



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 11:33 AM EDT

PDB ID : 8BP6 / pdb_00008bp6
Title : Structure of MHC-class I related molecule MR1 with bound M3Ade.
Authors : Berloff, G.; Jakob, R.P.; Maier, T.
Deposited on : 2022-11-16
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

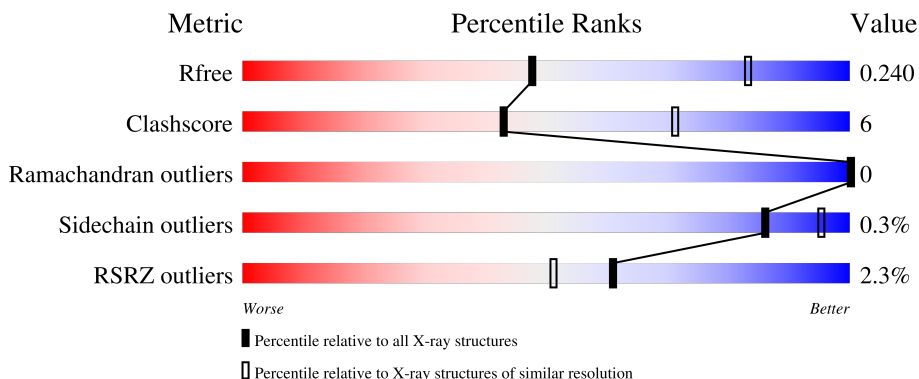
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

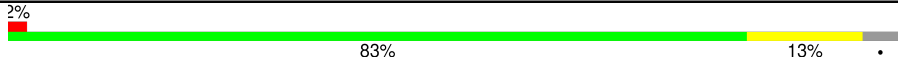
The reported resolution of this entry is 2.80 Å.

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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	384	
1	B	384	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6156 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 Beta-2-microglobulin, Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			3043	1944	521	565	13			
1	B	370	Total	C	N	O	S	0	0	0
			3063	1955	524	570	14			

There are 32 discrepancies between the modelled and reference sequences:

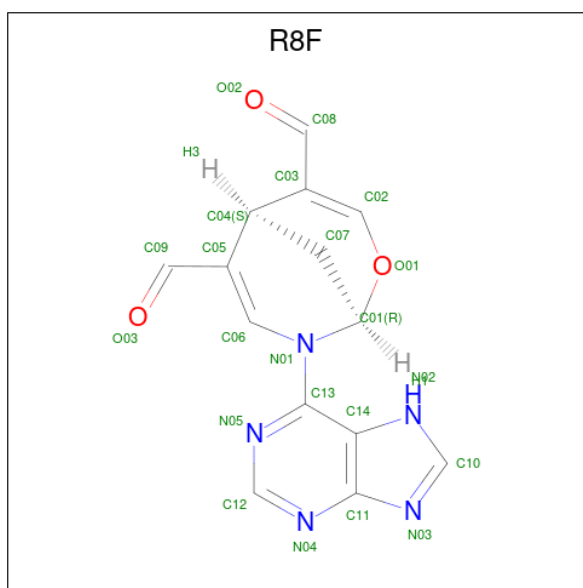
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	linker	UNP P61769
A	101	GLY	-	linker	UNP P61769
A	102	GLY	-	linker	UNP P61769
A	103	GLY	-	linker	UNP P61769
A	104	SER	-	linker	UNP P61769
A	105	GLY	-	linker	UNP P61769
A	106	GLY	-	linker	UNP P61769
A	107	GLY	-	linker	UNP P61769
A	108	GLY	-	linker	UNP P61769
A	109	SER	-	linker	UNP P61769
A	110	GLY	-	linker	UNP P61769
A	111	GLY	-	linker	UNP P61769
A	112	GLY	-	linker	UNP P61769
A	113	GLY	-	linker	UNP P61769
A	114	SER	-	linker	UNP P61769
A	115	GLU	-	linker	UNP P61769
B	100	GLY	-	linker	UNP P61769
B	101	GLY	-	linker	UNP P61769
B	102	GLY	-	linker	UNP P61769
B	103	GLY	-	linker	UNP P61769
B	104	SER	-	linker	UNP P61769
B	105	GLY	-	linker	UNP P61769
B	106	GLY	-	linker	UNP P61769
B	107	GLY	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	GLY	-	linker	UNP P61769
B	109	SER	-	linker	UNP P61769
B	110	GLY	-	linker	UNP P61769
B	111	GLY	-	linker	UNP P61769
B	112	GLY	-	linker	UNP P61769
B	113	GLY	-	linker	UNP P61769
B	114	SER	-	linker	UNP P61769
B	115	GLU	-	linker	UNP P61769

- Molecule 2 is (1R,5S)-8-(9H-purin-6-yl)-2-oxa-8-azabicyclo[3.3.1]nona-3,6-diene-4,6-dicarbaldehyde (CCD ID: R8F) (formula: $C_{14}H_{11}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	14	5	2		
2	B	1	Total	C	N	O	0	0
			21	14	5	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	5	Total	O	0	0
			5	5		

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.

- Chain A:
-
- 2% 83% 13%
- I1 L23 I35 D38 N42 G43 E44 R45 D53 F56 S57 K58 D59 W60 Y67 E77 H84 V85 T86 R97 ASP MET GLY GLY GLY SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY SER E115 R116 F123 S128 T131 H132 V134 P135 I138 Y151 T155 R156 Q157 K159 R161 L181 R182 F188 S204 Q208 E217 Q226 D233 L236 H252 Q256 E264 Q268 T294 L298 V301 E305 V310 G315 R316 A317 H318 P322 W329 E335 I359 L382 Q383 V384

- Chain B:
-
- 2% 81% 15%
- I1 S33 D34 I35 R45 L54 S55 F56 S67 K58 D59 W60 L64 E89 T73 E74 K75 M99 GLY GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY E114 E115 H118 S119 F123 D129 D144 T148 T149 T155 R156 Q157 W164 W165 L169 Y177 F188 K189 K193 H205 Q208 R209 M210 E217 Q226 Y227 A228 Y229 D230 D233 L236 V250 A253 H252 T253 L254 K255 Q256 E264 Q268 R300 E305 V310 T311 A317 M327 T328 W329 N332 E335 D341 Y342

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.35Å 143.53Å 77.03Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	49.28 – 2.80 49.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.28-2.80) 98.8 (49.28-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.237 , 0.247 0.235 , 0.240	Depositor DCC
R_{free} test set	1244 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6156	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R8F

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	0.21	0/3134	0.41	0/4257
1	B	0.23	0/3154	0.44	1/4283 (0.0%)
All	All	0.22	0/6288	0.43	1/8540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	SER	N-CA-C	-5.73	101.42	109.96

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	A	3043	0	2894	37	1
1	B	3063	0	2908	38	2
2	A	21	0	0	0	0
2	B	21	0	0	1	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
All	All	6156	0	5802	74	2

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 6.

The worst 5 of 74 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:53:ASP:OD2	1:A:161:ARG:NH2	2.19	0.76
1:B:362:ASP:HB2	1:B:364:GLN:HG2	1.70	0.73
1:A:335:GLU:N	1:A:335:GLU:OE2	2.30	0.65
1:B:118:HIS:ND1	1:B:144:ASP:OD2	2.27	0.65
1:B:374:GLU:OE1	1:B:379:HIS:ND1	2.30	0.65

All (2) 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)
1:B:69:GLU:OE1	1:B:365:SER:OG[1_655]	2.02	0.18
1:A:182:ARG:NH1	1:B:129:ASP:OD2[2_555]	2.16	0.04

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	363/384 (94%)	359 (99%)	4 (1%)	0	100	100
1	B	366/384 (95%)	359 (98%)	7 (2%)	0	100	100
All	All	729/768 (95%)	718 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	332/337 (98%)	331 (100%)	1 (0%)	86	95
1	B	334/337 (99%)	333 (100%)	1 (0%)	86	95
All	All	666/674 (99%)	664 (100%)	2 (0%)	86	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	PHE
1	B	188	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	186	GLN
1	B	252	HIS
1	B	367	ASN
1	B	318	HIS
1	B	364	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](#)

2 ligands are 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	R8F	B	401	1	22,24,25	3.27	6 (27%)	22,35,36	2.27	10 (45%)
2	R8F	A	401	1	22,24,25	3.38	7 (31%)	22,35,36	2.12	7 (31%)

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	R8F	B	401	1	-	2/4/31/33	0/4/4/4
2	R8F	A	401	1	-	2/4/31/33	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	R8F	C06-N01	9.49	1.50	1.34
2	B	401	R8F	C06-N01	9.30	1.49	1.34
2	A	401	R8F	C11-N03	-8.50	1.31	1.38
2	B	401	R8F	C11-N03	-7.42	1.32	1.38
2	B	401	R8F	O01-C02	6.24	1.47	1.35

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	R8F	C11-N03-C10	5.00	107.02	103.84
2	A	401	R8F	C11-N03-C10	4.00	106.38	103.84
2	B	401	R8F	C12-N05-C13	3.86	121.26	111.83
2	A	401	R8F	C12-N05-C13	3.65	120.74	111.83
2	A	401	R8F	C14-C11-N04	3.64	127.37	124.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

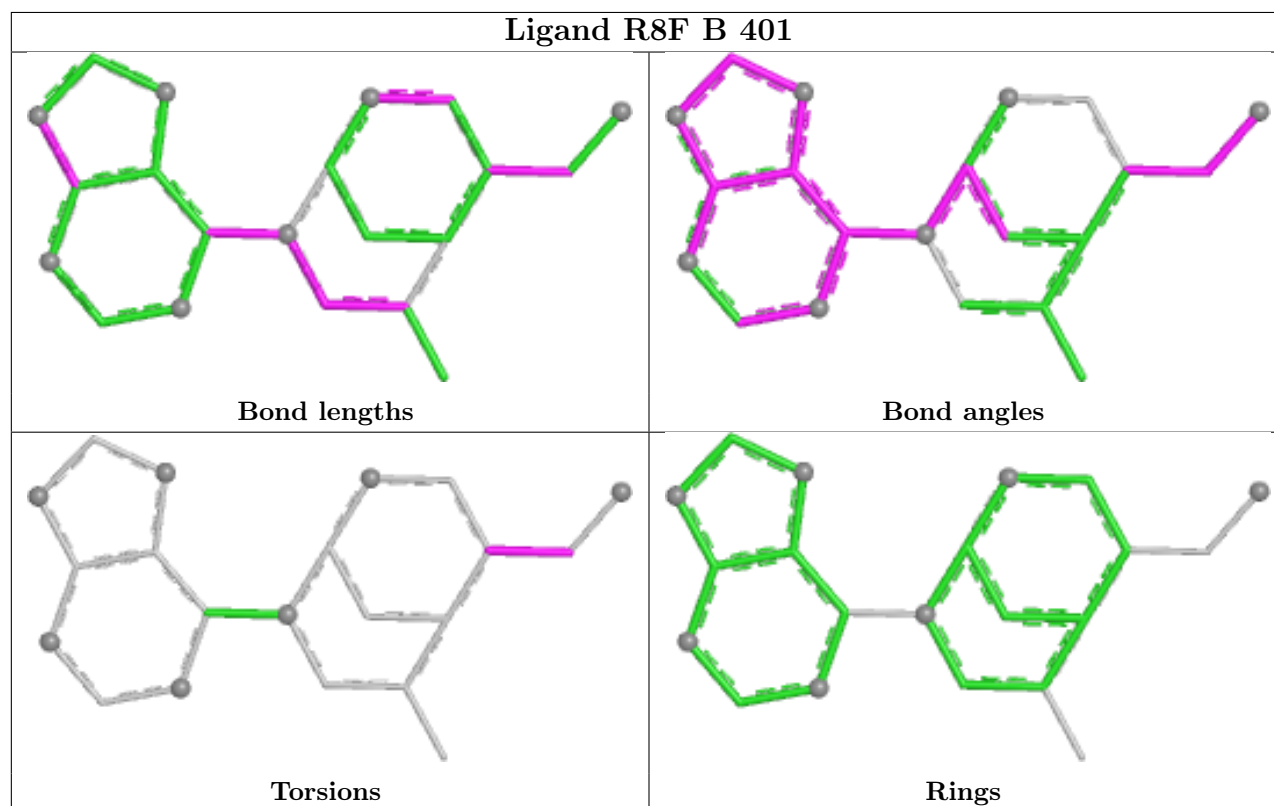
Mol	Chain	Res	Type	Atoms
2	A	401	R8F	C02-C03-C08-O02
2	A	401	R8F	C04-C03-C08-O02
2	B	401	R8F	C02-C03-C08-O02
2	B	401	R8F	C04-C03-C08-O02

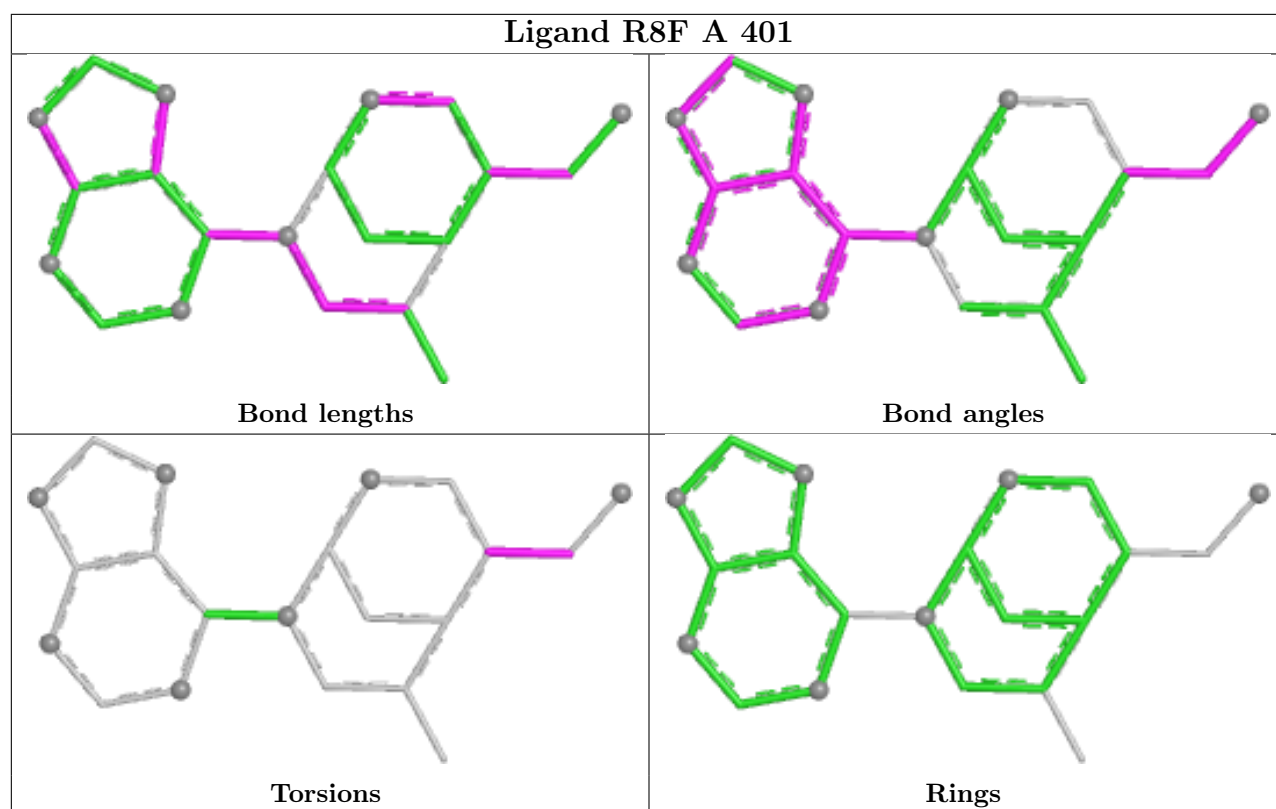
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	R8F	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 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 [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, 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	367/384 (95%)	0.24	8 (2%) 62 52	77, 110, 186, 214	0
1	B	370/384 (96%)	0.34	9 (2%) 59 49	73, 116, 191, 226	0
All	All	737/768 (95%)	0.29	17 (2%) 61 51	73, 113, 187, 226	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	384	VAL	3.9
1	B	56	PHE	3.2
1	A	58	LYS	2.6
1	A	384	VAL	2.5
1	B	327	MET	2.5

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](#)

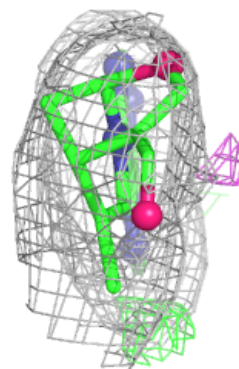
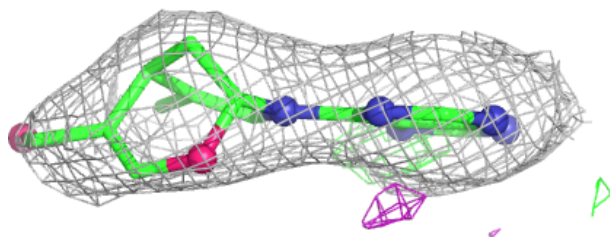
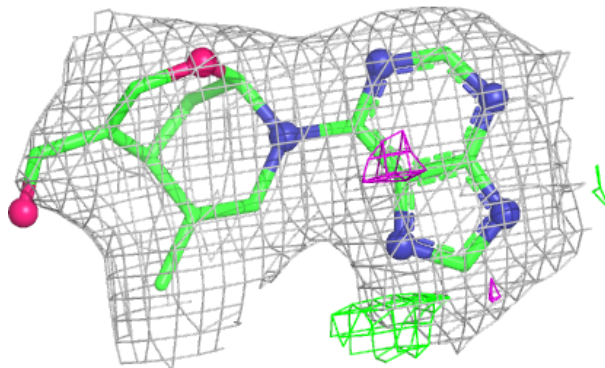
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	R8F	A	401	21/22	0.88	0.14	93,94,95,96	0
2	R8F	B	401	21/22	0.89	0.13	93,98,101,103	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.

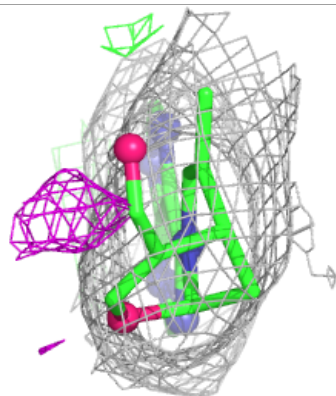
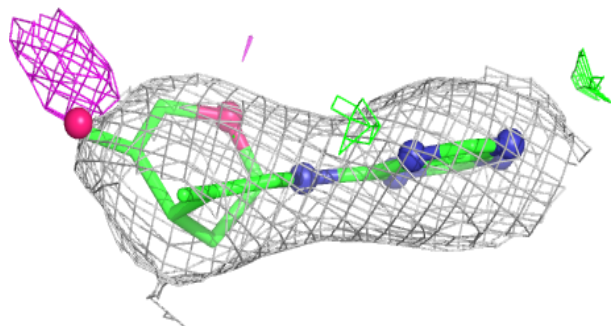
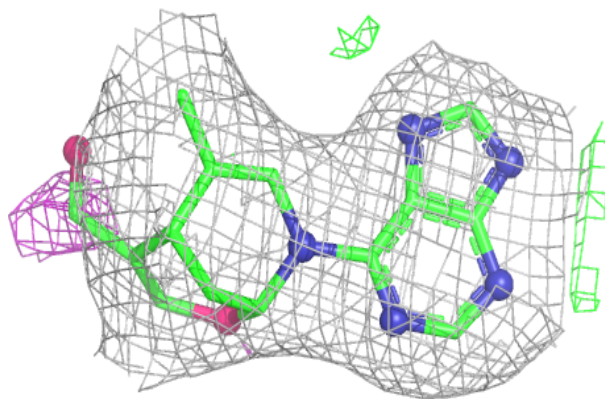
Electron density around R8F A 401:

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



Electron density around R8F B 401:

$2mF_o-DF_c$ (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.