



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:05 PM UTC

PDB ID : 9ETR / pdb_00009etr
Title : Crystal structure of PARP1 catalytic domain bound to AZD9574
Authors : Schimpl, M.
Deposited on : 2024-03-26
Resolution : 1.82 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

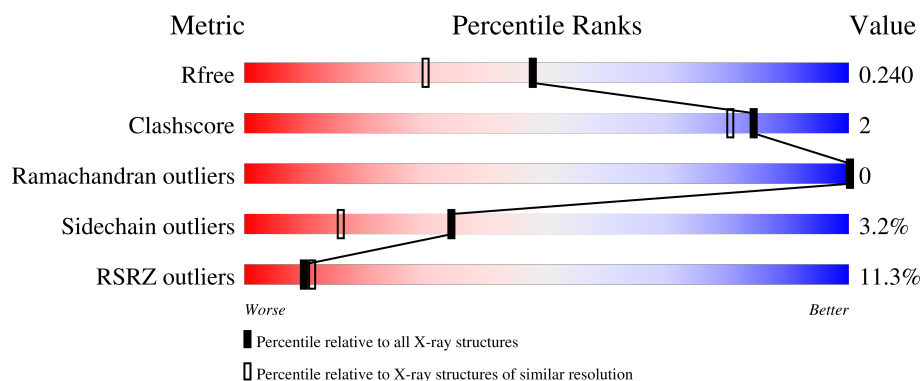
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	355	
1	B	355	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5644 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.

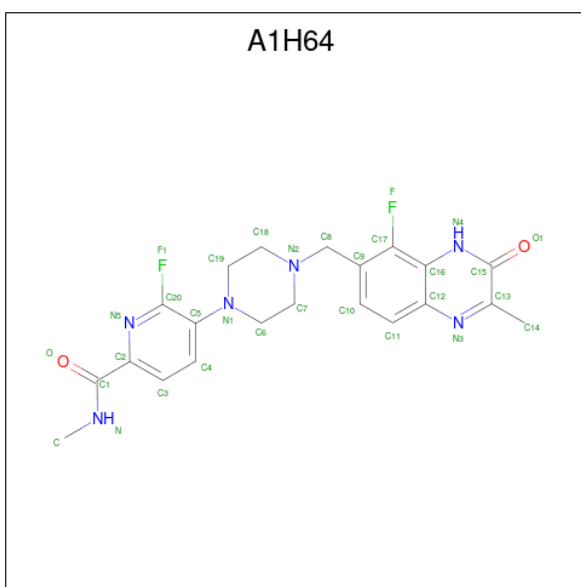
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1, processed C-terminus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2731	1738	461	521	11			
1	B	350	Total	C	N	O	S	0	0	0
			2733	1741	460	521	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	657	GLY	-	expression tag	UNP P09874
A	658	PRO	-	expression tag	UNP P09874
A	659	LEU	-	expression tag	UNP P09874
A	660	GLY	-	expression tag	UNP P09874
A	661	SER	-	expression tag	UNP P09874
A	762	ALA	VAL	engineered mutation	UNP P09874
B	657	GLY	-	expression tag	UNP P09874
B	658	PRO	-	expression tag	UNP P09874
B	659	LEU	-	expression tag	UNP P09874
B	660	GLY	-	expression tag	UNP P09874
B	661	SER	-	expression tag	UNP P09874
B	762	ALA	VAL	engineered mutation	UNP P09874

- Molecule 2 is 6-fluoranyl-5-[4-[(5-fluoranyl-2-methyl-3-oxidanylidene-4 {H}-quinoxalin-6-yl)methyl]piperazin-1-yl]- {N}-methyl-pyridine-2-carboxamide (CCD ID: A1H64) (formula: C₂₁H₂₂F₂N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	21	2	6	2		
2	B	1	Total	C	F	N	O	0	0
			31	21	2	6	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

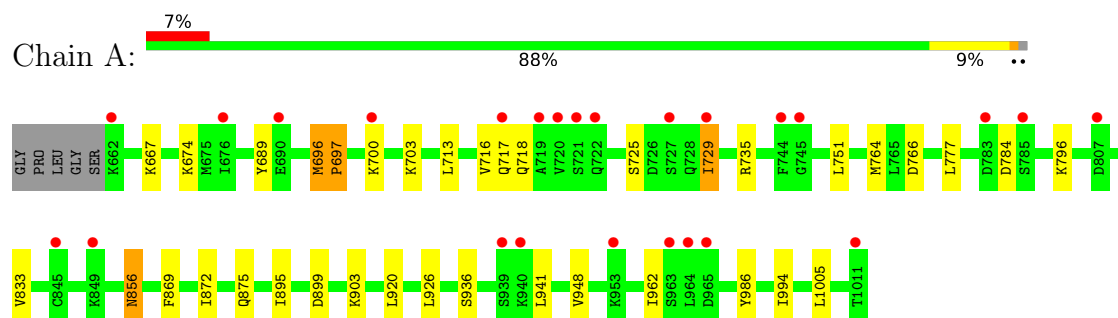
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total 52	O 52	0	0
4	B	56	Total 56	O 56	0	0

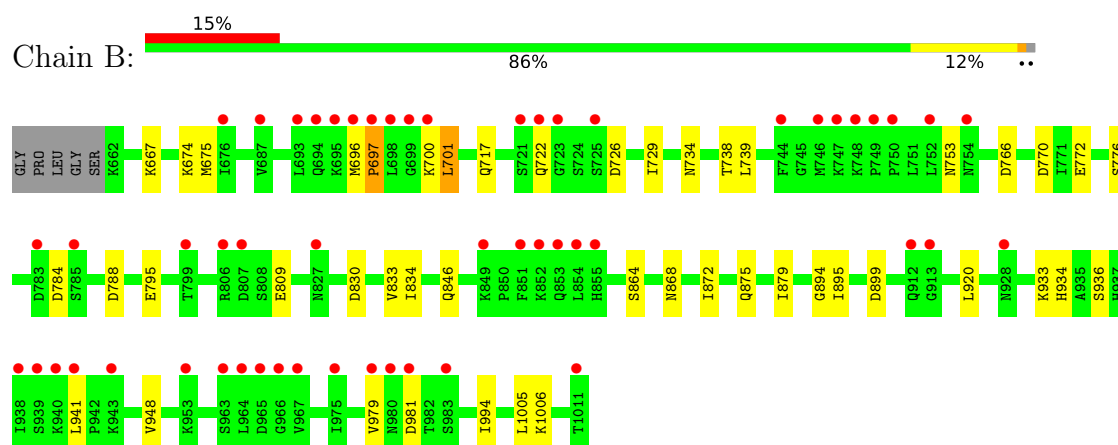
3 Residue-property plots [i](#)

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: Poly [ADP-ribose] polymerase 1, processed C-terminus



- Molecule 1: Poly [ADP-ribose] polymerase 1, processed C-terminus



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.27Å 92.58Å 165.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.40 – 1.82 26.40 – 1.82	Depositor EDS
% Data completeness (in resolution range)	61.9 (26.40-1.82) 63.2 (26.40-1.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.80Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.213 , 0.252 0.237 , 0.240	Depositor DCC
R_{free} test set	2160 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5644	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: SO4, A1H64

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	0.87	0/2783	1.34	13/3760 (0.3%)
1	B	0.89	0/2785	1.35	18/3762 (0.5%)
All	All	0.88	0/5568	1.34	31/7522 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	703	LYS	CA-C-N	6.54	130.62	120.82
1	A	703	LYS	C-N-CA	6.54	130.62	120.82
1	B	697	PRO	CA-C-N	6.21	128.60	120.28
1	B	697	PRO	C-N-CA	6.21	128.60	120.28
1	B	674	LYS	CA-C-N	5.84	128.03	120.44
1	B	674	LYS	C-N-CA	5.84	128.03	120.44
1	B	784	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	899	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	784	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	734	ASN	CA-CB-CG	5.47	118.07	112.60
1	B	830	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	869	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	717	GLN	CA-C-N	5.33	127.42	120.28
1	B	717	GLN	C-N-CA	5.33	127.42	120.28
1	A	674	LYS	CA-C-N	5.27	127.29	120.44
1	A	674	LYS	C-N-CA	5.27	127.29	120.44
1	B	899	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	675	MET	CA-C-N	5.24	128.90	120.30
1	B	675	MET	C-N-CA	5.24	128.90	120.30
1	A	856	ASN	CA-CB-CG	5.23	117.83	112.60
1	B	776	SER	CA-C-N	5.15	127.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	776	SER	C-N-CA	5.15	127.14	120.44
1	A	697	PRO	CA-C-N	5.13	127.41	120.38
1	A	697	PRO	C-N-CA	5.13	127.41	120.38
1	A	716	VAL	CA-C-N	5.13	127.41	120.38
1	A	716	VAL	C-N-CA	5.13	127.41	120.38
1	B	738	THR	N-CA-C	-5.08	105.38	112.45
1	B	788	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	795	GLU	CB-CG-CD	5.05	121.18	112.60
1	B	766	ASP	CA-CB-CG	5.02	117.62	112.60

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	2731	0	2753	12	0
1	B	2733	0	2754	14	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	52	0	0	0	0
4	B	56	0	0	0	0
All	All	5644	0	5507	25	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.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.88	0.56
1:B:872:ILE:HG21	1:B:920:LEU:HD11	1.90	0.54
1:A:697:PRO:HD2	1:A:700:LYS:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:SER:HA	1:B:936:SER:HA	1.94	0.49
1:B:697:PRO:HD2	1:B:700:LYS:HD2	1.95	0.49
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.95	0.48
1:A:856:ASN:HB3	1:A:926:LEU:HB2	1.95	0.48
1:A:725:SER:O	1:A:729:ILE:HG13	2.13	0.48
1:B:770:ASP:HB3	1:B:868:ASN:HA	1.96	0.48
1:A:941:LEU:HD21	1:A:948:VAL:HG23	1.97	0.47
1:B:941:LEU:HD21	1:B:948:VAL:HG23	1.96	0.47
1:B:701:LEU:HD13	1:B:772:GLU:HB2	1.98	0.45
1:B:879:ILE:HG12	1:B:894:GLY:HA2	1.98	0.45
1:A:903:LYS:HD2	1:A:986:TYR:HB2	2.00	0.44
1:A:777:LEU:HG	1:A:796:LYS:HB3	2.00	0.44
1:A:833:VAL:HA	1:A:1005:LEU:HD23	1.99	0.43
1:A:895:ILE:HD11	1:A:994:ILE:HG22	2.01	0.43
1:A:689:TYR:CG	1:A:764:MET:HG3	2.54	0.42
1:B:934:HIS:HE1	1:B:981:ASP:O	2.02	0.42
1:B:726:ASP:HA	1:B:729:ILE:HD12	2.00	0.42
1:A:696:MET:HE2	1:A:696:MET:HB3	1.83	0.42
1:B:833:VAL:HA	1:B:1005:LEU:HD23	2.01	0.42
1:B:895:ILE:HD11	1:B:994:ILE:HG22	2.01	0.42
1:B:933:LYS:HE2	1:B:979:VAL:HG13	2.03	0.41
1:B:729:ILE:HG21	1:B:753:ASN:HA	2.03	0.41

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	348/355 (98%)	347 (100%)	1 (0%)	0	100	100
1	B	348/355 (98%)	347 (100%)	1 (0%)	0	100	100
All	All	696/710 (98%)	694 (100%)	2 (0%)	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	302/310 (97%)	292 (97%)	10 (3%)	33	15
1	B	301/310 (97%)	292 (97%)	9 (3%)	36	17
All	All	603/620 (97%)	584 (97%)	19 (3%)	34	16

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	667	LYS
1	A	696	MET
1	A	713	LEU
1	A	717	GLN
1	A	718	GLN
1	A	729	ILE
1	A	735	ARG
1	A	751	LEU
1	A	875	GLN
1	A	962	ILE
1	B	667	LYS
1	B	696	MET
1	B	701	LEU
1	B	722	GLN
1	B	739	LEU
1	B	809	GLU
1	B	846	GLN
1	B	864	SER
1	B	875	GLN

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

Mol	Chain	Res	Type
1	A	694	GLN

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Mol	Chain	Res	Type
1	A	705	GLN
1	A	875	GLN
1	A	906	ASN
1	A	998	ASN
1	A	1008	ASN
1	B	875	GLN
1	B	906	ASN
1	B	934	HIS

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](#)

4 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	A1H64	A	1101	-	33,34,34	0.55	1 (3%)	48,49,49	0.64	1 (2%)
2	A1H64	B	1101	-	33,34,34	0.59	1 (3%)	48,49,49	0.69	1 (2%)
3	SO4	A	1102	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	B	1102	-	4,4,4	0.35	0	6,6,6	0.34	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
2	A1H64	A	1101	-	-	0/14/24/24	0/4/4/4
2	A1H64	B	1101	-	-	0/14/24/24	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	A1H64	C15-C13	2.53	1.53	1.47
2	B	1101	A1H64	C15-C13	2.36	1.53	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1H64	C9-C8-N2	2.40	117.01	112.75
2	B	1101	A1H64	C20-C5-N1	2.08	122.87	120.39

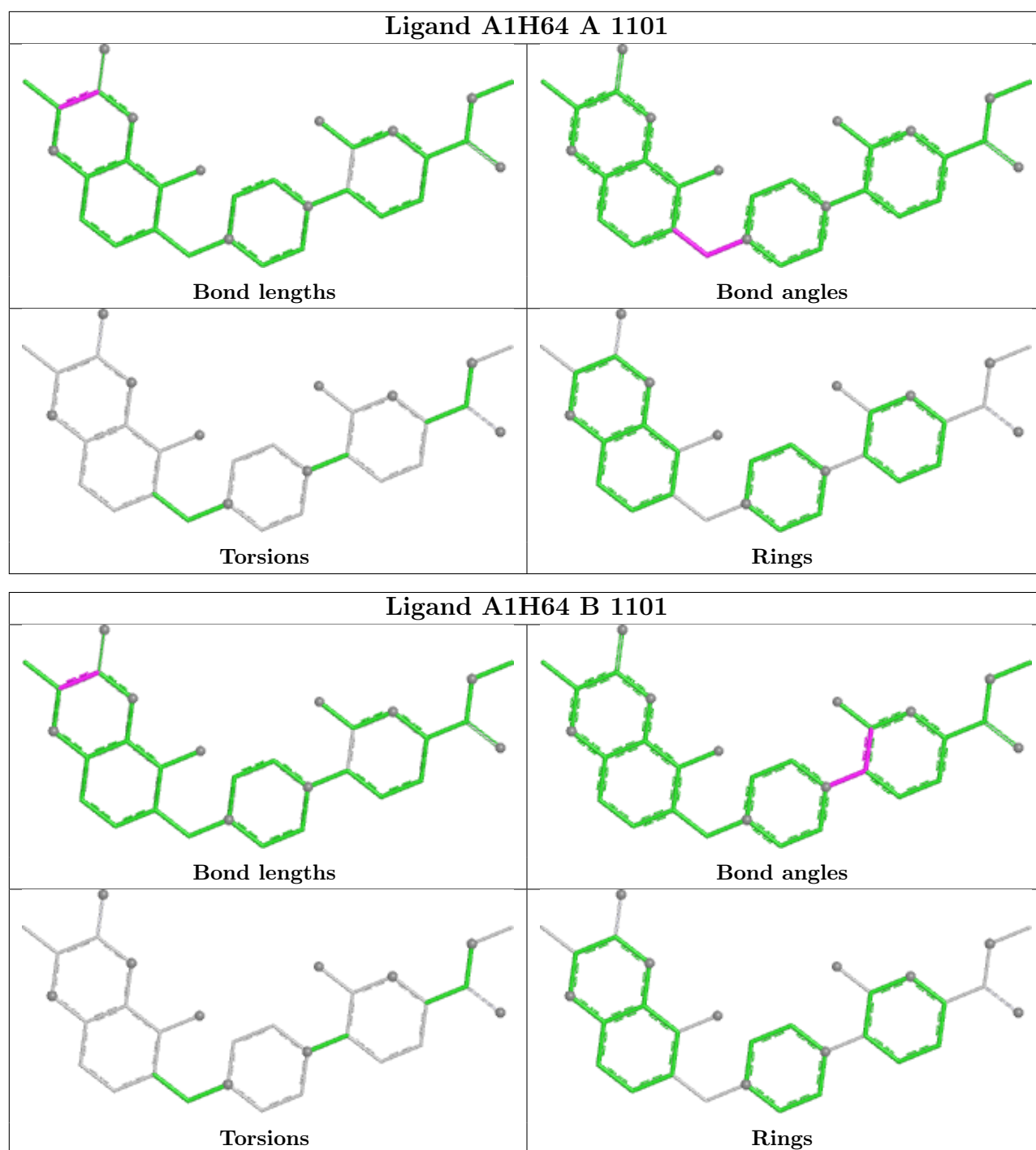
There are no chirality outliers.

There are no torsion outliers.

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	350/355 (98%)	0.57	25 (7%) 22 25	15, 29, 53, 68	0
1	B	350/355 (98%)	0.88	54 (15%) 5 5	17, 35, 61, 85	0
All	All	700/710 (98%)	0.73	79 (11%) 10 11	15, 32, 59, 85	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	854	LEU	6.1
1	B	1011	THR	6.0
1	B	981	ASP	5.1
1	B	964	LEU	4.7
1	B	747	LYS	4.0
1	B	963	SER	3.9
1	B	975	ILE	3.5
1	B	783	ASP	3.4
1	B	943	LYS	3.4
1	A	807	ASP	3.4
1	B	785	SER	3.3
1	B	687	VAL	3.3
1	A	1011	THR	3.2
1	B	980	ASN	3.2
1	A	953	LYS	3.2
1	B	744	PHE	3.2
1	A	729	ILE	3.1
1	B	746	MET	3.0
1	B	723	GLY	3.0
1	B	694	GLN	3.0
1	B	748	LYS	3.0
1	B	983	SER	2.9
1	A	849	LYS	2.9
1	A	785	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	754	ASN	2.8
1	B	939	SER	2.7
1	A	662	LYS	2.7
1	B	852	LYS	2.7
1	A	744	PHE	2.7
1	B	725	SER	2.7
1	B	912	GLN	2.7
1	B	849	LYS	2.7
1	B	913	GLY	2.6
1	A	845	CYS	2.6
1	A	721	SER	2.6
1	A	727	SER	2.6
1	B	721	SER	2.6
1	B	693	LEU	2.6
1	A	719	ALA	2.6
1	B	749	PRO	2.6
1	B	965	ASP	2.6
1	B	851	PHE	2.5
1	A	783	ASP	2.5
1	B	966	GLY	2.4
1	B	696	MET	2.4
1	B	698	LEU	2.4
1	B	700	LYS	2.4
1	A	690	GLU	2.4
1	B	722	GLN	2.4
1	B	752	LEU	2.4
1	B	807	ASP	2.4
1	A	720	VAL	2.4
1	A	965	ASP	2.3
1	B	853	GLN	2.3
1	B	827	ASN	2.3
1	B	928	ASN	2.3
1	A	700	LYS	2.3
1	A	964	LEU	2.3
1	B	855	HIS	2.2
1	B	695	LYS	2.2
1	B	806	ARG	2.2
1	B	967	VAL	2.2
1	A	717	GLN	2.2
1	A	939	SER	2.2
1	A	940	LYS	2.2
1	A	722	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	963	SER	2.2
1	B	676	ILE	2.1
1	B	940	LYS	2.1
1	B	938	ILE	2.1
1	A	676	ILE	2.1
1	B	750	PRO	2.1
1	B	953	LYS	2.0
1	A	745	GLY	2.0
1	B	979	VAL	2.0
1	B	941	LEU	2.0
1	B	699	GLY	2.0
1	B	799	THR	2.0
1	B	697	PRO	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](#)

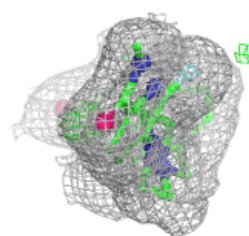
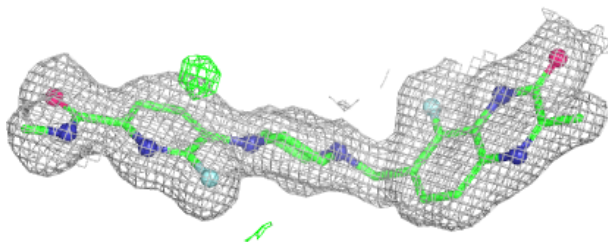
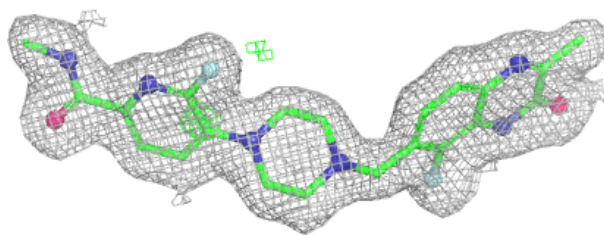
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1H64	B	1101	31/31	0.94	0.06	16,19,21,22	0
2	A1H64	A	1101	31/31	0.95	0.06	10,19,25,27	0
3	SO4	B	1102	5/5	0.98	0.07	25,29,31,33	0
3	SO4	A	1102	5/5	0.99	0.05	23,23,26,28	0

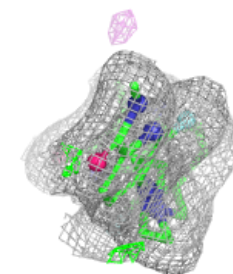
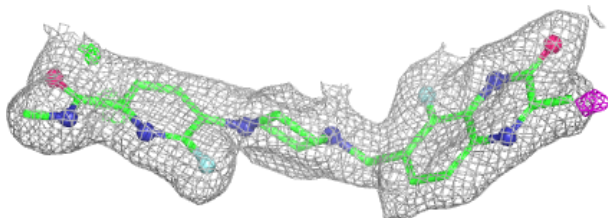
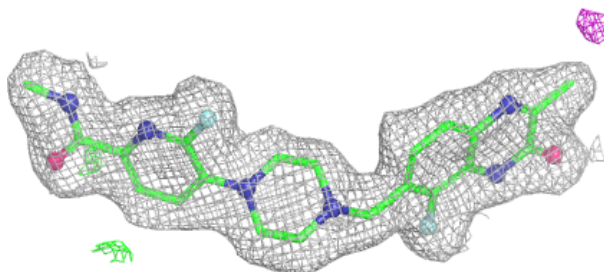
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H64 B 1101:

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

**Electron density around A1H64 A 1101:**

$2mF_o-DF_c$ (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.