



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:35 AM UTC

PDB ID : 8RFA / pdb_00008rfa
Title : Arginase 2 in complex with an inhibitor
Authors : Petersen, J.
Deposited on : 2023-12-12
Resolution : 1.76 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

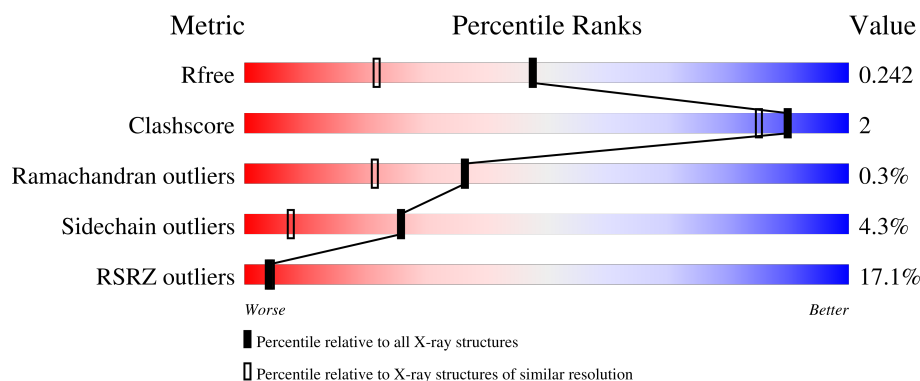
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	336	6% 88% 6% • 5%
1	B	336	37% 79% 9% • 12%
1	C	336	4% 86% 8% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7548 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 Arginase-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2430	1536	422	463	9			
1	B	296	Total	C	N	O	S	0	0	0
			2263	1434	389	431	9			
1	C	318	Total	C	N	O	S	0	0	0
			2430	1536	422	463	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	initiating methionine	UNP P78540
A	7	HIS	-	expression tag	UNP P78540
A	8	HIS	-	expression tag	UNP P78540
A	9	HIS	-	expression tag	UNP P78540
A	10	HIS	-	expression tag	UNP P78540
A	11	HIS	-	expression tag	UNP P78540
A	12	HIS	-	expression tag	UNP P78540
A	13	GLY	-	expression tag	UNP P78540
A	14	GLY	-	expression tag	UNP P78540
A	15	GLY	-	expression tag	UNP P78540
A	16	GLU	-	expression tag	UNP P78540
A	17	ASN	-	expression tag	UNP P78540
A	18	LEU	-	expression tag	UNP P78540
A	19	TYR	-	expression tag	UNP P78540
A	20	PHE	-	expression tag	UNP P78540
A	21	GLN	-	expression tag	UNP P78540
B	6	MET	-	initiating methionine	UNP P78540
B	7	HIS	-	expression tag	UNP P78540
B	8	HIS	-	expression tag	UNP P78540
B	9	HIS	-	expression tag	UNP P78540
B	10	HIS	-	expression tag	UNP P78540
B	11	HIS	-	expression tag	UNP P78540
B	12	HIS	-	expression tag	UNP P78540

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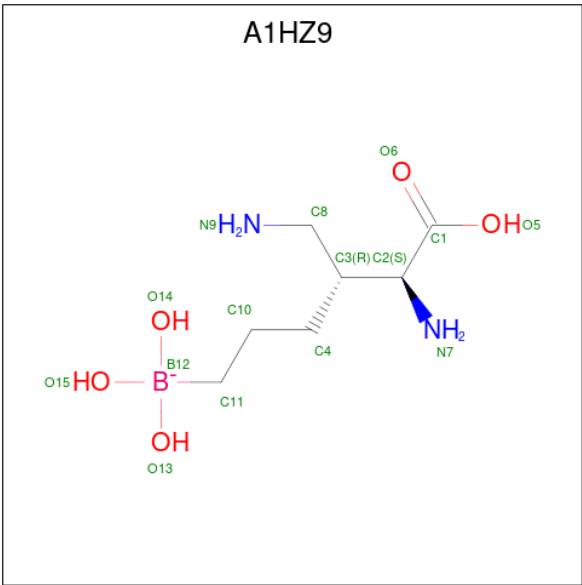
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Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLY	-	expression tag	UNP P78540
B	14	GLY	-	expression tag	UNP P78540
B	15	GLY	-	expression tag	UNP P78540
B	16	GLU	-	expression tag	UNP P78540
B	17	ASN	-	expression tag	UNP P78540
B	18	LEU	-	expression tag	UNP P78540
B	19	TYR	-	expression tag	UNP P78540
B	20	PHE	-	expression tag	UNP P78540
B	21	GLN	-	expression tag	UNP P78540
C	6	MET	-	initiating methionine	UNP P78540
C	7	HIS	-	expression tag	UNP P78540
C	8	HIS	-	expression tag	UNP P78540
C	9	HIS	-	expression tag	UNP P78540
C	10	HIS	-	expression tag	UNP P78540
C	11	HIS	-	expression tag	UNP P78540
C	12	HIS	-	expression tag	UNP P78540
C	13	GLY	-	expression tag	UNP P78540
C	14	GLY	-	expression tag	UNP P78540
C	15	GLY	-	expression tag	UNP P78540
C	16	GLU	-	expression tag	UNP P78540
C	17	ASN	-	expression tag	UNP P78540
C	18	LEU	-	expression tag	UNP P78540
C	19	TYR	-	expression tag	UNP P78540
C	20	PHE	-	expression tag	UNP P78540
C	21	GLN	-	expression tag	UNP P78540

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

- Molecule 3 is [(4 {R},5 {S})-4-(aminomethyl)-5-azanyl-6-oxidanyl-6-oxidanylidene-hexyl]-tris(oxidanyl)boron (CCD ID: A1HZ9) (formula: C₇H₁₈BN₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			15	1	7	2	5		

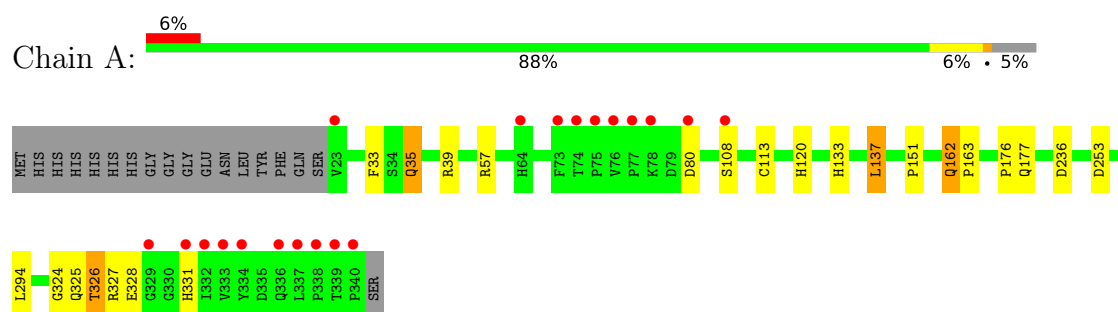
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	87	Total	O	0	0
			87	87		
4	C	174	Total	O	0	0
			174	174		

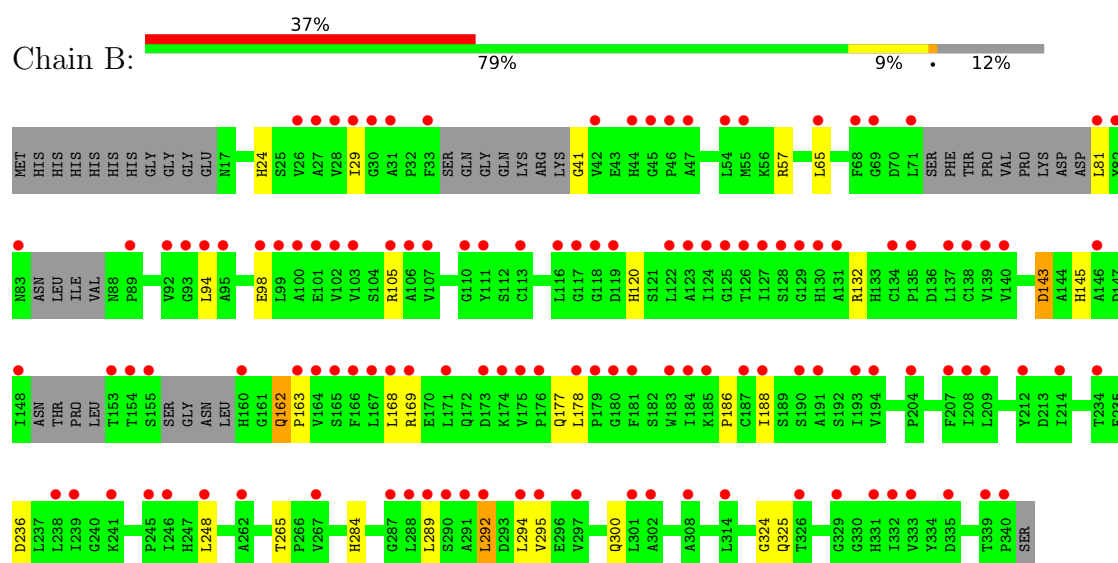
3 Residue-property plots [i](#)

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 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.

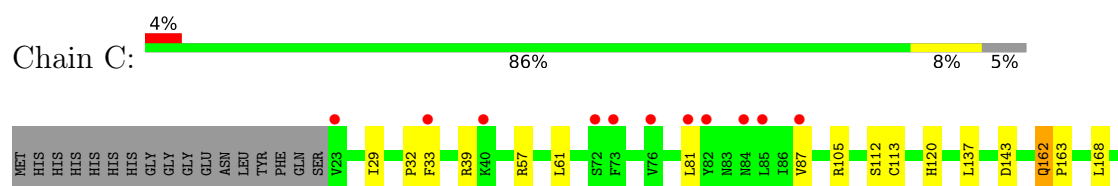
- Molecule 1: Arginase-2, mitochondrial

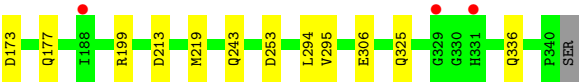


- Molecule 1: Arginase-2, mitochondrial



- Molecule 1: Arginase-2, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.66Å 134.87Å 144.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 1.76 44.40 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.40-1.76) 99.9 (44.40-1.76)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.76Å)	Xtriage
Refinement program	BUSTER 2.11.7 PACIOREK	Depositor
R, R_{free}	0.222 , 0.252 0.211 , 0.242	Depositor DCC
R_{free} test set	4377 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7548	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: A1HZ9, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.83	0/2484	1.14	3/3382 (0.1%)
1	B	0.86	0/2308	1.26	3/3133 (0.1%)
1	C	0.87	0/2484	1.17	9/3382 (0.3%)
All	All	0.85	0/7276	1.19	15/9897 (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	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ASP	CA-CB-CG	8.85	121.45	112.60
1	C	33	PHE	CA-CB-CG	7.71	121.51	113.80
1	C	32	PRO	CA-C-N	6.87	131.32	121.50
1	C	32	PRO	C-N-CA	6.87	131.32	121.50
1	C	143	ASP	CA-CB-CG	6.83	119.44	112.60
1	C	253	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	112	SER	N-CA-C	-5.86	100.29	109.25
1	C	87	VAL	CA-C-N	5.84	128.71	123.10
1	C	87	VAL	C-N-CA	5.84	128.71	123.10
1	A	253	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	324	GLY	N-CA-C	5.49	121.01	114.48
1	B	324	GLY	N-CA-C	5.33	120.82	114.48
1	B	236	ASP	CA-CB-CG	5.32	117.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	CYS	N-CA-C	5.08	116.59	108.41
1	C	173	ASP	CA-CB-CG	5.06	117.66	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	132	ARG	Mainchain

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	2430	0	2410	8	0
1	B	2263	0	2225	10	0
1	C	2430	0	2410	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	15	0	0	0	0
4	A	143	0	0	0	0
4	B	87	0	0	0	0
4	C	174	0	0	1	0
All	All	7548	0	7045	26	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 2.

All (26) 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:289:LEU:HD21	1:B:292:LEU:HD12	1.70	0.73
1:C:57:ARG:HH21	1:C:325:GLN:HE22	1.35	0.71
1:A:57:ARG:HH21	1:A:325:GLN:HE22	1.42	0.67
1:B:41:GLY:HA3	1:B:300:GLN:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:HH21	1:B:325:GLN:HE22	1.54	0.55
1:C:199:ARG:HD3	1:C:219:MET:HG3	1.91	0.53
1:A:137:LEU:C	1:A:137:LEU:HD12	2.35	0.50
1:A:108:SER:HB3	1:A:133:HIS:CE1	2.48	0.48
1:C:120:HIS:CG	1:C:295:VAL:HG21	2.50	0.47
1:A:151:PRO:HD2	1:A:176:PRO:HD2	1.96	0.46
1:A:33:PHE:CZ	1:A:35:GLN:HB2	2.49	0.46
1:B:169:ARG:HG2	1:B:186:PRO:HB2	1.96	0.46
1:A:57:ARG:NH2	1:A:325:GLN:HE22	2.12	0.45
1:C:29:ILE:HD12	1:C:113:CYS:SG	2.57	0.45
1:C:137:LEU:HD12	1:C:137:LEU:C	2.42	0.45
1:B:120:HIS:CG	1:B:295:VAL:HG21	2.53	0.44
1:B:248:LEU:HD23	1:B:292:LEU:HD11	2.01	0.42
1:C:243:GLN:HG2	4:C:771:HOH:O	2.18	0.42
1:A:326:THR:HG23	1:A:328:GLU:H	1.83	0.42
1:B:162:GLN:N	1:B:163:PRO:CD	2.82	0.42
1:A:162:GLN:N	1:A:163:PRO:CD	2.83	0.42
1:B:143:ASP:HB3	1:B:145:HIS:O	2.20	0.41
1:B:24:HIS:NE2	1:B:284:HIS:HE1	2.19	0.41
1:C:120:HIS:CD2	1:C:295:VAL:HG21	2.55	0.41
1:B:162:GLN:N	1:B:163:PRO:HD2	2.36	0.41
1:C:162:GLN:N	1:C:163:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	316/336 (94%)	310 (98%)	5 (2%)	1 (0%)	36	21
1	B	283/336 (84%)	274 (97%)	8 (3%)	1 (0%)	30	15
1	C	316/336 (94%)	311 (98%)	4 (1%)	1 (0%)	36	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	915/1008 (91%)	895 (98%)	17 (2%)	3 (0%)	36 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	B	162	GLN
1	C	162	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/283 (95%)	257 (96%)	11 (4%)	27 8
1	B	247/283 (87%)	234 (95%)	13 (5%)	20 5
1	C	268/283 (95%)	258 (96%)	10 (4%)	30 11
All	All	783/849 (92%)	749 (96%)	34 (4%)	26 8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	39	ARG
1	A	80	ASP
1	A	120	HIS
1	A	137	LEU
1	A	177	GLN
1	A	236	ASP
1	A	294	LEU
1	A	326	THR
1	A	327	ARG
1	A	331	HIS
1	B	29	ILE
1	B	65	LEU

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Mol	Chain	Res	Type
1	B	81	LEU
1	B	94	LEU
1	B	98	GLU
1	B	105	ARG
1	B	168	LEU
1	B	177	GLN
1	B	178	LEU
1	B	188	ILE
1	B	265	THR
1	B	292	LEU
1	B	294	LEU
1	C	39	ARG
1	C	61	LEU
1	C	81	LEU
1	C	105	ARG
1	C	168	LEU
1	C	177	GLN
1	C	213	ASP
1	C	294	LEU
1	C	306	GLU
1	C	336	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	206	HIS
1	A	300	GLN
1	A	325	GLN
1	B	44	HIS
1	B	83	ASN
1	B	284	HIS
1	B	300	GLN
1	B	325	GLN
1	C	177	GLN
1	C	228	GLN
1	C	284	HIS
1	C	325	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 7 ligands modelled in this entry, 6 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$
3	A1HZ9	A	403	2	14,14,14	2.56	3 (21%)	12,19,19	0.81	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
3	A1HZ9	A	403	2	-	1/14/17/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	A1HZ9	B12-O14	-5.47	1.36	1.47
3	A	403	A1HZ9	B12-O15	-5.38	1.36	1.47
3	A	403	A1HZ9	B12-O13	-4.69	1.38	1.47

There are no bond angle outliers.

There are no chirality outliers.

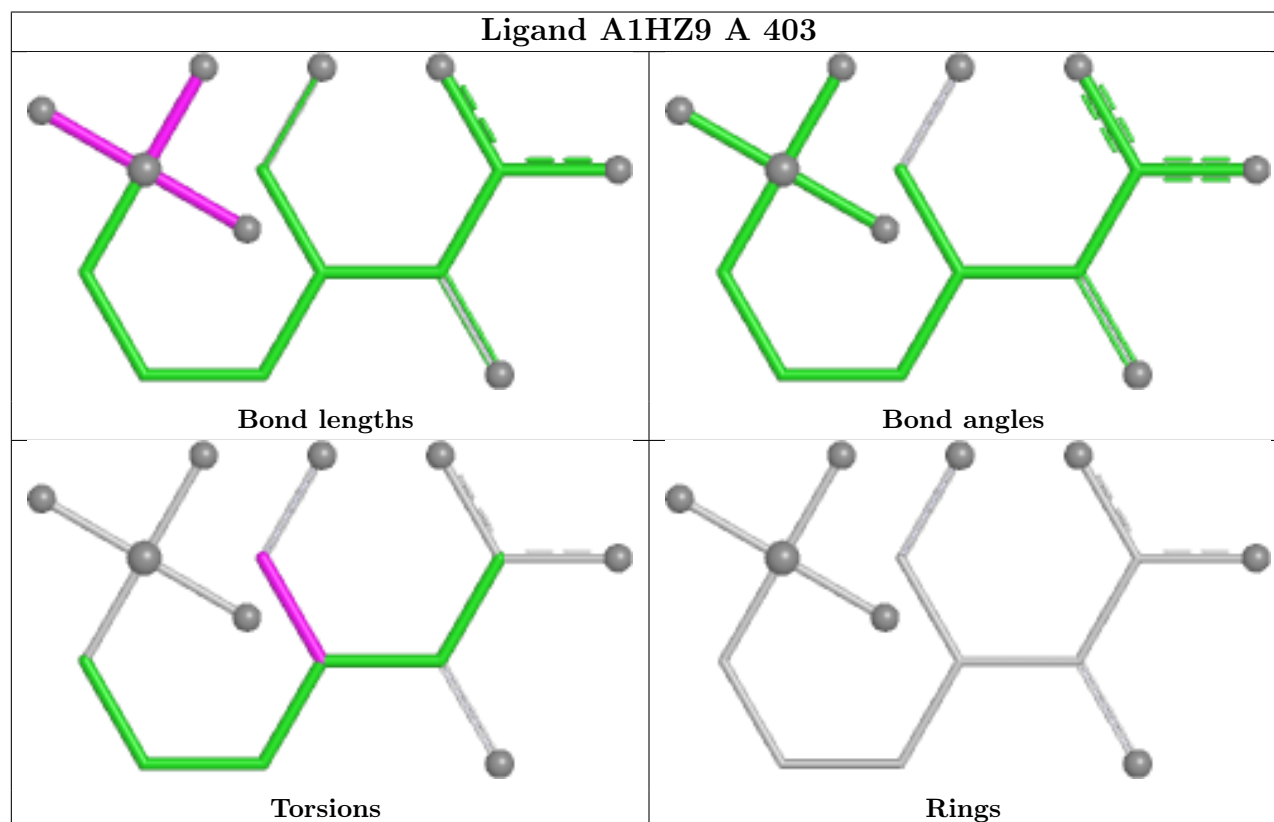
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	A1HZ9	C2-C3-C8-N9

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

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	318/336 (94%)	0.51	20 (6%) 26 30	23, 34, 68, 129	0
1	B	296/336 (88%)	1.93	125 (42%) 0 1	27, 51, 97, 157	0
1	C	318/336 (94%)	0.43	14 (4%) 39 45	22, 33, 60, 86	0
All	All	932/1008 (92%)	0.94	159 (17%) 4 4	22, 38, 78, 157	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	PHE	6.8
1	A	337	LEU	6.7
1	B	71	LEU	6.3
1	B	81	LEU	6.2
1	A	338	PRO	6.1
1	A	339	THR	6.0
1	B	92	VAL	5.9
1	B	166	PHE	5.9
1	B	33	PHE	5.6
1	B	171	LEU	5.2
1	B	175	VAL	5.1
1	B	168	LEU	5.0
1	B	184	ILE	5.0
1	B	167	LEU	4.9
1	A	334	TYR	4.8
1	B	207	PHE	4.6
1	B	188	ILE	4.6
1	B	183	TRP	4.6
1	B	29	ILE	4.6
1	B	94	LEU	4.4
1	A	332	ILE	4.4
1	B	118	GLY	4.4
1	B	95	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	178	LEU	4.3
1	B	125	GLY	4.2
1	B	82	TYR	4.2
1	A	77	PRO	4.2
1	B	119	ASP	4.1
1	A	333	VAL	4.1
1	B	187	CYS	4.1
1	B	181	PHE	4.0
1	B	297	VAL	4.0
1	B	113	CYS	3.9
1	B	137	LEU	3.9
1	B	164	VAL	3.8
1	B	148	ILE	3.8
1	B	111	TYR	3.8
1	B	99	LEU	3.8
1	B	153	THR	3.8
1	B	245	PRO	3.7
1	B	134	CYS	3.7
1	B	46	PRO	3.6
1	B	138	CYS	3.6
1	B	294	LEU	3.6
1	B	103	VAL	3.5
1	B	212	TYR	3.5
1	A	340	PRO	3.5
1	B	124	ILE	3.5
1	B	127	ILE	3.5
1	B	83	ASN	3.5
1	A	23	VAL	3.5
1	B	65	LEU	3.4
1	B	98	GLU	3.4
1	B	155	SER	3.4
1	B	292	LEU	3.4
1	B	31	ALA	3.3
1	B	68	PHE	3.3
1	B	102	VAL	3.3
1	A	80	ASP	3.3
1	B	105	ARG	3.2
1	B	107	VAL	3.2
1	B	122	LEU	3.2
1	B	154	THR	3.2
1	B	239	ILE	3.2
1	B	194	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	329	GLY	3.1
1	C	331	HIS	3.0
1	C	84	ASN	3.0
1	C	85	LEU	3.0
1	B	204	PRO	3.0
1	B	246	ILE	3.0
1	B	130	HIS	2.9
1	B	331	HIS	2.9
1	C	82	TYR	2.9
1	B	209	LEU	2.9
1	B	165	SER	2.9
1	B	93	GLY	2.9
1	B	117	GLY	2.9
1	B	129	GLY	2.9
1	B	340	PRO	2.9
1	A	76	VAL	2.8
1	A	64	HIS	2.8
1	B	179	PRO	2.8
1	B	238	LEU	2.8
1	B	262	ALA	2.7
1	B	176	PRO	2.7
1	B	26	VAL	2.7
1	B	185	LYS	2.7
1	B	116	LEU	2.7
1	A	331	HIS	2.7
1	B	160	HIS	2.7
1	B	326	THR	2.6
1	B	123	ALA	2.6
1	B	308	ALA	2.6
1	B	174	LYS	2.6
1	C	81	LEU	2.6
1	A	74	THR	2.6
1	B	128	SER	2.6
1	B	180	GLY	2.5
1	B	42	VAL	2.5
1	B	214	ILE	2.5
1	B	135	PRO	2.5
1	B	146	ALA	2.5
1	A	73	PHE	2.5
1	B	267	VAL	2.5
1	B	208	ILE	2.5
1	B	44	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	2.5
1	B	332	ILE	2.5
1	B	101	GLU	2.4
1	B	100	ALA	2.4
1	B	301	LEU	2.4
1	C	76	VAL	2.4
1	B	131	ALA	2.4
1	B	191	ALA	2.4
1	C	188	ILE	2.4
1	B	163	PRO	2.3
1	B	27	ALA	2.3
1	B	54	LEU	2.3
1	B	288	LEU	2.3
1	B	333	VAL	2.3
1	B	173	ASP	2.3
1	B	89	PRO	2.3
1	B	110	GLY	2.3
1	B	339	THR	2.3
1	B	289	LEU	2.3
1	B	169	ARG	2.3
1	B	69	GLY	2.3
1	B	335	ASP	2.3
1	C	329	GLY	2.2
1	A	336	GLN	2.2
1	B	295	VAL	2.2
1	B	47	ALA	2.2
1	B	190	SER	2.2
1	A	75	PRO	2.2
1	A	78	LYS	2.2
1	A	108	SER	2.2
1	B	55	MET	2.2
1	B	291	ALA	2.2
1	B	45	GLY	2.2
1	B	193	ILE	2.2
1	B	126	THR	2.2
1	B	234	THR	2.2
1	B	28	VAL	2.1
1	B	30	GLY	2.1
1	B	287	GLY	2.1
1	B	248	LEU	2.1
1	C	87	VAL	2.1
1	B	241	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	2.1
1	C	23	VAL	2.1
1	B	290	SER	2.1
1	C	73	PHE	2.1
1	B	106	ALA	2.0
1	B	314	LEU	2.0
1	C	40	LYS	2.0
1	B	302	ALA	2.0
1	C	72	SER	2.0
1	B	139	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

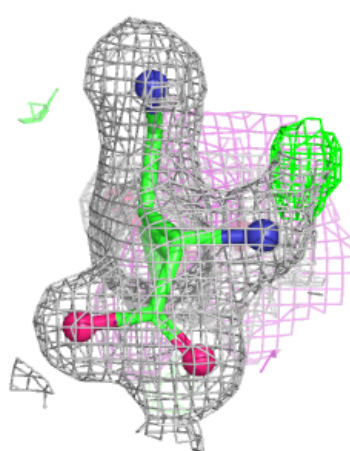
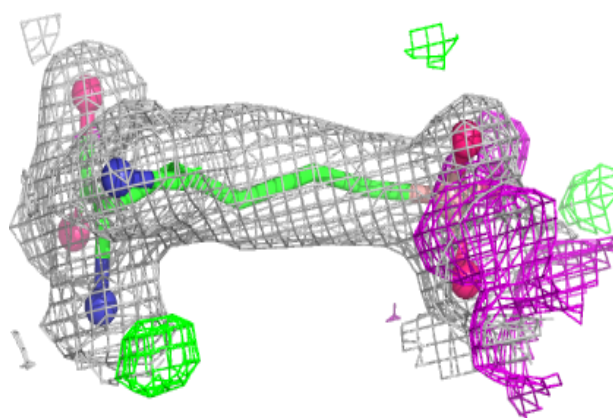
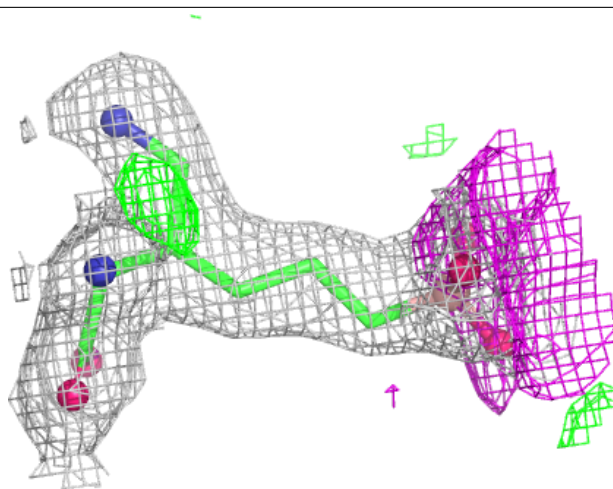
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1HZ9	A	403	15/15	0.84	0.12	34,37,47,52	0
2	MN	B	500	1/1	0.89	0.12	57,57,57,57	0
2	MN	B	501	1/1	0.96	0.13	47,47,47,47	0
2	MN	A	402	1/1	0.97	0.12	39,39,39,39	0
2	MN	C	500	1/1	0.98	0.07	33,33,33,33	0
2	MN	C	501	1/1	0.98	0.05	33,33,33,33	0
2	MN	A	401	1/1	0.98	0.16	37,37,37,37	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 A1HZ9 A 403:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.