Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 09:55 PM JST

PDB ID	:	8YWZ
Title	:	Crystal structure of SARS-Cov-2 main protease H163A mutant in complex with Bofutrelvir
Authors	:	Zou, X.F.; Wang, W.W.; Zhang, J.; Li, J.
Deposited on	:	2024-04-01
Resolution	:	1.91 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:

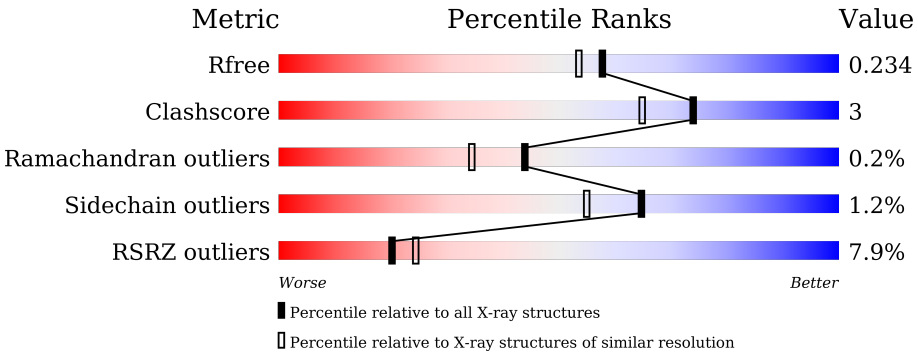
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	A	296	7% 94% 5% •
1	B	296	9% 91% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4840 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.

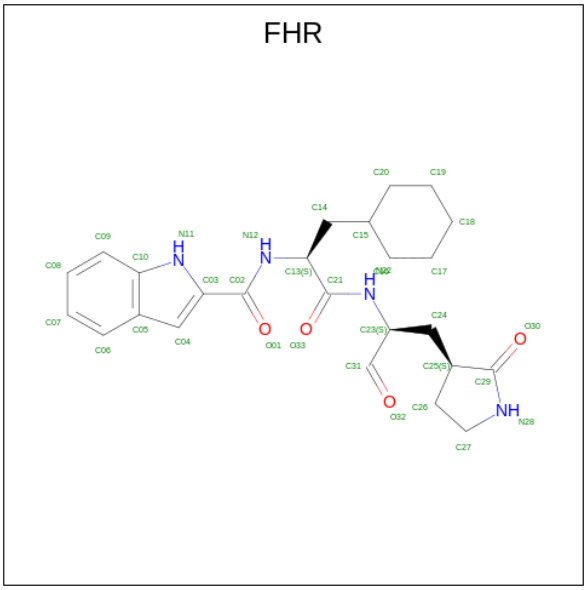
- Molecule 1 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2237	1420	376	421	20			
1	B	296	Total	C	N	O	S	0	0	0
			2229	1414	375	421	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ALA	ASN	conflict	UNP P0DTD1
A	163	ALA	HIS	engineered mutation	UNP P0DTD1
B	142	ALA	ASN	conflict	UNP P0DTD1
B	163	ALA	HIS	engineered mutation	UNP P0DTD1

- Molecule 2 is {N}-[(2 {S})-3-cyclohexyl-1-oxidanylidene-1-[[(2 {S})-1-oxidanylidene-3-[(3 {S})-2-oxidanylidenepyrrolidin-3-yl]propan-2-yl]amino]propan-2-yl]-1 {H}-indole-2-carbox amide (three-letter code: FHR) (formula: $C_{25}H_{32}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			33	25	4	4		

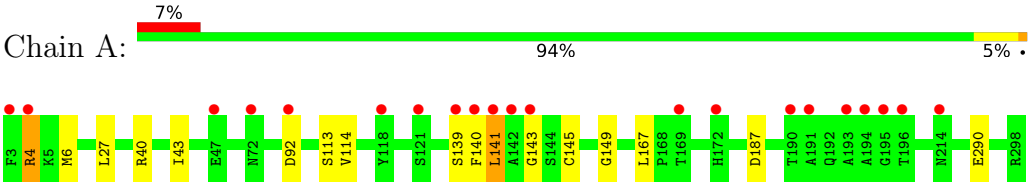
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total	O	0	0
			195	195		
3	B	146	Total	O	0	0
			146	146		

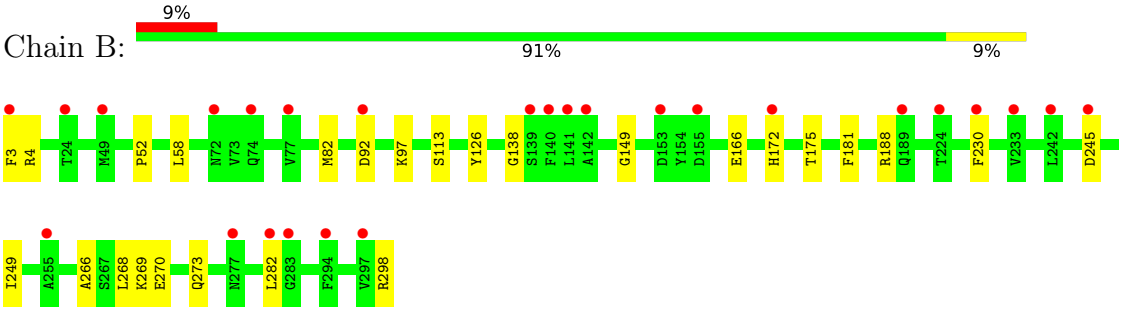
3 Residue-property plots (i)

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: 3C-like proteinase nsp5



• Molecule 1: 3C-like proteinase nsp5



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.83Å 102.80Å 102.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.63 – 1.91 30.63 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.63-1.91) 98.9 (30.63-1.91)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.196 , 0.233 0.197 , 0.234	Depositor DCC
R_{free} test set	3252 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FHR

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	0.40	0/2286	0.59	1/3115 (0.0%)
1	B	0.38	0/2278	0.56	0/3107
All	All	0.39	0/4564	0.57	1/6222 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	ASP	CB-CG-OD1	6.07	123.76	118.30

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	2237	0	2156	12	0
1	B	2229	0	2135	17	0
2	B	33	0	0	1	0
3	A	195	0	0	3	1
3	B	146	0	0	3	1
All	All	4840	0	4291	26	1

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 3.

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:A:6:MET:SD	3:B:472:HOH:O	2.36	0.83
1:A:290:GLU:OE2	3:A:301:HOH:O	2.14	0.65
1:A:145:CYS:SG	3:A:452:HOH:O	2.56	0.63
1:A:114:VAL:HG11	1:A:140:PHE:HZ	1.63	0.63
1:B:138:GLY:HA2	1:B:172:HIS:HD2	1.66	0.60
1:B:52:PRO:HD2	1:B:188:ARG:HG2	1.85	0.59
1:A:114:VAL:HG11	1:A:140:PHE:CZ	2.39	0.56
1:B:58:LEU:HD22	1:B:82:MET:HE2	1.86	0.56
1:A:139:SER:HB3	1:B:4:ARG:H	1.73	0.52
1:B:138:GLY:HA2	1:B:172:HIS:CD2	2.45	0.51
1:A:143:GLY:HA2	3:A:310:HOH:O	2.10	0.50
1:B:97:LYS:HD2	3:B:438:HOH:O	2.12	0.50
1:B:298:ARG:O	3:B:401:HOH:O	2.20	0.50
1:A:139:SER:HB3	1:B:3:PHE:HA	1.93	0.49
1:A:114:VAL:CG1	1:A:140:PHE:HZ	2.27	0.48
1:B:266:ALA:O	1:B:270:GLU:HG2	2.15	0.47
1:B:230:PHE:HZ	1:B:268:LEU:HD23	1.83	0.43
1:A:40:ARG:O	1:A:43:ILE:HG12	2.19	0.42
1:A:113:SER:O	1:A:149:GLY:HA2	2.19	0.42
1:B:113:SER:O	1:B:149:GLY:HA2	2.20	0.42
1:A:4:ARG:HD2	1:B:126:TYR:CD2	2.54	0.42
1:B:269:LYS:HE3	1:B:273:GLN:HE22	1.85	0.42
1:B:166:GLU:O	2:B:301:FHR:N11	2.53	0.42
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.90	0.41
1:B:175:THR:HG22	1:B:181:PHE:HA	2.02	0.40
1:B:245:ASP:O	1:B:249:ILE:HG23	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:434:HOH:O	3:B:492:HOH:O[2_554]	2.12	0.08

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	294/296 (99%)	286 (97%)	7 (2%)	1 (0%)	37 26
1	B	294/296 (99%)	290 (99%)	4 (1%)	0	100 100
All	All	588/592 (99%)	576 (98%)	11 (2%)	1 (0%)	44 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	LEU

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	241/253 (95%)	236 (98%)	5 (2%)	48 34
1	B	239/253 (94%)	238 (100%)	1 (0%)	89 88
All	All	480/506 (95%)	474 (99%)	6 (1%)	65 55

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	27	LEU
1	A	92	ASP
1	A	141	LEU
1	A	167	LEU

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Mol	Chain	Res	Type
1	B	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FHR	B	301	1	33,36,36	6.31	15 (45%)	40,49,49	2.02	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FHR	B	301	1	-	7/22/44/44	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FHR	C29-N28	25.98	1.61	1.33
2	B	301	FHR	C26-C27	11.41	1.70	1.53
2	B	301	FHR	C09-C10	9.43	1.58	1.41
2	B	301	FHR	C26-C25	-8.44	1.31	1.54
2	B	301	FHR	C06-C05	6.99	1.58	1.41
2	B	301	FHR	C27-N28	-6.93	1.31	1.46
2	B	301	FHR	C08-C09	6.66	1.51	1.36
2	B	301	FHR	C25-C29	6.55	1.60	1.52
2	B	301	FHR	C07-C06	6.50	1.51	1.36
2	B	301	FHR	C02-N12	6.02	1.47	1.34
2	B	301	FHR	C21-N22	5.11	1.45	1.34
2	B	301	FHR	C08-C07	4.10	1.48	1.38
2	B	301	FHR	C24-C25	3.98	1.62	1.53
2	B	301	FHR	O33-C21	-3.17	1.17	1.23
2	B	301	FHR	O30-C29	-2.09	1.19	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	FHR	C15-C14-C13	-8.72	102.79	114.52
2	B	301	FHR	C26-C27-N28	3.82	109.03	103.43
2	B	301	FHR	C27-N28-C29	-3.57	106.83	113.84
2	B	301	FHR	C26-C25-C29	3.22	107.07	102.88
2	B	301	FHR	O32-C31-C23	-2.37	118.57	124.78
2	B	301	FHR	C31-C23-N22	-2.24	105.69	109.73
2	B	301	FHR	C23-N22-C21	-2.06	119.36	123.15

There are no chirality outliers.

All (7) torsion outliers are listed below:

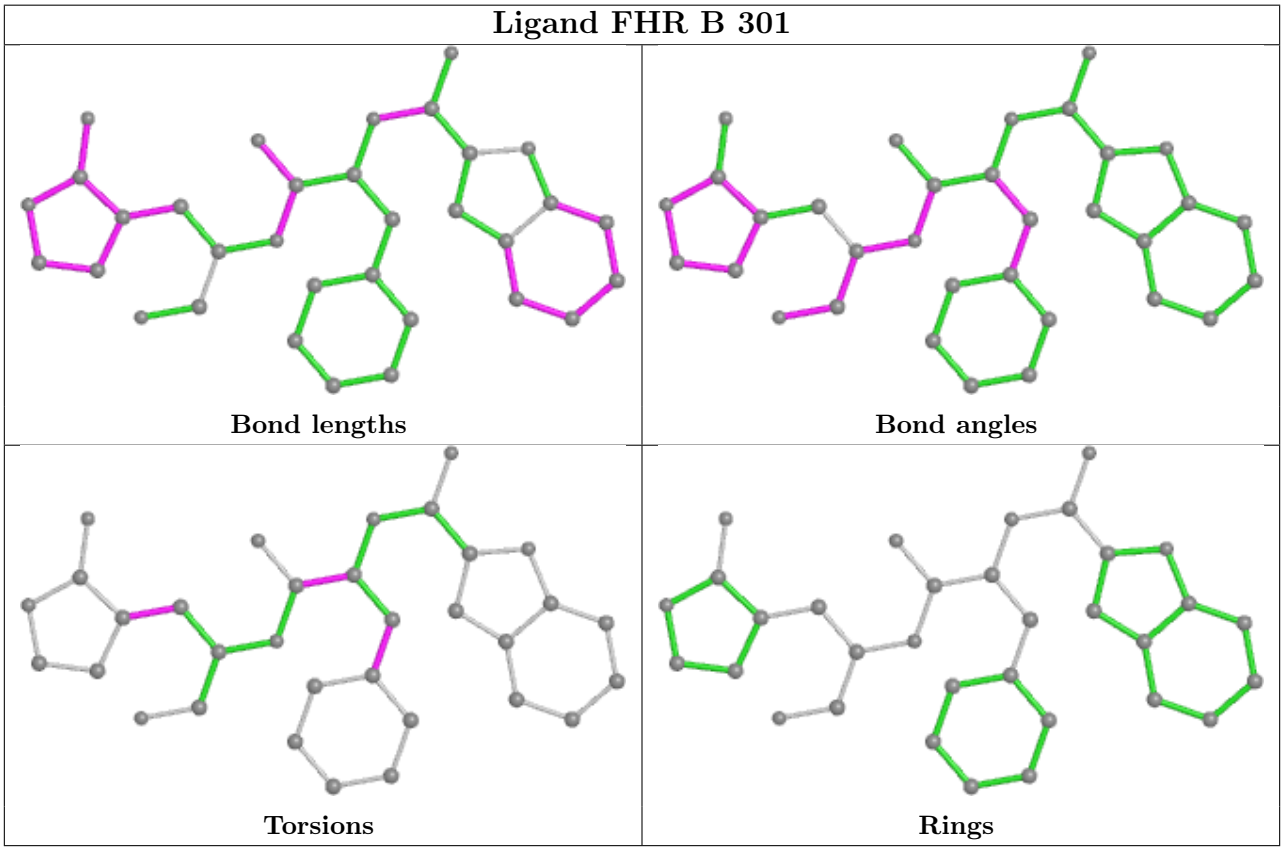
Mol	Chain	Res	Type	Atoms
2	B	301	FHR	C13-C14-C15-C20
2	B	301	FHR	C13-C14-C15-C16
2	B	301	FHR	N12-C13-C21-N22
2	B	301	FHR	N12-C13-C21-O33
2	B	301	FHR	C23-C24-C25-C29
2	B	301	FHR	C14-C13-C21-O33
2	B	301	FHR	C14-C13-C21-N22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	FHR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	296/296 (100%)	0.25	21 (7%)	23	29	22, 32, 48, 66	0
1	B	296/296 (100%)	0.55	26 (8%)	17	22	23, 38, 54, 63	0
All	All	592/592 (100%)	0.40	47 (7%)	20	24	22, 34, 52, 66	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PHE	8.2
1	A	141	LEU	5.2
1	A	142	ALA	4.9
1	B	141	LEU	4.0
1	B	72	ASN	3.9
1	A	3	PHE	3.8
1	A	139	SER	3.8
1	B	283	GLY	3.7
1	A	191	ALA	3.5
1	A	72	ASN	3.3
1	B	24	THR	3.1
1	B	155	ASP	3.0
1	B	140	PHE	2.9
1	B	92	ASP	2.9
1	B	282	LEU	2.9
1	A	143	GLY	2.9
1	A	196	THR	2.8
1	B	189	GLN	2.7
1	A	190	THR	2.7
1	B	277	ASN	2.6
1	B	245	ASP	2.6
1	A	194	ALA	2.6
1	B	3	PHE	2.6
1	B	224	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	92	ASP	2.5
1	B	74	GLN	2.5
1	B	255	ALA	2.4
1	A	169	THR	2.3
1	A	47	GLU	2.3
1	B	172	HIS	2.2
1	B	230	PHE	2.2
1	B	49	MET	2.2
1	B	139	SER	2.1
1	B	233	VAL	2.1
1	A	193	ALA	2.1
1	B	142	ALA	2.1
1	A	172	HIS	2.1
1	A	195	GLY	2.1
1	B	77	VAL	2.1
1	B	297	VAL	2.1
1	B	153	ASP	2.1
1	B	242	LEU	2.1
1	A	121	SER	2.1
1	B	294	PHE	2.0
1	A	118	TYR	2.0
1	A	4	ARG	2.0
1	A	214	ASN	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 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.

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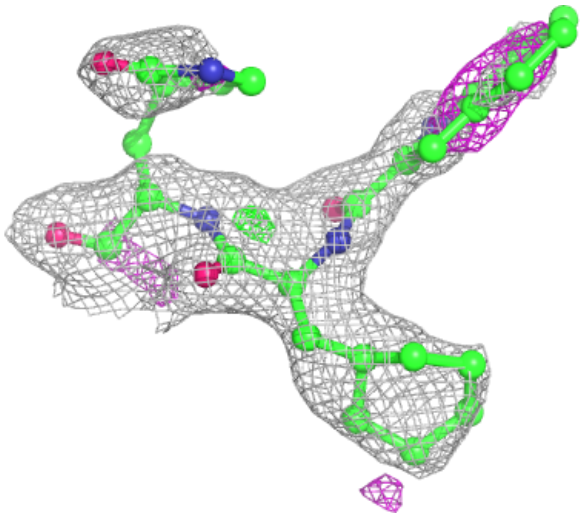
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

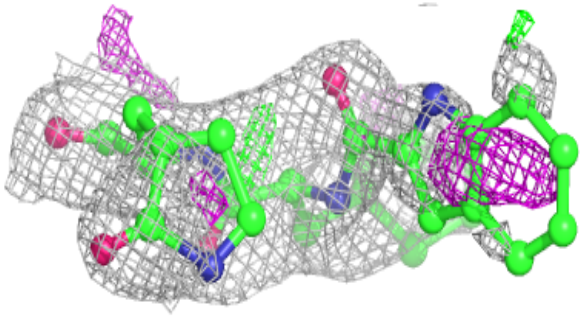
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FHR	B	301	33/33	0.78	0.16	43,55,68,71	0

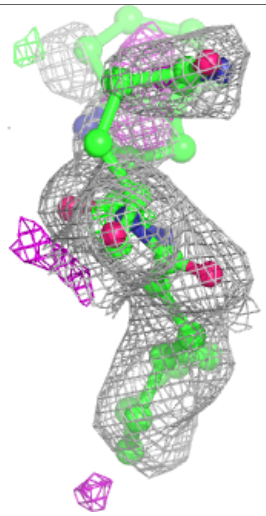
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FHR B 301:

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







6.5 Other polymers

There are no such residues in this entry.