



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:09 PM UTC

PDB ID : 7V3E / pdb_00007v3e
Title : The complex structure of soBcmB and its intermediate product 1a
Authors : Wu, L.; Zhou, J.H.
Deposited on : 2021-08-10
Resolution : 2.12 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

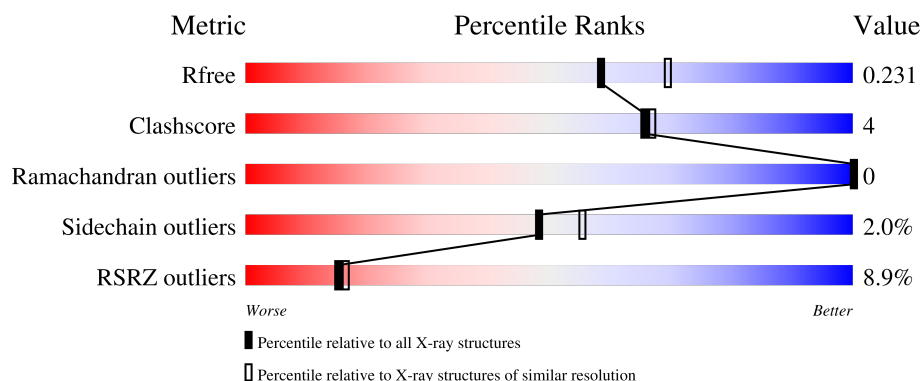
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	328	5% 78% 8% 15%
1	B	328	8% 77% 7% 15%
1	C	328	10% 76% 9% 15%

2 Entry composition [i](#)

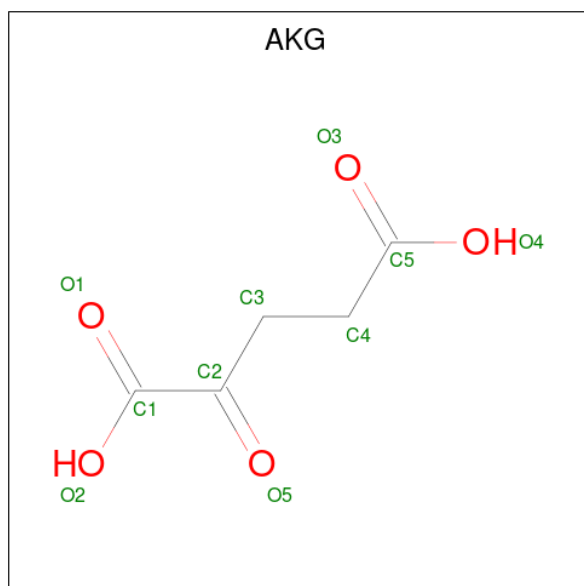
There are 7 unique types of molecules in this entry. The entry contains 7013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 dioxygenase.

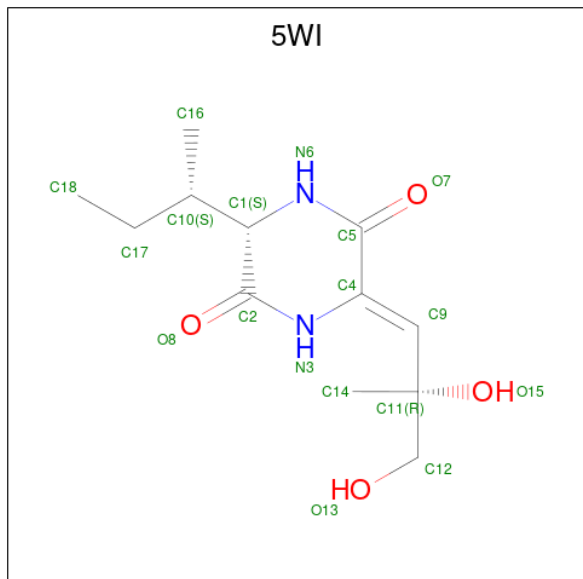
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	1	0
			2227	1394	395	430	8			
1	B	280	Total	C	N	O	S	0	1	0
			2228	1396	395	429	8			
1	C	280	Total	C	N	O	S	0	0	0
			2223	1391	395	429	8			

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



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

- Molecule 3 is (3S,6Z)-3-[(2S)-butan-2-yl]-6-[(2R)-2-methyl-2,3-bis(oxidanyl)propylidene]piperazine-2,5-dione (CCD ID: 5WI) (formula: $C_{12}H_{20}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	12	2	4		
3	B	1	Total	C	N	O	0	0
			18	12	2	4		
3	C	1	Total	C	N	O	0	0
			18	12	2	4		

- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

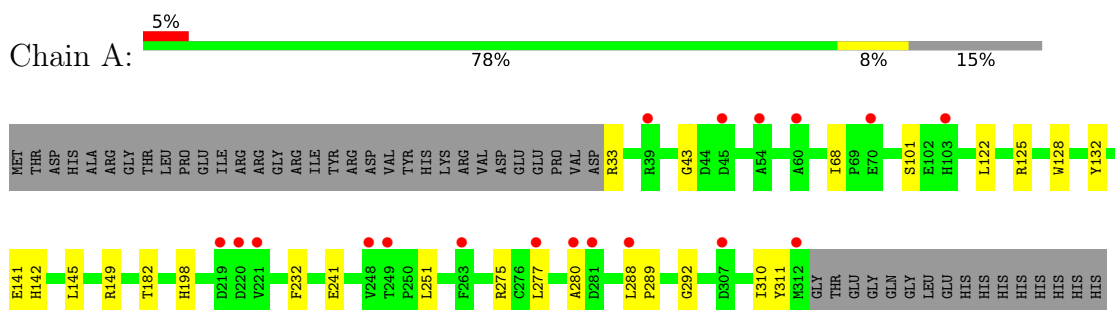
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	91	Total	O	0	0
			91	91		
7	B	79	Total	O	0	0
			79	79		
7	C	71	Total	O	0	0
			71	71		

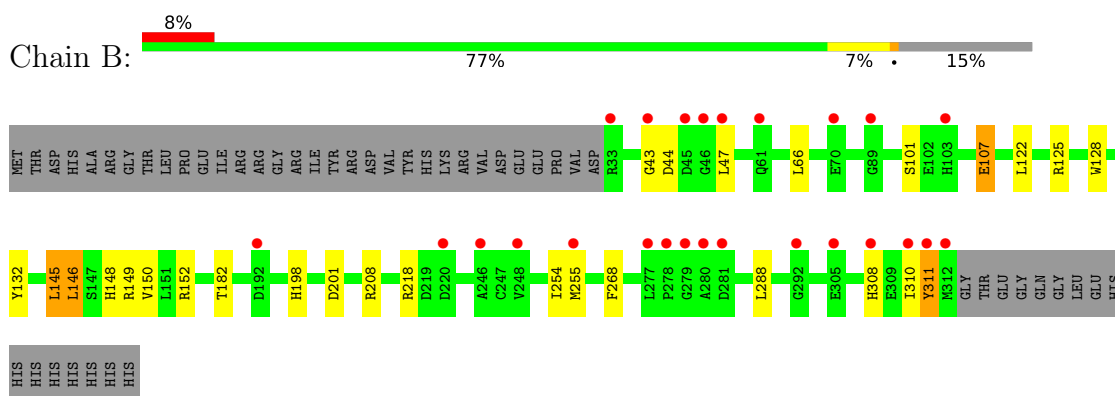
3 Residue-property plots [i](#)

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.

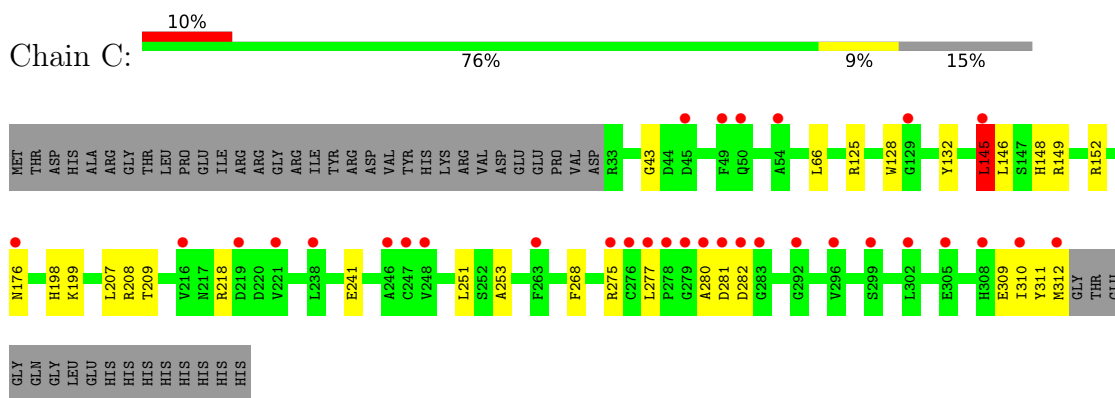
- Molecule 1: dioxygenase



- Molecule 1: dioxygenase



- Molecule 1: dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.88Å 180.53Å 133.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.46 – 2.12 17.46 – 2.12	Depositor EDS
% Data completeness (in resolution range)	100.0 (17.46-2.12) 99.8 (17.46-2.12)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.217 , 0.229 0.219 , 0.231	Depositor DCC
R_{free} test set	3384 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: AKG, FE2, 5WI, GOL, CL

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	0.20	0/2284	0.45	0/3093
1	B	0.20	0/2285	0.47	2/3094 (0.1%)
1	C	0.23	0/2277	0.48	1/3083 (0.0%)
All	All	0.21	0/6846	0.47	3/9270 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	CB-CG-CD2	-7.78	87.36	110.70
1	B	311	TYR	CA-C-N	5.89	132.30	121.70
1	B	311	TYR	C-N-CA	5.89	132.30	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2227	0	2096	15	0
1	B	2228	0	2100	16	0
1	C	2223	0	2089	19	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	4	0	0
3	A	18	0	0	1	0
3	B	18	0	0	2	0
3	C	18	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
6	B	6	0	8	1	0
7	A	91	0	0	1	0
7	B	79	0	0	1	0
7	C	71	0	0	1	0
All	All	7013	0	6305	50	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 4.

All (50) 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:C:176:ASN:O	1:C:275:ARG:NH1	2.15	0.79
1:C:66:LEU:HD21	1:C:146:LEU:HD21	1.66	0.77
1:B:44:ASP:OD1	7:B:501:HOH:O	2.13	0.64
1:C:198:HIS:HB2	1:C:310:ILE:HG12	1.79	0.62
1:C:311:TYR:OH	3:C:402:5WI:O13	2.18	0.59
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.85	0.57
1:B:311:TYR:OH	3:B:403:5WI:O13	2.15	0.55
1:A:198:HIS:HB2	1:A:310:ILE:HG12	1.89	0.55
1:A:198:HIS:CB	1:A:310:ILE:HG12	2.37	0.54
1:A:142:HIS:NE2	1:B:145:LEU:HD23	2.24	0.53
1:C:66:LEU:CD2	1:C:146:LEU:HD21	2.37	0.53
1:B:101:SER:HB2	1:B:107:GLU:HA	1.90	0.53
1:C:241:GLU:HA	1:C:251:LEU:O	2.09	0.51
1:B:152:ARG:HH21	6:B:407:GOL:H32	1.76	0.51
1:B:66:LEU:HD21	1:B:146:LEU:HD21	1.92	0.51
1:C:198:HIS:CB	1:C:310:ILE:HG12	2.41	0.49
1:A:277:LEU:HB2	1:A:280:ALA:HB3	1.95	0.48
1:A:43:GLY:O	1:A:149:ARG:NH2	2.46	0.48
1:B:125:ARG:HA	1:B:128:TRP:CD2	2.48	0.48
1:A:311:TYR:OH	3:A:403:5WI:O13	2.24	0.48
1:C:199:LYS:HD3	1:C:253:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLY:O	1:B:149:ARG:NH2	2.48	0.47
1:C:148:HIS:CE1	1:C:152:ARG:HD2	2.50	0.47
1:B:125:ARG:HA	1:B:128:TRP:CE2	2.50	0.47
1:C:208:ARG:HG2	1:C:268:PHE:CE1	2.50	0.46
1:C:125:ARG:HA	1:C:128:TRP:CD2	2.51	0.46
1:C:207:LEU:HG	1:C:209:THR:HG23	1.96	0.46
1:B:201:ASP:OD1	3:B:403:5WI:N6	2.48	0.46
1:C:176:ASN:C	1:C:275:ARG:HH12	2.24	0.46
1:C:145:LEU:C	1:C:145:LEU:HD12	2.42	0.45
1:C:277:LEU:HB2	1:C:280:ALA:HB3	1.98	0.45
1:A:125:ARG:HA	1:A:128:TRP:CD2	2.52	0.44
1:C:281:ASP:OD1	7:C:501:HOH:O	2.21	0.44
1:A:101:SER:N	7:A:507:HOH:O	2.50	0.44
1:A:141:GLU:O	1:A:145:LEU:HD13	2.18	0.44
1:A:68:ILE:HG12	1:A:232:PHE:CE2	2.53	0.43
1:C:43:GLY:O	1:C:149:ARG:NH2	2.51	0.43
3:C:402:5WI:N3	3:C:402:5WI:O15	2.52	0.43
1:B:122:LEU:HG	1:B:182:THR:HG23	2.00	0.43
1:A:241:GLU:HA	1:A:251:LEU:O	2.20	0.42
1:B:148:HIS:CE1	1:B:152:ARG:HD2	2.55	0.42
1:B:198:HIS:HB2	1:B:310:ILE:HG12	2.01	0.42
1:A:122:LEU:HG	1:A:182:THR:HG23	2.02	0.42
1:C:125:ARG:HA	1:C:128:TRP:CE2	2.54	0.41
1:B:218:ARG:HG2	1:B:254:ILE:HD11	2.02	0.41
1:B:47:LEU:HD11	1:B:150:VAL:HG13	2.02	0.41
1:A:275:ARG:NH1	1:A:280:ALA:HB1	2.35	0.41
1:A:288:LEU:O	1:A:292:GLY:N	2.47	0.41
1:B:208:ARG:HG2	1:B:268:PHE:CE1	2.57	0.40
1:C:275:ARG:HB3	1:C:282:ASP:CG	2.47	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	279/328 (85%)	270 (97%)	9 (3%)	0	100	100
1	B	279/328 (85%)	269 (96%)	10 (4%)	0	100	100
1	C	278/328 (85%)	270 (97%)	8 (3%)	0	100	100
All	All	836/984 (85%)	809 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/278 (85%)	235 (99%)	2 (1%)	73	80
1	B	237/278 (85%)	230 (97%)	7 (3%)	36	40
1	C	236/278 (85%)	231 (98%)	5 (2%)	47	54
All	All	710/834 (85%)	696 (98%)	14 (2%)	48	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	132	TYR
1	B	107	GLU
1	B	132	TYR
1	B	145	LEU
1	B	146	LEU
1	B	255	MET
1	B	288	LEU
1	B	308	HIS
1	C	132	TYR
1	C	145	LEU
1	C	218	ARG
1	C	309	GLU
1	C	312	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	C	55	GLN
1	C	103	HIS
1	C	235	ASN
1	C	262	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	5WI	B	403	-	16,18,18	2.83	6 (37%)	17,26,26	1.44	2 (11%)
2	AKG	B	404	4	9,9,9	1.66	1 (11%)	11,11,11	1.96	4 (36%)
3	5WI	A	403	-	16,18,18	2.75	5 (31%)	17,26,26	2.16	3 (17%)
3	5WI	C	402	-	16,18,18	2.90	6 (37%)	17,26,26	1.46	2 (11%)
6	GOL	B	407	-	5,5,5	0.40	0	5,5,5	0.22	0
2	AKG	A	402	4	9,9,9	1.69	1 (11%)	11,11,11	1.62	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AKG	C	404	4	9,9,9	1.76	2 (22%)	11,11,11	1.90	5 (45%)

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	5WI	B	403	-	-	3/13/30/30	0/1/1/1
2	AKG	B	404	4	-	0/9/9/9	-
3	5WI	A	403	-	-	7/13/30/30	0/1/1/1
3	5WI	C	402	-	-	4/13/30/30	0/1/1/1
6	GOL	B	407	-	-	4/4/4/4	-
2	AKG	A	402	4	-	0/9/9/9	-
2	AKG	C	404	4	-	0/9/9/9	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	5WI	C5-N6	9.09	1.49	1.34
3	B	403	5WI	C5-N6	8.82	1.48	1.34
3	A	403	5WI	C5-N6	8.40	1.48	1.34
3	A	403	5WI	C2-N3	4.54	1.45	1.37
3	C	402	5WI	C2-N3	4.47	1.45	1.37
3	B	403	5WI	C2-N3	4.43	1.45	1.37
2	C	404	AKG	C2-C1	-4.26	1.47	1.53
2	A	402	AKG	C2-C1	-4.08	1.47	1.53
2	B	404	AKG	C2-C1	-4.06	1.47	1.53
3	C	402	5WI	O15-C11	-2.99	1.40	1.44
3	A	403	5WI	O15-C11	-2.91	1.40	1.44
3	B	403	5WI	O15-C11	-2.91	1.40	1.44
3	A	403	5WI	O7-C5	-2.89	1.18	1.23
3	C	402	5WI	C1-N6	2.63	1.49	1.46
3	B	403	5WI	O7-C5	-2.62	1.18	1.23
3	C	402	5WI	O7-C5	-2.53	1.18	1.23
3	B	403	5WI	O8-C2	-2.50	1.18	1.23
3	A	403	5WI	O8-C2	-2.43	1.18	1.23
3	B	403	5WI	C1-N6	2.39	1.49	1.46
3	C	402	5WI	O8-C2	-2.35	1.18	1.23
2	C	404	AKG	O2-C1	-2.02	1.25	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	5WI	C10-C1-N6	-5.93	101.37	111.97
3	A	403	5WI	C2-N3-C4	-4.51	119.21	124.85
3	B	403	5WI	C5-C4-N3	3.49	119.79	116.65
2	B	404	AKG	O2-C1-C2	3.08	122.13	113.59
3	C	402	5WI	C2-N3-C4	-3.05	121.04	124.85
3	C	402	5WI	C5-C4-N3	2.94	119.29	116.65
2	B	404	AKG	O1-C1-C2	-2.92	118.17	121.81
2	C	404	AKG	O1-C1-C2	-2.72	118.43	121.81
2	C	404	AKG	O2-C1-C2	2.64	120.91	113.59
3	A	403	5WI	C9-C4-C5	-2.58	116.61	121.38
3	B	403	5WI	C2-N3-C4	-2.40	121.85	124.85
2	C	404	AKG	O5-C2-C1	2.38	123.06	119.67
2	C	404	AKG	C3-C4-C5	-2.36	107.40	113.67
2	A	402	AKG	C3-C2-C1	2.34	119.84	115.86
2	B	404	AKG	O5-C2-C1	2.21	122.83	119.67
2	A	402	AKG	C4-C3-C2	-2.20	108.78	112.91
2	B	404	AKG	C4-C3-C2	-2.08	109.01	112.91
2	C	404	AKG	C4-C3-C2	-2.04	109.08	112.91

There are no chirality outliers.

All (18) torsion outliers are listed below:

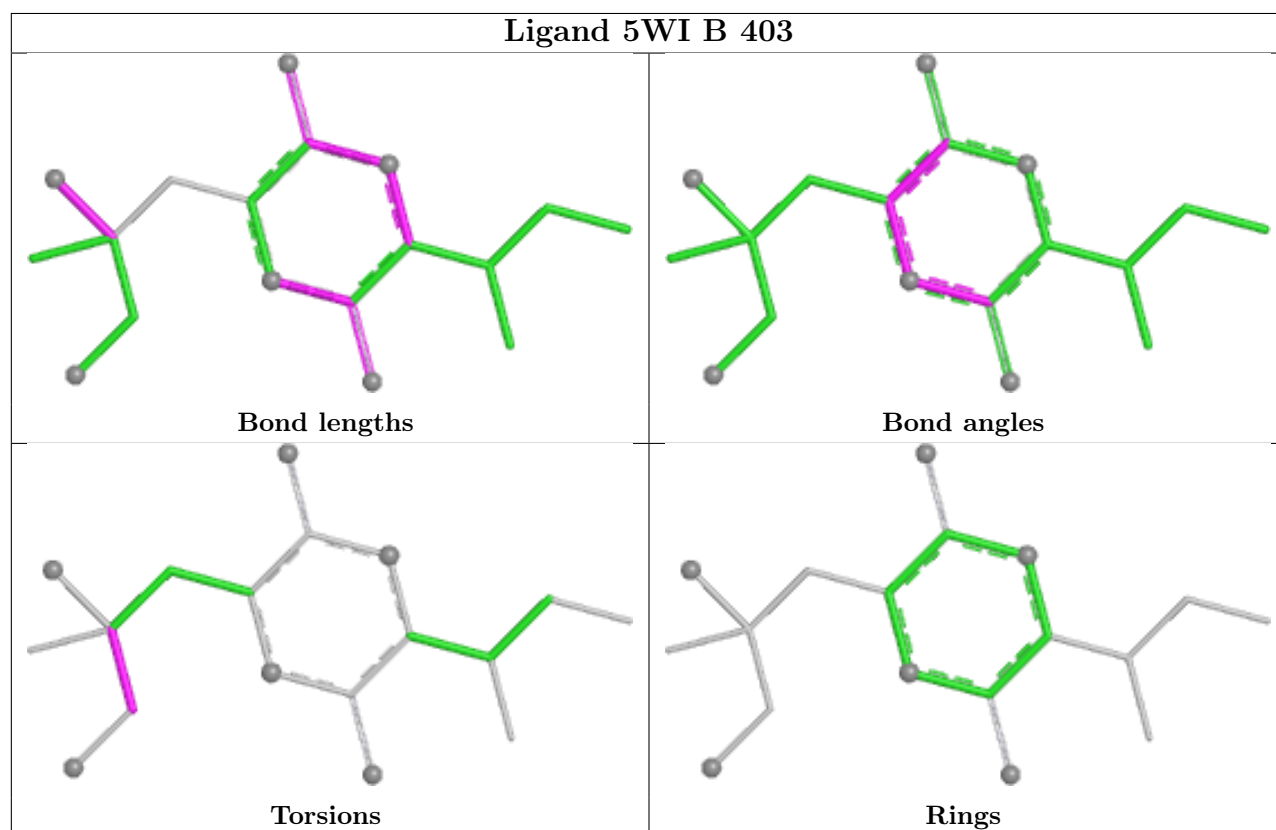
Mol	Chain	Res	Type	Atoms
3	A	403	5WI	C2-C1-C10-C16
3	A	403	5WI	C2-C1-C10-C17
3	A	403	5WI	N6-C1-C10-C16
3	A	403	5WI	N6-C1-C10-C17
3	A	403	5WI	C9-C11-C12-O13
3	A	403	5WI	C14-C11-C12-O13
3	A	403	5WI	O15-C11-C12-O13
3	B	403	5WI	C9-C11-C12-O13
3	B	403	5WI	C14-C11-C12-O13
3	B	403	5WI	O15-C11-C12-O13
3	C	402	5WI	N3-C4-C9-C11
3	C	402	5WI	C9-C11-C12-O13
3	C	402	5WI	C14-C11-C12-O13
3	C	402	5WI	O15-C11-C12-O13
6	B	407	GOL	O1-C1-C2-C3
6	B	407	GOL	C1-C2-C3-O3
6	B	407	GOL	O2-C2-C3-O3
6	B	407	GOL	O1-C1-C2-O2

There are no ring outliers.

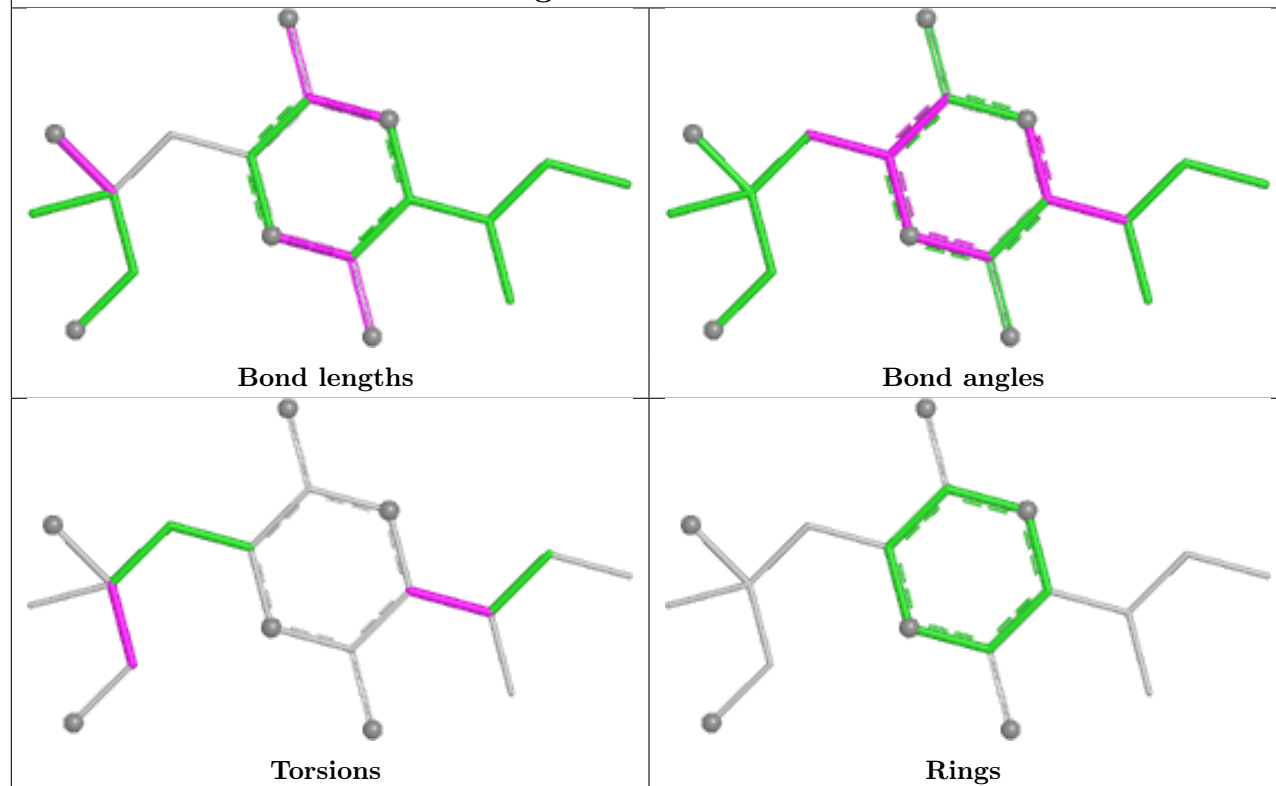
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	5WI	2	0
3	A	403	5WI	1	0
3	C	402	5WI	2	0
6	B	407	GOL	1	0

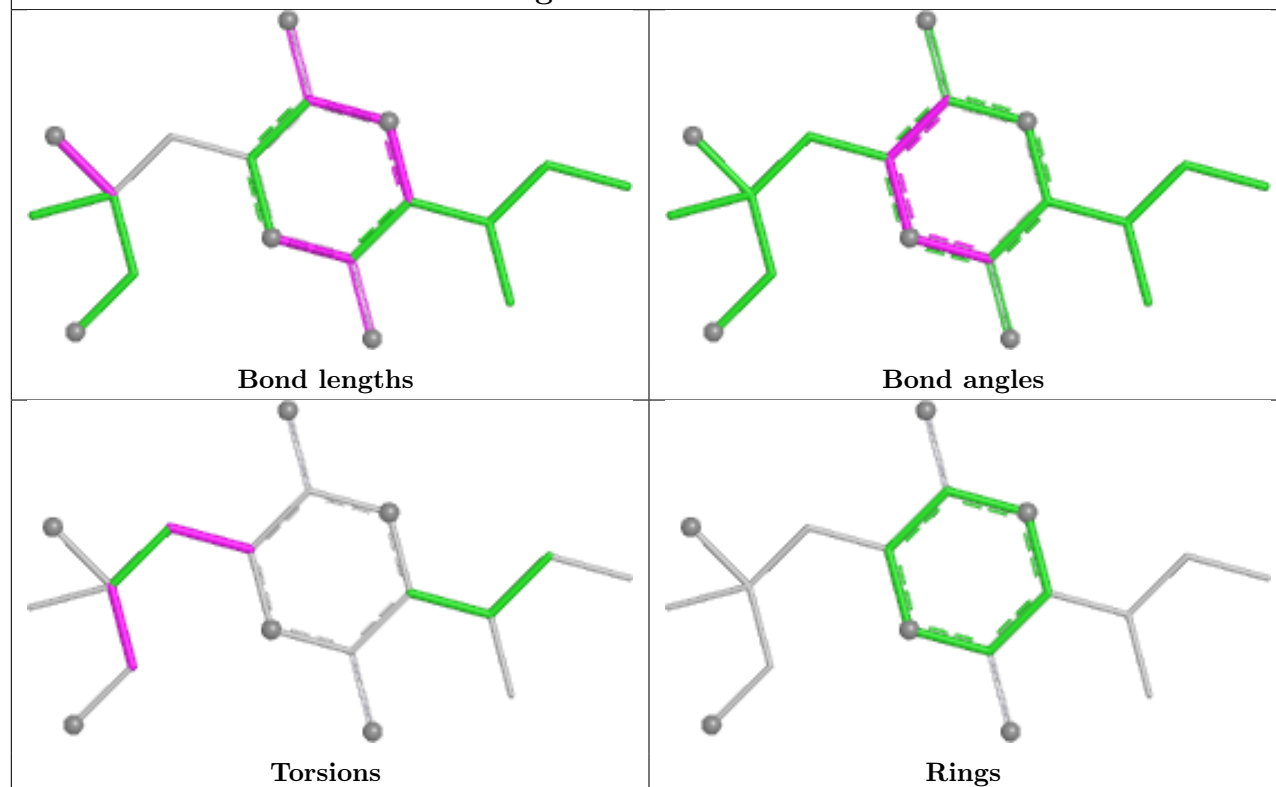
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand 5WI A 403



Ligand 5WI C 402



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	280/328 (85%)	0.49	18 (6%)	25 28	24, 41, 71, 85	1 (0%)
1	B	280/328 (85%)	0.58	25 (8%)	15 16	18, 41, 72, 83	1 (0%)
1	C	280/328 (85%)	0.84	32 (11%)	10 10	27, 48, 75, 82	0
All	All	840/984 (85%)	0.64	75 (8%)	15 16	18, 43, 72, 85	2 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	ALA	5.3
1	C	278	PRO	4.4
1	A	280	ALA	4.3
1	B	248	VAL	4.2
1	B	280	ALA	3.7
1	B	311	TYR	3.6
1	C	248	VAL	3.5
1	C	277	LEU	3.5
1	C	299	SER	3.4
1	C	50	GLN	3.4
1	C	263	PHE	3.4
1	C	279	GLY	3.4
1	B	278	PRO	3.3
1	C	145	LEU	3.3
1	A	248	VAL	3.3
1	C	312	MET	3.2
1	C	282	ASP	3.2
1	C	296	VAL	3.1
1	C	308	HIS	3.1
1	B	277	LEU	3.1
1	B	310	ILE	3.0
1	C	276	CYS	3.0
1	B	312	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	220	ASP	2.9
1	C	310	ILE	2.8
1	B	43	GLY	2.8
1	A	281	ASP	2.7
1	C	219	ASP	2.7
1	A	249	THR	2.7
1	A	312	MET	2.6
1	A	307	ASP	2.6
1	B	45	ASP	2.6
1	B	308	HIS	2.6
1	C	45	ASP	2.6
1	B	192	ASP	2.6
1	B	46	GLY	2.6
1	B	89	GLY	2.6
1	A	288	LEU	2.6
1	C	305	GLU	2.5
1	A	263	PHE	2.5
1	C	283	GLY	2.5
1	A	60	ALA	2.5
1	A	70	GLU	2.5
1	C	54	ALA	2.5
1	B	61	GLN	2.4
1	B	305	GLU	2.3
1	C	49	PHE	2.3
1	C	221	VAL	2.3
1	A	103	HIS	2.3
1	A	54	ALA	2.3
1	B	70	GLU	2.3
1	C	302	LEU	2.3
1	C	281	ASP	2.2
1	C	292	GLY	2.2
1	A	277	LEU	2.2
1	A	45	ASP	2.2
1	B	279	GLY	2.2
1	B	292	GLY	2.2
1	C	129	GLY	2.2
1	B	47	LEU	2.2
1	A	221	VAL	2.1
1	C	246	ALA	2.1
1	C	238	LEU	2.1
1	B	220	ASP	2.1
1	B	281	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	275	ARG	2.1
1	C	247	CYS	2.1
1	A	39	ARG	2.1
1	A	219	ASP	2.1
1	B	33	ARG	2.1
1	B	246	ALA	2.1
1	B	103	HIS	2.0
1	C	216	VAL	2.0
1	B	255	MET	2.0
1	C	176	ASN	2.0

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

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

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.

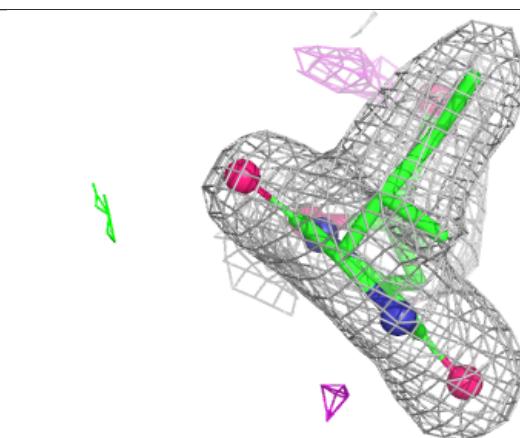
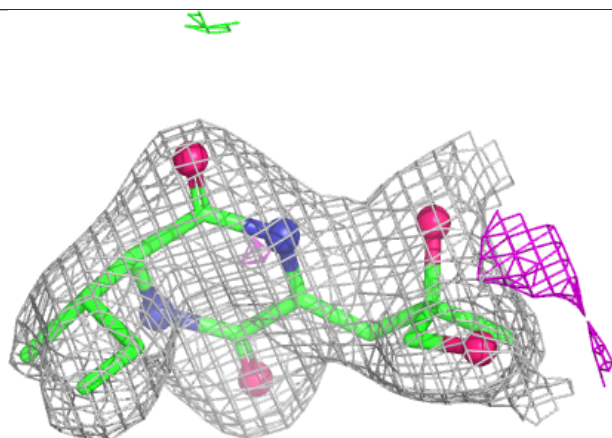
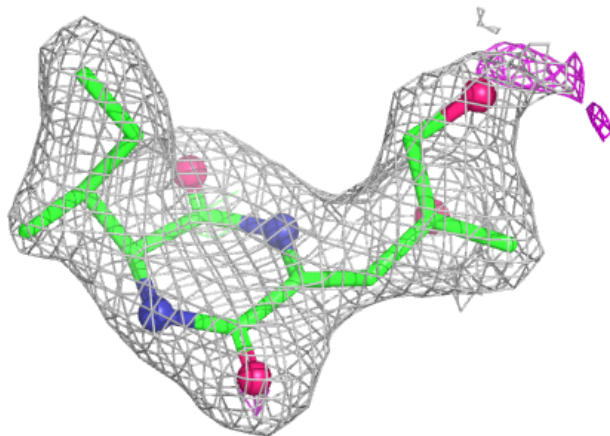
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	407	6/6	0.80	0.14	58,66,67,69	0
3	5WI	B	403	18/18	0.88	0.10	35,41,57,62	0
2	AKG	A	402	10/10	0.89	0.11	31,34,37,38	0
3	5WI	A	403	18/18	0.89	0.11	37,41,57,60	0
3	5WI	C	402	18/18	0.90	0.09	38,44,62,68	0
2	AKG	C	404	10/10	0.93	0.08	35,36,39,41	0
2	AKG	B	404	10/10	0.96	0.06	33,36,38,39	0
5	CL	B	406	1/1	0.97	0.10	47,47,47,47	0
4	FE2	C	406	1/1	0.99	0.10	41,41,41,41	0
4	FE2	A	406	1/1	0.99	0.06	31,31,31,31	0
4	FE2	B	405	1/1	0.99	0.06	34,34,34,34	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.

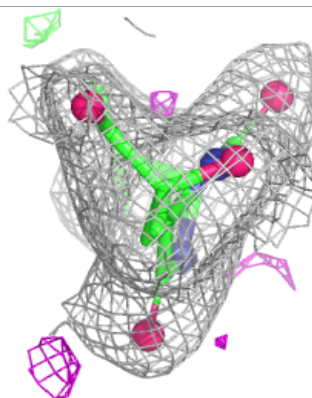
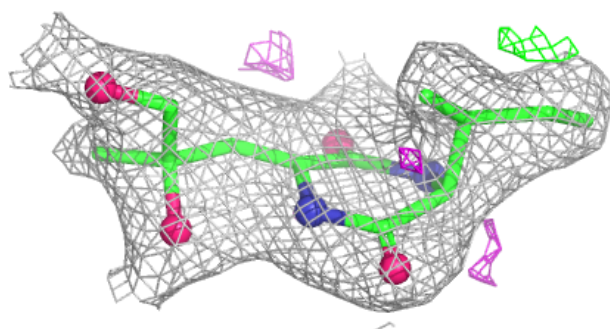
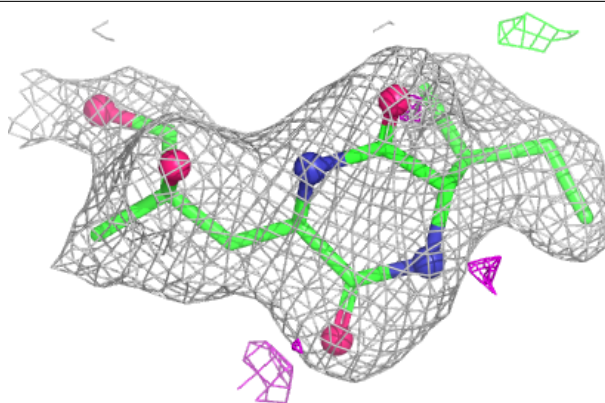
Electron density around 5WI B 403:

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

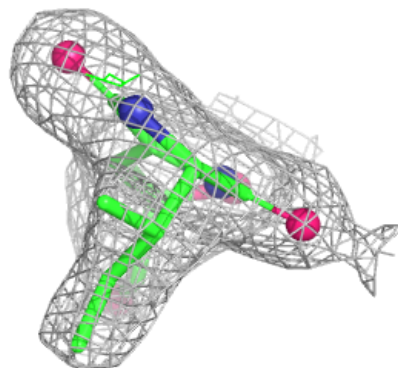
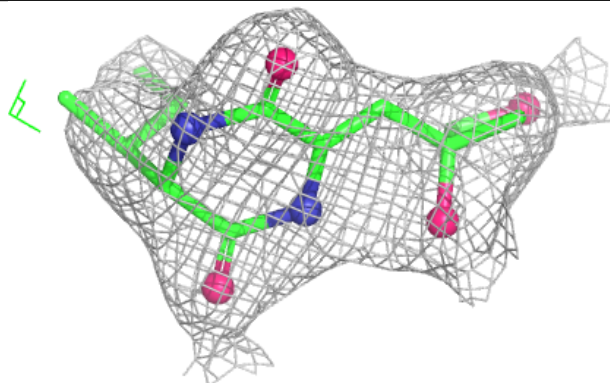
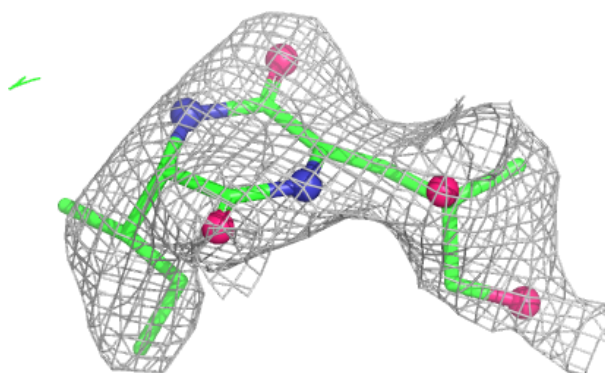


Electron density around 5WI A 403:

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

**Electron density around 5WI C 402:**

$2mF_o-DF_c$ (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.