



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:14 AM UTC

PDB ID : 9EIS / pdb_00009eis
Title : Ethylene forming enzyme in complex with manganese and 2-oxoglutarate from *Penicillium digitatum*
Authors : Chatterjee, S.; Rankin, J.A.; Farrugia, M.A.; Hu, J.; Hausinger, R.P.
Deposited on : 2024-11-26
Resolution : 2.80 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

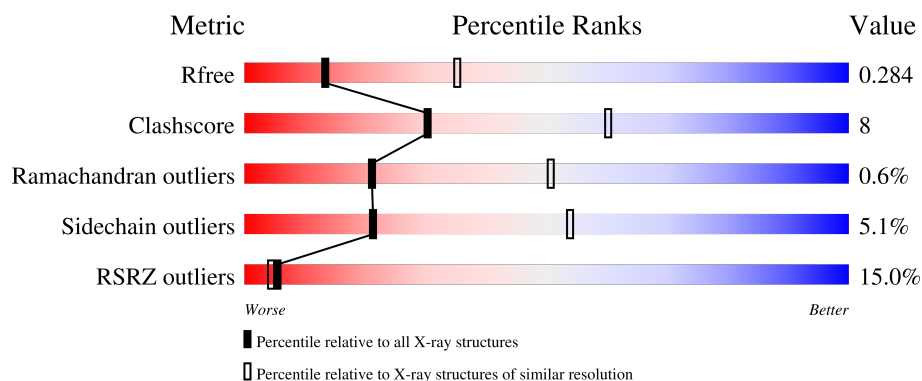
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	407	2% 65% 14% 19%
1	B	407	3% 66% 14% 19%
1	C	407	3% 68% 13% 18%
1	D	407	40% 58% 16% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AKG	A	501	-	-	X	-

2 Entry composition [i](#)

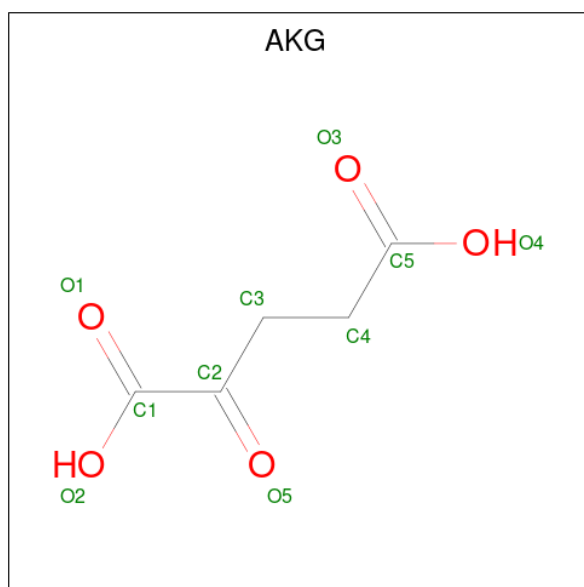
There are 6 unique types of molecules in this entry. The entry contains 10275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-oxoglutarate-dependent ethylene/succinate-forming enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	2	0
			2559	1640	441	464	14			
1	B	329	Total	C	N	O	S	0	0	0
			2563	1638	441	470	14			
1	C	335	Total	C	N	O	S	0	0	0
			2578	1652	443	469	14			
1	D	310	Total	C	N	O	S	0	0	0
			2233	1420	389	412	12			

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).



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

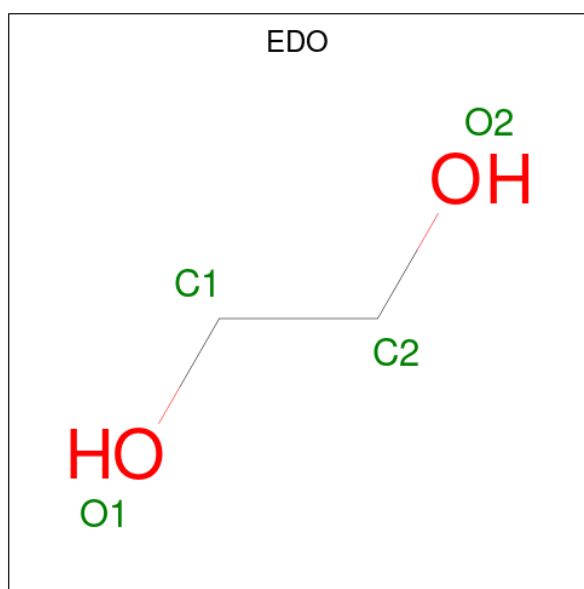
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

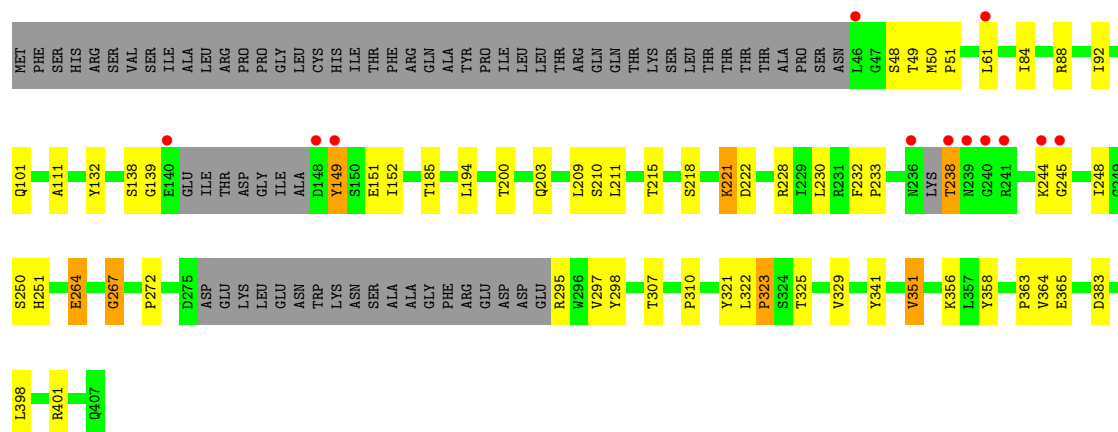
- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



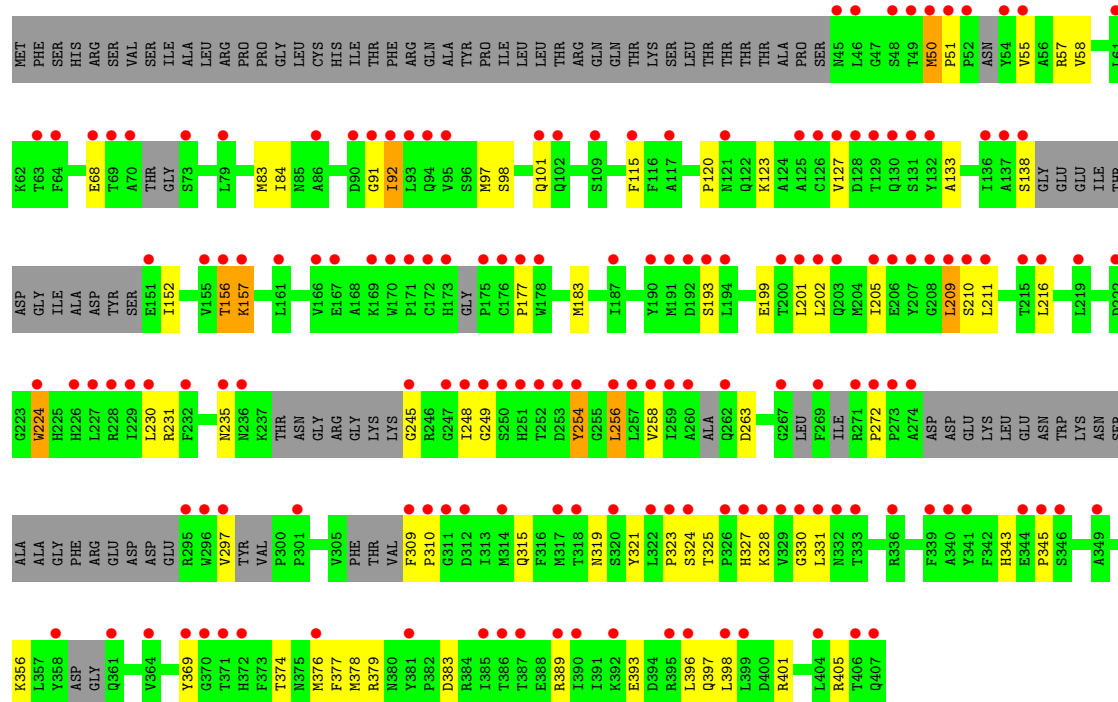
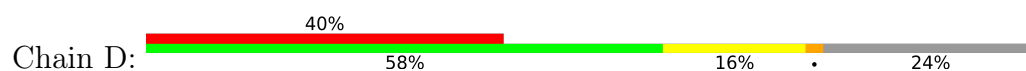
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	94	Total 94	O 94	0	0
6	B	94	Total 94	O 94	0	0
6	C	78	Total 78	O 78	0	0
6	D	46	Total 46	O 46	0	0



● Molecule 1: 2-oxoglutarate-dependent ethylene/succinate-forming enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.16Å 117.40Å 140.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.85 – 2.80 22.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (22.85-2.80) 99.2 (22.85-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.250 , 0.286 0.250 , 0.284	Depositor DCC
R_{free} test set	2089 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.1	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	0.88	EDS
Total number of atoms	10275	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, AKG, EDO, MN

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	0.57	3/2632 (0.1%)	0.87	10/3587 (0.3%)
1	B	0.46	0/2635	0.75	4/3587 (0.1%)
1	C	0.69	2/2652 (0.1%)	1.01	11/3613 (0.3%)
1	D	0.80	0/2290	1.23	12/3121 (0.4%)
All	All	0.64	5/10209 (0.0%)	0.97	37/13908 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	ALA	C-N	-9.21	1.22	1.33
1	C	250	SER	C-N	-8.39	1.21	1.33
1	A	252	THR	C-N	6.47	1.42	1.33
1	A	358	TYR	C-N	-6.18	1.25	1.33
1	C	251	HIS	C-N	-5.59	1.25	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	SER	N-CA-C	-7.32	103.49	113.30
1	A	355	ALA	CA-C-N	7.19	130.23	120.38
1	A	355	ALA	C-N-CA	7.19	130.23	120.38
1	D	224	TRP	N-CA-C	-7.11	98.91	109.15
1	A	49	THR	N-CA-C	-6.83	104.82	113.02
1	A	209	LEU	N-CA-C	-6.43	105.01	112.92
1	D	248	ILE	N-CA-C	-6.30	106.05	113.42
1	C	323	PRO	N-CA-C	6.27	120.49	110.40
1	D	327	HIS	CB-CA-C	-6.15	100.69	112.43
1	A	378	MET	N-CA-C	-6.06	102.26	110.68
1	C	321	TYR	N-CA-C	-5.97	104.69	111.14
1	A	122	GLN	N-CA-C	-5.95	104.92	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	PHE	CB-CA-C	5.94	116.90	108.76
1	D	68	GLU	N-CA-C	-5.93	106.20	113.50
1	C	48	SER	N-CA-C	-5.92	105.81	113.16
1	D	263	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	380	ASN	N-CA-C	-5.69	106.17	113.23
1	C	251	HIS	O-C-N	-5.68	117.14	123.04
1	C	358	TYR	N-CA-C	-5.66	106.18	112.57
1	D	50	MET	N-CA-C	5.60	122.18	109.81
1	D	328	LYS	CB-CA-C	-5.48	102.53	114.10
1	B	265	VAL	CA-C-N	-5.42	116.83	122.69
1	B	265	VAL	C-N-CA	-5.42	116.83	122.69
1	D	272	PRO	N-CA-C	5.40	117.28	110.70
1	B	253	ASP	CB-CA-C	5.29	119.27	109.54
1	A	358	TYR	CA-C-N	5.29	131.63	121.54
1	A	358	TYR	C-N-CA	5.29	131.63	121.54
1	C	264	GLU	N-CA-CB	-5.22	102.46	110.44
1	B	404	LEU	N-CA-C	-5.18	106.74	113.16
1	D	254	TYR	CA-C-N	-5.16	117.32	122.69
1	D	254	TYR	C-N-CA	-5.16	117.32	122.69
1	D	345	PRO	N-CA-C	5.11	118.38	111.22
1	C	221	LYS	CB-CA-C	5.10	117.92	110.26
1	A	182	ASP	CB-CA-C	5.10	119.90	109.55
1	C	222	ASP	CA-C-N	-5.05	115.54	120.34
1	C	222	ASP	C-N-CA	-5.05	115.54	120.34
1	D	177	PRO	N-CA-C	5.00	119.23	112.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	0	2458	41	0
1	B	2563	0	2468	43	0
1	C	2578	0	2464	35	0
1	D	2233	0	1944	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	4	4	0
2	C	10	0	4	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
5	D	4	0	6	0	0
6	A	94	0	0	8	0
6	B	94	0	0	3	0
6	C	78	0	0	6	0
6	D	46	0	0	11	0
All	All	10275	0	9348	162	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 8.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD23	1:A:351:VAL:HG22	1.23	1.20
1:A:219:LEU:CD2	1:A:351:VAL:HG22	1.73	1.19
1:B:230:LEU:HD13	1:B:232:PHE:CE2	1.81	1.15
1:D:258:VAL:HG23	6:D:632:HOH:O	1.68	0.93
1:B:230:LEU:CD1	1:B:232:PHE:CE2	2.56	0.89
1:A:378:MET:HG3	1:A:387:THR:HG23	1.53	0.88
1:A:184:ARG:O	1:A:188:GLN:HG2	1.72	0.88
1:A:219:LEU:HD23	1:A:351:VAL:CG2	2.05	0.85
1:C:152:ILE:HD11	1:C:228:ARG:HB3	1.58	0.85
1:B:230:LEU:HD12	1:B:230:LEU:O	1.75	0.84
1:D:330:GLY:O	1:D:331:LEU:HG	1.77	0.84
1:A:336:ARG:HH22	2:A:501:AKG:C1	1.93	0.81
1:B:229:ILE:HG22	1:B:339:PHE:CE1	2.15	0.81
1:B:379:ARG:HD3	6:B:628:HOH:O	1.82	0.80
1:D:97:MET:HE1	6:D:639:HOH:O	1.84	0.78
1:B:229:ILE:HG22	1:B:339:PHE:CD1	2.21	0.76
1:C:248:ILE:HG22	1:C:329:VAL:HB	1.68	0.74
1:B:230:LEU:HD11	1:B:338:ALA:HB3	1.73	0.70
1:B:219:LEU:HD13	1:B:351:VAL:HG22	1.74	0.69
1:A:336:ARG:NH1	2:A:501:AKG:O1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:THR:HA	6:C:622:HOH:O	1.92	0.69
1:A:264:GLU:HG3	6:A:622:HOH:O	1.95	0.67
1:D:224:TRP:HB3	1:D:369:TYR:HE2	1.61	0.66
1:D:254:TYR:HB3	1:D:376:MET:HE1	1.77	0.66
1:B:51:PRO:HG2	1:B:267:GLY:HA2	1.76	0.65
1:B:272:PRO:HG3	6:B:607:HOH:O	1.97	0.65
1:D:55:VAL:O	1:D:55:VAL:HG12	1.96	0.65
1:C:132:TYR:O	4:C:503:CL:CL	2.53	0.63
1:C:139:GLY:HA3	1:C:149:TYR:HB3	1.81	0.62
1:D:51:PRO:HG2	1:D:235:ASN:HB3	1.82	0.62
1:B:390:ILE:HG23	1:B:395:ARG:HB2	1.82	0.62
1:B:230:LEU:HD13	1:B:232:PHE:CZ	2.32	0.60
1:B:218:SER:HA	1:B:221:LYS:HE2	1.84	0.60
1:C:210:SER:O	1:C:356:LYS:NZ	2.35	0.60
1:D:101:GLN:HG2	1:D:193:SER:OG	2.03	0.59
1:B:230:LEU:CD1	1:B:232:PHE:HE2	2.10	0.59
1:A:378:MET:CG	1:A:387:THR:HG23	2.31	0.59
1:B:209:LEU:O	1:B:356:LYS:NZ	2.30	0.58
1:B:154:THR:HG1	1:B:228:ARG:HH21	1.51	0.58
1:B:154:THR:OG1	1:B:228:ARG:NH2	2.35	0.58
1:D:224:TRP:HB3	1:D:369:TYR:CE2	2.39	0.57
1:A:219:LEU:HD21	1:A:351:VAL:HG22	1.77	0.56
1:A:184:ARG:HG2	1:A:188:GLN:OE1	2.05	0.56
1:B:229:ILE:HG22	1:B:339:PHE:HE1	1.66	0.56
1:C:139:GLY:HA3	1:C:149:TYR:CG	2.40	0.56
1:B:238:THR:O	1:B:239:ASN:OD1	2.23	0.56
1:B:78:GLU:HA	1:B:81:LYS:NZ	2.21	0.56
1:D:152:ILE:HA	6:D:610:HOH:O	2.06	0.56
1:D:315:GLN:NE2	6:D:605:HOH:O	2.38	0.55
1:B:219:LEU:HD22	1:B:351:VAL:HG22	1.87	0.55
1:D:324:SER:CB	6:D:605:HOH:O	2.55	0.55
1:A:300:PRO:HD2	6:A:614:HOH:O	2.05	0.55
1:B:356:LYS:HG2	1:B:357:LEU:HD12	1.87	0.55
1:C:398:LEU:HD23	1:C:401:ARG:HD2	1.88	0.55
1:D:258:VAL:CG2	6:D:632:HOH:O	2.37	0.55
1:B:78:GLU:HA	1:B:81:LYS:HZ3	1.73	0.54
1:C:50:MET:HE2	1:C:298:TYR:HB2	1.89	0.54
1:C:139:GLY:HA3	1:C:149:TYR:CB	2.38	0.54
1:D:57:ARG:O	1:D:58:VAL:C	2.52	0.54
1:D:92:ILE:HG22	1:D:309:PHE:HB3	1.89	0.53
1:D:374:THR:HG22	1:D:378:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:LEU:HD23	1:C:401:ARG:HE	1.74	0.53
1:A:376:MET:O	1:A:379:ARG:HB3	2.09	0.52
1:D:120:PRO:HA	1:D:123:LYS:HE3	1.90	0.52
1:A:94:GLN:NE2	6:A:614:HOH:O	2.43	0.52
1:D:245:GLY:HA2	1:D:249:GLY:HA2	1.91	0.52
1:C:398:LEU:HD23	1:C:401:ARG:NE	2.24	0.52
1:D:83:MET:HE1	1:D:201:LEU:HD23	1.93	0.51
1:A:94:GLN:HG2	1:A:307:THR:HG22	1.91	0.51
1:A:264:GLU:CG	6:A:622:HOH:O	2.56	0.51
1:C:139:GLY:HA3	1:C:149:TYR:CD2	2.46	0.51
1:B:94:GLN:HG2	1:B:307:THR:HG22	1.92	0.50
1:D:199:GLU:HG3	1:D:343:HIS:NE2	2.27	0.50
1:C:111:ALA:CB	6:C:607:HOH:O	2.60	0.50
1:D:330:GLY:O	1:D:331:LEU:CG	2.55	0.50
1:A:210:SER:O	1:A:356:LYS:NZ	2.45	0.49
1:C:307:THR:CG2	6:C:611:HOH:O	2.60	0.49
1:D:230:LEU:HA	6:D:610:HOH:O	2.12	0.49
1:B:50:MET:HE3	1:B:269:PHE:HE1	1.78	0.49
1:B:310:PRO:HG2	1:B:323:PRO:O	2.12	0.49
1:C:398:LEU:CD2	1:C:401:ARG:HD2	2.42	0.49
1:C:351:VAL:HA	6:C:608:HOH:O	2.14	0.48
1:D:57:ARG:O	1:D:57:ARG:HG2	2.13	0.48
1:B:379:ARG:HB3	6:B:628:HOH:O	2.13	0.48
1:C:194:LEU:HD13	1:C:341:TYR:HB2	1.96	0.48
1:D:97:MET:CE	6:D:639:HOH:O	2.50	0.48
1:C:209:LEU:HB2	1:C:211:LEU:HG	1.95	0.48
1:C:398:LEU:HD23	1:C:401:ARG:CD	2.43	0.48
1:C:51:PRO:HG2	1:C:267:GLY:HA2	1.95	0.48
1:A:219:LEU:HD21	1:A:351:VAL:HA	1.96	0.48
1:B:219:LEU:HD13	1:B:351:VAL:CG2	2.43	0.47
1:B:153:PHE:HB3	1:B:229:ILE:HD11	1.97	0.47
1:C:61:LEU:HD21	1:C:92:ILE:HG23	1.95	0.47
1:A:162:ASP:OD1	1:A:162:ASP:N	2.36	0.47
1:A:344:GLU:HA	1:A:344:GLU:OE1	2.15	0.47
1:D:84:ILE:HD13	1:D:209:LEU:HD13	1.96	0.47
1:A:336:ARG:NH2	2:A:501:AKG:O1	2.48	0.47
1:B:233:PRO:O	1:B:331:LEU:HD22	2.14	0.47
1:A:194:LEU:HD22	1:A:259:ILE:HG21	1.96	0.46
1:D:91:GLY:CA	1:D:325:THR:HG21	2.45	0.46
1:A:374:THR:HG22	1:A:378:MET:HE3	1.97	0.46
1:B:230:LEU:CD1	1:B:338:ALA:HB3	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:PRO:HG2	1:C:323:PRO:O	2.16	0.46
1:B:132:TYR:O	4:B:502:CL:CL	2.71	0.46
1:D:310:PRO:HB2	1:D:323:PRO:O	2.15	0.46
1:C:272:PRO:HD2	1:C:295:ARG:O	2.16	0.46
1:A:102:GLN:OE1	1:A:304:GLY:HA2	2.16	0.45
1:D:389:ARG:O	1:D:393:GLU:HB2	2.16	0.45
1:B:229:ILE:HG22	1:B:339:PHE:HD1	1.78	0.45
1:D:209:LEU:HD11	1:D:321:TYR:CE2	2.52	0.45
1:C:363:PRO:HB2	1:C:365:GLU:HG2	1.98	0.45
1:B:84:ILE:HD12	1:B:208:GLY:HA3	1.98	0.45
1:D:157:LYS:HB3	1:D:157:LYS:HE2	1.78	0.44
1:A:243:LYS:HB3	1:A:246:ARG:HG2	1.98	0.44
1:C:111:ALA:HA	6:C:607:HOH:O	2.16	0.44
1:D:91:GLY:HA3	1:D:325:THR:HG21	1.99	0.44
1:C:233:PRO:HB2	1:C:238:THR:HG21	1.98	0.44
1:A:265:VAL:HB	1:A:336:ARG:HG3	1.99	0.44
1:B:250:SER:HB2	1:B:296:TRP:HZ2	1.83	0.44
1:A:259:ILE:HG23	1:A:306:PHE:CD1	2.53	0.44
1:A:66:LEU:HD11	1:A:201:LEU:HG	2.00	0.44
1:A:375:ASN:O	1:A:379:ARG:HB2	2.18	0.44
1:C:51:PRO:CG	1:C:267:GLY:HA2	2.47	0.44
1:C:264:GLU:CD	1:C:264:GLU:H	2.26	0.44
1:C:101:GLN:HB3	6:C:639:HOH:O	2.18	0.43
1:D:202:LEU:HD22	1:D:216:LEU:HD13	2.00	0.43
1:A:365:GLU:HG3	1:C:185:THR:HG21	1.99	0.43
1:D:115:PHE:CD1	1:D:183:MET:HE1	2.53	0.43
1:B:194:LEU:HD22	1:B:259:ILE:HG21	2.00	0.43
1:A:253:ASP:OD2	1:A:258:VAL:HG21	2.18	0.43
1:A:378:MET:HE2	1:A:390:ILE:HG21	2.00	0.43
1:A:375:ASN:HA	6:A:616:HOH:O	2.18	0.43
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.80	0.43
1:B:229:ILE:CG2	1:B:339:PHE:HE1	2.31	0.43
1:B:352:SER:HB3	1:B:366:LYS:HE3	2.01	0.43
1:A:407:GLN:NE2	6:A:620:HOH:O	2.52	0.42
1:C:218:SER:HA	1:C:221:LYS:HD2	2.00	0.42
1:A:253:ASP:OD1	1:A:327:HIS:CE1	2.71	0.42
1:D:231:ARG:N	6:D:610:HOH:O	2.53	0.42
1:D:315:GLN:CD	6:D:605:HOH:O	2.62	0.42
1:D:210:SER:HB3	1:D:356:LYS:NZ	2.34	0.42
1:C:244:LYS:O	1:C:245:GLY:C	2.63	0.42
1:B:118:MET:HE2	1:B:122:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:O	1:B:229:ILE:HG12	2.19	0.41
1:D:50:MET:O	1:D:51:PRO:C	2.63	0.41
1:D:133:ALA:HB2	1:D:156:THR:H	1.85	0.41
1:C:230:LEU:HD13	2:C:501:AKG:H31	2.02	0.41
1:D:84:ILE:HD11	1:D:205:ILE:HA	2.02	0.41
1:D:398:LEU:HA	1:D:401:ARG:HG3	2.02	0.41
1:B:115:PHE:O	1:B:118:MET:HB2	2.20	0.41
1:A:63:THR:N	6:A:617:HOH:O	2.46	0.41
1:D:209:LEU:HA	1:D:209:LEU:HD12	1.67	0.41
1:A:361:GLN:CB	6:A:603:HOH:O	2.68	0.41
1:B:51:PRO:CG	1:B:267:GLY:HA2	2.48	0.40
1:D:57:ARG:H	1:D:297:VAL:HA	1.87	0.40
1:B:50:MET:HE2	1:B:54:TYR:O	2.22	0.40
1:A:61:LEU:HD23	1:A:94:GLN:HG3	2.03	0.40
1:A:336:ARG:CZ	2:A:501:AKG:O1	2.70	0.40
1:A:378:MET:HE1	1:A:396:LEU:HD21	2.02	0.40
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.87	0.40
1:C:84:ILE:O	1:C:88:ARG:HG3	2.22	0.40
1:D:319:ASN:HB3	6:D:602:HOH:O	2.22	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	322/407 (79%)	307 (95%)	12 (4%)	3 (1%)	14	41
1	B	319/407 (78%)	306 (96%)	11 (3%)	2 (1%)	21	51
1	C	327/407 (80%)	312 (95%)	13 (4%)	2 (1%)	21	51
1	D	285/407 (70%)	256 (90%)	29 (10%)	0	100	100
All	All	1253/1628 (77%)	1181 (94%)	65 (5%)	7 (1%)	21	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	364	VAL
1	A	379	ARG
1	A	267	GLY
1	B	267	GLY
1	C	267	GLY
1	A	245	GLY
1	B	247	GLY

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	268/352 (76%)	253 (94%)	15 (6%)	19	50
1	B	272/352 (77%)	261 (96%)	11 (4%)	28	63
1	C	267/352 (76%)	256 (96%)	11 (4%)	27	62
1	D	205/352 (58%)	190 (93%)	15 (7%)	13	38
All	All	1012/1408 (72%)	960 (95%)	52 (5%)	21	54

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	60	GLN
1	A	62	LYS
1	A	71	THR
1	A	109	SER
1	A	151	GLU
1	A	185	THR
1	A	186	PRO
1	A	187	ILE
1	A	264	GLU
1	A	313	ILE
1	A	385	ILE
1	A	388	GLU

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Mol	Chain	Res	Type
1	A	397	GLN
1	A	398	LEU
1	B	55	VAL
1	B	81	LYS
1	B	136	ILE
1	B	138	SER
1	B	152	ILE
1	B	248	ILE
1	B	271	ARG
1	B	383	ASP
1	B	386	THR
1	B	400	ASP
1	B	403	GLU
1	C	49	THR
1	C	149	TYR
1	C	151	GLU
1	C	203	GLN
1	C	215	THR
1	C	238	THR
1	C	297	VAL
1	C	322	LEU
1	C	325	THR
1	C	351	VAL
1	C	383	ASP
1	D	92	ILE
1	D	98	SER
1	D	127	VAL
1	D	138	SER
1	D	156	THR
1	D	157	LYS
1	D	209	LEU
1	D	211	LEU
1	D	256	LEU
1	D	377	PHE
1	D	379	ARG
1	D	383	ASP
1	D	396	LEU
1	D	397	GLN
1	D	405	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	94	GLN
1	A	236	ASN
1	A	348	GLN
1	A	407	GLN
1	B	380	ASN
1	D	101	GLN
1	D	188	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
2	AKG	C	501	3	9,9,9	1.34	1 (11%)	11,11,11	2.51	2 (18%)
5	EDO	D	501	-	3,3,3	0.13	0	2,2,2	0.08	0
2	AKG	A	501	3	9,9,9	2.44	2 (22%)	11,11,11	2.28	4 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AKG	C	501	3	-	4/9/9/9	-
5	EDO	D	501	-	-	0/1/1/1	-
2	AKG	A	501	3	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AKG	C2-C1	-6.28	1.44	1.53
2	A	501	AKG	O2-C1	-2.85	1.22	1.30
2	C	501	AKG	O2-C1	-2.78	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	AKG	C3-C2-C1	6.81	127.42	115.86
2	A	501	AKG	C3-C2-C1	4.59	123.66	115.86
2	A	501	AKG	O1-C1-C2	-3.74	117.16	121.81
2	C	501	AKG	O5-C2-C1	-3.20	115.10	119.67
2	A	501	AKG	O4-C5-C4	2.58	122.16	114.00
2	A	501	AKG	O5-C2-C1	-2.08	116.70	119.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	AKG	O2-C1-C2-C3
2	C	501	AKG	O1-C1-C2-O5
2	C	501	AKG	O1-C1-C2-C3
2	C	501	AKG	O2-C1-C2-O5

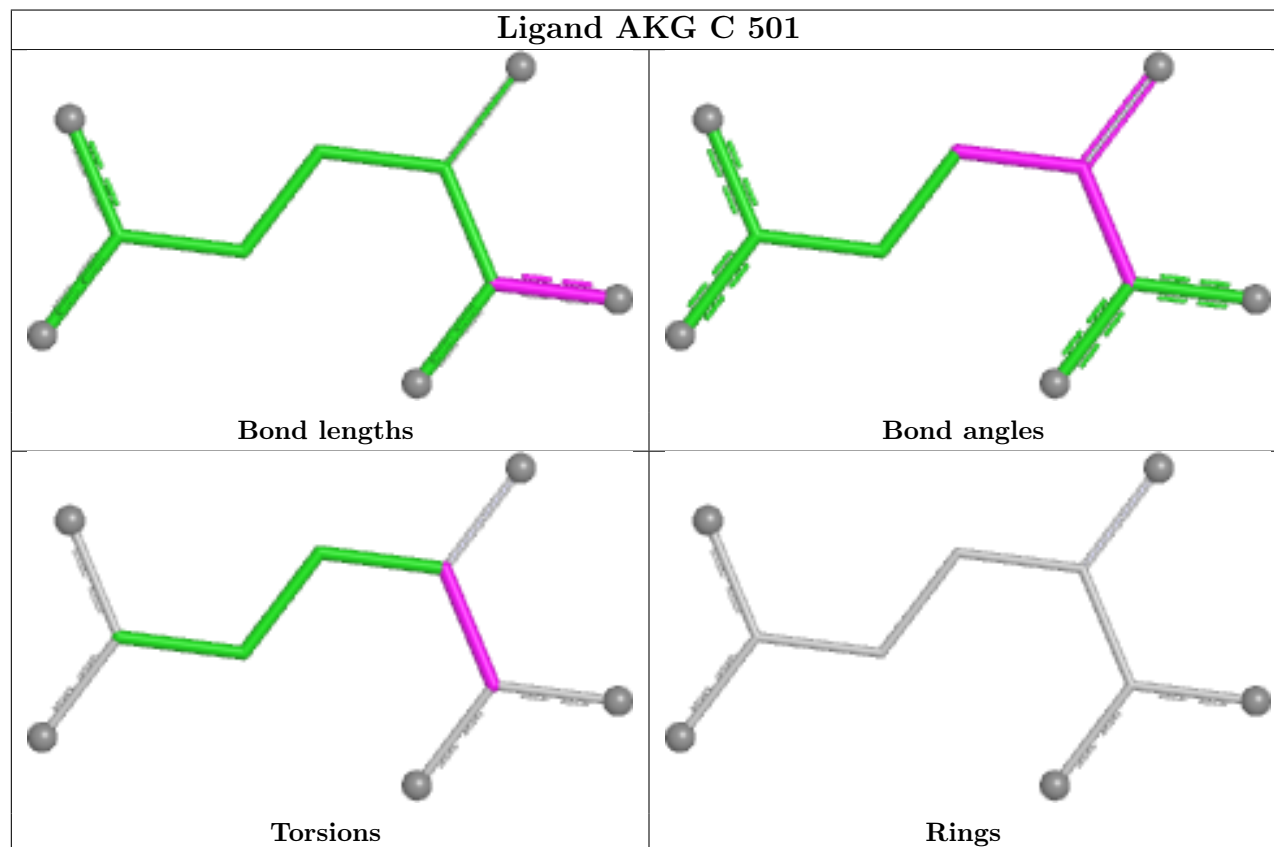
There are no ring outliers.

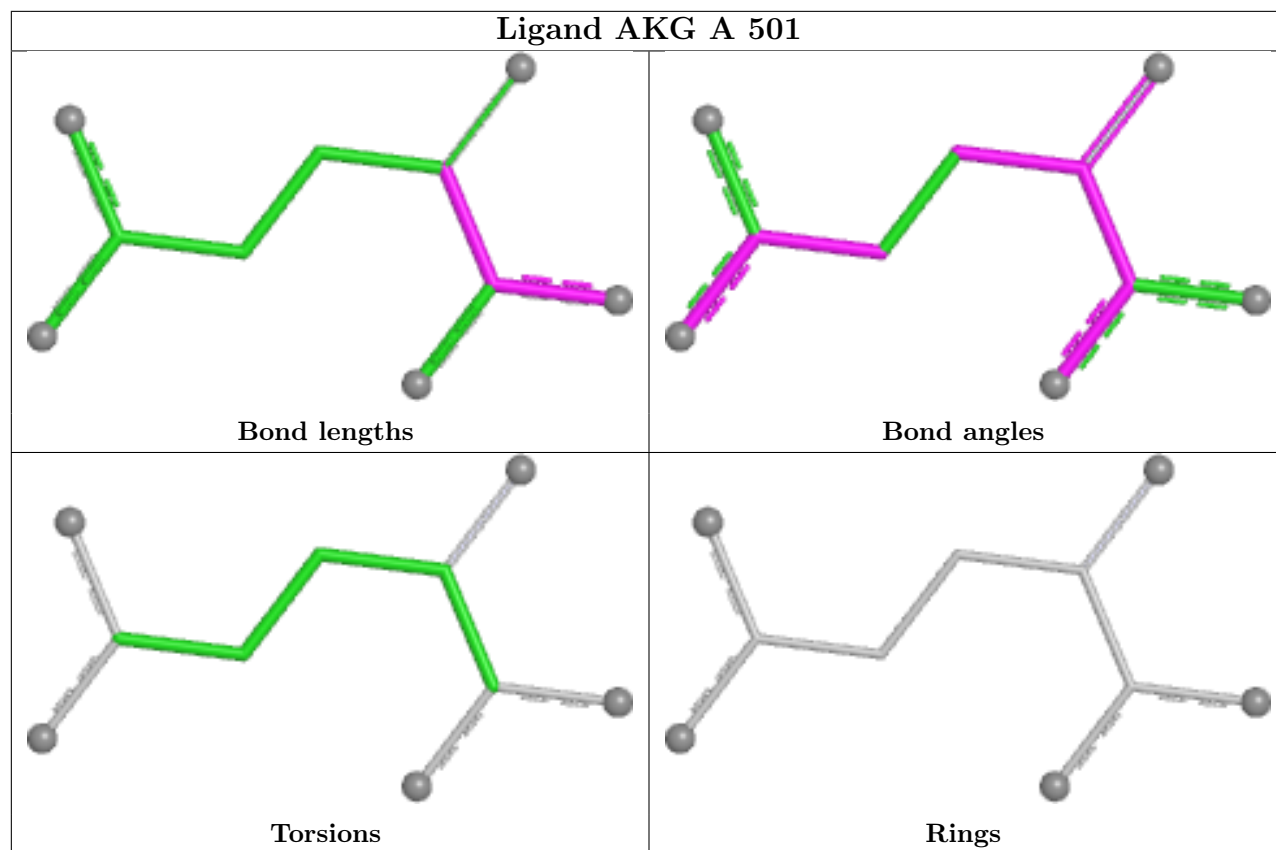
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	AKG	1	0
2	A	501	AKG	4	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	328/407 (80%)	0.25	10 (3%)	52 42	16, 35, 66, 98	2 (0%)
1	B	329/407 (80%)	0.18	12 (3%)	46 37	23, 35, 66, 130	0
1	C	335/407 (82%)	0.34	12 (3%)	46 37	21, 38, 80, 133	0
1	D	310/407 (76%)	2.13	161 (51%)	0 0	48, 75, 102, 128	0
All	All	1302/1628 (79%)	0.70	195 (14%)	5 4	16, 41, 92, 133	2 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	241	ARG	5.0
1	D	207	TYR	4.8
1	C	238	THR	4.8
1	C	245	GLY	4.8
1	D	310	PRO	4.7
1	D	205	ILE	4.6
1	D	256	LEU	4.5
1	D	331	LEU	4.5
1	D	49	THR	4.4
1	C	239	ASN	4.4
1	D	309	PHE	4.4
1	D	259	ILE	4.4
1	D	257	LEU	4.4
1	C	240	GLY	4.4
1	D	253	ASP	4.3
1	D	70	ALA	4.3
1	B	295	ARG	4.3
1	D	339	PHE	4.3
1	D	329	VAL	4.3
1	D	399	LEU	4.3
1	D	50	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	4.2
1	D	254	TYR	4.2
1	D	156	THR	4.1
1	C	244	LYS	4.1
1	D	236	ASN	4.1
1	A	149	TYR	3.9
1	B	230	LEU	3.9
1	D	404	LEU	3.9
1	D	248	ILE	3.9
1	D	330	GLY	3.9
1	D	235	ASN	3.8
1	D	208	GLY	3.8
1	D	172	CYS	3.8
1	D	52	PRO	3.8
1	D	129	THR	3.7
1	D	90	ASP	3.7
1	D	250	SER	3.6
1	D	201	LEU	3.6
1	D	245	GLY	3.6
1	D	192	ASP	3.6
1	D	274	ALA	3.5
1	D	389	ARG	3.5
1	D	93	LEU	3.5
1	D	51	PRO	3.5
1	D	95	VAL	3.5
1	B	48	SER	3.5
1	D	324	SER	3.4
1	C	149	TYR	3.4
1	D	295	ARG	3.4
1	D	125	ALA	3.4
1	D	138	SER	3.4
1	D	314	MET	3.4
1	D	361	GLN	3.4
1	D	45	ASN	3.3
1	D	173	HIS	3.3
1	D	301	PRO	3.3
1	D	200	THR	3.3
1	D	252	THR	3.3
1	D	336	ARG	3.3
1	A	244	LYS	3.3
1	B	146	ILE	3.3
1	D	136	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	215	THR	3.2
1	B	147	ALA	3.2
1	A	245	GLY	3.2
1	C	46	LEU	3.1
1	D	46	LEU	3.1
1	D	269	PHE	3.1
1	D	371	THR	3.1
1	D	262	GLN	3.1
1	B	239	ASN	3.1
1	D	219	LEU	3.1
1	D	332	ASN	3.1
1	D	296	TRP	3.0
1	B	237	LYS	3.0
1	D	385	ILE	3.0
1	D	202	LEU	3.0
1	D	216	LEU	3.0
1	D	258	VAL	3.0
1	D	297	VAL	3.0
1	D	131	SER	2.9
1	D	271	ARG	2.9
1	B	247	GLY	2.9
1	D	91	GLY	2.9
1	D	224	TRP	2.9
1	D	323	PRO	2.9
1	D	157	LYS	2.9
1	D	349	ALA	2.9
1	D	390	ILE	2.9
1	D	396	LEU	2.9
1	D	407	GLN	2.9
1	A	378	MET	2.9
1	D	230	LEU	2.9
1	C	236	ASN	2.8
1	D	232	PHE	2.8
1	D	320	SER	2.8
1	D	317	MET	2.8
1	D	102	GLN	2.8
1	D	386	THR	2.8
1	D	249	GLY	2.8
1	D	54	TYR	2.8
1	D	358	TYR	2.8
1	D	64	PHE	2.8
1	D	137	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	2.8
1	D	229	ILE	2.8
1	D	327	HIS	2.8
1	D	170	TRP	2.7
1	D	178	TRP	2.7
1	D	345	PRO	2.7
1	B	364	VAL	2.7
1	D	92	ILE	2.6
1	D	387	THR	2.6
1	A	180	ASP	2.6
1	D	260	ALA	2.6
1	D	376	MET	2.6
1	D	132	TYR	2.6
1	D	190	TYR	2.6
1	D	311	GLY	2.6
1	D	392	LYS	2.6
1	D	63	THR	2.6
1	D	251	HIS	2.5
1	D	273	PRO	2.5
1	D	369	TYR	2.5
1	D	73	SER	2.5
1	D	171	PRO	2.5
1	D	247	GLY	2.5
1	D	128	ASP	2.5
1	D	312	ASP	2.5
1	C	61	LEU	2.5
1	D	55	VAL	2.5
1	D	267	GLY	2.4
1	D	48	SER	2.4
1	D	211	LEU	2.4
1	D	210	SER	2.4
1	D	130	GLN	2.4
1	D	395	ARG	2.4
1	D	227	LEU	2.4
1	B	49	THR	2.4
1	D	333	THR	2.4
1	D	406	THR	2.4
1	D	209	LEU	2.4
1	B	248	ILE	2.4
1	D	166	VAL	2.3
1	A	48	SER	2.3
1	D	79	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	169	LYS	2.3
1	D	115	PHE	2.3
1	D	94	GLN	2.3
1	D	101	GLN	2.3
1	D	193	SER	2.3
1	D	372	HIS	2.3
1	D	341	TYR	2.3
1	D	175	PRO	2.3
1	D	127	VAL	2.3
1	D	370	GLY	2.3
1	D	326	PRO	2.3
1	D	191	MET	2.3
1	D	161	LEU	2.3
1	D	203	GLN	2.3
1	D	222	ASP	2.3
1	D	322	LEU	2.3
1	D	109	SER	2.3
1	D	86	ALA	2.2
1	D	151	GLU	2.2
1	D	340	ALA	2.2
1	D	344	GLU	2.2
1	A	129	THR	2.2
1	B	265	VAL	2.2
1	D	68	GLU	2.2
1	D	69	THR	2.2
1	C	140	GLU	2.2
1	D	167	GLU	2.2
1	D	226	HIS	2.2
1	A	394	ASP	2.2
1	D	318	THR	2.2
1	D	176	CYS	2.2
1	D	381	TYR	2.2
1	A	236	ASN	2.1
1	D	272	PRO	2.1
1	D	398	LEU	2.1
1	D	187	ILE	2.1
1	D	328	LYS	2.1
1	D	194	LEU	2.1
1	D	206	GLU	2.1
1	D	155	VAL	2.1
1	D	121	ASN	2.1
1	D	228	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	117	ALA	2.1
1	D	126	CYS	2.0
1	D	61	LEU	2.0
1	D	346	SER	2.0
1	D	364	VAL	2.0
1	D	177	PRO	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](#)

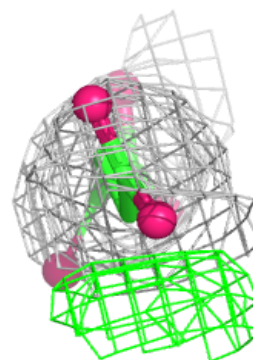
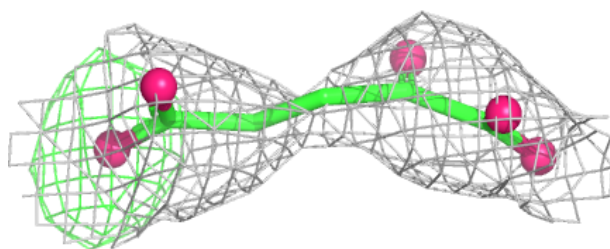
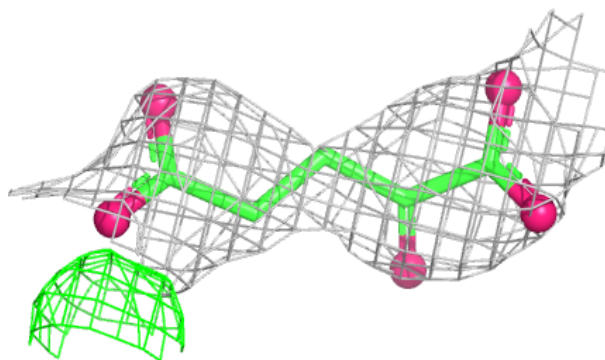
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	D	501	4/4	0.76	0.24	58,59,60,72	0
4	CL	B	502	1/1	0.77	0.15	42,42,42,42	1
2	AKG	C	501	10/10	0.80	0.17	41,46,48,53	0
3	MN	C	502	1/1	0.81	0.10	36,36,36,36	0
3	MN	D	502	1/1	0.83	0.11	80,80,80,80	0
2	AKG	A	501	10/10	0.86	0.19	31,41,48,52	0
4	CL	C	503	1/1	0.88	0.16	41,41,41,41	1
3	MN	B	501	1/1	0.92	0.10	35,35,35,35	0
3	MN	A	502	1/1	0.92	0.06	25,25,25,25	0

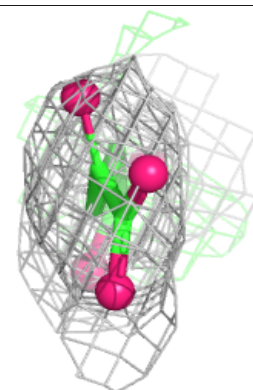
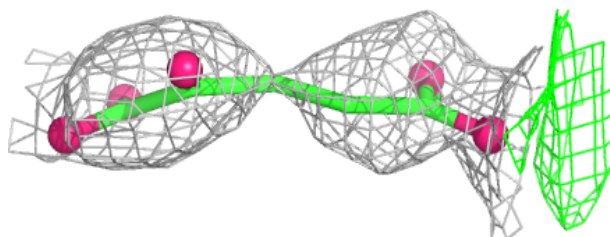
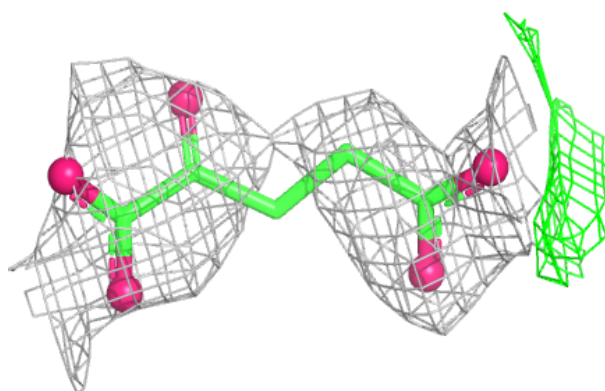
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AKG C 501:

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

**Electron density around AKG A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.