



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 08:10 PM JST

PDB ID : 8ZKA / pdb_00008zka
Title : Crystal structure of the Decarboxylase KDC4427 in complex with phenylpyruvic acid intermediate
Authors : Dong, S.; Liu, L.; Zhang, H.
Deposited on : 2024-05-15
Resolution : 1.95 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

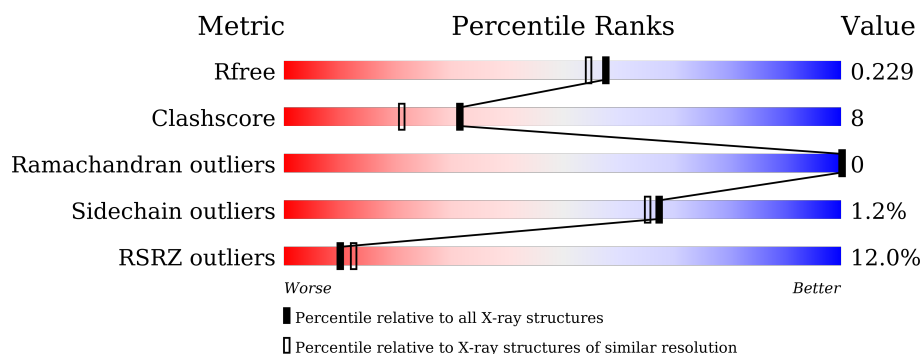
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	566	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	B	566	<div> <div>13%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9303 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 Indolepyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4092	2595	712	763	22			
1	B	539	Total	C	N	O	S	0	0	0
			4118	2611	716	769	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A2U3EYQ2
A	-12	GLY	-	expression tag	UNP A0A2U3EYQ2
A	-11	SER	-	expression tag	UNP A0A2U3EYQ2
A	-10	SER	-	expression tag	UNP A0A2U3EYQ2
A	-9	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-8	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-7	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-6	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-5	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-4	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-3	SER	-	expression tag	UNP A0A2U3EYQ2
A	-2	GLN	-	expression tag	UNP A0A2U3EYQ2
A	-1	ASP	-	expression tag	UNP A0A2U3EYQ2
A	0	PRO	-	expression tag	UNP A0A2U3EYQ2
B	-13	MET	-	initiating methionine	UNP A0A2U3EYQ2
B	-12	GLY	-	expression tag	UNP A0A2U3EYQ2
B	-11	SER	-	expression tag	UNP A0A2U3EYQ2
B	-10	SER	-	expression tag	UNP A0A2U3EYQ2
B	-9	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-8	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-7	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-6	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-5	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-4	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-3	SER	-	expression tag	UNP A0A2U3EYQ2

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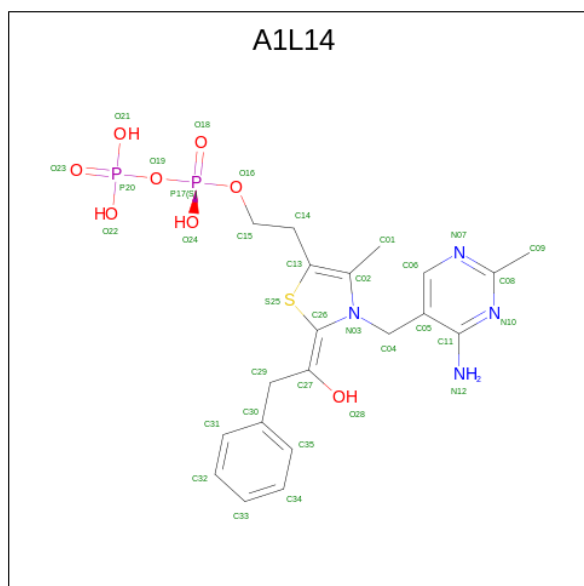
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP A0A2U3EYQ2
B	-1	ASP	-	expression tag	UNP A0A2U3EYQ2
B	0	PRO	-	expression tag	UNP A0A2U3EYQ2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 2-[(2 {E})-3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-2-(1-oxidanyl-2-phenyl-ethylidene)-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (CCD ID: A1L14) (formula: C₂₀H₂₆N₄O₈P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			35	20	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			35	20	4	8	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	524	Total 524	O 524	0	0
4	B	497	Total 497	O 497	0	0

- Molecule 1: Indolepyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.41Å 170.12Å 115.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.06 – 1.95 85.06 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.4 (85.06-1.95) 85.8 (85.06-1.95)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.207 , 0.230 0.208 , 0.229	Depositor DCC
R_{free} test set	96074 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9303	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MG, A1L14

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	6/4185 (0.1%)	0.48	3/5703 (0.1%)
1	B	0.43	4/4213 (0.1%)	0.53	4/5743 (0.1%)
All	All	0.42	10/8398 (0.1%)	0.51	7/11446 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	515	GLU	C-O	-8.13	1.14	1.24
1	B	289	ASP	C-O	-7.04	1.16	1.24
1	A	340	HIS	CA-C	6.14	1.55	1.52
1	A	339	VAL	C-O	-5.61	1.18	1.23
1	B	478	TYR	C-O	-5.57	1.16	1.24
1	A	198	PHE	C-O	-5.40	1.17	1.24
1	A	199	ARG	C-O	-5.39	1.17	1.24
1	B	454	HIS	C-O	-5.07	1.17	1.24
1	A	444	GLU	C-O	-5.07	1.17	1.24
1	A	469	ARG	C-O	-5.07	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	VAL	N-CA-C	-8.45	102.10	110.30
1	B	442	ILE	N-CA-C	6.97	118.56	110.62
1	A	339	VAL	CB-CA-C	-6.52	104.25	111.35
1	A	442	ILE	N-CA-C	6.40	117.92	110.62
1	A	341	ASP	N-CA-C	6.33	118.46	110.24
1	B	472	HIS	N-CA-C	5.78	117.19	108.46
1	B	445	LEU	N-CA-C	-5.32	104.89	111.33

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	4092	0	4024	59	0
1	B	4118	0	4049	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	35	0	0	1	0
3	B	35	0	0	3	0
4	A	524	0	0	16	1
4	B	497	0	0	14	1
All	All	9303	0	8073	131	1

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 (131) 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:546:LEU:HD21	4:B:1135:HOH:O	1.45	1.17
1:A:344:VAL:HG22	1:A:345:PRO:HD2	1.14	1.12
1:A:344:VAL:HG22	1:A:345:PRO:CD	1.99	0.91
1:A:344:VAL:CG2	1:A:345:PRO:HD2	2.01	0.91
1:A:466:THR:HA	1:A:469:ARG:HG3	1.50	0.91
1:B:546:LEU:CD2	4:B:1135:HOH:O	2.11	0.85
1:A:469:ARG:NH2	1:A:532:LYS:HE2	2.00	0.77
1:B:211:ARG:HA	4:B:785:HOH:O	1.87	0.75
1:B:454:HIS:NE2	1:B:498:GLN:OE1	2.19	0.73
1:A:272:GLU:OE2	4:A:701:HOH:O	2.06	0.72
1:A:124:ARG:NH1	4:A:706:HOH:O	2.23	0.70
1:B:122:GLU:OE1	4:B:701:HOH:O	2.10	0.70
1:B:476:GLN:HA	1:B:476:GLN:OE1	1.92	0.69
1:B:21:ASP:OD2	1:B:66:LYS:NZ	2.26	0.69
1:A:275:GLU:OE1	4:A:702:HOH:O	2.11	0.68
1:A:466:THR:OG1	3:A:602:A1L14:O21	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLN:OE1	4:A:703:HOH:O	2.12	0.66
1:A:143:GLN:HG3	4:A:1031:HOH:O	1.96	0.66
1:B:539:LEU:O	1:B:543:THR:HG23	1.97	0.64
1:B:467:VAL:HG11	3:B:602:A1L14:S25	2.38	0.64
1:A:105:THR:O	1:A:109:GLN:HG3	1.98	0.64
1:B:464:GLY:HA2	1:B:481:ILE:HG12	1.80	0.63
1:A:396:PRO:HG3	4:A:1101:HOH:O	1.98	0.63
1:B:544:LYS:NZ	4:B:707:HOH:O	2.33	0.62
1:A:158:ARG:NH1	4:A:704:HOH:O	2.14	0.61
1:A:464:GLY:HA2	1:A:481:ILE:HG12	1.82	0.60
1:B:54:ASN:HB3	1:B:444:GLU:HG2	1.84	0.59
1:A:16:THR:OG1	4:A:705:HOH:O	2.16	0.59
1:B:539:LEU:HA	1:B:542:ILE:HG22	1.83	0.59
1:B:33:GLN:HE22	1:B:173:LYS:NZ	2.02	0.58
1:B:194:CYS:HB3	4:B:1007:HOH:O	2.04	0.56
1:A:396:PRO:HD2	1:A:399:VAL:HG21	1.88	0.56
1:B:444:GLU:O	1:B:447:SER:N	2.39	0.55
1:B:506:GLU:HB2	1:B:509:GLN:HG3	1.88	0.55
1:A:226:LYS:HE3	4:A:971:HOH:O	2.07	0.55
1:A:344:VAL:CG2	1:A:345:PRO:CD	2.74	0.55
1:A:131:GLU:HB2	1:A:137:GLN:HE22	1.72	0.54
1:A:223:HIS:CD2	1:A:324:MET:HE1	2.43	0.54
1:B:255:VAL:HG22	1:B:343:PRO:HG2	1.90	0.53
1:B:131:GLU:HG2	1:B:137:GLN:HE22	1.73	0.53
1:A:83:MET:SD	1:B:83:MET:SD	3.07	0.53
1:A:33:GLN:HB3	1:A:173:LYS:HE2	1.91	0.53
1:A:293:ALA:HA	1:A:542:ILE:HD13	1.91	0.52
1:B:226:LYS:O	1:B:230:GLN:HG3	2.08	0.52
1:B:122:GLU:HG2	1:B:125:HIS:CE1	2.45	0.52
1:A:536:PRO:HD2	1:A:539:LEU:HB3	1.92	0.52
1:B:131:GLU:HG2	1:B:137:GLN:NE2	2.24	0.51
1:B:196:LYS:NZ	1:B:200:ASP:OD2	2.42	0.51
1:B:522:ARG:NH2	4:B:718:HOH:O	2.43	0.51
1:A:341:ASP:N	1:A:341:ASP:OD1	2.44	0.50
1:A:245:MET:HG3	1:A:405:PRO:HG2	1.94	0.50
1:A:122:GLU:HG2	1:A:125:HIS:CE1	2.45	0.50
1:B:97:LEU:HD22	1:B:153:LEU:HD21	1.94	0.50
1:B:128:HIS:O	1:B:131:GLU:HG3	2.12	0.50
1:B:373:ILE:HD12	1:B:396:PRO:HD3	1.93	0.49
1:B:534:ASP:HB3	4:B:724:HOH:O	2.12	0.49
1:B:122:GLU:HB2	4:B:701:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLY:HA3	1:B:545:ALA:HB1	1.93	0.49
1:A:338:HIS:C	4:A:710:HOH:O	2.56	0.48
1:A:535:ILE:HG23	1:A:539:LEU:HB3	1.93	0.48
1:B:465:TYR:O	1:B:469:ARG:HG3	2.12	0.48
1:A:339:VAL:O	1:A:339:VAL:HG12	2.11	0.48
1:A:203:GLU:HB2	1:A:334:LEU:HD22	1.96	0.48
1:B:173:LYS:NZ	4:B:726:HOH:O	2.47	0.47
1:B:466:THR:HA	1:B:469:ARG:HG3	1.96	0.47
1:B:498:GLN:O	1:B:522:ARG:HB3	2.13	0.47
1:A:218:PHE:CG	1:A:245:MET:HE2	2.50	0.47
1:A:544:LYS:HA	1:A:544:LYS:HD3	1.61	0.47
1:B:266:SER:HB2	1:B:271:LYS:HG3	1.97	0.47
1:A:10:TYR:CE2	1:A:179:PRO:HG3	2.50	0.47
1:A:336:LYS:HA	1:A:339:VAL:HG23	1.97	0.47
1:B:385:THR:HG23	3:B:602:A1L14:O22	2.14	0.46
1:A:340:HIS:CE1	4:A:985:HOH:O	2.67	0.46
1:A:218:PHE:HB3	1:A:245:MET:HB3	1.96	0.46
1:B:211:ARG:HD3	4:B:759:HOH:O	2.15	0.46
1:A:218:PHE:CD1	1:A:245:MET:HE2	2.51	0.46
1:A:293:ALA:HA	1:A:542:ILE:CD1	2.46	0.46
1:B:160:ARG:HD2	1:B:222:ARG:O	2.16	0.45
1:B:498:GLN:O	1:B:498:GLN:HG2	2.17	0.45
1:B:128:HIS:HA	1:B:131:GLU:HG3	1.99	0.45
1:B:5:TYR:CD2	1:B:178:PRO:HG3	2.52	0.45
1:A:287:PHE:HB3	1:A:292:THR:HG21	1.99	0.44
1:A:339:VAL:HA	4:A:710:HOH:O	2.17	0.44
1:B:396:PRO:HD2	1:B:399:VAL:HG21	1.98	0.44
1:B:503:ARG:HD3	1:B:527:GLU:OE1	2.17	0.44
1:B:232:TRP:HE1	1:B:238:MET:HE1	1.82	0.44
1:A:425:PRO:HB3	4:A:774:HOH:O	2.17	0.44
1:A:160:ARG:HD2	1:A:222:ARG:O	2.18	0.44
1:A:15:LEU:HD11	1:A:70:ALA:HB2	1.99	0.43
1:A:506:GLU:HB2	1:A:509:GLN:HG3	1.99	0.43
1:A:214:LEU:O	1:A:240:HIS:HA	2.19	0.43
4:A:1169:HOH:O	1:B:546:LEU:HD11	2.17	0.43
1:B:218:PHE:HB3	1:B:245:MET:HB3	2.00	0.43
1:A:210:LYS:HA	1:A:210:LYS:HD2	1.75	0.43
1:B:346:SER:OG	1:B:394:ARG:NH2	2.50	0.43
1:B:355:GLN:N	1:B:356:PRO:HD2	2.32	0.43
1:B:322:ILE:HG13	4:B:1007:HOH:O	2.18	0.43
1:B:279:THR:HA	1:B:303:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:HG13	1:B:345:PRO:HD2	2.01	0.43
1:B:544:LYS:HB3	1:B:544:LYS:HE3	1.67	0.43
1:A:12:LEU:HD22	1:A:44:ILE:HG21	2.01	0.43
1:B:56:SER:OG	1:B:85:GLY:HA3	2.18	0.43
1:B:245:MET:HG3	1:B:405:PRO:HG2	2.01	0.43
1:B:470:ALA:HB1	1:B:543:THR:HG21	2.00	0.43
1:B:223:HIS:CD2	1:B:324:MET:HE1	2.53	0.42
1:A:503:ARG:HD3	1:A:527:GLU:OE1	2.19	0.42
1:B:467:VAL:HG12	3:B:602:A1L14:O23	2.20	0.42
1:B:144:ASN:HA	1:B:147:TYR:CE2	2.55	0.42
1:B:208:MET:HE2	1:B:208:MET:HB3	1.91	0.42
1:A:435:ASP:OD1	1:A:435:ASP:N	2.50	0.42
1:B:10:TYR:CE1	1:B:179:PRO:HG3	2.55	0.42
1:B:214:LEU:O	1:B:240:HIS:HA	2.20	0.42
1:B:388:PHE:CD2	1:B:539:LEU:HD13	2.55	0.42
1:B:16:THR:HG22	1:B:44:ILE:HD11	2.01	0.42
1:A:205:ARG:NH1	1:A:279:THR:OG1	2.53	0.41
1:A:106:ALA:O	1:A:110:ARG:HG3	2.21	0.41
1:B:212:THR:O	4:B:702:HOH:O	2.22	0.41
1:B:232:TRP:NE1	1:B:238:MET:HE1	2.36	0.41
1:B:435:ASP:OD1	1:B:435:ASP:N	2.52	0.41
1:B:522:ARG:O	4:B:703:HOH:O	2.22	0.41
1:B:542:ILE:HA	1:B:545:ALA:HB2	2.02	0.41
1:B:178:PRO:HA	1:B:179:PRO:HD3	1.98	0.41
1:B:232:TRP:CD2	1:B:332:VAL:HG22	2.56	0.41
1:B:469:ARG:HD3	1:B:474:PRO:O	2.21	0.41
1:B:532:LYS:HB2	1:B:532:LYS:HE2	1.64	0.41
1:A:462:ASN:ND2	1:A:466:THR:OG1	2.54	0.41
1:A:511:ALA:O	1:A:515:GLU:HG3	2.21	0.41
1:A:206:LEU:HD21	1:A:281:LEU:HD21	2.03	0.40
1:A:421:GLN:HG2	1:A:453:GLN:HB3	2.03	0.40
1:A:83:MET:HB2	4:A:872:HOH:O	2.20	0.40
1:A:254:HIS:CE1	4:A:799:HOH:O	2.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1138:HOH:O	4:B:1130:HOH:O[8_555]	2.12	0.08

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	531/566 (94%)	519 (98%)	12 (2%)	0	100	100
1	B	535/566 (94%)	525 (98%)	10 (2%)	0	100	100
All	All	1066/1132 (94%)	1044 (98%)	22 (2%)	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	426/458 (93%)	420 (99%)	6 (1%)	62	59
1	B	430/458 (94%)	426 (99%)	4 (1%)	75	75
All	All	856/916 (93%)	846 (99%)	10 (1%)	67	65

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

Mol	Chain	Res	Type
1	A	199	ARG
1	A	341	ASP
1	A	344	VAL
1	A	444	GLU
1	A	467	VAL
1	A	542	ILE
1	B	359	SER
1	B	444	GLU

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Mol	Chain	Res	Type
1	B	467	VAL
1	B	468	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	137	GLN
1	A	181	ASN
1	A	254	HIS
1	A	337	GLN
1	A	340	HIS
1	B	33	GLN
1	B	137	GLN
1	B	230	GLN
1	B	254	HIS
1	B	439	GLN
1	B	519	HIS

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	A1L14	B	602	2	34,37,37	1.58	7 (20%)	40,54,54	1.75	8 (20%)
3	A1L14	A	602	2	34,37,37	1.56	5 (14%)	40,54,54	1.83	7 (17%)

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	A1L14	B	602	2	-	4/20/25/25	0/3/3/3
3	A1L14	A	602	2	-	5/20/25/25	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	A1L14	C11-N12	4.25	1.44	1.34
3	A	602	A1L14	C11-N12	4.08	1.44	1.34
3	A	602	A1L14	C02-N03	-3.60	1.33	1.39
3	B	602	A1L14	C02-N03	-3.49	1.33	1.39
3	B	602	A1L14	O28-C27	3.23	1.41	1.32
3	A	602	A1L14	O28-C27	3.14	1.40	1.32
3	B	602	A1L14	C01-C02	2.72	1.53	1.49
3	A	602	A1L14	C29-C27	2.61	1.53	1.49
3	A	602	A1L14	C01-C02	2.39	1.53	1.49
3	B	602	A1L14	C29-C27	2.31	1.53	1.49
3	B	602	A1L14	C11-N10	-2.23	1.31	1.35
3	B	602	A1L14	C05-C11	-2.01	1.39	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	A1L14	C02-C13-S25	-6.70	104.59	110.59
3	B	602	A1L14	C02-C13-S25	-6.16	105.07	110.59
3	A	602	A1L14	C04-N03-C02	-4.69	119.12	125.01
3	B	602	A1L14	C04-N03-C02	-4.08	119.88	125.01
3	A	602	A1L14	C14-C13-S25	4.02	127.84	119.20
3	B	602	A1L14	C14-C13-S25	3.71	127.18	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	A1L14	C06-N07-C08	2.91	120.92	115.96
3	A	602	A1L14	C06-N07-C08	2.88	120.86	115.96
3	A	602	A1L14	C09-C08-N07	2.70	120.11	117.14
3	B	602	A1L14	P17-O19-P20	-2.68	123.63	132.83
3	A	602	A1L14	N07-C08-N10	-2.64	121.00	125.54
3	B	602	A1L14	C05-C06-N07	-2.44	119.75	123.82
3	B	602	A1L14	C09-C08-N07	2.39	119.77	117.14
3	B	602	A1L14	N07-C08-N10	-2.34	121.51	125.54
3	A	602	A1L14	P17-O19-P20	-2.06	125.76	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	A1L14	P17-O19-P20-O21
3	B	602	A1L14	P17-O19-P20-O21
3	B	602	A1L14	O28-C27-C29-C30
3	A	602	A1L14	O28-C27-C29-C30
3	A	602	A1L14	C27-C29-C30-C35
3	A	602	A1L14	P17-O19-P20-O22
3	B	602	A1L14	P17-O19-P20-O22
3	A	602	A1L14	C15-O16-P17-O18
3	B	602	A1L14	C15-O16-P17-O18

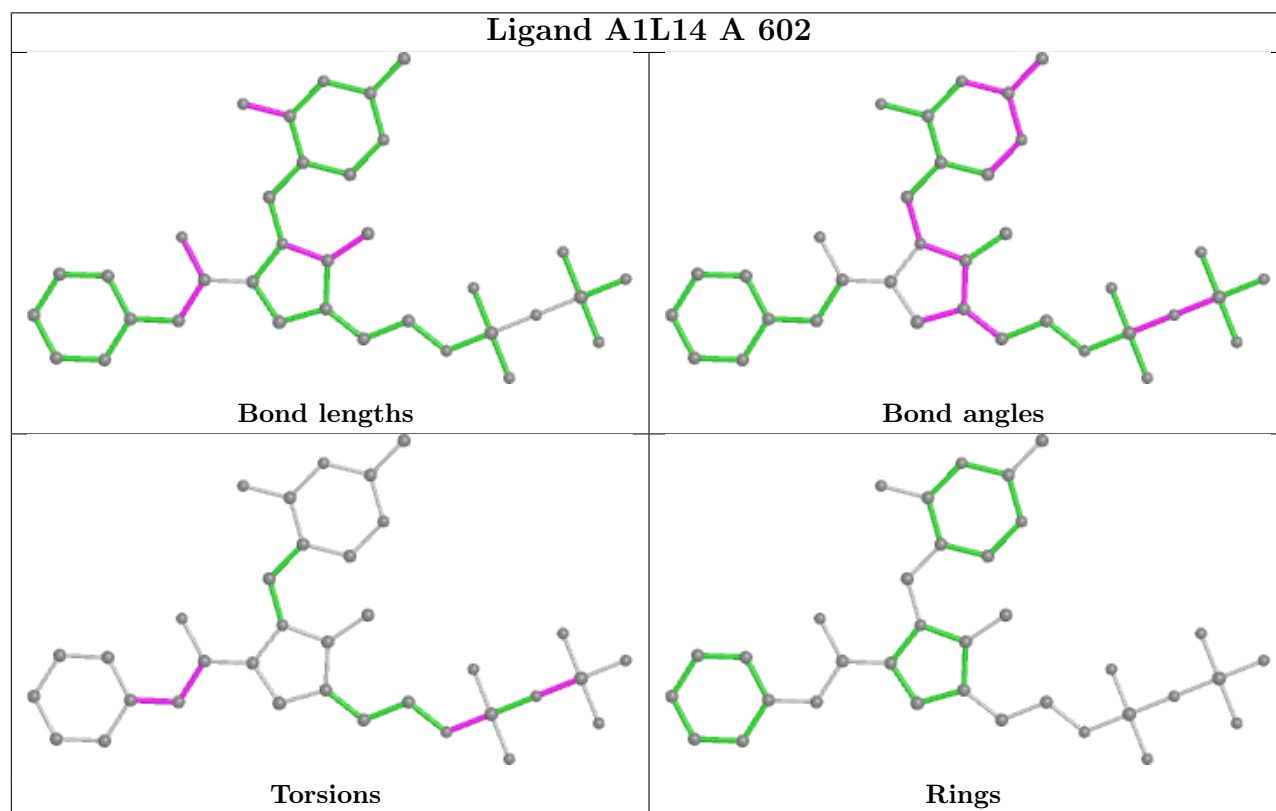
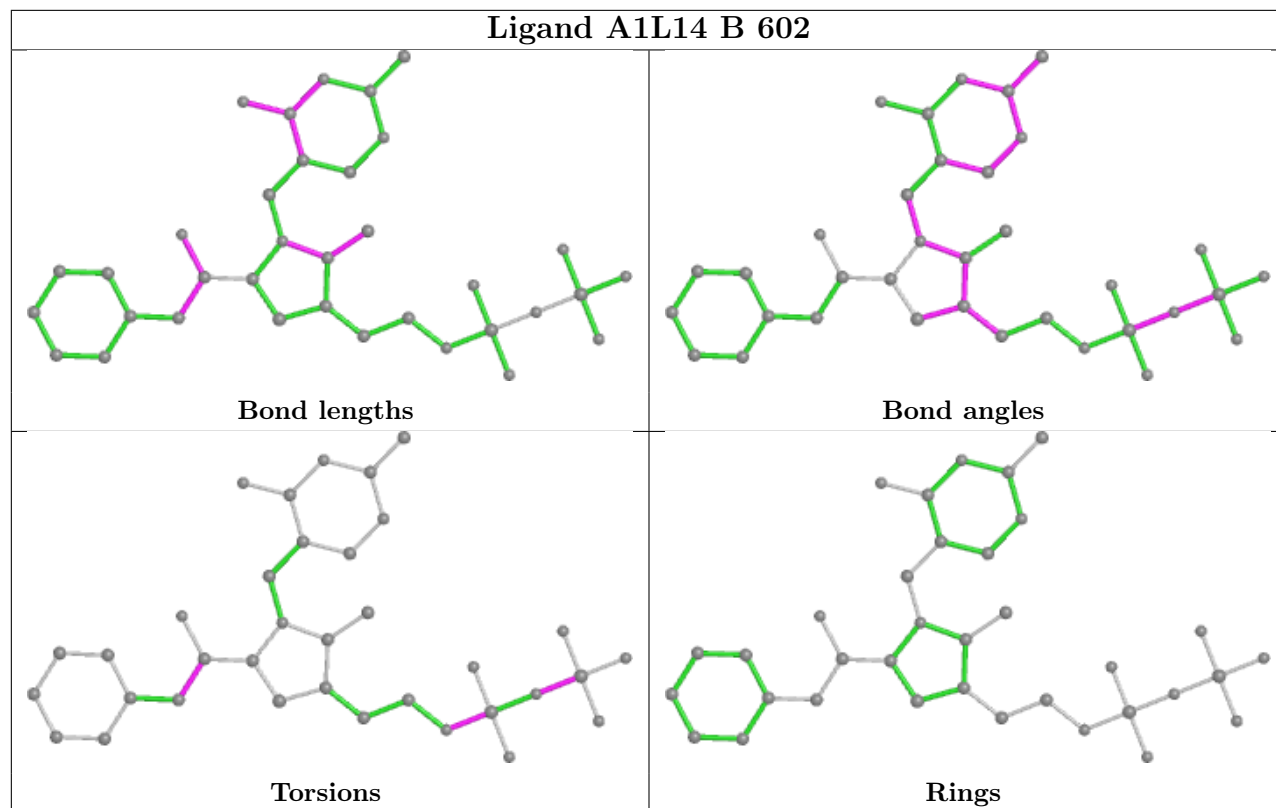
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	A1L14	3	0
3	A	602	A1L14	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	535/566 (94%)	0.78	58 (10%) 12 15	12, 23, 52, 105	0
1	B	539/566 (95%)	0.91	71 (13%) 8 10	12, 24, 57, 107	0
All	All	1074/1132 (94%)	0.85	129 (12%) 10 12	12, 23, 54, 107	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	ALA	9.8
1	A	546	LEU	9.0
1	A	344	VAL	9.0
1	B	548	ALA	8.5
1	B	546	LEU	8.3
1	A	343	PRO	8.2
1	B	539	LEU	7.9
1	A	345	PRO	7.7
1	B	541	ALA	7.5
1	B	542	ILE	7.1
1	B	538	LEU	7.0
1	B	540	GLY	6.9
1	B	467	VAL	6.4
1	A	542	ILE	6.3
1	B	545	ALA	6.3
1	B	3	THR	6.3
1	B	357	ASP	6.1
1	A	339	VAL	6.1
1	A	342	THR	6.0
1	B	537	PRO	5.8
1	A	470	ALA	5.7
1	A	341	ASP	5.7
1	A	541	ALA	5.6
1	A	535	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	356	PRO	5.4
1	A	539	LEU	5.3
1	B	470	ALA	5.3
1	B	477	ARG	5.3
1	A	543	THR	5.2
1	B	388	PHE	5.2
1	A	467	VAL	5.2
1	B	471	ILE	5.1
1	B	547	GLU	4.9
1	A	544	LYS	4.9
1	B	466	THR	4.9
1	A	547	GLU	4.8
1	B	474	PRO	4.7
1	A	471	ILE	4.7
1	A	340	HIS	4.7
1	B	544	LYS	4.7
1	A	540	GLY	4.6
1	B	543	THR	4.5
1	B	535	ILE	4.5
1	A	545	ALA	4.5
1	A	475	GLU	4.4
1	B	355	GLN	4.4
1	B	345	PRO	4.4
1	B	185	LEU	4.4
1	B	475	GLU	4.4
1	A	3	THR	4.4
1	B	187	HIS	4.4
1	B	533	ALA	4.4
1	A	187	HIS	4.3
1	A	388	PHE	4.2
1	A	536	PRO	4.1
1	B	346	SER	4.0
1	B	347	SER	4.0
1	B	498	GLN	4.0
1	A	537	PRO	3.9
1	B	478	TYR	3.9
1	A	538	LEU	3.9
1	A	254	HIS	3.8
1	A	533	ALA	3.8
1	A	466	THR	3.7
1	B	385	THR	3.7
1	B	186	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	516	LYS	3.6
1	A	357	ASP	3.6
1	B	4	PRO	3.6
1	A	227	HIS	3.5
1	B	532	LYS	3.4
1	B	536	PRO	3.4
1	B	344	VAL	3.3
1	B	387	ALA	3.3
1	B	473	GLY	3.3
1	A	473	GLY	3.2
1	A	189	HIS	3.2
1	A	188	ALA	3.2
1	B	472	HIS	3.2
1	A	474	PRO	3.1
1	B	468	GLU	3.1
1	B	469	ARG	3.0
1	B	394	ARG	3.0
1	B	534	ASP	3.0
1	B	183	LEU	2.9
1	A	185	LEU	2.8
1	B	476	GLN	2.7
1	A	531	PRO	2.7
1	B	211	ARG	2.6
1	B	343	PRO	2.6
1	B	398	ASP	2.6
1	B	465	TYR	2.6
1	B	254	HIS	2.6
1	A	532	LYS	2.5
1	B	452	LYS	2.5
1	B	204	ASN	2.5
1	A	358	GLY	2.5
1	A	507	ALA	2.5
1	B	15	LEU	2.4
1	B	479	ASN	2.4
1	A	387	ALA	2.4
1	A	186	ARG	2.4
1	A	477	ARG	2.4
1	B	531	PRO	2.4
1	B	255	VAL	2.4
1	A	398	ASP	2.3
1	A	472	HIS	2.3
1	A	464	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	338	HIS	2.2
1	B	40	ASP	2.2
1	B	386	SER	2.2
1	A	478	TYR	2.2
1	A	468	GLU	2.2
1	B	188	ALA	2.1
1	A	4	PRO	2.1
1	B	481	ILE	2.1
1	A	83	MET	2.1
1	B	190	ALA	2.1
1	B	179	PRO	2.1
1	A	465	TYR	2.1
1	A	359	SER	2.1
1	A	302	SER	2.1
1	B	342	THR	2.1
1	B	234	LYS	2.0
1	B	298	GLN	2.0
1	A	264	SER	2.0
1	B	147	TYR	2.0
1	B	189	HIS	2.0
1	A	394	ARG	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 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(\AA^2)	Q<0.9
3	A1L14	B	602	35/35	0.94	0.12	10,24,55,59	0
3	A1L14	A	602	35/35	0.95	0.12	15,26,59,66	0

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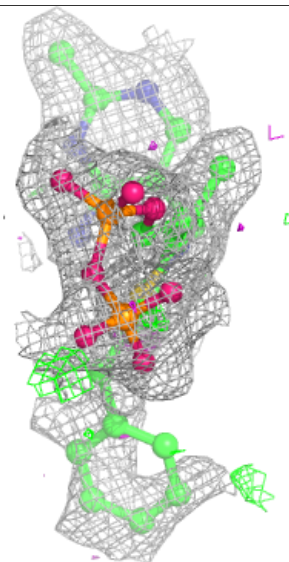
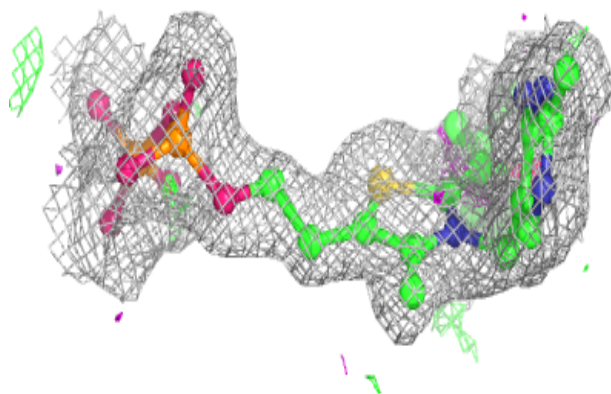
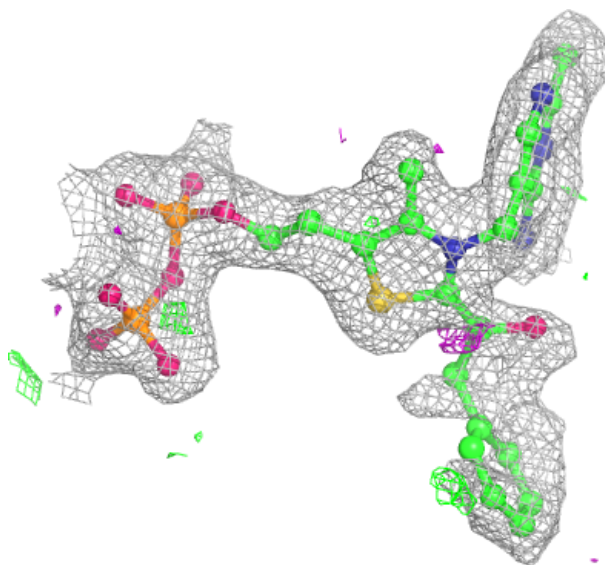
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	601	1/1	0.97	0.11	20,20,20,20	0
2	MG	B	601	1/1	0.98	0.08	15,15,15,15	0

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.

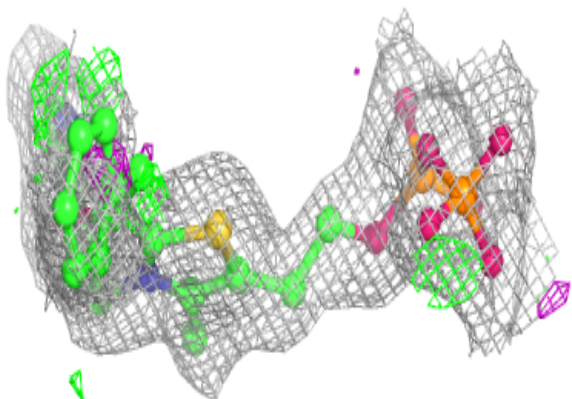
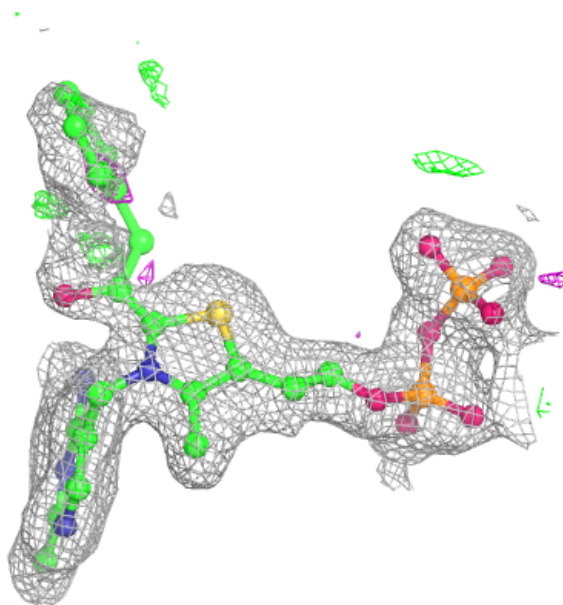
Electron density around A1L14 B 602:

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



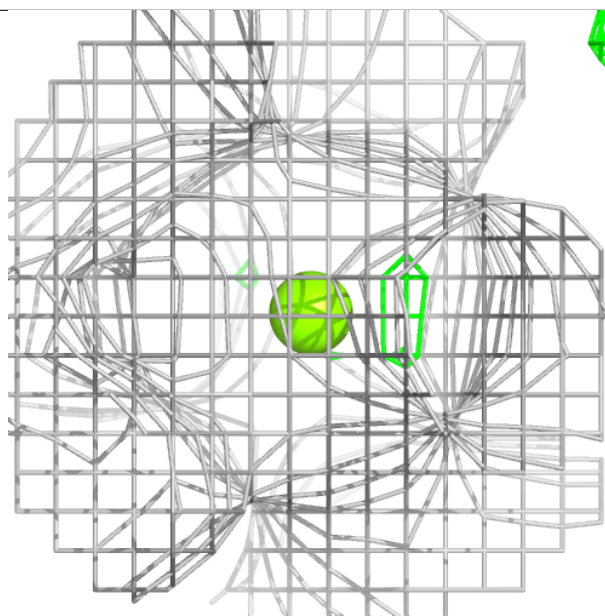
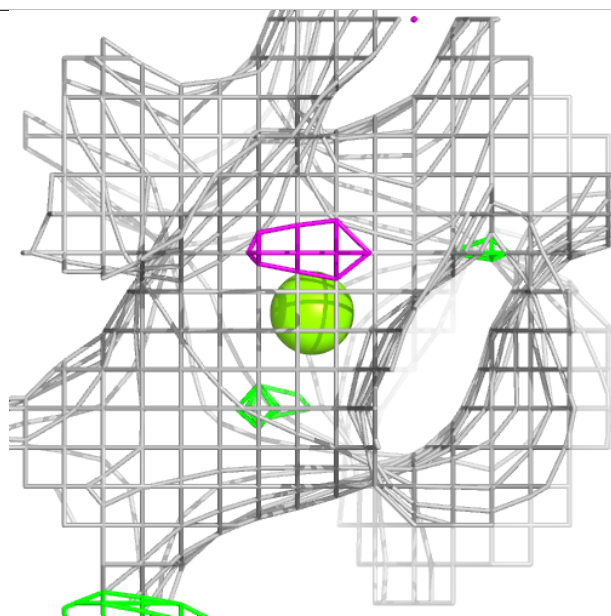
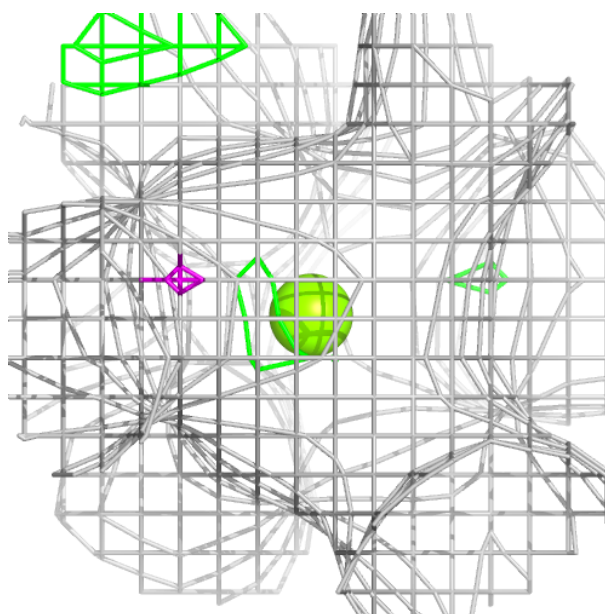
Electron density around A1L14 A 602:

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



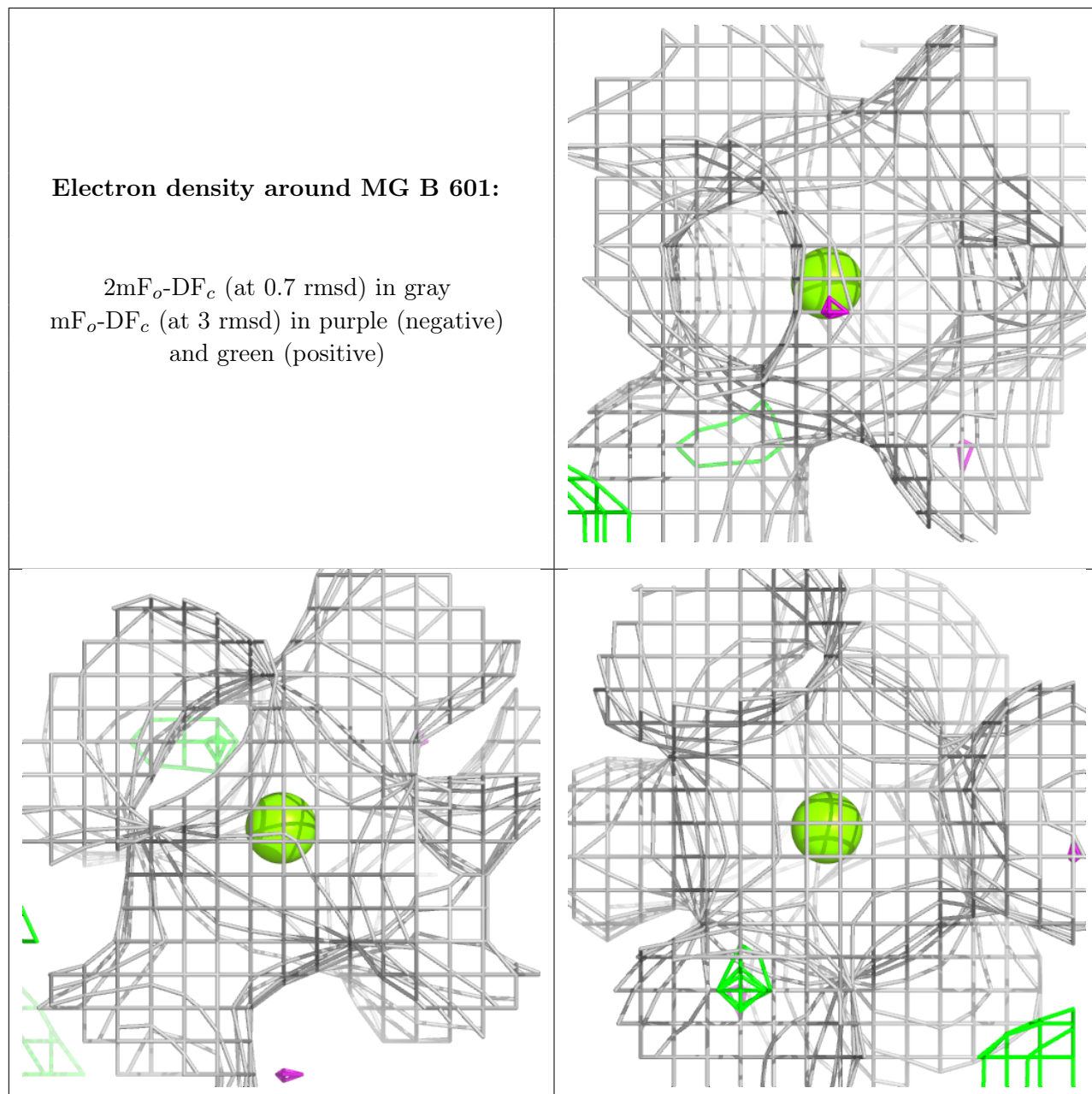
Electron density around MG A 601:

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



Electron density around MG B 601:

$2mF_o-DF_c$ (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.