



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 10:23 AM EDT

PDB ID : 10PI / pdb_000010pi
Title : JAK1 kinase (JH1 domain) in complex with povorcitinib
Authors : Epling, L.B.; Fenalti, G.
Deposited on : 2026-01-30
Resolution : 1.54 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

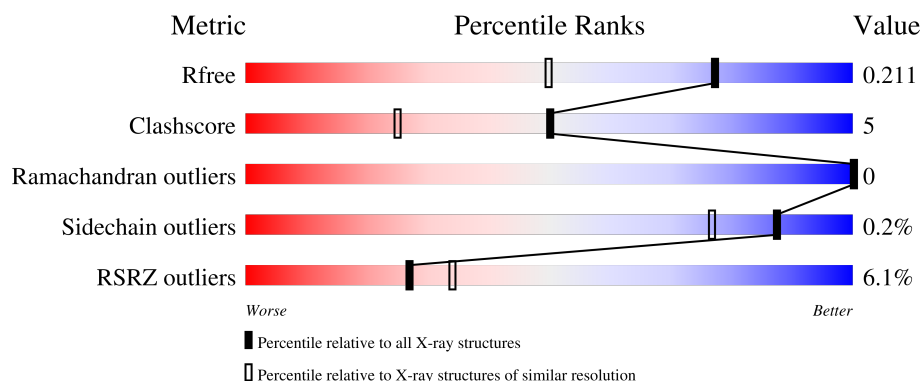
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	297	<div> <div>7%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	B	297	<div> <div>5%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	1503	-	-	X	-
2	EDO	B	1512	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5744 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 Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	8	0
			2332	1490	400	425	17			
1	B	291	Total	C	N	O	S	0	21	0
			2462	1582	418	444	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	864	ACE	-	acetylation	UNP P23458
A	865	MET	-	expression tag	UNP P23458
A	1155	HIS	-	expression tag	UNP P23458
A	1156	HIS	-	expression tag	UNP P23458
A	1157	HIS	-	expression tag	UNP P23458
A	1158	HIS	-	expression tag	UNP P23458
A	1159	HIS	-	expression tag	UNP P23458
A	1160	HIS	-	expression tag	UNP P23458
B	864	ACE	-	acetylation	UNP P23458
B	865	MET	-	expression tag	UNP P23458
B	1155	HIS	-	expression tag	UNP P23458
B	1156	HIS	-	expression tag	UNP P23458
B	1157	HIS	-	expression tag	UNP P23458
B	1158	HIS	-	expression tag	UNP P23458
B	1159	HIS	-	expression tag	UNP P23458
B	1160	HIS	-	expression tag	UNP P23458

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



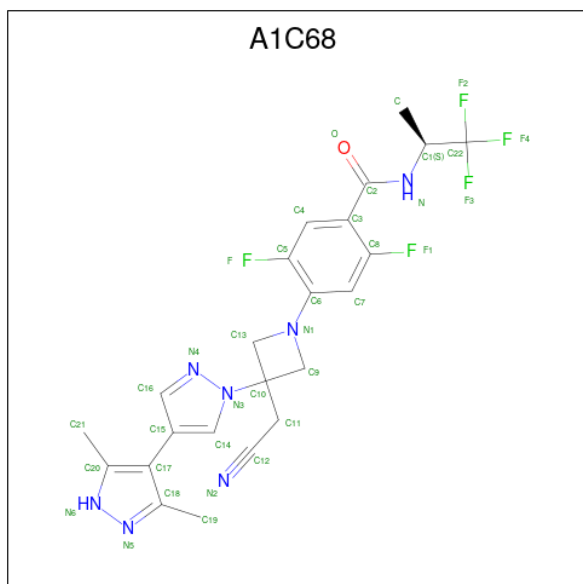
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is 4-{3-(cyanomethyl)-3-[(4M)-3',5'-dimethyl-1H,1'H-[4,4'-bipyrazol]-1-yl]azetid-1-yl}-2,5-difluoro-N-[(2S)-1,1,1-trifluoropropan-2-yl]benzamide (CCD ID: A1C68) (formula: C₂₃H₂₂F₅N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	23	5	7	1		
3	B	1	Total	C	F	N	O	0	0
			36	23	5	7	1		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

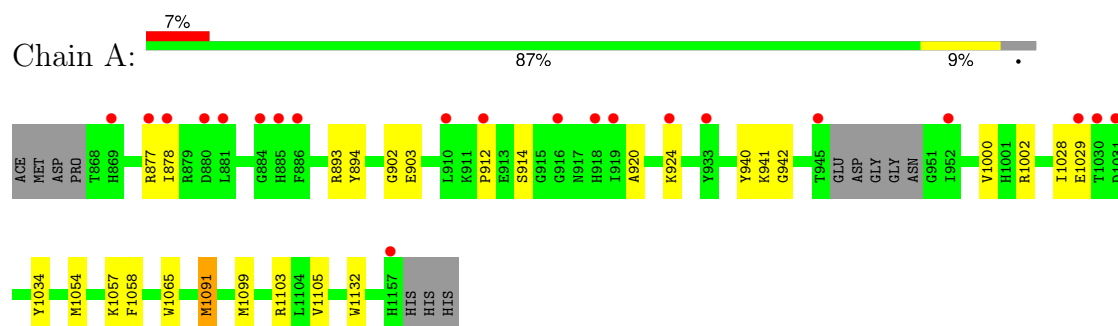
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	375	Total	O	0	0
			375	375		
5	B	423	Total	O	0	0
			423	423		

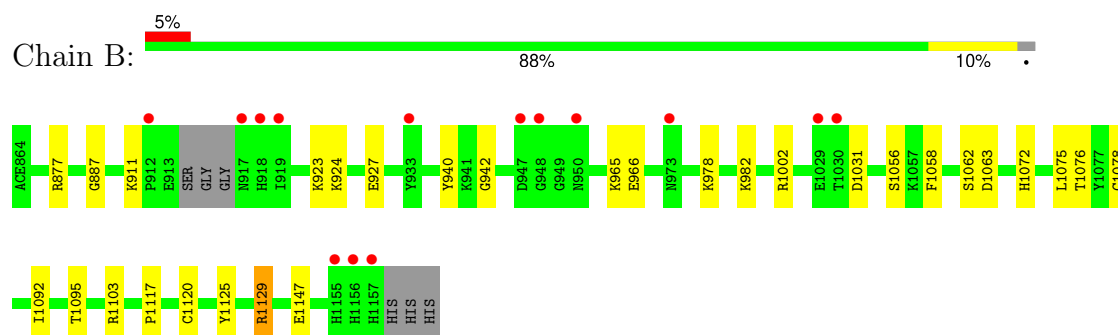
3 Residue-property plots

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: Tyrosine-protein kinase JAK1



• Molecule 1: Tyrosine-protein kinase JAK1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.90Å 49.49Å 85.81Å 90.00° 118.43° 90.00°	Depositor
Resolution (Å)	29.34 – 1.54 29.34 – 1.54	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.34-1.54) 97.4 (29.34-1.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.178 , 0.212 0.177 , 0.211	Depositor DCC
R_{free} test set	4674 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5744	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: EDO, A1C68, DMS, ACE

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	0.66	0/2407	0.81	1/3242 (0.0%)
1	B	0.68	0/2577	0.79	0/3467
All	All	0.67	0/4984	0.80	1/6709 (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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1091	MET	CG-SD-CE	-7.65	84.08	100.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1129[A]	ARG	Sidechain
1	B	1129[B]	ARG	Sidechain

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	2332	0	2337	21	0
1	B	2462	0	2522	30	0
2	A	32	0	48	3	0
2	B	44	0	66	13	0
3	A	36	0	0	0	0
3	B	36	0	0	0	0
4	B	4	0	6	1	0
5	A	375	0	0	6	0
5	B	423	0	0	5	0
All	All	5744	0	4979	53	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 5.

All (53) 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:B:1002:ARG:HA	2:B:1512:EDO:H12	1.44	0.99
1:B:1063:ASP:OD1	2:B:1512:EDO:H21	1.73	0.88
1:B:1058:PHE:HD2	2:B:1512:EDO:H11	1.42	0.83
1:B:1062:SER:HB2	2:B:1512:EDO:H22	1.66	0.78
1:A:877:ARG:HG2	5:A:1601:HOH:O	1.85	0.77
1:A:1099:MET:HE2	2:A:1508:EDO:H11	1.71	0.71
1:B:1095[B]:THR:HG23	5:B:1653:HOH:O	1.94	0.68
1:B:1058:PHE:CD2	2:B:1512:EDO:H11	2.27	0.67
1:B:923:LYS:O	1:B:927:GLU:HG3	1.97	0.65
1:B:1062:SER:CB	2:B:1512:EDO:H22	2.26	0.64
1:A:878:ILE:HD11	1:A:893:ARG:HB2	1.80	0.62
1:A:920:ALA:HB2	5:A:1809:HOH:O	2.00	0.61
1:B:1056:SER:OG	2:B:1503:EDO:H11	2.03	0.59
1:A:894:TYR:O	1:A:902:GLY:HA3	2.04	0.58
1:B:877[A]:ARG:CZ	4:B:1509:DMS:H23	2.34	0.57
1:A:903:GLU:OE2	1:A:941:LYS:HE2	2.07	0.55
1:A:1034:TYR:CZ	1:A:1057:LYS:HE3	2.44	0.53
1:B:1058:PHE:CZ	2:B:1503:EDO:H12	2.45	0.51
2:B:1502:EDO:H22	2:B:1510:EDO:H22	1.93	0.51
1:B:924:LYS:N	1:B:924:LYS:HD2	2.27	0.50
1:A:940:TYR:CZ	1:A:942:GLY:HA2	2.45	0.50
1:B:1147[B]:GLU:HG3	5:B:1776:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1502:EDO:C2	2:B:1510:EDO:H22	2.46	0.46
1:B:978:LYS:HE3	1:B:982[A]:LYS:NZ	2.31	0.46
1:B:1058:PHE:HZ	2:B:1503:EDO:H12	1.81	0.46
1:B:1062:SER:HB2	2:B:1512:EDO:C2	2.39	0.46
1:B:1072:HIS:O	1:B:1076[A]:THR:HG23	2.16	0.45
1:B:1075[B]:LEU:HD13	1:B:1120:CYS:SG	2.56	0.45
1:A:924:LYS:HE3	5:A:1674:HOH:O	2.17	0.45
1:B:940:TYR:CZ	1:B:942:GLY:HA2	2.53	0.44
1:B:1076[A]:THR:HG22	1:B:1117:PRO:HB3	1.99	0.44
1:B:1092[B]:ILE:HG23	1:B:1103:ARG:HB3	2.00	0.44
1:B:1031:ASP:HB2	5:B:1704:HOH:O	2.17	0.43
1:A:1034:TYR:CE2	1:A:1057:LYS:HE3	2.53	0.43
1:A:1029:GLU:HG3	5:A:1612:HOH:O	2.18	0.43
1:A:1091:MET:HB3	1:A:1091:MET:HE2	1.86	0.43
1:A:1065:TRP:CE3	1:A:1132:TRP:HA	2.55	0.42
1:A:1099:MET:HE2	2:A:1508:EDO:C1	2.47	0.42
1:A:1000:VAL:HG13	1:A:1028:ILE:HD11	2.01	0.42
1:A:1002[A]:ARG:HD2	1:A:1058:PHE:CG	2.54	0.42
1:A:924:LYS:HG2	5:A:1608:HOH:O	2.20	0.41
1:A:1103:ARG:HE	2:A:1508:EDO:H12	1.85	0.41
1:B:1129[A]:ARG:HD2	1:B:1129[A]:ARG:HA	1.81	0.41
1:A:1054[B]:MET:SD	1:A:1105:VAL:HG11	2.61	0.41
1:B:887:GLY:HA2	1:B:911:LYS:HG3	2.02	0.41
1:B:1002:ARG:NH2	5:B:1606:HOH:O	2.54	0.41
1:B:965[B]:LYS:HE3	5:B:1657:HOH:O	2.20	0.41
1:B:965[B]:LYS:HD2	1:B:1078:CYS:HB3	2.03	0.40
1:A:924:LYS:CE	5:A:1674:HOH:O	2.69	0.40
1:B:1125:TYR:CZ	1:B:1129[A]:ARG:HD3	2.57	0.40
1:B:1056:SER:HA	2:B:1503:EDO:H11	2.03	0.40
1:A:912:PRO:O	1:A:914:SER:HB2	2.20	0.40

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	289/297 (97%)	285 (99%)	4 (1%)	0	100	100
1	B	308/297 (104%)	303 (98%)	5 (2%)	0	100	100
All	All	597/594 (100%)	588 (98%)	9 (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	258/265 (97%)	258 (100%)	0	100	100
1	B	279/265 (105%)	277 (99%)	2 (1%)	76	55
All	All	537/530 (101%)	535 (100%)	2 (0%)	87	70

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

Mol	Chain	Res	Type
1	B	966[A]	GLU
1	B	966[B]	GLU

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	904	GLN
1	A	931	ASN
1	A	971	ASN
1	A	1126	GLN
1	B	885	HIS
1	B	918	HIS
1	B	1055	GLN
1	B	1098	GLN

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 ⓘ

22 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	EDO	A	1507	-	3,3,3	0.18	0	2,2,2	0.29	0
3	A1C68	A	1509	-	37,39,39	1.74	8 (21%)	47,60,60	1.78	9 (19%)
2	EDO	A	1503	-	3,3,3	0.27	0	2,2,2	0.24	0
2	EDO	B	1511	-	3,3,3	0.28	0	2,2,2	0.77	0
4	DMS	B	1509	-	3,3,3	0.56	0	3,3,3	0.97	0
2	EDO	A	1504	-	3,3,3	0.15	0	2,2,2	1.14	0
2	EDO	B	1512	-	3,3,3	0.44	0	2,2,2	1.63	1 (50%)
2	EDO	B	1508	-	3,3,3	0.25	0	2,2,2	0.70	0
2	EDO	A	1508	-	3,3,3	0.32	0	2,2,2	0.29	0
2	EDO	B	1505	-	3,3,3	0.39	0	2,2,2	0.12	0
2	EDO	A	1505	-	3,3,3	0.25	0	2,2,2	0.33	0
2	EDO	B	1507	-	3,3,3	0.25	0	2,2,2	0.30	0
2	EDO	A	1501	-	3,3,3	0.36	0	2,2,2	0.13	0
2	EDO	B	1510	-	3,3,3	0.35	0	2,2,2	0.66	0
2	EDO	B	1503	-	3,3,3	0.26	0	2,2,2	0.74	0
2	EDO	A	1502	-	3,3,3	0.31	0	2,2,2	0.31	0
2	EDO	B	1506	-	3,3,3	0.23	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	1501	-	3,3,3	0.30	0	2,2,2	0.15	0
2	EDO	A	1506	-	3,3,3	0.26	0	2,2,2	0.53	0
3	A1C68	B	1513	-	37,39,39	1.94	9 (24%)	47,60,60	2.05	12 (25%)
2	EDO	B	1504	-	3,3,3	0.42	0	2,2,2	0.12	0
2	EDO	B	1502	-	3,3,3	0.35	0	2,2,2	0.45	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	EDO	A	1507	-	-	0/1/1/1	-
3	A1C68	A	1509	-	-	12/30/42/42	0/4/4/4
2	EDO	A	1503	-	-	0/1/1/1	-
2	EDO	B	1511	-	-	0/1/1/1	-
2	EDO	A	1504	-	-	1/1/1/1	-
2	EDO	B	1512	-	-	1/1/1/1	-
2	EDO	B	1508	-	-	1/1/1/1	-
2	EDO	A	1508	-	-	1/1/1/1	-
2	EDO	B	1505	-	-	0/1/1/1	-
2	EDO	A	1505	-	-	0/1/1/1	-
2	EDO	B	1507	-	-	1/1/1/1	-
2	EDO	A	1501	-	-	0/1/1/1	-
2	EDO	B	1510	-	-	1/1/1/1	-
2	EDO	B	1503	-	-	1/1/1/1	-
2	EDO	A	1502	-	-	0/1/1/1	-
2	EDO	B	1506	-	-	0/1/1/1	-
2	EDO	B	1501	-	-	1/1/1/1	-
2	EDO	A	1506	-	-	1/1/1/1	-
3	A1C68	B	1513	-	-	8/30/42/42	0/4/4/4
2	EDO	B	1504	-	-	0/1/1/1	-
2	EDO	B	1502	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1509	A1C68	C14-N3	5.25	1.40	1.35
3	B	1513	A1C68	C14-N3	5.23	1.40	1.35
3	B	1513	A1C68	C16-N4	4.83	1.40	1.32
3	A	1509	A1C68	C9-C10	4.48	1.59	1.55
3	B	1513	A1C68	C10-N3	-3.79	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1513	A1C68	C13-N1	3.64	1.53	1.48
3	A	1509	A1C68	C16-N4	3.19	1.37	1.32
3	A	1509	A1C68	C10-N3	-2.97	1.43	1.48
3	B	1513	A1C68	C18-N5	2.73	1.39	1.34
3	B	1513	A1C68	N3-N4	2.71	1.40	1.36
3	B	1513	A1C68	C7-C8	2.55	1.42	1.37
3	A	1509	A1C68	C20-N6	2.46	1.39	1.34
3	B	1513	A1C68	C11-C12	2.42	1.49	1.46
3	A	1509	A1C68	C7-C8	2.30	1.41	1.37
3	A	1509	A1C68	C19-C18	-2.25	1.45	1.49
3	A	1509	A1C68	C2-N	2.11	1.39	1.34
3	B	1513	A1C68	F2-C22	2.03	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1513	A1C68	F2-C22-C1	5.95	120.41	112.11
3	A	1509	A1C68	C22-C1-N	-5.35	104.58	110.25
3	A	1509	A1C68	C15-C14-N3	-5.25	102.90	107.75
3	B	1513	A1C68	C14-C15-C16	5.02	108.66	104.22
3	B	1513	A1C68	C-C1-N	4.64	118.17	109.19
3	B	1513	A1C68	C22-C1-N	-4.17	105.83	110.25
3	A	1509	A1C68	C14-C15-C16	3.85	107.62	104.22
3	B	1513	A1C68	C10-C13-N1	-3.73	83.52	87.90
3	A	1509	A1C68	C-C1-N	3.54	116.05	109.19
3	B	1513	A1C68	F4-C22-C1	-3.38	107.39	112.11
3	B	1513	A1C68	C15-C14-N3	-3.01	104.97	107.75
3	B	1513	A1C68	C10-C9-N1	-2.79	84.63	87.90
3	B	1513	A1C68	C9-C10-C13	2.78	91.47	86.43
3	B	1513	A1C68	C10-N3-N4	-2.70	116.03	119.37
3	A	1509	A1C68	C19-C18-N5	-2.54	117.15	120.99
3	A	1509	A1C68	C7-C6-C5	2.49	119.12	116.53
3	A	1509	A1C68	F2-C22-C1	2.47	115.55	112.11
3	A	1509	A1C68	C4-C5-C6	-2.43	121.20	123.35
3	B	1513	A1C68	F4-C22-F2	-2.36	101.74	106.87
2	B	1512	EDO	O2-C2-C1	2.28	129.73	112.39
3	B	1513	A1C68	C7-C6-C5	2.07	118.69	116.53
3	A	1509	A1C68	C7-C8-C3	-2.01	121.26	123.48

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1509	A1C68	C16-C15-C17-C20
3	A	1509	A1C68	C16-C15-C17-C18
3	A	1509	A1C68	C-C1-C22-F2
3	A	1509	A1C68	N-C1-C22-F3
3	A	1509	A1C68	C-C1-C22-F3
3	A	1509	A1C68	N-C1-C22-F4
3	A	1509	A1C68	C-C1-C22-F4
3	B	1513	A1C68	C16-C15-C17-C20
3	B	1513	A1C68	C16-C15-C17-C18
3	B	1513	A1C68	N-C1-C22-F3
3	B	1513	A1C68	N-C1-C22-F4
3	B	1513	A1C68	C-C1-C22-F4
2	A	1508	EDO	O1-C1-C2-O2
2	A	1506	EDO	O1-C1-C2-O2
2	B	1512	EDO	O1-C1-C2-O2
2	B	1503	EDO	O1-C1-C2-O2
3	A	1509	A1C68	C22-C1-N-C2
3	A	1509	A1C68	N-C1-C22-F2
3	B	1513	A1C68	N-C1-C22-F2
3	A	1509	A1C68	C14-C15-C17-C18
3	B	1513	A1C68	C14-C15-C17-C18
3	A	1509	A1C68	C-C1-N-C2
2	B	1501	EDO	O1-C1-C2-O2
2	B	1508	EDO	O1-C1-C2-O2
2	B	1510	EDO	O1-C1-C2-O2
2	A	1504	EDO	O1-C1-C2-O2
2	B	1507	EDO	O1-C1-C2-O2
3	A	1509	A1C68	C14-C15-C17-C20
3	B	1513	A1C68	C14-C15-C17-C20

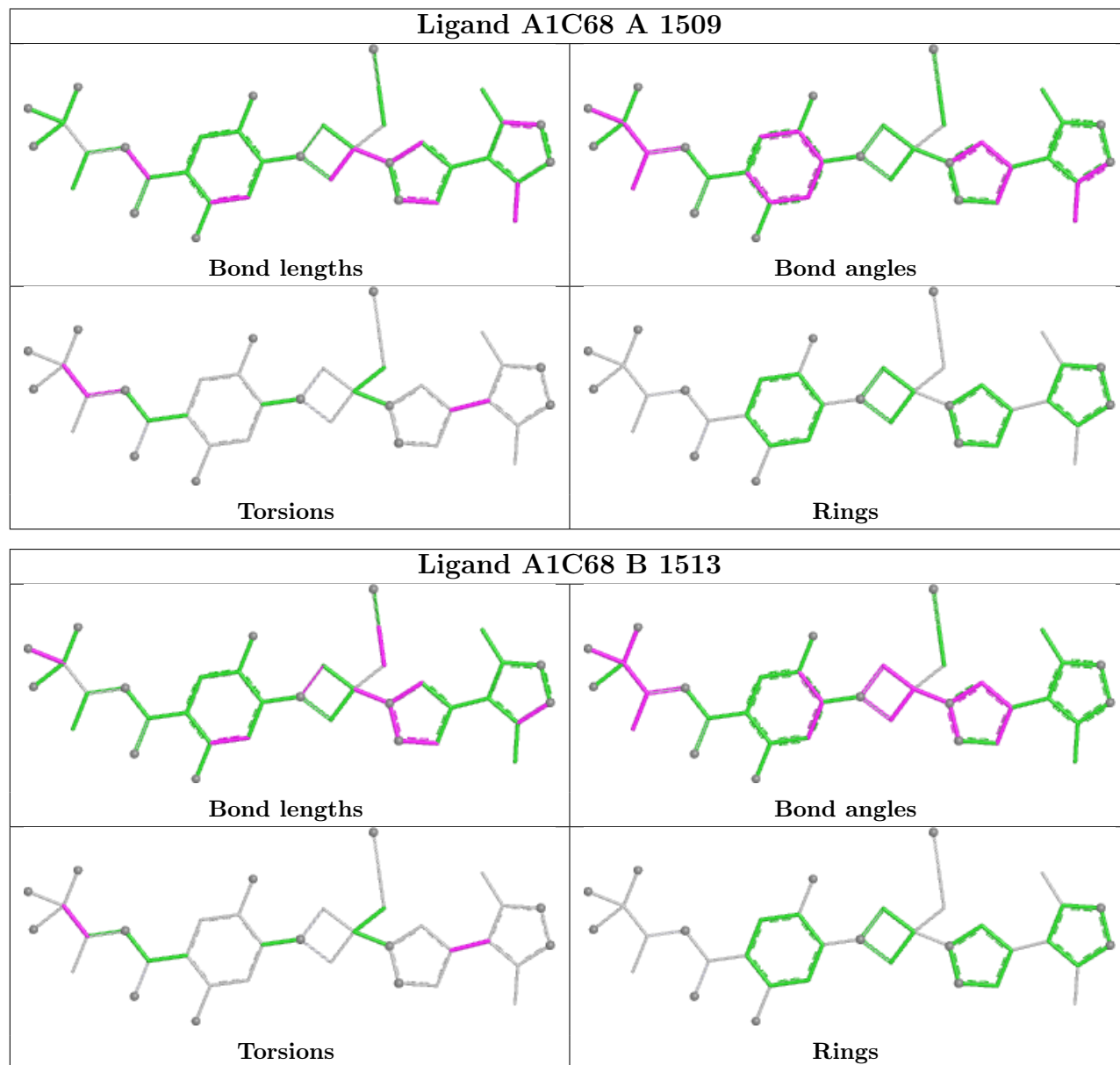
There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1509	DMS	1	0
2	B	1512	EDO	7	0
2	A	1508	EDO	3	0
2	B	1510	EDO	2	0
2	B	1503	EDO	4	0
2	B	1502	EDO	2	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 ⓘ

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	285/297 (95%)	0.39	21 (7%) 20 25	12, 27, 57, 83	8 (2%)
1	B	290/297 (97%)	0.23	14 (4%) 35 44	11, 23, 52, 86	21 (7%)
All	All	575/594 (96%)	0.31	35 (6%) 27 34	11, 25, 57, 86	29 (5%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	933	TYR	4.1
1	B	917	ASN	3.7
1	B	950	ASN	3.2
1	B	1030	THR	3.2
1	B	1155	HIS	3.2
1	A	910	LEU	3.1
1	A	1030	THR	3.0
1	B	1029	GLU	3.0
1	B	948	GLY	3.0
1	A	869	HIS	2.9
1	A	878	ILE	2.9
1	A	912	PRO	2.8
1	A	952	ILE	2.8
1	A	1157	HIS	2.7
1	A	1031	ASP	2.7
1	B	973	ASN	2.6
1	A	885	HIS	2.6
1	B	919	ILE	2.5
1	B	1156	HIS	2.5
1	A	919	ILE	2.5
1	A	1029	GLU	2.4
1	A	884	GLY	2.4
1	A	886	PHE	2.4
1	A	945	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1157	HIS	2.4
1	B	933	TYR	2.3
1	A	924	LYS	2.3
1	B	947	ASP	2.3
1	A	881	LEU	2.3
1	B	912	PRO	2.2
1	A	880	ASP	2.2
1	B	918	HIS	2.2
1	A	916	GLY	2.1
1	A	918	HIS	2.0
1	A	877	ARG	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(Å ²)	Q<0.9
2	EDO	A	1506	4/4	0.71	0.18	50,64,67,67	0
2	EDO	B	1510	4/4	0.82	0.16	31,44,51,52	0
2	EDO	A	1505	4/4	0.84	0.12	39,57,62,68	0
2	EDO	B	1508	4/4	0.85	0.12	45,50,52,54	0
2	EDO	A	1503	4/4	0.87	0.12	48,52,60,75	0
2	EDO	A	1508	4/4	0.87	0.12	23,38,41,49	0
2	EDO	B	1503	4/4	0.88	0.12	24,25,36,52	0
2	EDO	B	1511	4/4	0.89	0.12	32,42,42,55	0
2	EDO	B	1512	4/4	0.89	0.20	24,24,39,44	0
4	DMS	B	1509	4/4	0.89	0.11	42,47,48,63	0
2	EDO	B	1505	4/4	0.90	0.10	31,33,35,53	0
2	EDO	B	1501	4/4	0.90	0.11	40,43,48,50	0

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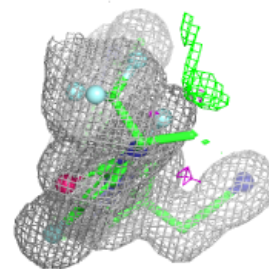
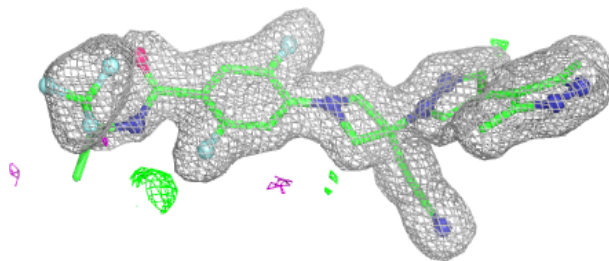
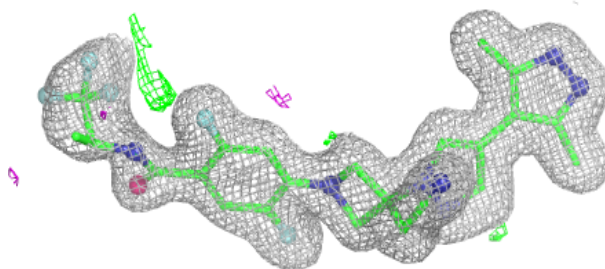
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	1507	4/4	0.91	0.09	35,40,41,57	0
2	EDO	A	1502	4/4	0.91	0.10	37,38,41,47	0
2	EDO	B	1506	4/4	0.91	0.11	25,26,26,27	0
2	EDO	A	1501	4/4	0.93	0.10	28,35,37,38	0
2	EDO	A	1504	4/4	0.93	0.10	35,48,49,50	0
2	EDO	B	1502	4/4	0.93	0.11	27,35,37,38	0
2	EDO	A	1507	4/4	0.93	0.10	36,38,53,53	0
3	A1C68	A	1509	36/36	0.96	0.08	17,23,70,81	0
3	A1C68	B	1513	36/36	0.96	0.08	15,18,51,67	0
2	EDO	B	1504	4/4	0.96	0.07	22,24,25,26	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.

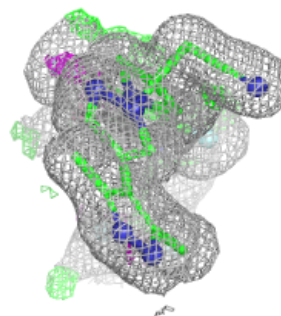
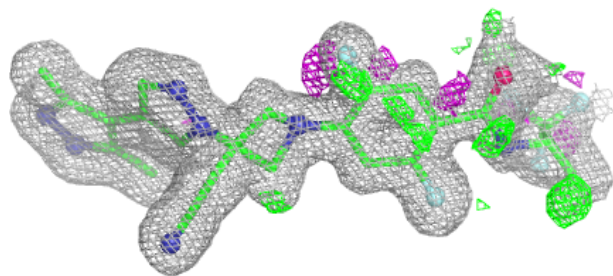
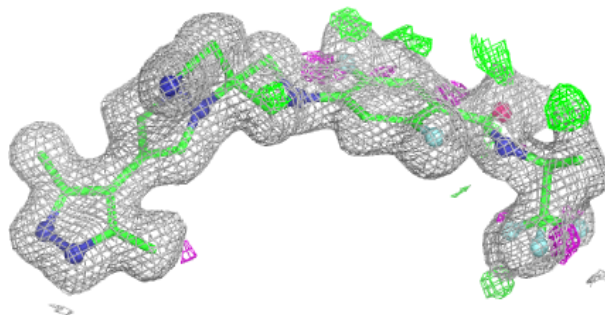
Electron density around A1C68 A 1509:

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 A1C68 B 1513:

$2mF_o - DF_c$ (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.