



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 10:23 AM EDT

PDB ID : 7LUN
Title : Human PARP14 (ARTD8), catalytic fragment in complex with RBN011980
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 : 2021-02-22
Resolution : 2.57 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

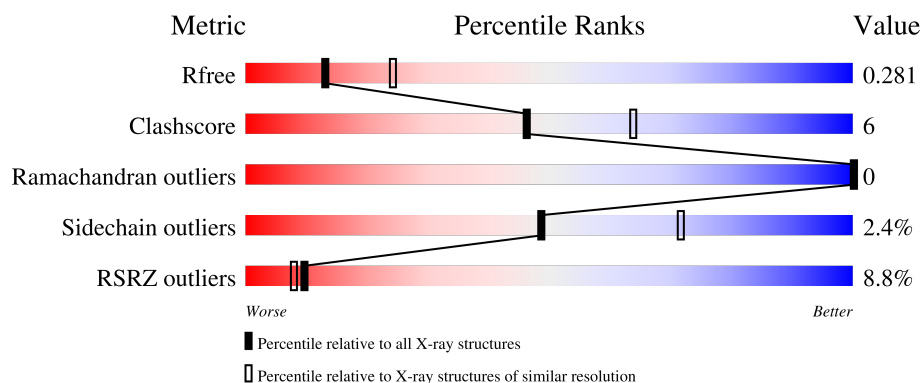
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>..</div> </div>
1	B	194	<div> <div>3%</div> <div>88%</div> <div>7%</div> <div>..</div> </div>
1	C	194	<div> <div>3%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	194	<div> <div>11%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
1	E	194	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	194	<div> <div>14%</div> <div>83%</div> <div>11%</div> <div>• •</div> </div>
1	G	194	<div> <div>15%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	H	194	<div> <div>17%</div> <div>85%</div> <div>11%</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
4	GOL	F	1902	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12718 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	186	Total	C	N	O	S	0	1	0
			1510	956	267	283	4			
1	B	186	Total	C	N	O	S	0	0	0
			1503	951	265	283	4			
1	C	186	Total	C	N	O	S	0	2	0
			1518	960	269	285	4			
1	D	186	Total	C	N	O	S	0	1	0
			1510	956	267	283	4			
1	E	186	Total	C	N	O	S	0	1	0
			1510	956	267	283	4			
1	F	186	Total	C	N	O	S	0	0	0
			1503	951	265	283	4			
1	G	186	Total	C	N	O	S	0	1	0
			1511	955	267	285	4			
1	H	186	Total	C	N	O	S	0	2	0
			1519	960	269	285	5			

There are 24 discrepancies between the modelled and reference sequences:

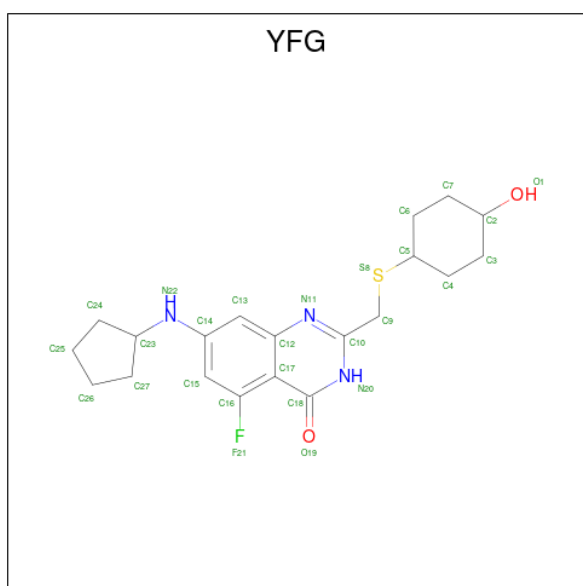
Chain	Residue	Modelled	Actual	Comment	Reference
A	1608	SER	-	expression tag	UNP Q460N5
A	1609	ASN	-	expression tag	UNP Q460N5
A	1610	ALA	-	expression tag	UNP Q460N5
B	1608	SER	-	expression tag	UNP Q460N5
B	1609	ASN	-	expression tag	UNP Q460N5
B	1610	ALA	-	expression tag	UNP Q460N5
C	1608	SER	-	expression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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1609	ASN	-	expression tag	UNP Q460N5
E	1610	ALA	-	expression tag	UNP Q460N5
F	1608	SER	-	expression tag	UNP Q460N5
F	1609	ASN	-	expression tag	UNP Q460N5
F	1610	ALA	-	expression tag	UNP Q460N5
G	1608	SER	-	expression tag	UNP Q460N5
G	1609	ASN	-	expression tag	UNP Q460N5
G	1610	ALA	-	expression tag	UNP Q460N5
H	1608	SER	-	expression tag	UNP Q460N5
H	1609	ASN	-	expression tag	UNP Q460N5
H	1610	ALA	-	expression tag	UNP Q460N5

- Molecule 2 is 7-(cyclopentylamino)-5-fluoro-2-[[[(trans-4-hydroxycyclohexyl)sulfanyl]methyl]quinazolin-4(3H)-one (three-letter code: YFG) (formula: C₂₀H₂₆FN₃O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			27	20	1	3	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			27	20	1	3	2	1		
2	C	1	Total	C	F	N	O	S	0	0
			27	20	1	3	2	1		
2	D	1	Total	C	F	N	O	S	0	0
			27	20	1	3	2	1		
2	E	1	Total	C	F	N	O	S	0	0
			27	20	1	3	2	1		

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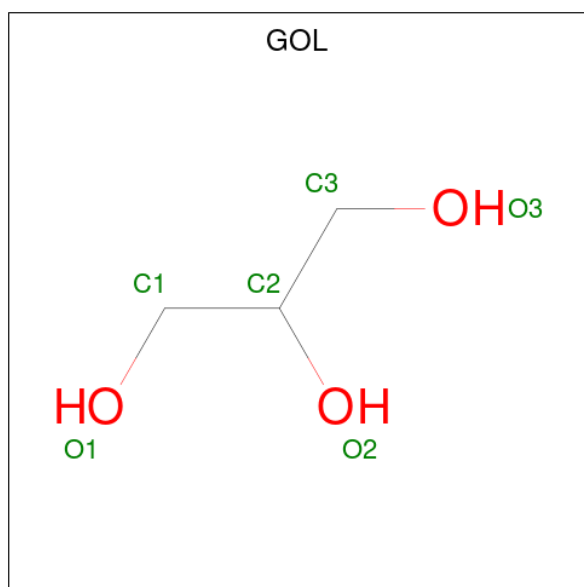
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	F	N	O	S	
			27	20	1	3	2	1	
2	G	1	Total	C	F	N	O	S	
			27	20	1	3	2	1	
2	H	1	Total	C	F	N	O	S	
			27	20	1	3	2	1	

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cl		
			1	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O		
			6	3	3	0	0
4	H	1	Total	C	O		
			6	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O		
			68	68	0	0

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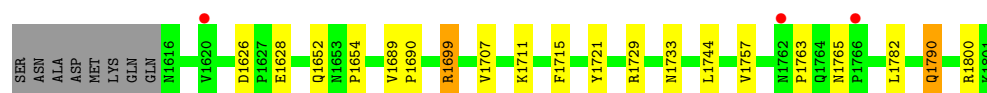
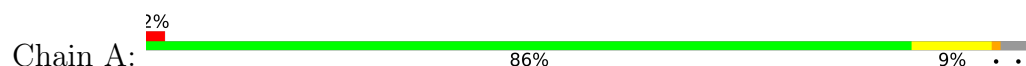
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	52	Total 52	O 52	0	0
5	C	47	Total 47	O 47	0	0
5	D	49	Total 49	O 49	0	0
5	E	53	Total 53	O 53	0	0
5	F	56	Total 56	O 56	0	0
5	G	35	Total 35	O 35	0	0
5	H	45	Total 45	O 45	0	0

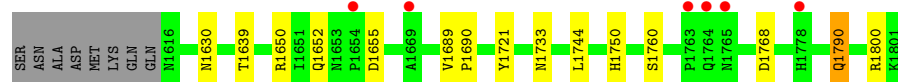
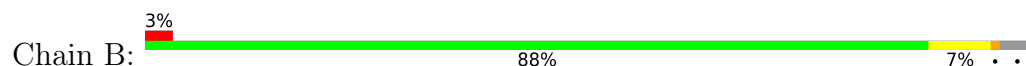
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

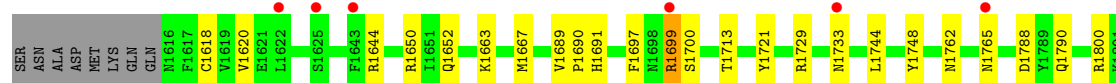
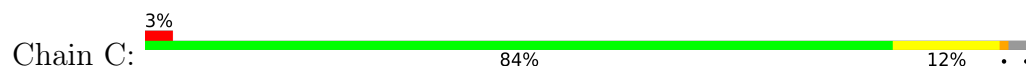
- Molecule 1: Protein mono-ADP-ribosyltransferase PARP14



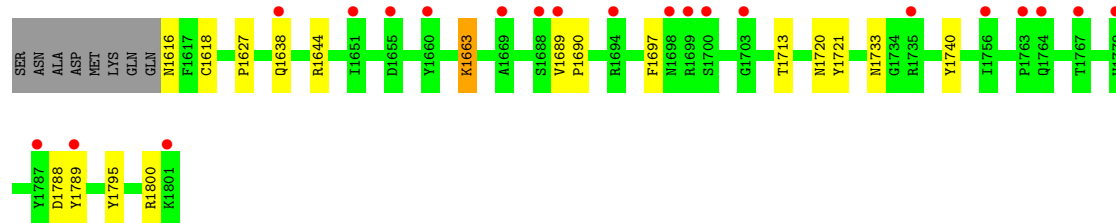
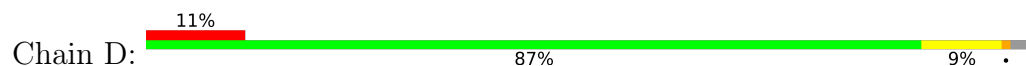
- Molecule 1: Protein mono-ADP-ribosyltransferase PARP14



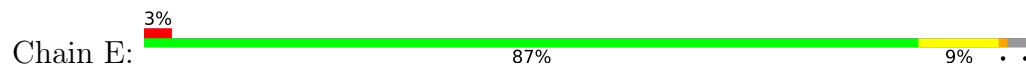
- Molecule 1: Protein mono-ADP-ribosyltransferase PARP14

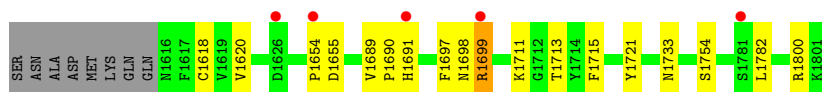


- Molecule 1: Protein mono-ADP-ribosyltransferase PARP14

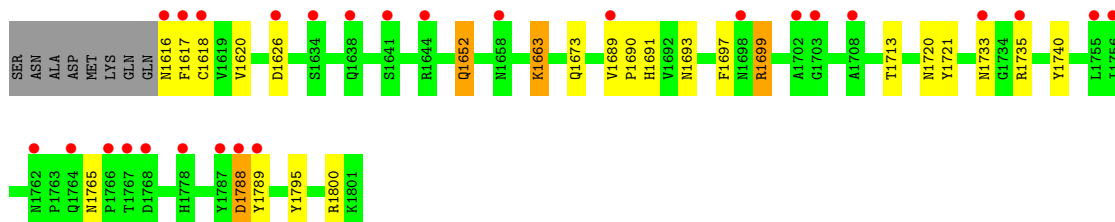
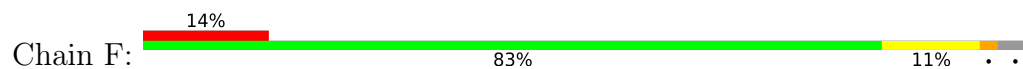


- Molecule 1: Protein mono-ADP-ribosyltransferase PARP14

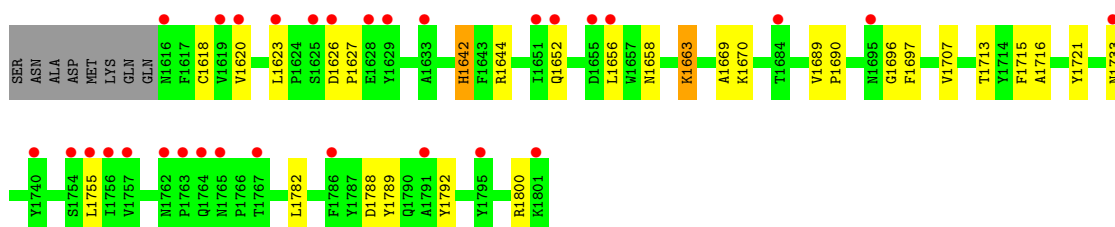
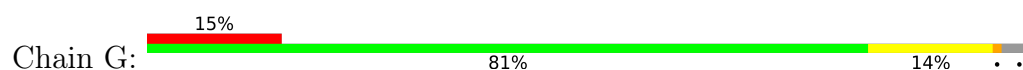




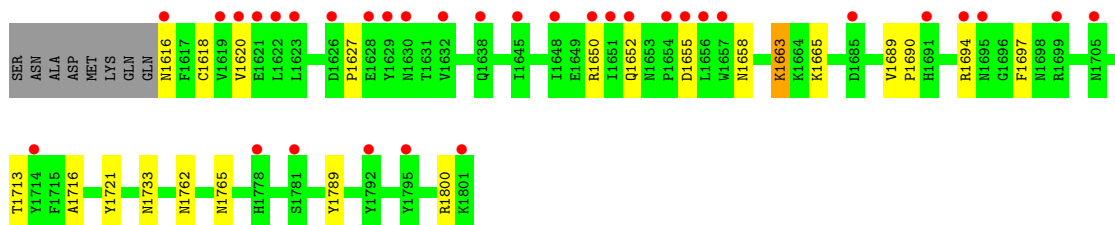
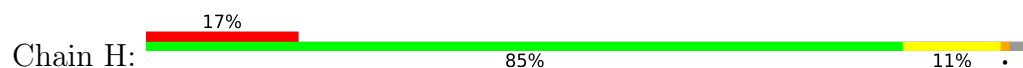
- Molecule 1: Protein mono-ADP-ribosyltransferase PARP14



- 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.99Å 153.66Å 87.46Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	48.53 – 2.57 48.49 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.53-2.57) 99.8 (48.49-2.57)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.232 , 0.278 0.237 , 0.281	Depositor DCC
R_{free} test set	2765 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12718	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	0/1558	0.88	0/2120
1	B	0.76	0/1547	0.85	0/2105
1	C	0.71	0/1566	0.86	0/2131
1	D	0.71	0/1558	0.86	0/2120
1	E	0.71	0/1558	0.85	0/2120
1	F	0.71	0/1547	0.87	0/2105
1	G	0.71	0/1555	0.86	0/2116
1	H	0.73	0/1564	0.84	0/2128
All	All	0.72	0/12453	0.86	0/16945

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1510	0	1430	18	0
1	B	1503	0	1423	12	0
1	C	1518	0	1436	24	0
1	D	1510	0	1431	15	0
1	E	1510	0	1431	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1503	0	1424	36	0
1	G	1511	0	1429	35	0
1	H	1519	0	1434	24	0
2	A	27	0	0	0	0
2	B	27	0	0	0	0
2	C	27	0	0	0	0
2	D	27	0	0	0	0
2	E	27	0	0	0	0
2	F	27	0	0	1	0
2	G	27	0	0	1	0
2	H	27	0	0	1	0
3	E	1	0	0	0	0
4	F	6	0	8	6	0
4	H	6	0	8	2	0
5	A	68	0	0	2	0
5	B	52	0	0	3	0
5	C	47	0	0	3	0
5	D	49	0	0	3	0
5	E	53	0	0	2	0
5	F	56	0	0	5	0
5	G	35	0	0	12	0
5	H	45	0	0	7	0
All	All	12718	0	11454	149	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 6.

All (149) 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:C:1765:ASN:HD21	1:F:1765:ASN:ND2	1.59	1.00
1:C:1765:ASN:ND2	1:F:1765:ASN:HD21	1.64	0.94
1:G:1627:PRO:HG3	1:H:1658:ASN:ND2	1.81	0.94
1:B:1750:HIS:HD2	5:B:2046:HOH:O	1.57	0.85
1:C:1765:ASN:HD21	1:F:1765:ASN:HD21	0.85	0.85
1:G:1656:LEU:HD22	1:G:1792:TYR:CD1	2.13	0.84
1:H:1694:ARG:HD2	5:H:2043:HOH:O	1.76	0.84
1:C:1650:ARG:HH21	1:C:1652:GLN:NE2	1.76	0.83
5:B:2042:HOH:O	1:D:1638:GLN:HG2	1.78	0.83
1:F:1652:GLN:HE21	4:F:1902:GOL:C1	1.91	0.82
1:A:1763:PRO:HD2	5:A:2022:HOH:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1627:PRO:HG3	1:H:1658:ASN:HD22	1.46	0.78
1:G:1707:VAL:CG2	5:G:2031:HOH:O	2.32	0.77
1:G:1656:LEU:HD22	1:G:1792:TYR:HD1	1.51	0.74
1:A:1707:VAL:HG12	1:A:1711:LYS:HE3	1.71	0.71
1:G:1663:LYS:HG2	1:G:1789:TYR:CD1	2.25	0.69
1:F:1663:LYS:HG2	1:F:1789:TYR:CD1	2.26	0.69
1:H:1663:LYS:HG2	1:H:1789:TYR:CD1	2.28	0.69
1:C:1650:ARG:HH21	1:C:1652:GLN:HE22	1.41	0.68
1:F:1617:PHE:CE1	1:F:1693:ASN:HB3	2.28	0.68
1:C:1618:CYS:HG	1:D:1618:CYS:HG	1.30	0.67
1:G:1652:GLN:HE22	1:H:1652:GLN:HE22	1.42	0.67
1:D:1663:LYS:HG2	1:D:1789:TYR:CD1	2.30	0.67
1:C:1650:ARG:HE	1:C:1652:GLN:HE21	1.43	0.66
1:G:1707:VAL:HG23	5:G:2031:HOH:O	1.93	0.66
1:E:1754:SER:HA	5:E:2038:HOH:O	1.97	0.65
2:F:1901:YFG:N11	5:F:2001:HOH:O	2.28	0.65
1:F:1617:PHE:CZ	1:F:1693:ASN:CB	2.81	0.64
1:F:1652:GLN:HE21	4:F:1902:GOL:H12	1.61	0.64
1:F:1652:GLN:NE2	4:F:1902:GOL:O2	2.31	0.63
1:B:1733:ASN:OD1	1:H:1690:PRO:HG2	1.98	0.63
1:F:1617:PHE:CZ	1:F:1693:ASN:HB3	2.34	0.62
1:F:1699:ARG:HD3	1:F:1699:ARG:O	1.98	0.62
1:G:1656:LEU:CD2	1:G:1792:TYR:HD1	2.11	0.62
1:F:1626:ASP:HB3	5:F:2020:HOH:O	1.99	0.62
1:C:1699:ARG:HH22	1:C:1788:ASP:N	1.98	0.61
1:A:1699:ARG:NH1	1:C:1699:ARG:HD2	2.16	0.59
1:G:1620:VAL:HG11	5:H:2041:HOH:O	2.03	0.59
1:H:1650:ARG:NH2	5:H:2002:HOH:O	2.36	0.58
1:F:1617:PHE:CZ	1:F:1693:ASN:HB2	2.39	0.58
1:A:1711:LYS:HD2	5:C:2005:HOH:O	2.04	0.57
1:E:1620:VAL:CG2	1:F:1616:ASN:HB2	2.34	0.57
1:A:1757:VAL:CG1	1:C:1699:ARG:HB3	2.36	0.55
1:H:1665:LYS:NZ	5:H:2003:HOH:O	2.39	0.55
1:H:1716:ALA:HB2	2:H:1901:YFG:F21	1.97	0.55
1:F:1691:HIS:HB2	5:F:2047:HOH:O	2.06	0.54
1:G:1669:ALA:C	5:G:2003:HOH:O	2.47	0.53
1:G:1658:ASN:ND2	1:H:1627:PRO:HD2	2.24	0.52
1:G:1620:VAL:HG13	1:H:1618[A]:CYS:SG	2.49	0.52
1:E:1620:VAL:CG2	1:F:1616:ASN:CB	2.88	0.52
1:A:1733:ASN:O	1:A:1800:ARG:NH2	2.44	0.51
1:G:1670:LYS:N	5:G:2003:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1733:ASN:O	1:D:1800:ARG:NH2	2.43	0.51
1:A:1628:GLU:HB2	5:A:2020:HOH:O	2.11	0.51
1:G:1623:LEU:HD11	1:H:1616:ASN:HD22	1.76	0.51
1:F:1663:LYS:HG2	1:F:1789:TYR:CE1	2.46	0.50
1:G:1644:ARG:NH1	5:G:2004:HOH:O	2.44	0.50
1:B:1733:ASN:O	1:B:1800:ARG:NH2	2.43	0.50
1:F:1733:ASN:O	1:F:1800:ARG:NH2	2.45	0.50
1:C:1733:ASN:O	1:C:1800:ARG:NH2	2.45	0.50
1:A:1690:PRO:HG2	1:G:1733:ASN:HD21	1.77	0.50
1:G:1618:CYS:SG	1:H:1620:VAL:HG22	2.51	0.50
1:G:1733:ASN:O	1:G:1800:ARG:NH2	2.45	0.50
1:E:1733:ASN:O	1:E:1800:ARG:NH2	2.45	0.49
1:A:1652:GLN:OE1	1:B:1652:GLN:HB3	2.12	0.49
1:F:1788:ASP:CB	5:F:2028:HOH:O	2.60	0.49
1:G:1689:VAL:HB	1:G:1690:PRO:HD3	1.95	0.49
1:E:1620:VAL:HG21	1:F:1616:ASN:HB2	1.94	0.49
1:E:1699:ARG:NH2	1:E:1711:LYS:O	2.46	0.49
1:D:1689:VAL:HB	1:D:1690:PRO:HD3	1.95	0.49
1:H:1620:VAL:HG11	5:H:2002:HOH:O	2.12	0.49
1:H:1650:ARG:HE	1:H:1652:GLN:NE2	2.11	0.49
1:D:1644:ARG:CD	5:D:2024:HOH:O	2.60	0.49
1:H:1689:VAL:HB	1:H:1690:PRO:HD3	1.94	0.48
1:B:1630:ASN:OD1	1:D:1627:PRO:HA	2.13	0.48
1:C:1699:ARG:HH22	1:C:1788:ASP:H	1.59	0.48
1:E:1618:CYS:SG	1:F:1618:CYS:SG	3.05	0.48
1:F:1689:VAL:HB	1:F:1690:PRO:HD3	1.96	0.48
1:E:1620:VAL:HG22	1:F:1616:ASN:CB	2.43	0.48
1:H:1733:ASN:O	1:H:1800:ARG:NH2	2.47	0.48
1:A:1626:ASP:OD1	1:B:1655:ASP:OD2	2.32	0.48
1:F:1697:PHE:HB3	1:F:1713:THR:HG21	1.96	0.48
1:A:1652:GLN:HB3	1:B:1652:GLN:OE1	2.14	0.47
1:G:1652:GLN:HE22	1:H:1652:GLN:NE2	2.10	0.47
1:F:1652:GLN:HE21	4:F:1902:GOL:H11	1.78	0.47
1:G:1626:ASP:HB3	5:G:2009:HOH:O	2.14	0.47
1:H:1655:ASP:HB2	5:H:2039:HOH:O	2.14	0.47
1:F:1788:ASP:HB3	5:F:2028:HOH:O	2.14	0.47
1:D:1697:PHE:HB3	1:D:1713:THR:HG21	1.98	0.46
1:G:1627:PRO:CD	5:G:2009:HOH:O	2.62	0.46
1:C:1689:VAL:HB	1:C:1690:PRO:HD3	1.97	0.46
1:B:1639:THR:HA	5:B:2043:HOH:O	2.15	0.46
1:G:1652:GLN:NE2	1:H:1652:GLN:HE22	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1697:PHE:HB3	1:G:1713:THR:HG21	1.98	0.45
1:A:1689:VAL:HB	1:A:1690:PRO:HD3	1.98	0.45
1:H:1697:PHE:HB3	1:H:1713:THR:HG21	1.98	0.45
1:E:1620:VAL:HG22	1:F:1616:ASN:HB2	1.97	0.45
1:F:1663:LYS:HG2	1:F:1789:TYR:HD1	1.79	0.45
1:G:1656:LEU:HD11	1:G:1696:GLY:HA3	1.98	0.45
1:G:1707:VAL:HG22	5:G:2031:HOH:O	2.07	0.45
1:F:1663:LYS:CG	1:F:1789:TYR:CD1	3.00	0.45
1:C:1729:ARG:HD2	5:C:2010:HOH:O	2.17	0.45
1:G:1755:LEU:HD22	5:G:2001:HOH:O	2.17	0.45
1:H:1762:ASN:HB3	1:H:1765:ASN:HB3	1.99	0.45
1:D:1663:LYS:HG2	1:D:1789:TYR:CE1	2.51	0.44
1:E:1691[A]:HIS:CE1	1:E:1698:ASN:HD21	2.35	0.44
1:F:1663:LYS:CG	1:F:1789:TYR:HD1	2.30	0.44
1:E:1754:SER:CA	5:E:2038:HOH:O	2.60	0.44
1:C:1650:ARG:NH2	1:C:1652:GLN:NE2	2.57	0.44
1:B:1689:VAL:HB	1:B:1690:PRO:HD3	1.99	0.44
1:D:1644:ARG:HD3	5:D:2024:HOH:O	2.16	0.44
1:G:1656:LEU:HD11	1:G:1696:GLY:CA	2.47	0.44
1:E:1689:VAL:HB	1:E:1690:PRO:HD3	1.98	0.44
1:G:1663:LYS:CG	1:G:1789:TYR:CD1	3.00	0.44
1:C:1748:TYR:CE1	1:F:1673:GLN:HB3	2.53	0.44
1:B:1760:SER:HA	1:B:1768:ASP:O	2.18	0.43
1:D:1663:LYS:CG	1:D:1789:TYR:HD1	2.31	0.43
1:C:1699:ARG:N	1:C:1699:ARG:HD3	2.32	0.43
1:C:1691[B]:HIS:CE1	5:C:2019:HOH:O	2.71	0.43
1:H:1789:TYR:HB3	5:H:2005:HOH:O	2.18	0.43
1:A:1757:VAL:HG11	1:C:1699:ARG:HB3	1.99	0.43
1:A:1757:VAL:HG21	1:C:1700:SER:HA	2.01	0.43
1:C:1620:VAL:HG22	1:D:1616:ASN:HD22	1.83	0.43
1:G:1627:PRO:HD2	5:G:2009:HOH:O	2.18	0.43
1:G:1642:HIS:CD2	1:G:1642:HIS:O	2.71	0.43
1:A:1744:LEU:HB2	1:A:1790:GLN:HG2	2.01	0.43
1:F:1740:TYR:HB3	1:F:1795:TYR:HB2	2.01	0.42
5:G:2014:HOH:O	4:H:1902:GOL:C1	2.66	0.42
1:D:1644:ARG:HD2	5:D:2024:HOH:O	2.18	0.42
1:H:1663:LYS:HG2	1:H:1789:TYR:CE1	2.54	0.42
1:D:1740:TYR:HB3	1:D:1795:TYR:HB2	2.01	0.42
1:E:1697:PHE:HB3	1:E:1713:THR:HG21	2.00	0.42
1:E:1654:PRO:CB	1:F:1620:VAL:HG21	2.50	0.42
1:G:1663:LYS:HG2	1:G:1789:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:VAL:HG12	1:A:1711:LYS:CE	2.47	0.41
1:C:1663:LYS:HE3	1:C:1667:MET:HE2	2.02	0.41
1:G:1715:PHE:O	1:G:1782:LEU:HA	2.21	0.41
1:D:1663:LYS:HG2	1:D:1789:TYR:HD1	1.80	0.41
1:E:1654:PRO:HB2	1:F:1620:VAL:HG21	2.03	0.41
1:C:1744:LEU:HB2	1:C:1790:GLN:HG2	2.01	0.41
1:F:1652:GLN:NE2	4:F:1902:GOL:C1	2.71	0.41
1:E:1715:PHE:O	1:E:1782:LEU:HA	2.21	0.41
1:C:1697:PHE:HB3	1:C:1713:THR:HG21	2.02	0.41
1:F:1652:GLN:NE2	4:F:1902:GOL:C2	2.84	0.41
1:G:1716:ALA:HB2	2:G:1901:YFG:F21	2.11	0.41
1:A:1715:PHE:O	1:A:1782:LEU:HA	2.21	0.40
1:B:1744:LEU:HB2	1:B:1790:GLN:HG2	2.03	0.40
5:G:2014:HOH:O	4:H:1902:GOL:H12	2.21	0.40
1:A:1654:PRO:HG3	1:B:1650:ARG:HD2	2.03	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	185/194 (95%)	180 (97%)	5 (3%)	0	100	100
1	B	184/194 (95%)	179 (97%)	5 (3%)	0	100	100
1	C	186/194 (96%)	182 (98%)	4 (2%)	0	100	100
1	D	185/194 (95%)	179 (97%)	6 (3%)	0	100	100
1	E	185/194 (95%)	181 (98%)	4 (2%)	0	100	100
1	F	184/194 (95%)	179 (97%)	5 (3%)	0	100	100
1	G	185/194 (95%)	180 (97%)	5 (3%)	0	100	100
1	H	186/194 (96%)	180 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1480/1552 (95%)	1440 (97%)	40 (3%)	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	164/170 (96%)	159 (97%)	5 (3%)	41	65
1	B	163/170 (96%)	161 (99%)	2 (1%)	71	86
1	C	165/170 (97%)	161 (98%)	4 (2%)	49	72
1	D	164/170 (96%)	160 (98%)	4 (2%)	49	72
1	E	164/170 (96%)	161 (98%)	3 (2%)	59	78
1	F	163/170 (96%)	156 (96%)	7 (4%)	29	52
1	G	164/170 (96%)	160 (98%)	4 (2%)	49	72
1	H	165/170 (97%)	163 (99%)	2 (1%)	71	86
All	All	1312/1360 (96%)	1281 (98%)	31 (2%)	49	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1699	ARG
1	A	1721	TYR
1	A	1729	ARG
1	A	1765	ASN
1	A	1790	GLN
1	B	1721	TYR
1	B	1790	GLN
1	C	1644	ARG
1	C	1699	ARG
1	C	1721	TYR
1	C	1762	ASN
1	D	1663	LYS

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Mol	Chain	Res	Type
1	D	1720	ASN
1	D	1721	TYR
1	D	1788	ASP
1	E	1655	ASP
1	E	1699	ARG
1	E	1721	TYR
1	F	1652	GLN
1	F	1663	LYS
1	F	1699	ARG
1	F	1720	ASN
1	F	1721	TYR
1	F	1735	ARG
1	F	1788	ASP
1	G	1642	HIS
1	G	1663	LYS
1	G	1721	TYR
1	G	1788	ASP
1	H	1663	LYS
1	H	1721	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1661	GLN
1	A	1764	GLN
1	A	1779	HIS
1	A	1790	GLN
1	B	1750	HIS
1	B	1790	GLN
1	C	1652	GLN
1	C	1679	GLN
1	C	1695	ASN
1	E	1658	ASN
1	E	1679	GLN
1	E	1753	HIS
1	F	1652	GLN
1	F	1661	GLN
1	F	1765	ASN
1	G	1642	HIS
1	G	1661	GLN
1	G	1733	ASN
1	H	1652	GLN

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Mol	Chain	Res	Type
1	H	1658	ASN
1	H	1779	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	YFG	G	1901	-	29,30,30	1.19	2 (6%)	30,42,42	2.54	9 (30%)
2	YFG	H	1901	-	29,30,30	1.58	7 (24%)	30,42,42	3.59	8 (26%)
2	YFG	D	1901	-	29,30,30	1.52	4 (13%)	30,42,42	2.89	10 (33%)
2	YFG	B	1901	-	29,30,30	1.52	6 (20%)	30,42,42	2.88	9 (30%)
2	YFG	A	1901	-	29,30,30	1.41	3 (10%)	30,42,42	2.71	12 (40%)
2	YFG	F	1901	-	29,30,30	1.64	6 (20%)	30,42,42	3.10	10 (33%)
4	GOL	F	1902	-	5,5,5	0.29	0	5,5,5	0.56	0
2	YFG	C	1901	-	29,30,30	1.35	3 (10%)	30,42,42	2.98	11 (36%)
2	YFG	E	1901	-	29,30,30	1.40	3 (10%)	30,42,42	2.83	9 (30%)
4	GOL	H	1902	-	5,5,5	0.19	0	5,5,5	0.42	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	YFG	G	1901	-	-	0/9/26/26	0/4/4/4
2	YFG	H	1901	-	-	1/9/26/26	0/4/4/4
2	YFG	D	1901	-	-	0/9/26/26	0/4/4/4
2	YFG	B	1901	-	-	1/9/26/26	0/4/4/4
2	YFG	A	1901	-	-	0/9/26/26	0/4/4/4
2	YFG	F	1901	-	-	2/9/26/26	0/4/4/4
4	GOL	F	1902	-	-	3/4/4/4	-
2	YFG	C	1901	-	-	0/9/26/26	0/4/4/4
2	YFG	E	1901	-	-	1/9/26/26	0/4/4/4
4	GOL	H	1902	-	-	4/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	YFG	C16-C17	-4.74	1.36	1.42
2	D	1901	YFG	C16-C17	-4.42	1.36	1.42
2	D	1901	YFG	C10-N11	-4.26	1.27	1.33
2	F	1901	YFG	C9-C10	4.25	1.54	1.50
2	C	1901	YFG	C10-N11	-3.91	1.28	1.33
2	E	1901	YFG	C10-N11	-3.69	1.28	1.33
2	H	1901	YFG	C10-N11	-3.45	1.28	1.33
2	H	1901	YFG	F21-C16	3.45	1.42	1.36
2	B	1901	YFG	C10-N11	-3.38	1.28	1.33
2	F	1901	YFG	C9-S8	3.21	1.88	1.81
2	E	1901	YFG	F21-C16	3.04	1.41	1.36
2	C	1901	YFG	C12-N11	-2.98	1.32	1.37
2	B	1901	YFG	C10-N20	2.95	1.37	1.33
2	H	1901	YFG	C15-C16	2.88	1.41	1.36
2	F	1901	YFG	F21-C16	-2.85	1.30	1.36
2	B	1901	YFG	C16-C17	-2.82	1.38	1.42
2	F	1901	YFG	C10-N20	2.75	1.37	1.33
2	H	1901	YFG	C9-C10	2.61	1.53	1.50
2	D	1901	YFG	C13-C12	-2.57	1.37	1.41
2	G	1901	YFG	C9-C10	2.56	1.53	1.50
2	C	1901	YFG	C16-C17	-2.39	1.39	1.42
2	A	1901	YFG	F21-C16	-2.35	1.31	1.36
2	H	1901	YFG	C9-S8	2.35	1.86	1.81
2	G	1901	YFG	C12-N11	-2.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	YFG	C5-S8	2.27	1.87	1.83
2	F	1901	YFG	C18-N20	2.27	1.37	1.33
2	B	1901	YFG	C13-C12	-2.23	1.38	1.41
2	F	1901	YFG	C13-C12	-2.20	1.38	1.41
2	B	1901	YFG	C9-C10	2.19	1.52	1.50
2	D	1901	YFG	C17-C12	-2.19	1.39	1.42
2	E	1901	YFG	C15-C16	2.18	1.39	1.36
2	B	1901	YFG	F21-C16	-2.12	1.32	1.36
2	H	1901	YFG	C12-N11	-2.10	1.34	1.37
2	H	1901	YFG	C27-C23	2.08	1.58	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1901	YFG	C10-N11-C12	12.80	125.22	116.54
2	C	1901	YFG	C17-C18-N20	-11.90	113.53	124.09
2	B	1901	YFG	C17-C18-N20	-11.03	114.31	124.09
2	H	1901	YFG	C15-C16-C17	-9.71	116.53	124.54
2	D	1901	YFG	C17-C18-N20	-9.58	115.59	124.09
2	E	1901	YFG	C15-C16-C17	-8.59	117.45	124.54
2	G	1901	YFG	C10-N11-C12	7.95	121.93	116.54
2	F	1901	YFG	C10-N11-C12	7.63	121.71	116.54
2	A	1901	YFG	C17-C18-N20	-7.62	117.32	124.09
2	F	1901	YFG	C17-C18-N20	-7.44	117.49	124.09
2	F	1901	YFG	F21-C16-C17	6.93	126.08	118.56
2	E	1901	YFG	C17-C18-N20	-6.73	118.11	124.09
2	B	1901	YFG	C10-N11-C12	6.73	121.10	116.54
2	H	1901	YFG	C14-C15-C16	6.00	123.66	118.76
2	F	1901	YFG	C4-C3-C2	-5.91	101.50	111.61
2	D	1901	YFG	C15-C16-C17	-5.87	119.69	124.54
2	A	1901	YFG	C9-S8-C5	5.80	112.03	101.67
2	G	1901	YFG	C15-C16-C17	-5.79	119.77	124.54
2	D	1901	YFG	C9-S8-C5	5.29	111.13	101.67
2	C	1901	YFG	C15-C16-C17	-5.11	120.32	124.54
2	E	1901	YFG	C10-N11-C12	4.90	119.86	116.54
2	G	1901	YFG	C17-C18-N20	-4.82	119.81	124.09
2	H	1901	YFG	F21-C16-C17	4.78	123.75	118.56
2	A	1901	YFG	C10-N11-C12	4.74	119.75	116.54
2	E	1901	YFG	C9-S8-C5	4.43	109.59	101.67
2	A	1901	YFG	C15-C16-C17	-4.33	120.97	124.54
2	H	1901	YFG	C17-C18-N20	-4.29	120.28	124.09
2	D	1901	YFG	C10-N11-C12	4.28	119.44	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1901	YFG	N11-C10-N20	-4.26	120.44	126.06
2	D	1901	YFG	F21-C16-C17	4.20	123.11	118.56
2	E	1901	YFG	F21-C16-C17	4.11	123.02	118.56
2	F	1901	YFG	N11-C10-N20	-4.05	120.72	126.06
2	D	1901	YFG	C14-C15-C16	3.90	121.95	118.76
2	F	1901	YFG	F21-C16-C15	-3.90	111.03	117.70
2	B	1901	YFG	C15-C16-C17	-3.79	121.41	124.54
2	F	1901	YFG	C9-S8-C5	3.68	108.25	101.67
2	C	1901	YFG	C18-C17-C16	-3.65	119.89	125.58
2	E	1901	YFG	N11-C10-N20	-3.62	121.28	126.06
2	C	1901	YFG	F21-C16-C15	3.60	123.86	117.70
2	G	1901	YFG	F21-C16-C17	3.59	122.45	118.56
2	A	1901	YFG	O1-C2-C3	3.59	119.30	110.16
2	C	1901	YFG	C9-S8-C5	3.52	107.96	101.67
2	G	1901	YFG	C9-S8-C5	3.40	107.74	101.67
2	C	1901	YFG	C10-N11-C12	3.37	118.82	116.54
2	A	1901	YFG	C13-C12-N11	3.31	123.76	118.72
2	G	1901	YFG	N11-C10-N20	-3.31	121.69	126.06
2	B	1901	YFG	N11-C10-N20	-3.30	121.70	126.06
2	F	1901	YFG	C27-C23-C24	3.29	109.87	103.34
2	A	1901	YFG	C3-C2-C7	-3.26	103.00	111.20
2	H	1901	YFG	C6-C7-C2	-3.19	106.16	111.61
2	D	1901	YFG	N11-C10-N20	-3.03	122.05	126.06
2	A	1901	YFG	C6-C5-C4	-2.94	103.15	110.73
2	F	1901	YFG	C7-C6-C5	-2.93	104.89	113.34
2	E	1901	YFG	C14-C15-C16	2.86	121.09	118.76
2	A	1901	YFG	C18-C17-C16	-2.79	121.22	125.58
2	D	1901	YFG	C7-C6-C5	-2.77	105.36	113.34
2	C	1901	YFG	C14-C15-C16	2.72	120.98	118.76
2	C	1901	YFG	C27-C23-N22	-2.70	106.00	111.76
2	B	1901	YFG	C3-C2-C7	-2.64	104.56	111.20
2	G	1901	YFG	C7-C6-C5	-2.64	105.73	113.34
2	A	1901	YFG	C14-C15-C16	2.56	120.85	118.76
2	C	1901	YFG	F21-C16-C17	-2.53	115.81	118.56
2	B	1901	YFG	C14-C15-C16	2.53	120.82	118.76
2	B	1901	YFG	F21-C16-C15	2.52	122.02	117.70
2	G	1901	YFG	C4-C3-C2	2.52	115.91	111.61
2	H	1901	YFG	C14-C13-C12	-2.40	117.88	120.50
2	C	1901	YFG	C6-C7-C2	2.32	115.57	111.61
2	A	1901	YFG	C4-C3-C2	2.31	115.55	111.61
2	B	1901	YFG	C6-C7-C2	-2.29	107.70	111.61
2	D	1901	YFG	C4-C3-C2	-2.28	107.71	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	YFG	F21-C16-C15	2.27	121.58	117.70
2	B	1901	YFG	C25-C26-C27	-2.25	98.42	105.99
2	D	1901	YFG	C3-C4-C5	-2.22	106.94	113.34
2	E	1901	YFG	O1-C2-C3	-2.18	104.61	110.16
2	G	1901	YFG	C13-C12-N11	2.05	121.84	118.72
2	C	1901	YFG	C25-C26-C27	-2.04	99.12	105.99
2	F	1901	YFG	C15-C16-C17	-2.02	122.87	124.54
2	E	1901	YFG	C18-C17-C16	-2.01	122.44	125.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1901	YFG	C6-C5-S8-C9
4	F	1902	GOL	O1-C1-C2-O2
4	F	1902	GOL	O1-C1-C2-C3
4	H	1902	GOL	O1-C1-C2-C3
4	H	1902	GOL	C1-C2-C3-O3
4	H	1902	GOL	O2-C2-C3-O3
2	B	1901	YFG	C10-C9-S8-C5
4	F	1902	GOL	O2-C2-C3-O3
2	F	1901	YFG	C6-C5-S8-C9
4	H	1902	GOL	O1-C1-C2-O2
2	F	1901	YFG	C10-C9-S8-C5
2	H	1901	YFG	N20-C10-C9-S8

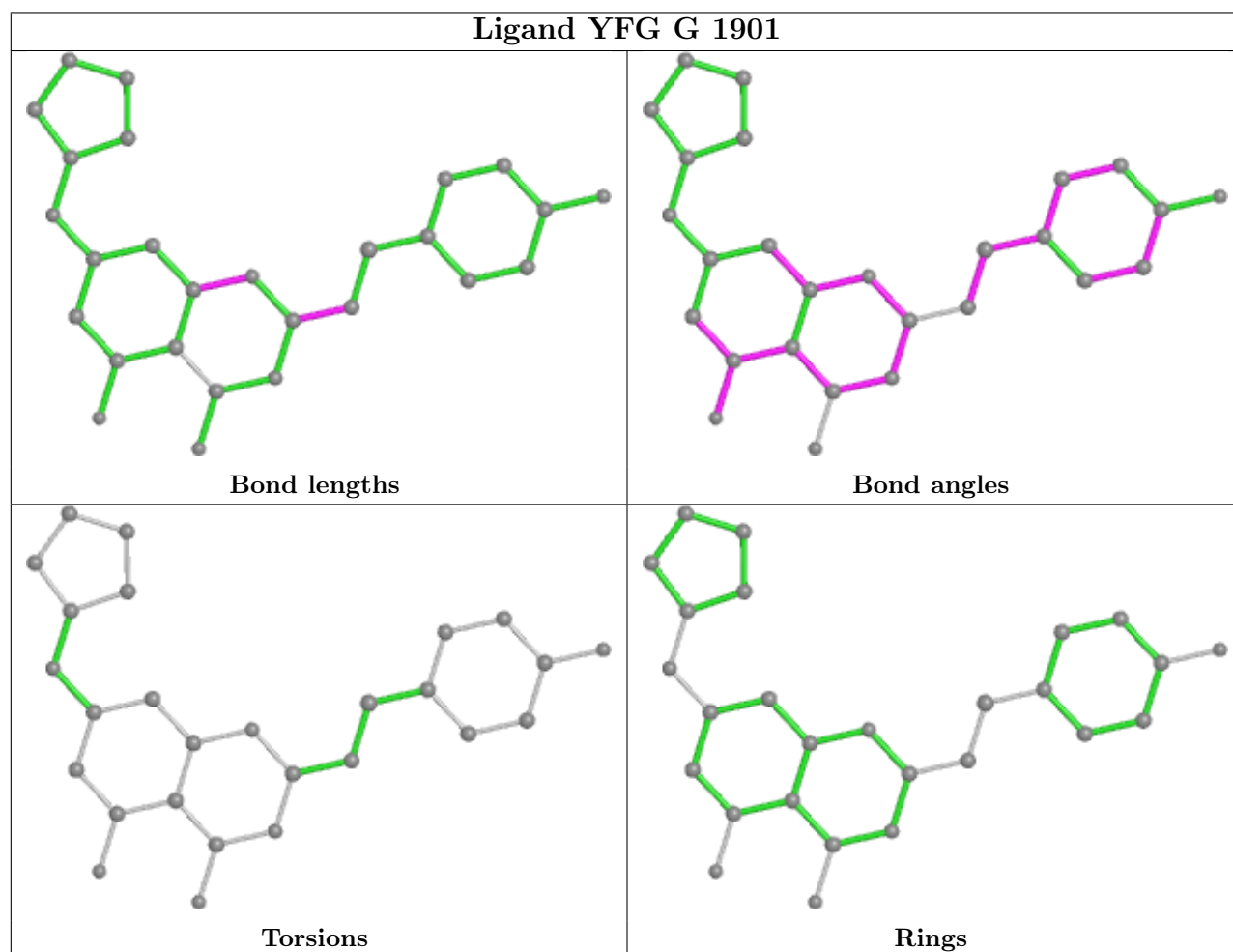
There are no ring outliers.

5 monomers are involved in 11 short contacts:

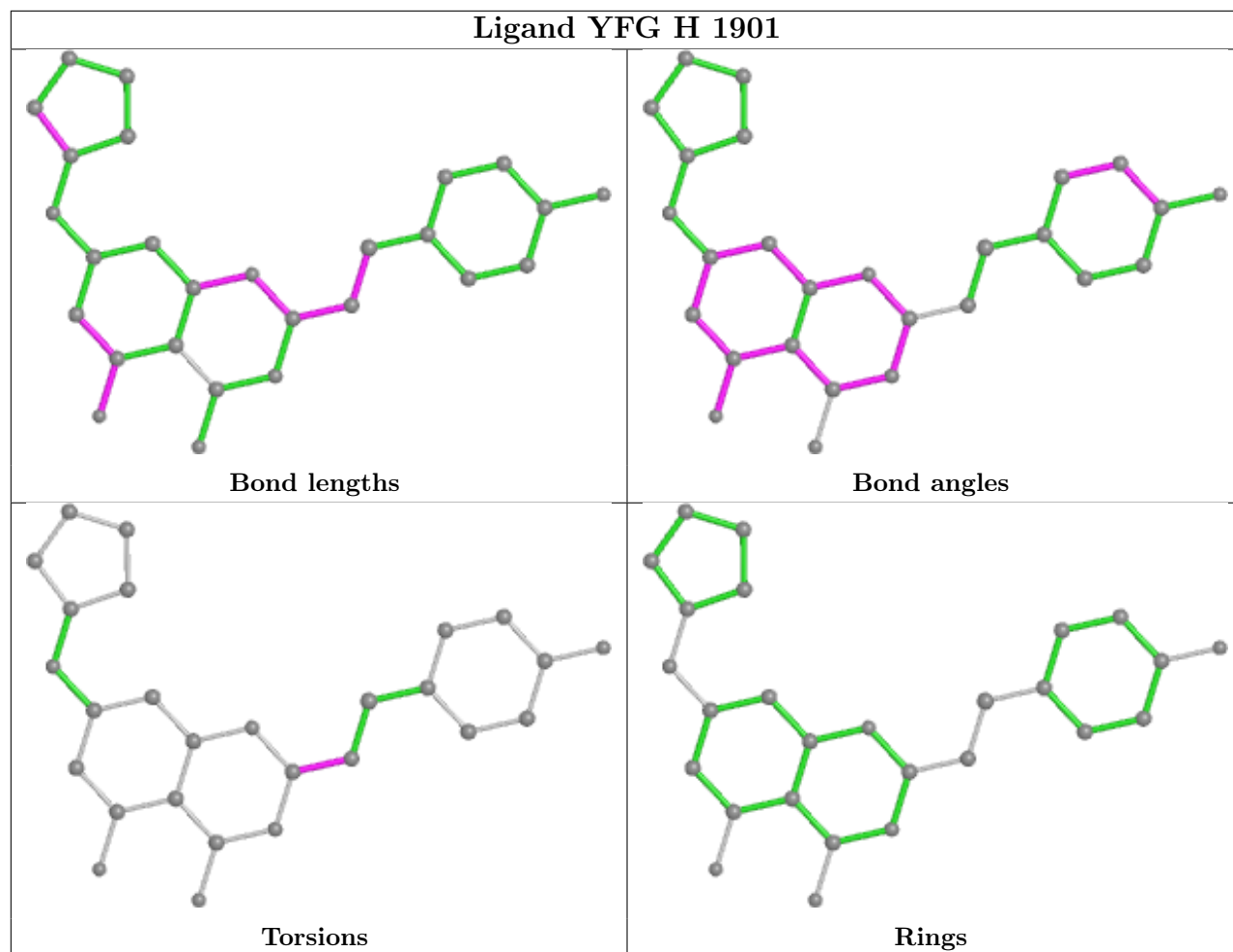
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1901	YFG	1	0
2	H	1901	YFG	1	0
2	F	1901	YFG	1	0
4	F	1902	GOL	6	0
4	H	1902	GOL	2	0

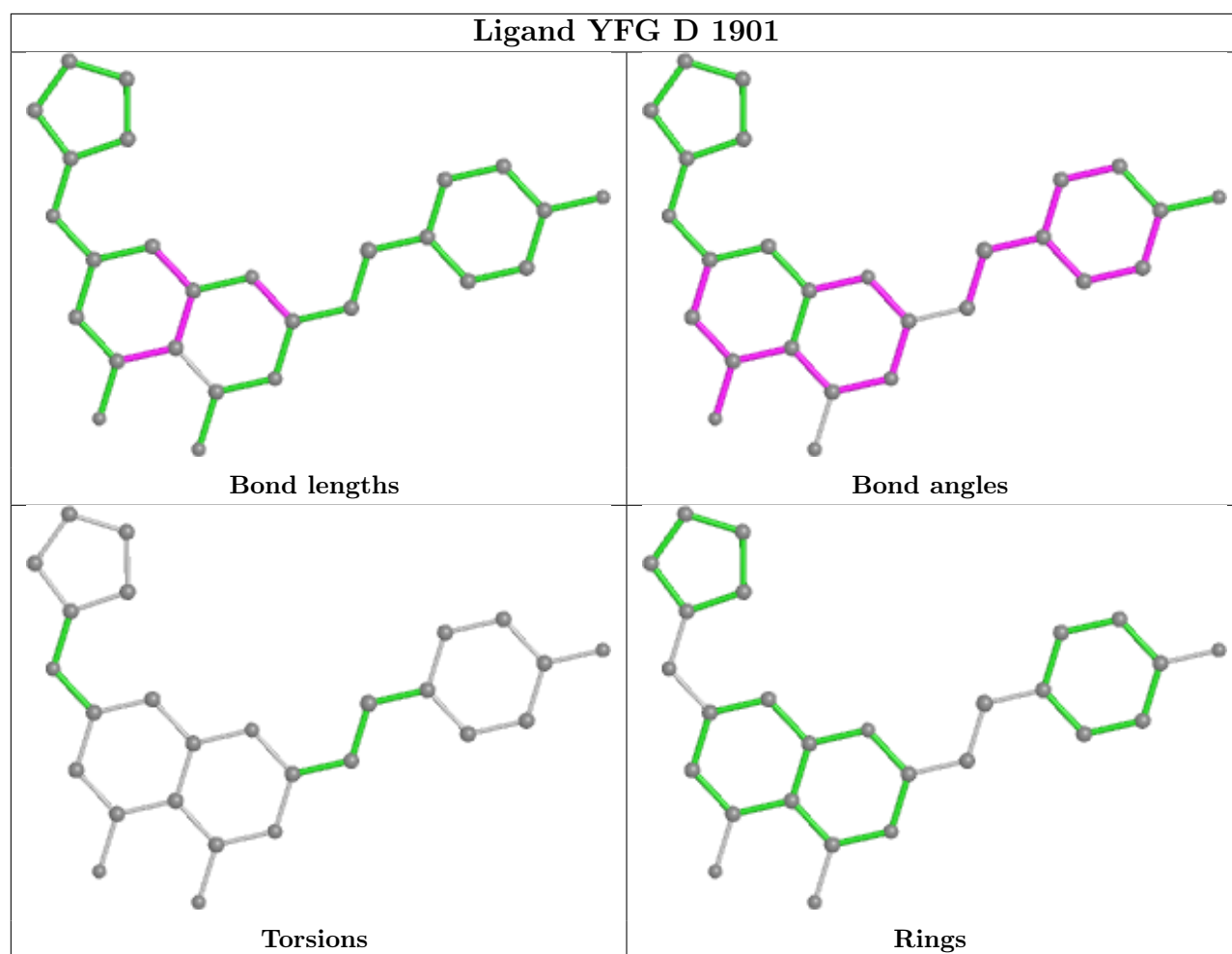
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

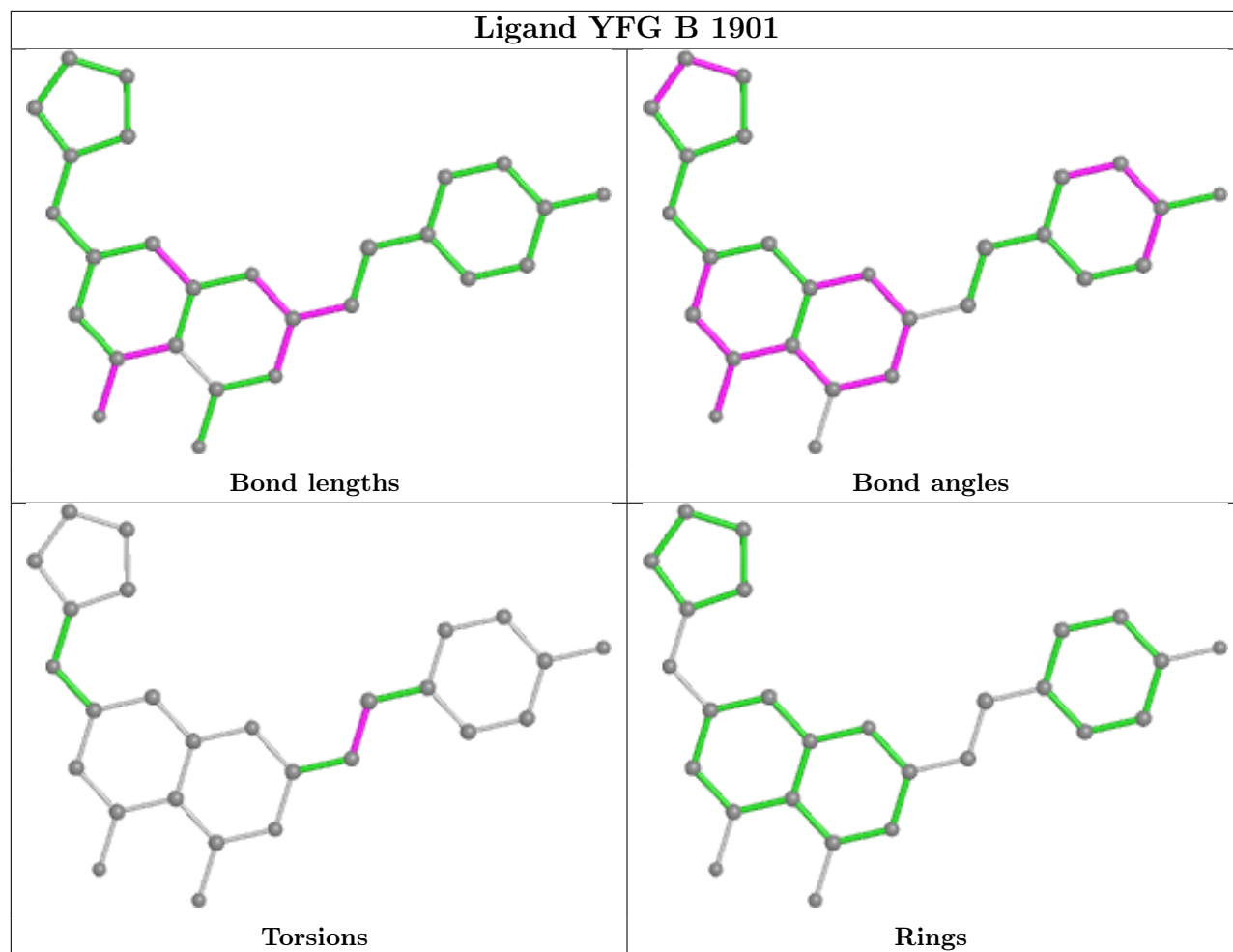
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

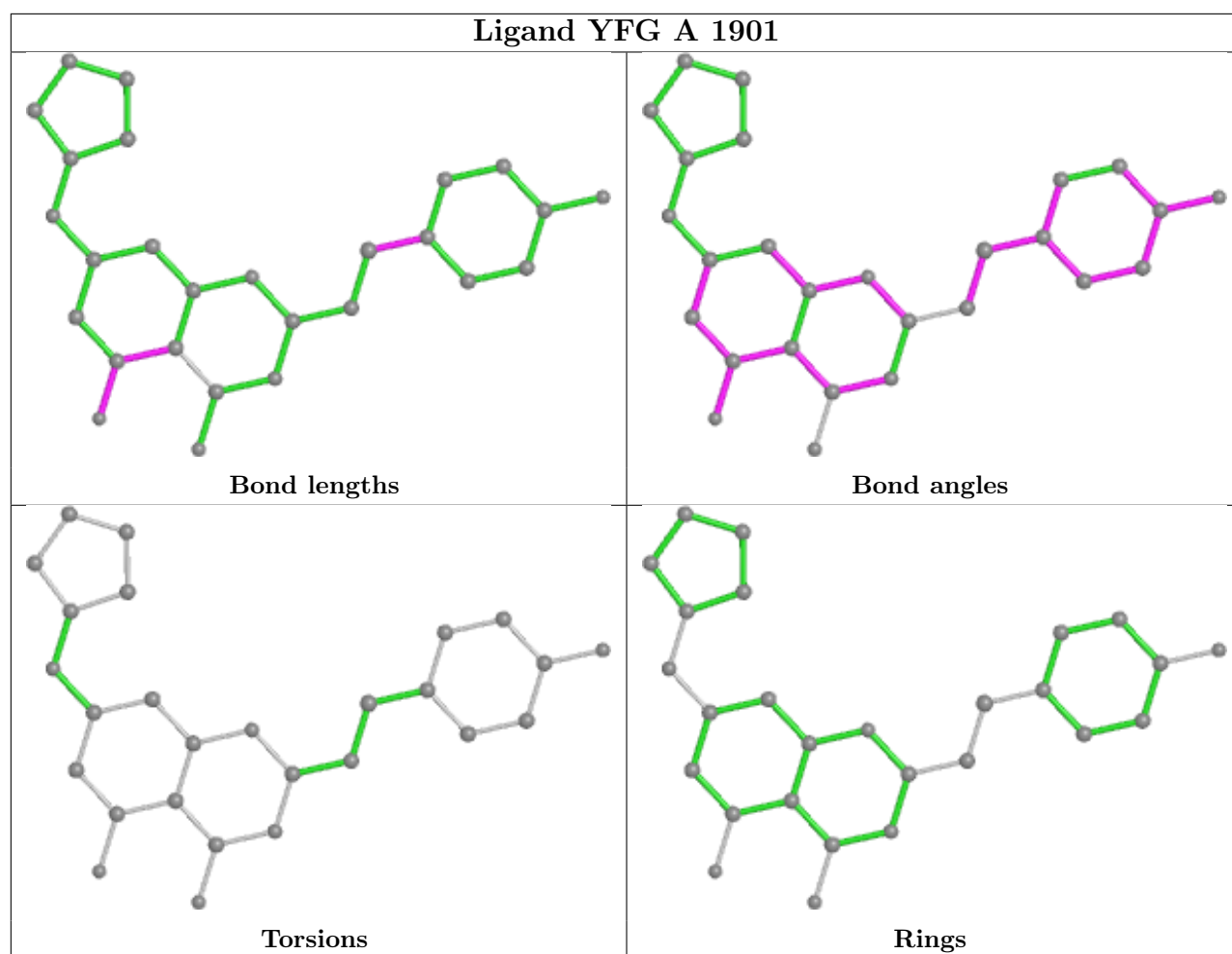


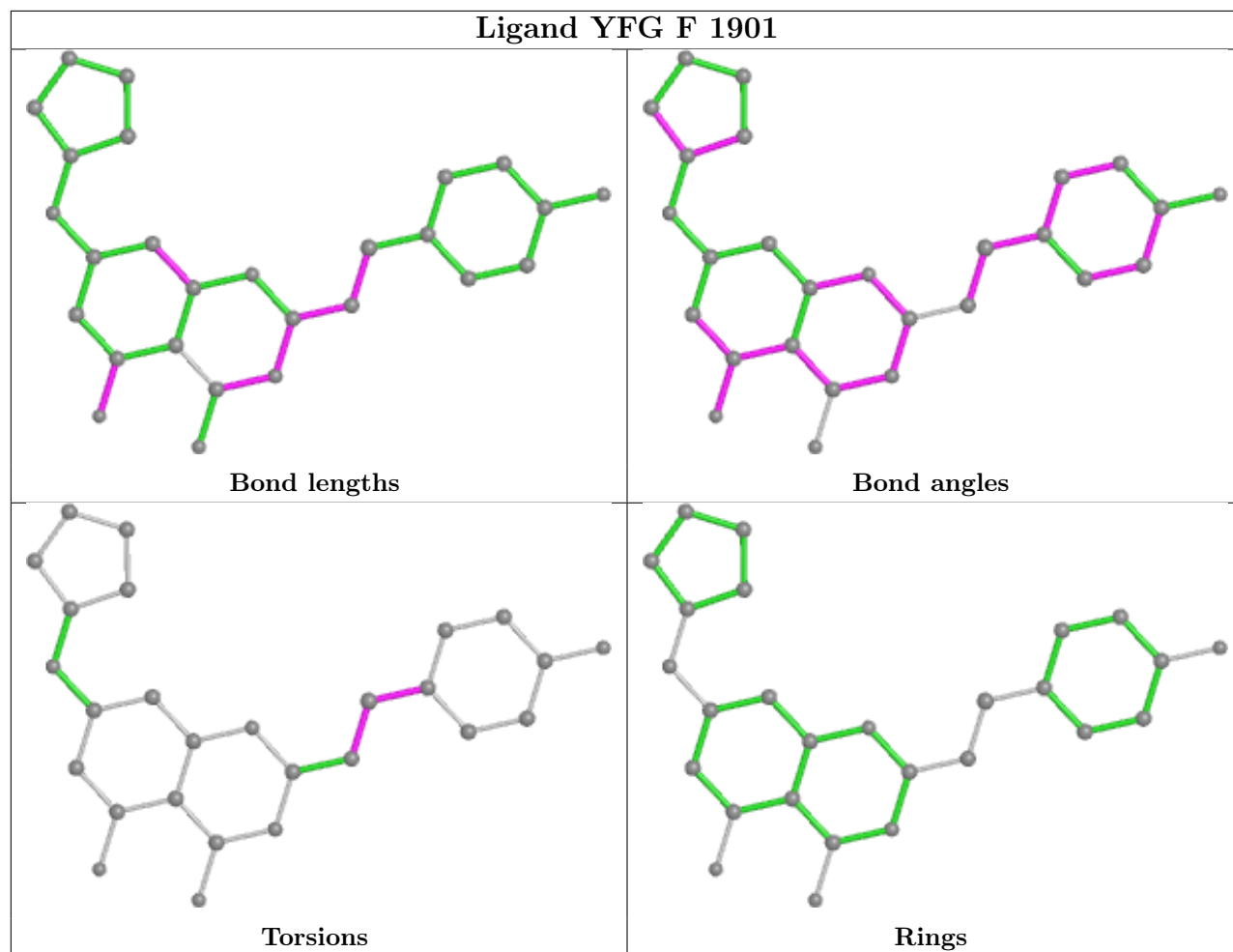
Ligand YFG H 1901

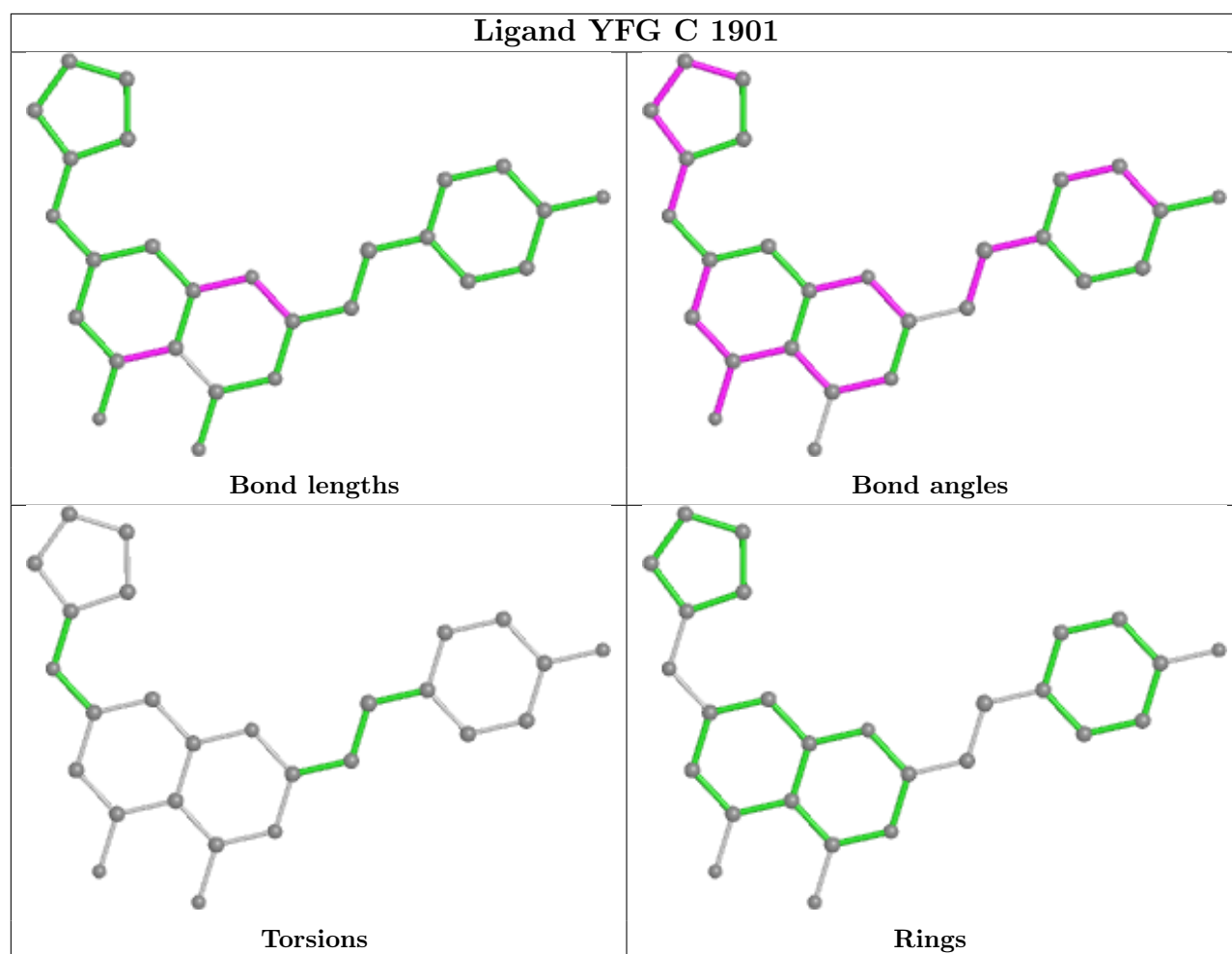


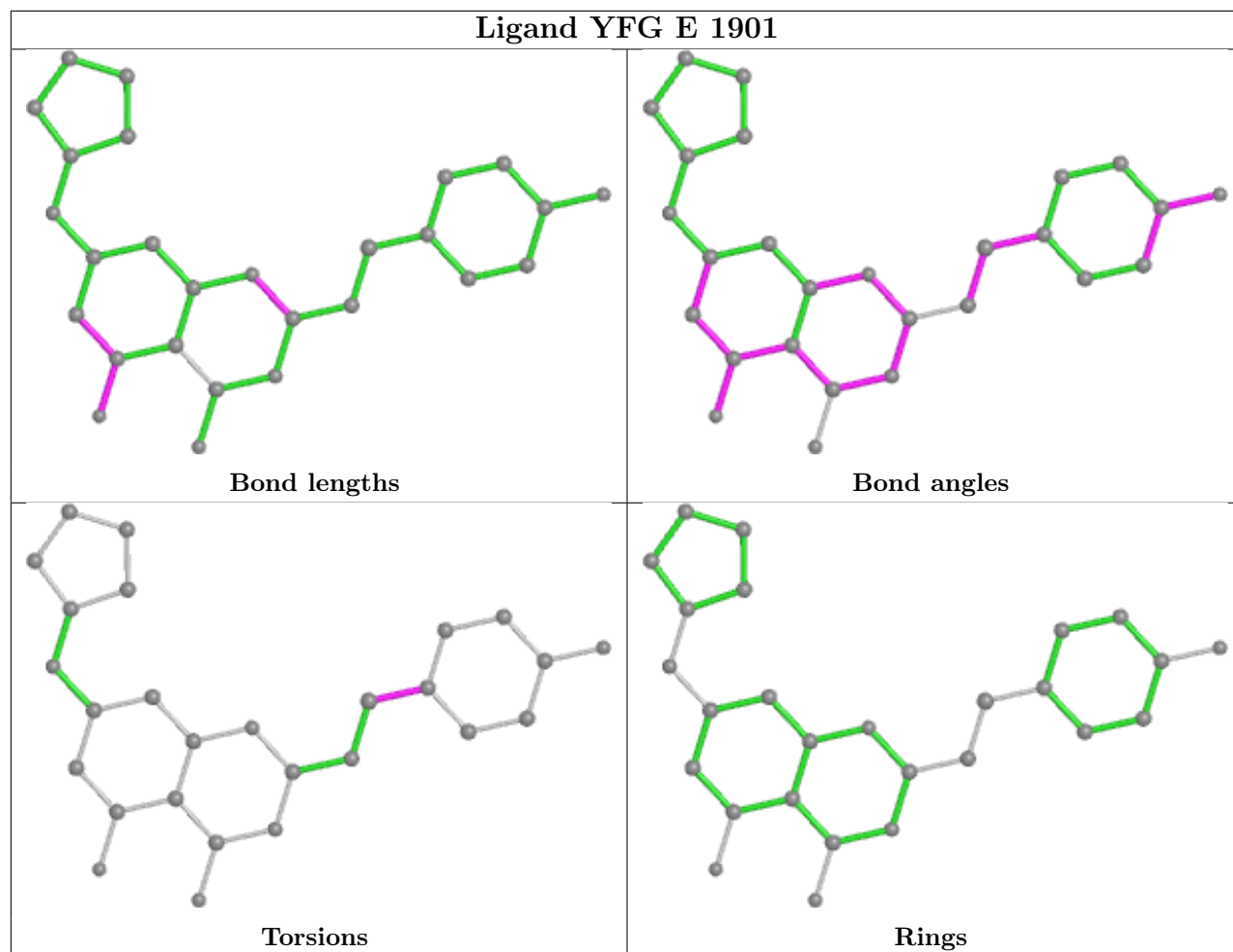












5.7 Other polymers [i](#)

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	186/194 (95%)	0.45	3 (1%) 72 69	20, 30, 49, 71	0
1	B	186/194 (95%)	0.52	6 (3%) 47 43	18, 32, 63, 124	0
1	C	186/194 (95%)	0.66	6 (3%) 47 43	21, 37, 71, 94	0
1	D	186/194 (95%)	1.02	21 (11%) 5 4	24, 42, 75, 116	0
1	E	186/194 (95%)	0.62	5 (2%) 54 51	20, 36, 67, 106	0
1	F	186/194 (95%)	0.96	27 (14%) 2 1	19, 40, 74, 117	0
1	G	186/194 (95%)	1.16	30 (16%) 1 1	24, 45, 84, 149	0
1	H	186/194 (95%)	1.06	33 (17%) 1 1	22, 42, 75, 91	0
All	All	1488/1552 (95%)	0.80	131 (8%) 10 8	18, 38, 72, 149	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1763	PRO	5.4
1	H	1629	TYR	5.2
1	G	1756	ILE	5.2
1	G	1767	THR	4.7
1	G	1619	VAL	4.5
1	F	1698	ASN	4.4
1	F	1617	PHE	4.3
1	G	1763	PRO	4.3
1	F	1764	GLN	4.1
1	G	1764	GLN	4.0
1	H	1655	ASP	4.0
1	H	1619	VAL	3.9
1	G	1626	ASP	3.9
1	D	1767	THR	3.9
1	D	1778	HIS	3.9
1	H	1626	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	1767	THR	3.8
1	H	1623	LEU	3.5
1	B	1764	GLN	3.5
1	D	1700	SER	3.5
1	H	1628	GLU	3.5
1	H	1695	ASN	3.5
1	D	1651	ILE	3.4
1	H	1685	ASP	3.3
1	F	1689	VAL	3.2
1	G	1629	TYR	3.2
1	B	1765	ASN	3.2
1	F	1762	ASN	3.2
1	D	1660	TYR	3.1
1	H	1622	LEU	3.2
1	G	1765	ASN	3.1
1	F	1755	LEU	3.1
1	H	1801	LYS	3.1
1	F	1778	HIS	3.0
1	A	1620	VAL	3.0
1	D	1735	ARG	3.0
1	D	1669	ALA	2.9
1	G	1762	ASN	2.9
1	G	1625	SER	2.8
1	G	1684	THR	2.8
1	F	1618	CYS	2.8
1	G	1655	ASP	2.8
1	F	1787	TYR	2.8
1	B	1654	PRO	2.8
1	B	1763	PRO	2.8
1	B	1669	ALA	2.7
1	G	1623	LEU	2.7
1	H	1694	ARG	2.7
1	H	1621	GLU	2.7
1	D	1638	GLN	2.7
1	F	1768	ASP	2.7
1	F	1766	PRO	2.7
1	F	1735	ARG	2.6
1	G	1755	LEU	2.6
1	H	1691	HIS	2.6
1	G	1695	ASN	2.6
1	D	1694	ARG	2.6
1	D	1789	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1764	GLN	2.6
1	F	1788	ASP	2.6
1	E	1691[A]	HIS	2.5
1	H	1620	VAL	2.5
1	D	1689	VAL	2.5
1	C	1622	LEU	2.5
1	F	1756	ILE	2.5
1	G	1652	GLN	2.5
1	F	1626	ASP	2.4
1	H	1792	TYR	2.4
1	H	1654	PRO	2.4
1	H	1795	TYR	2.4
1	H	1778	HIS	2.4
1	H	1632	VAL	2.4
1	H	1648	ILE	2.4
1	G	1754	SER	2.4
1	G	1656	LEU	2.4
1	D	1801	LYS	2.3
1	G	1757	VAL	2.3
1	H	1651	ILE	2.3
1	F	1616	ASN	2.3
1	H	1705	ASN	2.3
1	E	1626	ASP	2.3
1	F	1638	GLN	2.3
1	G	1620	VAL	2.3
1	G	1801	LYS	2.3
1	G	1651	ILE	2.3
1	F	1733	ASN	2.3
1	D	1703	GLY	2.3
1	F	1702	ALA	2.3
1	D	1787	TYR	2.3
1	H	1656	LEU	2.3
1	A	1766	PRO	2.3
1	H	1645	ILE	2.3
1	C	1625	SER	2.2
1	F	1708	ALA	2.2
1	D	1756	ILE	2.2
1	H	1652	GLN	2.2
1	D	1655	ASP	2.2
1	H	1781	SER	2.2
1	C	1733	ASN	2.2
1	H	1657	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	1633	ALA	2.1
1	C	1699	ARG	2.1
1	H	1616	ASN	2.1
1	E	1654	PRO	2.1
1	F	1634	SER	2.1
1	F	1789	TYR	2.1
1	G	1795	TYR	2.1
1	F	1703	GLY	2.1
1	G	1786	PHE	2.1
1	B	1778	HIS	2.1
1	F	1644	ARG	2.1
1	H	1699	ARG	2.1
1	A	1762	ASN	2.1
1	H	1714	TYR	2.1
1	F	1641	SER	2.1
1	G	1616	ASN	2.1
1	G	1791	ALA	2.1
1	D	1688	SER	2.1
1	C	1765	ASN	2.1
1	G	1740	TYR	2.1
1	C	1643	PHE	2.1
1	E	1699	ARG	2.1
1	H	1650	ARG	2.1
1	F	1658	ASN	2.0
1	H	1630	ASN	2.0
1	E	1781	SER	2.0
1	D	1699	ARG	2.0
1	G	1628	GLU	2.0
1	D	1698	ASN	2.0
1	G	1733	ASN	2.0
1	H	1638	GLN	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 monosaccharides in this entry.

6.4 Ligands

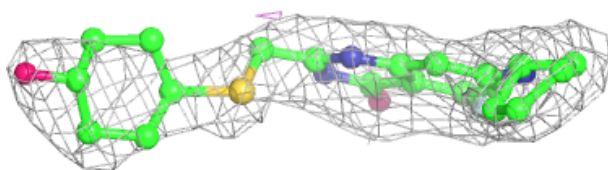
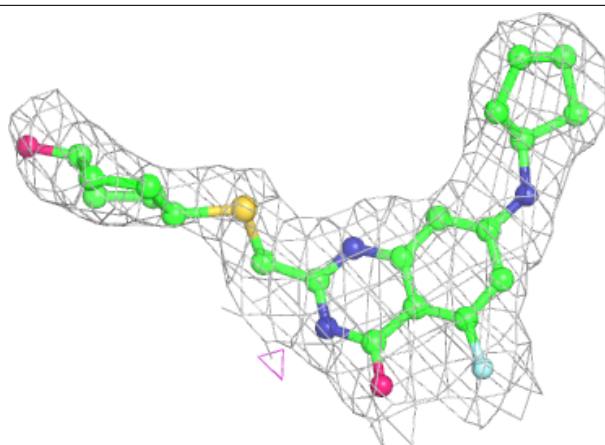
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	F	1902	6/6	0.83	0.21	39,45,46,47	0
4	GOL	H	1902	6/6	0.84	0.14	41,46,47,47	0
3	CL	E	1902	1/1	0.92	0.21	56,56,56,56	0
2	YFG	H	1901	27/27	0.94	0.20	18,23,66,67	0
2	YFG	E	1901	27/27	0.94	0.20	23,28,51,57	0
2	YFG	F	1901	27/27	0.94	0.17	22,28,40,43	0
2	YFG	G	1901	27/27	0.94	0.16	22,28,47,57	0
2	YFG	B	1901	27/27	0.95	0.18	22,27,42,46	0
2	YFG	C	1901	27/27	0.95	0.17	18,25,37,41	0
2	YFG	A	1901	27/27	0.95	0.19	18,21,30,31	0
2	YFG	D	1901	27/27	0.96	0.18	19,26,48,57	0

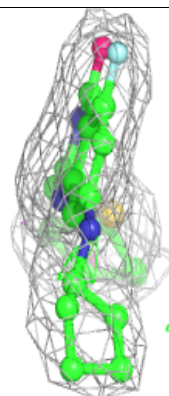
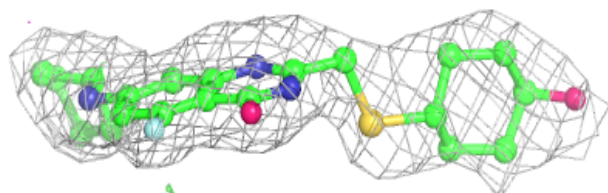
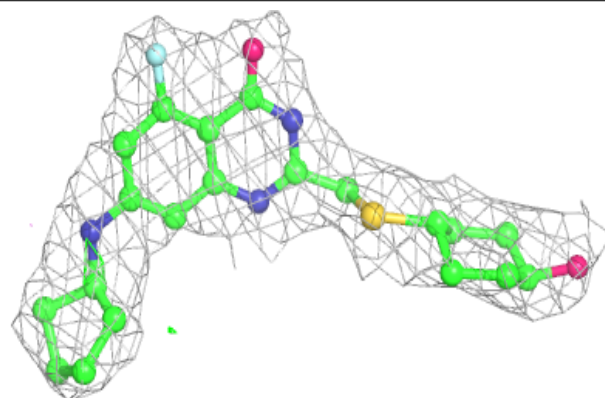
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YFG H 1901:

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

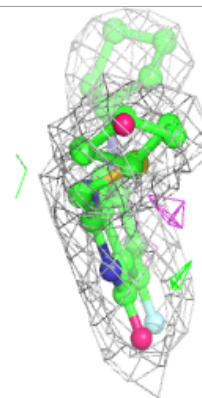
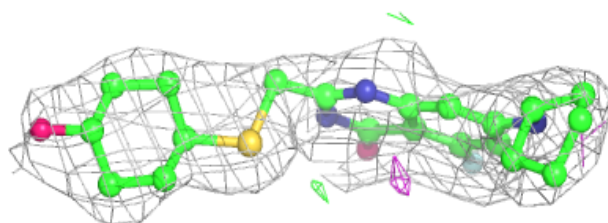
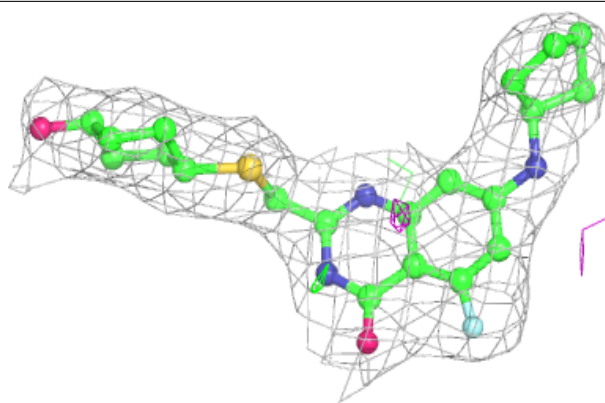
**Electron density around YFG E 1901:**

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

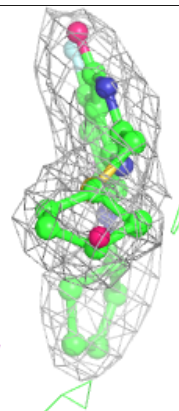
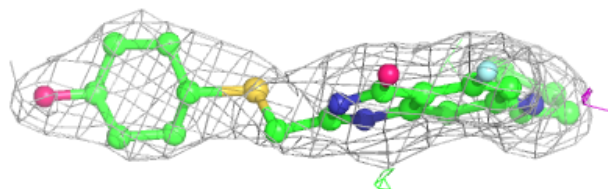
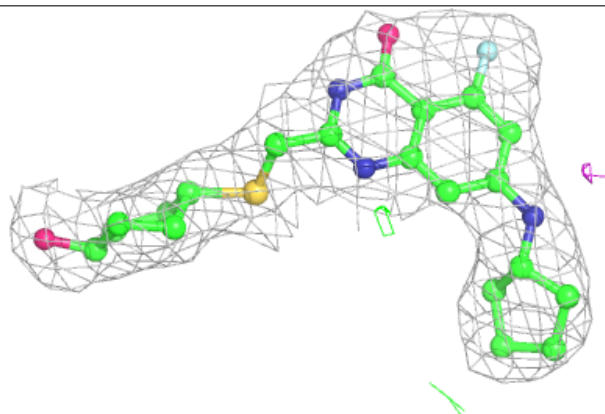


Electron density around YFG F 1901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

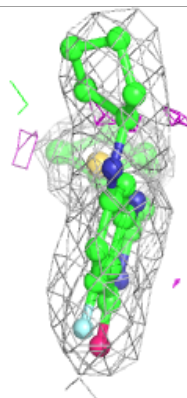
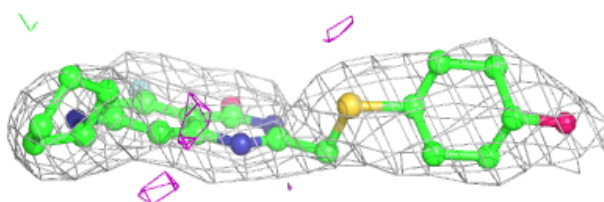
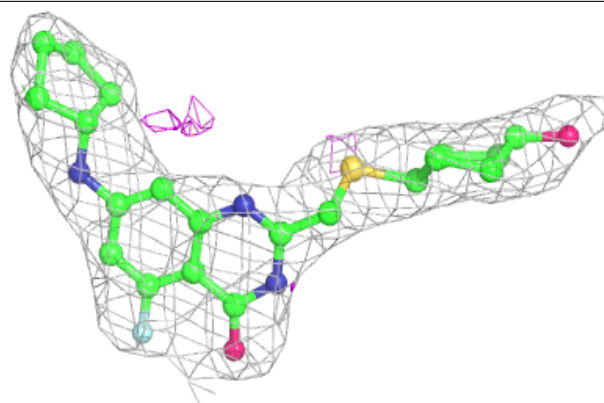
**Electron density around YFG G 1901:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

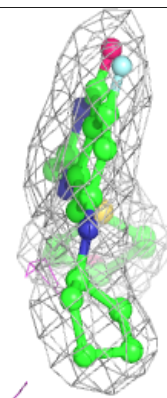
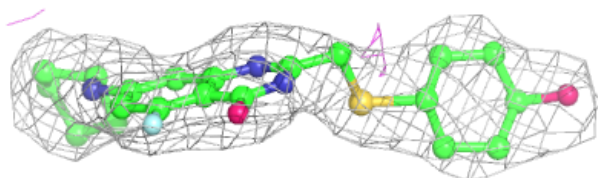
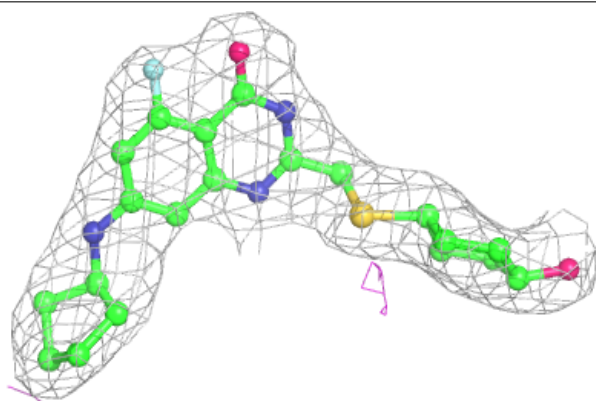


Electron density around YFG B 1901:

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

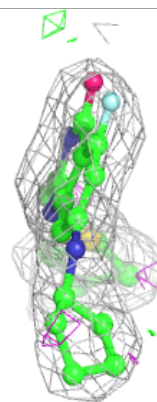
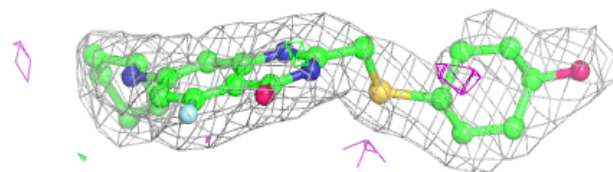
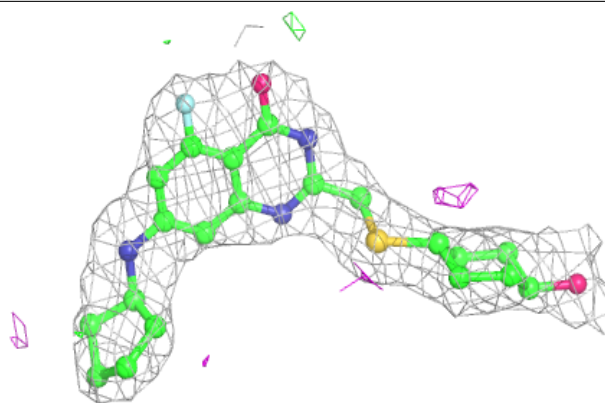
**Electron density around YFG C 1901:**

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

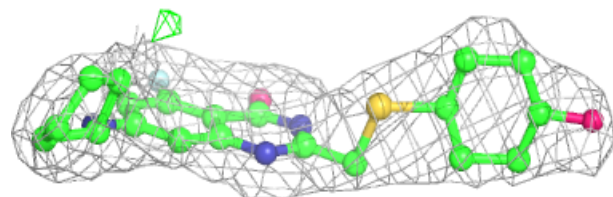
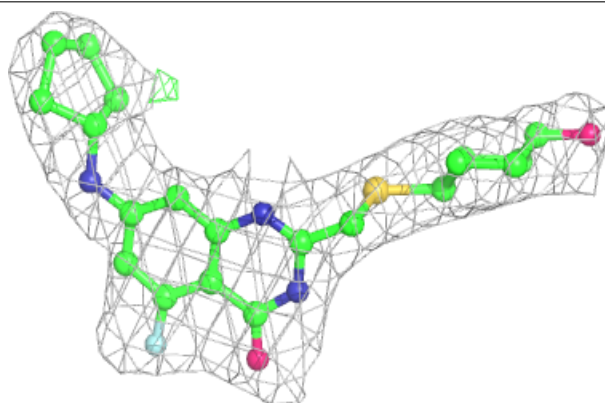


Electron density around YFG A 1901:

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

**Electron density around YFG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.