



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:03 PM UTC

PDB ID : 4V04 / pdb_00004v04
Title : FGFR1 in complex with ponatinib.
Authors : Tucker, J.; Klein, T.; Breed, J.; Breeze, A.; Overman, R.; Phillips, C.; Norman, R.A.
Deposited on : 2014-09-10
Resolution : 2.12 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

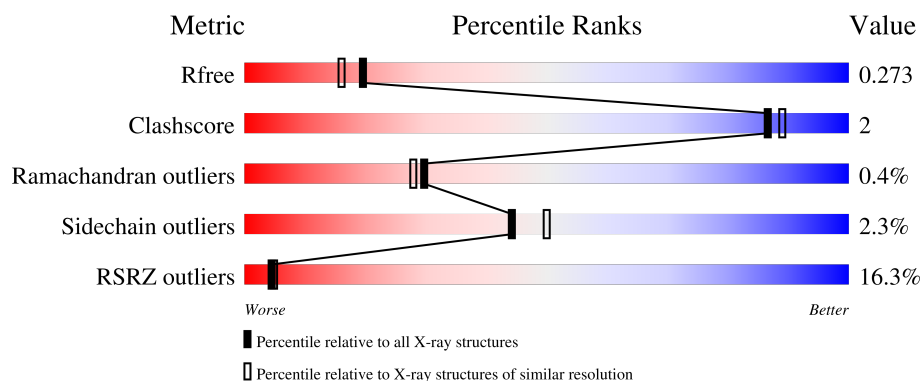
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	309	23% 88% 6% 5%
1	B	309	7% 88% 5% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5161 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.

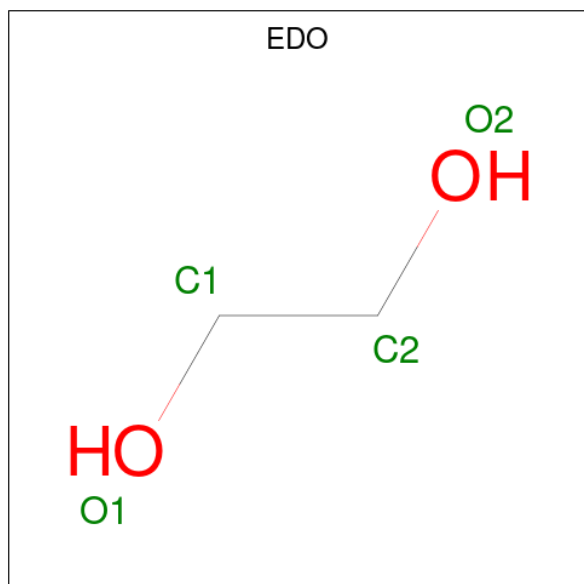
- Molecule 1 is a protein called FIBROBLAST GROWTH FACTOR RECEPTOR 1 (FMS-RELATED TYROSINE KINASE 2, PFEIFFER SYNDROME), ISOFORM CRA_B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	8	1
			2318	1476	395	428	19			
1	B	289	Total	C	N	O	S	0	6	0
			2276	1451	386	421	18			

There are 6 discrepancies between the modelled and reference sequences:

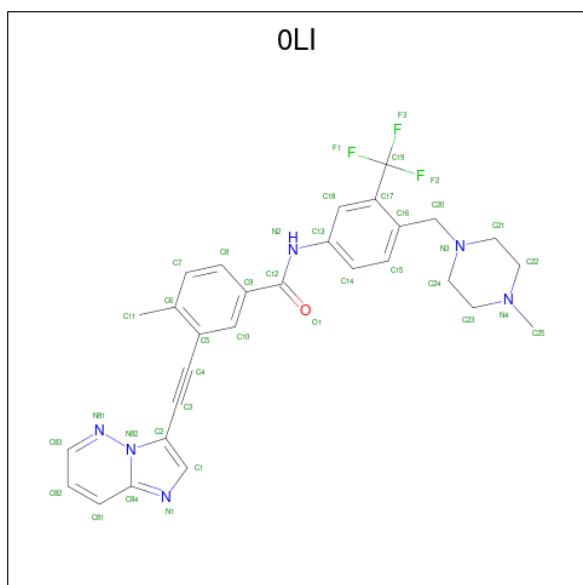
Chain	Residue	Modelled	Actual	Comment	Reference
A	457	GLY	-	expression tag	UNP D3DSX2
A	488	ALA	CYS	engineered mutation	UNP D3DSX2
A	584	SER	CYS	engineered mutation	UNP D3DSX2
B	457	GLY	-	expression tag	UNP D3DSX2
B	488	ALA	CYS	engineered mutation	UNP D3DSX2
B	584	SER	CYS	engineered mutation	UNP D3DSX2

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



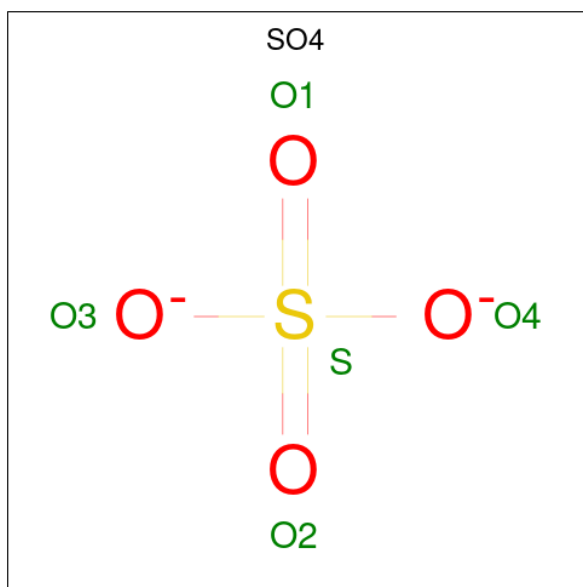
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0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

- Molecule 3 is 3-(imidazo[1,2-b]pyridazin-3-ylethynyl)-4-methyl-N-{4-[(4-methylpiperazin-1-yl)methyl]-3-(trifluoromethyl)phenyl}benzamide (CCD ID: 0LI) (formula: C₂₉H₂₇F₃N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	1
			39	29	3	6	1		
3	B	1	Total	C	F	N	O	0	1
			39	29	3	6	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

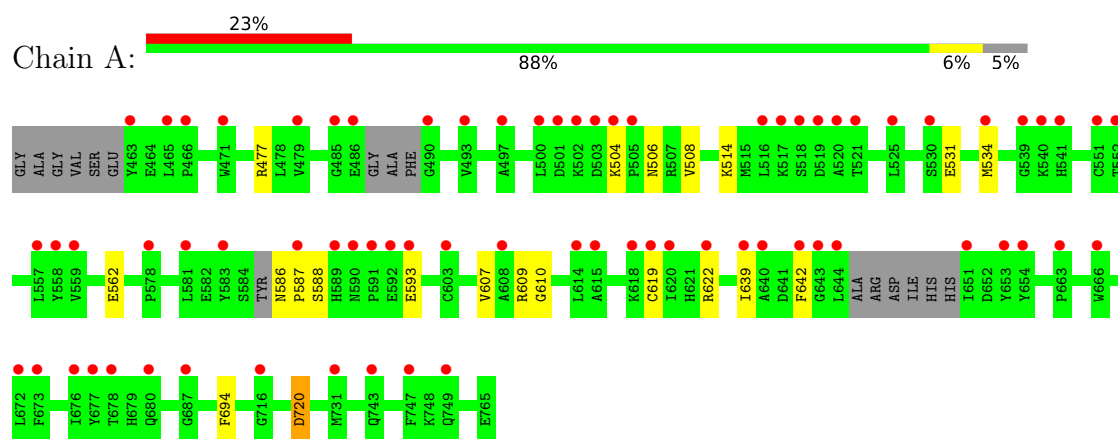
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	205	Total	O	0	0
			205	205		

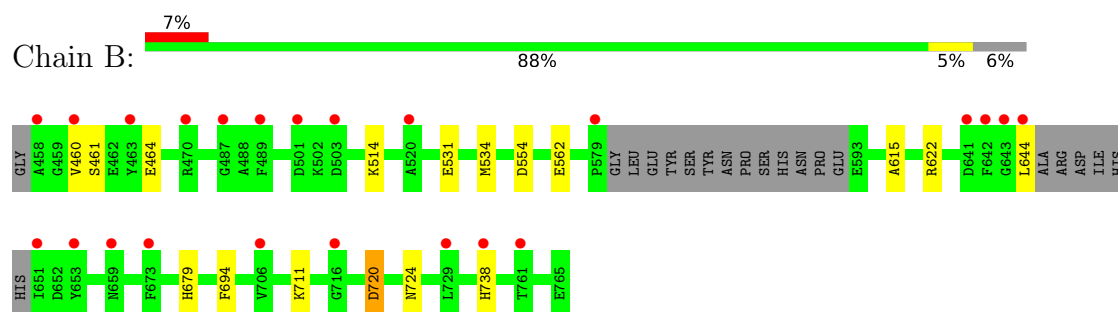
3 Residue-property plots

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: FIBROBLAST GROWTH FACTOR RECEPTOR 1 (FMS-RELATED TYROSINE KINASE 2, PFEIFFER SYNDROME), ISOFORM CRA_B



- Molecule 1: FIBROBLAST GROWTH FACTOR RECEPTOR 1 (FMS-RELATED TYROSINE KINASE 2, PFEIFFER SYNDROME), ISOFORM CRA_B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.25Å 58.09Å 65.23Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	21.37 – 2.12 21.37 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.6 (21.37-2.12) 96.6 (21.37-2.12)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.11Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.186 , 0.228 0.244 , 0.273	Depositor DCC
R_{free} test set	2076 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5161	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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, OLI, EDO

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	0/2364	1.17	3/3197 (0.1%)
1	B	0.83	0/2321	1.17	2/3139 (0.1%)
All	All	0.85	0/4685	1.17	5/6336 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	720	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	720	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	694	PHE	CA-CB-CG	-6.02	107.78	113.80
1	B	694	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	508	VAL	N-CA-CB	5.24	119.25	110.86

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	2318	0	2274	13	0
1	B	2276	0	2221	6	1
2	A	24	0	36	0	0
2	B	20	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	39	0	27	8	0
3	B	39	0	27	4	0
4	A	20	0	0	1	0
4	B	5	0	0	0	0
5	A	215	0	0	1	3
5	B	205	0	0	0	0
All	All	5161	0	4615	20	3

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)
4:A:1773:SO4:O2	5:A:2209:HOH:O	2.00	0.79
1:A:622:ARG:HH11	3:A:1772[A]:OLI:H25	1.52	0.74
1:B:622:ARG:HH11	3:B:1771[A]:OLI:H25	1.62	0.64
1:A:619[A]:CYS:SG	3:A:1772[A]:OLI:H24A	2.46	0.56
1:A:562:GLU:O	3:A:1772[A]:OLI:H1	2.11	0.50
1:A:607:VAL:HG13	1:A:639[A]:ILE:HD11	1.96	0.48
1:A:531:GLU:HG3	3:A:1772[A]:OLI:H14	1.97	0.46
1:B:514:LYS:HB2	3:B:1771[A]:OLI:C11	2.45	0.46
1:B:562:GLU:O	3:B:1771[A]:OLI:H1	2.16	0.46
1:A:610:GLY:HA3	1:A:639[B]:ILE:HD12	1.97	0.46
1:A:622:ARG:NH1	3:A:1772[A]:OLI:H25	2.27	0.45
1:A:504:LYS:HG2	1:A:506:ASN:H	1.82	0.45
1:A:477:ARG:HA	1:A:477:ARG:NE	2.33	0.44
1:A:586:ASN:C	1:A:588:SER:H	2.27	0.43
1:A:619[A]:CYS:SG	3:A:1772[A]:OLI:C24	3.07	0.43
1:A:514:LYS:HB2	3:A:1772[A]:OLI:C11	2.48	0.42
1:A:514:LYS:HB2	3:A:1772[A]:OLI:H11	2.00	0.42
1:B:615:ALA:HA	1:B:679:HIS:CE1	2.55	0.42
1:B:461:SER:HA	1:B:464:GLU:O	2.20	0.41
1:B:531:GLU:HG3	3:B:1771[A]:OLI:H14	2.03	0.40

All (3) 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)
5:A:2036:HOH:O	5:A:2036:HOH:O[2_656]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2034:HOH:O	5:A:2034:HOH:O[2_656]	2.18	0.02
1:B:554:ASP:O	5:A:2190:HOH:O[4_556]	2.18	0.02

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	291/309 (94%)	286 (98%)	4 (1%)	1 (0%)	36	36
1	B	287/309 (93%)	283 (99%)	3 (1%)	1 (0%)	36	36
All	All	578/618 (94%)	569 (98%)	7 (1%)	2 (0%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	460	VAL
1	A	587	PRO

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	247/269 (92%)	241 (98%)	6 (2%)	43	48
1	B	237/269 (88%)	231 (98%)	6 (2%)	42	47
All	All	484/538 (90%)	472 (98%)	12 (2%)	44	47

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	MET
1	A	593	GLU
1	A	609	ARG
1	A	642[A]	PHE
1	A	642[B]	PHE
1	A	720	ASP
1	B	534	MET
1	B	644[B]	LEU
1	B	711	LYS
1	B	720	ASP
1	B	724	ASN
1	B	738	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	589	HIS
1	A	594	GLN
1	A	717	HIS
1	A	743	GLN
1	B	594	GLN
1	B	717	HIS
1	B	743	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

18 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
3	OLI	A	1772[A]	-	43,43,43	0.71	0	59,62,62	1.35	2 (3%)
2	EDO	A	1767	-	3,3,3	0.45	0	2,2,2	0.90	0
2	EDO	A	1768	-	3,3,3	0.75	0	2,2,2	0.04	0
2	EDO	B	1769	-	3,3,3	0.53	0	2,2,2	0.43	0
2	EDO	B	1770	-	3,3,3	0.62	0	2,2,2	0.34	0
4	SO4	A	1775	-	4,4,4	0.28	0	6,6,6	0.20	0
3	OLI	B	1771[A]	-	43,43,43	0.81	0	59,62,62	1.45	3 (5%)
4	SO4	A	1776	-	4,4,4	0.39	0	6,6,6	0.17	0
2	EDO	B	1766	-	3,3,3	0.29	0	2,2,2	0.61	0
4	SO4	A	1773	-	4,4,4	0.57	0	6,6,6	0.32	0
2	EDO	B	1768	-	3,3,3	0.48	0	2,2,2	0.50	0
2	EDO	A	1770	-	3,3,3	0.76	0	2,2,2	0.09	0
2	EDO	A	1771	-	3,3,3	0.57	0	2,2,2	0.38	0
4	SO4	B	1772	-	4,4,4	0.34	0	6,6,6	0.34	0
2	EDO	A	1769	-	3,3,3	0.63	0	2,2,2	0.18	0
4	SO4	A	1774	-	4,4,4	0.30	0	6,6,6	0.44	0
2	EDO	B	1767	-	3,3,3	0.49	0	2,2,2	0.44	0
2	EDO	A	1766	-	3,3,3	0.40	0	2,2,2	0.31	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
3	OLI	A	1772[A]	-	-	3/21/33/33	0/5/5/5
2	EDO	A	1767	-	-	1/1/1/1	-
2	EDO	A	1768	-	-	1/1/1/1	-
2	EDO	B	1769	-	-	0/1/1/1	-
2	EDO	B	1770	-	-	0/1/1/1	-
3	OLI	B	1771[A]	-	-	2/21/33/33	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	1766	-	-	0/1/1/1	-
2	EDO	B	1768	-	-	0/1/1/1	-
2	EDO	A	1770	-	-	0/1/1/1	-
2	EDO	A	1771	-	-	1/1/1/1	-
2	EDO	A	1769	-	-	1/1/1/1	-
2	EDO	B	1767	-	-	0/1/1/1	-
2	EDO	A	1766	-	-	0/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1771[A]	0LI	C1-C2-N82	8.64	106.67	103.61
3	A	1772[A]	0LI	C1-C2-N82	8.60	106.65	103.61
3	B	1771[A]	0LI	C19-C17-C16	3.18	124.11	121.06
3	A	1772[A]	0LI	C2-C1-N1	-2.14	110.06	112.35
3	B	1771[A]	0LI	C8-C9-C12	2.02	127.14	120.60

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1772[A]	0LI	C2-C3-C4-C5
3	A	1772[A]	0LI	C3-C4-C5-C10
3	A	1772[A]	0LI	C3-C4-C5-C6
3	B	1771[A]	0LI	C3-C4-C5-C10
2	A	1769	EDO	O1-C1-C2-O2
3	B	1771[A]	0LI	C3-C4-C5-C6
2	A	1768	EDO	O1-C1-C2-O2
2	A	1771	EDO	O1-C1-C2-O2
2	A	1767	EDO	O1-C1-C2-O2

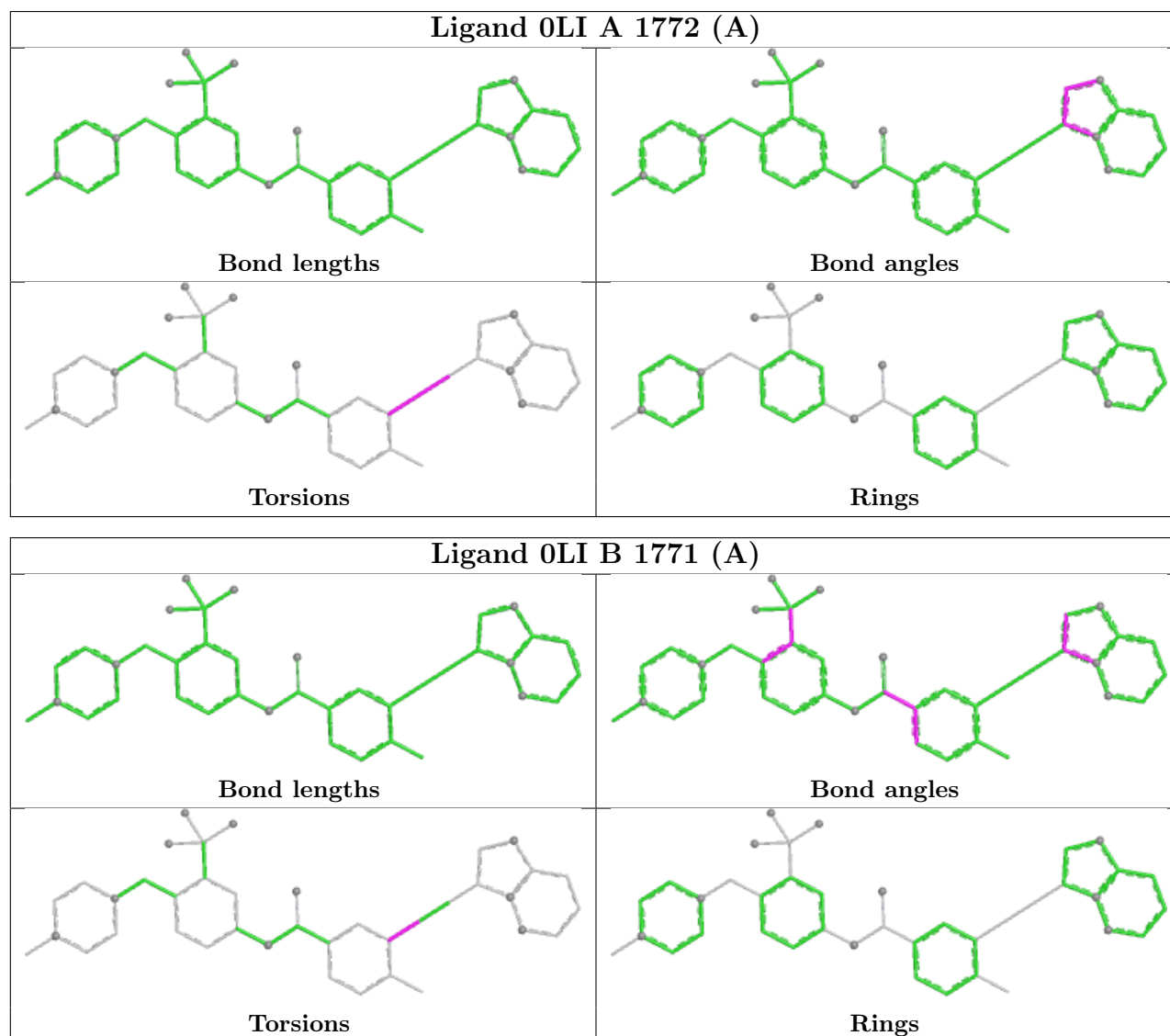
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1772[A]	0LI	8	0
3	B	1771[A]	0LI	4	0
4	A	1773	SO4	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 ⓘ

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	293/309 (94%)	1.54	72 (24%) 2 2	16, 45, 87, 110	8 (2%)
1	B	289/309 (93%)	0.82	23 (7%) 18 20	16, 48, 82, 105	6 (2%)
All	All	582/618 (94%)	1.18	95 (16%) 4 5	16, 47, 86, 110	14 (2%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644[B]	LEU	7.3
1	B	644[B]	LEU	7.2
1	A	642[A]	PHE	5.6
1	A	587	PRO	4.4
1	A	643[B]	GLY	4.3
1	A	653	TYR	4.2
1	A	516	LEU	4.2
1	A	471	TRP	4.1
1	A	583	TYR	4.0
1	A	463	TYR	3.7
1	A	557	LEU	3.7
1	B	673	PHE	3.5
1	B	463	TYR	3.5
1	B	460	VAL	3.4
1	A	520	ALA	3.3
1	A	590	ASN	3.3
1	A	651	ILE	3.3
1	A	534	MET	3.2
1	A	731	MET	3.2
1	A	503	ASP	3.2
1	A	519	ASP	3.2
1	A	486	GLU	3.2
1	A	672	LEU	3.1
1	A	465	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	653	TYR	3.1
1	B	642[A]	PHE	3.1
1	A	581	LEU	3.0
1	A	501	ASP	3.0
1	A	747	PHE	3.0
1	B	503	ASP	3.0
1	B	458	ALA	2.9
1	B	579	PRO	2.9
1	A	615	ALA	2.9
1	A	466	PRO	2.9
1	B	651	ILE	2.8
1	A	673	PHE	2.8
1	A	504	LYS	2.8
1	A	603[A]	CYS	2.8
1	A	622	ARG	2.8
1	B	643[B]	GLY	2.8
1	A	517	LYS	2.7
1	A	539	GLY	2.7
1	A	743	GLN	2.6
1	A	608	ALA	2.6
1	A	678	THR	2.6
1	A	619[A]	CYS	2.5
1	A	530	SER	2.5
1	A	639[A]	ILE	2.5
1	A	518	SER	2.5
1	A	497	ALA	2.5
1	A	500	LEU	2.5
1	A	589	HIS	2.5
1	A	485	GLY	2.5
1	A	680	GLN	2.4
1	A	654	TYR	2.4
1	A	677	TYR	2.4
1	A	591	PRO	2.4
1	A	687	GLY	2.4
1	B	501	ASP	2.4
1	A	676	ILE	2.4
1	B	738	HIS	2.4
1	B	520	ALA	2.3
1	A	540	LYS	2.3
1	A	618	LYS	2.3
1	A	663	PRO	2.3
1	A	490	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	716	GLY	2.3
1	A	521	THR	2.2
1	A	558	TYR	2.2
1	A	552	THR	2.2
1	A	592	GLU	2.2
1	A	525	LEU	2.2
1	B	487	GLY	2.2
1	A	666	TRP	2.2
1	A	559	VAL	2.1
1	A	749[A]	GLN	2.1
1	B	489	PHE	2.1
1	A	541	HIS	2.1
1	B	470	ARG	2.1
1	A	640	ALA	2.1
1	B	729	LEU	2.1
1	B	761	THR	2.1
1	A	716	GLY	2.1
1	A	493	VAL	2.1
1	B	706	VAL	2.1
1	A	614	LEU	2.1
1	A	578	PRO	2.1
1	A	479	VAL	2.1
1	B	659	ASN	2.0
1	A	620	ILE	2.0
1	A	593	GLU	2.0
1	B	641[A]	ASP	2.0
1	A	551	CYS	2.0
1	A	502	LYS	2.0
1	A	505	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

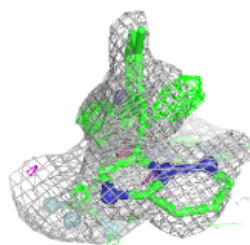
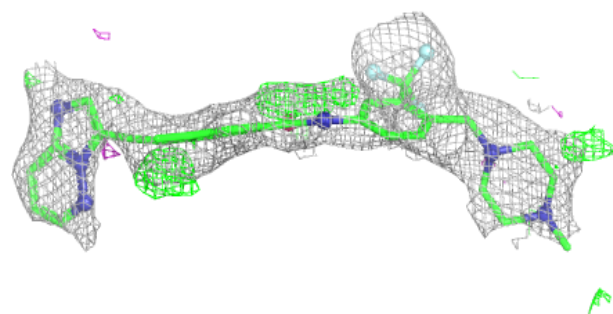
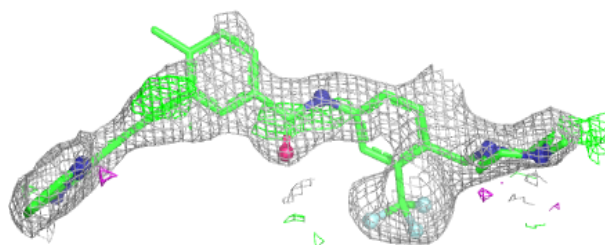
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1768	4/4	0.67	0.26	59,61,62,65	0
2	EDO	B	1768	4/4	0.70	0.13	66,69,70,70	0
2	EDO	A	1770	4/4	0.71	0.16	57,57,59,60	0
2	EDO	A	1769	4/4	0.73	0.19	70,70,71,71	0
4	SO4	A	1776	5/5	0.74	0.18	69,70,73,75	5
3	OLI	A	1772[A]	39/39	0.75	0.19	27,37,42,43	39
3	OLI	B	1771[A]	39/39	0.77	0.20	30,38,45,49	39
2	EDO	B	1769	4/4	0.79	0.18	62,65,69,70	0
2	EDO	A	1771	4/4	0.80	0.12	58,61,62,64	0
4	SO4	A	1773	5/5	0.81	0.15	33,41,42,44	5
2	EDO	B	1770	4/4	0.81	0.15	65,68,69,69	0
2	EDO	B	1767	4/4	0.82	0.14	61,61,62,62	0
2	EDO	A	1767	4/4	0.83	0.15	39,41,41,43	0
4	SO4	A	1775	5/5	0.84	0.12	89,89,92,93	0
2	EDO	B	1766	4/4	0.88	0.12	50,51,51,53	0
4	SO4	A	1774	5/5	0.88	0.11	65,72,76,78	0
2	EDO	A	1766	4/4	0.90	0.10	30,31,33,34	0
4	SO4	B	1772	5/5	0.91	0.16	48,58,61,64	0

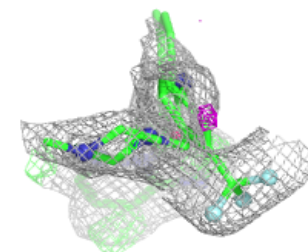
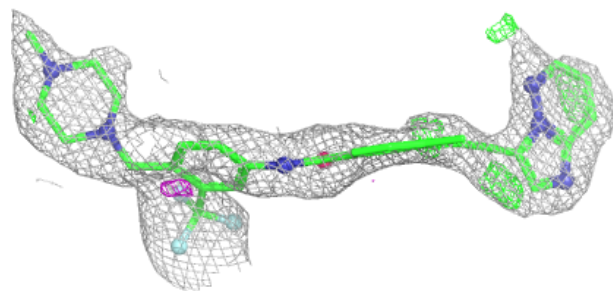
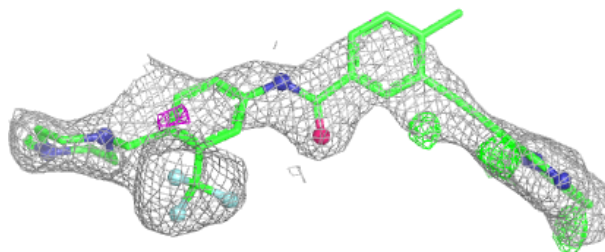
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0LI A 1772 (A):

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

**Electron density around 0LI B 1771 (A):**

$2mF_o-DF_c$ (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.