



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:37 PM UTC

PDB ID : 1M0Q / pdb_00001m0q
Title : Structure of Dialkylglycine Decarboxylase Complexed with S-1-aminoethanephosphonate
Authors : Liu, W.; Rogers, C.J.; Fisher, A.J.; Toney, M.D.
Deposited on : 2002-06-13
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

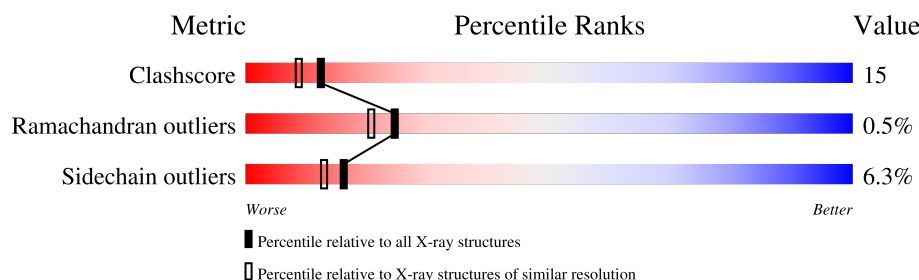
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	58% 32% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3511 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 2,2-Dialkylglycine Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3252	2051	576	607	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	GLN	SEE REMARK 999	UNP P16932
A	81	GLU	GLY	SEE REMARK 999	UNP P16932

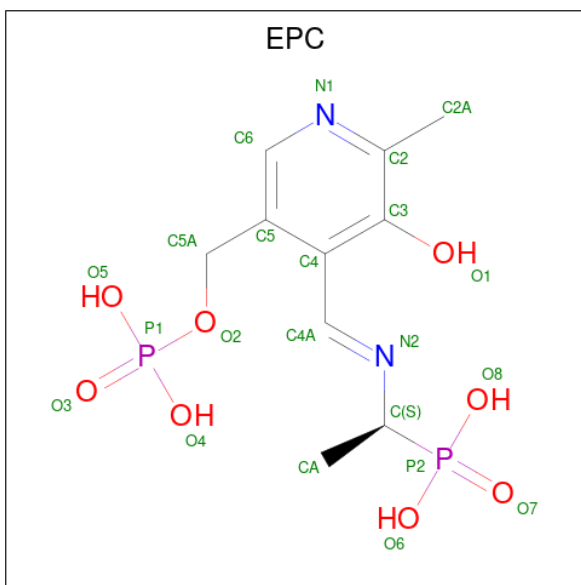
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is (1S)-1-(((1E)-{3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYLENE)AMINO)ETHYLPHOSPHONIC ACID (CCD ID: EPC) (formula: C₁₀H₁₆N₂O₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	2	8	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	235	Total	O	0	0
			235	235		

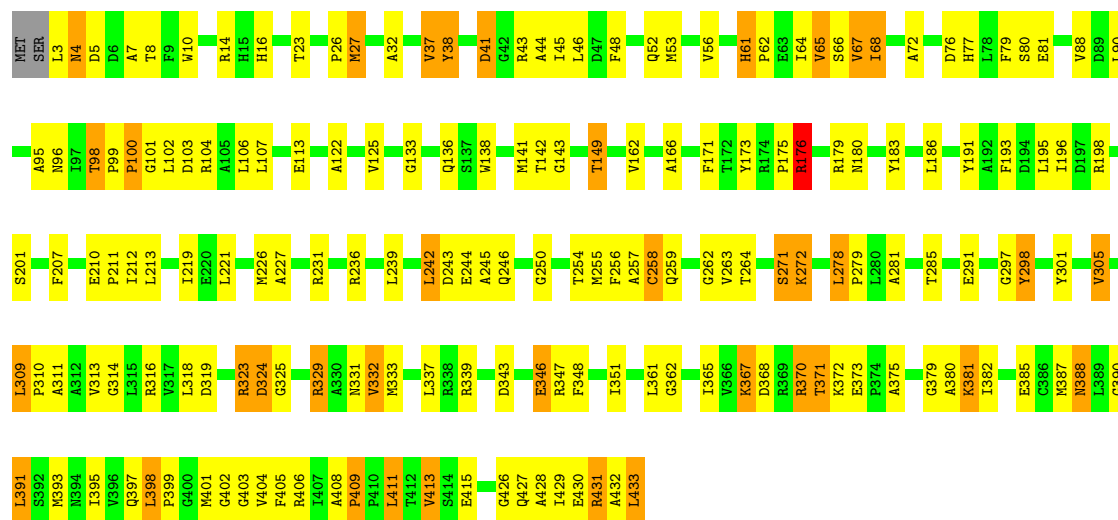
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 2,2-Dialkylglycine Decarboxylase

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.81Å 150.81Å 85.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.2 (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, CNS	Depositor
R, R_{free}	0.191 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3511	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPC, NA, K

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	2.00	69/3309 (2.1%)	1.48	24/4478 (0.5%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	ALA	CA-CB	9.62	1.68	1.53
1	A	380	ALA	CA-CB	-9.11	1.39	1.53
1	A	7	ALA	CA-CB	-8.44	1.40	1.53
1	A	219	ILE	CA-CB	-7.99	1.44	1.53
1	A	26	PRO	C-O	-7.66	1.14	1.24
1	A	314	GLY	CA-C	7.20	1.60	1.52
1	A	4	ASN	N-CA	-7.19	1.36	1.46
1	A	180	ASN	CA-C	-7.02	1.44	1.53
1	A	380	ALA	CA-C	-6.91	1.43	1.52
1	A	387	MET	SD-CE	6.89	1.96	1.79
1	A	176	ARG	CZ-NH2	6.85	1.42	1.33
1	A	262	GLY	CA-C	6.82	1.60	1.51
1	A	371	THR	CA-CB	6.69	1.64	1.53
1	A	365	ILE	CA-CB	-6.65	1.46	1.54
1	A	65	VAL	CA-C	6.53	1.60	1.52
1	A	258	CYS	CA-C	6.50	1.61	1.52
1	A	88	VAL	CA-C	6.50	1.61	1.52
1	A	415	GLU	CG-CD	6.41	1.68	1.52
1	A	176	ARG	CG-CD	6.32	1.71	1.52
1	A	113	GLU	C-O	-6.29	1.16	1.24
1	A	191	TYR	CA-C	6.28	1.60	1.52
1	A	90	LEU	C-O	6.24	1.31	1.24
1	A	388	ASN	CA-C	-6.21	1.44	1.52
1	A	212	ILE	CA-C	6.19	1.60	1.52
1	A	430	GLU	CG-CD	6.17	1.67	1.52
1	A	176	ARG	CB-CG	6.16	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	GLY	CA-C	6.10	1.58	1.52
1	A	285	THR	CA-C	6.08	1.60	1.52
1	A	64	ILE	CA-CB	-6.08	1.46	1.54
1	A	264	THR	CA-C	-6.05	1.45	1.52
1	A	100	PRO	N-CA	-5.98	1.39	1.47
1	A	298	TYR	CA-CB	-5.96	1.43	1.53
1	A	243	ASP	CA-CB	5.94	1.60	1.52
1	A	395	ILE	C-O	-5.87	1.18	1.24
1	A	393	MET	SD-CE	5.86	1.94	1.79
1	A	227	ALA	CA-CB	-5.77	1.44	1.53
1	A	64	ILE	CA-C	-5.72	1.45	1.52
1	A	45	ILE	N-CA	-5.72	1.39	1.46
1	A	305	VAL	CA-CB	5.71	1.60	1.54
1	A	231	ARG	C-O	5.64	1.30	1.24
1	A	351	ILE	CA-CB	-5.56	1.47	1.53
1	A	61	HIS	CA-C	5.52	1.60	1.52
1	A	236	ARG	CZ-NH1	5.51	1.40	1.32
1	A	324	ASP	CA-C	-5.51	1.44	1.52
1	A	390	GLY	CA-C	5.51	1.59	1.51
1	A	38	TYR	CA-C	-5.50	1.45	1.52
1	A	8	THR	CA-CB	-5.48	1.44	1.53
1	A	272	LYS	N-CA	5.47	1.52	1.46
1	A	106	LEU	CA-C	5.44	1.58	1.52
1	A	142	THR	CA-C	-5.43	1.45	1.52
1	A	379	GLY	C-O	5.42	1.30	1.23
1	A	313	VAL	CA-CB	5.38	1.60	1.54
1	A	102	LEU	CA-C	-5.33	1.46	1.52
1	A	176	ARG	NE-CZ	5.31	1.38	1.33
1	A	242	LEU	CA-CB	5.28	1.60	1.53
1	A	413	VAL	C-O	-5.23	1.18	1.24
1	A	278	LEU	CA-C	-5.23	1.45	1.52
1	A	243	ASP	CA-C	5.20	1.59	1.52
1	A	244	GLU	C-O	5.19	1.30	1.23
1	A	149	THR	CA-CB	-5.18	1.46	1.53
1	A	391	LEU	CA-C	-5.15	1.46	1.52
1	A	125	VAL	CA-CB	-5.14	1.47	1.54
1	A	122	ALA	C-O	5.12	1.30	1.24
1	A	258	CYS	N-CA	5.08	1.52	1.46
1	A	409	PRO	CA-C	5.07	1.56	1.52
1	A	67	VAL	CA-CB	-5.07	1.48	1.54
1	A	37	VAL	C-O	5.03	1.29	1.23
1	A	331	ASN	CA-C	5.02	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	ASP	CA-C	-5.00	1.45	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	GLY	N-CA-C	-8.36	99.72	112.51
1	A	415	GLU	N-CA-C	-8.03	102.51	111.82
1	A	16	HIS	N-CA-C	7.20	123.09	112.94
1	A	96	ASN	N-CA-C	6.46	119.31	111.82
1	A	403	GLY	N-CA-C	-6.14	104.22	112.14
1	A	332	VAL	N-CA-CB	-6.04	103.83	110.65
1	A	411	LEU	N-CA-C	-5.96	105.26	112.54
1	A	207	PHE	N-CA-C	-5.96	99.69	109.40
1	A	348	PHE	N-CA-C	5.90	118.14	108.52
1	A	226	MET	CG-SD-CE	-5.79	88.16	100.90
1	A	72	ALA	N-CA-C	-5.67	105.10	111.28
1	A	95	ALA	N-CA-C	-5.62	105.16	111.28
1	A	101	GLY	N-CA-C	-5.52	106.91	114.64
1	A	201	SER	N-CA-C	-5.52	106.39	113.02
1	A	431	ARG	N-CA-C	5.52	118.06	111.71
1	A	5	ASP	N-CA-C	5.47	119.66	113.15
1	A	98	THR	N-CA-C	-5.44	103.78	110.31
1	A	193	PHE	CA-C-N	-5.43	112.46	120.28
1	A	193	PHE	C-N-CA	-5.43	112.46	120.28
1	A	210	GLU	N-CA-C	-5.31	102.98	110.31
1	A	103	ASP	N-CA-C	5.24	120.53	114.04
1	A	254	THR	N-CA-C	-5.16	101.44	109.24
1	A	250	GLY	N-CA-C	5.16	121.22	115.08
1	A	311	ALA	N-CA-C	-5.14	105.57	111.07

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	3252	0	3279	101	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	22	0	12	0	0
5	A	235	0	0	3	0
All	All	3511	0	3291	101	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 15.

All (101) 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:3:LEU:HD12	1:A:4:ASN:H	1.17	1.08
1:A:278:LEU:HG	1:A:279:PRO:HD2	1.38	1.02
1:A:370:ARG:HH11	1:A:370:ARG:HG3	1.30	0.94
1:A:79:PHE:CE2	1:A:81:GLU:HB2	2.08	0.88
1:A:278:LEU:HG	1:A:279:PRO:CD	2.08	0.83
1:A:368:ASP:HB3	1:A:371:THR:OG1	1.82	0.80
1:A:333:MET:HA	1:A:333:MET:HE2	1.65	0.77
1:A:10:TRP:O	1:A:14:ARG:HG3	1.87	0.75
1:A:61:HIS:ND1	1:A:62:PRO:HD2	2.01	0.75
1:A:67:VAL:HB	1:A:316:ARG:NH1	2.02	0.74
1:A:332:VAL:HG12	1:A:333:MET:HE3	1.71	0.73
1:A:3:LEU:HD13	1:A:41:ASP:OD2	1.90	0.71
1:A:246:GLN:HG2	1:A:272:LYS:HE2	1.74	0.70
1:A:371:THR:OG1	1:A:373:GLU:HB2	1.91	0.70
1:A:79:PHE:CD2	1:A:81:GLU:HB2	2.27	0.70
1:A:3:LEU:CD1	1:A:4:ASN:H	2.00	0.69
1:A:3:LEU:HD12	1:A:4:ASN:N	2.01	0.69
1:A:401:MET:HE3	1:A:404:VAL:HG23	1.74	0.69
1:A:138:TRP:CZ2	1:A:141:MET:HE3	2.29	0.68
1:A:329:ARG:HB3	1:A:329:ARG:CZ	2.24	0.67
1:A:278:LEU:CG	1:A:279:PRO:HD2	2.21	0.66
1:A:332:VAL:HG12	1:A:333:MET:CE	2.27	0.65
1:A:370:ARG:NH1	5:A:533:HOH:O	2.30	0.65
1:A:309:LEU:C	1:A:309:LEU:HD12	2.23	0.64
1:A:370:ARG:HG3	1:A:370:ARG:NH1	2.06	0.63
1:A:138:TRP:HA	1:A:149:THR:HG23	1.82	0.61
1:A:246:GLN:HG2	1:A:272:LYS:CE	2.31	0.60
1:A:368:ASP:O	1:A:372:LYS:N	2.27	0.59
1:A:333:MET:HE2	1:A:333:MET:CA	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLN:CG	1:A:272:LYS:HE2	2.33	0.58
1:A:255:MET:HB3	1:A:259:GLN:HE22	1.69	0.57
1:A:38:TYR:CE1	1:A:44:ALA:HB2	2.40	0.56
1:A:171:PHE:CE1	1:A:173:TYR:HB3	2.41	0.56
1:A:397:GLN:C	1:A:398:LEU:HD12	2.32	0.55
1:A:211:PRO:O	1:A:221:LEU:HG	2.07	0.54
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.72	0.54
1:A:56:VAL:HB	1:A:411:LEU:HG	1.89	0.53
1:A:76:ASP:CG	1:A:77:HIS:H	2.16	0.53
1:A:343:ASP:O	1:A:346:GLU:HB2	2.08	0.53
1:A:242:LEU:CD1	1:A:258:CYS:HB3	2.39	0.52
1:A:362:GLY:HA2	1:A:405:PHE:O	2.10	0.52
1:A:337:LEU:HD23	1:A:361:LEU:HD12	1.92	0.52
1:A:98:THR:HB	1:A:99:PRO:HD2	1.90	0.51
1:A:61:HIS:CE1	1:A:62:PRO:HD2	2.45	0.51
1:A:38:TYR:HA	1:A:43:ARG:O	2.10	0.50
1:A:67:VAL:HG13	1:A:68:ILE:N	2.25	0.50
1:A:239:LEU:HD12	1:A:239:LEU:N	2.25	0.50
1:A:398:LEU:HD12	1:A:398:LEU:N	2.28	0.49
1:A:256:PHE:H	1:A:259:GLN:NE2	2.09	0.49
1:A:133:GLY:O	1:A:166:ALA:HA	2.12	0.49
1:A:381:LYS:HE2	1:A:432:ALA:HA	1.95	0.48
1:A:325:GLY:HA2	5:A:580:HOH:O	2.13	0.48
1:A:255:MET:HG3	1:A:256:PHE:CE2	2.48	0.48
1:A:213:LEU:HD12	1:A:213:LEU:N	2.28	0.48
1:A:258:CYS:HB2	1:A:263:VAL:O	2.14	0.47
1:A:309:LEU:HB3	1:A:310:PRO:HD3	1.96	0.47
1:A:278:LEU:HG	1:A:279:PRO:N	2.30	0.47
1:A:375:ALA:N	5:A:670:HOH:O	2.44	0.47
1:A:67:VAL:HB	1:A:316:ARG:HH12	1.77	0.47
1:A:175:PRO:O	1:A:176:ARG:HD3	2.15	0.46
1:A:398:LEU:HB3	1:A:399:PRO:HD2	1.98	0.46
1:A:32:ALA:HA	1:A:37:VAL:HA	1.97	0.46
1:A:38:TYR:HE1	1:A:44:ALA:HB2	1.81	0.46
1:A:297:GLY:O	1:A:298:TYR:C	2.57	0.46
1:A:382:ILE:HD13	1:A:429:ILE:HG12	1.98	0.46
1:A:80:SER:HB2	1:A:301:TYR:CZ	2.50	0.46
1:A:245:ALA:O	1:A:272:LYS:HB2	2.15	0.46
1:A:61:HIS:O	1:A:65:VAL:HG23	2.16	0.46
1:A:401:MET:HE3	1:A:404:VAL:CG2	2.43	0.46
1:A:323:ARG:HG2	1:A:323:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD23	1:A:391:LEU:HD13	1.98	0.45
1:A:68:ILE:HD13	1:A:68:ILE:HG23	1.62	0.45
1:A:107:LEU:O	1:A:305:VAL:HA	2.16	0.45
1:A:385:GLU:HB2	1:A:428:ALA:HB1	1.98	0.45
1:A:408:ALA:N	1:A:409:PRO:HD3	2.31	0.44
1:A:323:ARG:HH11	1:A:323:ARG:CG	2.30	0.44
1:A:61:HIS:CG	1:A:62:PRO:HD2	2.52	0.44
1:A:23:THR:O	1:A:23:THR:HG23	2.17	0.44
1:A:175:PRO:HB3	1:A:183:TYR:CD2	2.53	0.44
1:A:367:LYS:HG3	1:A:375:ALA:HA	1.99	0.44
1:A:76:ASP:OD1	1:A:77:HIS:N	2.39	0.44
1:A:429:ILE:O	1:A:433:LEU:HD12	2.18	0.43
1:A:53:MET:HE1	1:A:406:ARG:HB3	2.00	0.43
1:A:43:ARG:NH2	1:A:388:ASN:O	2.44	0.43
1:A:175:PRO:HB3	1:A:183:TYR:CG	2.53	0.43
1:A:27:MET:HE3	1:A:27:MET:HB3	1.94	0.42
1:A:398:LEU:N	1:A:398:LEU:CD1	2.82	0.42
1:A:99:PRO:HA	1:A:100:PRO:HD3	1.69	0.42
1:A:52:GLN:O	1:A:53:MET:HB2	2.19	0.42
1:A:76:ASP:CG	1:A:77:HIS:N	2.77	0.42
1:A:413:VAL:O	1:A:413:VAL:HG13	2.20	0.41
1:A:162:VAL:H	1:A:162:VAL:HG23	1.54	0.41
1:A:61:HIS:HA	1:A:62:PRO:HD3	1.78	0.41
1:A:324:ASP:O	1:A:325:GLY:C	2.63	0.41
1:A:195:LEU:O	1:A:196:ILE:C	2.60	0.41
1:A:318:LEU:O	1:A:319:ASP:C	2.62	0.41
1:A:271:SER:HA	1:A:281:ALA:HA	2.02	0.41
1:A:179:ARG:HD3	1:A:179:ARG:HA	1.92	0.41
1:A:427:GLN:O	1:A:431:ARG:HG3	2.22	0.40
1:A:3:LEU:HD12	1:A:4:ASN:HB2	2.03	0.40
1:A:332:VAL:CG1	1:A:333:MET:HE3	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	429/433 (99%)	411 (96%)	16 (4%)	2 (0%)	24	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY
1	A	271	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	334/336 (99%)	313 (94%)	21 (6%)	16	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	MET
1	A	48	PHE
1	A	66	SER
1	A	68	ILE
1	A	104	ARG
1	A	136	GLN
1	A	176	ARG
1	A	186	LEU
1	A	198	ARG
1	A	291	GLU
1	A	309	LEU
1	A	323	ARG
1	A	329	ARG
1	A	339	ARG
1	A	346	GLU
1	A	347	ARG
1	A	367	LYS

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Mol	Chain	Res	Type
1	A	370	ARG
1	A	381	LYS
1	A	398	LEU
1	A	433	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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$
4	EPC	A	435	-	21,22,22	3.85	9 (42%)	27,33,33	1.62	4 (14%)

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
4	EPC	A	435	-	-	1/15/17/17	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	435	EPC	P2-C	-9.66	1.68	1.84
4	A	435	EPC	C4-C3	7.67	1.53	1.41
4	A	435	EPC	C6-C5	7.40	1.52	1.37
4	A	435	EPC	C2-N1	5.46	1.43	1.33
4	A	435	EPC	P2-O7	5.01	1.58	1.49
4	A	435	EPC	P2-O6	3.91	1.61	1.54
4	A	435	EPC	CA-C	3.18	1.60	1.52
4	A	435	EPC	C4-C4A	2.64	1.52	1.46
4	A	435	EPC	C2A-C2	2.64	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	435	EPC	C-N2-C4A	5.73	127.19	117.87
4	A	435	EPC	O4-P1-O2	3.04	114.59	106.67
4	A	435	EPC	C6-N1-C2	2.34	123.44	119.20
4	A	435	EPC	CA-C-N2	2.10	112.60	108.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

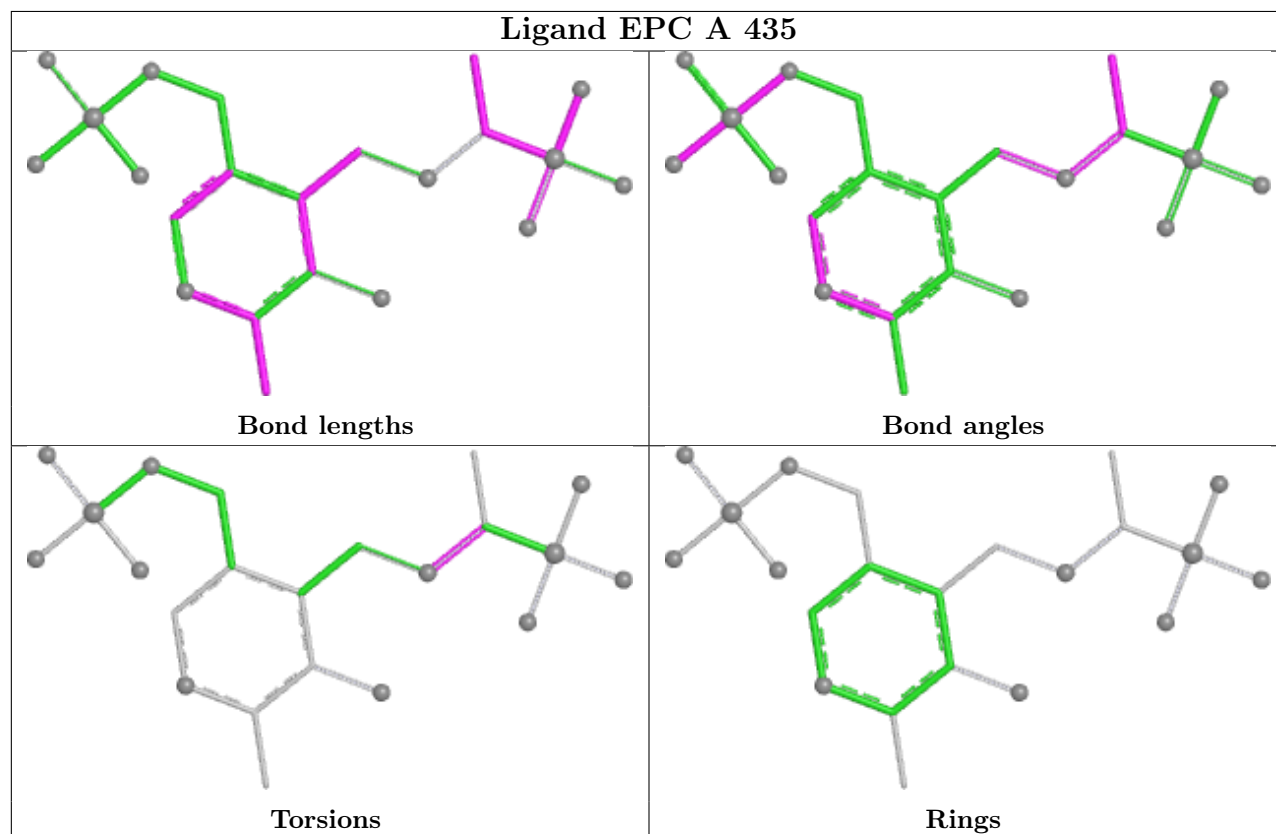
Mol	Chain	Res	Type	Atoms
4	A	435	EPC	CA-C-N2-C4A

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.