



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 03:43 PM UTC

PDB ID : 8BX9 / pdb_00008bx9
Title : Crystal structure of JAK2 JH1 in complex with ilginatinib
Authors : Haikarainen, T.
Deposited on : 2022-12-08
Resolution : 1.40 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

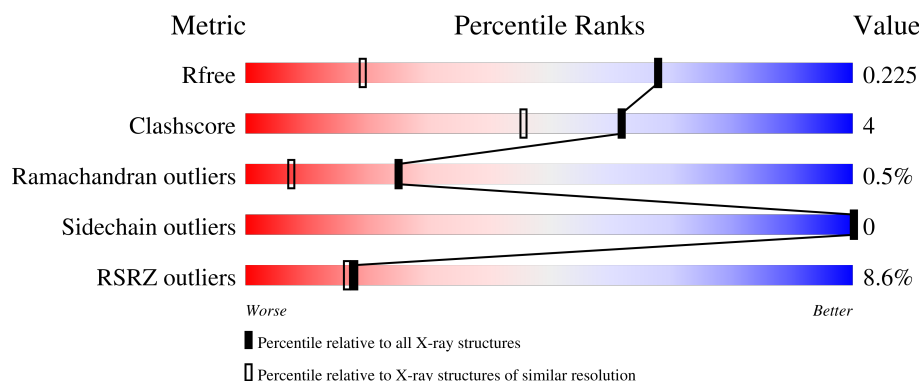
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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	316	8% 86% 9% 5%
1	B	316	8% 84% 10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10562 atoms, of which 4982 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 JAK2.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	300	Total	C	H	N	O	P	S		0	12	0
			5006	1606	2487	433	463	2	15				
1	B	300	Total	C	H	N	O	P	S		0	9	0
			4939	1588	2443	426	465	2	15				

There are 46 discrepancies between the modelled and reference sequences:

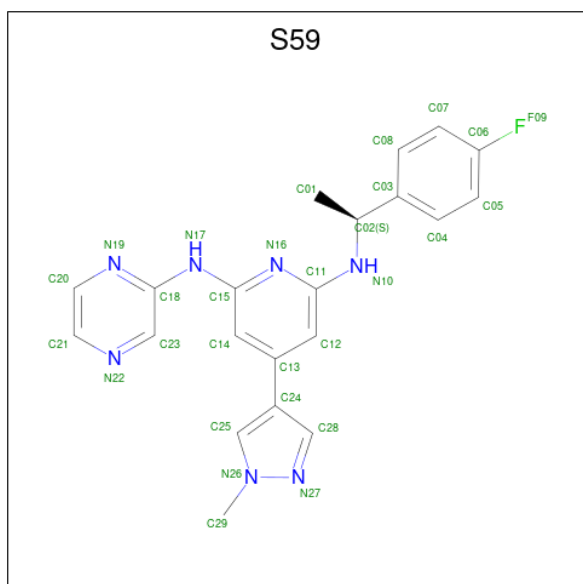
Chain	Residue	Modelled	Actual	Comment	Reference
A	817	MET	-	initiating methionine	UNP O60674
A	818	HIS	-	expression tag	UNP O60674
A	819	HIS	-	expression tag	UNP O60674
A	820	HIS	-	expression tag	UNP O60674
A	821	HIS	-	expression tag	UNP O60674
A	822	HIS	-	expression tag	UNP O60674
A	823	HIS	-	expression tag	UNP O60674
A	824	SER	-	expression tag	UNP O60674
A	825	SER	-	expression tag	UNP O60674
A	826	GLY	-	expression tag	UNP O60674
A	827	VAL	-	expression tag	UNP O60674
A	828	ASP	-	expression tag	UNP O60674
A	829	LEU	-	expression tag	UNP O60674
A	830	GLY	-	expression tag	UNP O60674
A	831	THR	-	expression tag	UNP O60674
A	832	GLU	-	expression tag	UNP O60674
A	833	ASN	-	expression tag	UNP O60674
A	834	LEU	-	expression tag	UNP O60674
A	835	TYR	-	expression tag	UNP O60674
A	836	PHE	-	expression tag	UNP O60674
A	837	GLN	-	expression tag	UNP O60674
A	838	SER	-	expression tag	UNP O60674
A	839	MET	-	expression tag	UNP O60674
B	817	MET	-	initiating methionine	UNP O60674
B	818	HIS	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	819	HIS	-	expression tag	UNP O60674
B	820	HIS	-	expression tag	UNP O60674
B	821	HIS	-	expression tag	UNP O60674
B	822	HIS	-	expression tag	UNP O60674
B	823	HIS	-	expression tag	UNP O60674
B	824	SER	-	expression tag	UNP O60674
B	825	SER	-	expression tag	UNP O60674
B	826	GLY	-	expression tag	UNP O60674
B	827	VAL	-	expression tag	UNP O60674
B	828	ASP	-	expression tag	UNP O60674
B	829	LEU	-	expression tag	UNP O60674
B	830	GLY	-	expression tag	UNP O60674
B	831	THR	-	expression tag	UNP O60674
B	832	GLU	-	expression tag	UNP O60674
B	833	ASN	-	expression tag	UNP O60674
B	834	LEU	-	expression tag	UNP O60674
B	835	TYR	-	expression tag	UNP O60674
B	836	PHE	-	expression tag	UNP O60674
B	837	GLN	-	expression tag	UNP O60674
B	838	SER	-	expression tag	UNP O60674
B	839	MET	-	expression tag	UNP O60674

- Molecule 2 is Ilginatinib (CCD ID: S59) (formula: C₂₁H₂₀FN₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	0	0
			49	21	1	20	7		
2	B	1	Total	C	F	H	N	0	0
			49	21	1	20	7		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

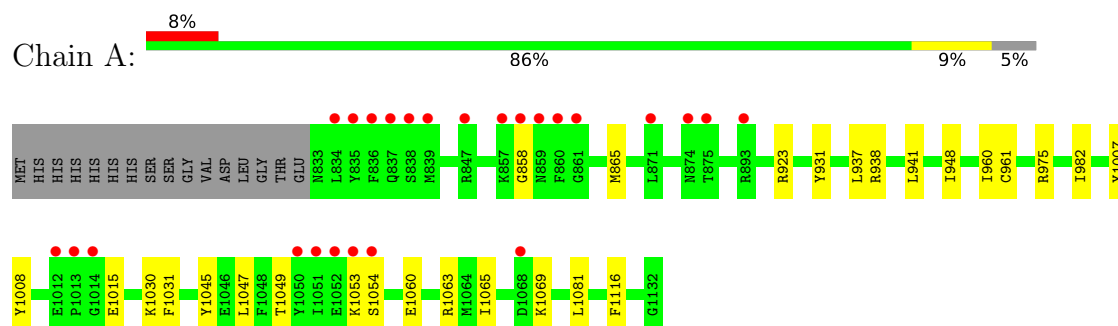
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	242	Total	O	0	11
			253	253		
4	B	239	Total	O	0	7
			246	246		

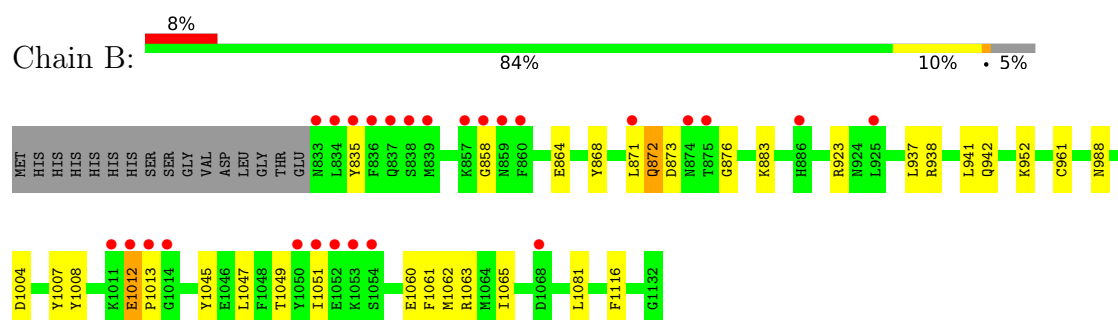
3 Residue-property plots [i](#)

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: Tyrosine-protein kinase JAK2



• Molecule 1: Tyrosine-protein kinase JAK2



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.53Å 68.88Å 107.96Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	67.14 – 1.40 67.14 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (67.14-1.40) 99.8 (67.14-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.191 , 0.223 0.194 , 0.225	Depositor DCC
R_{free} test set	7078 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10562	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0977e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, DMS, S59

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	0.46	0/2574	0.61	0/3467
1	B	0.45	0/2542	0.62	0/3426
All	All	0.46	0/5116	0.61	0/6893

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	923	ARG	Sidechain
1	B	923	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2519	2487	2512	19	0
1	B	2496	2443	2461	21	0
2	A	29	20	0	0	0
2	B	29	20	0	0	0
3	A	4	6	6	1	0
3	B	4	6	6	1	0
4	A	253	0	0	3	0
4	B	246	0	0	2	0
All	All	5580	4982	4985	40	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 4.

All (40) 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:1061:PHE:O	1:B:1065[B]:ILE:HG23	1.81	0.81
1:B:871:LEU:O	1:B:873:ASP:N	2.22	0.73
1:B:952:LYS:NZ	1:B:988:ASN:OD1	2.26	0.68
1:B:1060:GLU:OE2	1:B:1063:ARG:NH2	2.29	0.61
1:A:1065[B]:ILE:HG22	1:A:1069:LYS:HD2	1.82	0.60
1:A:938:ARG:NH2	4:A:1305:HOH:O	2.38	0.55
1:A:1060:GLU:OE2	1:A:1063:ARG:NH2	2.34	0.54
1:A:975[B]:ARG:HG2	1:A:1031:PHE:CD2	2.44	0.52
1:B:1045:TYR:CZ	1:B:1049[A]:THR:HG21	2.45	0.51
1:B:938:ARG:NH2	4:B:1306:HOH:O	2.44	0.51
1:A:1045:TYR:CZ	1:A:1049[A]:THR:HG21	2.47	0.50
1:B:871:LEU:O	1:B:872:GLN:C	2.55	0.50
1:A:941:LEU:HD11	1:A:1047:LEU:HD23	1.92	0.49
1:B:961[B]:CYS:SG	1:B:1116:PHE:O	2.70	0.49
1:A:865:MET:HE2	1:A:931:TYR:CZ	2.48	0.49
1:B:864:GLU:OE2	1:B:883:LYS:NZ	2.39	0.47
1:A:937:LEU:HD21	1:A:1047:LEU:HD21	1.97	0.47
1:B:1045:TYR:CE2	1:B:1049[A]:THR:HG21	2.50	0.47
1:A:1081:LEU:C	1:A:1081:LEU:HD23	2.39	0.47
1:B:1012:GLU:N	1:B:1013:PRO:HD3	2.30	0.46
1:B:1045:TYR:O	1:B:1049[A]:THR:HG23	2.16	0.46
1:B:937:LEU:HD21	1:B:1047:LEU:HD21	1.97	0.45
1:A:1045:TYR:CE1	1:A:1049[A]:THR:HG21	2.51	0.45
1:B:942:GLN:CG	1:B:1051:ILE:HB	2.47	0.45
1:B:1062:MET:SD	1:B:1065[B]:ILE:HD11	2.56	0.44
1:B:941:LEU:HD11	1:B:1047:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:ARG:CZ	4:A:1305:HOH:O	2.65	0.44
1:A:1015:GLU:HB3	1:B:835:TYR:HB3	2.00	0.44
1:A:1045:TYR:O	1:A:1049[A]:THR:HG23	2.17	0.44
1:A:1053:LYS:O	1:A:1054:SER:OG	2.26	0.43
1:A:941:LEU:HD23	1:A:948:ILE:HD13	2.01	0.43
1:B:1081:LEU:C	1:B:1081:LEU:HD23	2.44	0.43
1:A:961[B]:CYS:SG	1:A:1116:PHE:O	2.77	0.42
1:B:1004:ASP:OD1	1:B:1004:ASP:N	2.52	0.42
1:A:1030:LYS:NZ	4:A:1312:HOH:O	2.52	0.42
1:B:868:TYR:O	1:B:876:GLY:HA3	2.20	0.41
1:A:858:GLY:CA	3:A:1202:DMS:O	2.69	0.41
1:B:942:GLN:HG2	1:B:1051:ILE:HB	2.03	0.41
3:B:1202:DMS:H12	4:B:1464:HOH:O	2.21	0.40
1:A:960:ILE:CD1	1:A:982[B]:ILE:HD13	2.51	0.40

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	308/316 (98%)	297 (96%)	11 (4%)	0	100	100
1	B	305/316 (96%)	291 (95%)	11 (4%)	3 (1%)	13	2
All	All	613/632 (97%)	588 (96%)	22 (4%)	3 (0%)	25	7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	872	GLN
1	B	858	GLY
1	B	1012	GLU

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	276/286 (96%)	276 (100%)	0	100	100
1	B	272/286 (95%)	272 (100%)	0	100	100
All	All	548/572 (96%)	548 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1067	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	PTR	A	1008	1	15,16,17	1.00	1 (6%)	17,22,24	1.00	2 (11%)
1	PTR	B	1008	1	15,16,17	1.22	1 (6%)	17,22,24	0.69	0
1	PTR	B	1007	1	15,16,17	1.22	1 (6%)	17,22,24	0.55	0
1	PTR	A	1007	1	15,16,17	1.44	1 (6%)	17,22,24	0.53	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
1	PTR	A	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1007	PTR	OH-CZ	-4.63	1.30	1.40
1	B	1007	PTR	OH-CZ	-4.28	1.31	1.40
1	B	1008	PTR	OH-CZ	-4.11	1.31	1.40
1	A	1008	PTR	OH-CZ	-3.53	1.32	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	PTR	P-OH-CZ	2.47	132.68	123.88
1	A	1008	PTR	O2P-P-OH	2.40	112.42	105.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	S59	B	1201	-	29,32,32	3.39	4 (13%)	39,44,44	2.15	8 (20%)
2	S59	A	1201	-	29,32,32	3.35	6 (20%)	39,44,44	1.67	5 (12%)
3	DMS	A	1202	-	3,3,3	0.61	0	3,3,3	0.39	0
3	DMS	B	1202	-	3,3,3	0.66	0	3,3,3	1.04	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	S59	B	1201	-	-	0/16/16/16	0/4/4/4
2	S59	A	1201	-	-	0/16/16/16	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	S59	C29-N26	17.07	1.60	1.47
2	A	1201	S59	C29-N26	16.76	1.60	1.47
2	A	1201	S59	C05-C06	2.98	1.43	1.37
2	B	1201	S59	F09-C06	-2.56	1.30	1.36
2	A	1201	S59	C03-C02	2.48	1.58	1.52
2	B	1201	S59	C07-C06	2.40	1.41	1.37
2	B	1201	S59	C08-C03	2.27	1.42	1.39
2	A	1201	S59	C07-C06	2.25	1.41	1.37
2	A	1201	S59	C04-C03	2.17	1.42	1.39
2	A	1201	S59	F09-C06	-2.16	1.31	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	S59	C23-C18-N19	-9.68	116.94	121.26
2	A	1201	S59	C23-C18-N19	-6.51	118.36	121.26
2	A	1201	S59	C07-C06-C05	-3.43	118.30	122.80
2	B	1201	S59	C07-C06-C05	-3.28	118.50	122.80
2	A	1201	S59	C28-N27-N26	3.17	107.54	104.23
2	B	1201	S59	C20-C21-N22	-2.87	118.39	121.96
2	B	1201	S59	C28-N27-N26	2.82	107.17	104.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	S59	C25-N26-N27	-2.36	109.51	111.56
2	B	1201	S59	C05-C04-C03	2.16	123.34	121.18
2	A	1201	S59	C08-C07-C06	2.11	120.54	118.38
2	B	1201	S59	C13-C14-C15	2.10	121.70	118.55
2	A	1201	S59	F09-C06-C05	2.07	121.86	118.55
2	B	1201	S59	C20-N19-C18	2.03	120.11	117.21

There are no chirality outliers.

There are no torsion outliers.

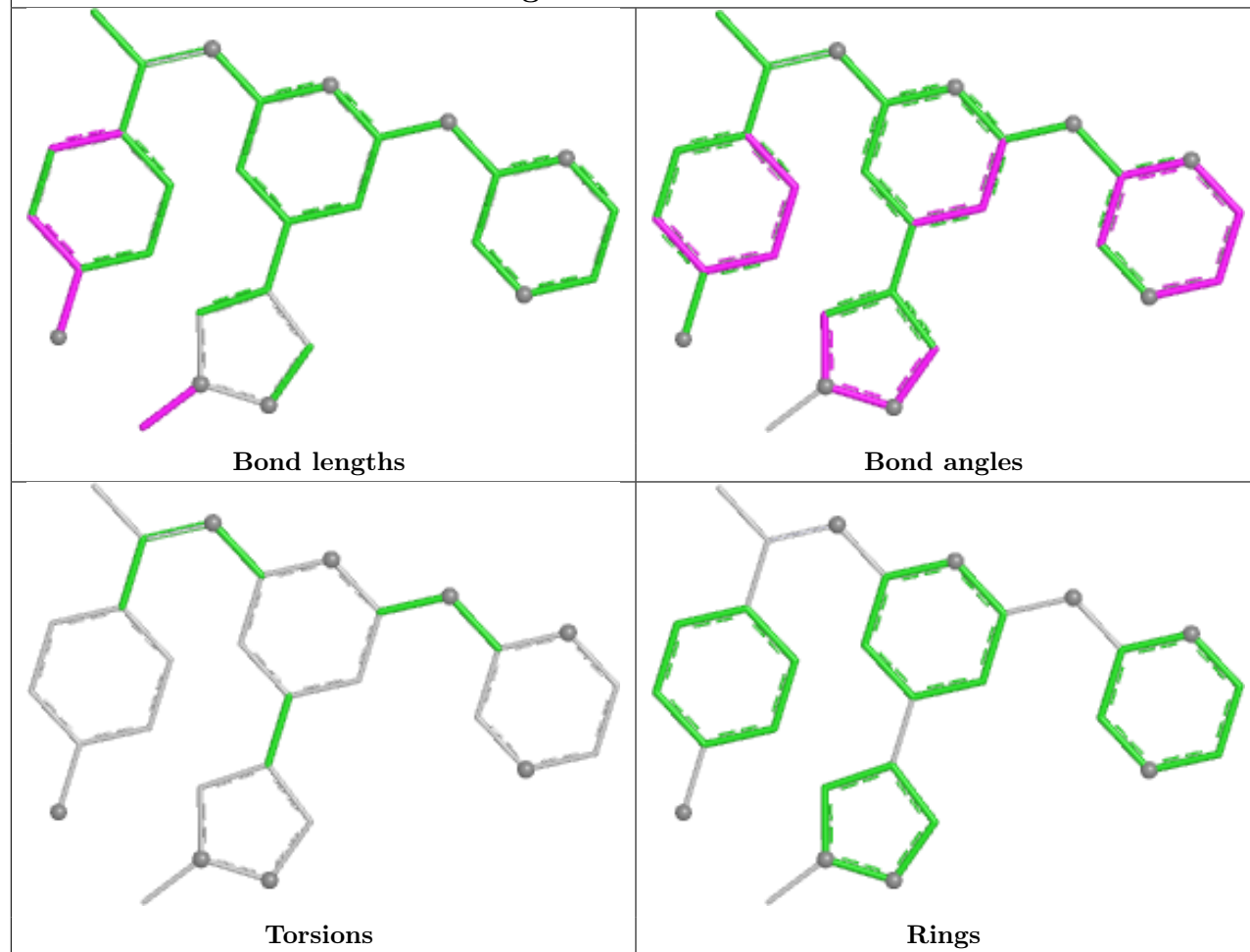
There are no ring outliers.

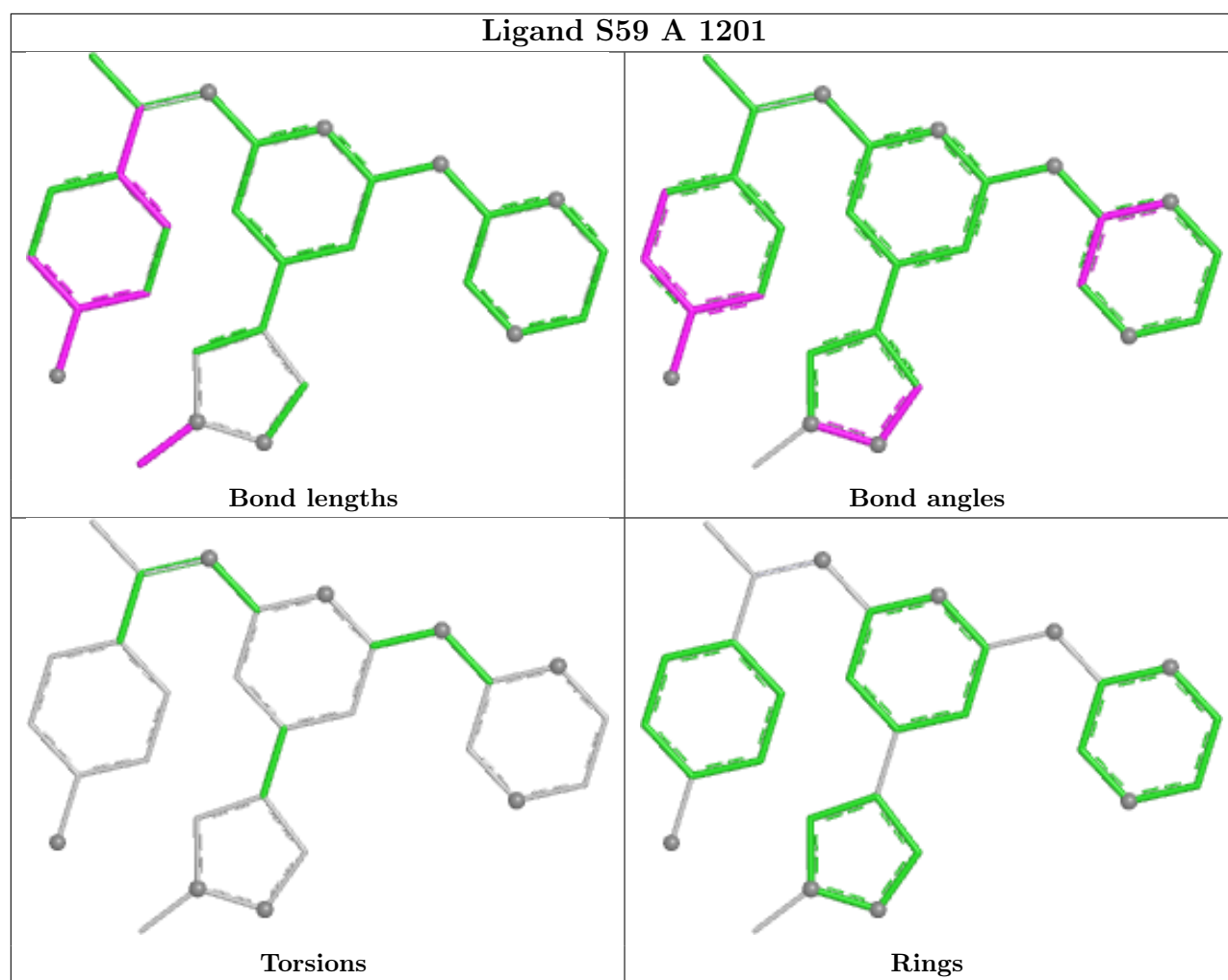
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	DMS	1	0
3	B	1202	DMS	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.

Ligand S59 B 1201





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	298/316 (94%)	0.02	25 (8%)	18 17	8, 20, 54, 71	12 (4%)
1	B	298/316 (94%)	0.00	26 (8%)	17 16	8, 19, 53, 71	9 (3%)
All	All	596/632 (94%)	0.01	51 (8%)	18 17	8, 20, 53, 71	21 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1051	ILE	6.0
1	A	859	ASN	5.6
1	A	1050	TYR	5.2
1	A	1051	ILE	5.1
1	A	1054	SER	5.1
1	B	859	ASN	4.8
1	B	860	PHE	4.7
1	B	1054	SER	4.5
1	A	1013	PRO	4.4
1	A	860	PHE	4.3
1	A	1053	LYS	4.3
1	A	839	MET	4.2
1	B	1013	PRO	4.1
1	B	1050	TYR	4.1
1	A	836	PHE	4.1
1	B	839	MET	4.1
1	B	1053	LYS	3.7
1	A	858	GLY	3.7
1	B	875	THR	3.7
1	B	858	GLY	3.6
1	B	837	GLN	3.5
1	A	834	LEU	3.4
1	A	875	THR	3.4
1	A	837	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	893[A]	ARG	3.3
1	A	857	LYS	3.2
1	B	871	LEU	3.1
1	B	834	LEU	3.0
1	B	1012	GLU	3.0
1	B	836	PHE	3.0
1	B	857	LYS	2.9
1	A	871	LEU	2.9
1	B	874	ASN	2.7
1	B	1068	ASP	2.6
1	B	1011	LYS	2.6
1	B	835	TYR	2.6
1	B	833	ASN	2.5
1	A	838	SER	2.5
1	A	1052	GLU	2.5
1	A	835	TYR	2.5
1	A	847	ARG	2.4
1	B	838	SER	2.3
1	A	1012	GLU	2.3
1	A	1014	GLY	2.1
1	B	925	LEU	2.1
1	A	874	ASN	2.1
1	B	1014	GLY	2.1
1	B	1052	GLU	2.1
1	B	886	HIS	2.1
1	A	861	GLY	2.1
1	A	1068	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	1008	16/17	0.93	0.12	17,26,53,57	0
1	PTR	B	1008	16/17	0.93	0.13	18,29,58,61	0
1	PTR	B	1007	16/17	0.95	0.08	18,26,53,55	0
1	PTR	A	1007	16/17	0.96	0.07	17,27,50,53	0

6.3 Carbohydrates [i](#)

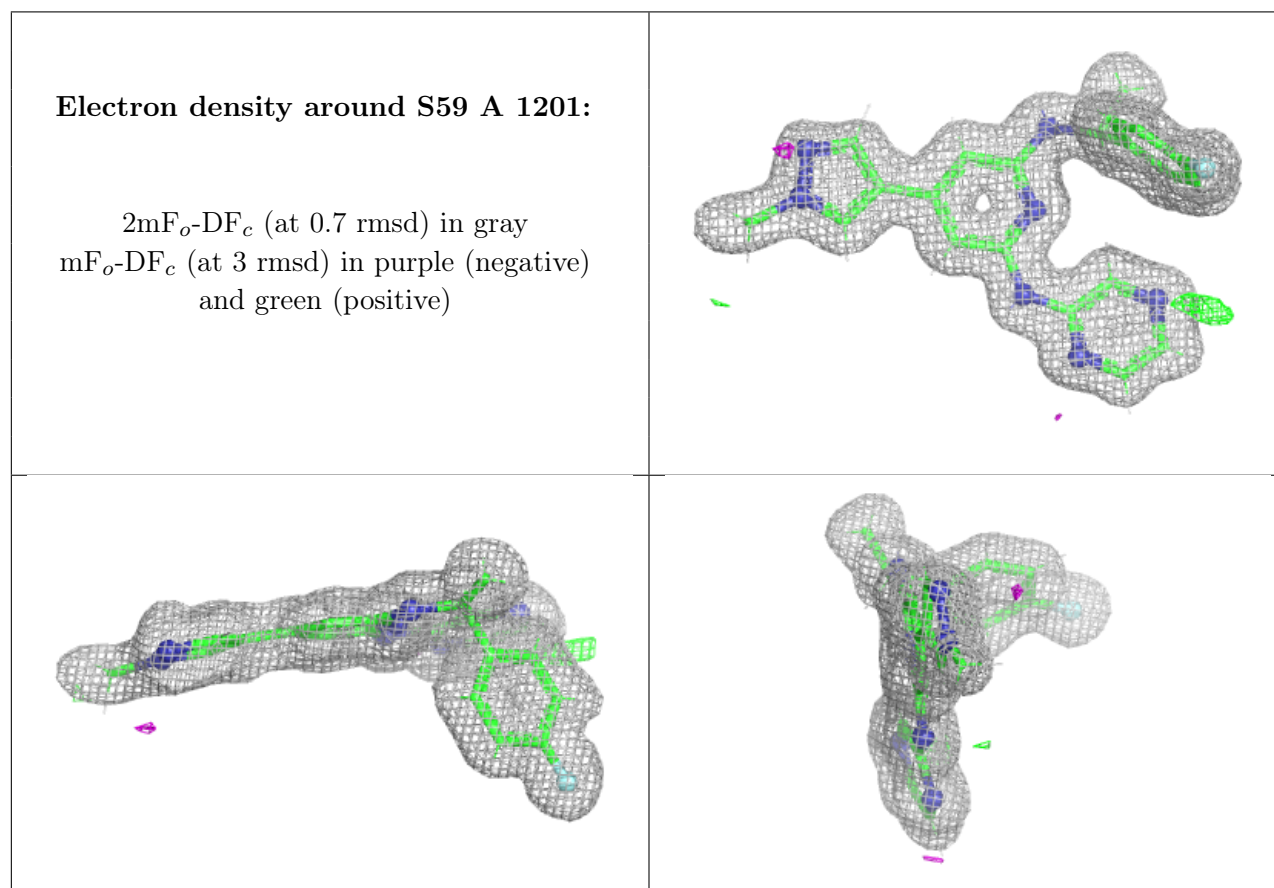
There are no oligosaccharides in this entry.

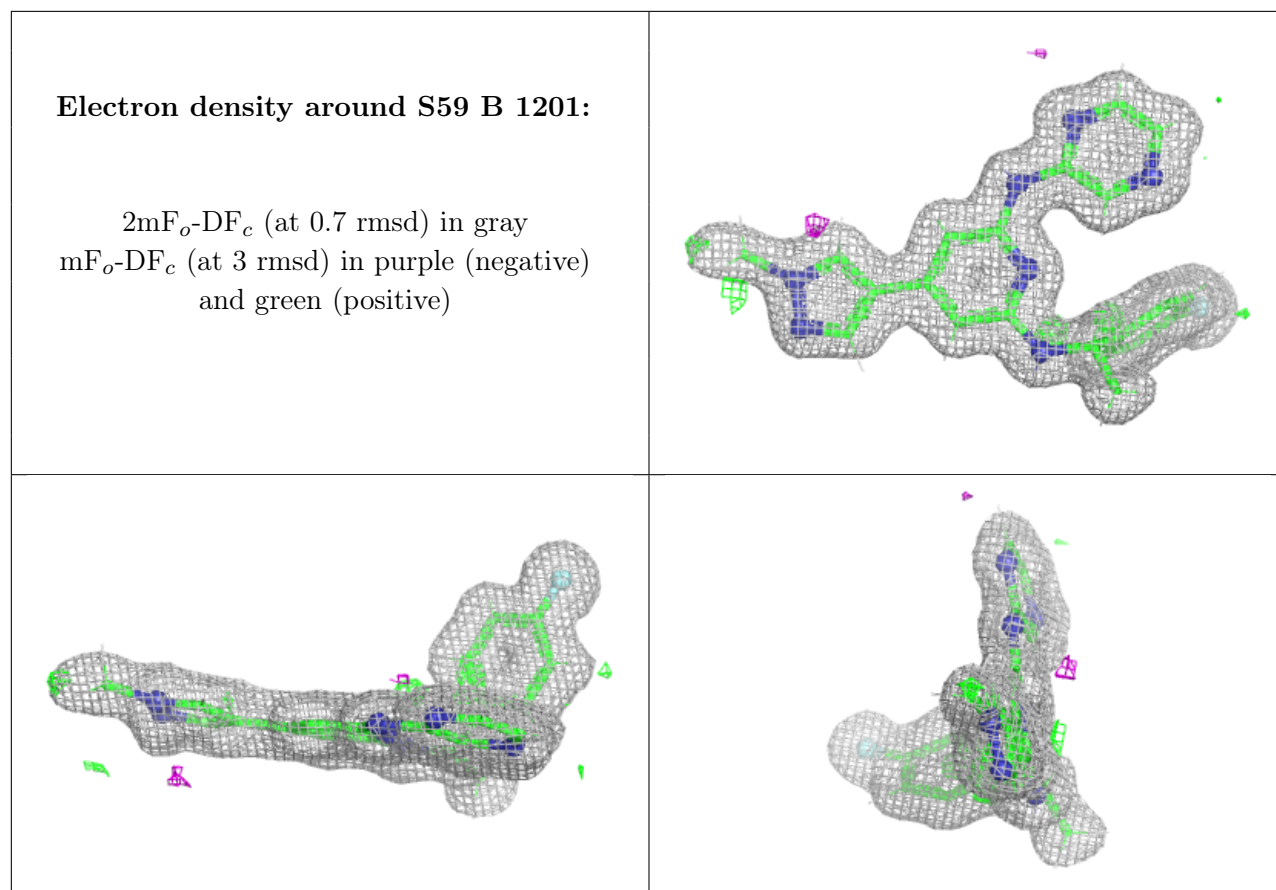
6.4 Ligands [i](#)

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
3	DMS	B	1202	4/4	0.88	0.16	43,56,62,62	0
3	DMS	A	1202	4/4	0.89	0.15	40,48,57,57	0
2	S59	A	1201	29/29	0.98	0.05	11,15,25,29	0
2	S59	B	1201	29/29	0.98	0.05	11,14,27,27	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.