



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:36 PM UTC

PDB ID : 7PVU / pdb_00007pvu
Title : Crystal structure of p38alpha C162S in complex with CAS2094511-69-8, P 1
21 1
Authors : Baginski, B.; Pous, J.; Gonzalez, L.; Macias, M.J.; Nebreda, A.R.
Deposited on : 2021-10-05
Resolution : 2.15 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

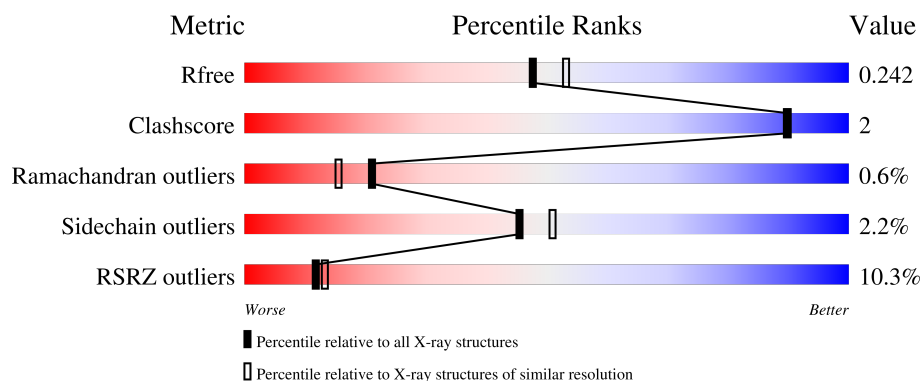
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	359	8% 88% 5% 6%
1	B	359	12% 86% 7% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5660 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.

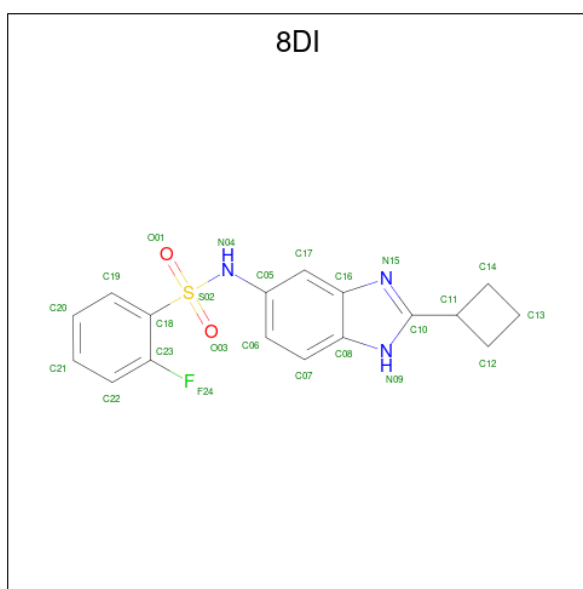
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	17	1	0
			2728	1751	469	497	11			
1	B	336	Total	C	N	O	S	24	1	0
			2722	1750	465	496	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	CYS	conflict	UNP P47811
B	162	SER	CYS	conflict	UNP P47811

- Molecule 2 is N-(2-cyclobutyl-1H-1,3-benzodiazol-5-yl)-2-fluorobenzene-1-sulfonamide (CCD ID: 8DI) (formula: C₁₇H₁₆FN₃O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	S	0	0
			24	17	1	3	2	1		

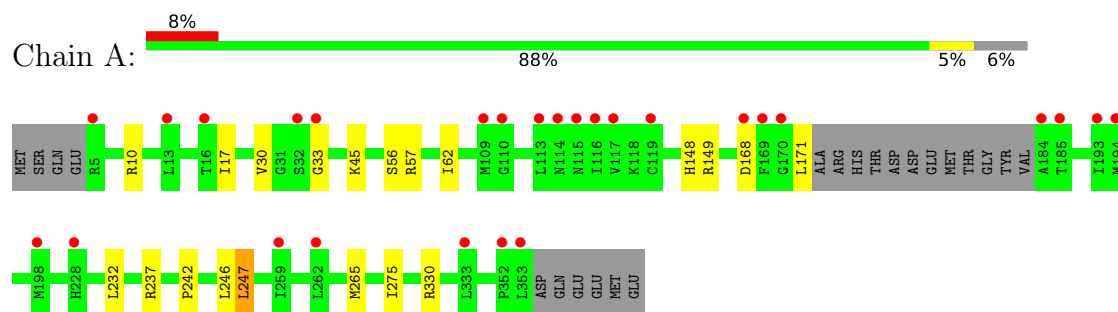
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total 130	O 130	0	0
3	B	56	Total 56	O 56	0	0

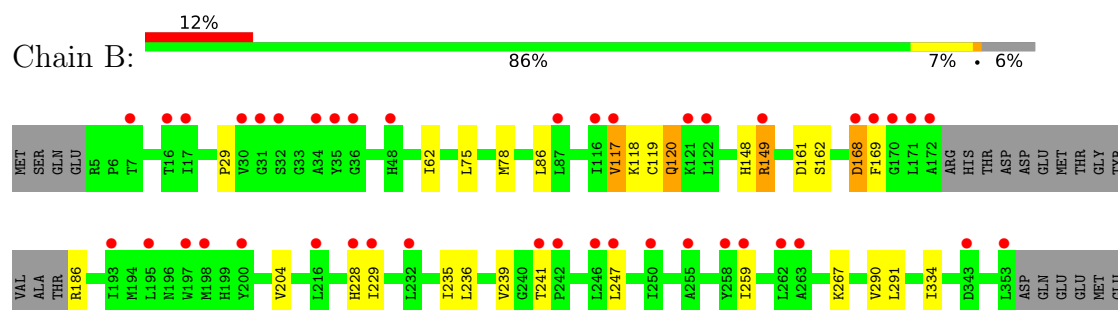
3 Residue-property plots [i](#)

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: Mitogen-activated protein kinase 14



- Molecule 1: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.14Å 68.07Å 79.98Å 90.00° 94.78° 90.00°	Depositor
Resolution (Å)	79.70 – 2.15 79.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (79.70-2.15) 99.3 (79.70-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.205 , 0.239 0.211 , 0.242	Depositor DCC
R_{free} test set	2015 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5660	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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: 8DI

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	0.47	1/2795 (0.0%)	0.79	0/3793
1	B	0.48	2/2790 (0.1%)	0.77	1/3787 (0.0%)
All	All	0.48	3/5585 (0.1%)	0.78	1/7580 (0.0%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	VAL	C-N	-8.66	1.21	1.33
1	A	33	GLY	C-N	-7.07	1.24	1.34
1	B	120	GLN	C-N	6.26	1.42	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	VAL	O-C-N	-5.58	115.60	122.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	VAL	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	2728	0	2734	9	0
1	B	2722	0	2723	12	0
2	B	24	0	0	0	0
3	A	130	0	0	0	0
3	B	56	0	0	0	0
All	All	5660	0	5457	20	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 (20) 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:10:ARG:HG3	1:A:17:ILE:HG23	1.78	0.65
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	1.68	0.59
1:A:62:ILE:HD12	1:B:162:SER:HB2	1.88	0.54
1:A:330[B]:ARG:HG2	1:A:330[B]:ARG:NH1	2.23	0.54
1:B:247:LEU:HD13	1:B:259:ILE:HD11	1.91	0.52
1:B:239:VAL:CG2	1:B:291:LEU:HD21	2.41	0.51
1:B:62:ILE:HD13	1:B:334:ILE:HG13	1.94	0.50
1:A:237:ARG:HD2	1:A:265:MET:HE2	1.94	0.49
1:B:149:ARG:HH11	1:B:204:VAL:HG21	1.77	0.49
1:B:148:HIS:NE2	1:B:168:ASP:O	2.47	0.47
1:B:78:MET:HG3	1:B:169:PHE:CE1	2.50	0.46
1:B:228:HIS:CE1	1:B:229:ILE:HG12	2.52	0.45
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.99	0.44
1:B:148:HIS:O	1:B:149:ARG:HB2	2.18	0.44
1:A:148:HIS:O	1:A:149:ARG:HB2	2.18	0.43
1:B:236:LEU:HD12	1:B:241:THR:HA	2.00	0.43
1:B:75:LEU:HB3	1:B:86:LEU:HG	2.00	0.42
1:A:247:LEU:HD13	1:A:247:LEU:HA	1.89	0.42
1:B:235:ILE:O	1:B:239:VAL:HG22	2.20	0.42
1:A:56:SER:O	1:A:57:ARG:C	2.63	0.41

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	334/359 (93%)	323 (97%)	11 (3%)	0	100	100
1	B	333/359 (93%)	317 (95%)	12 (4%)	4 (1%)	10	5
All	All	667/718 (93%)	640 (96%)	23 (3%)	4 (1%)	21	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	ASP
1	B	119	CYS
1	B	149	ARG
1	B	29	PRO

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	299/318 (94%)	292 (98%)	7 (2%)	44	49
1	B	298/318 (94%)	292 (98%)	6 (2%)	48	54
All	All	597/636 (94%)	584 (98%)	13 (2%)	45	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	45	LYS

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Mol	Chain	Res	Type
1	A	168	ASP
1	A	171	LEU
1	A	232	LEU
1	A	247	LEU
1	A	275	ILE
1	B	118	LYS
1	B	120	GLN
1	B	161	ASP
1	B	186	ARG
1	B	267	LYS
1	B	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	155	ASN
1	A	269	ASN
1	B	48	HIS
1	B	115	ASN
1	B	126	HIS
1	B	257	ASN
1	B	310	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](#)

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	8DI	B	401	-	27,27,27	2.67	5 (18%)	36,40,40	2.34	9 (25%)

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	8DI	B	401	-	-	4/11/21/21	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	8DI	C18-S02	-12.06	1.60	1.77
2	B	401	8DI	C05-N04	-4.28	1.36	1.43
2	B	401	8DI	C08-N09	-2.65	1.34	1.38
2	B	401	8DI	C10-N15	2.45	1.35	1.32
2	B	401	8DI	C16-N15	-2.33	1.35	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	8DI	O03-S02-O01	-8.95	108.66	119.52
2	B	401	8DI	C18-S02-N04	5.68	113.99	107.30
2	B	401	8DI	C22-C23-C18	-4.14	120.21	122.22
2	B	401	8DI	C23-C18-S02	-3.44	119.01	121.21
2	B	401	8DI	C19-C18-S02	2.69	121.38	117.51
2	B	401	8DI	F24-C23-C18	2.45	120.81	118.91
2	B	401	8DI	C13-C12-C11	2.38	90.52	88.48
2	B	401	8DI	C05-C17-C16	2.35	120.45	118.32
2	B	401	8DI	C13-C14-C11	2.28	90.44	88.48

There are no chirality outliers.

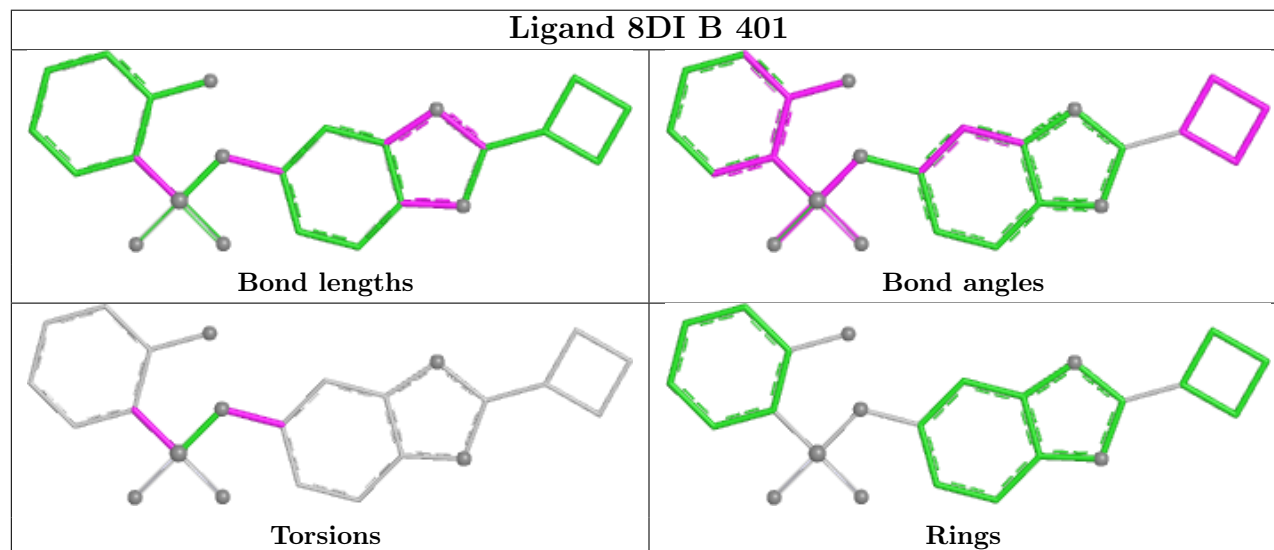
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	8DI	C23-C18-S02-N04
2	B	401	8DI	C19-C18-S02-N04
2	B	401	8DI	C06-C05-N04-S02
2	B	401	8DI	C17-C05-N04-S02

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	335/359 (93%)	0.39	27 (8%) 18 19	24, 44, 85, 108	1 (0%)
1	B	333/359 (92%)	0.92	42 (12%) 8 8	36, 65, 119, 139	1 (0%)
All	All	668/718 (93%)	0.66	69 (10%) 12 13	24, 55, 105, 139	2 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35[A]	TYR	8.9
1	B	169	PHE	7.2
1	B	34	ALA	4.8
1	B	171	LEU	4.5
1	A	113	LEU	4.3
1	A	116	ILE	4.2
1	B	172	ALA	4.2
1	A	184	ALA	4.1
1	B	117	VAL	4.0
1	B	36	GLY	3.8
1	B	197	TRP	3.6
1	B	170	GLY	3.4
1	A	119	CYS	3.2
1	A	353	LEU	3.2
1	B	353	LEU	3.1
1	B	258	TYR	3.1
1	B	263	ALA	3.1
1	B	262	LEU	3.1
1	B	122	LEU	3.0
1	B	247	LEU	3.0
1	A	115	ASN	3.0
1	B	121	LYS	3.0
1	B	195	LEU	3.0
1	B	250	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	2.9
1	B	343	ASP	2.8
1	A	117	VAL	2.8
1	B	259	ILE	2.8
1	A	333	LEU	2.8
1	B	229	ILE	2.8
1	B	149	ARG	2.7
1	B	7	THR	2.7
1	B	16	THR	2.7
1	B	193	ILE	2.6
1	B	228	HIS	2.6
1	A	185	THR	2.6
1	B	32	SER	2.6
1	B	116	ILE	2.6
1	B	168	ASP	2.6
1	A	262	LEU	2.5
1	B	255	ALA	2.5
1	A	170	GLY	2.5
1	B	241	THR	2.4
1	B	232	LEU	2.4
1	A	168	ASP	2.4
1	A	228	HIS	2.4
1	B	200	TYR	2.3
1	A	198	MET	2.3
1	B	48	HIS	2.2
1	A	259	ILE	2.2
1	A	169	PHE	2.2
1	B	216	LEU	2.2
1	A	194	MET	2.2
1	A	352	PRO	2.1
1	A	193	ILE	2.1
1	B	17	ILE	2.1
1	B	30	VAL	2.1
1	A	13	LEU	2.1
1	A	114	ASN	2.1
1	B	31	GLY	2.1
1	A	32	SER	2.1
1	B	87	LEU	2.1
1	A	16	THR	2.1
1	B	198	MET	2.1
1	B	246	LEU	2.0
1	A	5	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	MET	2.0
1	B	242	PRO	2.0
1	A	33	GLY	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](#)

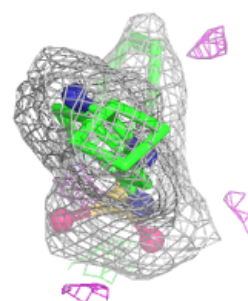
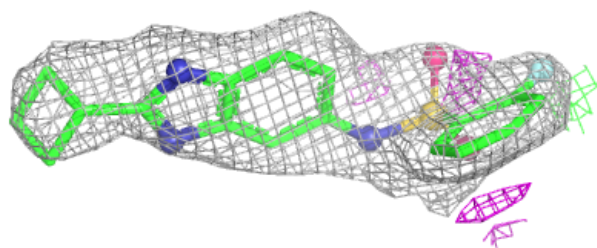
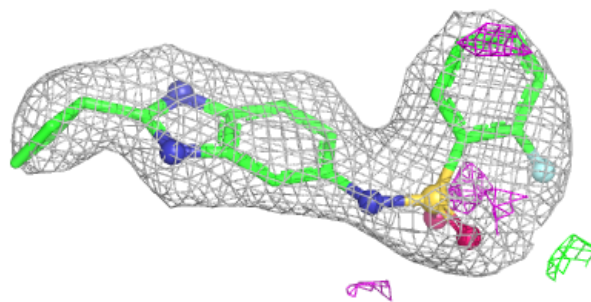
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8DI	B	401	24/24	0.86	0.14	74,81,86,87	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 8DI 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 ⓘ

There are no such residues in this entry.