



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:12 am BST

PDB ID : 1SR7  
Title : Progesterone Receptor Hormone Binding Domain with Bound Mometasone Furoate  
Authors : Madauss, K.P.; Deng, S.-J.; Austin, R.J.; Lambert, M.H.; McLay, I.; Pritchard, J.; Short, S.A.; Stewart, E.L.; Uings, I.J.; Williams, S.P.  
Deposited on : 2004-03-22  
Resolution : 1.46 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.

---

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

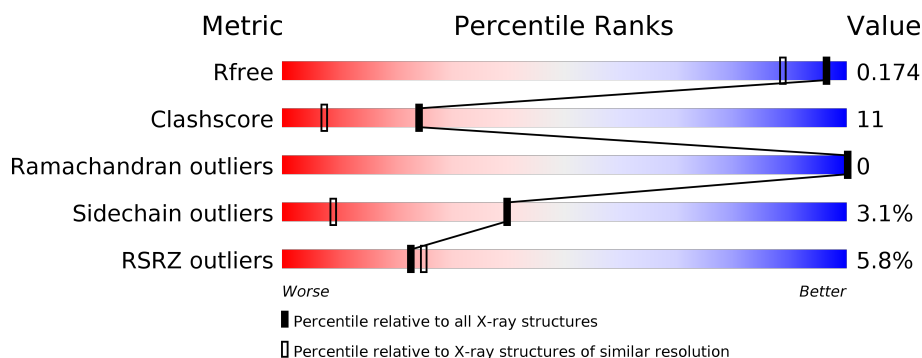
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.46 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	259	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	259	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>.</div> <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
3	SO4	B	402	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4374 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.

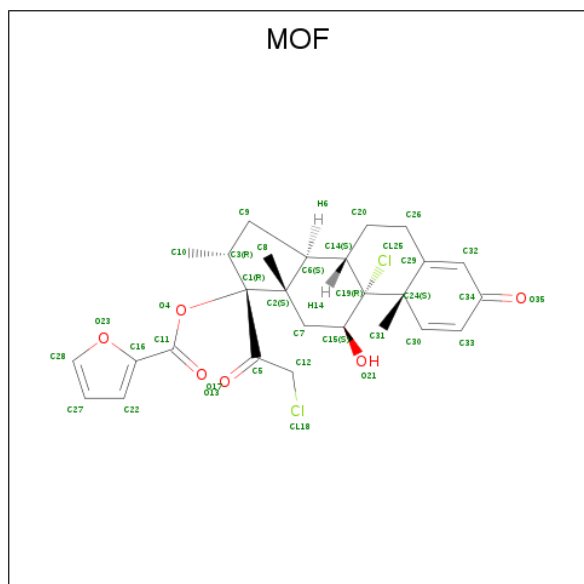
- Molecule 1 is a protein called Progesterone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	1	0
			2000	1298	329	359	14			
1	B	249	Total	C	N	O	S	0	1	0
			2007	1301	332	360	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	675	GLY	-	CLONING ARTIFACT	UNP P06401
B	675	GLY	-	CLONING ARTIFACT	UNP P06401

- Molecule 2 is MOMETASONE FUROATE (three-letter code: MOF) (formula:  $C_{27}H_{30}Cl_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			35	27	2	6		

*Continued on next page...*

*Continued from previous page...*

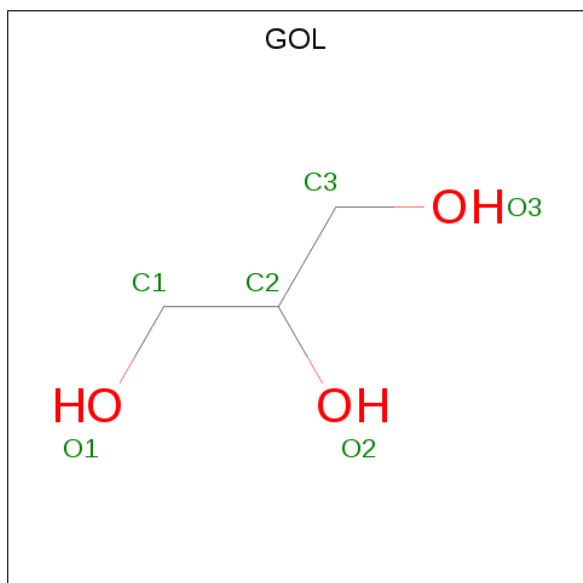
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	O	0	0
			35	27	2	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

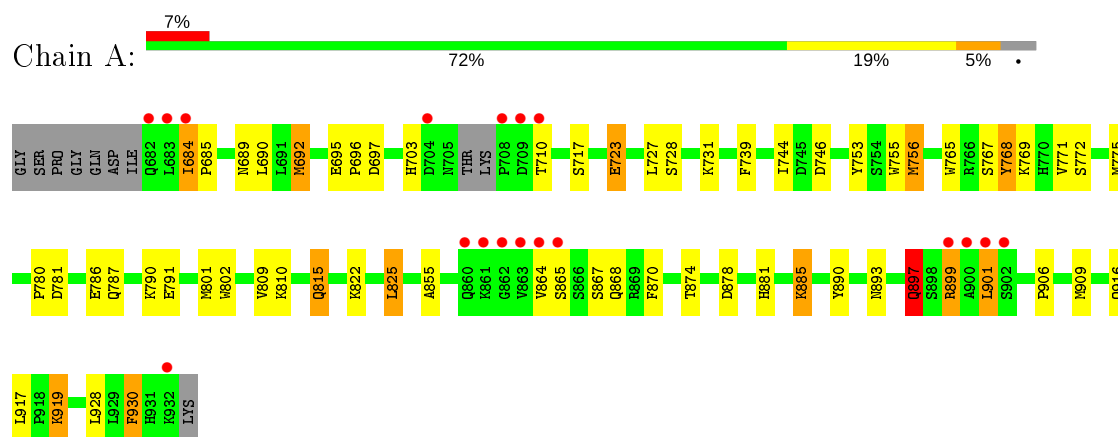
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	162	Total	O	0	0
			162	162		

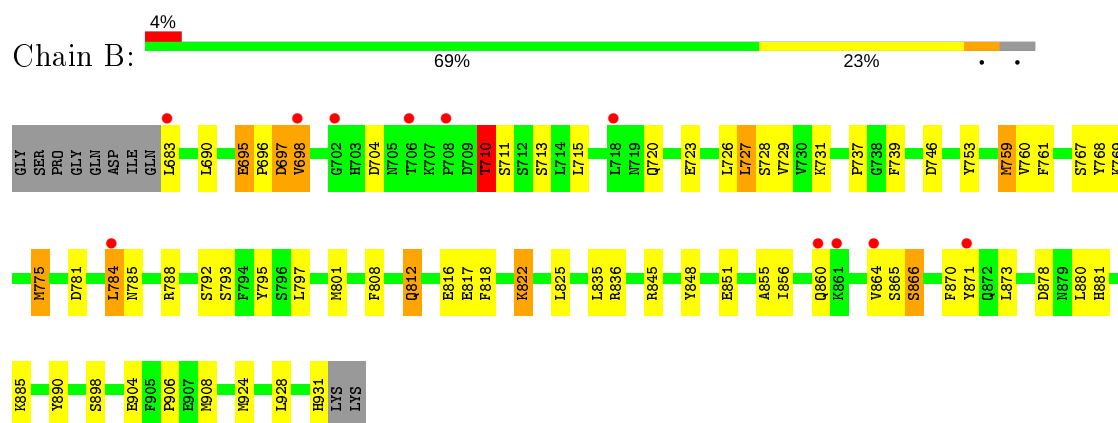
### 3 Residue-property plots [i](#)

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: Progesterone receptor



#### • Molecule 1: Progesterone receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.11Å 64.26Å 70.09Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	19.96 – 1.46 19.97 – 1.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.46) 90.5 (19.97-1.46)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.174 , 0.211 0.180 , 0.174	Depositor DCC
$R_{free}$ test set	5561 reflections (6.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, MOF

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	1.71	23/2047 (1.1%)	1.47	16/2770 (0.6%)
1	B	1.85	38/2055 (1.8%)	1.62	38/2782 (1.4%)
All	All	1.78	61/4102 (1.5%)	1.55	54/5552 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	822	LYS	CE-NZ	12.62	1.80	1.49
1	B	775	MET	SD-CE	-10.63	1.18	1.77
1	B	801	MET	SD-CE	-9.94	1.22	1.77
1	A	801	MET	SD-CE	-9.63	1.24	1.77
1	A	756	MET	CB-CG	9.05	1.80	1.51
1	B	768	TYR	CE2-CZ	-8.81	1.27	1.38
1	B	822	LYS	CD-CE	8.77	1.73	1.51
1	B	822	LYS	CG-CD	7.99	1.79	1.52
1	B	698	VAL	CB-CG2	7.51	1.68	1.52
1	A	753	TYR	CD1-CE1	7.46	1.50	1.39
1	B	890	TYR	CD1-CE1	7.29	1.50	1.39
1	B	768	TYR	CD1-CE1	7.10	1.50	1.39
1	B	904	GLU	CD-OE2	6.90	1.33	1.25
1	B	817	GLU	CD-OE1	6.78	1.33	1.25
1	B	845	ARG	NE-CZ	-6.76	1.24	1.33
1	B	795	TYR	CD1-CE1	6.64	1.49	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	924	MET	SD-CE	-6.62	1.40	1.77
1	B	898	SER	CB-OG	-6.57	1.33	1.42
1	B	818	PHE	CD1-CE1	6.39	1.52	1.39
1	A	768	TYR	CD1-CE1	6.39	1.49	1.39
1	A	695	GLU	CD-OE1	-6.38	1.18	1.25
1	A	772	SER	CA-CB	6.36	1.62	1.52
1	A	930	PHE	CE2-CZ	6.33	1.49	1.37
1	B	795	TYR	CE2-CZ	6.31	1.46	1.38
1	A	893	ASN	CB-CG	-6.30	1.36	1.51
1	B	767	SER	CB-OG	6.20	1.50	1.42
1	B	768	TYR	CZ-OH	6.11	1.48	1.37
1	B	851	GLU	CD-OE1	-5.97	1.19	1.25
1	A	786	GLU	CD-OE1	5.97	1.32	1.25
1	B	848	TYR	CD1-CE1	5.93	1.48	1.39
1	A	855	ALA	CA-CB	5.89	1.64	1.52
1	B	731	LYS	CD-CE	5.86	1.65	1.51
1	A	695	GLU	CD-OE2	5.85	1.32	1.25
1	A	897	GLN	CD-OE1	5.81	1.36	1.24
1	B	808	PHE	CE2-CZ	5.76	1.48	1.37
1	B	739	PHE	CE1-CZ	5.74	1.48	1.37
1	A	822	LYS	CD-CE	5.66	1.65	1.51
1	A	756	MET	CG-SD	-5.61	1.66	1.81
1	B	845	ARG	CZ-NH2	5.60	1.40	1.33
1	A	767	SER	CB-OG	5.60	1.49	1.42
1	A	692	MET	CG-SD	5.54	1.95	1.81
1	A	930	PHE	CG-CD1	5.50	1.47	1.38
1	A	885	LYS	CD-CE	5.50	1.65	1.51
1	B	695	GLU	CD-OE2	5.48	1.31	1.25
1	B	727	LEU	CG-CD1	5.45	1.72	1.51
1	A	739	PHE	CD1-CE1	5.44	1.50	1.39
1	A	809	VAL	CB-CG1	5.32	1.64	1.52
1	B	855	ALA	CA-CB	5.32	1.63	1.52
1	B	697	ASP	C-O	-5.23	1.13	1.23
1	A	787	GLN	CD-OE1	5.21	1.35	1.24
1	B	871	TYR	CD1-CE1	5.20	1.47	1.39
1	B	871	TYR	CE1-CZ	5.19	1.45	1.38
1	B	856	ILE	C-O	5.18	1.33	1.23
1	B	873	LEU	C-O	5.14	1.33	1.23
1	B	812	GLN	CB-CG	5.13	1.66	1.52
1	B	866	SER	C-O	5.09	1.33	1.23
1	A	723	GLU	CD-OE1	5.08	1.31	1.25
1	B	731	LYS	CE-NZ	-5.05	1.36	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	793	SER	CB-OG	-5.04	1.35	1.42
1	A	870	PHE	CE2-CZ	-5.01	1.27	1.37
1	B	760	VAL	CB-CG1	-5.00	1.42	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	727	LEU	CB-CG-CD1	12.78	132.73	111.00
1	B	845	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	A	753	TYR	CB-CG-CD2	-10.72	114.57	121.00
1	A	825	LEU	CB-CG-CD2	9.59	127.30	111.00
1	A	697	ASP	CB-CG-OD2	9.40	126.76	118.30
1	B	775	MET	CG-SD-CE	-8.88	86.00	100.20
1	B	753	TYR	CB-CG-CD2	-8.85	115.69	121.00
1	A	695	GLU	CG-CD-OE1	-8.50	101.30	118.30
1	A	692	MET	CG-SD-CE	-8.20	87.09	100.20
1	B	878	ASP	CB-CG-OD2	7.61	125.14	118.30
1	B	880	LEU	CB-CG-CD1	-7.58	98.12	111.00
1	B	759	MET	CA-CB-CG	-7.12	101.19	113.30
1	A	768	TYR	CG-CD2-CE2	6.88	126.81	121.30
1	B	781	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	768	TYR	CG-CD1-CE1	-6.58	116.04	121.30
1	A	690	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	B	768	TYR	OH-CZ-CE2	-6.45	102.69	120.10
1	B	695	GLU	CG-CD-OE1	-6.37	105.55	118.30
1	A	878	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	753	TYR	CD1-CE1-CZ	-6.33	114.10	119.80
1	B	768	TYR	CD1-CE1-CZ	-6.32	114.11	119.80
1	B	753	TYR	CB-CG-CD1	6.27	124.76	121.00
1	B	761	PHE	CG-CD1-CE1	-6.23	113.94	120.80
1	B	845	ARG	NH1-CZ-NH2	6.23	126.25	119.40
1	A	885	LYS	CD-CE-NZ	-6.22	97.38	111.70
1	B	784	LEU	CB-CG-CD2	6.14	121.43	111.00
1	A	890	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	B	836	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	781	ASP	CB-CG-OD2	6.06	123.76	118.30
1	B	797	LEU	CB-CG-CD1	-6.06	100.69	111.00
1	B	870	PHE	CZ-CE2-CD2	-6.04	112.86	120.10
1	A	695	GLU	CG-CD-OE2	6.03	130.36	118.30
1	B	711	SER	CB-CA-C	5.98	121.46	110.10
1	B	816	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	B	906	PRO	N-CD-CG	-5.96	94.26	103.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	B	885	LYS	CD-CE-NZ	-5.87	98.19	111.70
1	B	768	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	729	VAL	CA-CB-CG2	-5.74	102.30	110.90
1	B	759	MET	CB-CG-SD	-5.72	95.25	112.40
1	B	746	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	727	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	B	753	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
1	B	710	THR	N-CA-CB	-5.46	99.92	110.30
1	B	704	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	746	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	768	TYR	CE1-CZ-CE2	5.24	128.19	119.80
1	B	695	GLU	CG-CD-OE2	5.18	128.66	118.30
1	A	768	TYR	CZ-CE2-CD2	-5.17	115.14	119.80
1	B	792	SER	N-CA-C	5.11	124.81	111.00
1	B	822	LYS	CD-CE-NZ	-5.07	100.03	111.70
1	B	848	TYR	CD1-CE1-CZ	-5.05	115.25	119.80
1	B	704	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	B	835	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	768	TYR	Sidechain

## 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	2000	0	2035	40	2
1	B	2007	0	2049	45	5
2	A	35	0	29	2	0
2	B	35	0	29	5	0
3	B	5	0	0	0	3
4	B	6	0	8	1	0
5	A	124	0	0	16	8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	162	0	0	11	3
All	All	4374	0	4150	91	11

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 11.

All (91) 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:822:LYS:CD	1:B:822:LYS:CG	1.79	1.53
1:A:756:MET:CG	1:A:756:MET:CB	1.80	1.53
1:A:775:MET:CE	1:A:775:MET:SD	2.02	1.45
1:B:908:MET:CE	1:B:908:MET:SD	2.04	1.45
1:B:822:LYS:CE	1:B:822:LYS:NZ	1.80	1.41
1:B:728:SER:HB3	5:B:256:HOH:O	1.17	1.31
1:B:775:MET:SD	1:B:775:MET:CE	1.18	1.27
1:A:815:GLN:HG2	5:A:216:HOH:O	1.20	1.27
1:B:775:MET:CG	1:B:775:MET:CE	2.10	1.27
1:A:710:THR:HG21	5:A:127:HOH:O	1.02	1.18
1:B:775:MET:HE1	1:B:775:MET:SD	1.76	1.10
1:A:815:GLN:CG	5:A:216:HOH:O	1.82	1.08
1:B:775:MET:SD	1:B:775:MET:HE2	1.76	1.07
1:B:775:MET:SD	1:B:775:MET:HE3	1.76	1.07
1:A:815:GLN:NE2	5:A:216:HOH:O	1.88	1.05
1:A:692:MET:HG2	5:A:53:HOH:O	1.60	1.02
1:B:860:GLN:OE1	5:B:164:HOH:O	1.82	0.98
1:A:684:ILE:HG21	1:A:689:ASN:HD21	1.32	0.94
1:A:791:GLU:HB2	5:A:275:HOH:O	1.71	0.90
1:B:698:VAL:CG2	5:B:137:HOH:O	2.19	0.89
1:B:775:MET:HG2	1:B:775:MET:CE	2.11	0.81
1:B:860:GLN:NE2	1:B:865:SER:OG	2.13	0.81
1:A:756:MET:SD	1:A:756:MET:CB	2.69	0.80
1:B:775:MET:CG	1:B:775:MET:HE3	1.97	0.80
1:B:710:THR:HG22	1:B:713:SER:H	1.46	0.80
1:A:684:ILE:HG21	1:A:689:ASN:ND2	1.95	0.79
1:B:775:MET:HE2	1:B:785:ASN:HB3	1.64	0.78
1:B:775:MET:CE	1:B:785:ASN:HB3	2.16	0.76
1:A:885:LYS:HG2	5:A:146:HOH:O	1.88	0.73
1:A:815:GLN:CD	5:A:216:HOH:O	1.93	0.71
1:B:775:MET:HG2	1:B:775:MET:HE3	1.68	0.70
1:B:720:GLN:HG3	5:B:161:HOH:O	1.90	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:VAL:HG12	5:B:118:HOH:O	1.93	0.68
1:A:696:PRO:HB3	1:A:728:SER:OG	1.93	0.68
1:A:881:HIS:HD2	5:A:18:HOH:O	1.77	0.68
2:B:302:MOF:H71	2:B:302:MOF:H121	1.74	0.68
1:A:710:THR:CG2	5:A:127:HOH:O	1.84	0.67
1:A:916:GLN:OE1	1:A:919:LYS:HE3	1.96	0.66
1:B:822:LYS:CD	1:B:822:LYS:CB	2.72	0.66
1:B:822:LYS:CE	1:B:822:LYS:CG	2.75	0.65
1:B:698:VAL:HG23	5:B:137:HOH:O	1.88	0.65
1:A:684:ILE:CG2	1:A:689:ASN:ND2	2.60	0.64
1:B:881:HIS:HD2	4:B:501:GOL:O3	1.79	0.64
1:A:756:MET:CA	1:A:756:MET:CG	2.72	0.63
1:B:931:HIS:CE1	5:B:65:HOH:O	2.52	0.62
1:B:723:GLU:O	1:B:727:LEU:HD13	2.00	0.61
1:A:703:HIS:HD2	1:A:717:SER:OG	1.82	0.61
1:B:698:VAL:HG22	5:B:137:HOH:O	1.89	0.61
1:A:692:MET:CG	5:A:53:HOH:O	2.32	0.59
1:B:698:VAL:HA	5:B:137:HOH:O	2.03	0.58
1:B:695:GLU:OE2	1:B:822:LYS:HE2	2.03	0.58
1:B:775:MET:CG	1:B:775:MET:HE2	2.21	0.56
1:B:715:LEU:HD22	2:B:302:MOF:H122	1.88	0.55
1:A:775:MET:CG	1:A:775:MET:CE	2.84	0.54
2:B:302:MOF:H311	2:B:302:MOF:O21	2.08	0.54
1:B:822:LYS:CD	1:B:822:LYS:NZ	2.70	0.53
1:B:710:THR:HB	1:B:713:SER:OG	2.09	0.52
1:B:728:SER:CB	5:B:256:HOH:O	1.99	0.52
1:A:692:MET:CB	5:A:53:HOH:O	2.57	0.52
1:B:860:GLN:HB3	1:B:866:SER:OG	2.11	0.51
1:A:723:GLU:CD	1:A:906:PRO:HB2	2.32	0.50
2:B:302:MOF:C7	2:B:302:MOF:H121	2.41	0.50
1:B:908:MET:CG	1:B:908:MET:CE	2.89	0.50
1:A:897:GLN:HG3	1:A:901:LEU:HD22	1.94	0.49
1:A:780:PRO:HG3	5:A:266:HOH:O	2.12	0.49
1:B:931:HIS:HE1	5:B:65:HOH:O	1.90	0.49
2:A:301:MOF:O17	2:A:301:MOF:C5	2.58	0.49
1:A:771:VAL:HB	5:A:268:HOH:O	2.13	0.49
1:A:684:ILE:CG2	1:A:689:ASN:HD21	2.13	0.48
1:A:684:ILE:O	1:A:684:ILE:CG2	2.59	0.48
1:B:726:LEU:HD21	1:B:908:MET:HG2	1.94	0.48
1:B:696:PRO:HB3	1:B:728:SER:OG	2.14	0.48
1:B:881:HIS:HE1	1:B:928:LEU:O	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:GLN:HE21	1:B:865:SER:CB	2.28	0.47
1:A:810:LYS:NZ	5:A:204:HOH:O	2.46	0.47
1:B:784:LEU:HD22	1:B:788:ARG:HD3	1.97	0.46
1:A:864:VAL:O	1:A:868:GLN:HG3	2.16	0.46
1:A:684:ILE:HA	1:A:685:PRO:HD3	1.83	0.46
1:A:703:HIS:HE1	5:A:242:HOH:O	1.98	0.45
2:B:302:MOF:O17	2:B:302:MOF:C5	2.64	0.45
1:B:825:LEU:HD23	1:B:825:LEU:HA	1.87	0.44
1:A:765:TRP:CZ2	1:A:769:LYS:HD3	2.52	0.44
1:A:727:LEU:HG	1:A:731:LYS:HE2	1.98	0.44
1:A:917:LEU:HD12	1:A:917:LEU:HA	1.87	0.44
1:B:726:LEU:HG	1:B:908:MET:SD	2.57	0.43
1:A:899:ARG:HG3	1:A:899:ARG:HH11	1.83	0.43
1:A:881:HIS:HE1	1:A:928:LEU:O	2.02	0.43
2:A:301:MOF:H83	2:A:301:MOF:O21	2.18	0.43
1:B:690[A]:LEU:HD23	1:B:737:PRO:HG2	2.01	0.42
1:A:874:THR:HB	1:A:930:PHE:CG	2.54	0.42
1:A:755:TRP:CH2	1:A:909:MET:HE2	2.56	0.41

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:MET:CG	5:A:259:HOH:O[2_555]	1.18	1.02
3:B:402:SO4:S	5:A:173:HOH:O[1_554]	1.54	0.66
1:B:812:GLN:CG	5:B:253:HOH:O[2_655]	1.59	0.61
3:B:402:SO4:O3	5:A:173:HOH:O[1_554]	1.69	0.51
1:A:775:MET:CG	5:A:225:HOH:O[2_546]	1.74	0.46
1:A:744:ILE:CG1	5:A:245:HOH:O[2_556]	1.74	0.46
1:B:812:GLN:CB	5:B:253:HOH:O[2_655]	1.81	0.39
1:B:775:MET:SD	5:B:89:HOH:O[2_655]	1.92	0.28
5:A:225:HOH:O	5:A:268:HOH:O[2_556]	1.97	0.23
3:B:402:SO4:O4	5:A:173:HOH:O[1_554]	1.98	0.22
1:B:683:LEU:CA	5:A:260:HOH:O[1_554]	2.13	0.07

## 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	246/259 (95%)	239 (97%)	7 (3%)	0	100	100
1	B	248/259 (96%)	242 (98%)	6 (2%)	0	100	100
All	All	494/518 (95%)	481 (97%)	13 (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	227/240 (95%)	216 (95%)	11 (5%)	25	2
1	B	229/240 (95%)	226 (99%)	3 (1%)	69	40
All	All	456/480 (95%)	442 (97%)	14 (3%)	40	9

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	684	ILE
1	A	790	LYS
1	A	802	TRP
1	A	815	GLN
1	A	825	LEU
1	A	865	SER
1	A	867	SER
1	A	897	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	899	ARG
1	A	901	LEU
1	A	919	LYS
1	B	697	ASP
1	B	710	THR
1	B	769	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	689	ASN
1	A	703	HIS
1	A	725	GLN
1	A	741	ASN
1	A	747	GLN
1	A	787	GLN
1	A	812	GLN
1	A	881	HIS
1	A	897	GLN
1	B	689	ASN
1	B	703	HIS
1	B	705	ASN
1	B	725	GLN
1	B	741	ASN
1	B	747	GLN
1	B	860	GLN
1	B	881	HIS
1	B	931	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 carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	SO4	B	402	-	4,4,4	0.27	0	6,6,6	3.28	3 (50%)
4	GOL	B	501	-	5,5,5	0.45	0	5,5,5	1.97	2 (40%)
2	MOF	A	301	-	30,39,39	2.56	8 (26%)	43,64,64	2.82	20 (46%)
2	MOF	B	302	-	30,39,39	2.44	9 (30%)	43,64,64	3.57	23 (53%)

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
4	GOL	B	501	-	-	0/4/4/4	-
2	MOF	A	301	-	-	2/15/93/93	0/5/5/5
2	MOF	B	302	-	-	2/15/93/93	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MOF	C33-C30	10.08	1.49	1.33
2	B	302	MOF	C32-C29	6.85	1.44	1.34
2	B	302	MOF	C33-C30	6.49	1.43	1.33
2	A	301	MOF	C1-C5	-4.08	1.45	1.53
2	B	302	MOF	C24-C30	3.82	1.54	1.50
2	B	302	MOF	O4-C11	3.56	1.42	1.34
2	A	301	MOF	C32-C29	3.34	1.39	1.34
2	A	301	MOF	C7-C15	-3.20	1.48	1.53
2	A	301	MOF	C1-C3	-3.11	1.53	1.57
2	B	302	MOF	C1-C3	-2.94	1.53	1.57
2	A	301	MOF	C9-C3	-2.86	1.48	1.54
2	B	302	MOF	C6-C14	-2.85	1.48	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	MOF	C7-C15	-2.70	1.49	1.53
2	A	301	MOF	C26-C29	2.47	1.54	1.50
2	B	302	MOF	C33-C34	2.41	1.51	1.45
2	A	301	MOF	O13-C5	2.27	1.25	1.21
2	B	302	MOF	C20-C14	2.20	1.57	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	MOF	C30-C33-C34	-9.11	113.71	121.47
2	B	302	MOF	C29-C32-C34	-9.10	114.77	122.72
2	B	302	MOF	C33-C34-C32	8.49	125.79	117.13
2	A	301	MOF	C2-C6-C14	6.92	119.18	113.73
2	B	302	MOF	C7-C2-C6	6.30	113.61	108.03
2	A	301	MOF	C30-C33-C34	-6.22	116.18	121.47
3	B	402	SO4	O4-S-O3	5.89	134.19	109.06
2	B	302	MOF	C9-C6-C14	5.72	124.38	119.07
2	A	301	MOF	C26-C29-C24	5.54	119.02	115.61
2	A	301	MOF	C9-C6-C14	5.05	123.76	119.07
2	A	301	MOF	C30-C24-C29	4.87	114.94	112.36
2	B	302	MOF	C24-C29-C32	4.78	125.60	122.12
2	B	302	MOF	C26-C29-C24	4.61	118.45	115.61
2	B	302	MOF	O35-C34-C33	-4.57	114.20	121.56
3	B	402	SO4	O3-S-O2	-4.53	85.64	109.31
2	A	301	MOF	C9-C3-C1	4.53	109.75	105.52
2	A	301	MOF	C7-C2-C1	4.51	119.69	115.85
2	B	302	MOF	C9-C6-C2	4.44	108.55	103.97
2	B	302	MOF	C31-C24-C30	-4.28	102.15	106.63
2	B	302	MOF	O4-C11-O17	-4.04	118.35	124.67
2	B	302	MOF	C8-C2-C6	-3.73	104.58	111.80
4	B	501	GOL	O2-C2-C3	3.68	125.35	109.12
2	B	302	MOF	C2-C1-C3	3.64	107.11	104.47
2	A	301	MOF	C2-C7-C15	-3.31	108.44	113.19
2	A	301	MOF	O13-C5-C1	-3.31	117.16	121.91
2	A	301	MOF	C9-C6-C2	3.13	107.19	103.97
2	B	302	MOF	C2-C6-C14	3.04	116.13	113.73
3	B	402	SO4	O4-S-O2	-2.98	93.73	109.31
2	B	302	MOF	C26-C29-C32	-2.97	115.90	120.87
2	A	301	MOF	C7-C2-C6	2.91	110.62	108.03
2	A	301	MOF	O4-C1-C2	-2.87	100.15	105.19
2	A	301	MOF	O4-C11-C16	-2.85	107.23	111.12
2	B	302	MOF	C2-C7-C15	-2.80	109.16	113.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MOF	C20-C26-C29	-2.79	106.68	111.93
2	A	301	MOF	C10-C3-C1	2.79	126.61	117.15
2	B	302	MOF	C9-C3-C1	2.78	108.12	105.52
2	A	301	MOF	C33-C34-C32	2.76	119.95	117.13
2	B	302	MOF	C7-C2-C1	2.70	118.15	115.85
2	A	301	MOF	C10-C3-C9	-2.65	109.26	113.53
2	B	302	MOF	O21-C15-C7	2.64	116.47	110.19
2	B	302	MOF	O4-C11-C16	2.64	114.71	111.12
2	B	302	MOF	C19-C24-C29	2.60	109.45	106.81
2	A	301	MOF	C8-C2-C6	-2.47	107.02	111.80
2	B	302	MOF	C20-C26-C29	-2.41	107.39	111.93
2	A	301	MOF	C8-C2-C7	-2.38	107.83	111.11
2	A	301	MOF	C24-C29-C32	-2.36	120.41	122.12
2	B	302	MOF	C24-C30-C33	2.16	125.95	124.38
4	B	501	GOL	C3-C2-C1	-2.13	103.41	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MOF	C2-C1-C5-O13
2	B	302	MOF	C2-C1-C5-O13
2	A	301	MOF	C2-C1-C5-C12
2	B	302	MOF	C3-C1-C5-O13

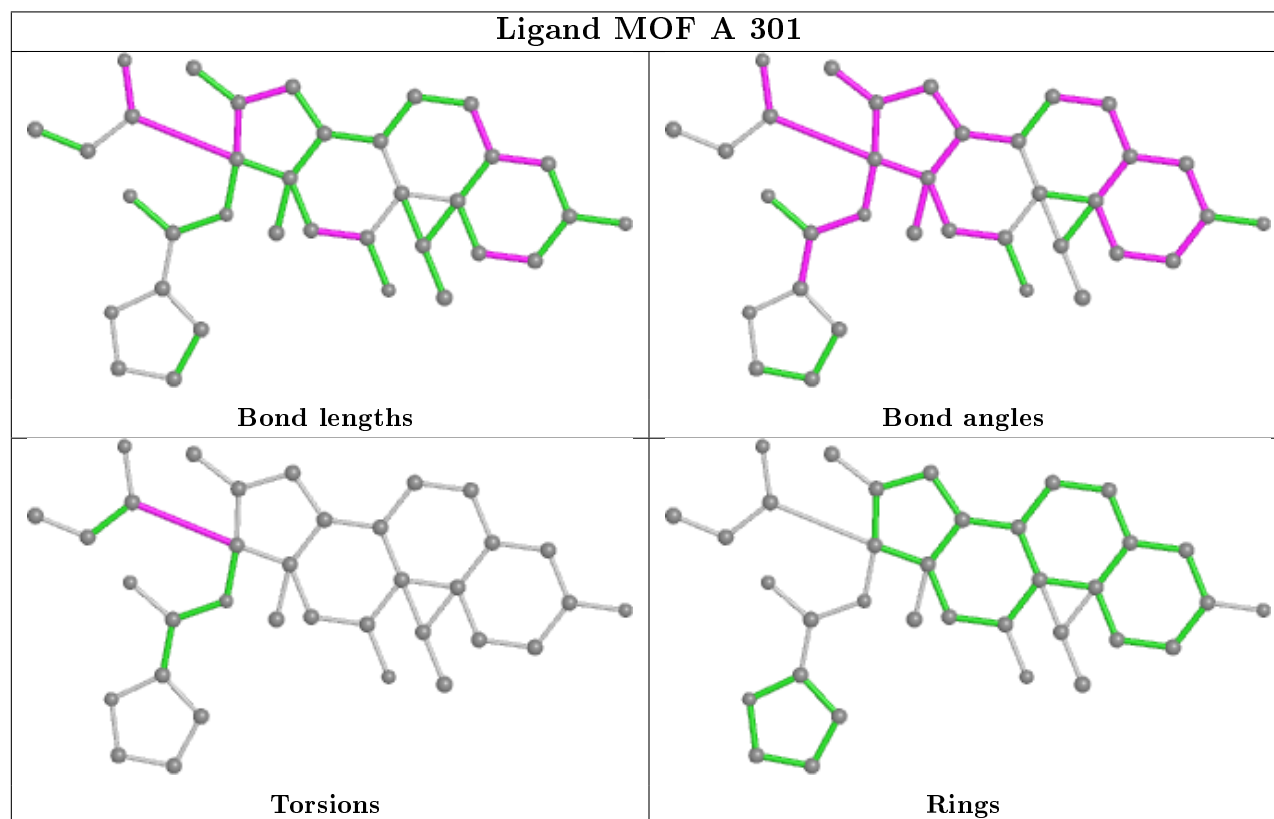
There are no ring outliers.

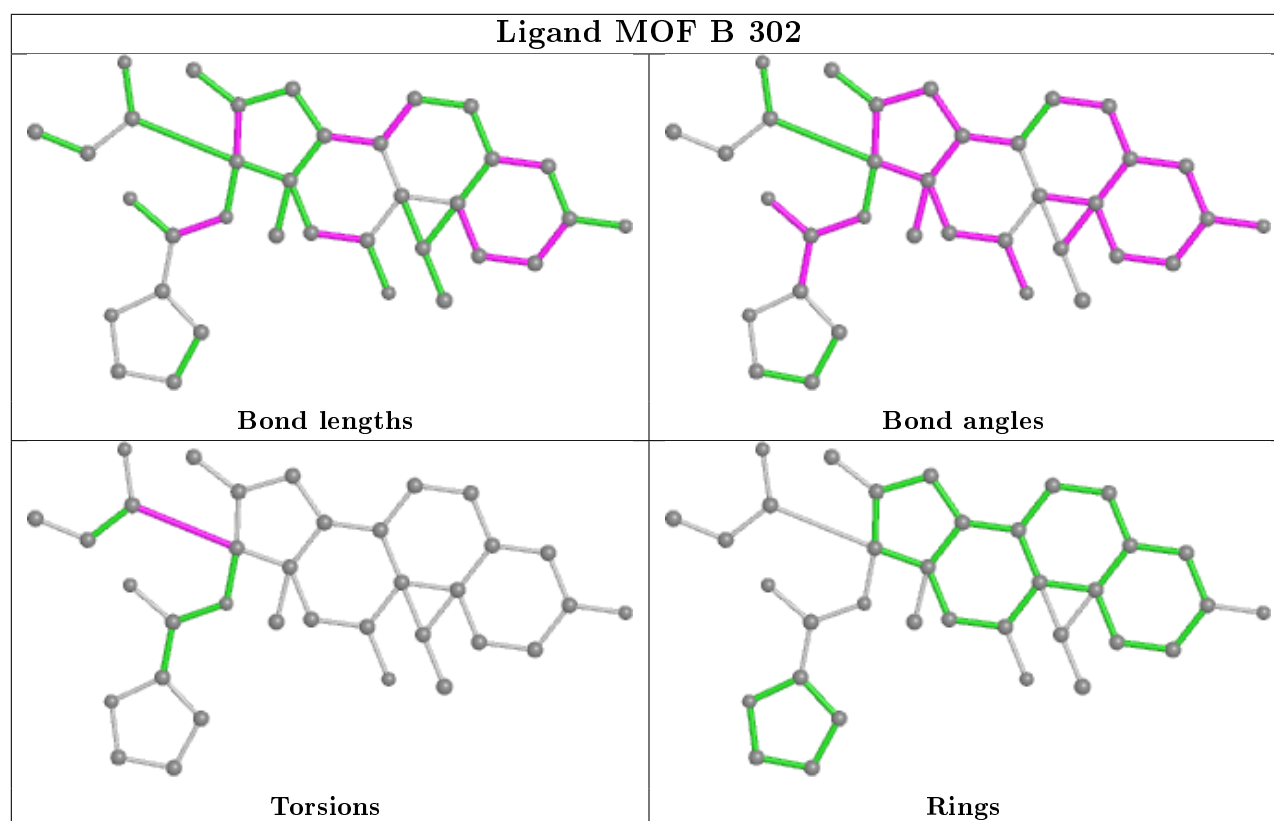
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SO4	0	3
4	B	501	GOL	1	0
2	A	301	MOF	2	0
2	B	302	MOF	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	249/259 (96%)	0.11	18 (7%) 15 17	12, 19, 41, 52	4 (1%)
1	B	249/259 (96%)	-0.02	11 (4%) 34 37	10, 17, 31, 43	2 (0%)
All	All	498/518 (96%)	0.05	29 (5%) 23 25	10, 18, 37, 52	6 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	LEU	7.0
1	A	864	VAL	6.9
1	A	708	PRO	5.1
1	A	901	LEU	4.9
1	A	863	VAL	4.9
1	A	862	GLY	4.2
1	B	708	PRO	4.2
1	B	860	GLN	4.1
1	A	682	GLN	3.9
1	A	900	ALA	3.8
1	A	932	LYS	3.6
1	A	902	SER	3.6
1	B	706	THR	3.5
1	B	871	TYR	3.3
1	A	704	ASP	3.1
1	A	861	LYS	3.1
1	A	709	ASP	3.0
1	B	784	LEU	2.9
1	A	684	ILE	2.9
1	A	710	THR	2.6
1	A	860	GLN	2.6
1	B	861	LYS	2.4
1	A	865	SER	2.4
1	A	899	ARG	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	718	LEU	2.3
1	B	702	GLY	2.2
1	B	698	VAL	2.1
1	B	864	VAL	2.1
1	B	683	LEU	2.1

## 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.

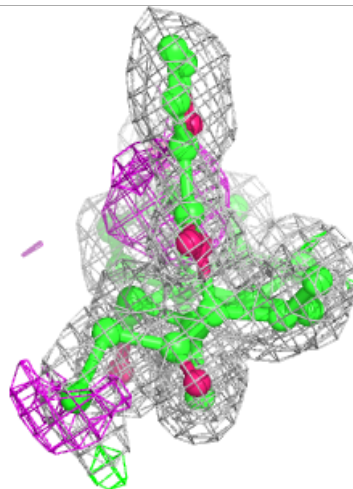
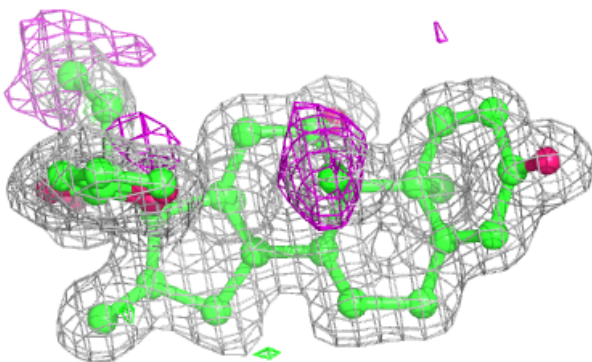
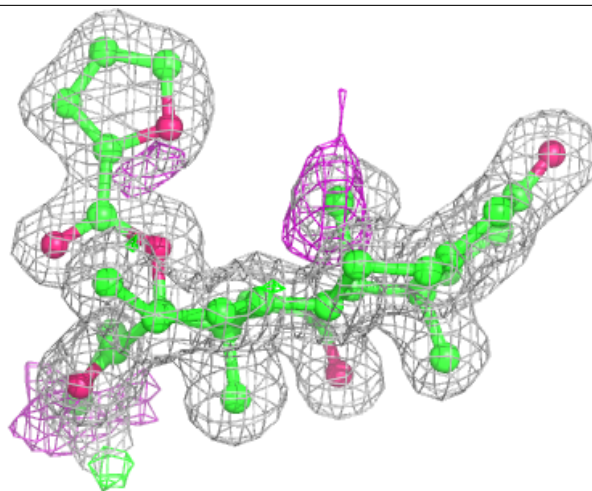
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MOF	B	302	35/35	0.91	0.10	15,18,26,44	0
2	MOF	A	301	35/35	0.93	0.08	13,18,23,36	0
4	GOL	B	501	6/6	0.96	0.07	21,22,26,28	0
3	SO4	B	402	5/5	0.99	0.06	20,20,26,31	0

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.



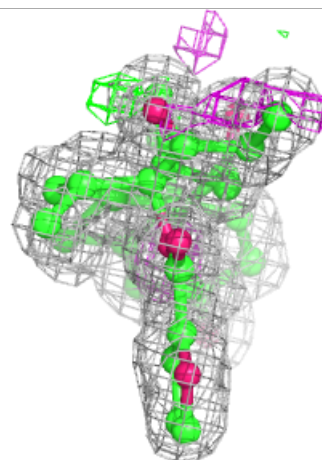
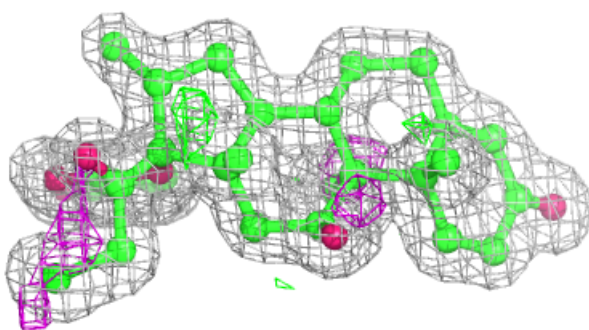
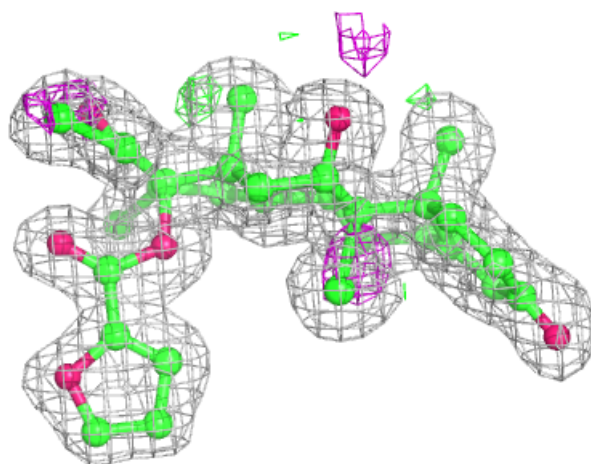
**Electron density around MOF B 302:**

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



**Electron density around MOF A 301:**

$2mF_o-DF_c$  (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.