



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:00 AM UTC

PDB ID : 1ACM / pdb_00001acm
Title : ARGININE 54 IN THE ACTIVE SITE OF ESCHERICHIA COLI ASPARTATE TRANSCARBAMOYLASE IS CRITICAL FOR CATALYSIS: A SITE-SPECIFIC MUTAGENESIS, NMR AND X-RAY CRYSTALLOGRAPHY STUDY
Authors : Stevens, R.C.; Kantrowitz, E.R.; Lipscomb, W.N.
Deposited on : 1992-07-08
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)
Xtrriage (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

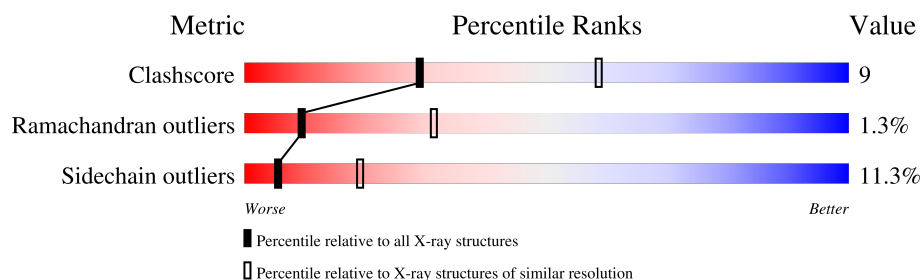
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7143 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 ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ALA	ARG	conflict	UNP P0A786
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
C	54	ALA	ARG	conflict	UNP P0A786
C	60	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLU	GLN	conflict	UNP P0A786
C	196	GLU	GLN	conflict	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

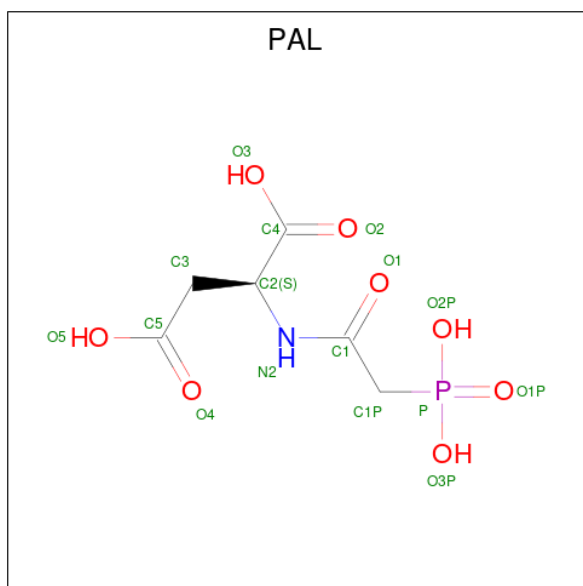
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLY	GLN	conflict	UNP P0A7F3

- Molecule 3 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (CCD ID: PAL) (formula: $C_6H_{10}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

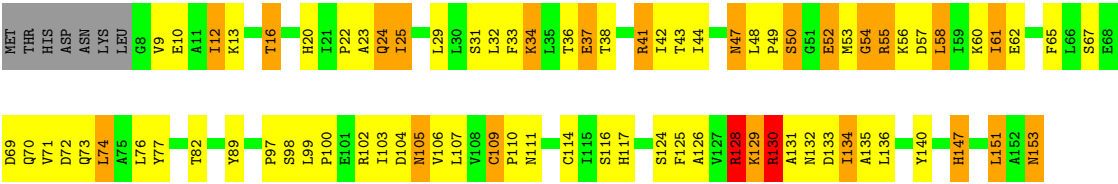
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	C	7	Total	O	0	0
			7	7		

Chain D: 43% 37% 14% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.20Å 122.20Å 156.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

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: PAL, ZN

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	1.07	15/2455 (0.6%)	1.83	62/3332 (1.9%)
1	C	1.14	14/2455 (0.6%)	1.81	48/3332 (1.4%)
2	B	0.93	3/1155 (0.3%)	1.83	29/1561 (1.9%)
2	D	0.94	4/1155 (0.3%)	1.81	25/1561 (1.6%)
All	All	1.05	36/7220 (0.5%)	1.82	164/9786 (1.7%)

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	3
1	C	0	3
2	B	0	2
2	D	0	3
All	All	0	11

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	117	HIS	CD2-NE2	-7.39	1.29	1.37
1	C	156	HIS	CD2-NE2	-7.37	1.29	1.37
1	C	212	HIS	CD2-NE2	-7.32	1.29	1.37
2	D	20	HIS	CD2-NE2	-6.79	1.30	1.37
2	B	117	HIS	CD2-NE2	-6.73	1.30	1.37
1	C	106	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	282	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	156	HIS	CD2-NE2	-6.44	1.30	1.37
1	C	265	HIS	CD2-NE2	-6.44	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	147	HIS	CD2-NE2	-6.43	1.30	1.37
2	B	147	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	265	HIS	CD2-NE2	-6.32	1.30	1.37
1	C	8	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	170	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.20	1.31	1.37
2	B	20	HIS	CD2-NE2	-6.15	1.31	1.37
1	C	170	HIS	CD2-NE2	-6.13	1.31	1.37
1	C	64	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	255	HIS	CD2-NE2	-6.07	1.31	1.37
1	C	212	HIS	CG-ND1	-5.83	1.31	1.38
1	C	41	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	64	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	106	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	134	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	8	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	212	HIS	CG-ND1	-5.51	1.32	1.38
1	A	41	HIS	CD2-NE2	-5.50	1.31	1.37
1	C	106	HIS	CG-ND1	-5.42	1.32	1.38
1	C	255	HIS	CD2-NE2	-5.32	1.31	1.37
1	C	282	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	282	HIS	CG-ND1	-5.17	1.32	1.38
1	C	8	HIS	CG-ND1	-5.11	1.32	1.38
1	A	265	HIS	CG-ND1	-5.06	1.32	1.38
1	A	106	HIS	CG-ND1	-5.01	1.32	1.38
2	D	117	HIS	CG-ND1	-5.00	1.32	1.38

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	153	ASN	CA-CB-CG	11.36	123.96	112.60
1	A	233	GLU	CA-CB-CG	10.56	135.22	114.10
1	A	200	ASP	CA-CB-CG	10.31	122.91	112.60
2	B	153	ASN	CA-CB-CG	9.27	121.87	112.60
1	A	271	ASP	CA-CB-CG	8.89	121.49	112.60
1	A	276	ASP	CA-CB-CG	8.68	121.28	112.60
2	B	19	ASP	CA-CB-CG	8.60	121.20	112.60
1	C	198	ILE	N-CA-C	-8.54	102.53	110.82
1	A	137	GLN	N-CA-C	-8.48	101.98	111.14
1	A	6	GLN	CA-CB-CG	-8.45	97.20	114.10
1	A	14	ASP	CA-CB-CG	8.03	120.63	112.60
1	C	137	GLN	N-CA-C	-7.93	101.72	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	291	ASN	OD1-CG-ND2	-7.87	114.73	122.60
1	C	271	ASP	CA-CB-CG	7.86	120.46	112.60
1	C	219	MET	N-CA-C	7.80	120.76	111.33
2	B	152	ALA	N-CA-C	7.66	127.11	110.80
1	C	78	ASN	CA-CB-CG	-7.60	105.00	112.60
1	C	297	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	A	200	ASP	CB-CA-C	-7.47	98.34	110.74
2	B	69	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	153	ASP	CA-CB-CG	7.31	119.91	112.60
2	B	34	LYS	N-CA-C	7.25	121.46	112.47
2	B	87	ASP	N-CA-C	-7.24	97.44	109.24
2	D	24	GLN	OE1-CD-NE2	-7.19	115.41	122.60
1	C	234	ARG	CG-CD-NE	-7.14	96.29	112.00
1	A	229	ARG	NE-CZ-NH1	7.11	128.61	121.50
2	B	57	ASP	CA-CB-CG	7.09	119.69	112.60
2	B	47	ASN	OD1-CG-ND2	-7.09	115.51	122.60
1	C	170	HIS	N-CA-C	-7.08	103.50	111.14
2	D	105	ASN	N-CA-C	7.04	125.79	110.80
1	A	255	HIS	CA-CB-CG	7.02	120.82	113.80
2	D	130	ARG	N-CA-C	7.02	120.73	108.52
1	C	200	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	54	ALA	N-CA-C	7.00	118.80	111.03
2	D	153	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	A	113	ARG	CA-C-O	-6.92	113.55	120.82
2	D	47	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	215	ILE	N-CA-C	-6.78	103.61	111.00
2	B	94	LYS	N-CA-C	-6.78	97.48	108.52
1	C	33	ASN	CA-C-N	6.66	126.57	119.85
1	C	33	ASN	C-N-CA	6.66	126.57	119.85
2	B	130	ARG	N-CA-C	6.65	121.06	113.15
1	A	236	ASP	CA-CB-CG	-6.59	106.01	112.60
1	A	233	GLU	CB-CA-C	-6.55	98.50	110.63
1	C	309	VAL	O-C-N	6.55	131.79	122.62
1	A	37	GLU	N-CA-C	-6.51	103.44	112.30
1	C	61	THR	N-CA-C	-6.49	103.48	111.40
1	C	42	LYS	CA-CB-CG	-6.49	101.12	114.10
1	C	141	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	35	GLN	CA-C-N	6.38	127.82	119.84
1	A	35	GLN	C-N-CA	6.38	127.82	119.84
2	B	133	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	81	LEU	N-CA-C	-6.38	103.62	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ASN	CA-CB-CG	-6.37	106.23	112.60
1	C	291	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	C	14	ASP	CA-CB-CG	6.36	118.96	112.60
2	B	153	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	33	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	117	GLU	CA-CB-CG	-6.31	101.47	114.10
2	D	41	ARG	N-CA-C	6.31	119.62	110.28
2	D	24	GLN	CG-CD-NE2	6.31	125.86	116.40
1	A	134	HIS	CA-CB-CG	6.25	120.05	113.80
1	C	242	ASN	OD1-CG-ND2	-6.23	116.37	122.60
2	B	103	ILE	CB-CA-C	-6.22	104.38	111.59
1	A	138	THR	N-CA-CB	-6.20	100.67	110.22
1	C	51	ALA	N-CA-C	6.19	119.02	110.35
2	D	153	ASN	CB-CG-ND2	6.19	125.69	116.40
2	D	24	GLN	CB-CG-CD	6.17	123.09	112.60
1	A	309	VAL	O-C-N	6.16	130.27	122.57
2	B	68	GLU	N-CA-C	-6.16	104.49	111.14
1	A	42	LYS	CA-CB-CG	-6.15	101.80	114.10
2	D	55	ARG	CA-CB-CG	6.14	126.38	114.10
1	A	21	ASN	OD1-CG-ND2	-6.14	116.46	122.60
2	D	128	ARG	CA-CB-CG	6.10	126.29	114.10
2	B	57	ASP	O-C-N	-6.09	116.21	123.27
2	D	105	ASN	CA-CB-CG	-6.08	106.52	112.60
1	C	276	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	84	ASN	CB-CG-ND2	5.98	125.37	116.40
1	C	41	HIS	CA-CB-CG	5.98	119.78	113.80
2	B	58	LEU	N-CA-C	5.97	117.92	108.79
1	A	234	ARG	CG-CD-NE	-5.92	98.99	112.00
1	C	73	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	147	GLN	CA-C-O	-5.86	114.34	120.55
2	B	128	ARG	CA-CB-CG	5.84	125.79	114.10
1	C	182	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	33	ASN	CA-C-N	5.82	126.63	120.11
1	A	33	ASN	C-N-CA	5.82	126.63	120.11
2	D	130	ARG	N-CA-CB	-5.82	102.20	110.58
1	A	79	THR	O-C-N	-5.80	116.44	122.94
2	D	132	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	C	71	VAL	CA-C-O	-5.72	115.97	121.63
1	A	251	ALA	N-CA-C	5.70	118.26	111.71
2	B	139	LYS	CA-CB-CG	5.70	125.50	114.10
1	C	35	GLN	O-C-N	-5.69	116.18	121.36
1	A	10	ILE	N-CA-C	5.69	116.51	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	25	ILE	N-CA-C	-5.67	107.29	112.96
1	A	7	LYS	CG-CD-CE	5.62	124.23	111.30
2	B	97	PRO	N-CA-C	5.61	120.02	111.15
1	C	134	HIS	CA-C-N	5.55	125.21	119.05
1	C	134	HIS	C-N-CA	5.55	125.21	119.05
2	D	57	ASP	N-CA-C	-5.55	101.54	110.14
1	C	56	ARG	CG-CD-NE	-5.54	99.82	112.00
1	A	223	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	153	ASP	N-CA-C	-5.51	101.19	109.95
1	C	232	LYS	CA-CB-CG	-5.51	103.08	114.10
1	C	151	ARG	CA-CB-CG	5.51	125.11	114.10
2	D	130	ARG	CA-CB-CG	5.49	125.07	114.10
2	B	10	GLU	N-CA-C	5.47	122.46	110.80
1	A	58	SER	N-CA-C	-5.46	104.97	111.69
1	C	111	ALA	N-CA-C	5.45	117.22	111.28
1	C	137	GLN	CG-CD-NE2	5.45	124.58	116.40
1	C	103	VAL	N-CA-C	-5.44	100.55	108.17
1	C	8	HIS	N-CA-C	-5.41	100.42	109.24
1	A	188	ALA	O-C-N	-5.40	118.05	121.88
1	C	17	ARG	CA-CB-CG	5.40	124.90	114.10
1	A	287	GLN	N-CA-C	-5.39	105.32	111.14
1	C	126	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	296	ARG	CA-CB-CG	-5.38	103.35	114.10
1	A	37	GLU	CA-CB-CG	5.37	124.85	114.10
2	D	50	SER	N-CA-C	-5.37	97.07	107.44
1	A	6	GLN	N-CA-C	5.36	119.40	112.86
1	C	222	VAL	N-CA-C	5.35	116.68	108.71
2	B	73	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	C	151	ARG	N-CA-CB	-5.33	101.55	110.99
2	B	69	ASP	N-CA-CB	-5.33	101.10	109.78
1	C	95	ILE	CB-CA-C	-5.33	105.06	112.04
1	C	122	VAL	N-CA-CB	-5.30	104.40	111.08
1	C	88	LEU	N-CA-C	-5.28	105.69	111.82
1	A	306	ARG	O-C-N	5.28	127.72	122.12
1	A	13	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	69	SER	CA-CB-OG	-5.26	100.57	111.10
2	D	33	PHE	CA-CB-CG	5.25	119.05	113.80
2	B	57	ASP	N-CA-C	-5.24	101.11	109.23
1	A	19	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	303	VAL	CG1-CB-CG2	-5.24	99.28	110.80
1	A	270	VAL	CA-C-O	-5.22	114.26	120.78
1	A	221	GLU	CA-CB-CG	5.21	124.52	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	C	15	LEU	O-C-N	-5.18	117.15	123.10
2	D	109	CYS	CA-C-N	5.16	124.82	119.56
2	D	109	CYS	C-N-CA	5.16	124.82	119.56
1	A	174	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	193	ALA	N-CA-C	5.14	116.73	110.41
2	B	147	HIS	CA-CB-CG	5.14	118.94	113.80
2	B	133	ASP	N-CA-C	-5.11	102.44	110.36
1	A	157	VAL	CA-C-O	5.11	125.70	120.39
2	B	48	LEU	CA-C-N	5.11	125.39	119.93
2	B	48	LEU	C-N-CA	5.11	125.39	119.93
1	A	229	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	D	53	MET	N-CA-C	5.09	118.81	112.59
1	A	247	PHE	N-CA-C	-5.09	100.22	108.52
1	A	78	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	114	LEU	CA-CB-CG	5.06	134.02	116.30
1	C	243	VAL	N-CA-C	5.06	115.78	110.62
1	C	113	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A	83	LYS	N-CA-C	5.05	119.71	113.50
1	A	233	GLU	N-CA-CB	5.05	118.00	110.22
2	B	39	ASP	CA-CB-CG	5.04	117.64	112.60
2	D	111	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	200	ASP	N-CA-CB	5.02	117.96	109.78
1	C	101	ALA	CA-C-O	-5.02	115.86	121.23
2	D	73	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	163	LEU	N-CA-C	-5.01	107.21	113.38

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	TYR	Sidechain
1	A	269	ARG	Sidechain
1	A	98	TYR	Sidechain
2	B	77	TYR	Sidechain
2	B	99	LEU	Peptide
1	C	165	TYR	Sidechain
1	C	234	ARG	Sidechain
1	C	240	TYR	Sidechain
2	D	125	PHE	Sidechain
2	D	140	TYR	Sidechain
2	D	77	TYR	Sidechain

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	2409	0	2414	29	0
1	C	2409	0	2414	21	0
2	B	1138	0	1154	36	0
2	D	1138	0	1154	42	0
3	A	16	0	6	0	0
3	C	16	0	6	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	0	0	0
5	C	7	0	0	0	0
All	All	7143	0	7148	124	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 9.

All (124) 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)
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.60	0.84
2:D:102:ARG:NH2	2:D:124:SER:HB3	1.94	0.83
2:D:99:LEU:HD11	2:D:134:ILE:HD12	1.64	0.78
2:D:102:ARG:HH21	2:D:124:SER:HB3	1.47	0.78
2:D:22:PRO:HB2	2:D:25:ILE:HD12	1.70	0.72
1:A:270:VAL:HG23	1:A:271:ASP:H	1.56	0.69
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.76	0.67
1:A:154:ASN:HA	1:A:181:GLY:O	1.95	0.67
2:D:74:LEU:HD23	2:D:97:PRO:HG2	1.76	0.66
1:A:35:GLN:HG2	1:A:38:LEU:HG	1.77	0.65
2:D:128:ARG:HD2	2:D:130:ARG:HB2	1.79	0.65
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.80	0.63
1:C:1:ALA:HA	1:C:306:ARG:HG2	1.81	0.61
2:B:12:ILE:HG13	2:B:62:GLU:HG3	1.82	0.61
1:A:130:GLY:O	1:A:167:ARG:HD3	2.00	0.60
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.82	0.60
1:A:157:VAL:HG12	1:A:224:ILE:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HD11	1:A:116:THR:HG21	1.84	0.60
2:B:42:ILE:HG12	2:B:61:ILE:HG23	1.83	0.59
1:A:257:ALA:HB1	1:A:261:MET:HE3	1.86	0.58
2:B:25:ILE:HA	2:B:28:LYS:HD3	1.86	0.56
2:D:49:PRO:HA	2:D:54:GLY:O	2.07	0.55
2:B:46:LEU:HD12	2:D:44:ILE:HD11	1.89	0.55
2:B:84:ASN:HD21	2:B:91:VAL:HG22	1.72	0.55
2:D:12:ILE:HG23	2:D:41:ARG:NH2	2.22	0.54
1:C:63:MET:SD	1:C:70:VAL:HG22	2.47	0.54
2:B:17:VAL:HG13	2:B:84:ASN:HB3	1.91	0.53
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.90	0.53
2:B:124:SER:HB3	2:B:139:LYS:HG2	1.91	0.53
1:C:254:LEU:HD11	1:C:277:VAL:HG13	1.90	0.53
1:A:77:ALA:O	1:A:83:LYS:HD3	2.08	0.52
1:A:10:ILE:HD11	1:A:116:THR:CG2	2.38	0.52
1:C:232:LYS:HE3	1:C:243:VAL:O	2.09	0.52
2:B:14:ARG:HG2	2:B:88:ASN:H	1.74	0.52
2:D:128:ARG:HG3	2:D:135:ALA:HB3	1.92	0.52
2:D:43:THR:HB	2:D:60:LYS:HB2	1.92	0.51
2:B:62:GLU:HG2	2:B:63:ASN:HD22	1.77	0.50
1:A:50:GLU:CD	1:A:234:ARG:HH22	2.20	0.50
2:B:82:THR:HG23	2:B:96:ARG:NH1	2.27	0.50
1:C:130:GLY:HA2	1:C:234:ARG:HH21	1.76	0.50
1:C:35:GLN:HB3	1:C:38:LEU:HG	1.93	0.49
2:D:50:SER:HB2	2:D:52:GLU:OE2	2.13	0.49
2:B:111:ASN:O	2:B:117:HIS:HE1	1.96	0.49
1:A:163:LEU:O	1:A:170:HIS:HE1	1.95	0.49
2:B:22:PRO:O	2:B:25:ILE:HB	2.13	0.48
2:D:13:LYS:HG2	2:D:89:TYR:CE1	2.48	0.48
1:A:223:ASP:O	1:A:261:MET:HA	2.14	0.48
2:D:126:ALA:O	2:D:136:LEU:HA	2.14	0.48
2:B:62:GLU:HG2	2:B:63:ASN:ND2	2.28	0.48
1:C:308:LEU:HG	1:C:310:LEU:HD12	1.96	0.48
1:A:215:ILE:HG22	1:A:219:MET:HE2	1.96	0.48
2:B:14:ARG:HA	2:B:86:ILE:O	2.14	0.48
2:D:16:THR:OG1	2:D:65:PHE:HA	2.14	0.48
2:B:75:ALA:HB2	2:B:97:PRO:HB2	1.96	0.48
2:D:106:VAL:HG23	2:D:107:LEU:HG	1.96	0.47
2:D:72:ASP:HB3	2:D:100:PRO:HD3	1.97	0.47
2:B:44:ILE:HB	2:D:44:ILE:HD13	1.97	0.47
1:A:229:ARG:HH22	1:A:233:GLU:CD	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:ILE:HG23	2:D:41:ARG:HH22	1.80	0.47
1:A:3:PRO:HD2	1:A:22:LEU:HD21	1.97	0.46
1:C:76:SER:HA	1:C:79:THR:HG23	1.97	0.46
2:B:84:ASN:ND2	2:B:86:ILE:HG23	2.30	0.46
1:C:164:LYS:NZ	1:C:239:GLU:OE2	2.48	0.46
2:D:10:GLU:HB2	2:D:43:THR:HG21	1.98	0.46
2:B:84:ASN:OD1	2:B:94:LYS:HD3	2.16	0.46
2:B:10:GLU:HG2	2:B:43:THR:HG21	1.98	0.46
2:B:102:ARG:HA	2:B:125:PHE:O	2.16	0.45
2:D:71:VAL:O	2:D:74:LEU:HB3	2.16	0.45
2:B:106:VAL:HG12	2:B:107:LEU:HD23	1.98	0.45
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.98	0.45
1:A:151:ARG:NH1	1:A:154:ASN:O	2.49	0.45
2:D:76:LEU:HD22	2:D:103:ILE:CD1	2.45	0.45
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.51	0.45
1:C:229:ARG:NH2	1:C:233:GLU:OE1	2.49	0.45
2:B:147:HIS:O	2:B:151:LEU:HG	2.16	0.45
2:D:12:ILE:HG21	2:D:62:GLU:HA	1.99	0.45
1:A:293:ILE:O	1:A:297:GLN:HB2	2.17	0.45
2:B:12:ILE:HD11	2:B:62:GLU:HA	1.98	0.44
1:C:279:LYS:N	1:C:279:LYS:HD2	2.32	0.44
2:D:128:ARG:NH1	2:D:130:ARG:HG3	2.33	0.44
2:B:96:ARG:NH1	2:B:96:ARG:HB2	2.32	0.44
2:D:9:VAL:O	2:D:60:LYS:NZ	2.50	0.44
2:D:23:ALA:HB2	2:D:55:ARG:HB3	1.98	0.44
2:D:114:CYS:SG	2:D:116:SER:HB3	2.58	0.44
1:A:261:MET:C	1:A:261:MET:SD	3.00	0.44
1:A:19:ASP:O	1:A:23:VAL:HG23	2.17	0.44
2:B:46:LEU:HB2	2:D:42:ILE:HB	2.00	0.44
1:C:223:ASP:O	1:C:261:MET:HA	2.18	0.44
2:B:82:THR:HG23	2:B:96:ARG:HH12	1.82	0.43
1:A:269:ARG:NH2	1:A:278:ASP:OD1	2.52	0.43
1:C:91:THR:O	1:C:95:ILE:HG12	2.18	0.43
2:B:134:ILE:O	2:B:147:HIS:HB3	2.19	0.43
2:D:109:CYS:HA	2:D:110:PRO:HD3	1.83	0.43
2:D:34:LYS:HZ2	2:D:37:GLU:CD	2.27	0.43
2:B:34:LYS:NZ	2:B:37:GLU:OE1	2.52	0.43
1:A:270:VAL:HG23	1:A:271:ASP:N	2.29	0.42
1:C:37:GLU:CD	1:C:40:LYS:NZ	2.78	0.42
2:B:66:LEU:HD12	2:B:71:VAL:HG22	2.01	0.42
2:D:147:HIS:O	2:D:151:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:TYR:CE2	1:A:306:ARG:HD3	2.55	0.42
1:A:164:LYS:NZ	1:A:239:GLU:OE2	2.52	0.42
2:B:82:THR:OG1	2:B:96:ARG:NH2	2.53	0.42
1:C:229:ARG:HH22	1:C:233:GLU:CD	2.28	0.42
1:C:275:THR:O	1:C:279:LYS:HE3	2.20	0.42
2:D:48:LEU:HD11	2:D:58:LEU:HD22	2.02	0.42
2:D:42:ILE:HG12	2:D:61:ILE:HG23	2.01	0.42
1:A:12:ILE:HD13	1:A:12:ILE:HA	1.81	0.41
1:C:37:GLU:OE2	1:C:40:LYS:NZ	2.53	0.41
2:D:69:ASP:CG	2:D:70:GLN:N	2.78	0.41
2:B:21:ILE:HD12	2:B:58:LEU:HA	2.02	0.41
1:C:23:VAL:HG11	1:C:139:LEU:HD13	2.02	0.41
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.66	0.41
2:B:68:GLU:O	2:B:71:VAL:HB	2.19	0.41
1:A:50:GLU:HB3	1:A:105:ARG:HG2	2.03	0.41
2:D:50:SER:O	2:D:54:GLY:N	2.54	0.41
2:D:58:LEU:HD21	2:D:60:LYS:NZ	2.35	0.41
1:C:137:GLN:O	1:C:140:LEU:HG	2.21	0.41
2:D:34:LYS:NZ	2:D:37:GLU:OE1	2.53	0.41
2:B:13:LYS:HE2	2:B:88:ASN:OD1	2.22	0.40
1:C:7:LYS:HD3	1:C:7:LYS:HA	1.94	0.40
1:A:114:LEU:HD21	2:B:119:GLU:HG3	2.04	0.40
2:D:23:ALA:CB	2:D:55:ARG:HD3	2.52	0.40
2:D:104:ASP:HA	2:D:124:SER:HA	2.04	0.40
2:D:129:LYS:HD2	2:D:129:LYS:H	1.87	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	308/310 (99%)	298 (97%)	7 (2%)	3 (1%)	12 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	308/310 (99%)	300 (97%)	7 (2%)	1 (0%)	36	66
2	B	144/153 (94%)	122 (85%)	16 (11%)	6 (4%)	2	7
2	D	144/153 (94%)	130 (90%)	12 (8%)	2 (1%)	9	30
All	All	904/926 (98%)	850 (94%)	42 (5%)	12 (1%)	9	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	VAL
2	B	10	GLU
2	B	152	ALA
2	B	131	ALA
2	D	131	ALA
2	D	54	GLY
1	A	307	ASP
2	B	88	ASN
2	B	54	GLY
1	A	309	VAL
1	A	270	VAL
1	C	270	VAL

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	260/260 (100%)	234 (90%)	26 (10%)	7	24
1	C	260/260 (100%)	240 (92%)	20 (8%)	12	36
2	B	129/136 (95%)	113 (88%)	16 (12%)	4	16
2	D	129/136 (95%)	103 (80%)	26 (20%)	1	4
All	All	778/792 (98%)	690 (89%)	88 (11%)	5	19

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	38	LEU
1	A	40	LYS
1	A	59	PHE
1	A	83	LYS
1	A	92	ILE
1	A	114	LEU
1	A	125	LEU
1	A	149	GLU
1	A	151	ARG
1	A	183	ARG
1	A	198	ILE
1	A	202	LEU
1	A	229	ARG
1	A	233	GLU
1	A	237	PRO
1	A	246	GLN
1	A	250	ARG
1	A	253	ASP
1	A	255	HIS
1	A	262	LYS
1	A	267	LEU
1	A	269	ARG
1	A	307	ASP
1	A	310	LEU
2	B	14	ARG
2	B	17	VAL
2	B	19	ASP
2	B	30	LEU
2	B	31	SER
2	B	52	GLU
2	B	53	MET
2	B	69	ASP
2	B	80	GLN
2	B	82	THR
2	B	84	ASN
2	B	86	ILE
2	B	128	ARG
2	B	136	LEU
2	B	139	LYS
2	B	153	ASN
1	C	15	LEU

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Mol	Chain	Res	Type
1	C	37	GLU
1	C	40	LYS
1	C	56	ARG
1	C	59	PHE
1	C	60	GLN
1	C	114	LEU
1	C	121	ASN
1	C	147	GLN
1	C	151	ARG
1	C	183	ARG
1	C	194	MET
1	C	204	GLU
1	C	205	LYS
1	C	213	SER
1	C	221	GLU
1	C	256	ASN
1	C	271	ASP
1	C	279	LYS
1	C	285	TYR
2	D	12	ILE
2	D	16	THR
2	D	24	GLN
2	D	29	LEU
2	D	31	SER
2	D	32	LEU
2	D	34	LYS
2	D	36	THR
2	D	37	GLU
2	D	38	THR
2	D	47	ASN
2	D	52	GLU
2	D	56	LYS
2	D	58	LEU
2	D	61	ILE
2	D	67	SER
2	D	74	LEU
2	D	82	THR
2	D	98	SER
2	D	105	ASN
2	D	128	ARG
2	D	129	LYS
2	D	130	ARG

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Mol	Chain	Res	Type
2	D	134	ILE
2	D	151	LEU
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	170	HIS
1	A	246	GLN
1	A	256	ASN
1	A	297	GLN
1	A	305	ASN
2	B	24	GLN
2	B	47	ASN
2	B	63	ASN
2	B	84	ASN
2	B	117	HIS
2	B	132	ASN
2	B	153	ASN
1	C	108	GLN
1	C	242	ASN
1	C	291	ASN
2	D	47	ASN
2	D	113	ASN
2	D	147	HIS
2	D	148	ASN

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

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	PAL	A	311	-	15,15,15	1.51	4 (26%)	20,21,21	1.31	2 (10%)
3	PAL	C	311	-	15,15,15	1.27	3 (20%)	20,21,21	1.81	2 (10%)

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	PAL	A	311	-	-	0/17/17/17	-
3	PAL	C	311	-	-	2/17/17/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	PAL	P-O1P	3.15	1.56	1.50
3	A	311	PAL	P-C1P	2.97	1.84	1.79
3	C	311	PAL	P-O1P	2.49	1.55	1.50
3	A	311	PAL	O3-C4	-2.46	1.22	1.30
3	C	311	PAL	O3-C4	-2.36	1.23	1.30
3	A	311	PAL	O5-C5	-2.29	1.23	1.30
3	C	311	PAL	O5-C5	-2.14	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	PAL	C4-C2-N2	6.04	124.59	110.57
3	C	311	PAL	C3-C2-N2	-3.45	104.05	110.64
3	A	311	PAL	C4-C2-N2	2.44	116.24	110.57
3	A	311	PAL	O3P-P-O1P	-2.16	106.80	112.39

There are no chirality outliers.

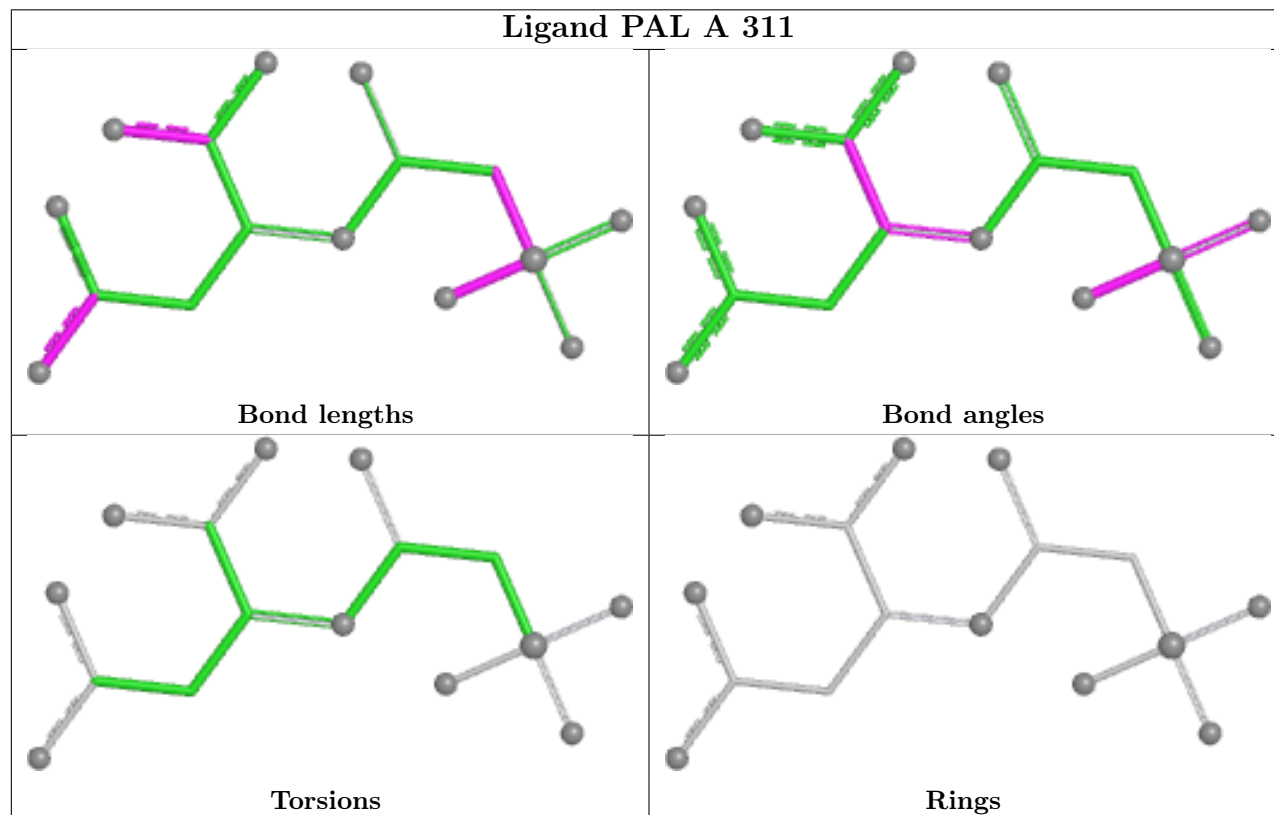
All (2) torsion outliers are listed below:

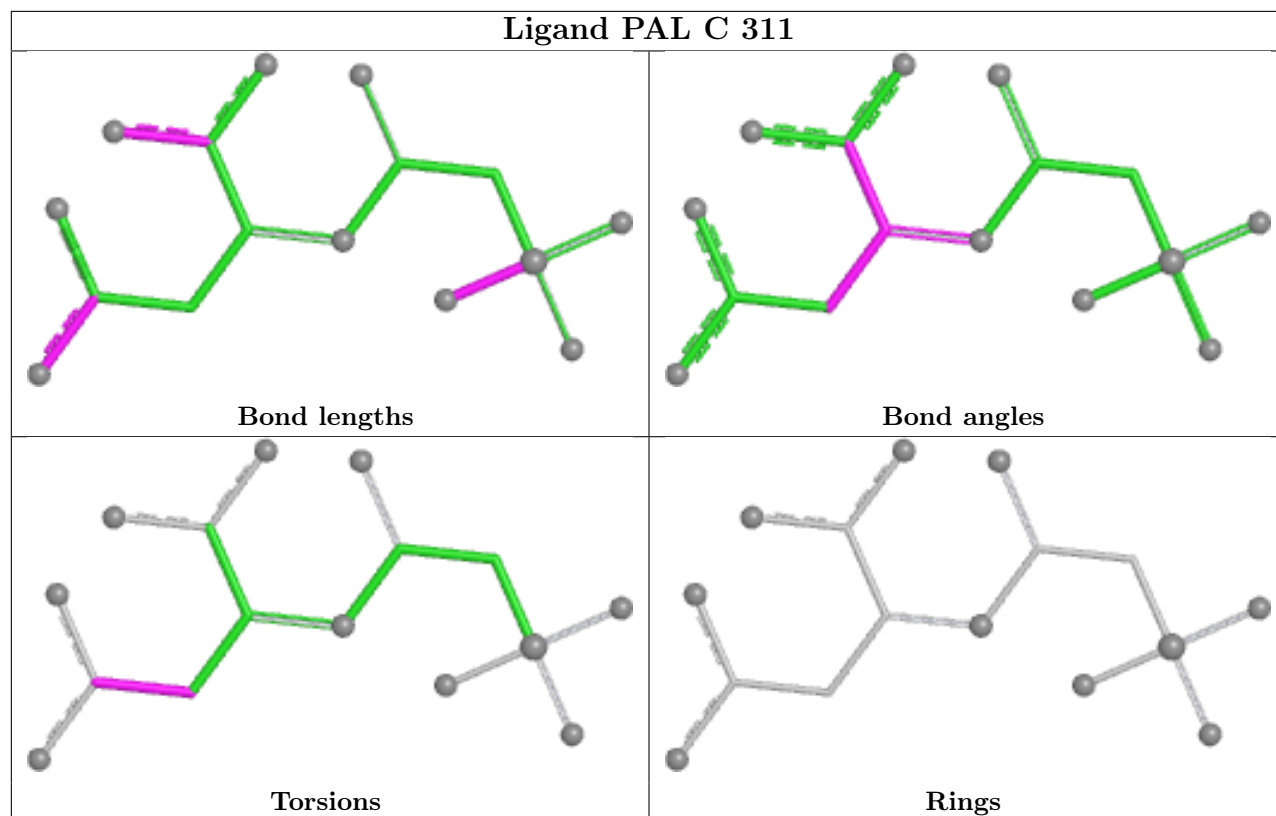
Mol	Chain	Res	Type	Atoms
3	C	311	PAL	C2-C3-C5-O5
3	C	311	PAL	C2-C3-C5-O4

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.