; Yan, W.P.
Deposited on : 2024-08-05
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

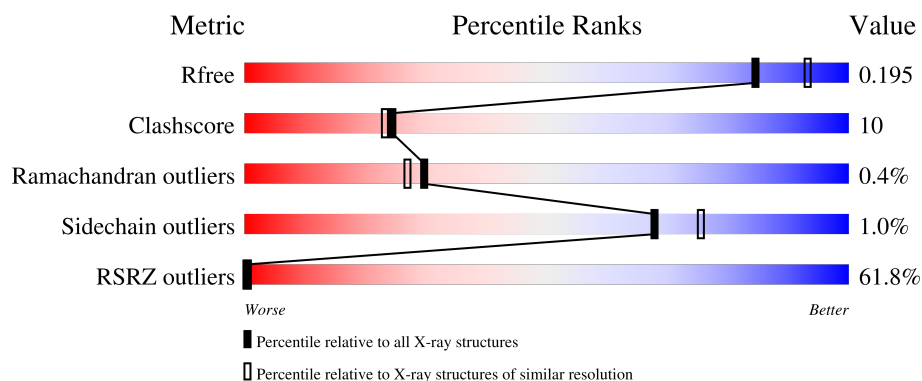
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	312	59% 70% 20% • 9%
1	B	312	53% 69% 21% • 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4919 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 Verruculogen synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	F	N	O	S	0	0	0
			2249	1427	2	394	413	13			
1	B	281	Total	C	F	N	O	S	0	0	0
			2217	1404	2	388	410	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	-	expression tag	UNP Q4WAW9
A	293	GLU	-	expression tag	UNP Q4WAW9
A	294	VAL	-	expression tag	UNP Q4WAW9
A	295	ASP	-	expression tag	UNP Q4WAW9
A	296	LEU	-	expression tag	UNP Q4WAW9
A	297	GLN	-	expression tag	UNP Q4WAW9
A	298	GLY	-	expression tag	UNP Q4WAW9
A	299	ASP	-	expression tag	UNP Q4WAW9
A	300	HIS	-	expression tag	UNP Q4WAW9
A	301	GLY	-	expression tag	UNP Q4WAW9
A	302	LEU	-	expression tag	UNP Q4WAW9
A	303	SER	-	expression tag	UNP Q4WAW9
A	304	ALA	-	expression tag	UNP Q4WAW9
A	305	TRP	-	expression tag	UNP Q4WAW9
A	306	SER	-	expression tag	UNP Q4WAW9
A	307	HIS	-	expression tag	UNP Q4WAW9
A	308	PRO	-	expression tag	UNP Q4WAW9
A	309	GLN	-	expression tag	UNP Q4WAW9
A	310	PHE	-	expression tag	UNP Q4WAW9
A	311	GLU	-	expression tag	UNP Q4WAW9
A	312	LYS	-	expression tag	UNP Q4WAW9
B	292	LEU	-	expression tag	UNP Q4WAW9
B	293	GLU	-	expression tag	UNP Q4WAW9
B	294	VAL	-	expression tag	UNP Q4WAW9
B	295	ASP	-	expression tag	UNP Q4WAW9

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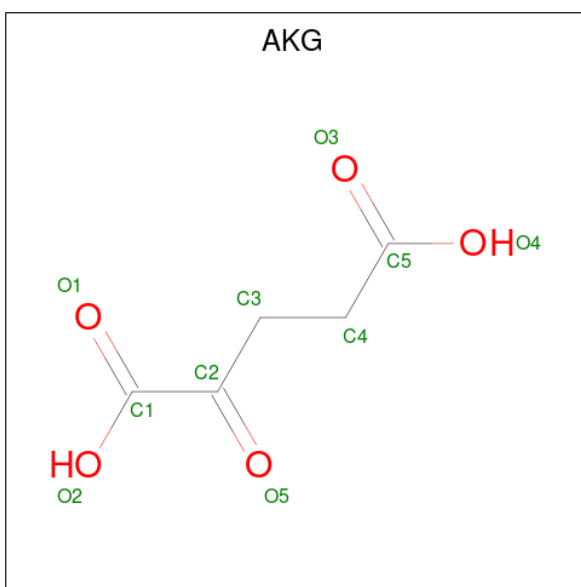
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Chain	Residue	Modelled	Actual	Comment	Reference
B	296	LEU	-	expression tag	UNP Q4WAW9
B	297	GLN	-	expression tag	UNP Q4WAW9
B	298	GLY	-	expression tag	UNP Q4WAW9
B	299	ASP	-	expression tag	UNP Q4WAW9
B	300	HIS	-	expression tag	UNP Q4WAW9
B	301	GLY	-	expression tag	UNP Q4WAW9
B	302	LEU	-	expression tag	UNP Q4WAW9
B	303	SER	-	expression tag	UNP Q4WAW9
B	304	ALA	-	expression tag	UNP Q4WAW9
B	305	TRP	-	expression tag	UNP Q4WAW9
B	306	SER	-	expression tag	UNP Q4WAW9
B	307	HIS	-	expression tag	UNP Q4WAW9
B	308	PRO	-	expression tag	UNP Q4WAW9
B	309	GLN	-	expression tag	UNP Q4WAW9
B	310	PHE	-	expression tag	UNP Q4WAW9
B	311	GLU	-	expression tag	UNP Q4WAW9
B	312	LYS	-	expression tag	UNP Q4WAW9

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	B	1	Total Co 1 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

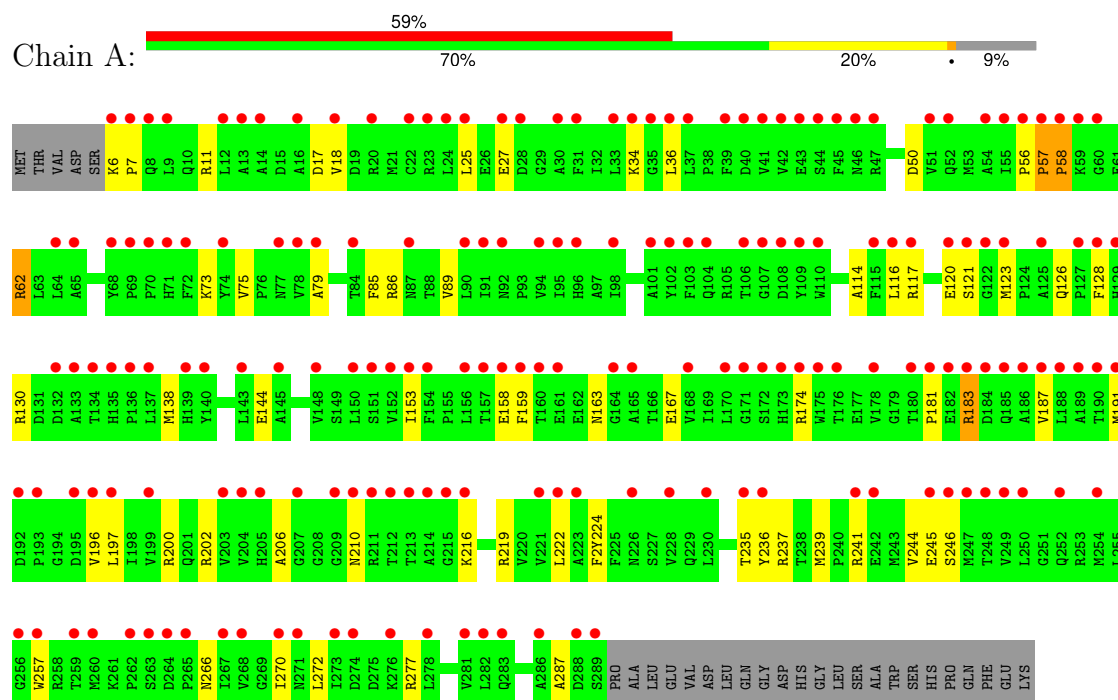
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	0
			229	229		
6	B	191	Total	O	0	0
			191	191		

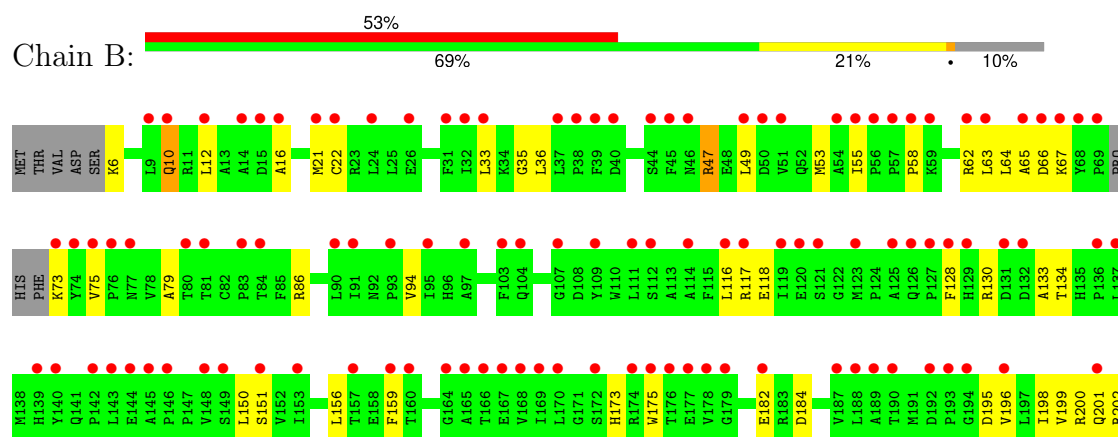
3 Residue-property plots [i](#)

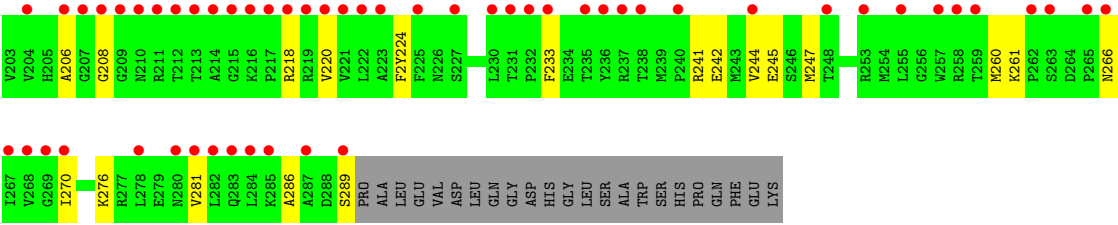
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Verruculogen synthase



• Molecule 1: Verruculogen synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.03Å 62.08Å 151.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 2.00 47.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.95-2.00) 98.9 (47.95-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.65 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.172 , 0.194 0.172 , 0.195	Depositor DCC
R_{free} test set	2003 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.447 for k,h,-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4919	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, GOL, AKG, SO4, F2Y

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	0.36	0/2288	0.58	0/3114
1	B	0.33	0/2252	0.53	0/3064
All	All	0.34	0/4540	0.56	0/6178

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ARG	Sidechain
1	A	62	ARG	Sidechain
1	B	47	ARG	Sidechain

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	2249	0	2236	49	0
1	B	2217	0	2201	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	4	3	0
3	B	10	0	4	1	0
4	A	6	0	8	1	0
5	B	5	0	0	0	0
6	A	229	0	0	4	0
6	B	191	0	0	4	0
All	All	4919	0	4453	89	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 10.

All (89) 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:B:276:LYS:HE2	1:B:281:VAL:HG22	1.73	0.69
1:A:222:LEU:HD21	3:A:402:AKG:H42	1.79	0.64
1:B:62:ARG:HB3	1:B:65:ALA:HB3	1.79	0.62
1:A:58:PRO:HB3	1:A:62:ARG:HD2	1.80	0.62
1:B:35:GLY:N	1:B:195:ASP:OD1	2.30	0.59
1:B:75:VAL:HB	1:B:116:LEU:HB3	1.83	0.59
1:A:120:GLU:O	1:A:123:MET:HG2	2.03	0.58
1:B:73:LYS:HB3	1:B:118:GLU:HB3	1.86	0.57
1:A:36:LEU:HD23	1:A:196:VAL:HG21	1.86	0.57
1:A:7:PRO:O	1:A:187:VAL:HG11	2.05	0.56
1:A:58:PRO:HG3	1:A:62:ARG:HD2	1.87	0.56
1:A:159:PHE:N	1:A:191:MET:O	2.33	0.55
1:B:286:ALA:N	1:B:289:SER:OG	2.35	0.55
1:A:277:ARG:HD3	6:A:618:HOH:O	2.08	0.54
1:B:128:PHE:HA	1:B:206:ALA:HB2	1.90	0.54
1:B:151:SER:HB2	1:B:199:VAL:HB	1.89	0.54
1:B:200:ARG:NH1	1:B:201:GLN:O	2.36	0.54
1:A:138:MET:O	1:A:202:ARG:NH2	2.40	0.54
1:B:10:GLN:HG2	6:B:686:HOH:O	2.08	0.53
1:A:167:GLU:OE1	1:A:183:ARG:NH1	2.41	0.52
1:A:50:ASP:OD1	1:A:219:ARG:NH2	2.30	0.52
1:A:27:GLU:HA	1:A:174:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HE	1:B:65:ALA:HB3	1.74	0.52
1:A:121:SER:HA	1:A:210:ASN:HB3	1.91	0.52
1:B:159:PHE:HZ	1:B:220:VAL:HB	1.75	0.51
1:A:11:ARG:HG2	1:A:34:LYS:HD3	1.93	0.51
1:A:246:SER:O	1:A:287:ALA:HB2	2.11	0.50
1:B:16:ALA:HB3	1:B:21:MET:HE2	1.93	0.50
1:B:150:LEU:HD11	1:B:198:ILE:HG22	1.94	0.50
1:B:201:GLN:HG2	1:B:202:ARG:HG3	1.94	0.50
1:A:266:ASN:HB2	1:B:133:ALA:O	2.12	0.49
1:A:128:PHE:CD2	1:A:181:PRO:HG2	2.48	0.49
1:B:130:ARG:NH2	1:B:175:TRP:O	2.34	0.49
1:A:235:THR:OG1	1:A:237:ARG:HD2	2.13	0.49
1:B:33:LEU:HD13	1:B:36:LEU:HD13	1.95	0.48
1:A:159:PHE:HB2	1:A:191:MET:H	1.77	0.48
1:A:239:MET:HE2	1:A:244:VAL:HG22	1.95	0.48
1:A:57:PRO:HB2	1:A:58:PRO:HD3	1.95	0.47
1:A:270:ILE:HG13	1:B:233:PHE:HA	1.96	0.47
1:A:123:MET:SD	4:A:403:GOL:O2	2.70	0.47
1:A:56:PRO:HA	1:A:57:PRO:HD3	1.70	0.47
1:A:126:GLN:HB3	1:A:206:ALA:HB1	1.96	0.47
1:B:36:LEU:HD11	1:B:94:VAL:HB	1.96	0.47
1:B:62:ARG:O	1:B:66:ASP:N	2.45	0.47
1:A:73:LYS:NZ	6:A:529:HOH:O	2.48	0.46
1:B:208:GLY:HA3	6:B:613:HOH:O	2.15	0.46
1:B:261:LYS:NZ	1:B:266:ASN:O	2.45	0.46
1:A:58:PRO:CB	1:A:62:ARG:HD2	2.44	0.46
1:A:75:VAL:HB	1:A:116:LEU:HB3	1.97	0.46
1:A:114:ALA:HA	1:A:222:LEU:O	2.16	0.46
1:B:6:LYS:N	6:B:629:HOH:O	2.48	0.46
1:B:49:LEU:O	1:B:53:MET:HG3	2.16	0.46
1:A:117:ARG:HE	3:A:402:AKG:H41	1.81	0.45
1:B:200:ARG:HG2	1:B:201:GLN:N	2.32	0.45
1:B:260:MET:O	1:B:270:ILE:N	2.50	0.45
1:A:241:ARG:NH1	1:A:245:GLU:OE2	2.42	0.45
1:A:272:LEU:HD11	1:B:233:PHE:CE2	2.51	0.45
1:A:244:VAL:HG21	1:A:257:TRP:CZ2	2.52	0.45
1:A:62:ARG:NH2	6:A:525:HOH:O	2.48	0.45
1:B:218:ARG:HH12	3:B:503:AKG:C5	2.30	0.44
1:B:79:ALA:O	1:B:86:ARG:NH1	2.36	0.44
1:B:117:ARG:HG2	6:B:713:HOH:O	2.17	0.43
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:NH1	1:B:245:GLU:OE2	2.51	0.43
1:B:58:PRO:HG3	1:B:62:ARG:HH11	1.83	0.43
1:A:57:PRO:CB	1:A:58:PRO:HD3	2.49	0.43
1:A:85:PHE:HA	1:A:89:VAL:HB	2.01	0.43
1:B:12:LEU:HD23	1:B:16:ALA:HB1	2.01	0.42
1:B:64:LEU:HD12	1:B:67:LYS:HE3	2.00	0.42
1:A:6:LYS:HA	1:A:7:PRO:HD3	1.88	0.42
1:A:25:LEU:O	1:A:200:ARG:HD2	2.19	0.42
1:B:242:GLU:CD	1:B:242:GLU:H	2.27	0.42
1:B:73:LYS:HB2	1:B:118:GLU:O	2.20	0.42
1:A:58:PRO:CG	1:A:62:ARG:HD2	2.49	0.42
1:A:130:ARG:CZ	1:A:202:ARG:HG2	2.49	0.42
1:A:266:ASN:ND2	1:B:134:THR:HA	2.35	0.42
1:A:17:ASP:OD1	1:A:18:VAL:N	2.52	0.41
1:A:120:GLU:HB2	6:A:665:HOH:O	2.20	0.41
1:B:173:HIS:HA	1:B:202:ARG:O	2.20	0.41
1:A:79:ALA:O	1:A:86:ARG:HD3	2.20	0.41
1:B:182:GLU:HG3	1:B:184:ASP:OD2	2.20	0.41
1:B:244:VAL:HA	1:B:247:MET:HE3	2.02	0.41
1:A:153:ILE:HB	1:A:197:LEU:HB3	2.03	0.41
1:B:36:LEU:HD22	1:B:196:VAL:HG21	2.02	0.41
1:B:47:ARG:HA	1:B:47:ARG:HD3	1.83	0.40
1:A:216:LYS:HA	1:A:216:LYS:HD3	1.77	0.40
1:A:236:TYR:HB3	1:A:239:MET:SD	2.62	0.40
1:A:117:ARG:NE	3:A:402:AKG:H41	2.35	0.40
1:A:158:GLU:O	1:A:163:ASN:ND2	2.55	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	281/312 (90%)	270 (96%)	9 (3%)	2 (1%)	18	14
1	B	276/312 (88%)	263 (95%)	13 (5%)	0	100	100
All	All	557/624 (89%)	533 (96%)	22 (4%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PRO
1	A	57	PRO

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	245/269 (91%)	244 (100%)	1 (0%)	84	89
1	B	241/269 (90%)	237 (98%)	4 (2%)	53	60
All	All	486/538 (90%)	481 (99%)	5 (1%)	68	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	GLU
1	B	10	GLN
1	B	22	CYS
1	B	55	ILE
1	B	156	LEU

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

Mol	Chain	Res	Type
1	B	8	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	F2Y	A	224	1	13,14,15	1.17	1 (7%)	14,19,21	1.91	2 (14%)
1	F2Y	B	224	1	13,14,15	1.12	0	14,19,21	2.26	5 (35%)

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	F2Y	A	224	1	-	2/5/6/8	0/1/1/1
1	F2Y	B	224	1	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	F2Y	CD2-CE2	2.42	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	F2Y	CD2-CE2-CZ	-4.78	120.05	123.79
1	B	224	F2Y	CD2-CE2-CZ	-4.77	120.06	123.79
1	B	224	F2Y	F2-CE2-CZ	4.32	120.25	117.13
1	B	224	F2Y	CD1-CE1-CZ	-3.77	120.84	123.79
1	A	224	F2Y	CD1-CE1-CZ	-3.33	121.18	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	F2Y	CG-CD2-CE2	2.49	121.00	119.37
1	B	224	F2Y	F1-CE1-CD1	2.08	122.79	118.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	224	F2Y	CA-CB-CG-CD2
1	A	224	F2Y	CA-CB-CG-CD1
1	B	224	F2Y	CA-CB-CG-CD1
1	B	224	F2Y	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	AKG	A	402	2	9,9,9	0.30	0	11,11,11	0.48	0
4	GOL	A	403	-	5,5,5	1.08	0	5,5,5	1.20	0
3	AKG	B	503	2	9,9,9	0.29	0	11,11,11	0.41	0
5	SO4	B	501	-	4,4,4	0.43	0	6,6,6	0.07	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	AKG	A	402	2	-	4/9/9/9	-
4	GOL	A	403	-	-	2/4/4/4	-
3	AKG	B	503	2	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

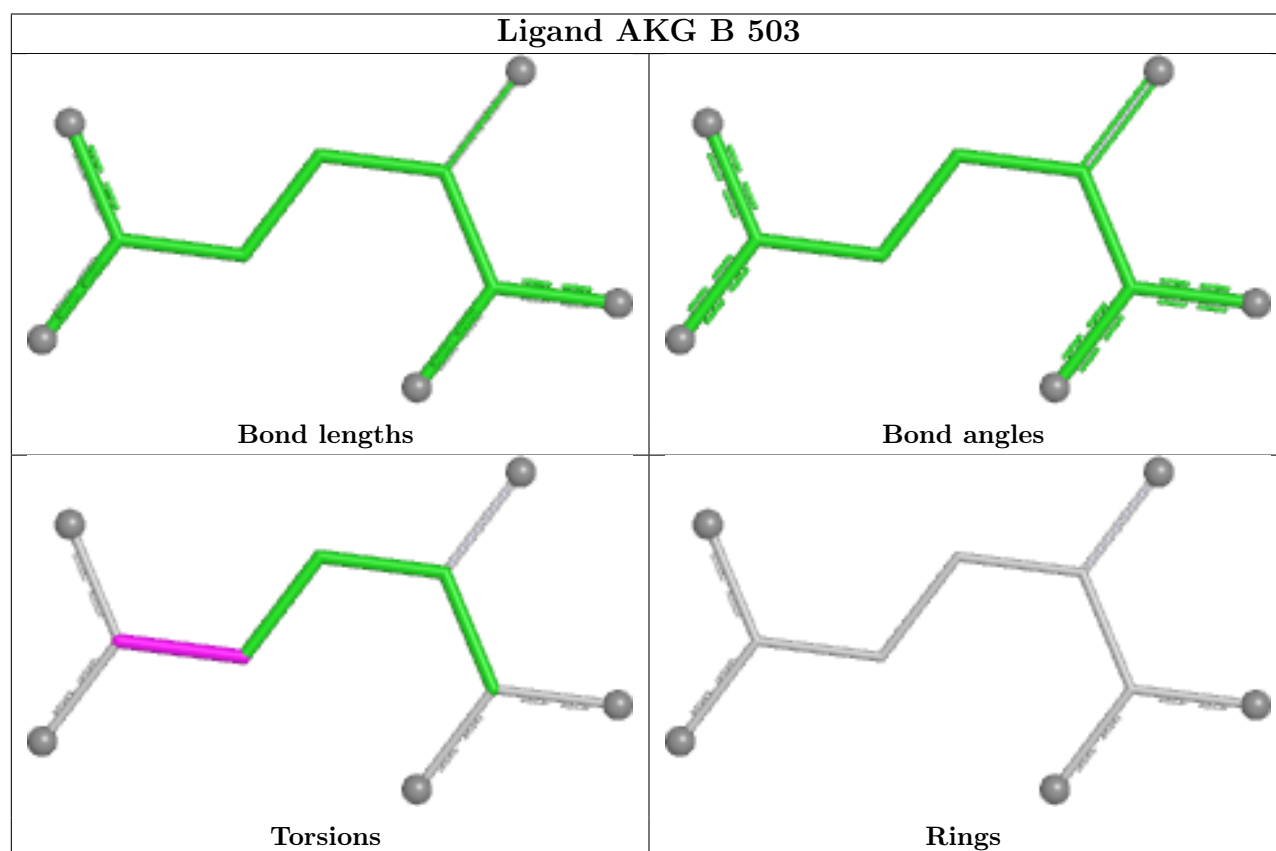
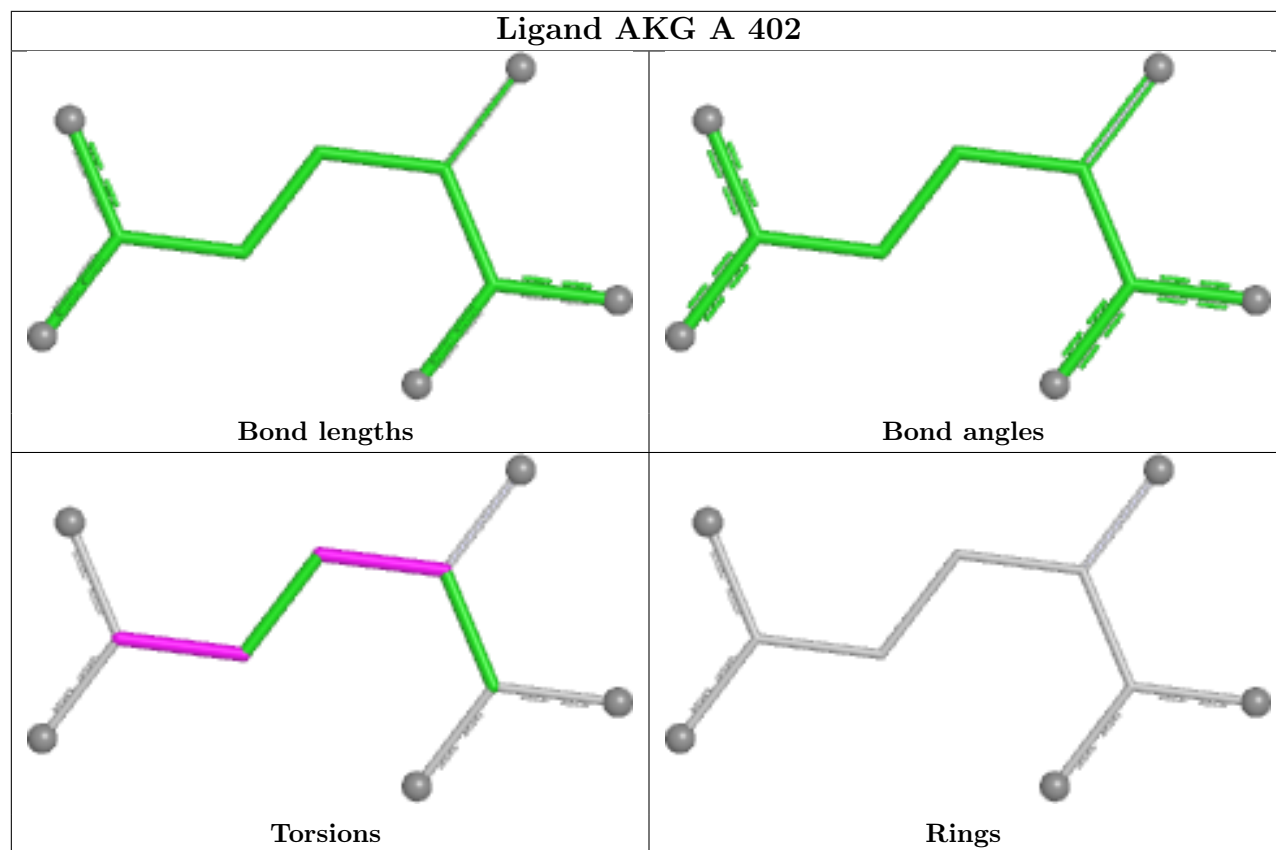
Mol	Chain	Res	Type	Atoms
3	A	402	AKG	C1-C2-C3-C4
4	A	403	GOL	O1-C1-C2-O2
4	A	403	GOL	O1-C1-C2-C3
3	A	402	AKG	O5-C2-C3-C4
3	A	402	AKG	C3-C4-C5-O4
3	A	402	AKG	C3-C4-C5-O3
3	B	503	AKG	C3-C4-C5-O3
3	B	503	AKG	C3-C4-C5-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	AKG	3	0
4	A	403	GOL	1	0
3	B	503	AKG	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 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, 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	283/312 (90%)	2.53	184 (65%) 0 0	18, 30, 44, 90	0
1	B	280/312 (89%)	2.34	164 (58%) 0 0	19, 29, 59, 84	0
All	All	563/624 (90%)	2.43	348 (61%) 0 0	18, 29, 50, 90	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ALA	6.6
1	A	128	PHE	6.4
1	A	18	VAL	6.2
1	B	140	TYR	5.7
1	A	133	ALA	5.6
1	B	169	ILE	5.0
1	A	42	VAL	5.0
1	B	69	PRO	5.0
1	A	160	THR	5.0
1	B	215	GLY	4.9
1	A	109	TYR	4.9
1	A	235	THR	4.8
1	A	140	TYR	4.8
1	A	51	VAL	4.8
1	A	64	LEU	4.7
1	B	217	PRO	4.7
1	B	68	TYR	4.7
1	A	13	ALA	4.7
1	A	209	GLY	4.6
1	B	159	PHE	4.6
1	A	35	GLY	4.6
1	A	74	TYR	4.5
1	B	194	GLY	4.5
1	B	49	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	39	PHE	4.4
1	A	236	TYR	4.3
1	A	134	THR	4.3
1	B	165	ALA	4.3
1	B	188	LEU	4.3
1	B	166	THR	4.3
1	A	52	GLN	4.3
1	A	223	ALA	4.3
1	A	212	THR	4.3
1	A	72	PHE	4.2
1	B	282	LEU	4.2
1	A	203	VAL	4.2
1	A	14	ALA	4.2
1	A	7	PRO	4.1
1	A	58	PRO	4.1
1	A	92	ASN	4.1
1	A	186	ALA	4.1
1	B	97	ALA	4.1
1	B	209	GLY	4.1
1	B	65	ALA	4.0
1	B	269	GLY	4.0
1	A	101	ALA	4.0
1	A	71	HIS	4.0
1	A	139	HIS	4.0
1	B	137	LEU	4.0
1	A	207	GLY	4.0
1	A	256	GLY	4.0
1	B	50	ASP	4.0
1	A	281	VAL	4.0
1	B	265	PRO	4.0
1	B	119	ILE	4.0
1	A	27	GLU	4.0
1	B	107	GLY	4.0
1	B	149	SER	3.9
1	A	69	PRO	3.9
1	B	218	ARG	3.9
1	A	110	TRP	3.9
1	B	125	ALA	3.9
1	A	184	ASP	3.9
1	B	192	ASP	3.9
1	A	156	LEU	3.9
1	A	94	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	3.8
1	B	216	LYS	3.8
1	A	159	PHE	3.8
1	A	25	LEU	3.7
1	B	120	GLU	3.7
1	B	144	GLU	3.7
1	A	121	SER	3.7
1	A	210	ASN	3.7
1	B	31	PHE	3.7
1	A	273	ILE	3.7
1	B	211	ARG	3.7
1	A	172	SER	3.6
1	A	173	HIS	3.6
1	A	158	GLU	3.6
1	B	123	MET	3.6
1	A	165	ALA	3.6
1	B	14	ALA	3.6
1	B	287	ALA	3.6
1	B	240	PRO	3.6
1	B	213	THR	3.6
1	B	146	PRO	3.6
1	A	9	LEU	3.6
1	B	22	CYS	3.6
1	B	139	HIS	3.5
1	B	63	LEU	3.5
1	A	115	PHE	3.5
1	B	57	PRO	3.5
1	A	143	LEU	3.5
1	A	23	ARG	3.5
1	A	216	LYS	3.5
1	B	104	GLN	3.5
1	B	221	VAL	3.5
1	A	22	CYS	3.4
1	A	199	VAL	3.4
1	A	98	ILE	3.4
1	B	112	SER	3.4
1	B	175	TRP	3.4
1	A	45	PHE	3.4
1	A	250	LEU	3.4
1	B	148	VAL	3.4
1	B	212	THR	3.4
1	A	120	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	262	PRO	3.4
1	A	16	ALA	3.4
1	A	65	ALA	3.4
1	A	137	LEU	3.4
1	A	28	ASP	3.3
1	A	122	GLY	3.3
1	A	145	ALA	3.3
1	A	178	VAL	3.3
1	B	145	ALA	3.3
1	A	103	PHE	3.3
1	B	45	PHE	3.3
1	B	182	GLU	3.3
1	B	257	TRP	3.3
1	B	81	THR	3.3
1	A	265	PRO	3.3
1	A	245	GLU	3.3
1	B	233	PHE	3.3
1	A	213	THR	3.2
1	B	56	PRO	3.2
1	A	286	ALA	3.2
1	B	90	LEU	3.2
1	B	128	PHE	3.2
1	A	205	HIS	3.2
1	A	175	TRP	3.2
1	A	211	ARG	3.2
1	B	253	ARG	3.2
1	A	91	ILE	3.2
1	B	12	LEU	3.2
1	B	24	LEU	3.2
1	A	40	ASP	3.2
1	A	135	HIS	3.2
1	A	271	ASN	3.2
1	A	222	LEU	3.2
1	A	31	PHE	3.2
1	B	55	ILE	3.1
1	A	180	THR	3.1
1	B	73	LYS	3.1
1	B	190	THR	3.1
1	A	136	PRO	3.1
1	A	196	VAL	3.1
1	B	132	ASP	3.1
1	B	167	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	121	SER	3.1
1	B	160	THR	3.1
1	B	176	THR	3.1
1	B	16	ALA	3.1
1	A	150	LEU	3.1
1	A	123	MET	3.1
1	A	181	PRO	3.1
1	A	24	LEU	3.1
1	A	164	GLY	3.0
1	A	171	GLY	3.0
1	B	266	ASN	3.0
1	A	170	LEU	3.0
1	A	60	GLY	3.0
1	A	106	THR	3.0
1	A	59	LYS	3.0
1	A	20	ARG	3.0
1	A	230	LEU	3.0
1	A	246	SER	2.9
1	B	75	VAL	2.9
1	A	270	ILE	2.9
1	A	116	LEU	2.9
1	B	15	ASP	2.9
1	B	95	ILE	2.9
1	A	8	GLN	2.9
1	A	57	PRO	2.9
1	A	102	TYR	2.9
1	B	263	SER	2.9
1	B	21	MET	2.8
1	B	93	PRO	2.8
1	A	125	ALA	2.8
1	B	207	GLY	2.8
1	B	51	VAL	2.8
1	B	178	VAL	2.8
1	A	70	PRO	2.8
1	B	83	PRO	2.8
1	B	214	ALA	2.8
1	B	33	LEU	2.8
1	B	77	ASN	2.8
1	A	47	ARG	2.8
1	A	191	MET	2.8
1	B	225	PHE	2.8
1	B	74	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	58	PRO	2.8
1	A	221	VAL	2.8
1	B	268	VAL	2.8
1	A	267	ILE	2.8
1	A	46	ASN	2.7
1	A	262	PRO	2.7
1	B	174	ARG	2.7
1	A	152	VAL	2.7
1	B	208	GLY	2.7
1	A	54	ALA	2.7
1	A	176	THR	2.7
1	B	38	PRO	2.7
1	A	187	VAL	2.7
1	B	196	VAL	2.7
1	A	132	ASP	2.7
1	A	195	ASP	2.7
1	A	204	VAL	2.7
1	A	249	VAL	2.7
1	B	142	PRO	2.6
1	A	153	ILE	2.6
1	B	32	ILE	2.6
1	B	117	ARG	2.6
1	B	164	GLY	2.6
1	B	177	GLU	2.6
1	B	189	ALA	2.6
1	B	170	LEU	2.6
1	B	230	LEU	2.6
1	A	6	LYS	2.6
1	A	41	VAL	2.6
1	A	55	ILE	2.6
1	A	185	GLN	2.6
1	A	257	TRP	2.6
1	A	37	LEU	2.6
1	A	192	ASP	2.6
1	B	237	ARG	2.6
1	B	91	ILE	2.6
1	B	267	ILE	2.6
1	A	161	GLU	2.6
1	A	107	GLY	2.6
1	A	30	ALA	2.6
1	B	248	THR	2.6
1	B	44	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLN	2.5
1	A	78	VAL	2.5
1	A	268	VAL	2.5
1	B	204	VAL	2.5
1	A	214	ALA	2.5
1	B	111	LEU	2.5
1	A	190	THR	2.5
1	B	103	PHE	2.5
1	A	129	HIS	2.5
1	B	244	VAL	2.5
1	B	270	ILE	2.5
1	B	223	ALA	2.5
1	A	278	LEU	2.5
1	A	87	ASN	2.5
1	B	46	ASN	2.5
1	B	283	GLN	2.4
1	A	84	THR	2.4
1	B	172	SER	2.4
1	B	127	PRO	2.4
1	B	193	PRO	2.4
1	B	222	LEU	2.4
1	B	255	LEU	2.4
1	B	187	VAL	2.4
1	B	281	VAL	2.4
1	A	157	THR	2.4
1	A	259	THR	2.4
1	B	126	GLN	2.4
1	B	66	ASP	2.4
1	B	227	SER	2.4
1	B	236	TYR	2.4
1	A	96	HIS	2.4
1	A	189	ALA	2.4
1	A	117	ARG	2.4
1	B	114	ALA	2.3
1	B	143	LEU	2.3
1	A	154	PHE	2.3
1	B	59	LYS	2.3
1	B	258	ARG	2.3
1	A	168	VAL	2.3
1	A	263	SER	2.3
1	A	289	SER	2.3
1	B	168	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	289	SER	2.3
1	B	26	GLU	2.3
1	A	248	THR	2.3
1	B	157	THR	2.3
1	B	232	PRO	2.3
1	A	90	LEU	2.3
1	A	276	LYS	2.3
1	A	44	SER	2.3
1	B	10	GLN	2.3
1	B	62	ARG	2.3
1	A	274	ASP	2.3
1	B	179	GLY	2.3
1	B	284	LEU	2.3
1	A	43	GLU	2.2
1	A	228	VAL	2.2
1	A	226	ASN	2.2
1	B	210	ASN	2.2
1	A	34	LYS	2.2
1	A	33	LEU	2.2
1	B	278	LEU	2.2
1	A	242	GLU	2.2
1	A	77	ASN	2.2
1	B	259	THR	2.2
1	A	252	GLN	2.2
1	A	68	TYR	2.2
1	A	241	ARG	2.2
1	A	193	PRO	2.2
1	A	288	ASP	2.2
1	B	131	ASP	2.2
1	A	148	VAL	2.2
1	B	129	HIS	2.2
1	B	37	LEU	2.2
1	A	247	MET	2.2
1	A	127	PRO	2.1
1	B	40	ASP	2.2
1	B	220	VAL	2.1
1	A	183	ARG	2.1
1	B	219	ARG	2.1
1	A	260	MET	2.1
1	A	56	PRO	2.1
1	B	76	PRO	2.1
1	B	238	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLN	2.1
1	A	12	LEU	2.1
1	A	197	LEU	2.1
1	A	282	LEU	2.1
1	A	182	GLU	2.1
1	B	280	ASN	2.1
1	B	201	GLN	2.1
1	A	95	ILE	2.1
1	B	153	ILE	2.1
1	B	39	PHE	2.1
1	B	206	ALA	2.1
1	B	9	LEU	2.1
1	B	151	SER	2.1
1	A	254	MET	2.1
1	A	108	ASP	2.1
1	B	109	TYR	2.1
1	B	235	THR	2.1
1	A	79	ALA	2.1
1	A	151	SER	2.1
1	A	188	LEU	2.0
1	B	116	LEU	2.0
1	A	264	ASP	2.0
1	A	174	ARG	2.0
1	B	80	THR	2.0
1	B	231	THR	2.0
1	B	67	LYS	2.0
1	B	285	LYS	2.0
1	B	84	THR	2.0
1	B	136	PRO	2.0
1	A	215	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	F2Y	A	224	14/15	0.90	0.16	19,23,26,28	0
1	F2Y	B	224	14/15	0.90	0.16	20,24,26,29	0

6.3 Carbohydrates [i](#)

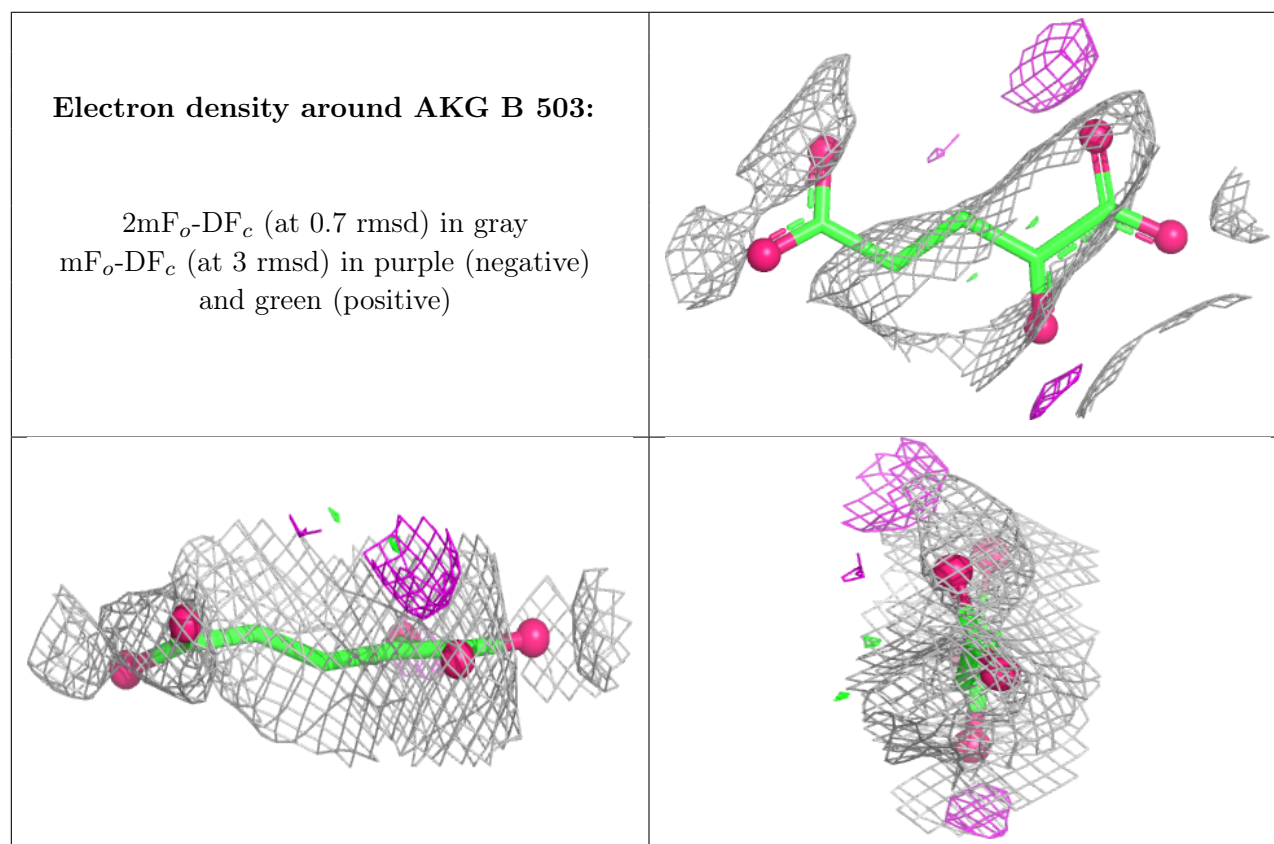
There are no oligosaccharides in this entry.

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, 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.

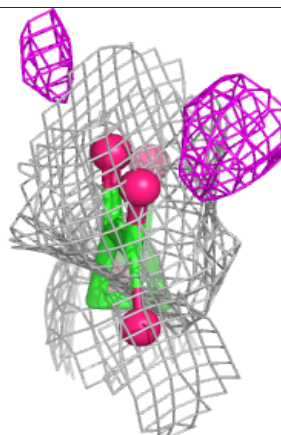
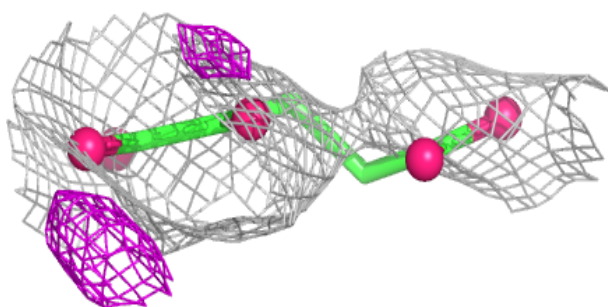
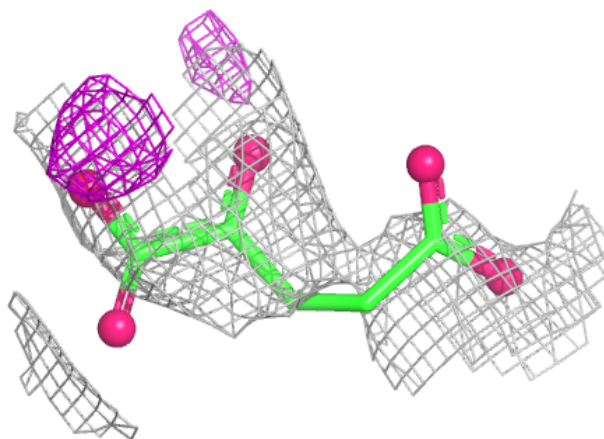
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AKG	B	503	10/10	0.92	0.15	26,29,29,29	0
5	SO4	B	501	5/5	0.93	0.15	26,26,31,36	0
3	AKG	A	402	10/10	0.96	0.18	31,32,32,33	0
4	GOL	A	403	6/6	0.98	0.12	32,35,37,39	0
2	CO	A	401	1/1	0.98	0.05	29,29,29,29	0
2	CO	B	502	1/1	0.99	0.04	27,27,27,27	0

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.



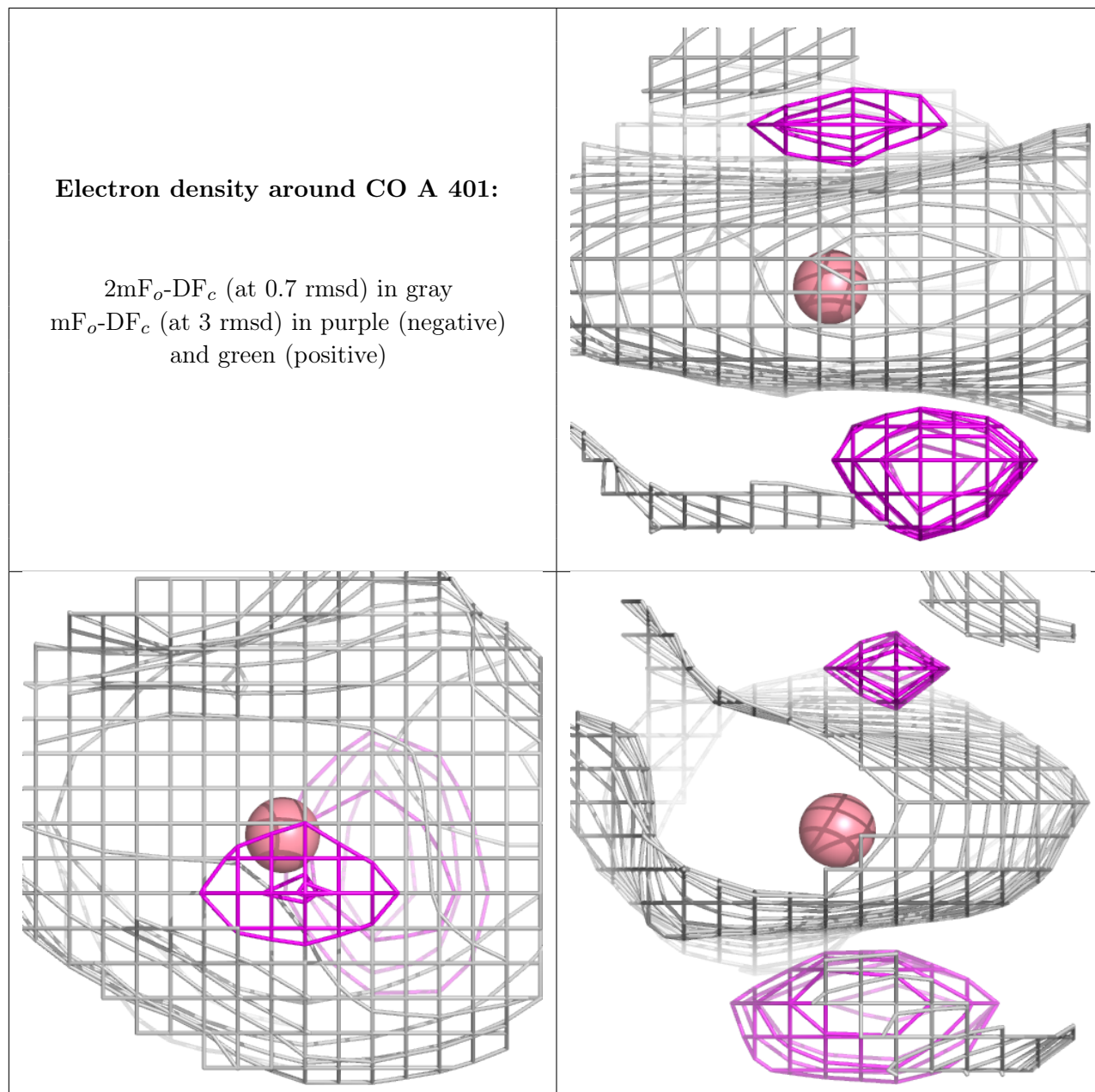
Electron density around AKG A 402:

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



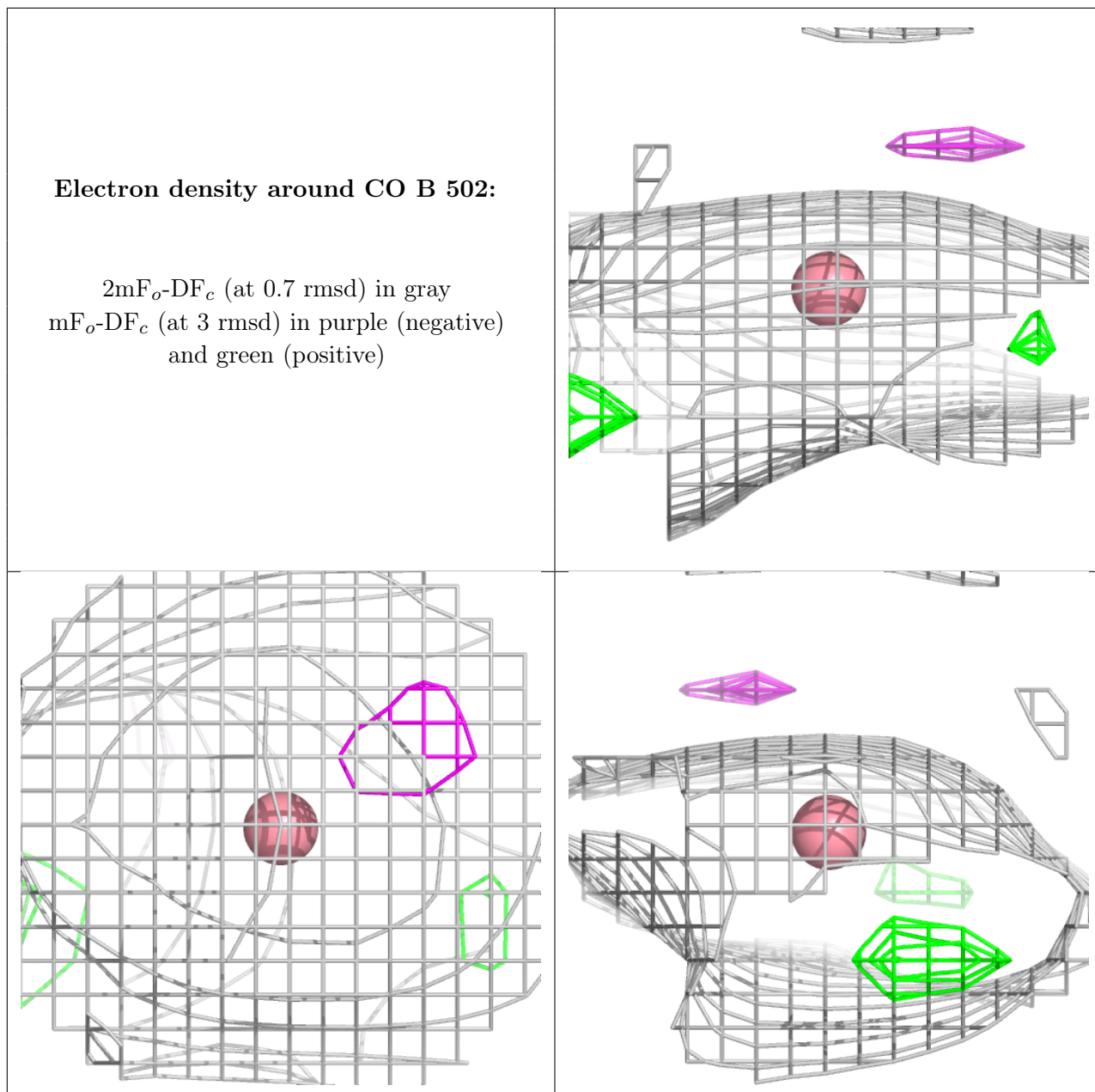
Electron density around CO A 401:

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



Electron density around CO B 502:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.