



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 7L9Y / pdb_0000719y
Title : Human PARP14 (ARTD8), catalytic fragment in complex with RBN012042
Authors : Dorsey, B.W.; Swinger, K.K.; Schenkel, L.B.; Church, W.D.; Perl, N.R.; Vasbinder, M.M.; Wigle, T.J.; Kuntz, K.W.
Deposited on : 2021-01-05
Resolution : 2.25 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

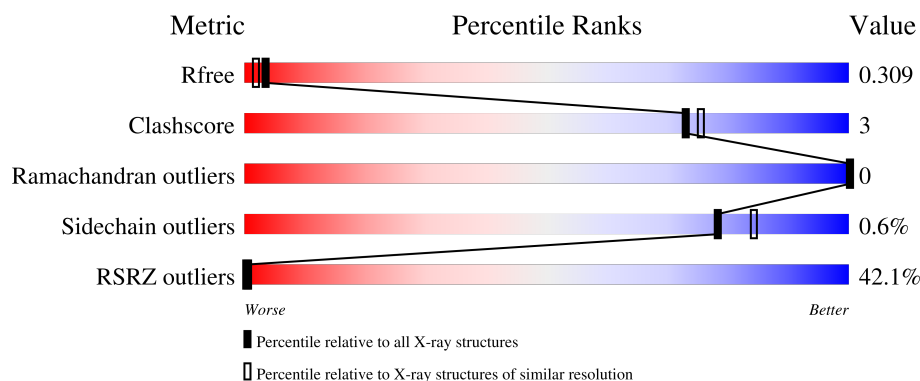
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	194	33% 87% 9% .
1	B	194	47% 88% 8% .
1	C	194	37% 86% 11% .
1	D	194	46% 88% 9% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6292 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.

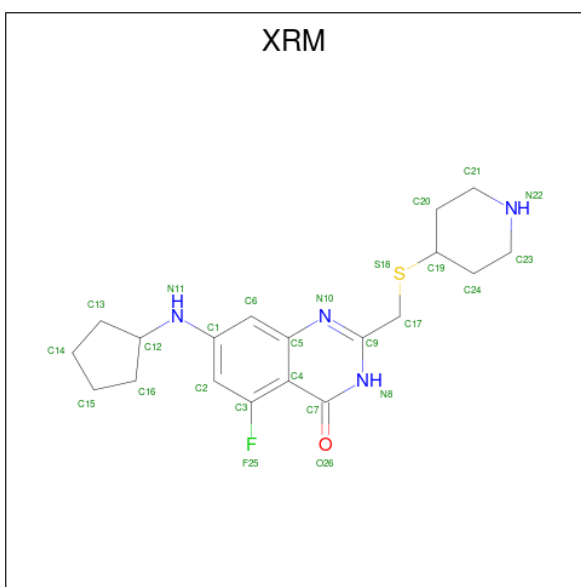
- Molecule 1 is a protein called Protein mono-ADP-ribosyltransferase PARP14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	2	0
			1521	961	268	288	4			
1	B	187	Total	C	N	O	S	0	2	0
			1521	961	268	288	4			
1	C	187	Total	C	N	O	S	0	2	0
			1521	961	268	288	4			
1	D	188	Total	C	N	O	S	0	1	0
			1527	964	270	289	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1608	SER	-	expression tag	UNP Q460N5
A	1609	ASN	-	expression tag	UNP Q460N5
A	1610	ALA	-	expression tag	UNP Q460N5
B	1608	SER	-	expression tag	UNP Q460N5
B	1609	ASN	-	expression tag	UNP Q460N5
B	1610	ALA	-	expression tag	UNP Q460N5
C	1608	SER	-	expression tag	UNP Q460N5
C	1609	ASN	-	expression tag	UNP Q460N5
C	1610	ALA	-	expression tag	UNP Q460N5
D	1608	SER	-	expression tag	UNP Q460N5
D	1609	ASN	-	expression tag	UNP Q460N5
D	1610	ALA	-	expression tag	UNP Q460N5

- Molecule 2 is 7-(cyclopentylamino)-5-fluoro-2-[[piperidin-4-yl)sulfanyl]methyl}quinazolin-4(3H)-one (CCD ID: XRM) (formula: C₁₉H₂₅FN₄OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 19	F 1	N 4	O 1	S 1	0	0
2	B	1	Total 26	C 19	F 1	N 4	O 1	S 1	0	0
2	C	1	Total 26	C 19	F 1	N 4	O 1	S 1	0	0
2	D	1	Total 26	C 19	F 1	N 4	O 1	S 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

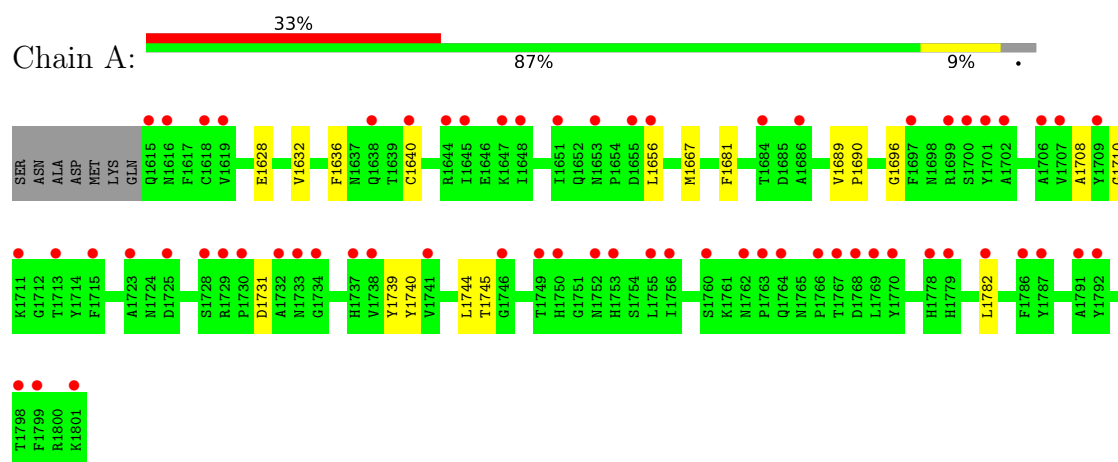
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	20	Total	O	0	0
			20	20		
5	C	16	Total	O	0	0
			16	16		
5	D	18	Total	O	0	0
			18	18		

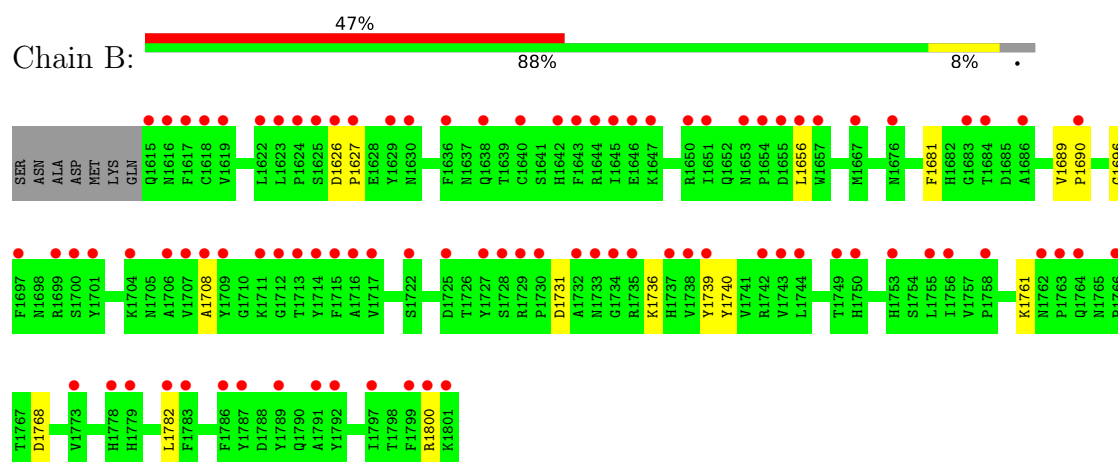
3 Residue-property plots

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.

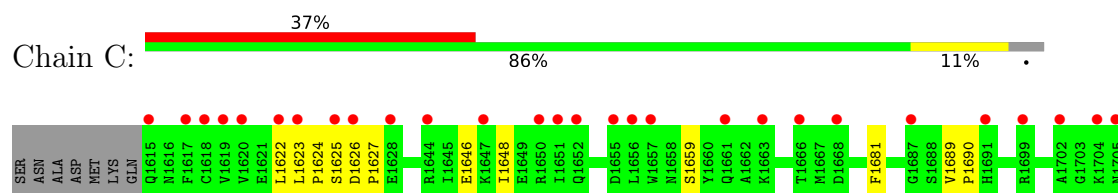
• Molecule 1: Protein mono-ADP-ribosyltransferase PARP14

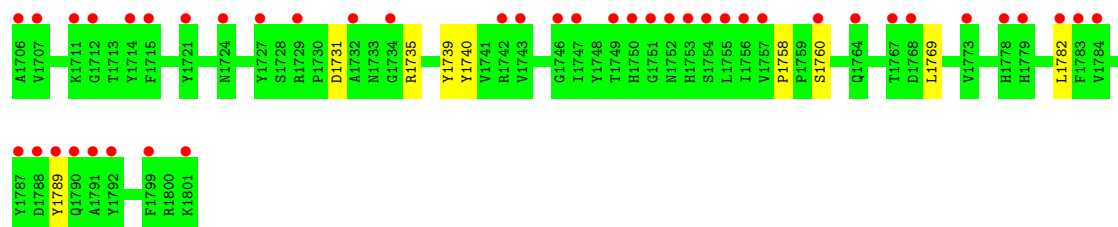


• Molecule 1: Protein mono-ADP-ribosyltransferase PARP14

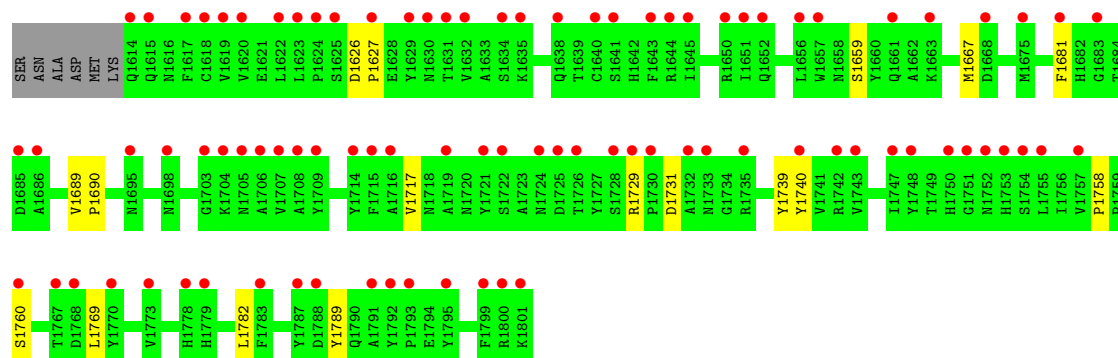
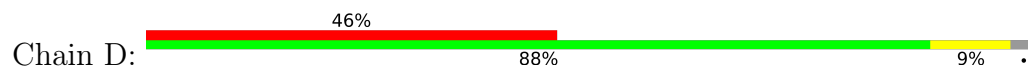


• Molecule 1: Protein mono-ADP-ribosyltransferase PARP14





● Molecule 1: Protein mono-ADP-ribosyltransferase PARP14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.65Å 92.23Å 144.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 2.25 46.16 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.16-2.25) 99.7 (46.16-2.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.266 , 0.298 0.285 , 0.309	Depositor DCC
R_{free} test set	2273 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	1.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 16.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6292	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 40.89 % 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 2.5599e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, XRM

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	1.02	0/1568	1.39	2/2133 (0.1%)
1	B	1.01	0/1568	1.40	1/2133 (0.0%)
1	C	1.01	0/1568	1.36	1/2133 (0.0%)
1	D	1.01	0/1571	1.37	1/2137 (0.0%)
All	All	1.01	0/6275	1.38	5/8536 (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	C	1731	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	1731	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	1731	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	1710	GLY	CA-C-O	-5.24	118.08	122.33
1	B	1731	ASP	CA-CB-CG	5.22	117.82	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	1521	0	1440	9	0
1	B	1521	0	1440	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1521	0	1440	12	0
1	D	1527	0	1443	9	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
2	D	26	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	D	4	0	6	0	0
5	A	23	0	0	0	0
5	B	20	0	0	1	0
5	C	16	0	0	0	0
5	D	18	0	0	0	0
All	All	6292	0	5787	38	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 3.

All (38) 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:1656:LEU:HD21	1:A:1696:GLY:CA	2.32	0.59
1:D:1717:VAL:O	3:D:1902:CL:CL	2.58	0.58
1:C:1624:PRO:O	1:C:1625:SER:OG	2.22	0.51
1:C:1681:PHE:HA	1:C:1739:TYR:O	2.12	0.49
1:C:1659:SER:HB3	1:C:1789:TYR:CG	2.48	0.49
1:D:1681:PHE:HA	1:D:1739:TYR:O	2.13	0.49
1:B:1681:PHE:HA	1:B:1739:TYR:O	2.13	0.49
1:A:1681:PHE:HA	1:A:1739:TYR:O	2.13	0.48
1:D:1758:PRO:O	1:D:1769:LEU:HD22	2.14	0.48
1:D:1659:SER:HB3	1:D:1789:TYR:CG	2.49	0.48
1:D:1782:LEU:C	1:D:1782:LEU:HD12	2.39	0.48
1:A:1782:LEU:C	1:A:1782:LEU:HD12	2.39	0.47
1:C:1622:LEU:HD12	1:C:1648:ILE:HG22	1.96	0.47
1:B:1761:LYS:HD3	1:B:1768:ASP:CG	2.39	0.47
1:C:1782:LEU:HD12	1:C:1782:LEU:C	2.39	0.47
1:B:1782:LEU:C	1:B:1782:LEU:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1656:LEU:HD11	1:B:1696:GLY:N	2.29	0.46
1:A:1667:MET:SD	1:A:1744:LEU:HB3	2.57	0.45
1:B:1689:VAL:N	1:B:1690:PRO:CD	2.80	0.44
1:A:1689:VAL:N	1:A:1690:PRO:CD	2.81	0.44
1:C:1689:VAL:N	1:C:1690:PRO:CD	2.80	0.44
1:C:1623:LEU:O	1:C:1626:ASP:HB2	2.17	0.44
1:B:1736:LYS:HA	5:B:2006:HOH:O	2.18	0.43
1:C:1760:SER:HA	1:C:1769:LEU:HA	2.01	0.43
1:D:1689:VAL:N	1:D:1690:PRO:CD	2.82	0.43
1:D:1760:SER:HA	1:D:1769:LEU:HA	2.00	0.42
1:A:1708:ALA:HB2	1:B:1708:ALA:HA	2.01	0.42
1:C:1646:GLU:OE1	1:C:1735:ARG:NH1	2.53	0.42
1:C:1681:PHE:CE1	1:C:1740:TYR:CD1	3.08	0.42
1:A:1636:PHE:O	1:A:1640:CYS:HB2	2.21	0.41
1:C:1758:PRO:O	1:C:1769:LEU:HG	2.19	0.41
1:A:1628:GLU:O	1:A:1632:VAL:HG23	2.19	0.41
1:C:1626:ASP:O	1:C:1627:PRO:C	2.63	0.41
1:D:1681:PHE:CE1	1:D:1740:TYR:CD1	3.09	0.41
1:A:1681:PHE:CE1	1:A:1740:TYR:CD1	3.09	0.41
1:B:1681:PHE:CE1	1:B:1740:TYR:CD1	3.09	0.40
1:D:1626:ASP:O	1:D:1627:PRO:C	2.63	0.40
1:B:1626:ASP:O	1:B:1627:PRO:C	2.65	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	187/194 (96%)	184 (98%)	3 (2%)	0	100	100
1	B	187/194 (96%)	183 (98%)	4 (2%)	0	100	100
1	C	187/194 (96%)	182 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	187/194 (96%)	183 (98%)	4 (2%)	0	100	100
All	All	748/776 (96%)	732 (98%)	16 (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	166/170 (98%)	165 (99%)	1 (1%)	78	84
1	B	166/170 (98%)	165 (99%)	1 (1%)	78	84
1	C	166/170 (98%)	166 (100%)	0	100	100
1	D	166/170 (98%)	164 (99%)	2 (1%)	63	74
All	All	664/680 (98%)	660 (99%)	4 (1%)	78	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1745	THR
1	B	1800	ARG
1	D	1667	MET
1	D	1729	ARG

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	1724	ASN
1	A	1733	ASN
1	A	1764	GLN
1	B	1724	ASN
1	B	1733	ASN
1	D	1638	GLN
1	D	1652	GLN

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Mol	Chain	Res	Type
1	D	1720	ASN

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](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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	XRM	B	1901	-	27,29,29	0.80	0	30,40,40	1.92	3 (10%)
4	EDO	B	1904	-	3,3,3	0.09	0	2,2,2	0.11	0
2	XRM	A	1901	-	27,29,29	0.91	2 (7%)	30,40,40	1.79	5 (16%)
2	XRM	D	1901	-	27,29,29	0.95	1 (3%)	30,40,40	1.71	5 (16%)
2	XRM	C	1901	-	27,29,29	0.85	1 (3%)	30,40,40	2.05	8 (26%)
4	EDO	B	1903	-	3,3,3	0.16	0	2,2,2	0.12	0
4	EDO	D	1903	-	3,3,3	0.15	0	2,2,2	0.21	0
4	EDO	A	1904	-	3,3,3	0.09	0	2,2,2	0.12	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	XRM	B	1901	-	-	2/7/24/24	0/4/4/4
4	EDO	B	1904	-	-	0/1/1/1	-
2	XRM	A	1901	-	-	1/7/24/24	0/4/4/4
2	XRM	D	1901	-	-	1/7/24/24	0/4/4/4
2	XRM	C	1901	-	-	1/7/24/24	0/4/4/4
4	EDO	B	1903	-	-	1/1/1/1	-
4	EDO	D	1903	-	-	1/1/1/1	-
4	EDO	A	1904	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1901	XRM	C17-S18	3.21	1.84	1.81
2	A	1901	XRM	C17-S18	3.17	1.84	1.81
2	C	1901	XRM	C17-S18	2.63	1.84	1.81
2	A	1901	XRM	C5-N10	-2.07	1.35	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1901	XRM	C17-S18-C19	6.44	113.23	101.75
2	D	1901	XRM	C17-S18-C19	6.24	112.87	101.75
2	B	1901	XRM	C17-S18-C19	6.19	112.78	101.75
2	A	1901	XRM	C17-S18-C19	6.10	112.62	101.75
2	B	1901	XRM	C2-C3-C4	-5.29	118.90	123.96
2	B	1901	XRM	C1-C2-C3	4.54	122.61	118.82
2	C	1901	XRM	C7-N8-C9	-4.16	121.49	123.90
2	A	1901	XRM	C2-C3-C4	-3.76	120.36	123.96
2	C	1901	XRM	C2-C3-C4	-3.13	120.96	123.96
2	D	1901	XRM	C2-C3-C4	-3.10	121.00	123.96
2	C	1901	XRM	C1-C6-C5	2.87	120.93	118.32
2	D	1901	XRM	C1-C2-C3	2.78	121.14	118.82
2	C	1901	XRM	C6-C5-N10	2.72	122.96	118.44
2	C	1901	XRM	C1-C2-C3	2.59	120.98	118.82
2	A	1901	XRM	C7-N8-C9	-2.57	122.42	123.90
2	A	1901	XRM	C23-N22-C21	2.40	117.19	110.40
2	D	1901	XRM	C7-N8-C9	-2.29	122.58	123.90
2	D	1901	XRM	C1-C6-C5	2.27	120.38	118.32
2	C	1901	XRM	C4-C7-N8	2.24	117.56	115.05
2	A	1901	XRM	C23-C24-C19	-2.12	105.10	109.71
2	C	1901	XRM	C2-C1-N11	-2.08	116.11	120.64

There are no chirality outliers.

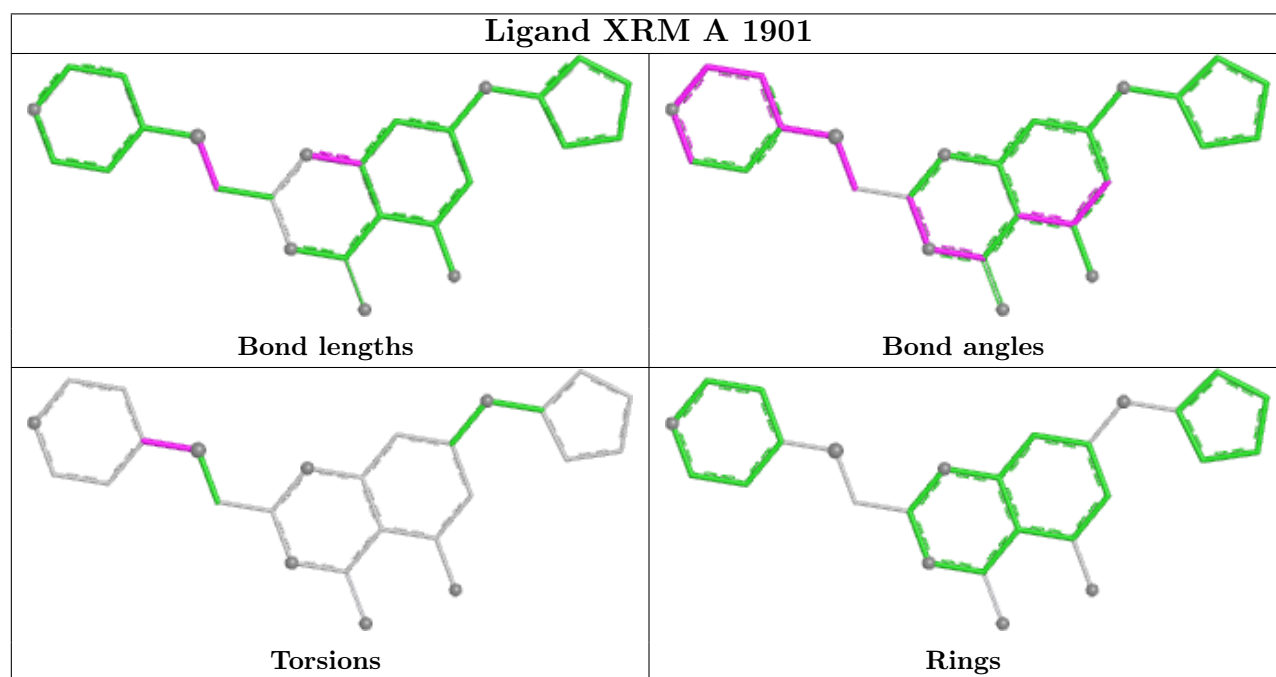
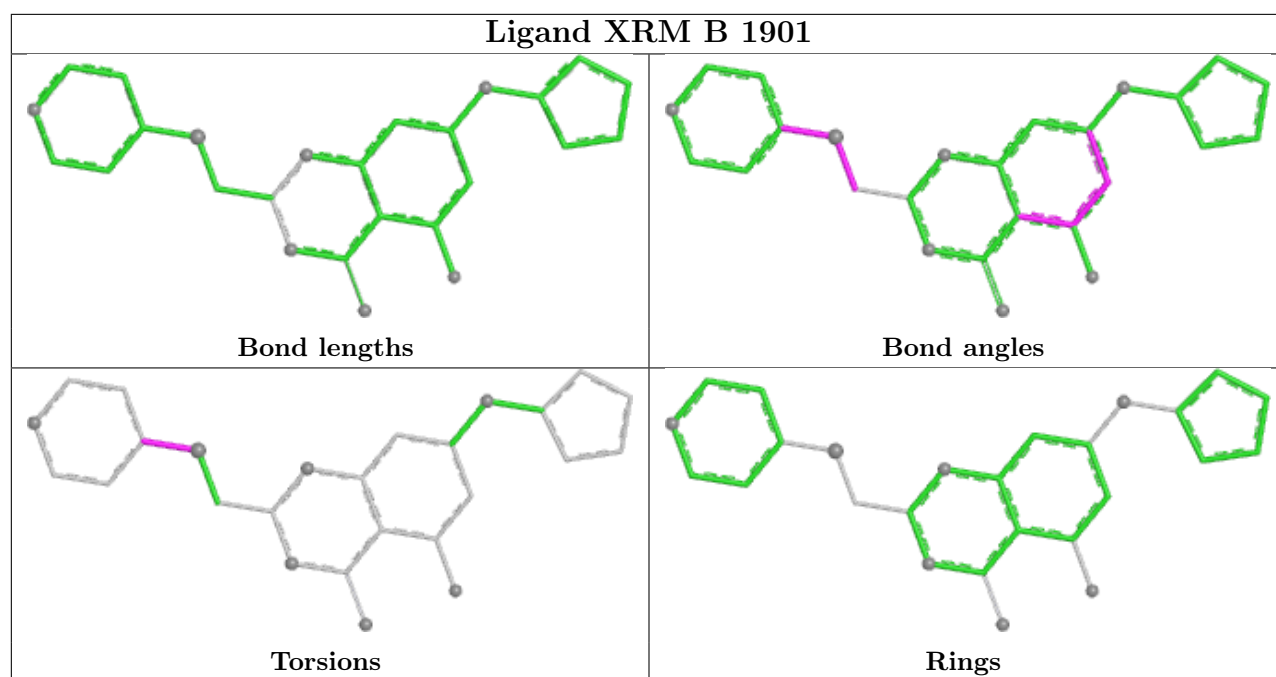
All (8) torsion outliers are listed below:

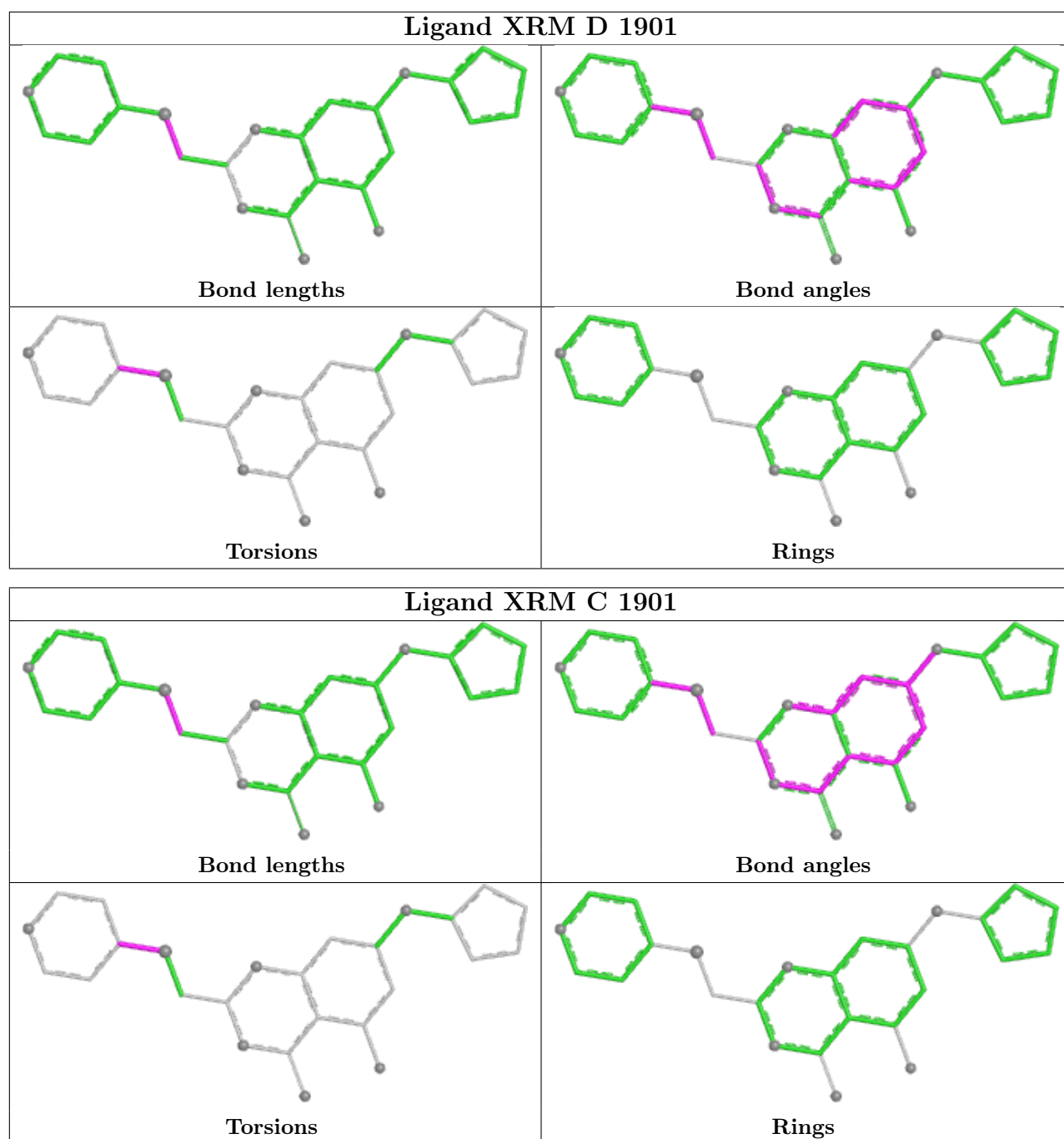
Mol	Chain	Res	Type	Atoms
2	A	1901	XRM	C20-C19-S18-C17
2	B	1901	XRM	C20-C19-S18-C17
2	C	1901	XRM	C20-C19-S18-C17
2	D	1901	XRM	C20-C19-S18-C17
4	B	1903	EDO	O1-C1-C2-O2
4	D	1903	EDO	O1-C1-C2-O2
2	B	1901	XRM	C24-C19-S18-C17
4	A	1904	EDO	O1-C1-C2-O2

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	187/194 (96%)	1.82	64 (34%) 1 0	22, 42, 62, 100	2 (1%)
1	B	187/194 (96%)	2.13	91 (48%) 0 0	22, 45, 78, 96	2 (1%)
1	C	187/194 (96%)	1.89	71 (37%) 1 0	19, 44, 64, 86	2 (1%)
1	D	188/194 (96%)	2.06	89 (47%) 0 0	23, 46, 71, 82	1 (0%)
All	All	749/776 (96%)	1.98	315 (42%) 0 0	19, 44, 71, 100	7 (0%)

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1729	ARG	5.5
1	D	1663	LYS	5.3
1	B	1699	ARG	5.1
1	B	1623	LEU	5.0
1	B	1734	GLY	5.0
1	D	1623	LEU	4.9
1	B	1627	PRO	4.8
1	A	1655	ASP	4.7
1	B	1644	ARG	4.6
1	A	1763	PRO	4.6
1	A	1699	ARG	4.6
1	A	1762	ASN	4.6
1	B	1655	ASP	4.5
1	D	1627	PRO	4.4
1	B	1762	ASN	4.4
1	D	1622	LEU	4.4
1	B	1732	ALA	4.3
1	A	1768	ASP	4.2
1	C	1618	CYS	4.1
1	B	1622	LEU	4.1
1	D	1704	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	1778	HIS	4.0
1	B	1763	PRO	3.9
1	A	1764	GLN	3.9
1	A	1791	ALA	3.9
1	D	1707	VAL	3.9
1	A	1618	CYS	3.9
1	D	1706	ALA	3.9
1	D	1787	TYR	3.8
1	D	1752	ASN	3.8
1	B	1779	HIS	3.8
1	D	1729	ARG	3.7
1	A	1779	HIS	3.7
1	B	1733	ASN	3.7
1	D	1624	PRO	3.7
1	B	1615	GLN	3.6
1	B	1799	PHE	3.6
1	B	1735	ARG	3.6
1	B	1707	VAL	3.6
1	C	1704	LYS	3.6
1	C	1753	HIS	3.6
1	B	1729	ARG	3.6
1	B	1773	VAL	3.6
1	B	1750	HIS	3.6
1	C	1767	THR	3.6
1	B	1645	ILE	3.5
1	D	1651	ILE	3.5
1	B	1684	THR	3.5
1	A	1741	VAL	3.5
1	C	1644	ARG	3.5
1	A	1801	LYS	3.4
1	B	1624	PRO	3.4
1	A	1769	LEU	3.4
1	B	1619	VAL	3.4
1	C	1750	HIS	3.4
1	C	1791	ALA	3.4
1	D	1640	CYS	3.4
1	D	1630	ASN	3.4
1	B	1709	TYR	3.3
1	D	1641	SER	3.3
1	D	1656	LEU	3.2
1	C	1779	HIS	3.2
1	D	1750	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	1787	TYR	3.2
1	C	1789	TYR	3.2
1	D	1644	ARG	3.2
1	D	1801	LYS	3.2
1	A	1615	GLN	3.2
1	A	1729	ARG	3.2
1	C	1752	ASN	3.2
1	B	1618	CYS	3.1
1	A	1686	ALA	3.1
1	D	1788	ASP	3.1
1	D	1795	TYR	3.1
1	D	1652	GLN	3.1
1	B	1801	LYS	3.1
1	D	1634	SER	3.1
1	C	1734	GLY	3.1
1	C	1652	GLN	3.1
1	B	1800	ARG	3.1
1	D	1650	ARG	3.1
1	D	1657	TRP	3.1
1	B	1640	CYS	3.1
1	D	1614	GLN	3.1
1	B	1727	TYR	3.0
1	A	1756	ILE	3.0
1	C	1615	GLN	3.0
1	B	1697	PHE	3.0
1	C	1727	TYR	3.0
1	D	1715	PHE	3.0
1	A	1766	PRO	3.0
1	C	1757	VAL	3.0
1	A	1645	ILE	3.0
1	D	1792	TYR	3.0
1	B	1625	SER	3.0
1	C	1773	VAL	3.0
1	A	1648	ILE	3.0
1	B	1647	LYS	3.0
1	D	1721	TYR	3.0
1	B	1730	PRO	3.0
1	D	1643	PHE	2.9
1	D	1703	GLY	2.9
1	A	1715	PHE	2.9
1	D	1757	VAL	2.9
1	C	1790	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	1756	ILE	2.9
1	D	1645	ILE	2.9
1	B	1766	PRO	2.9
1	A	1786	PHE	2.9
1	C	1801	LYS	2.9
1	C	1705	ASN	2.9
1	C	1792	TYR	2.9
1	B	1778	HIS	2.9
1	B	1706	ALA	2.9
1	C	1661	GLN	2.9
1	D	1716	ALA	2.9
1	B	1728	SER	2.8
1	A	1753	HIS	2.8
1	B	1656	LEU	2.8
1	C	1715	PHE	2.8
1	A	1738	VAL	2.8
1	A	1767	THR	2.8
1	C	1663	LYS	2.8
1	C	1712	GLY	2.8
1	D	1742	ARG	2.8
1	D	1779	HIS	2.8
1	A	1750	HIS	2.8
1	D	1722	SER	2.8
1	D	1778	HIS	2.8
1	C	1721	TYR	2.8
1	D	1755	LEU	2.8
1	C	1706	ALA	2.8
1	A	1778	HIS	2.8
1	D	1631	THR	2.8
1	A	1760	SER	2.8
1	B	1716	ALA	2.8
1	B	1791	ALA	2.8
1	B	1783	PHE	2.8
1	C	1666	THR	2.7
1	D	1760	SER	2.7
1	A	1755	LEU	2.7
1	C	1755	LEU	2.7
1	C	1650	ARG	2.7
1	B	1713	THR	2.7
1	C	1724	ASN	2.7
1	D	1747	ILE	2.7
1	B	1704	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1719	ALA	2.7
1	B	1715	PHE	2.7
1	C	1782	LEU	2.7
1	C	1620	VAL	2.7
1	A	1684	THR	2.7
1	A	1746	GLY	2.6
1	D	1683	GLY	2.6
1	B	1711	LYS	2.6
1	B	1686	ALA	2.6
1	B	1626	ASP	2.6
1	B	1743	VAL	2.6
1	C	1746	GLY	2.6
1	B	1722	SER	2.6
1	C	1617	PHE	2.6
1	A	1792	TYR	2.6
1	B	1792	TYR	2.6
1	C	1707	VAL	2.6
1	D	1709	TYR	2.6
1	D	1793	PRO	2.6
1	A	1651	ILE	2.6
1	B	1756	ILE	2.6
1	C	1764	GLN	2.6
1	A	1701	TYR	2.6
1	B	1642	HIS	2.6
1	D	1618	CYS	2.5
1	D	1705	ASN	2.5
1	A	1730	PRO	2.5
1	B	1643	PHE	2.5
1	D	1799	PHE	2.5
1	D	1773	VAL	2.5
1	D	1748	TYR	2.5
1	B	1782	LEU	2.5
1	A	1640	CYS	2.5
1	B	1630	ASN	2.5
1	A	1734	GLY	2.5
1	B	1749	THR	2.5
1	A	1619	VAL	2.5
1	A	1707	VAL	2.5
1	B	1764	GLN	2.5
1	B	1739	TYR	2.5
1	C	1628	GLU	2.5
1	D	1770	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1706	ALA	2.5
1	C	1788	ASP	2.5
1	C	1687	GLY	2.5
1	D	1783	PHE	2.5
1	C	1651	ILE	2.5
1	C	1768	ASP	2.5
1	D	1791	ALA	2.5
1	B	1786	PHE	2.4
1	C	1783	PHE	2.4
1	B	1657	TRP	2.4
1	B	1667	MET	2.4
1	B	1737	HIS	2.4
1	C	1743	VAL	2.4
1	B	1629	TYR	2.4
1	C	1749	THR	2.4
1	C	1623	LEU	2.4
1	B	1758	PRO	2.4
1	A	1732	ALA	2.4
1	B	1712	GLY	2.4
1	D	1625	SER	2.4
1	C	1619	VAL	2.4
1	D	1619	VAL	2.4
1	C	1656	LEU	2.4
1	A	1616	ASN	2.3
1	A	1709	TYR	2.3
1	B	1616	ASN	2.3
1	B	1701	TYR	2.3
1	D	1725	ASP	2.3
1	C	1751	GLY	2.3
1	D	1708	ALA	2.3
1	A	1700	SER	2.3
1	B	1617	PHE	2.3
1	B	1636	PHE	2.3
1	B	1738	VAL	2.3
1	D	1753	HIS	2.3
1	C	1647	LYS	2.3
1	D	1730	PRO	2.3
1	C	1702	ALA	2.3
1	A	1798	THR	2.3
1	D	1620	VAL	2.3
1	D	1768	ASP	2.3
1	B	1650	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1742	ARG	2.3
1	C	1742	ARG	2.3
1	D	1732	ALA	2.3
1	B	1753	HIS	2.3
1	C	1668	ASP	2.2
1	D	1751	GLY	2.2
1	A	1787	TYR	2.2
1	B	1787	TYR	2.2
1	D	1638	GLN	2.2
1	D	1726	THR	2.2
1	C	1625	SER	2.2
1	C	1711	LYS	2.2
1	A	1782	LEU	2.2
1	C	1622	LEU	2.2
1	A	1697	PHE	2.2
1	D	1617	PHE	2.2
1	B	1654	PRO	2.2
1	B	1638	GLN	2.2
1	D	1635	LYS	2.2
1	D	1767	THR	2.2
1	C	1657	TRP	2.2
1	A	1799	PHE	2.2
1	A	1644	ARG	2.2
1	A	1733	ASN	2.2
1	B	1646	GLU	2.2
1	D	1686	ALA	2.2
1	C	1760	SER	2.2
1	D	1728	SER	2.2
1	C	1714	TYR	2.2
1	D	1714	TYR	2.2
1	D	1740	TYR	2.2
1	D	1632	VAL	2.2
1	D	1733	ASN	2.2
1	B	1690	PRO	2.2
1	A	1737	HIS	2.2
1	B	1683	GLY	2.2
1	A	1749	THR	2.2
1	D	1754	SER	2.2
1	A	1770	TYR	2.1
1	B	1744	LEU	2.1
1	B	1676	ASN	2.1
1	C	1784	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1728	SER	2.1
1	B	1708	ALA	2.1
1	D	1735	ARG	2.1
1	D	1629	TYR	2.1
1	C	1747	ILE	2.1
1	A	1752	ASN	2.1
1	D	1724	ASN	2.1
1	C	1799	PHE	2.1
1	D	1681	PHE	2.1
1	A	1713	THR	2.1
1	C	1699	ARG	2.1
1	A	1723	ALA	2.1
1	A	1653	ASN	2.1
1	B	1714	TYR	2.1
1	D	1698	ASN	2.1
1	A	1638	GLN	2.1
1	D	1615	GLN	2.1
1	D	1661	GLN	2.1
1	B	1700	SER	2.1
1	C	1754	SER	2.1
1	C	1732	ALA	2.1
1	C	1691	HIS	2.1
1	B	1797	ILE	2.1
1	B	1789	TYR	2.1
1	D	1743	VAL	2.1
1	A	1702	ALA	2.0
1	A	1656	LEU	2.0
1	A	1725	ASP	2.0
1	B	1725	ASP	2.0
1	B	1755	LEU	2.0
1	D	1668	ASP	2.0
1	D	1685	ASP	2.0
1	D	1695	ASN	2.0
1	B	1651	ILE	2.0
1	B	1717	VAL	2.0
1	D	1800	ARG	2.0
1	A	1647	LYS	2.0
1	D	1675	MET	2.0
1	B	1653	ASN	2.0
1	C	1626	ASP	2.0
1	C	1655	ASP	2.0
1	A	1711	LYS	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](#)

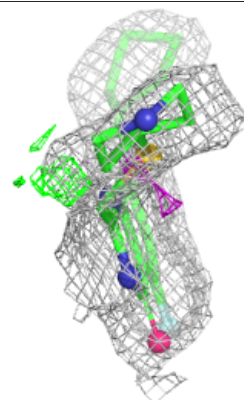
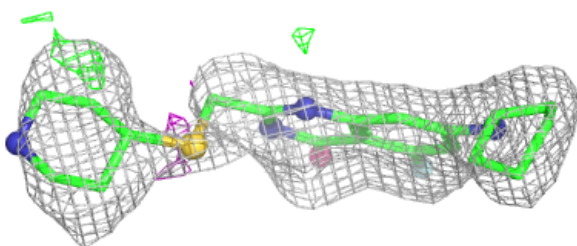
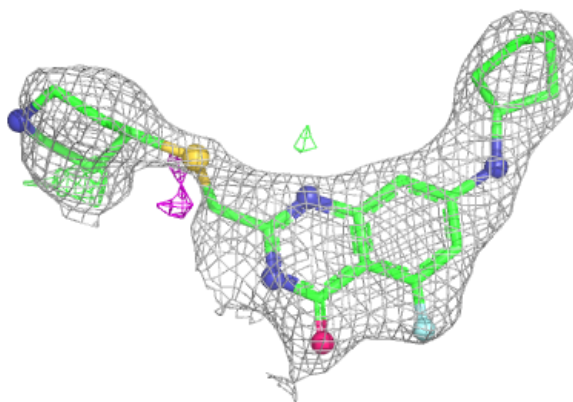
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	A	1904	4/4	0.71	0.24	51,52,54,56	0
4	EDO	B	1904	4/4	0.75	0.21	48,50,51,52	0
2	XRM	C	1901	26/26	0.77	0.21	48,55,73,80	0
4	EDO	B	1903	4/4	0.80	0.23	47,49,51,53	0
2	XRM	D	1901	26/26	0.80	0.23	41,55,83,94	0
4	EDO	D	1903	4/4	0.81	0.20	50,52,53,55	0
2	XRM	A	1901	26/26	0.84	0.15	38,44,61,63	0
2	XRM	B	1901	26/26	0.86	0.15	37,46,66,75	0
3	CL	C	1902	1/1	0.86	0.11	53,53,53,53	0
3	CL	A	1903	1/1	0.90	0.14	51,51,51,51	0
3	CL	A	1902	1/1	0.91	0.11	49,49,49,49	0
3	CL	D	1902	1/1	0.93	0.11	58,58,58,58	0
3	CL	B	1902	1/1	0.94	0.09	46,46,46,46	0

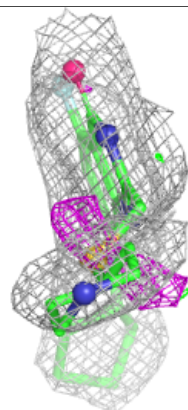
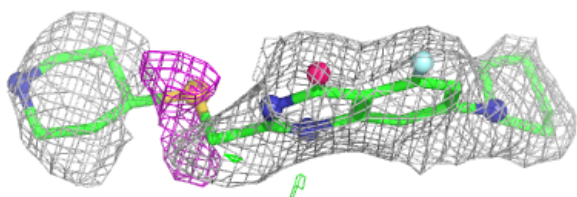
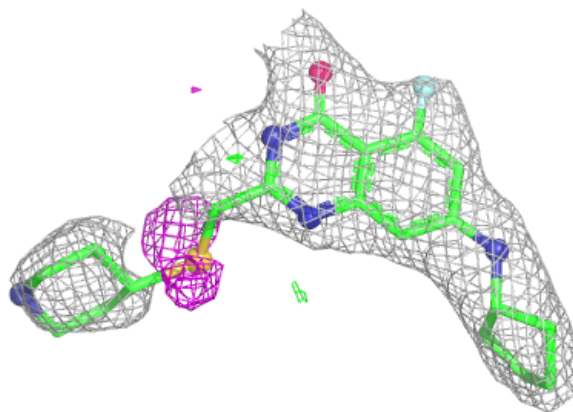
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XRM C 1901:

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

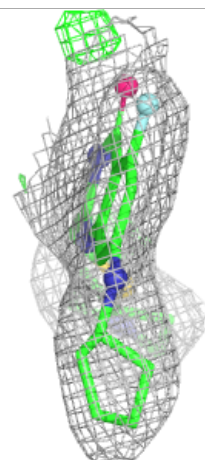
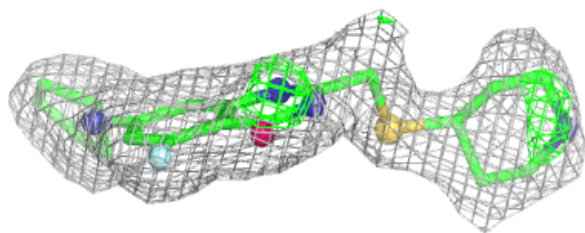
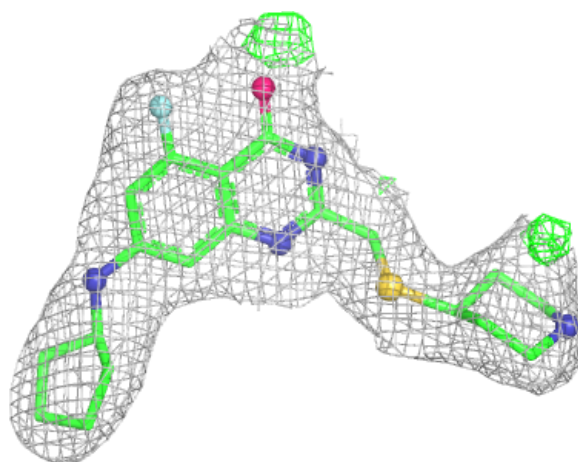
**Electron density around XRM D 1901:**

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



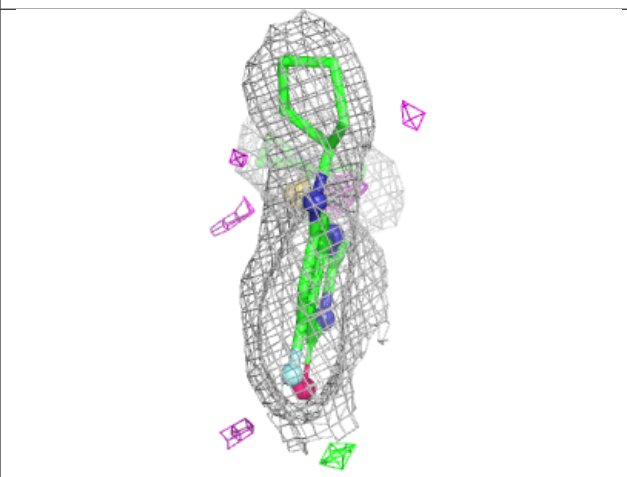
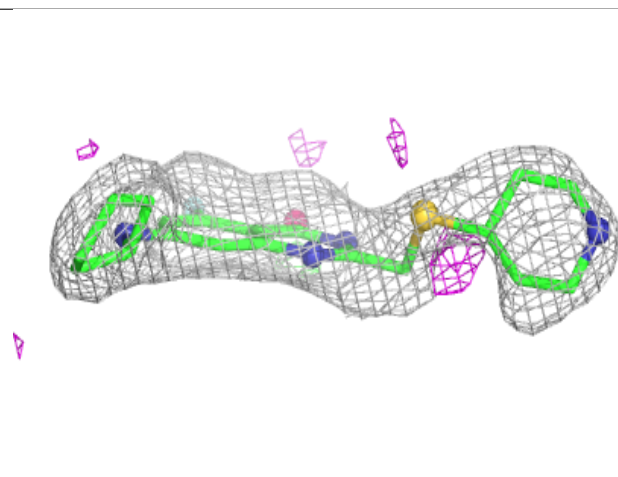
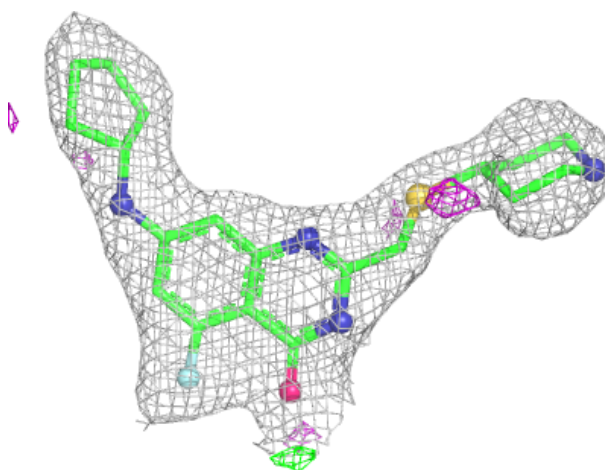
Electron density around XRM A 1901:

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



Electron density around XRM B 1901:

$2mF_o-DF_c$ (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.