

Full wwPDB X-ray Structure Validation Report (i)

Nov 25, 2024 – 12:10 pm GMT

PDB ID	:	8RG6
Title	:	Arginase 2 in complex with inhibitor
Authors	:	Petersen, J.
Deposited on	:	2023-12-13
Resolution	:	1.62 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

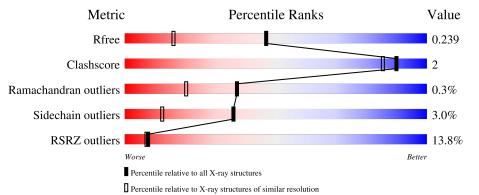
The following versions of software and data (see references (1)) were used in the production of this report:

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.62 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	164625	6077 (1.64-1.60)
Clashscore	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)
RSRZ outliers	164620	6075 (1.64-1.60)

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 <=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	А	336	8%	7% • 5%
-	D		8%	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
	В	336	91%	5% • •
1	С	336	88%	6% • 5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7751 atoms, of which 6 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	318	Total 2430	C 1536	N 422	0 463	S 9	0	0	0
1	В	324	Total 2477	C 1567	N 428	0 473	S 9	0	0	0
1	С	318	Total 2430	C 1536	N 422	0 463	S 9	0	0	0

• Molecule 1 is a protein called Arginase-2, mitochondrial.

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

There are 48 discrepancies between the modelled and reference sequences:



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

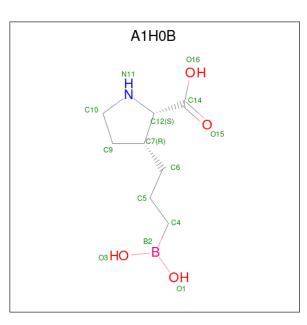
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• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mn 2 2	0	0
2	В	2	Total Mn 2 2	0	0
2	С	2	Total Mn 2 2	0	0

• Molecule 3 is $(2 \{S\}, 3 \{R\})$ -3-[3-(dihydroxyboranyl)propyl]pyrrolidine-2-carboxylic acid (three-letter code: A1H0B) (formula: $C_8H_{16}BNO_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total B C H N O 16 1 8 2 1 4	0	0
3	В	1	Total B C H N O 16 1 8 2 1 4	0	0
3	С	1	Total B C H N O 16 1 8 2 1 4	0	0

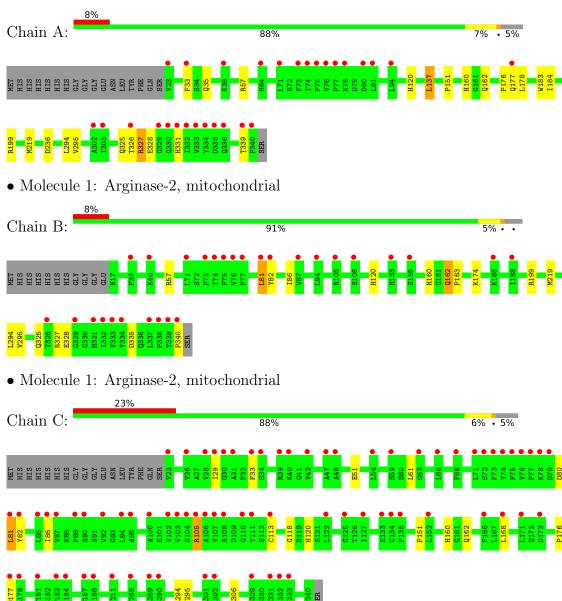
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	127	Total O 127 127	0	0
4	В	137	Total O 137 137	0	0
4	С	96	Total O 96 96	0	0



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.51Å 134.29Å 145.02Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 - 1.62	Depositor
Resolution (A)	49.27 - 1.62	EDS
% Data completeness	99.9 (49.27-1.62)	Depositor
(in resolution range)	99.9 (49.27 - 1.62)	EDS
R _{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.99 (at 1.62 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.7 PACIOREK	Depositor
D D.	0.228 , 0.249	Depositor
R, R_{free}	0.212 , 0.239	DCC
R_{free} test set	6076 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.7	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 31.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7751	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: A1H0B, 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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.50	0/2484	0.62	0/3382
1	В	0.50	0/2531	0.62	0/3444
1	С	0.49	0/2484	0.64	0/3382
All	All	0.50	0/7499	0.62	0/10208

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	А	2430	0	2410	10	0
1	В	2477	0	2451	10	0
1	С	2430	0	2410	8	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	А	14	2	0	0	0
3	В	14	2	0	0	0
3	С	14	2	0	0	0
4	А	127	0	0	0	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 (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:57:ARG:HH21	1:B:325:GLN:HE22	1.39	0.70
1:A:326:THR:HG23	1:A:328:GLU:H	1.56	0.69
1:A:57:ARG:HH21	1:A:325:GLN:HE22	1.45	0.64
1:C:29:ILE:HD12	1:C:113:CYS:SG	2.40	0.62
1:C:81:LEU:H	1:C:81:LEU:HD23	1.72	0.53
1:C:105:ARG:HB3	4:C:565:HOH:O	2.12	0.50
1:B:340:PRO:HB3	1:C:176:PRO:HB3	1.93	0.49
1:A:137:LEU:C	1:A:137:LEU:HD12	2.33	0.48
1:C:82:TYR:HB3	1:C:86:ILE:HB	1.94	0.48
1:A:33:PHE:CZ	1:A:35:GLN:HB2	2.49	0.48
1:A:151:PRO:HD2	1:A:176:PRO:HD2	1.95	0.47
1:B:57:ARG:NH2	1:B:325:GLN:HE22	2.09	0.47
1:C:120:HIS:CG	1:C:295:VAL:HG21	2.51	0.46
1:B:82:TYR:HB3	1:B:86:ILE:HB	1.98	0.46
1:B:81:LEU:H	1:B:81:LEU:HD23	1.82	0.45
1:B:120:HIS:CG	1:B:295:VAL:HG21	2.52	0.45
1:A:199:ARG:HD3	1:A:219:MET:HG3	1.99	0.44
1:B:199:ARG:HD3	1:B:219:MET:HG3	1.99	0.43
1:A:339:THR:HG22	1:B:174:LYS:HE2	2.00	0.42
1:C:33:PHE:O	1:C:118:GLY:HA2	2.19	0.42
1:B:162:GLN:N	1:B:163:PRO:CD	2.83	0.41
1:A:120:HIS:CG	1:A:295:VAL:HG21	2.55	0.41
1:A:327:ARG:O	1:B:199:ARG:HA	2.20	0.41
1:A:183:TRP:CE2	1:A:184:ILE:HG13	2.56	0.41
1:C:151:PRO:HD2	1:C:176:PRO:HD2	2.03	0.41

There are no symmetry-related clashes.



Chain Non-H H(model) H(added) Clashes Symm-Clashes Mol В 137 0 4 0 0 0 4 С 96 0 0 1 0 All All 7745 6 7271 250

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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	Perce	ntiles
1	А	316/336~(94%)	310~(98%)	5(2%)	1 (0%)	37	20
1	В	321/336~(96%)	313 (98%)	7~(2%)	1 (0%)	37	20
1	С	316/336~(94%)	307~(97%)	8 (2%)	1 (0%)	37	20
All	All	953/1008~(94%)	930~(98%)	20 (2%)	3~(0%)	37	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	162	GLN
1	В	162	GLN
1	С	162	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	268/283~(95%)	260~(97%)	8~(3%)	36 12
1	В	273/283~(96%)	267~(98%)	6 (2%)	47 22
1	С	268/283~(95%)	258~(96%)	10 (4%)	29 8
All	All	809/849~(95%)	785~(97%)	24 (3%)	36 12

All (24) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	137	LEU
1	А	160	HIS
1	А	177	GLN
1	А	178	LEU
1	А	236	ASP
1	А	294	LEU
1	А	327	ARG
1	A A A A A B	331	HIS
1		81	LEU
1	В	160	HIS
1	В	294	LEU
1	В	327	ARG
1	В	328	GLU
1	В	335	ASP
1	С	51	GLU
1	С	61	LEU
1	С	80	ASP
1	С	81	LEU
1	С	105	ARG
1	С	160	HIS
1	B C C C C C C C C C C	168	LEU
1	С	177	GLN
1	С	294	LEU
1	С	306	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	88	ASN
1	А	228	GLN
1	А	325	GLN
1	В	228	GLN
1	В	284	HIS
1	В	325	GLN
1	С	206	HIS
1	С	228	GLN
1	С	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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	Trune	Chain	Res Link		Bo	ond leng	$_{\rm ths}$	В	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1H0B	А	403	2	11,14,14	1.00	1 (9%)	$12,\!18,\!18$	1.17	1 (8%)
3	A1H0B	С	403	2	11,14,14	1.68	2 (18%)	12,18,18	1.55	2 (16%)
3	A1H0B	В	403	2	11,14,14	0.84	0	12,18,18	1.26	1 (8%)

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	A1H0B	А	403	2	-	1/8/20/20	0/1/1/1
3	A1H0B	С	403	2	-	1/8/20/20	0/1/1/1
3	A1H0B	В	403	2	-	1/8/20/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
3	С	403	A1H0B	O15-C14	3.91	1.34	1.22
3	С	403	A1H0B	O16-C14	-2.82	1.21	1.30
3	А	403	A1H0B	C9-C10	2.11	1.56	1.53



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	403	A1H0B	C9-C7-C12	-3.93	98.26	103.14
3	В	403	A1H0B	C9-C7-C12	-3.58	98.70	103.14
3	А	403	A1H0B	C9-C7-C12	-3.19	99.17	103.14
3	С	403	A1H0B	O16-C14-C12	2.05	121.43	114.21

All (4) bond angle outliers are listed below:

There are no chirality outliers.

All (3) torsion outliers are listed below:

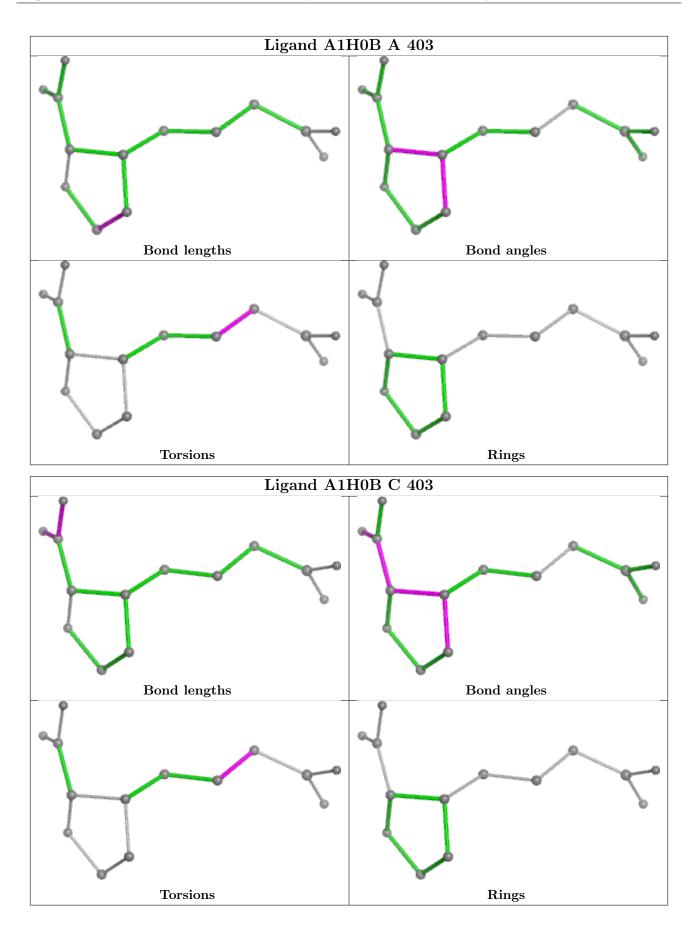
Mol	Chain	Res	Type	Atoms
3	А	403	A1H0B	B2-C4-C5-C6
3	В	403	A1H0B	B2-C4-C5-C6
3	С	403	A1H0B	B2-C4-C5-C6

There are no ring outliers.

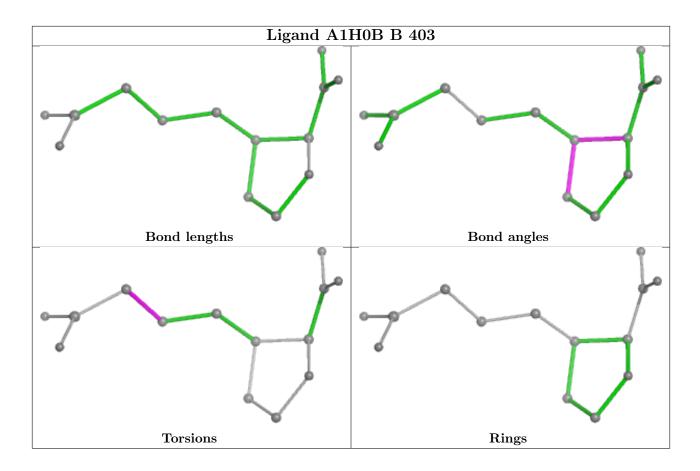
No monomer is involved in short contacts.

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 then 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 (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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	318/336~(94%)	0.60	28 (8%) 17 17	21, 34, 62, 87	0
1	В	324/336~(96%)	0.48	28 (8%) 18 17	21, 32, 60, 89	0
1	С	318/336~(94%)	1.37	76 (23%) 2 2	24, 41, 75, 106	0
All	All	960/1008~(95%)	0.81	132 (13%) 8 7	21, 35, 65, 106	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	33	PHE	6.2
1	С	107	VAL	5.3
1	С	122	LEU	4.9
1	С	110	GLY	4.7
1	С	106	ALA	4.6
1	В	73	PHE	4.4
1	С	26	VAL	4.4
1	С	81	LEU	4.4
1	С	30	GLY	4.3
1	С	76	VAL	4.3
1	В	339	THR	4.2
1	В	33	PHE	4.2
1	А	334	TYR	4.1
1	С	188	ILE	4.0
1	С	103	VAL	4.0
1	С	73	PHE	3.9
1	В	77	PRO	3.9
1	В	76	VAL	3.9
1	А	332	ILE	3.8
1	С	113	CYS	3.8
1	С	111	TYR	3.7
1	А	335	ASP	3.7
1	С	71	LEU	3.7



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Mol	Chain	Res	ous page. Type	RSRZ
1	С	102	VAL	3.6
1	C	77	PRO	3.6
1	C	42	VAL	3.5
1	C	92	VAL	3.4
1	C C	29	ILE	3.4
1	C	65	LEU	3.3
1	C C	178	LEU	3.3
1	B	340	PRO	3.3
1	B	133	HIS	3.3
1	A	80	ASP	3.2
1	B	329	GLY	$\frac{3.2}{3.2}$
1	B	94	LEU	$\frac{3.2}{3.2}$
1	A	94 333	VAL	3.2 3.1
$\frac{1}{1}$	A C	82 82	TYR	3.1 3.1
1	C	68 68	PHE	3.1 3.1
$\frac{1}{1}$	A		VAL	
<u> </u>	A C	23 125	GLY VAL	3.1 3.0
			HIS	3.0
1	A	331		
1	C A	181	PHE	3.0
1	A C	340	PRO	3.0
1	C	331	HIS	3.0
1	C	184	ILE	3.0
1	C C	78	LYS	3.0
1		108	SER	3.0
1	B	81	LEU	2.9
1	C	85	LEU	2.9
1	A	76	VAL	2.9
1	C	177	GLN	2.9
1	B	331	HIS	2.9
1	C	94	LEU	2.9
1	A	78	LYS	2.9
1	A	77	PRO	2.9
1	A	302	ALA	2.9
1	A	74	THR	2.9
1	С	166	PHE	2.8
1	С	105	ARG	2.8
1	В	105	ARG	2.8
1	C	23	VAL	2.8
1	С	95	ALA	2.8
1	С	183	TRP	2.7
1	С	48	ALA	2.7
1	В	74	THR	2.7

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Mol	nuea fron Chain	Res	Type	RSRZ
1	С	265	THR	2.7
1	С	59	SER	2.7
1	В	326	THR	2.7
1	В	338	PRO	2.7
1	С	90	ARG	2.7
1	В	185	LYS	2.7
1	С	171	LEU	2.6
1	А	336	GLN	2.6
1	А	326	THR	2.6
1	С	74	THR	2.6
1	С	152	LEU	2.6
1	В	334	TYR	2.6
1	С	187	CYS	2.6
1	A	71	LEU	2.5
1	C	302	ALA	2.5
1	C	89	PRO	2.5
1	A	73	PHE	2.5
1	С	28	VAL	2.5
1	С	127	ILE	2.5
1	С	104	SER	2.4
1	В	333	VAL	2.4
1	А	94	LEU	2.4
1	С	34	SER	2.4
1	В	87	VAL	2.4
1	А	177	GLN	2.4
1	С	72	SER	2.4
1	В	71	LEU	2.4
1	С	62	GLY	2.4
1	С	86	ILE	2.4
1	С	75	PRO	2.4
1	А	81	LEU	2.4
1	С	79	ASP	2.4
1	C C	39	ARG	2.3
1	С	289	LEU	2.3
1	C C	301	LEU	2.3
1	С	133	HIS	2.3
1	С	290	SER	2.3
1	С	54	LEU	2.3
1	А	33	PHE	2.3
1	С	31	ALA	2.3
1	А	329	GLY	2.3

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Mol	Chain	Res Type		RSRZ	
1	В	337	LEU	2.3	
1	В	75	PRO	2.2	
1	С	100	ALA	2.2	
1	С	40	LYS	2.2	
1	А	75	PRO	2.2	
1	А	303	THR	2.2	
1	В	40	LYS	2.2	
1	В	188	ILE	2.2	
1	С	333	VAL	2.2	
1	В	332	ILE	2.1	
1	С	135	PRO	2.1	
1	С	329	GLY	2.1	
1	В	82	TYR	2.1	
1	С	173	ASP	2.1	
1	С	87	VAL	2.1	
1	С	168	LEU	2.1	
1	А	38	LYS	2.1	
1	С	47	ALA	2.0	
1	А	64	HIS	2.0	
1	С	332	ILE	2.0	
1	В	108	SER	2.0	
1	С	134	CYS	2.0	
1	А	330	GLY	2.0	
1	В	155	SER	2.0	
1	С	211	ASN	2.0	

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

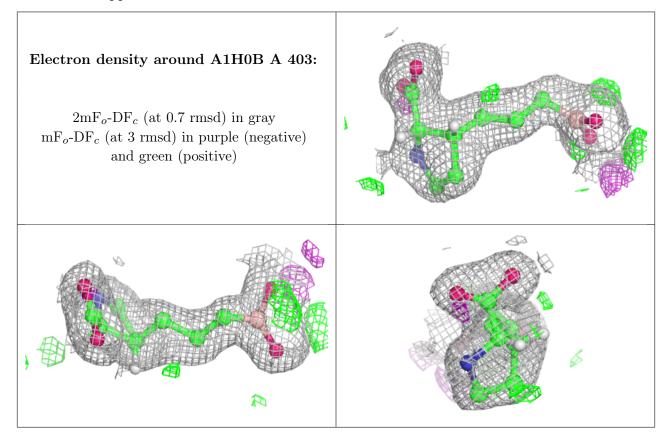
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

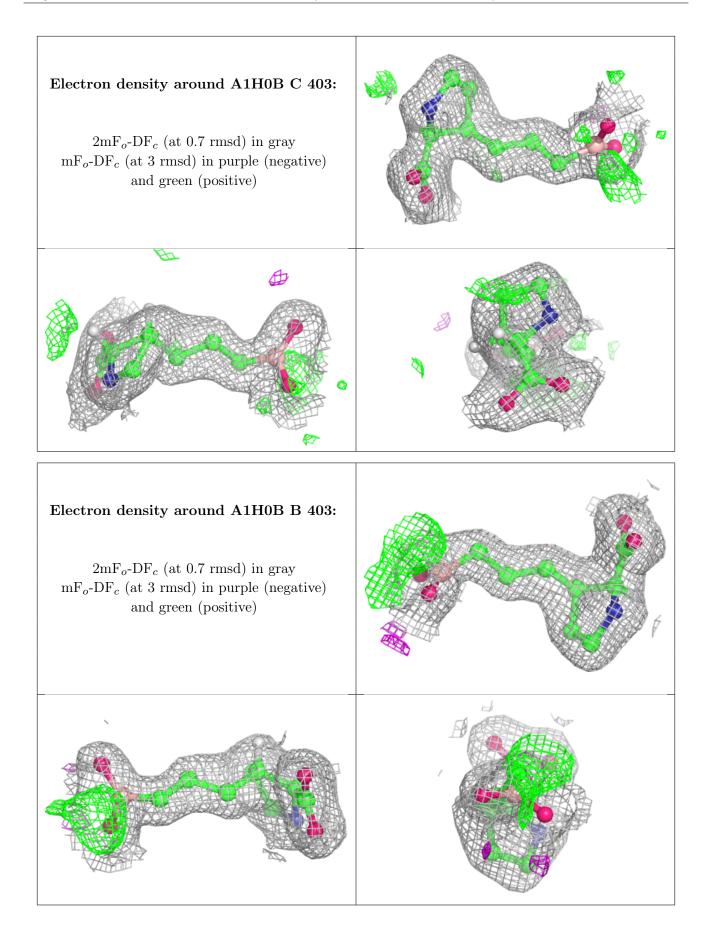


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	$Q{<}0.9$
3	A1H0B	А	403	14/14	0.89	0.10	33,34,36,37	0
3	A1H0B	С	403	14/14	0.91	0.10	$31,\!33,\!35,\!36$	0
3	A1H0B	В	403	14/14	0.92	0.08	$25,\!30,\!32,\!32$	0
2	MN	А	402	1/1	0.97	0.05	$31,\!31,\!31,\!31$	0
2	MN	А	401	1/1	0.98	0.04	29,29,29,29	0
2	MN	В	402	1/1	0.98	0.03	$25,\!25,\!25,\!25$	0
2	MN	С	401	1/1	0.98	0.05	32,32,32,32	0
2	MN	С	402	1/1	0.99	0.04	31,31,31,31	0
2	MN	В	401	1/1	0.99	0.02	26,26,26,26	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.









6.5 Other polymers (i)

There are no such residues in this entry.

