



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:47 PM UTC

PDB ID : 9DUI / pdb_00009dui
Title : Re-refined of Crystal structure of dopa decarboxylase in complex with the inhibitor carbidopa (1JS3) with ketoenamine form of carbidopa
Authors : Doukov, I.T.; Berkowitz, B.D.
Deposited on : 2024-10-03
Resolution : 2.25 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

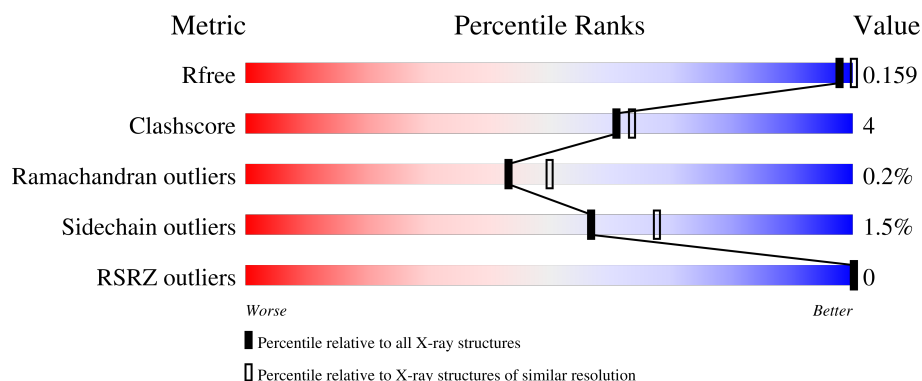
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	487	 84% 11% . .
1	B	487	 84% 10% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7996 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.

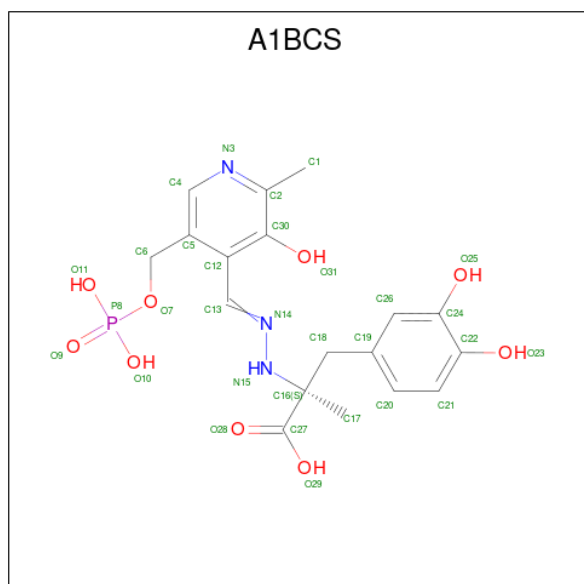
- Molecule 1 is a protein called Aromatic-L-amino-acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	5	0
			3668	2356	635	651	26			
1	B	467	Total	C	N	O	S	0	5	0
			3667	2355	633	653	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P80041
B	0	ACE	-	acetylation	UNP P80041

- Molecule 2 is (2S)-3-(3,4-dihydroxyphenyl)-2-[(2E)-2-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene)hydrazin-1-yl]-2-methylpropanoic acid (CCD ID: A1BCS) (formula: C₁₈H₂₂N₃O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	18	3	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	18	3	9	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

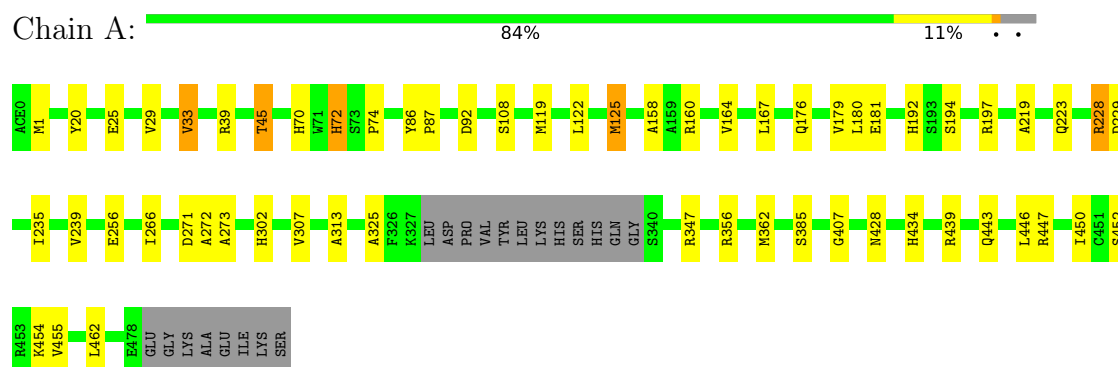
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	284	Total	O	0	0
			284	284		

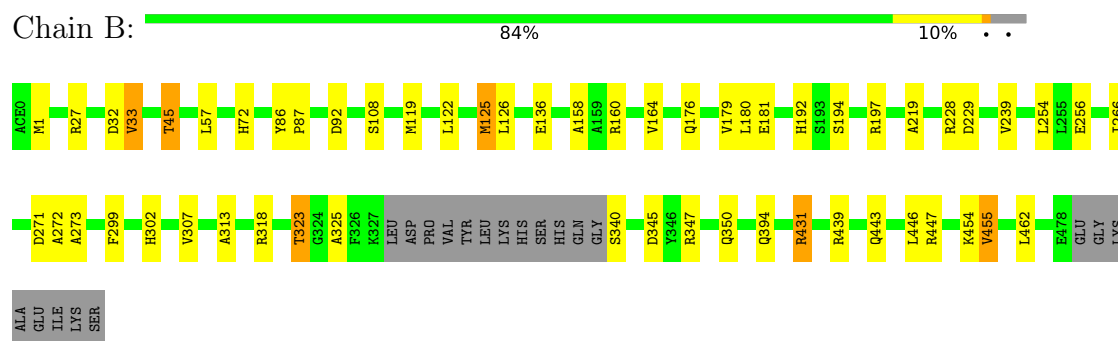
3 Residue-property plots

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: Aromatic-L-amino-acid decarboxylase



• Molecule 1: Aromatic-L-amino-acid decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	154.36Å 154.36Å 86.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.61 – 2.25 19.61 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.61-2.25) 95.8 (19.61-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.117 , 0.154 0.129 , 0.159	Depositor DCC
R_{free} test set	2540 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: SO4, ACE, A1BCS

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	0.70	0/3770	1.06	9/5104 (0.2%)
1	B	0.71	1/3769 (0.0%)	1.07	11/5103 (0.2%)
All	All	0.70	1/7539 (0.0%)	1.07	20/10207 (0.2%)

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	4
1	B	0	5
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	C-N	6.02	1.42	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	THR	CA-CB-OG1	-7.53	98.31	109.60
1	A	45	THR	CA-CB-OG1	-7.24	98.74	109.60
1	A	125	MET	CG-SD-CE	-7.19	85.09	100.90
1	A	72	HIS	CA-CB-CG	-7.03	106.77	113.80
1	B	136	GLU	CB-CG-CD	6.98	124.47	112.60
1	B	394	GLN	CB-CA-C	-6.85	96.57	109.72
1	B	125	MET	CG-SD-CE	-6.42	86.78	100.90
1	A	181	GLU	CB-CA-C	-6.39	98.80	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	O-C-N	-6.31	112.91	123.00
1	B	33	VAL	N-CA-CB	-6.19	98.39	110.45
1	A	33	VAL	N-CA-CB	-5.94	98.86	110.45
1	B	72	HIS	CA-CB-CG	-5.93	107.86	113.80
1	B	45	THR	CA-CB-OG1	-5.86	100.81	109.60
1	B	181	GLU	CB-CA-C	-5.74	100.02	110.63
1	A	45	THR	OG1-CB-CG2	5.73	120.76	109.30
1	B	45	THR	N-CA-CB	-5.70	100.92	111.53
1	B	455	VAL	N-CA-CB	5.36	119.14	110.13
1	A	228	ARG	CD-NE-CZ	5.20	131.67	124.40
1	A	39	ARG	CD-NE-CZ	5.10	131.53	124.40
1	B	45	THR	OG1-CB-CG2	5.03	119.37	109.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ARG	Sidechain
1	A	347	ARG	Sidechain
1	A	356	ARG	Sidechain
1	A	447	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	27	ARG	Sidechain
1	B	318	ARG	Sidechain
1	B	347	ARG	Sidechain
1	B	447	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	3668	0	3658	34	0
1	B	3667	0	3652	29	0
2	A	31	0	0	1	0
2	B	31	0	0	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	295	0	0	5	0
4	B	284	0	0	4	0
All	All	7996	0	7310	62	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 (62) 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:428:ASN:OD1	4:A:601:HOH:O	2.00	0.79
1:B:160:ARG:O	1:B:164:VAL:HG23	1.87	0.74
1:A:160:ARG:O	1:A:164:VAL:HG23	1.89	0.72
1:B:164:VAL:HG22	1:B:179:VAL:HG11	1.76	0.68
1:B:164:VAL:HG21	1:B:176:GLN:HE22	1.59	0.68
1:A:164:VAL:HG21	1:A:176[A]:GLN:HE22	1.59	0.67
1:A:164:VAL:HG22	1:A:179:VAL:HG11	1.78	0.65
1:A:20:TYR:OH	1:A:70:HIS:HD2	1.80	0.63
1:A:434:HIS:HE1	4:A:647:HOH:O	1.83	0.60
1:A:70:HIS:HE1	4:A:618:HOH:O	1.84	0.58
1:B:340:SER:N	4:B:604:HOH:O	2.37	0.57
1:B:219:ALA:HB2	1:B:256:GLU:HB3	1.89	0.54
1:B:119:MET:HE1	1:B:313:ALA:HB1	1.90	0.53
1:A:219:ALA:HB2	1:A:256:GLU:HB3	1.92	0.52
1:A:119:MET:HE1	1:A:313:ALA:HB1	1.92	0.51
1:B:158:ALA:HA	1:B:325:ALA:HB2	1.92	0.51
1:B:302:HIS:HA	1:B:307:VAL:O	2.10	0.51
1:A:302:HIS:HA	1:A:307:VAL:O	2.11	0.50
1:A:164:VAL:HG21	1:A:176[A]:GLN:NE2	2.25	0.50
1:A:192:HIS:HD2	1:A:194:SER:OG	1.95	0.50
1:B:32:ASP:OD1	1:B:431:ARG:NH1	2.43	0.49
1:A:452:SER:O	1:A:455:VAL:HG12	2.14	0.48
1:A:158:ALA:HA	1:A:325:ALA:HB2	1.95	0.48
1:B:192:HIS:HD2	1:B:194:SER:OG	1.96	0.47
1:B:271:ASP:OD2	2:B:501:A1BCS:N3	2.46	0.47
1:A:25:GLU:HG2	1:A:74:PRO:HG2	1.97	0.46
1:A:450:ILE:HG23	1:A:455:VAL:HG11	1.98	0.45
1:A:72:HIS:HD2	4:A:841:HOH:O	1.99	0.45
1:B:454:LYS:HE2	1:B:454:LYS:HA	1.98	0.45
1:A:446:LEU:N	1:A:446:LEU:HD12	2.33	0.45
1:B:228:ARG:HD2	1:B:229:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TYR:N	1:A:87:PRO:CD	2.81	0.44
1:B:164:VAL:CG2	1:B:176:GLN:HE22	2.29	0.44
1:B:350:GLN:OE1	4:B:601:HOH:O	2.21	0.44
1:B:122:LEU:HA	1:B:125:MET:HE3	1.99	0.44
1:A:239:VAL:HG23	1:A:266:ILE:HG21	1.99	0.43
1:B:86:TYR:N	1:B:87:PRO:CD	2.81	0.43
1:A:228:ARG:HD2	1:A:229:ASP:OD1	2.17	0.43
1:B:446:LEU:HD12	1:B:446:LEU:N	2.34	0.43
1:B:126:LEU:HD11	1:B:299:PHE:CE1	2.54	0.43
1:A:180:LEU:HD22	1:B:180:LEU:HD12	1.99	0.43
1:B:192:HIS:CD2	1:B:194:SER:H	2.37	0.43
1:B:462[B]:LEU:HG	4:B:774:HOH:O	2.19	0.42
1:B:239:VAL:HG23	1:B:266:ILE:HG21	2.00	0.42
1:A:167:LEU:HD11	1:A:235:ILE:HD13	2.00	0.42
1:A:439:ARG:HA	1:A:443:GLN:O	2.19	0.42
1:A:272:ALA:O	1:A:273:ALA:C	2.62	0.42
1:A:164:VAL:CG2	1:A:176[A]:GLN:HE22	2.29	0.41
1:B:345:ASP:O	1:B:345:ASP:CG	2.60	0.41
1:B:454:LYS:HA	1:B:454:LYS:CE	2.51	0.41
1:A:271:ASP:OD2	2:A:501:A1BCS:N3	2.53	0.41
1:A:122:LEU:HA	1:A:125:MET:HE3	2.03	0.41
1:A:454:LYS:CE	1:A:454:LYS:HA	2.50	0.41
1:B:272:ALA:O	1:B:273:ALA:C	2.64	0.41
1:B:439:ARG:HA	1:B:443:GLN:O	2.21	0.41
1:B:340:SER:CA	4:B:604:HOH:O	2.68	0.41
1:A:122:LEU:HD22	1:A:362:MET:HE3	2.03	0.41
1:A:192:HIS:CD2	1:A:194:SER:H	2.38	0.41
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.93	0.41
1:A:29:VAL:HG23	4:A:777:HOH:O	2.20	0.40
1:A:385:SER:HB2	1:A:407:GLY:HA2	2.04	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	468/487 (96%)	456 (97%)	11 (2%)	1 (0%)	43	50
1	B	468/487 (96%)	452 (97%)	15 (3%)	1 (0%)	43	50
All	All	936/974 (96%)	908 (97%)	26 (3%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	SER
1	A	108	SER

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	381/393 (97%)	376 (99%)	5 (1%)	61	72
1	B	381/393 (97%)	374 (98%)	7 (2%)	51	63
All	All	762/786 (97%)	750 (98%)	12 (2%)	57	66

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	45	THR
1	A	92	ASP
1	A	223[A]	GLN
1	A	223[B]	GLN
1	B	33	VAL
1	B	45	THR
1	B	92	ASP
1	B	254	LEU
1	B	323	THR
1	B	431	ARG

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Mol	Chain	Res	Type
1	B	455	VAL

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	70	HIS
1	A	72	HIS
1	A	192	HIS
1	A	428	ASN
1	A	434	HIS
1	B	28	GLN
1	B	176	GLN
1	B	192	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](#)

6 ligands 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
3	SO4	A	503	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.38	0
2	A1BCS	B	501	-	32,32,32	1.12	2 (6%)	41,47,47	1.50	6 (14%)
3	SO4	B	503	-	4,4,4	0.27	0	6,6,6	0.15	0
2	A1BCS	A	501	-	32,32,32	1.15	3 (9%)	41,47,47	1.46	6 (14%)
3	SO4	B	502	-	4,4,4	0.21	0	6,6,6	0.42	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
2	A1BCS	A	501	-	-	9/21/24/24	0/2/2/2
2	A1BCS	B	501	-	-	6/21/24/24	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1BCS	O31-C30	-3.69	1.28	1.36
2	A	501	A1BCS	C12-C13	-3.45	1.39	1.46
2	A	501	A1BCS	C13-N14	-3.09	1.24	1.28
2	A	501	A1BCS	O31-C30	-2.68	1.30	1.36
2	B	501	A1BCS	C12-C13	-2.48	1.41	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1BCS	C12-C30-C2	-5.29	117.17	120.14
2	B	501	A1BCS	C12-C30-C2	-4.79	117.44	120.14
2	B	501	A1BCS	C17-C16-N15	3.94	116.59	109.22
2	B	501	A1BCS	O28-C27-C16	-3.04	117.32	122.78
2	A	501	A1BCS	O28-C27-C16	-3.01	117.38	122.78
2	B	501	A1BCS	O7-C6-C5	-2.89	103.94	109.36
2	A	501	A1BCS	C5-C12-C13	-2.79	117.16	121.47
2	A	501	A1BCS	C17-C16-N15	2.74	114.35	109.22
2	A	501	A1BCS	O7-C6-C5	-2.66	104.36	109.36
2	B	501	A1BCS	C5-C12-C13	-2.45	117.69	121.47
2	B	501	A1BCS	C18-C16-N15	-2.36	104.02	109.74
2	A	501	A1BCS	C12-C13-N14	2.05	125.49	120.69

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1BCS	N15-C16-C27-O28
2	A	501	A1BCS	N15-C16-C27-O29
2	A	501	A1BCS	C17-C16-C27-O28
2	A	501	A1BCS	C17-C16-C27-O29
2	A	501	A1BCS	C6-O7-P8-O10
2	A	501	A1BCS	C6-O7-P8-O11
2	A	501	A1BCS	C12-C13-N14-N15
2	B	501	A1BCS	C6-O7-P8-O9
2	B	501	A1BCS	C6-O7-P8-O10
2	B	501	A1BCS	C6-O7-P8-O11
2	B	501	A1BCS	C12-C13-N14-N15
2	A	501	A1BCS	C18-C16-C27-O28
2	A	501	A1BCS	C18-C16-C27-O29
2	B	501	A1BCS	C17-C16-C27-O28
2	B	501	A1BCS	C17-C16-C27-O29

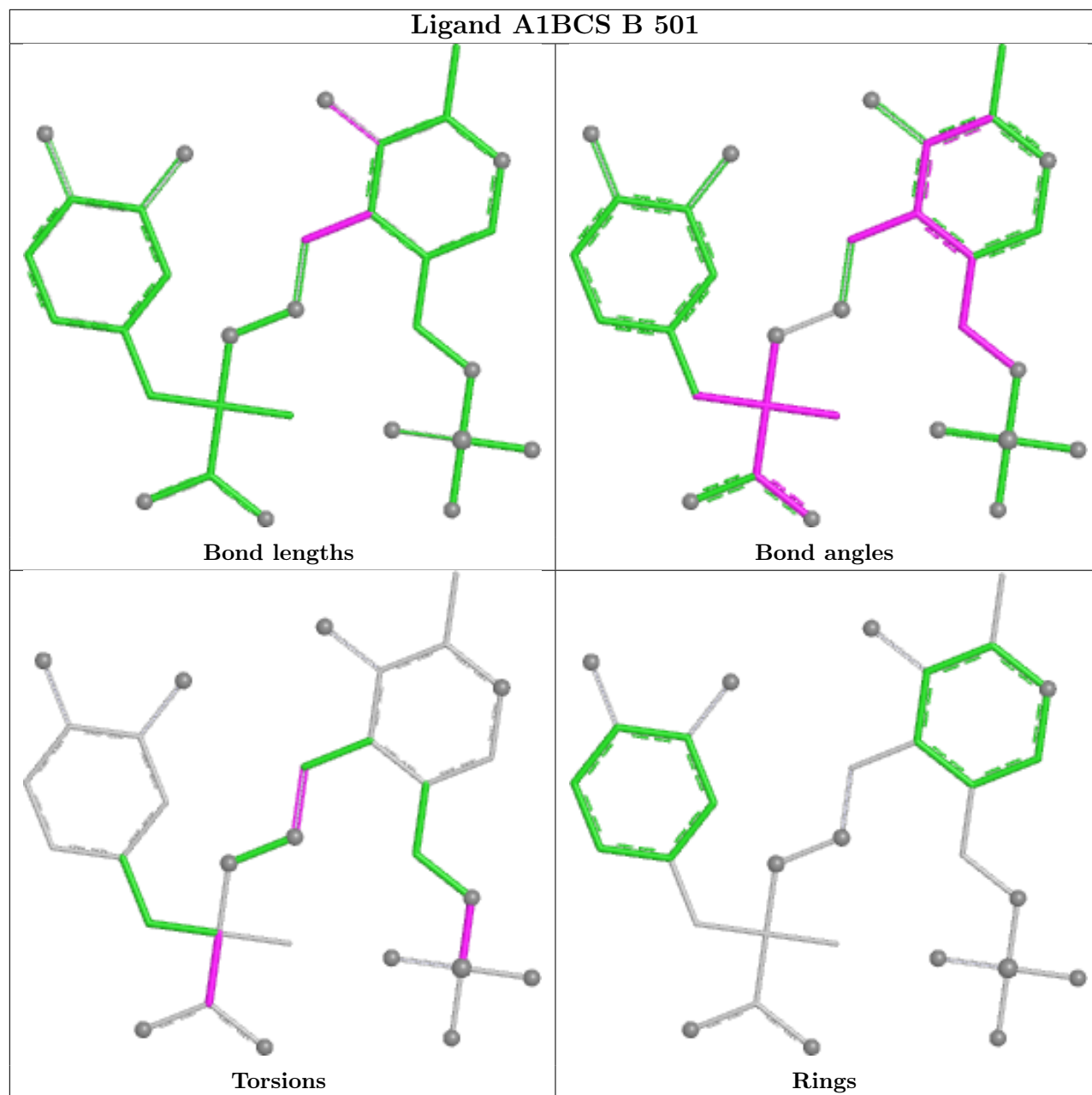
There are no ring outliers.

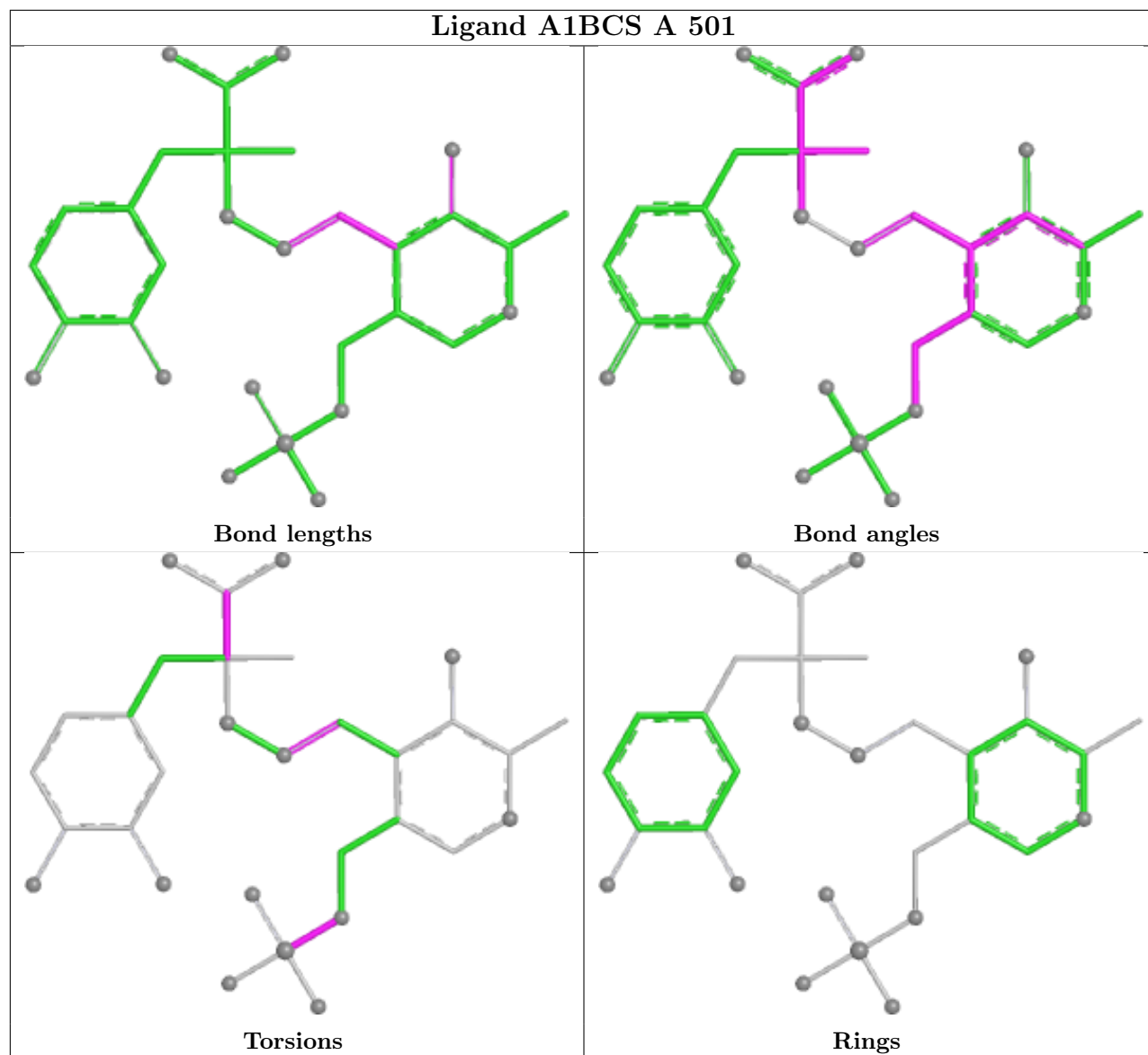
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	A1BCS	1	0
2	A	501	A1BCS	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 A1BCS B 501





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	466/487 (95%)	-0.83	0 100 100	11, 21, 47, 101	5 (1%)
1	B	466/487 (95%)	-0.84	0 100 100	10, 22, 44, 84	5 (1%)
All	All	932/974 (95%)	-0.84	0 100 100	10, 21, 46, 101	10 (1%)

There are no RSRZ outliers to report.

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](#)

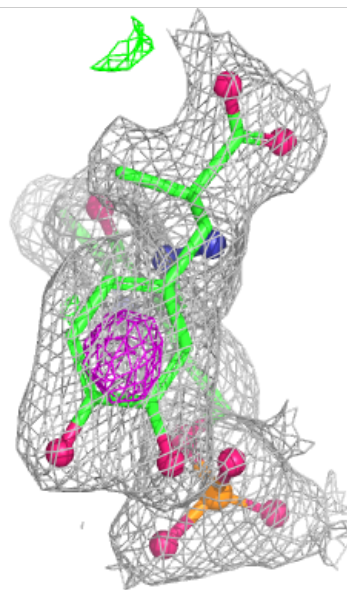
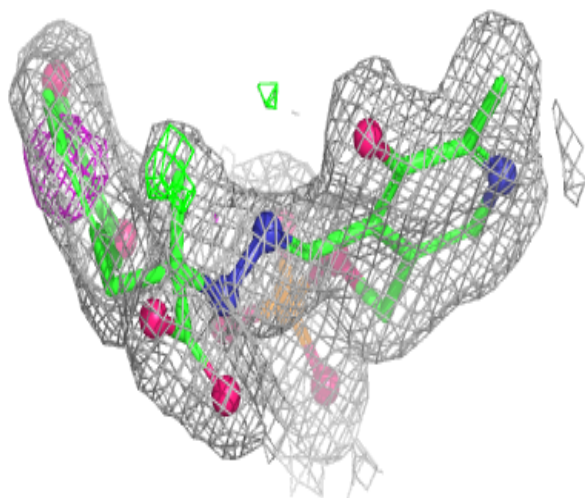
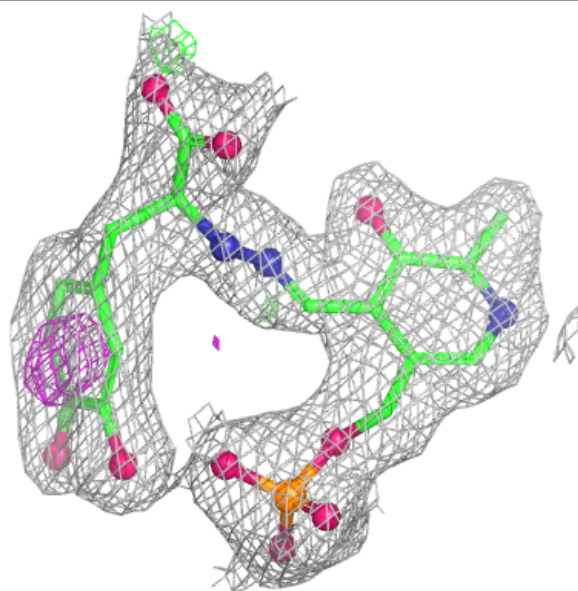
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	503	5/5	0.87	0.13	60,66,85,104	0
3	SO4	B	502	5/5	0.92	0.12	40,49,81,82	0
3	SO4	A	503	5/5	0.93	0.12	56,64,71,76	0
3	SO4	A	502	5/5	0.94	0.10	37,45,70,70	0
2	A1BCS	B	501	31/31	0.98	0.06	11,23,32,45	0
2	A1BCS	A	501	31/31	0.99	0.05	11,21,34,38	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.

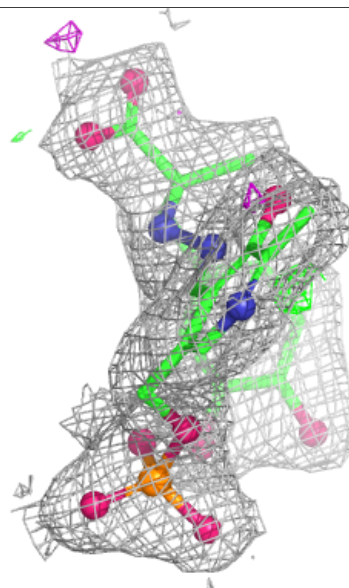
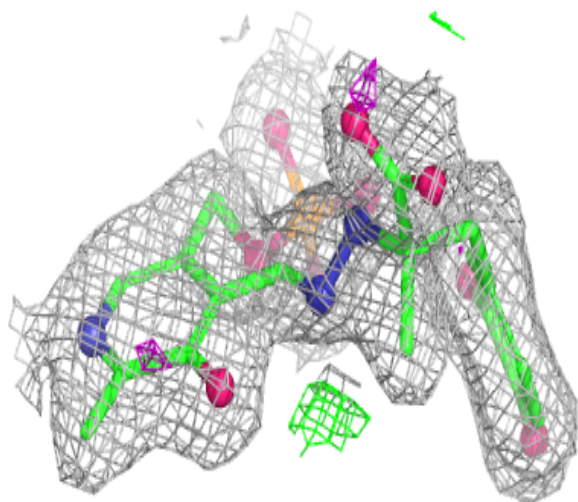
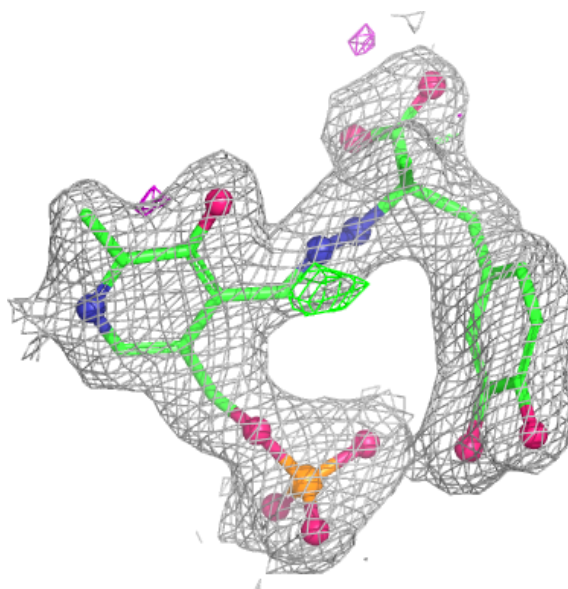
Electron density around A1BCS B 501:

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



Electron density around A1BCS 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 ⓘ

There are no such residues in this entry.