



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 10:21 PM JST

PDB ID : 9J1H
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

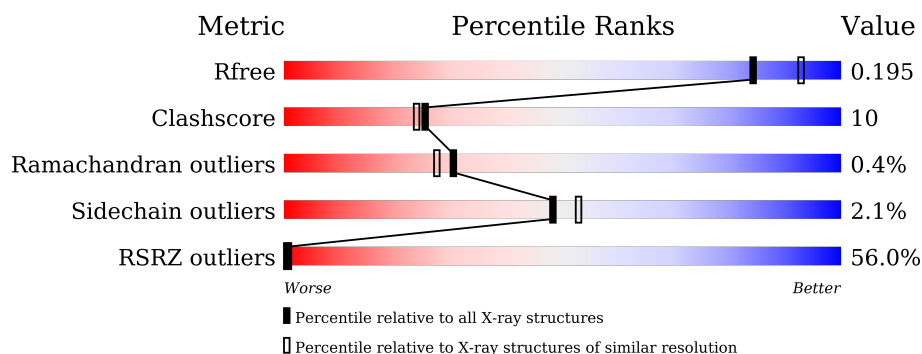
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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	<div> <div>54%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>9%</div> </div> </div>
1	B	312	<div> <div>47%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>10%</div> </div> </div>

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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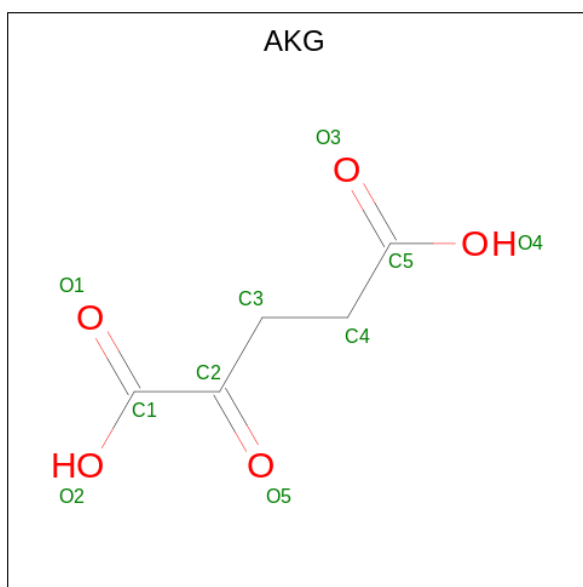
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Chain	Residue	Modelled	Actual	Comment	Reference
B	296	LEU	-	expression tag	UNP Q4WAW9
B	297	GLN	-	expression tag	UNP Q4WAW9
B	298	GLY	-	expression tag	UNP Q4WAW9
B	299	ASP	-	expression tag	UNP Q4WAW9
B	300	HIS	-	expression tag	UNP Q4WAW9
B	301	GLY	-	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 (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

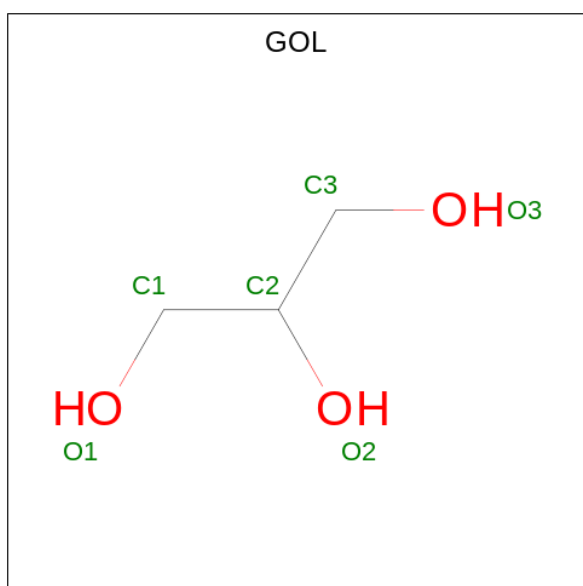
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	B	1	Total Co 1 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: 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 (three-letter code: 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 (three-letter code: SO4) (formula: O_4S).



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

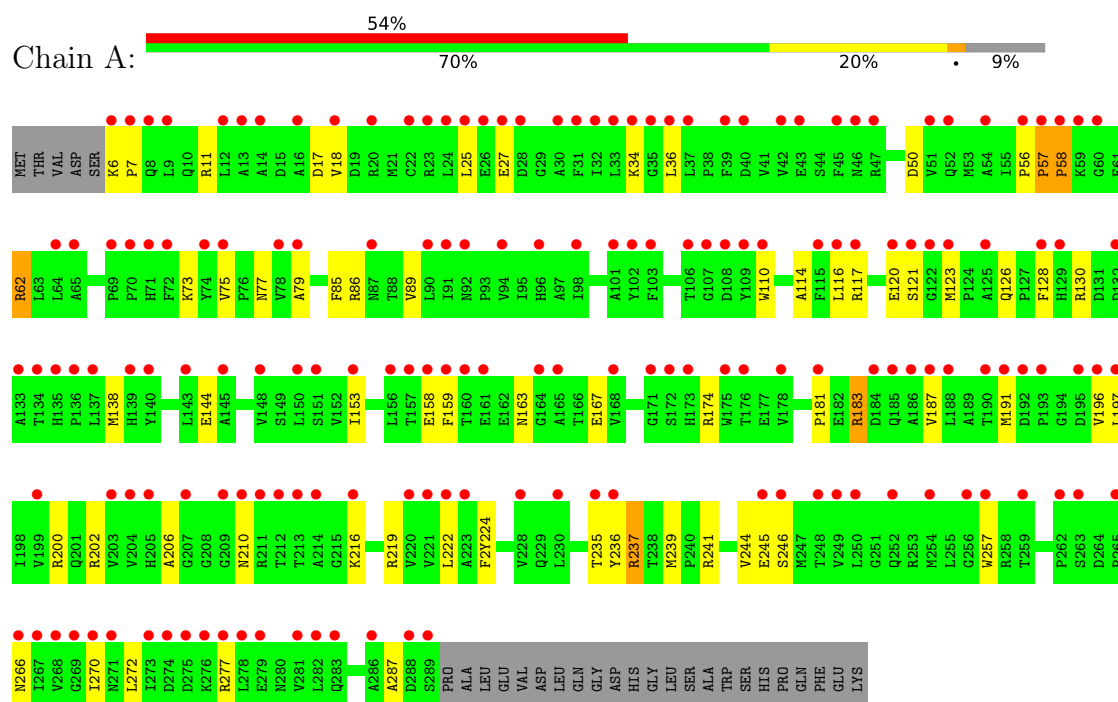
- Molecule 6 is water.

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

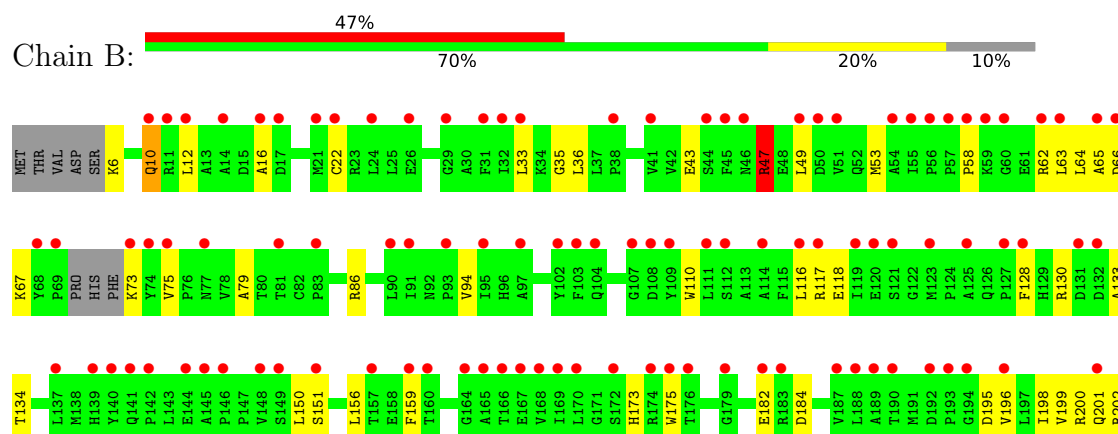
3 Residue-property plots

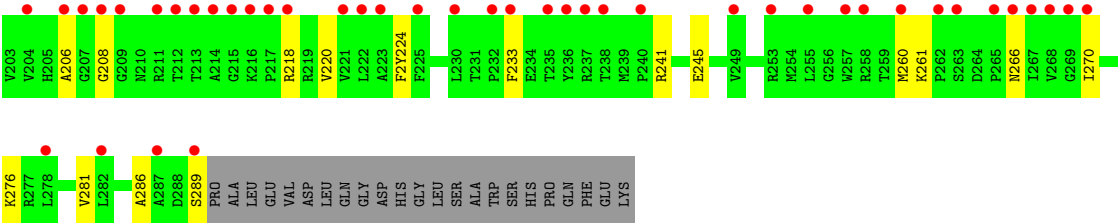
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	1992 reflections (5.13%)	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 , 56.3	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	0.81	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: GOL, F2Y, SO4, AKG, CO

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	0.40	0/2288	0.67	0/3114
1	B	0.37	0/2252	0.67	0/3064
All	All	0.39	0/4540	0.67	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	48	0
1	B	2217	0	2201	41	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	85	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 (85) 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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:261:LYS:NZ	1:B:266:ASN:O	2.45	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%)	19	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 [i](#)

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%)	241 (98%)	4 (2%)	58	64
1	B	241/269 (90%)	235 (98%)	6 (2%)	42	45
All	All	486/538 (90%)	476 (98%)	10 (2%)	48	53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	110	TRP
1	A	144	GLU
1	A	237	ARG
1	B	10	GLN
1	B	22	CYS
1	B	43	GLU
1	B	47	ARG
1	B	110	TRP
1	B	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

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	1.15	1 (7%)	16,19,21	1.85	3 (18%)
1	F2Y	B	224	1	13,14,15	1.11	0	16,19,21	2.17	5 (31%)

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	2.45	1.41	1.37

All (8) 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	4.20	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
1	B	224	F2Y	CG-CD2-CE2	2.52	121.00	119.37
1	B	224	F2Y	F1-CE1-CD1	2.10	122.79	118.61
1	A	224	F2Y	CG-CD2-CE2	2.00	120.67	119.37

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	0.29	0	11,11,11	0.43	0
5	SO4	B	501	-	4,4,4	0.50	0	6,6,6	0.07	0
4	GOL	A	403	-	5,5,5	1.05	0	5,5,5	1.12	0
3	AKG	B	503	2	9,9,9	0.27	0	11,11,11	0.40	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:

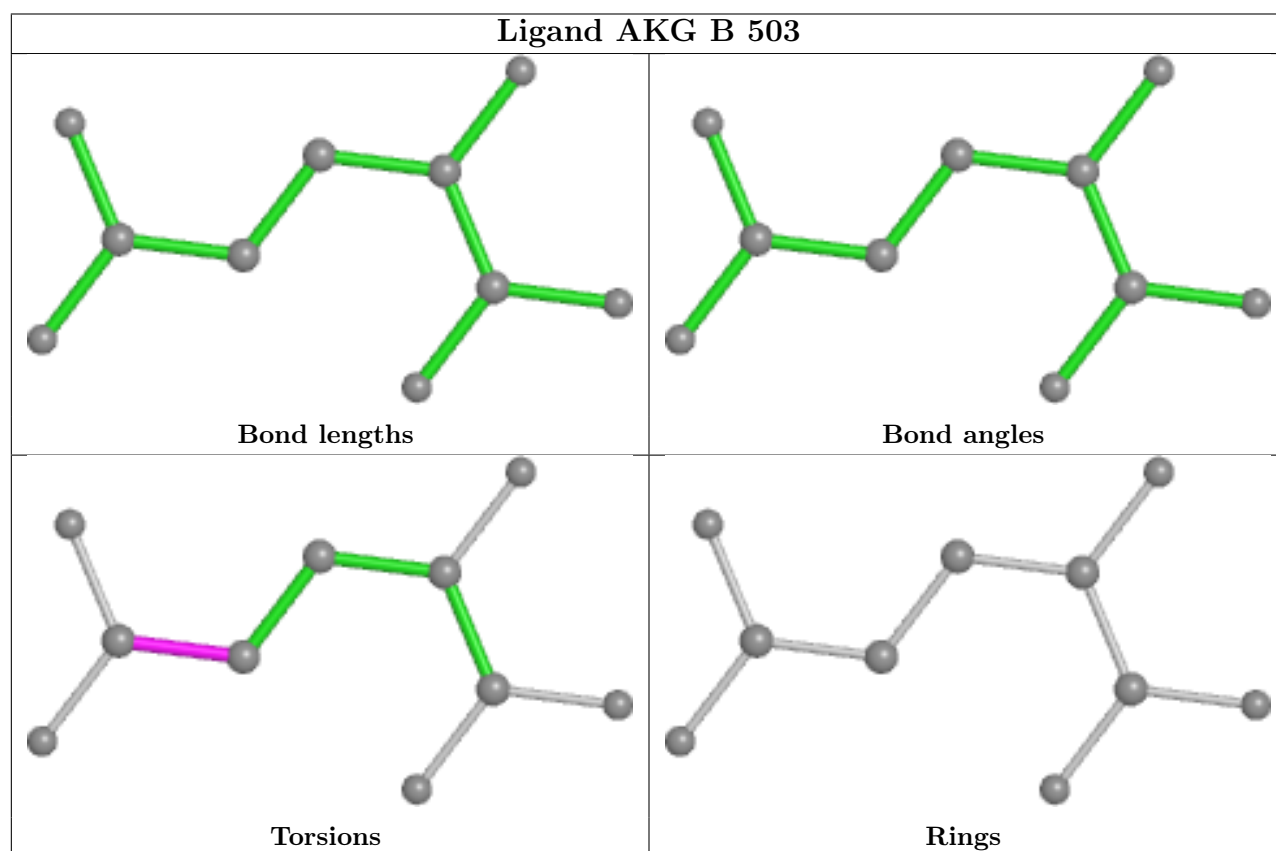
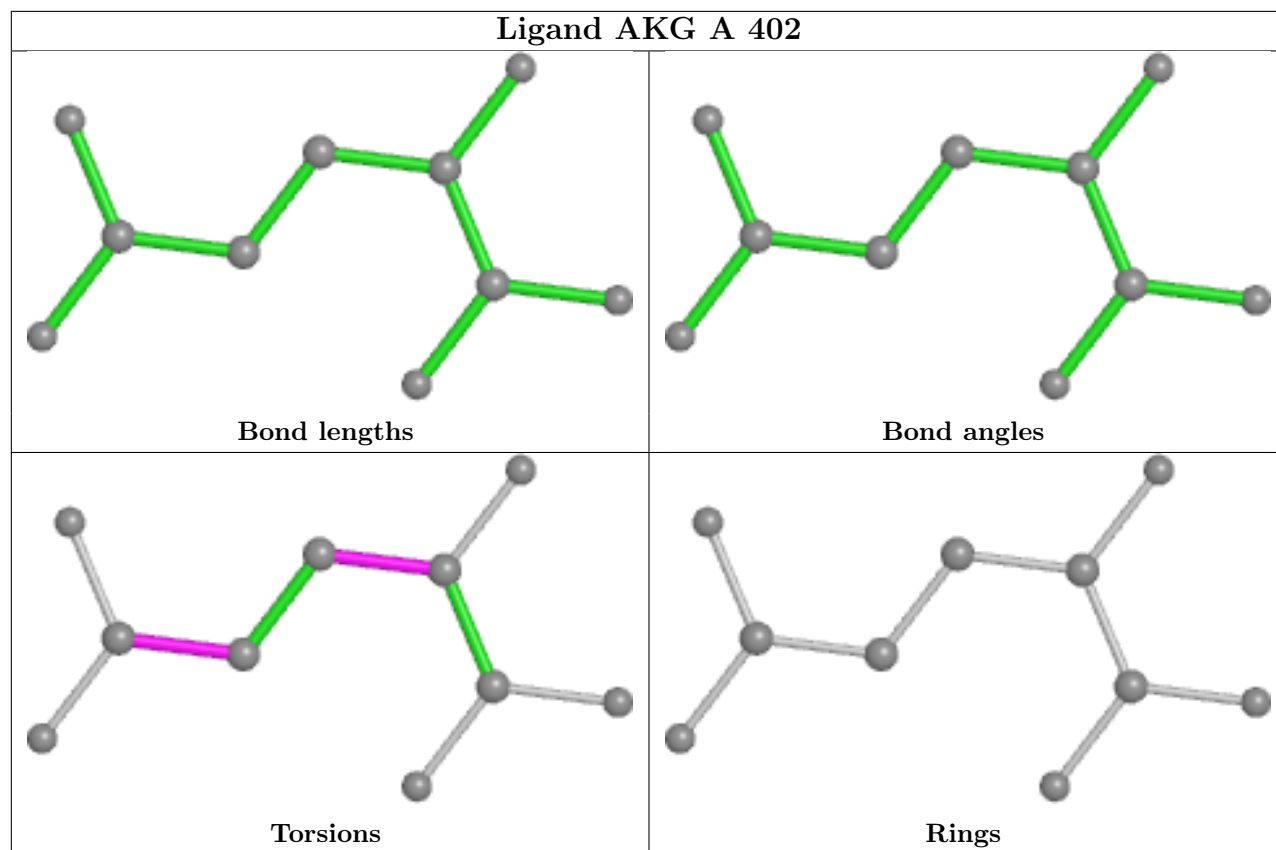
Mol	Chain	Res	Type	Atoms
3	A	402	AKG	C1-C2-C3-C4
4	A	403	GOL	O1-C1-C2-O2
4	A	403	GOL	O1-C1-C2-C3
3	A	402	AKG	C3-C4-C5-O3
3	A	402	AKG	C3-C4-C5-O4
3	A	402	AKG	O5-C2-C3-C4
3	B	503	AKG	C3-C4-C5-O3
3	B	503	AKG	C3-C4-C5-O4

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%)	2.42	169 (59%) 0 1	18, 30, 44, 90	0
1	B	280/312 (89%)	2.18	146 (52%) 0 1	19, 29, 59, 84	0
All	All	563/624 (90%)	2.30	315 (55%) 0 1	18, 29, 50, 90	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	VAL	6.2
1	B	54	ALA	6.1
1	A	128	PHE	5.7
1	B	217	PRO	5.5
1	B	215	GLY	5.4
1	B	265	PRO	5.4
1	A	160	THR	5.3
1	A	235	THR	5.1
1	B	140	TYR	5.0
1	B	169	ILE	4.7
1	A	209	GLY	4.7
1	A	133	ALA	4.7
1	B	159	PHE	4.6
1	A	39	PHE	4.6
1	A	42	VAL	4.5
1	A	64	LEU	4.5
1	B	69	PRO	4.5
1	B	188	LEU	4.4
1	A	13	ALA	4.4
1	A	58	PRO	4.4
1	B	282	LEU	4.4
1	A	14	ALA	4.4
1	A	7	PRO	4.3
1	A	140	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	236	TYR	4.3
1	A	74	TYR	4.3
1	A	25	LEU	4.3
1	A	110	TRP	4.3
1	B	125	ALA	4.3
1	A	178	VAL	4.2
1	A	106	THR	4.2
1	B	68	TYR	4.2
1	B	192	ASP	4.2
1	A	203	VAL	4.2
1	A	207	GLY	4.2
1	A	109	TYR	4.2
1	A	51	VAL	4.2
1	A	256	GLY	4.1
1	B	65	ALA	4.1
1	A	212	THR	4.1
1	B	240	PRO	4.0
1	B	112	SER	4.0
1	A	69	PRO	4.0
1	B	165	ALA	4.0
1	A	210	ASN	4.0
1	B	209	GLY	4.0
1	A	136	PRO	3.9
1	A	184	ASP	3.9
1	A	92	ASN	3.9
1	A	223	ALA	3.9
1	B	22	CYS	3.9
1	A	27	GLU	3.8
1	A	71	HIS	3.8
1	B	166	THR	3.8
1	A	156	LEU	3.8
1	A	72	PHE	3.8
1	B	97	ALA	3.8
1	A	28	ASP	3.7
1	A	173	HIS	3.7
1	A	281	VAL	3.7
1	B	216	LYS	3.7
1	B	119	ILE	3.6
1	B	49	LEU	3.6
1	B	194	GLY	3.6
1	B	269	GLY	3.6
1	A	134	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	143	LEU	3.6
1	B	137	LEU	3.5
1	A	122	GLY	3.5
1	A	273	ILE	3.5
1	A	36	LEU	3.5
1	B	123	MET	3.5
1	B	120	GLU	3.5
1	B	50	ASP	3.5
1	A	270	ILE	3.5
1	A	137	LEU	3.5
1	A	94	VAL	3.5
1	B	289	SER	3.4
1	B	148	VAL	3.4
1	B	63	LEU	3.4
1	A	125	ALA	3.4
1	A	158	GLU	3.4
1	B	144	GLU	3.4
1	B	211	ARG	3.4
1	A	116	LEU	3.4
1	A	101	ALA	3.4
1	B	218	ARG	3.4
1	B	45	PHE	3.3
1	B	146	PRO	3.3
1	A	91	ILE	3.3
1	A	115	PHE	3.3
1	A	23	ARG	3.3
1	B	59	LYS	3.3
1	B	139	HIS	3.3
1	A	65	ALA	3.2
1	A	16	ALA	3.2
1	A	286	ALA	3.2
1	A	161	GLU	3.2
1	B	176	THR	3.2
1	A	172	SER	3.2
1	B	287	ALA	3.2
1	A	175	TRP	3.2
1	B	31	PHE	3.2
1	A	132	ASP	3.2
1	B	57	PRO	3.2
1	A	186	ALA	3.2
1	B	182	GLU	3.2
1	A	52	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	213	THR	3.1
1	B	221	VAL	3.1
1	B	233	PHE	3.1
1	A	9	LEU	3.1
1	A	230	LEU	3.1
1	A	216	LYS	3.1
1	A	22	CYS	3.1
1	A	271	ASN	3.1
1	A	31	PHE	3.1
1	A	262	PRO	3.1
1	A	135	HIS	3.1
1	B	160	THR	3.1
1	B	253	ARG	3.1
1	A	205	HIS	3.0
1	A	30	ALA	3.0
1	B	55	ILE	3.0
1	B	262	PRO	3.0
1	A	103	PHE	3.0
1	A	150	LEU	3.0
1	B	128	PHE	3.0
1	A	145	ALA	3.0
1	A	199	VAL	3.0
1	B	127	PRO	3.0
1	A	8	GLN	3.0
1	A	98	ILE	3.0
1	A	6	LYS	3.0
1	A	24	LEU	3.0
1	B	16	ALA	3.0
1	B	73	LYS	3.0
1	A	40	ASP	2.9
1	B	257	TRP	2.9
1	B	24	LEU	2.9
1	A	245	GLU	2.9
1	A	191	MET	2.9
1	B	104	GLN	2.9
1	B	212	THR	2.9
1	B	208	GLY	2.9
1	B	38	PRO	2.9
1	A	250	LEU	2.9
1	B	214	ALA	2.9
1	A	121	SER	2.9
1	A	153	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	149	SER	2.9
1	A	164	GLY	2.9
1	B	263	SER	2.9
1	B	12	LEU	2.8
1	B	90	LEU	2.8
1	A	139	HIS	2.8
1	A	165	ALA	2.8
1	A	120	GLU	2.8
1	B	213	THR	2.8
1	A	123	MET	2.8
1	A	171	GLY	2.8
1	A	265	PRO	2.8
1	B	56	PRO	2.8
1	B	33	LEU	2.8
1	B	58	PRO	2.8
1	B	255	LEU	2.8
1	A	46	ASN	2.7
1	A	59	LYS	2.7
1	A	45	PHE	2.7
1	B	95	ILE	2.7
1	B	132	ASP	2.7
1	A	54	ALA	2.7
1	B	21	MET	2.7
1	B	60	GLY	2.7
1	A	187	VAL	2.7
1	A	35	GLY	2.7
1	A	159	PHE	2.7
1	B	107	GLY	2.7
1	B	44	SER	2.7
1	A	168	VAL	2.7
1	A	47	ARG	2.7
1	A	211	ARG	2.7
1	A	192	ASP	2.7
1	A	195	ASP	2.7
1	A	57	PRO	2.6
1	A	222	LEU	2.6
1	A	249	VAL	2.6
1	B	206	ALA	2.6
1	B	81	THR	2.6
1	B	175	TRP	2.6
1	B	142	PRO	2.6
1	B	266	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	246	SER	2.6
1	A	37	LEU	2.6
1	B	111	LEU	2.6
1	A	268	VAL	2.6
1	B	145	ALA	2.6
1	B	268	VAL	2.6
1	A	289	SER	2.6
1	A	278	LEU	2.6
1	A	214	ALA	2.6
1	A	228	VAL	2.6
1	B	204	VAL	2.6
1	B	267	ILE	2.6
1	B	14	ALA	2.5
1	A	148	VAL	2.5
1	B	74	TYR	2.5
1	B	83	PRO	2.5
1	B	131	ASP	2.5
1	A	75	VAL	2.5
1	A	196	VAL	2.5
1	A	221	VAL	2.5
1	A	248	THR	2.5
1	A	283	GLN	2.5
1	B	151	SER	2.5
1	A	274	ASP	2.5
1	A	220	VAL	2.5
1	B	77	ASN	2.5
1	A	117	ARG	2.4
1	A	79	ALA	2.4
1	B	223	ALA	2.4
1	A	87	ASN	2.4
1	A	190	THR	2.4
1	A	26	GLU	2.4
1	A	181	PRO	2.4
1	B	237	ARG	2.4
1	B	114	ALA	2.4
1	A	34	LYS	2.4
1	B	51	VAL	2.4
1	A	193	PRO	2.4
1	A	252	GLN	2.4
1	A	33	LEU	2.4
1	B	222	LEU	2.4
1	B	26	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	190	THR	2.4
1	B	235	THR	2.4
1	B	187	VAL	2.4
1	B	62	ARG	2.4
1	B	103	PHE	2.4
1	B	207	GLY	2.4
1	B	236	TYR	2.4
1	A	108	ASP	2.4
1	A	90	LEU	2.3
1	A	78	VAL	2.3
1	B	121	SER	2.3
1	B	168	VAL	2.3
1	A	185	GLN	2.3
1	B	164	GLY	2.3
1	A	20	ARG	2.3
1	A	70	PRO	2.3
1	B	93	PRO	2.3
1	B	10	GLN	2.3
1	B	108	ASP	2.3
1	B	230	LEU	2.3
1	B	278	LEU	2.3
1	B	174	ARG	2.3
1	A	254	MET	2.3
1	A	259	THR	2.3
1	B	179	GLY	2.3
1	A	32	ILE	2.3
1	A	176	THR	2.3
1	B	157	THR	2.3
1	B	232	PRO	2.2
1	B	66	ASP	2.2
1	B	41	VAL	2.2
1	B	46	ASN	2.2
1	A	267	ILE	2.2
1	B	91	ILE	2.2
1	A	197	LEU	2.2
1	B	17	ASP	2.2
1	A	269	GLY	2.2
1	A	129	HIS	2.2
1	A	102	TYR	2.2
1	A	56	PRO	2.2
1	A	276	LYS	2.2
1	B	11	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	117	ARG	2.2
1	A	204	VAL	2.2
1	B	270	ILE	2.2
1	B	183	ARG	2.2
1	B	32	ILE	2.1
1	A	263	SER	2.1
1	A	277	ARG	2.1
1	B	258	ARG	2.1
1	B	29	GLY	2.1
1	A	266	ASN	2.1
1	B	167	GLU	2.1
1	A	12	LEU	2.1
1	B	170	LEU	2.1
1	A	151	SER	2.1
1	B	189	ALA	2.1
1	B	102	TYR	2.1
1	A	279	GLU	2.1
1	B	116	LEU	2.1
1	B	225	PHE	2.1
1	B	238	THR	2.1
1	A	96	HIS	2.1
1	B	260	MET	2.1
1	A	257	TRP	2.1
1	A	43	GLU	2.1
1	B	75	VAL	2.1
1	B	249	VAL	2.1
1	B	172	SER	2.1
1	A	60	GLY	2.0
1	B	141	GLN	2.1
1	B	193	PRO	2.0
1	B	109	TYR	2.0
1	B	196	VAL	2.0
1	A	157	THR	2.0
1	A	188	LEU	2.0
1	A	282	LEU	2.0
1	B	201	GLN	2.0
1	A	107	GLY	2.0
1	A	275	ASP	2.0
1	A	288	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B	224	14/15	0.89	0.15	20,24,26,29	0
1	F2Y	A	224	14/15	0.90	0.16	19,23,26,28	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

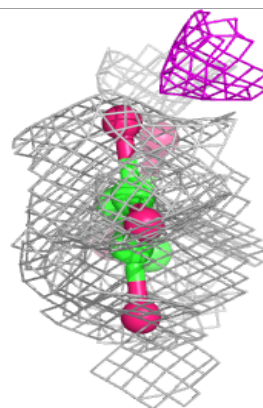
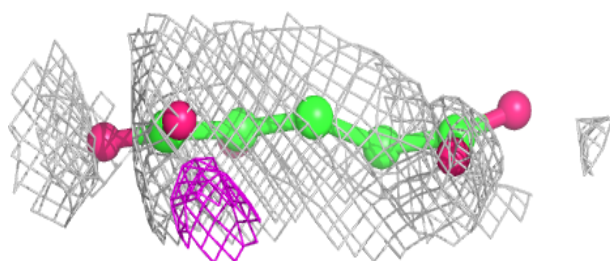
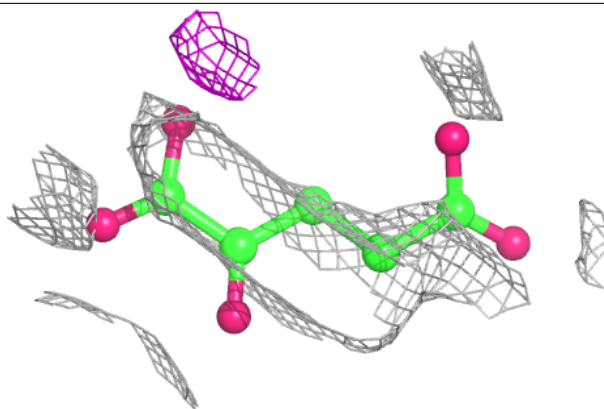
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.89	0.17	26,29,29,29	0
5	SO4	B	501	5/5	0.91	0.18	26,26,31,36	0
4	GOL	A	403	6/6	0.97	0.14	32,35,37,39	0
3	AKG	A	402	10/10	0.97	0.17	31,32,32,33	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

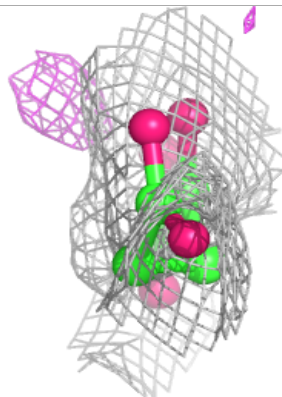
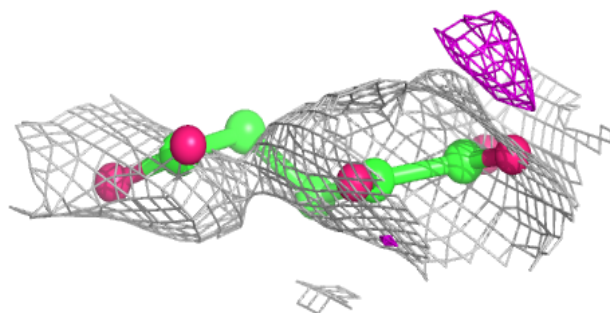
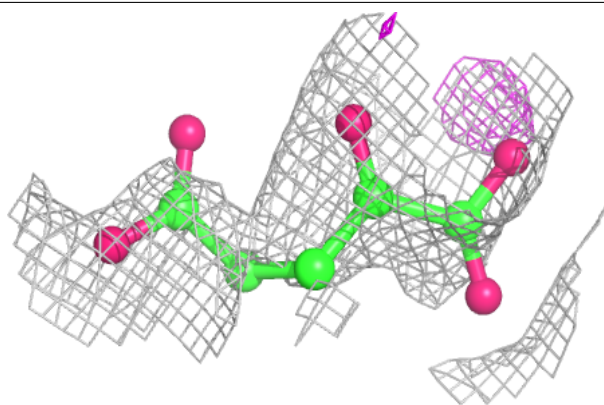
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AKG B 503:

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

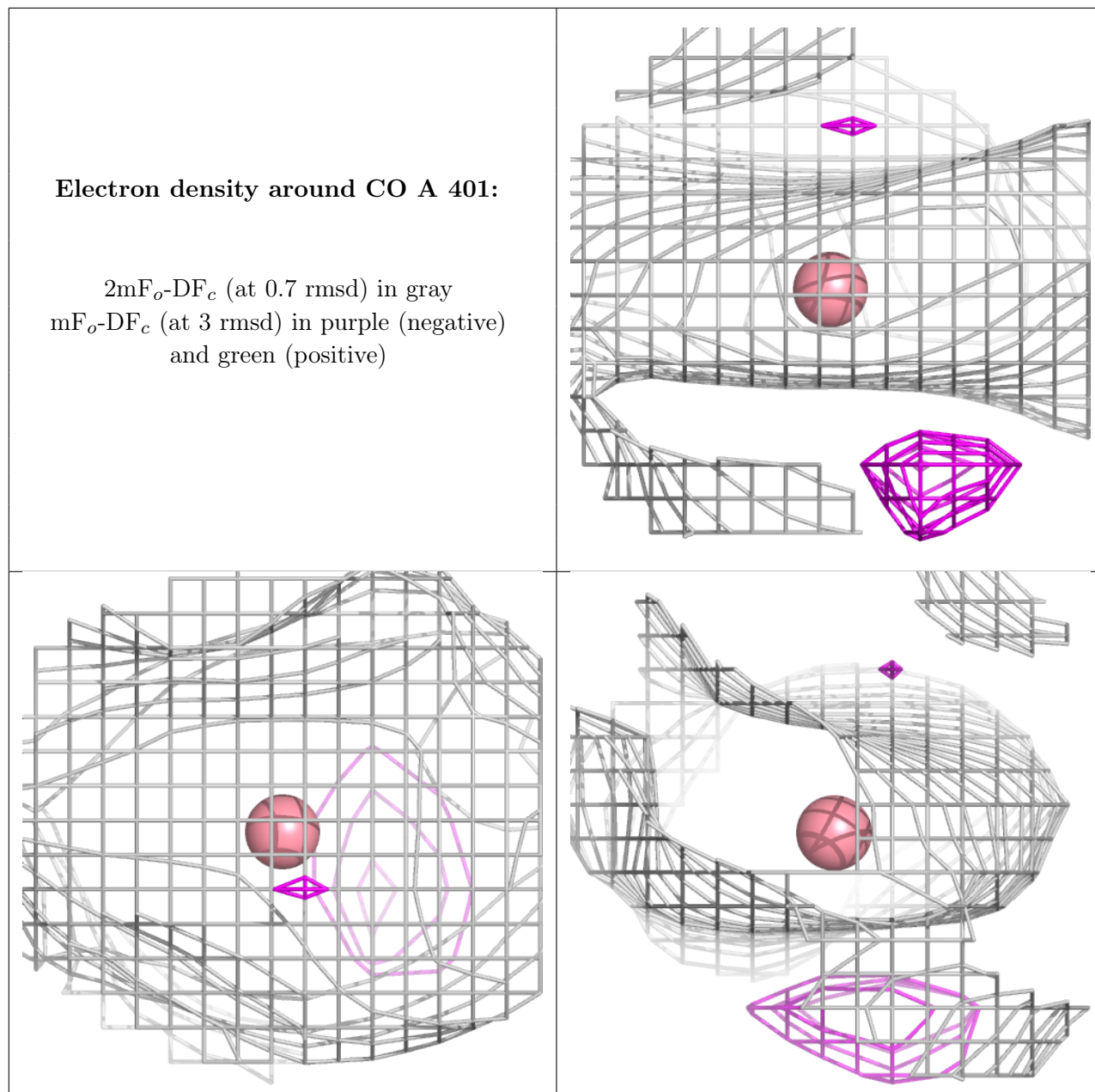
**Electron density around AKG A 402:**

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



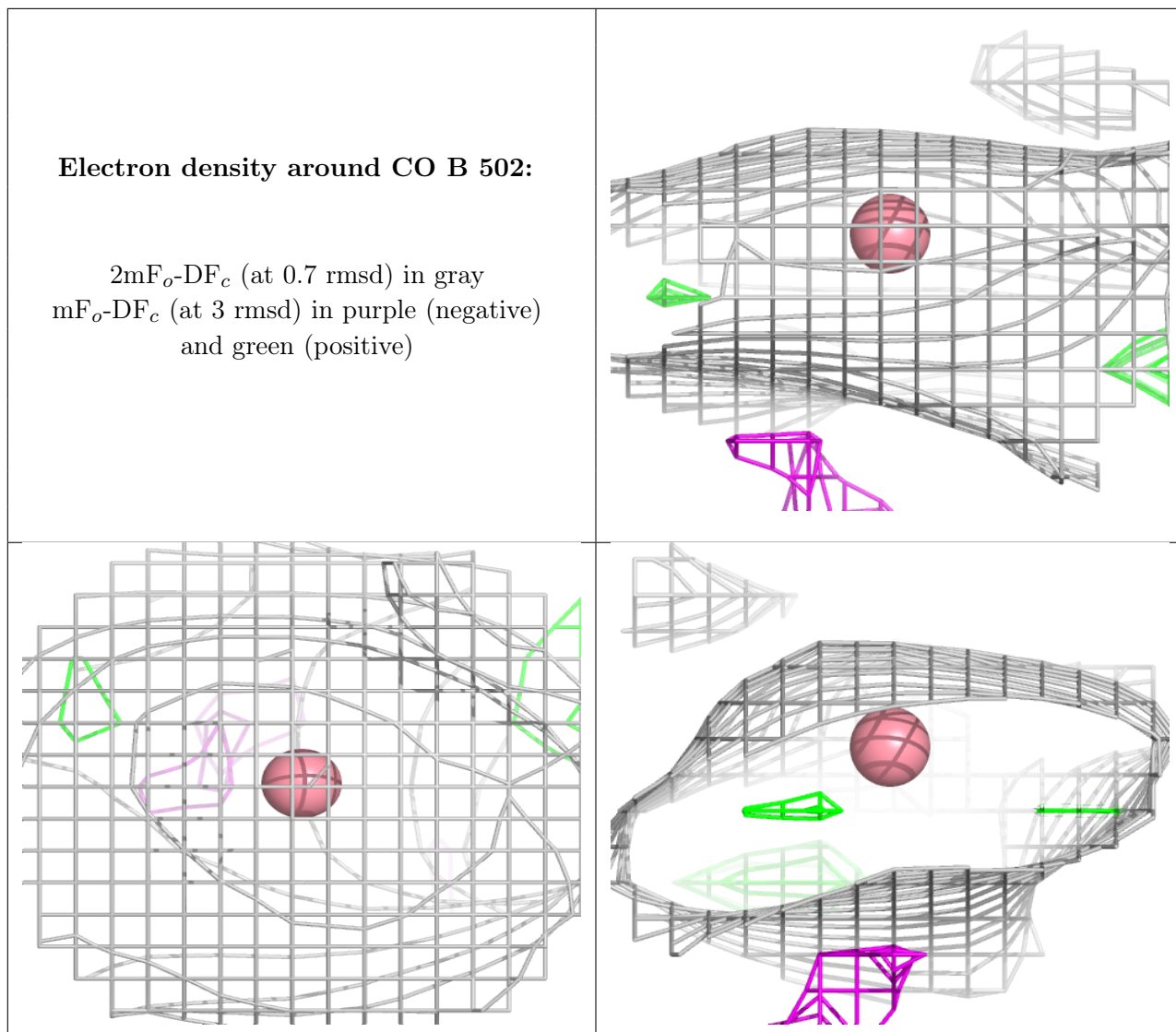
Electron density around CO A 401:

$2mF_o-DF_c$ (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.