



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:10 am BST

PDB ID : 4PJT  
Title : Structure of PARP1 catalytic domain bound to inhibitor BMN 673  
Authors : Aoyagi-Scharber, M.; Gardberg, A.S.; Arakaki, T.L.  
Deposited on : 2014-05-12  
Resolution : 2.35 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](mailto: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.

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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 : 2.11  
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) : 2.11

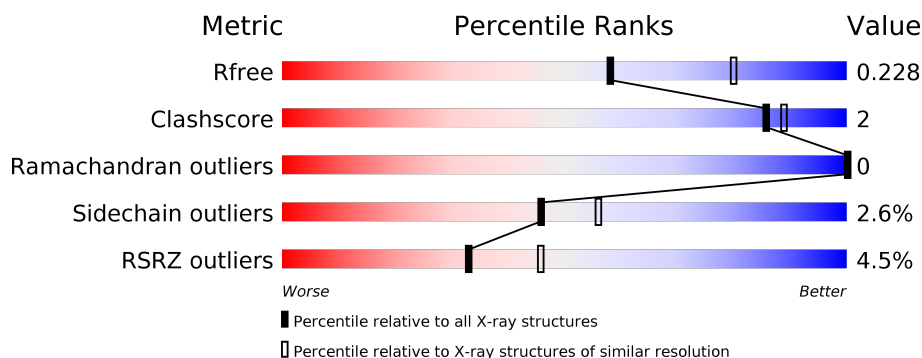
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	370	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 85%, yellow 85%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>6% • 9%</span> </div> </div>
1	B	370	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 84%, yellow 84%, yellow 89%, grey 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>84%</span> <span>5% • 10%</span> </div> </div>
1	C	370	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 87%, yellow 87%, yellow 92%, grey 92%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>87%</span> <span>5% • 6%</span> </div> </div>
1	D	370	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 9%, green 9%, green 81%, yellow 81%, yellow 87%, grey 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>9%</span> <span>81%</span> <span>6% 12%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10711 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	1	0
			2595	1657	428	500	10			
1	B	332	Total	C	N	O	S	0	0	0
			2504	1603	412	479	10			
1	C	346	Total	C	N	O	S	0	2	0
			2647	1690	440	506	11			
1	D	326	Total	C	N	O	S	0	0	0
			2444	1562	408	464	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	MET	-	expression tag	UNP P09874
A	643	GLY	-	expression tag	UNP P09874
A	644	SER	-	expression tag	UNP P09874
A	645	SER	-	expression tag	UNP P09874
A	646	HIS	-	expression tag	UNP P09874
A	647	HIS	-	expression tag	UNP P09874
A	648	HIS	-	expression tag	UNP P09874
A	649	HIS	-	expression tag	UNP P09874
A	650	HIS	-	expression tag	UNP P09874
A	651	HIS	-	expression tag	UNP P09874
A	652	SER	-	expression tag	UNP P09874
A	653	GLY	-	expression tag	UNP P09874
A	654	LEU	-	expression tag	UNP P09874
A	655	VAL	-	expression tag	UNP P09874
A	656	PRO	-	expression tag	UNP P09874
A	657	ARG	-	expression tag	UNP P09874
A	658	GLY	-	expression tag	UNP P09874
A	659	SER	-	expression tag	UNP P09874
A	660	HIS	-	expression tag	UNP P09874
A	661	MET	-	expression tag	UNP P09874
B	642	MET	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	643	GLY	-	expression tag	UNP P09874
B	644	SER	-	expression tag	UNP P09874
B	645	SER	-	expression tag	UNP P09874
B	646	HIS	-	expression tag	UNP P09874
B	647	HIS	-	expression tag	UNP P09874
B	648	HIS	-	expression tag	UNP P09874
B	649	HIS	-	expression tag	UNP P09874
B	650	HIS	-	expression tag	UNP P09874
B	651	HIS	-	expression tag	UNP P09874
B	652	SER	-	expression tag	UNP P09874
B	653	GLY	-	expression tag	UNP P09874
B	654	LEU	-	expression tag	UNP P09874
B	655	VAL	-	expression tag	UNP P09874
B	656	PRO	-	expression tag	UNP P09874
B	657	ARG	-	expression tag	UNP P09874
B	658	GLY	-	expression tag	UNP P09874
B	659	SER	-	expression tag	UNP P09874
B	660	HIS	-	expression tag	UNP P09874
B	661	MET	-	expression tag	UNP P09874
C	642	MET	-	expression tag	UNP P09874
C	643	GLY	-	expression tag	UNP P09874
C	644	SER	-	expression tag	UNP P09874
C	645	SER	-	expression tag	UNP P09874
C	646	HIS	-	expression tag	UNP P09874
C	647	HIS	-	expression tag	UNP P09874
C	648	HIS	-	expression tag	UNP P09874
C	649	HIS	-	expression tag	UNP P09874
C	650	HIS	-	expression tag	UNP P09874
C	651	HIS	-	expression tag	UNP P09874
C	652	SER	-	expression tag	UNP P09874
C	653	GLY	-	expression tag	UNP P09874
C	654	LEU	-	expression tag	UNP P09874
C	655	VAL	-	expression tag	UNP P09874
C	656	PRO	-	expression tag	UNP P09874
C	657	ARG	-	expression tag	UNP P09874
C	658	GLY	-	expression tag	UNP P09874
C	659	SER	-	expression tag	UNP P09874
C	660	HIS	-	expression tag	UNP P09874
C	661	MET	-	expression tag	UNP P09874
D	642	MET	-	expression tag	UNP P09874
D	643	GLY	-	expression tag	UNP P09874
D	644	SER	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
D	645	SER	-	expression tag	UNP P09874
D	646	HIS	-	expression tag	UNP P09874
D	647	HIS	-	expression tag	UNP P09874
D	648	HIS	-	expression tag	UNP P09874
D	649	HIS	-	expression tag	UNP P09874
D	650	HIS	-	expression tag	UNP P09874
D	651	HIS	-	expression tag	UNP P09874
D	652	SER	-	expression tag	UNP P09874
D	653	GLY	-	expression tag	UNP P09874
D	654	LEU	-	expression tag	UNP P09874
D	655	VAL	-	expression tag	UNP P09874
D	656	PRO	-	expression tag	UNP P09874
D	657	ARG	-	expression tag	UNP P09874
D	658	GLY	-	expression tag	UNP P09874
D	659	SER	-	expression tag	UNP P09874
D	660	HIS	-	expression tag	UNP P09874
D	661	MET	-	expression tag	UNP P09874

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



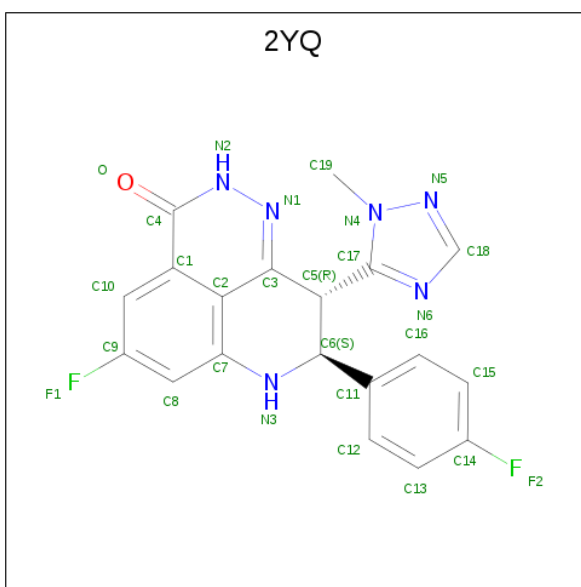
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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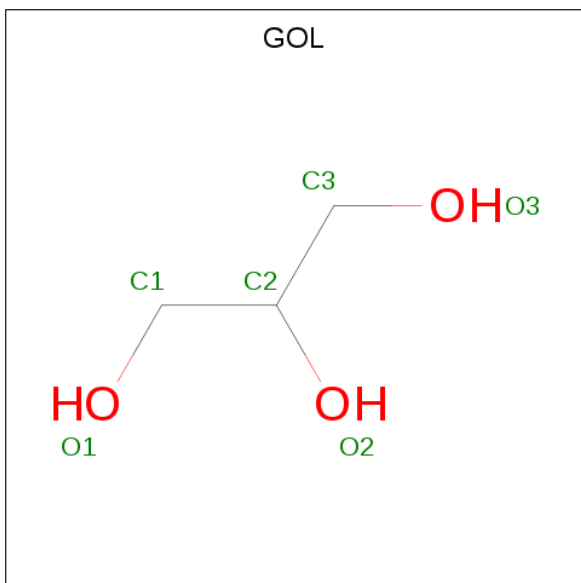
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- Molecule 3 is (8S,9R)-5-fluoro-8-(4-fluorophenyl)-9-(1-methyl-1H-1,2,4-triazol-5-yl)-2,7,8,9-tetrahydro-3H-pyrido[4,3,2-de]phthalazin-3-one (three-letter code: 2YQ) (formula: C<sub>19</sub>H<sub>14</sub>F<sub>2</sub>N<sub>6</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
3	B	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
3	C	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
3	D	1	Total	C	F	N	O	0	0
			28	19	2	6	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is water.

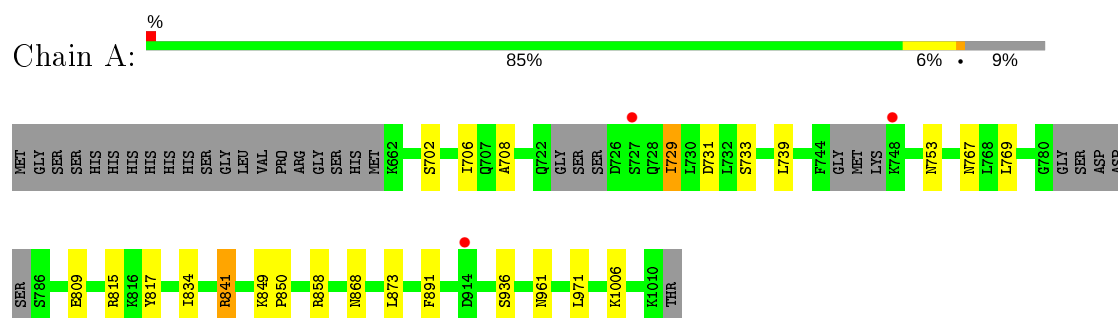
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	55	Total	O	0	0
			55	55		
5	C	100	Total	O	0	0
			100	100		
5	D	53	Total	O	0	0
			53	53		



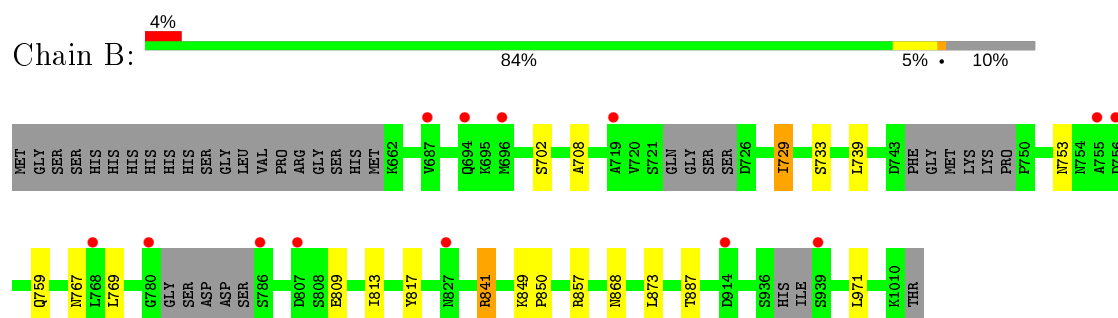
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

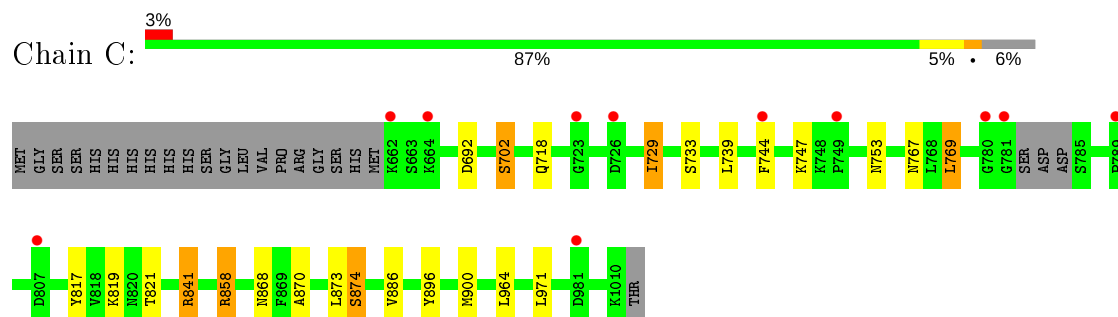
- Molecule 1: Poly [ADP-ribose] polymerase 1



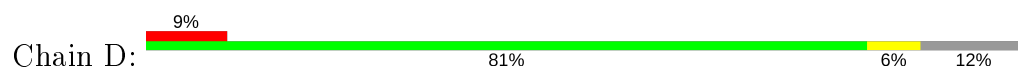
- Molecule 1: Poly [ADP-ribose] polymerase 1

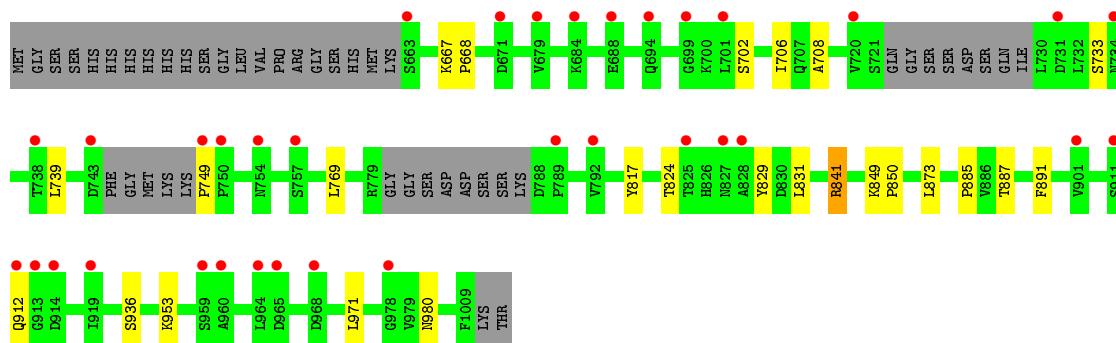


- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 1: Poly [ADP-ribose] polymerase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.69Å 108.15Å 142.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.35 19.94 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.94-2.35) 99.8 (19.94-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.188 , 0.228 0.192 , 0.228	Depositor DCC
$R_{free}$ test set	3387 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, SO4, 2YQ

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	0.65	0/2647	0.78	2/3590 (0.1%)
1	B	0.58	0/2549	0.74	3/3462 (0.1%)
1	C	0.63	0/2706	0.77	5/3675 (0.1%)
1	D	0.53	0/2490	0.71	3/3388 (0.1%)
All	All	0.60	0/10392	0.75	13/14115 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	841	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	C	841	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	C	841	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	D	841	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	841	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	841	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	D	841	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	D	749	PRO	N-CA-CB	6.00	110.50	103.30
1	C	692	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	857	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	858	ARG	CG-CD-NE	-5.42	100.42	111.80
1	C	964	LEU	CA-CB-CG	5.12	127.08	115.30

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	2595	0	2532	15	0
1	B	2504	0	2412	9	0
1	C	2647	0	2575	13	0
1	D	2444	0	2340	10	0
2	A	20	0	0	1	0
2	B	25	0	0	0	0
2	C	15	0	0	3	0
2	D	15	0	0	0	0
3	A	28	0	14	0	0
3	B	28	0	14	0	0
3	C	28	0	14	0	0
3	D	28	0	14	0	0
4	A	12	0	16	0	0
4	C	6	0	8	1	0
5	A	108	0	0	1	0
5	B	55	0	0	0	0
5	C	100	0	0	2	0
5	D	53	0	0	0	0
All	All	10711	0	9939	44	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 2.

All (44) 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:759:GLN:HG3	1:B:887:THR:HG22	1.48	0.92
1:B:841:ARG:HD2	1:B:873:LEU:O	1.83	0.78
1:A:809:GLU:CD	1:C:886:VAL:HG11	2.06	0.76
1:A:841:ARG:HD2	1:A:873:LEU:O	1.86	0.74
1:A:809:GLU:OE1	1:C:886:VAL:HG11	1.87	0.73
1:C:841:ARG:HD2	1:C:873:LEU:O	1.87	0.73
1:D:841:ARG:HD2	1:D:873:LEU:O	1.88	0.73
1:C:769:LEU:HD22	5:C:1283:HOH:O	1.94	0.67
1:B:729:ILE:HD11	1:B:753:ASN:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ILE:HD11	1:B:753:ASN:HB3	1.78	0.64
1:C:702:SER:HB2	2:C:1103:SO4:O1	2.01	0.61
1:B:759:GLN:CG	1:B:887:THR:HG22	2.27	0.59
1:D:829:TYR:HE1	1:D:831:LEU:HD21	1.69	0.56
1:D:885:PRO:HB2	1:D:887:THR:HG22	1.87	0.55
1:A:961:ASN:ND2	5:A:1243:HOH:O	2.39	0.55
1:C:744:PHE:HB2	1:C:747:LYS:O	2.09	0.52
1:A:767:ASN:HA	1:A:868:ASN:HD21	1.75	0.52
2:C:1101:SO4:O2	5:C:1266:HOH:O	2.18	0.50
1:A:729:ILE:HD11	1:A:753:ASN:CB	2.43	0.49
2:C:1102:SO4:O3	1:D:849:LYS:NZ	2.41	0.49
1:A:708:ALA:HB3	1:A:739:LEU:HD21	1.95	0.48
1:B:767:ASN:HA	1:B:868:ASN:HD21	1.78	0.48
1:C:767:ASN:HA	1:C:868:ASN:HD21	1.79	0.48
1:A:858:ARG:NH2	2:A:1102:SO4:O3	2.46	0.45
1:B:849:LYS:HB3	1:B:850:PRO:HD3	1.98	0.45
1:C:896:TYR:CE2	4:C:1105:GOL:H32	2.51	0.45
1:B:809:GLU:O	1:B:813:ILE:HG13	2.17	0.45
1:B:708:ALA:HB3	1:B:739:LEU:HD21	1.98	0.44
1:C:870:ALA:O	1:C:874:SER:HB3	2.18	0.44
1:D:849:LYS:HB3	1:D:850:PRO:HD3	1.99	0.44
1:A:849:LYS:HB3	1:A:850:PRO:HD3	1.99	0.43
1:A:729:ILE:HD11	1:A:753:ASN:HB3	1.99	0.42
1:C:821:THR:HB	1:C:900:MET:HA	2.02	0.42
1:A:815:ARG:NH1	1:C:718:GLN:HG2	2.35	0.42
1:D:708:ALA:HB3	1:D:739:LEU:HD21	2.00	0.42
1:A:891:PHE:HA	1:A:936:SER:O	2.20	0.42
1:A:809:GLU:OE1	1:C:886:VAL:CG1	2.62	0.41
1:D:891:PHE:HA	1:D:936:SER:O	2.21	0.41
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	2.01	0.41
1:D:667:LYS:N	1:D:668:PRO:CD	2.84	0.41
1:D:953:LYS:NZ	1:D:980:ASN:O	2.51	0.41
1:D:706:ILE:HG21	1:D:769:LEU:HG	2.03	0.41
1:A:706:ILE:HG21	1:A:769:LEU:HG	2.03	0.40
1:C:729:ILE:HD11	1:C:753:ASN:CB	2.52	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	331/370 (90%)	329 (99%)	2 (1%)	0	100	100
1	B	322/370 (87%)	321 (100%)	1 (0%)	0	100	100
1	C	344/370 (93%)	342 (99%)	2 (1%)	0	100	100
1	D	318/370 (86%)	316 (99%)	2 (1%)	0	100	100
All	All	1315/1480 (89%)	1308 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/325 (86%)	273 (98%)	6 (2%)	52	63
1	B	260/325 (80%)	254 (98%)	6 (2%)	50	61
1	C	282/325 (87%)	272 (96%)	10 (4%)	36	44
1	D	252/325 (78%)	246 (98%)	6 (2%)	49	59
All	All	1073/1300 (82%)	1045 (97%)	28 (3%)	46	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	702	SER
1	A	729	ILE

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Mol	Chain	Res	Type
1	A	731	ASP
1	A	733	SER
1	A	817	TYR
1	A	971	LEU
1	B	702	SER
1	B	729	ILE
1	B	733	SER
1	B	769	LEU
1	B	817	TYR
1	B	971	LEU
1	C	702	SER
1	C	729	ILE
1	C	733	SER
1	C	739	LEU
1	C	769	LEU
1	C	817	TYR
1	C	819	LYS
1	C	858	ARG
1	C	874	SER
1	C	971	LEU
1	D	702	SER
1	D	733	SER
1	D	817	TYR
1	D	824	THR
1	D	912	GLN
1	D	971	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	767	ASN
1	A	868	ASN
1	A	961	ASN
1	B	767	ASN
1	B	868	ASN
1	C	767	ASN
1	C	868	ASN
1	D	998	ASN



### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	2YQ	A	1105	-	27,32,32	2.31	7 (25%)	30,48,48	2.19	10 (33%)
2	SO4	A	1104	-	4,4,4	0.32	0	6,6,6	0.61	0
2	SO4	C	1103	-	4,4,4	0.20	0	6,6,6	0.77	0
2	SO4	A	1103	-	4,4,4	0.64	0	6,6,6	1.21	1 (16%)
2	SO4	B	1102	-	4,4,4	0.34	0	6,6,6	0.56	0
2	SO4	D	1103	-	4,4,4	0.36	0	6,6,6	0.28	0
2	SO4	C	1101	-	4,4,4	0.98	0	6,6,6	0.83	0
2	SO4	B	1103	-	4,4,4	0.18	0	6,6,6	0.44	0
4	GOL	C	1105	-	5,5,5	0.86	0	5,5,5	1.48	2 (40%)
2	SO4	C	1102	-	4,4,4	0.32	0	6,6,6	0.38	0
2	SO4	B	1106	-	4,4,4	0.37	0	6,6,6	0.41	0
2	SO4	D	1102	-	4,4,4	0.77	0	6,6,6	0.63	0
3	2YQ	D	1104	-	27,32,32	2.37	8 (29%)	30,48,48	1.92	7 (23%)
3	2YQ	B	1105	-	27,32,32	2.12	6 (22%)	30,48,48	1.81	7 (23%)
4	GOL	A	1106	-	5,5,5	0.46	0	5,5,5	0.88	0
3	2YQ	C	1104	-	27,32,32	2.32	6 (22%)	30,48,48	1.90	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	1104	-	4,4,4	0.27	0	6,6,6	0.73	0
2	SO4	D	1101	-	4,4,4	0.40	0	6,6,6	0.58	0
2	SO4	B	1101	-	4,4,4	0.42	0	6,6,6	0.92	0
2	SO4	A	1101	-	4,4,4	1.10	1 (25%)	6,6,6	0.46	0
4	GOL	A	1107	-	5,5,5	0.51	0	5,5,5	0.44	0
2	SO4	A	1102	-	4,4,4	0.28	0	6,6,6	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2YQ	B	1105	-	-	0/4/20/20	0/4/5/5
4	GOL	A	1106	-	-	2/4/4/4	-
3	2YQ	A	1105	-	-	0/4/20/20	0/4/5/5
4	GOL	C	1105	-	-	0/4/4/4	-
3	2YQ	C	1104	-	-	0/4/20/20	0/4/5/5
3	2YQ	D	1104	-	-	0/4/20/20	0/4/5/5
4	GOL	A	1107	-	-	3/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1104	2YQ	C3-C5	-8.54	1.48	1.51
3	D	1104	2YQ	C3-C5	-8.48	1.48	1.51
3	B	1105	2YQ	C3-C5	-7.61	1.48	1.51
3	A	1105	2YQ	C3-C5	-6.93	1.48	1.51
3	A	1105	2YQ	C7-N3	-5.07	1.35	1.40
3	A	1105	2YQ	C3-C2	-4.97	1.38	1.43
3	C	1104	2YQ	C3-C2	-4.84	1.38	1.43
3	B	1105	2YQ	C7-N3	-3.80	1.36	1.40
3	D	1104	2YQ	N2-N1	3.73	1.43	1.34
3	D	1104	2YQ	C11-C6	-3.62	1.47	1.52
3	C	1104	2YQ	C7-N3	-3.44	1.36	1.40
3	A	1105	2YQ	C17-C5	-3.24	1.45	1.50
3	D	1104	2YQ	C10-C9	3.23	1.41	1.36
3	A	1105	2YQ	C7-C2	-2.91	1.38	1.42
3	D	1104	2YQ	C7-N3	-2.91	1.37	1.40
3	B	1105	2YQ	N2-N1	2.79	1.41	1.34
3	C	1104	2YQ	N2-N1	2.68	1.41	1.34
3	B	1105	2YQ	C10-C9	2.59	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	2YQ	N2-N1	2.52	1.40	1.34
3	B	1105	2YQ	C3-C2	-2.52	1.40	1.43
3	A	1105	2YQ	C10-C9	2.41	1.40	1.36
3	D	1104	2YQ	C17-N6	2.40	1.38	1.34
3	D	1104	2YQ	C3-C2	-2.32	1.41	1.43
3	C	1104	2YQ	C17-C5	-2.29	1.47	1.50
3	B	1105	2YQ	C19-N4	2.19	1.51	1.47
3	C	1104	2YQ	C19-N4	2.05	1.51	1.47
2	A	1101	SO4	O2-S	2.03	1.57	1.46
3	D	1104	2YQ	C8-C7	2.02	1.41	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	2YQ	C2-C7-N3	7.55	122.39	117.45
3	D	1104	2YQ	C2-C7-N3	5.72	121.19	117.45
3	C	1104	2YQ	C2-C7-N3	5.21	120.86	117.45
3	D	1104	2YQ	C10-C9-C8	-4.94	120.19	124.09
3	B	1105	2YQ	C2-C7-N3	4.83	120.61	117.45
3	B	1105	2YQ	C19-N4-C17	4.41	134.07	128.84
3	A	1105	2YQ	C19-N4-C17	3.81	133.36	128.84
3	C	1104	2YQ	C10-C9-C8	-3.54	121.30	124.09
3	C	1104	2YQ	C3-N1-N2	3.51	123.24	119.67
3	B	1105	2YQ	C2-C3-N1	-3.20	119.31	121.50
3	C	1104	2YQ	C4-C1-C2	3.12	121.50	119.18
3	A	1105	2YQ	C2-C3-N1	-3.06	119.40	121.50
3	A	1105	2YQ	C10-C9-C8	-2.98	121.74	124.09
3	D	1104	2YQ	C19-N4-C17	2.93	132.31	128.84
3	A	1105	2YQ	C16-C15-C14	2.75	121.21	118.36
3	B	1105	2YQ	C3-N1-N2	2.72	122.43	119.67
3	D	1104	2YQ	C5-C17-N6	2.71	130.25	125.08
3	C	1104	2YQ	C19-N4-C17	2.61	131.93	128.84
3	C	1104	2YQ	C2-C3-N1	-2.61	119.71	121.50
3	C	1104	2YQ	C3-C5-C6	2.52	114.28	109.81
3	D	1104	2YQ	F1-C9-C10	2.41	122.78	119.17
3	C	1104	2YQ	C7-C2-C1	2.38	121.78	117.49
4	C	1105	GOL	O2-C2-C3	-2.36	98.74	109.12
3	D	1104	2YQ	C3-C5-C6	2.35	113.97	109.81
3	B	1105	2YQ	C4-C1-C2	2.35	120.93	119.18
3	B	1105	2YQ	C7-C2-C1	2.29	121.62	117.49
3	B	1105	2YQ	C5-C3-N1	2.23	120.53	118.18
3	A	1105	2YQ	C15-C14-C13	-2.21	119.89	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	2YQ	C7-C2-C1	2.19	121.45	117.49
3	A	1105	2YQ	C3-N1-N2	2.13	121.83	119.67
4	C	1105	GOL	C3-C2-C1	2.11	119.91	111.70
2	A	1103	SO4	O3-S-O2	2.11	120.30	109.31
3	D	1104	2YQ	C5-C3-N1	2.09	120.38	118.18
3	C	1104	2YQ	C9-C10-C1	2.09	120.92	119.43
3	C	1104	2YQ	C11-C6-N3	2.09	114.22	110.93
3	A	1105	2YQ	C5-C17-N6	2.08	129.05	125.08
3	A	1105	2YQ	C3-C5-C6	2.04	113.43	109.81
3	C	1104	2YQ	C5-C3-N1	2.02	120.31	118.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1106	GOL	O1-C1-C2-C3
4	A	1107	GOL	O1-C1-C2-O2
4	A	1107	GOL	O1-C1-C2-C3
4	A	1106	GOL	O1-C1-C2-O2
4	A	1107	GOL	O2-C2-C3-O3

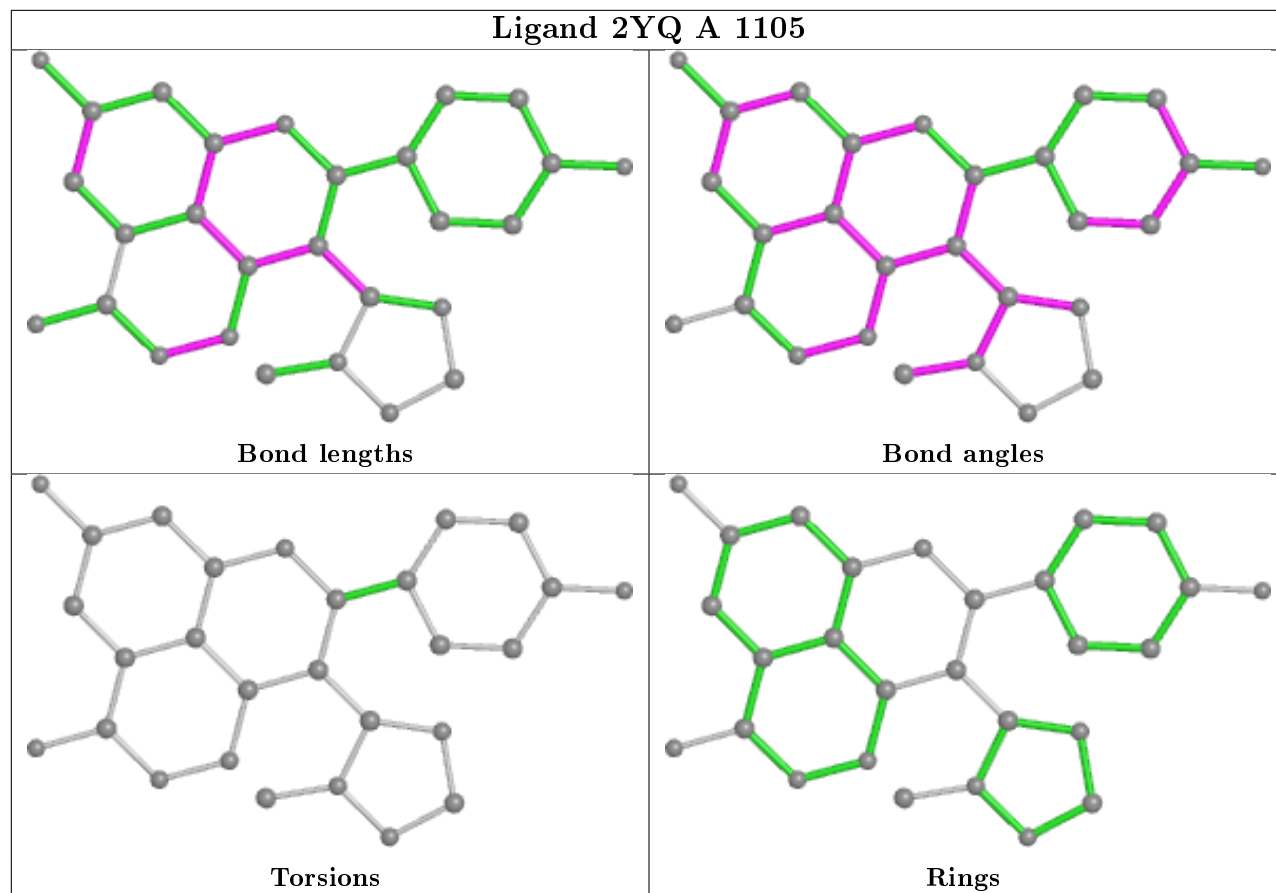
There are no ring outliers.

5 monomers are involved in 5 short contacts:

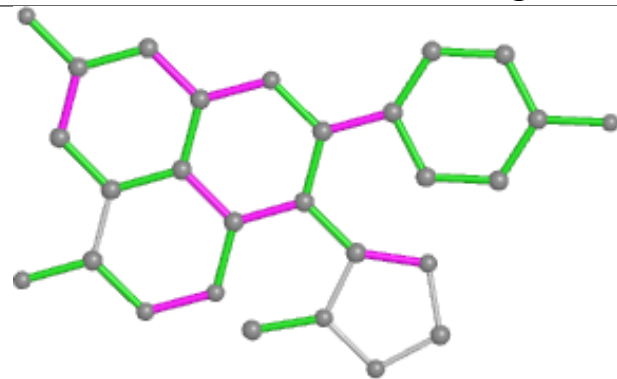
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1103	SO4	1	0
2	C	1101	SO4	1	0
4	C	1105	GOL	1	0
2	C	1102	SO4	1	0
2	A	1102	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

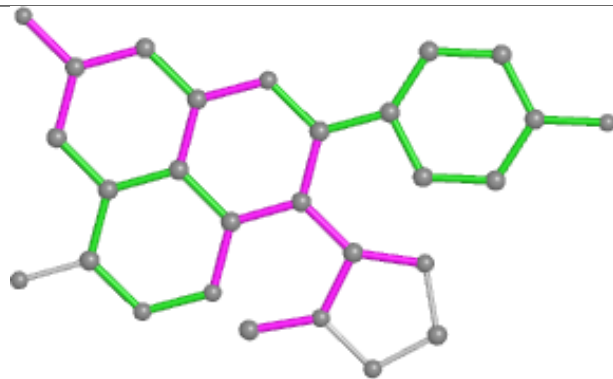
equivalents in the CSD to analyse the geometry.



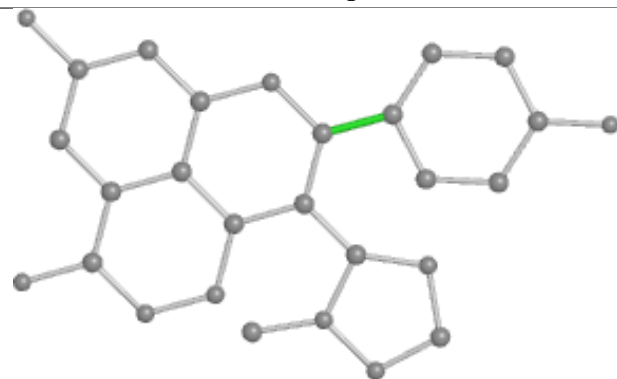
## Ligand 2YQ D 1104



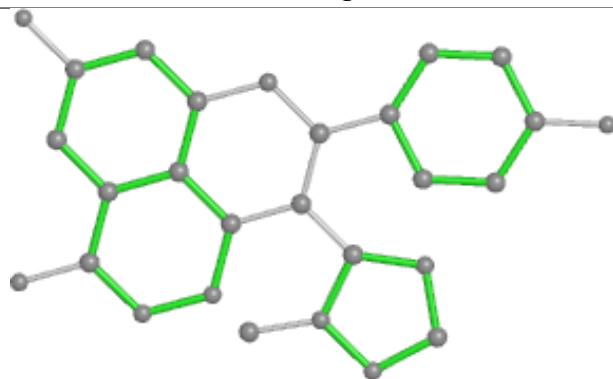
Bond lengths



Bond angles

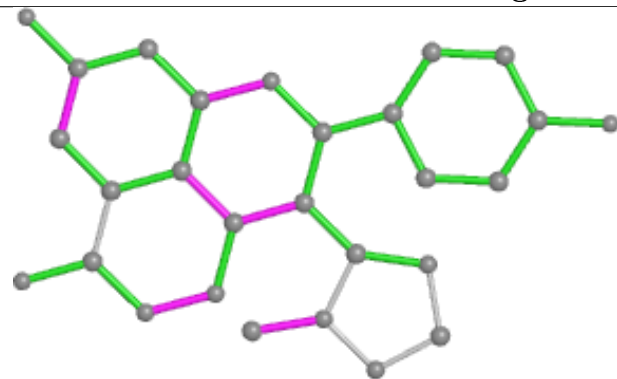


Torsions

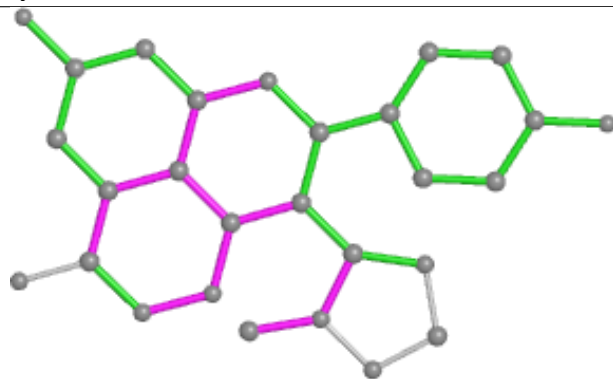


Rings

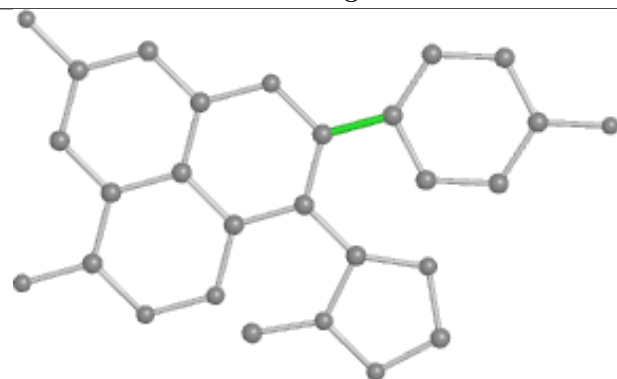
## Ligand 2YQ B 1105



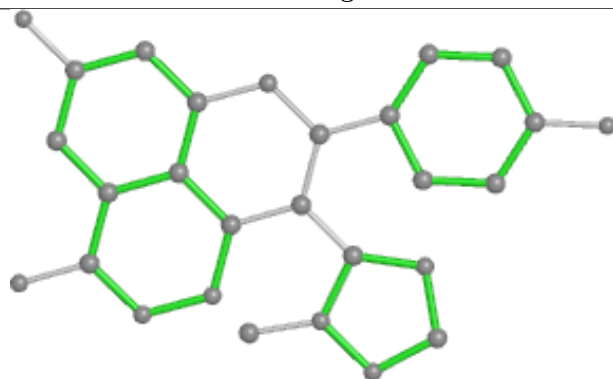
Bond lengths



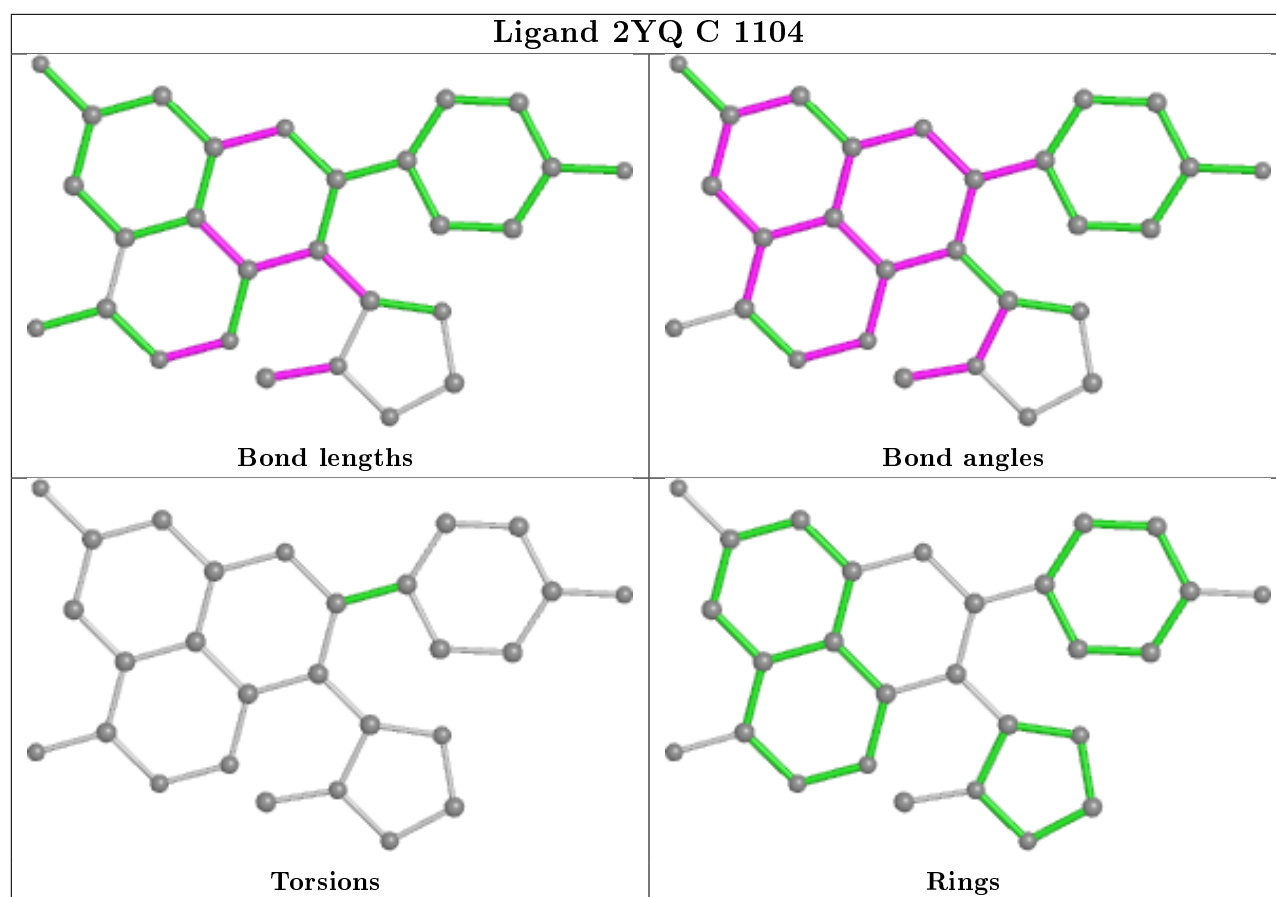
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	338/370 (91%)	-0.09	3 (0%) 84 90	17, 34, 61, 91	0
1	B	332/370 (89%)	0.20	13 (3%) 39 52	22, 46, 72, 86	0
1	C	346/370 (93%)	-0.01	11 (3%) 47 59	17, 34, 60, 81	0
1	D	326/370 (88%)	0.40	34 (10%) 6 10	26, 51, 80, 91	0
All	All	1342/1480 (90%)	0.12	61 (4%) 33 46	17, 40, 72, 91	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	939	SER	5.8
1	C	807	ASP	4.7
1	C	744	PHE	4.2
1	D	663	SER	4.0
1	B	786	SER	3.9
1	C	780	GLY	3.9
1	C	781	GLY	3.7
1	B	780	GLY	3.5
1	D	827	ASN	3.5
1	D	792	VAL	3.5
1	D	738	THR	3.4
1	D	965	ASP	3.3
1	B	687	VAL	3.3
1	D	749	PRO	3.3
1	B	807	ASP	3.2
1	B	768	LEU	3.2
1	D	913	GLY	3.2
1	A	727	SER	3.1
1	D	720	VAL	3.0
1	D	828	ALA	3.0
1	D	750	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	959	SER	2.8
1	D	743	ASP	2.8
1	D	914	ASP	2.8
1	D	960	ALA	2.8
1	B	755	ALA	2.8
1	B	756	ASP	2.7
1	B	827	ASN	2.7
1	C	664	LYS	2.6
1	D	964	LEU	2.6
1	D	911	SER	2.6
1	C	726	ASP	2.6
1	C	981	ASP	2.5
1	D	731	ASP	2.5
1	D	789	PRO	2.5
1	A	748	LYS	2.4
1	D	912	GLN	2.4
1	D	919	ILE	2.4
1	D	825	THR	2.4
1	B	694	GLN	2.4
1	D	701	LEU	2.3
1	B	696	MET	2.3
1	D	757	SER	2.3
1	D	699	GLY	2.3
1	B	914	ASP	2.3
1	D	901	VAL	2.2
1	D	734	ASN	2.2
1	D	671	ASP	2.2
1	C	662	LYS	2.1
1	D	679	VAL	2.1
1	C	789	PRO	2.1
1	D	754	ASN	2.0
1	B	719	ALA	2.0
1	D	978	GLY	2.0
1	C	749	PRO	2.0
1	A	914	ASP	2.0
1	D	968	ASP	2.0
1	C	723	GLY	2.0
1	D	688	GLU	2.0
1	D	694	GLN	2.0
1	D	684	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

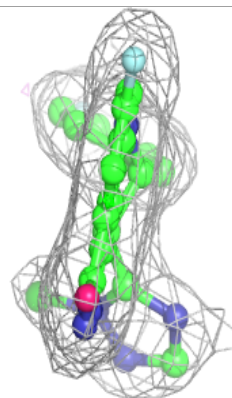
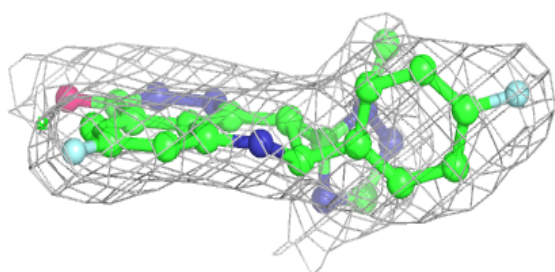
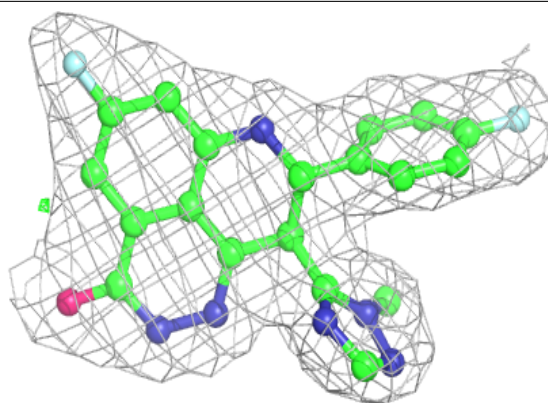
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GOL	A	1107	6/6	0.81	0.17	54,60,62,65	0
2	SO4	B	1106	5/5	0.86	0.24	46,49,54,54	5
2	SO4	D	1102	5/5	0.87	0.17	50,51,61,66	0
2	SO4	B	1101	5/5	0.88	0.16	47,54,56,60	0
2	SO4	A	1101	5/5	0.91	0.16	29,37,37,41	0
4	GOL	A	1106	6/6	0.91	0.21	42,53,56,62	0
2	SO4	C	1101	5/5	0.92	0.13	36,40,53,54	0
4	GOL	C	1105	6/6	0.94	0.11	28,31,35,36	0
2	SO4	A	1102	5/5	0.94	0.17	30,31,33,34	5
2	SO4	C	1103	5/5	0.95	0.12	30,31,33,33	5
3	2YQ	D	1104	28/28	0.95	0.11	23,27,32,34	0
2	SO4	A	1104	5/5	0.95	0.15	28,28,29,32	5
2	SO4	B	1104	5/5	0.95	0.20	25,26,28,29	5
3	2YQ	C	1104	28/28	0.96	0.10	17,19,23,28	0
2	SO4	D	1103	5/5	0.96	0.13	37,37,40,42	5
2	SO4	A	1103	5/5	0.97	0.14	37,39,44,50	0
3	2YQ	B	1105	28/28	0.97	0.09	22,27,37,45	0
3	2YQ	A	1105	28/28	0.97	0.10	18,19,23,24	0
2	SO4	B	1102	5/5	0.98	0.11	52,52,57,57	0
2	SO4	D	1101	5/5	0.98	0.17	43,44,50,51	0
2	SO4	C	1102	5/5	0.98	0.15	55,59,64,67	0
2	SO4	B	1103	5/5	0.99	0.16	31,31,34,34	5

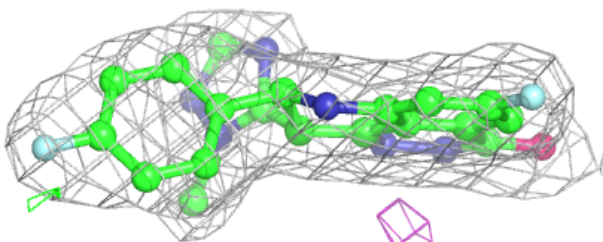
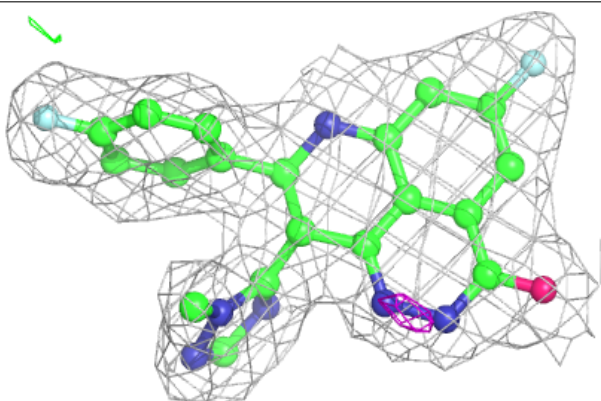
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2YQ D 1104:**

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

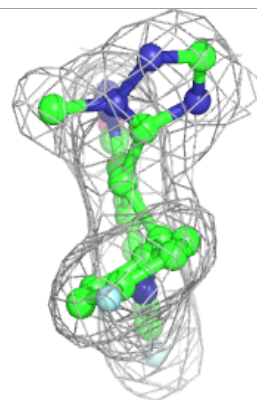
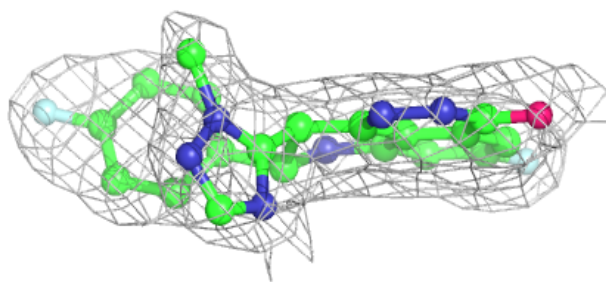
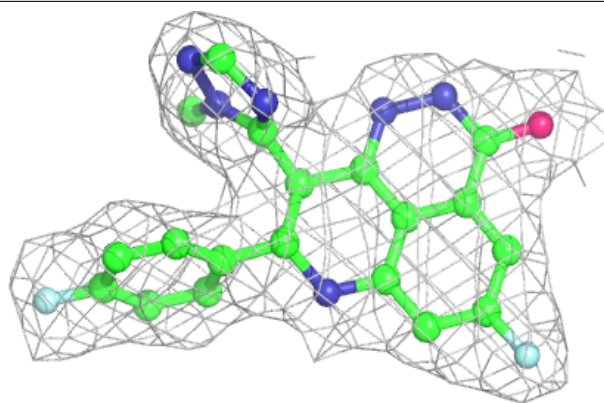
**Electron density around 2YQ C 1104:**

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

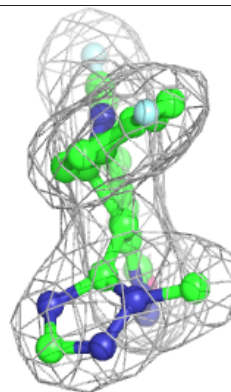
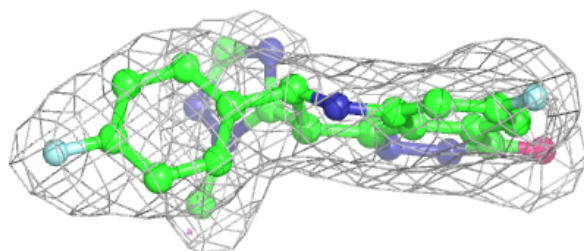
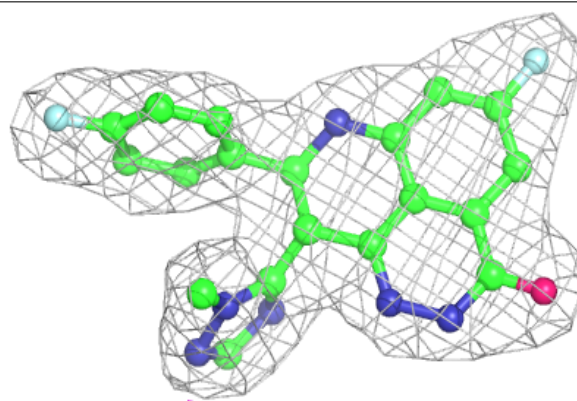


**Electron density around 2YQ B 1105:**

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

**Electron density around 2YQ A 1105:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.