



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:00 am BST

PDB ID : 5JJM  
Title : Crystal Structure of Homodimeric Androgen Receptor Ligand-Binding Domain bound to DHT and LxxLL peptide  
Authors : Estebanez-Perpina, E.; Fuentes-Prior, P.  
Deposited on : 2016-04-24  
Resolution : 2.15 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

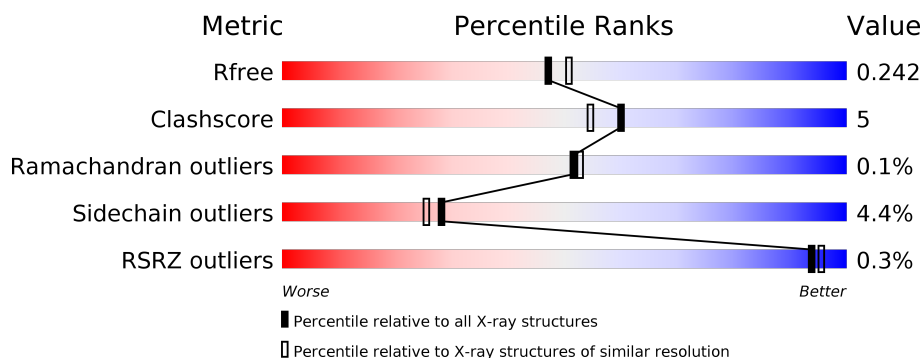
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	252	<div> <div style="width: 84%;"></div> <div style="width: 16%;"></div> </div>
1	C	252	<div> <div style="width: 80%;"></div> <div style="width: 18%;"></div> <div style="width: 2%;"></div> </div>
1	D	252	<div> <div style="width: 83%;"></div> <div style="width: 14%;"></div> <div style="width: 3%;"></div> </div>
2	F	3	<div> <div style="width: 67%;"></div> <div style="width: 33%;"></div> </div>
2	K	3	<div> <div style="width: 33%;"></div> <div style="width: 100%;"></div> </div>
2	L	3	<div> <div style="width: 100%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	M	3	
3	B	252	
4	G	8	
4	H	8	
4	I	8	
4	J	8	

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
2	FME	L	503	-	X	-	-
9	GOL	A	1005	-	X	-	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 8848 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 Androgen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	3	0
			2073	1340	356	358	19			
1	C	250	Total	C	N	O	S	0	3	0
			2052	1327	353	352	20			
1	D	249	Total	C	N	O	S	0	2	0
			2041	1320	351	350	20			

- Molecule 2 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	3	Total	C	N	O	S	0	0	0
			24	13	3	7	1			
2	F	3	Total	C	N	O	S	0	0	0
			24	13	3	7	1			
2	K	3	Total	C	N	O	S	0	0	0
			24	13	3	7	1			
2	L	3	Total	C	N	O	S	0	0	0
			24	13	3	7	1			

- Molecule 3 is a protein called Androgen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	251	Total	C	N	O	S	0	3	0
			2060	1329	354	356	21			

- Molecule 4 is a protein called uba3-derived peptide.

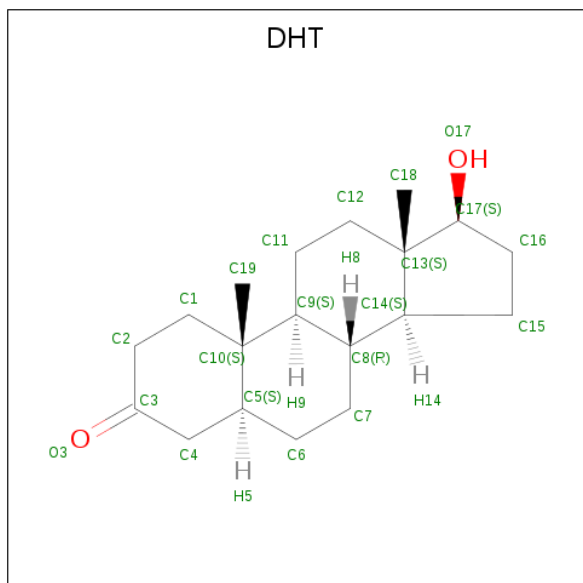
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			58	39	8	11			
4	H	8	Total	C	N	O	0	0	0
			65	43	9	13			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	8	Total	C	N	O	0	0	0
			65	43	9	13			
4	J	8	Total	C	N	O	0	0	0
			65	43	9	13			

- Molecule 5 is 5-ALPHA-DIHYDROTESTOSTERONE (three-letter code: DHT) (formula:  $C_{19}H_{30}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	19	2		
5	B	1	Total	C	O	0	0
			21	19	2		
5	C	1	Total	C	O	0	0
			21	19	2		
5	D	1	Total	C	O	0	0
			21	19	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

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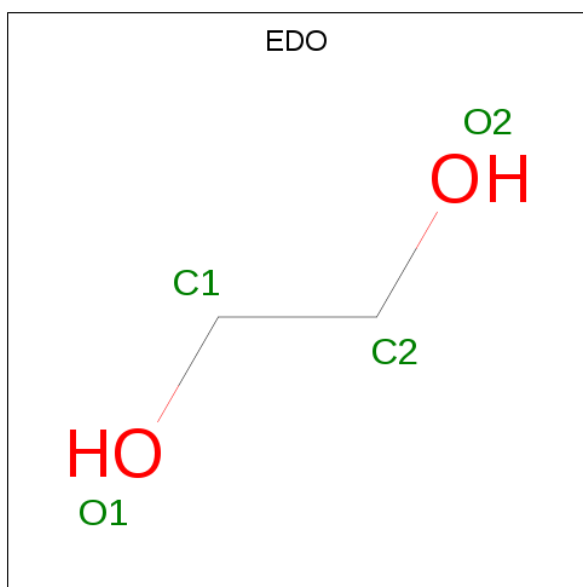
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



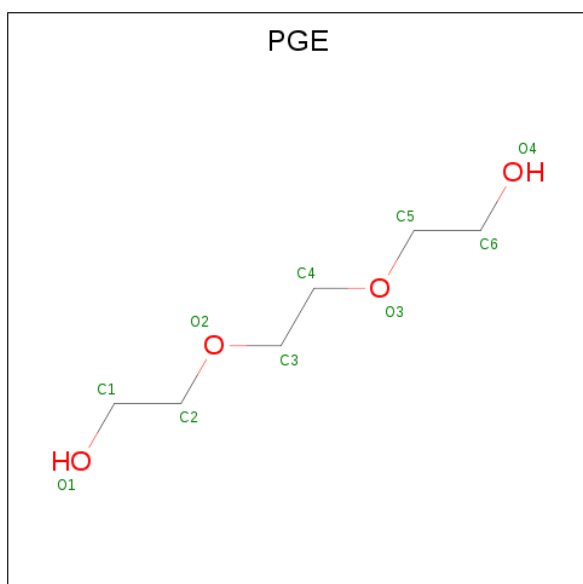
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

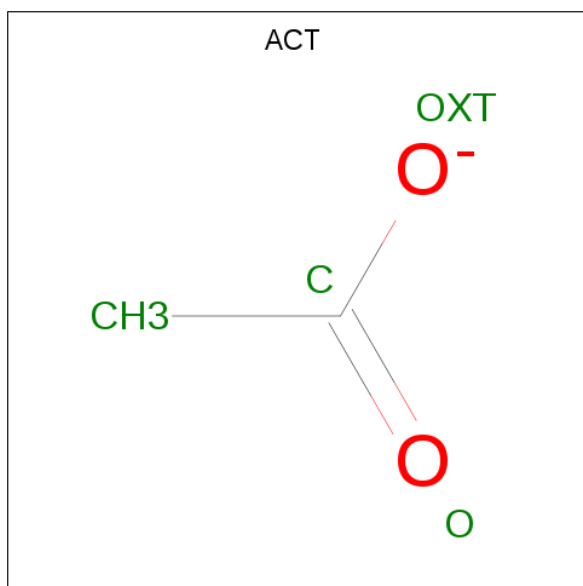
- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 12 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

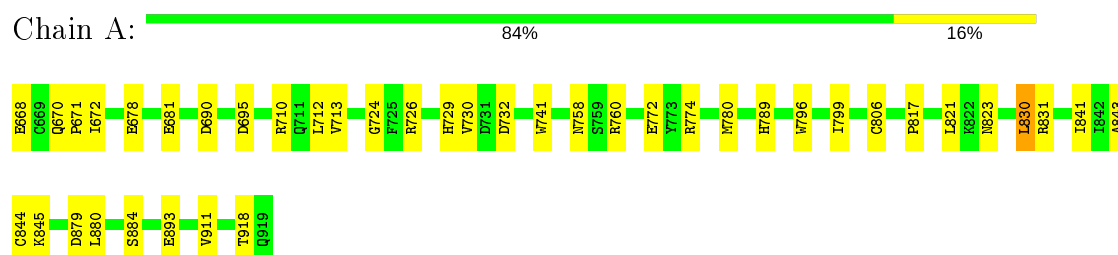
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	26	Total	O	0	0
			26	26		
13	B	21	Total	O	0	0
			21	21		
13	C	28	Total	O	0	0
			28	28		
13	D	24	Total	O	0	0
			24	24		

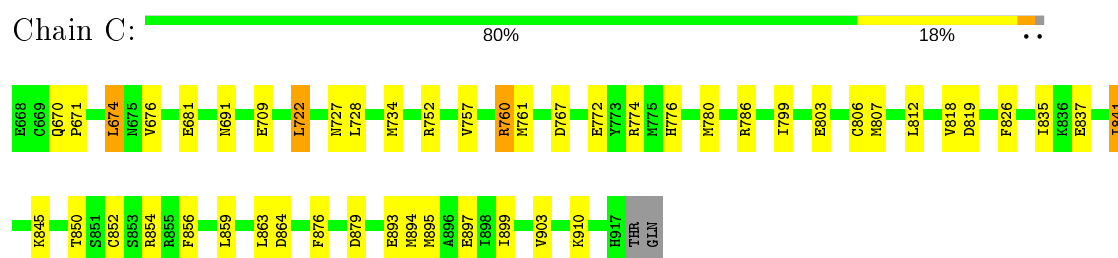
### 3 Residue-property plots

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.

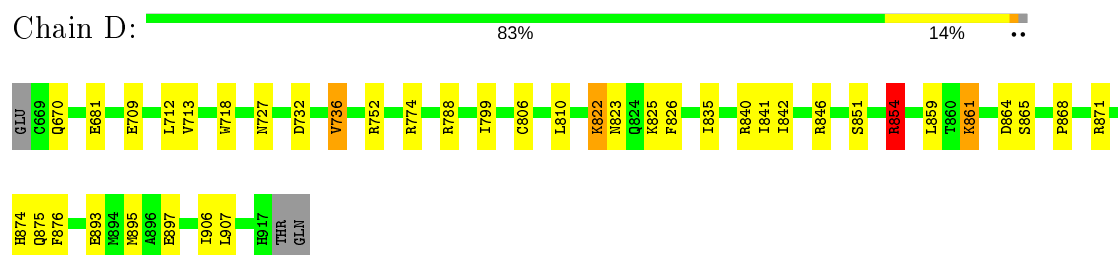
- Molecule 1: Androgen receptor



- Molecule 1: Androgen receptor



- Molecule 1: Androgen receptor



- Molecule 2: Unknown peptide



- Molecule 2: Unknown peptide

Chain F:  67% 33%



- Molecule 2: Unknown peptide

Chain K:  33% 100%




- Molecule 2: Unknown peptide

Chain L:  100%

There are no outlier residues recorded for this chain.

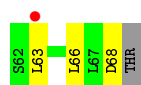
- Molecule 3: Androgen receptor

Chain B:  83% 14%



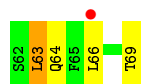
- Molecule 4: uba3-derived peptide

Chain G:  13% 50% 38% 13%



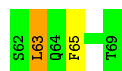
- Molecule 4: uba3-derived peptide

Chain H:  13% 50% 38% 13%



- Molecule 4: uba3-derived peptide

Chain I:  75% 13% 13%



- Molecule 4: uba3-derived peptide

Chain J:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.09Å 91.01Å 157.23Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	157.23 – 2.15 64.38 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (157.23-2.15) 99.4 (64.38-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.201 , 0.243 0.200 , 0.242	Depositor DCC
$R_{free}$ test set	3444 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.348 for k,h,-l 0.357 for -k,-h,-l 0.317 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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, ZN, PGE, SNC, CL, EDO, SO4, ACT, FME, DHT

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	1.30	4/2135 (0.2%)	1.22	9/2884 (0.3%)
1	C	1.30	5/2121 (0.2%)	1.23	14/2863 (0.5%)
1	D	1.30	4/2102 (0.2%)	1.18	11/2838 (0.4%)
2	F	1.19	0/13	1.77	0/16
2	K	1.77	0/13	1.26	0/16
2	L	1.53	0/13	1.33	0/16
2	M	0.70	0/13	0.88	0/16
3	B	1.22	4/2117 (0.2%)	1.18	9/2855 (0.3%)
4	G	1.01	0/58	1.24	0/77
4	H	0.96	0/65	1.02	0/87
4	I	0.91	0/65	1.01	0/87
4	J	0.96	0/65	1.25	0/87
All	All	1.27	17/8780 (0.2%)	1.20	43/11842 (0.4%)

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
3	B	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	852	CYS	C-N	14.04	1.66	1.34
1	A	741	TRP	CZ3-CH2	6.89	1.51	1.40
1	C	803	GLU	CD-OE1	6.27	1.32	1.25
1	A	681	GLU	CD-OE2	6.25	1.32	1.25
1	D	876	PHE	CG-CD2	5.88	1.47	1.38
1	D	681	GLU	CD-OE2	5.55	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	854	ARG	CZ-NH1	5.54	1.40	1.33
1	A	796	TRP	CG-CD1	5.44	1.44	1.36
1	A	678	GLU	CD-OE1	5.44	1.31	1.25
1	D	897	GLU	CG-CD	5.39	1.60	1.51
3	B	829	GLU	CG-CD	5.39	1.60	1.51
1	D	718	TRP	CE3-CZ3	5.39	1.47	1.38
3	B	718	TRP	CE3-CZ3	5.27	1.47	1.38
1	C	681	GLU	CD-OE2	5.24	1.31	1.25
3	B	897	GLU	CG-CD	5.20	1.59	1.51
3	B	796	TRP	CE3-CZ3	5.06	1.47	1.38
1	C	864	ASP	CB-CG	5.03	1.62	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	805	LEU	CB-CG-CD1	11.01	129.72	111.00
1	C	864	ASP	CB-CG-OD1	9.96	127.27	118.30
1	A	831	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	D	752	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	726	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	C	752	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	C	728	LEU	CB-CG-CD2	-8.35	96.81	111.00
1	A	726	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	C	854	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	D	774	ARG	NE-CZ-NH2	-7.29	116.66	120.30
3	B	787	MET	CG-SD-CE	7.17	111.68	100.20
1	A	690	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	830	LEU	CB-CG-CD1	-7.06	99.00	111.00
1	A	774	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	780	MET	CG-SD-CE	-6.80	89.32	100.20
1	C	879	ASP	CB-CG-OD1	6.76	124.39	118.30
1	C	774	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	D	774	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	D	864	ASP	CB-CG-OD1	6.41	124.06	118.30
1	C	774	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	879	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	788	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	861	LYS	CA-CB-CG	6.13	126.88	113.40
1	A	690	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	786	ARG	NE-CZ-NH2	-6.09	117.25	120.30
3	B	690	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	854	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	831	ARG	NE-CZ-NH1	-6.02	117.29	120.30
3	B	907	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	C	674	LEU	CA-CB-CG	5.74	128.51	115.30
3	B	855	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	712	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	C	761	MET	CG-SD-CE	-5.54	91.33	100.20
3	B	788	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	864	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	760	ARG	NE-CZ-NH1	5.33	122.97	120.30
3	B	883	LYS	CD-CE-NZ	5.32	123.93	111.70
1	D	752	ARG	CB-CA-C	-5.21	99.97	110.40
1	C	786	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	895	MET	CG-SD-CE	-5.21	91.87	100.20
1	D	846	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	840	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	B	838	LEU	CB-CG-CD1	5.00	119.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	685	VAL	Mainchain

## 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	2073	0	2089	21	1
1	C	2052	0	2062	21	0
1	D	2041	0	2060	20	0
2	F	24	0	18	1	0
2	K	24	0	18	0	0
2	L	24	0	18	0	0
2	M	24	0	18	4	0
3	B	2060	0	2076	18	0
4	G	58	0	58	1	0
4	H	65	0	65	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	65	0	65	1	0
4	J	65	0	65	2	0
5	A	21	0	30	0	0
5	B	21	0	30	0	0
5	C	21	0	30	0	0
5	D	21	0	30	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	1	0
8	A	4	0	6	2	0
8	B	12	0	18	0	0
8	C	4	0	6	0	0
8	D	12	0	18	0	0
9	A	6	0	8	1	0
9	C	6	0	8	1	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
10	C	10	0	0	0	0
10	D	5	0	0	0	0
11	C	10	0	14	1	0
12	D	4	0	3	0	0
13	A	26	0	0	1	1
13	B	21	0	0	0	0
13	C	28	0	0	2	0
13	D	24	0	0	0	0
All	All	8848	0	8813	81	1

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 5.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:CYS:SG	1:A:841:ILE:HD12	1.59	1.43
1:A:806:CYS:SG	1:A:841:ILE:CD1	2.28	1.21
1:A:843:ALA:HB2	2:M:503:FME:CE	2.12	0.80
1:A:710:ARG:HH12	8:A:1004:EDO:H22	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:GLU:HG3	1:C:676:VAL:HG21	1.73	0.68
3:B:734:MET:SD	4:H:63:LEU:HD13	2.33	0.68
1:D:871:ARG:O	1:D:875[A]:GLN:HG3	1.95	0.67
1:A:806:CYS:SG	1:A:841:ILE:HD11	2.34	0.67
1:A:843:ALA:HB2	2:M:503:FME:HE3	1.77	0.66
1:D:713:VAL:HG22	4:J:66:LEU:HD11	1.79	0.64
3:B:801:PRO:HB3	9:C:1004:GOL:H31	1.80	0.64
1:D:893:GLU:HG2	7:D:1003:CL:CL	2.38	0.61
1:A:806:CYS:HG	1:A:841:ILE:CD1	2.14	0.59
3:B:760:ARG:C	3:B:761[B]:MET:HG2	2.22	0.59
1:A:758:ASN:OD1	9:A:1005:GOL:H11	2.02	0.59
1:D:823:ASN:HD22	1:D:826:PHE:CB	2.17	0.58
3:B:780:MET:HG2	3:B:876:PHE:CZ	2.39	0.58
1:A:724:GLY:HA3	1:A:830:LEU:HD21	1.86	0.56
3:B:735:ALA:HB1	3:B:739:TYR:CE2	2.41	0.56
1:C:806[A]:CYS:SG	1:C:841:ILE:HG12	2.46	0.56
1:A:729:HIS:HB2	1:A:823[A]:ASN:OD1	2.06	0.56
1:D:851:SER:HA	1:D:854:ARG:HG3	1.89	0.55
1:A:710:ARG:NH1	8:A:1004:EDO:H22	2.20	0.55
1:A:789:HIS:HB2	13:A:1126:HOH:O	2.07	0.55
1:C:899:ILE:O	1:C:903:VAL:HB	2.07	0.55
1:A:843:ALA:HB2	2:M:503:FME:HE2	1.89	0.54
1:D:727:ASN:HB2	1:D:826:PHE:CE2	2.42	0.54
1:D:732:ASP:O	1:D:736:VAL:HG13	2.07	0.53
3:B:786:ARG:HH22	3:B:868:PRO:HB2	1.73	0.53
1:D:799:ILE:CD1	1:D:859:LEU:HD22	2.38	0.53
1:D:823:ASN:HD22	1:D:826:PHE:HB2	1.75	0.52
1:C:727:ASN:HB2	1:C:826:PHE:CE2	2.45	0.51
1:D:823:ASN:ND2	1:D:826:PHE:H	2.08	0.51
4:H:64:GLN:HA	4:H:64:GLN:OE1	2.10	0.51
3:B:843:ALA:HB2	2:F:503:FME:HE3	1.93	0.50
3:B:842:ILE:HD11	3:B:859:LEU:HD12	1.93	0.50
1:D:799:ILE:CD1	1:D:859:LEU:CD2	2.89	0.50
1:D:799:ILE:HD11	1:D:859:LEU:CD2	2.42	0.50
1:C:837:GLU:O	1:C:841:ILE:HD13	2.12	0.49
1:D:799:ILE:HD11	1:D:859:LEU:HD22	1.93	0.49
1:C:722:LEU:HD12	1:C:812:LEU:CD2	2.43	0.49
1:C:799:ILE:CD1	1:C:859:LEU:CD2	2.91	0.49
3:B:845:LYS:HE3	3:B:846:ARG:HH22	1.78	0.48
3:B:732:ASP:O	3:B:736:VAL:HG13	2.14	0.48
4:J:66:LEU:HA	4:J:66:LEU:HD23	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:780:MET:HG2	1:C:876:PHE:CZ	2.49	0.47
1:A:713:VAL:HG22	4:G:66:LEU:HD21	1.97	0.47
3:B:786:ARG:NH2	3:B:868:PRO:HB2	2.31	0.46
1:C:670:GLN:HA	1:C:671:PRO:HD3	1.86	0.46
1:D:875[A]:GLN:HG2	1:D:907:LEU:HD22	1.98	0.45
1:A:843:ALA:CB	2:M:503:FME:HE2	2.47	0.45
1:C:807:MET:HB3	1:C:863:LEU:HD21	1.99	0.45
1:D:865:SER:O	1:D:868:PRO:HD2	2.17	0.45
1:C:691:ASN:HB2	13:C:1118:HOH:O	2.17	0.44
3:B:673:PHE:N	3:B:837:GLU:OE1	2.39	0.44
1:C:845:LYS:HE3	13:C:1105:HOH:O	2.17	0.44
3:B:847:LYS:HD3	3:B:847:LYS:N	2.32	0.44
1:C:727:ASN:HB2	1:C:826:PHE:CZ	2.53	0.44
1:A:732:ASP:CG	1:A:821:LEU:HB3	2.38	0.44
1:C:709:GLU:OE1	1:C:894:MET:HB3	2.18	0.43
1:D:709:GLU:OE1	1:D:895:MET:HG2	2.18	0.43
1:C:835:ILE:HG23	1:C:856:PHE:CZ	2.54	0.43
3:B:772:GLU:H	3:B:772:GLU:CD	2.22	0.43
3:B:713:VAL:HG22	4:H:66:LEU:HD11	2.01	0.43
3:B:863:LEU:HA	3:B:863:LEU:HD23	1.91	0.42
1:D:806[A]:CYS:SG	1:D:841:ILE:HD13	2.60	0.42
1:C:767:ASP:N	1:C:767:ASP:OD1	2.53	0.42
1:A:817:PRO:HA	1:A:911:VAL:HA	2.02	0.41
1:A:670:GLN:HA	1:A:671:PRO:HD3	1.89	0.41
1:A:880:LEU:O	1:A:884:SER:HB3	2.20	0.41
1:C:671:PRO:HB3	1:C:841:ILE:HD11	2.02	0.41
1:D:822:LYS:HA	1:D:822:LYS:HD2	1.79	0.41
1:D:874:HIS:CE1	1:D:906:ILE:HD13	2.55	0.41
1:C:799:ILE:HD11	1:C:859:LEU:CD2	2.49	0.41
1:A:772:GLU:HG2	1:A:772:GLU:H	1.46	0.41
1:C:776:HIS:CE1	11:C:1005:PGE:H1	2.56	0.41
3:B:841:ILE:N	3:B:841:ILE:CD1	2.83	0.41
1:D:810:LEU:HD21	1:D:835:ILE:HG13	2.03	0.40
1:C:757:VAL:O	1:C:760:ARG:HG3	2.22	0.40
3:B:841:ILE:HD12	3:B:841:ILE:N	2.35	0.40
1:C:734:MET:SD	4:I:63:LEU:HD13	2.62	0.40

All (1) 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:A:760:ARG:NH1	13:A:1120:HOH:O[2_455]	2.13	0.07

## 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	253/252 (100%)	243 (96%)	9 (4%)	1 (0%)	34	29
1	C	251/252 (100%)	244 (97%)	7 (3%)	0	100	100
1	D	249/252 (99%)	240 (96%)	9 (4%)	0	100	100
2	F	1/3 (33%)	1 (100%)	0	0	100	100
2	K	1/3 (33%)	1 (100%)	0	0	100	100
2	L	1/3 (33%)	1 (100%)	0	0	100	100
2	M	1/3 (33%)	1 (100%)	0	0	100	100
3	B	251/252 (100%)	244 (97%)	7 (3%)	0	100	100
4	G	5/8 (62%)	5 (100%)	0	0	100	100
4	H	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
4	I	6/8 (75%)	6 (100%)	0	0	100	100
4	J	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
All	All	1031/1052 (98%)	995 (96%)	35 (3%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	695	ASP

### 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	233/230 (101%)	223 (96%)	10 (4%)	29	27
1	C	231/230 (100%)	221 (96%)	10 (4%)	29	27
1	D	229/230 (100%)	222 (97%)	7 (3%)	40	39
2	F	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
2	M	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	B	231/229 (101%)	223 (96%)	8 (4%)	36	34
4	G	7/8 (88%)	5 (71%)	2 (29%)	0	0
4	H	8/8 (100%)	6 (75%)	2 (25%)	0	0
4	I	8/8 (100%)	6 (75%)	2 (25%)	0	0
4	J	8/8 (100%)	7 (88%)	1 (12%)	4	1
All	All	963/959 (100%)	920 (96%)	43 (4%)	28	24

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	668	GLU
1	A	672	ILE
1	A	712[A]	LEU
1	A	712[B]	LEU
1	A	730	VAL
1	A	799	ILE
1	A	844	CYS
1	A	845	LYS
1	A	893	GLU
1	A	918	THR
2	M	505	ASP
3	B	736	VAL
3	B	772	GLU
3	B	805	LEU
3	B	822	LYS
3	B	825	LYS
3	B	845	LYS
3	B	847	LYS

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Mol	Chain	Res	Type
3	B	858	GLN
1	C	674	LEU
1	C	722	LEU
1	C	772	GLU
1	C	818	VAL
1	C	819	ASP
1	C	841	ILE
1	C	850	THR
1	C	893	GLU
1	C	897	GLU
1	C	910	LYS
1	D	670	GLN
1	D	736	VAL
1	D	822	LYS
1	D	825	LYS
1	D	842	ILE
1	D	854	ARG
1	D	861	LYS
4	G	63	LEU
4	G	68	ASP
4	H	63	LEU
4	H	69	THR
4	I	63	LEU
4	I	65	PHE
4	J	62	SER

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

Mol	Chain	Res	Type
1	D	874	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FME	K	503	2,6	8,9,10	1.15	1 (12%)	7,9,11	5.22	4 (57%)
2	FME	L	503	2,6	8,9,10	2.59	1 (12%)	7,9,11	4.87	6 (85%)
2	FME	M	503	2,6	8,9,10	2.13	1 (12%)	7,9,11	5.92	4 (57%)
2	FME	F	503	2,6	8,9,10	2.65	1 (12%)	7,9,11	3.60	1 (14%)
3	SNC	B	686	3	4,7,8	1.68	1 (25%)	1,7,9	0.29	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	FME	K	503	2,6	-	3/7/9/11	-
2	FME	L	503	2,6	-	5/7/9/11	-
2	FME	M	503	2,6	-	5/7/9/11	-
2	FME	F	503	2,6	-	1/7/9/11	-
3	SNC	B	686	3	-	0/0/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	503	FME	CA-N	7.20	1.56	1.46
2	L	503	FME	CA-N	7.00	1.56	1.46
2	M	503	FME	CA-N	5.52	1.54	1.46
3	B	686	SNC	CB-CA	2.29	1.58	1.53
2	K	503	FME	O1-CN	2.08	1.29	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	503	FME	CA-N-CN	14.80	145.59	122.82
2	K	503	FME	CA-N-CN	12.38	141.85	122.82
2	L	503	FME	CA-N-CN	10.59	139.11	122.82
2	F	503	FME	CA-N-CN	8.93	136.55	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	503	FME	O1-CN-N	3.97	135.72	125.27
2	L	503	FME	CE-SD-CG	3.95	113.95	100.40
2	K	503	FME	O1-CN-N	-3.79	115.28	125.27
2	M	503	FME	O1-CN-N	3.42	134.27	125.27
2	K	503	FME	C-CA-N	3.10	115.33	109.73
2	L	503	FME	C-CA-N	2.94	115.04	109.73
2	M	503	FME	CE-SD-CG	2.92	110.43	100.40
2	L	503	FME	CG-CB-CA	2.83	120.81	112.95
2	K	503	FME	O-C-CA	-2.80	117.45	124.78
2	L	503	FME	O-C-CA	-2.35	118.62	124.78
2	M	503	FME	O-C-CA	-2.20	119.01	124.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	503	FME	O1-CN-N-CA
2	L	503	FME	CB-CA-N-CN
2	L	503	FME	C-CA-CB-CG
2	L	503	FME	CA-CB-CG-SD
2	M	503	FME	CB-CA-N-CN
2	M	503	FME	N-CA-CB-CG
2	F	503	FME	CB-CA-N-CN
2	K	503	FME	CA-CB-CG-SD
2	M	503	FME	CA-CB-CG-SD
2	K	503	FME	CB-CG-SD-CE
2	L	503	FME	CB-CG-SD-CE
2	L	503	FME	N-CA-CB-CG
2	M	503	FME	C-CA-CB-CG
2	M	503	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	503	FME	4	0
2	F	503	FME	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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
10	SO4	D	1008	-	4,4,4	0.17	0	6,6,6	1.09	0
10	SO4	B	1007	-	4,4,4	0.32	0	6,6,6	0.43	0
5	DHT	B	1001	-	24,24,24	1.38	3 (12%)	39,39,39	2.05	12 (30%)
10	SO4	C	1006	-	4,4,4	0.36	0	6,6,6	0.80	0
8	EDO	B	1006	-	3,3,3	0.80	0	2,2,2	0.86	0
10	SO4	A	1006	-	4,4,4	0.41	0	6,6,6	0.75	0
11	PGE	C	1005	-	9,9,9	0.88	0	8,8,8	1.03	0
8	EDO	D	1005	-	3,3,3	0.38	0	2,2,2	1.17	0
8	EDO	B	1004	-	3,3,3	1.02	0	2,2,2	0.19	0
5	DHT	D	1001	-	24,24,24	1.56	3 (12%)	39,39,39	2.41	15 (38%)
5	DHT	C	1001	-	24,24,24	1.27	2 (8%)	39,39,39	2.25	15 (38%)
8	EDO	C	1003	-	3,3,3	0.72	0	2,2,2	0.14	0
8	EDO	B	1005	-	3,3,3	1.03	0	2,2,2	0.92	0
5	DHT	A	1001	-	24,24,24	1.73	3 (12%)	39,39,39	2.55	16 (41%)
8	EDO	D	1004	-	3,3,3	0.49	0	2,2,2	0.98	0
12	ACT	D	1006	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
10	SO4	C	1007	-	4,4,4	0.27	0	6,6,6	0.21	0
8	EDO	D	1007	-	3,3,3	1.49	0	2,2,2	1.04	0
9	GOL	C	1004	-	5,5,5	0.54	0	5,5,5	0.91	0
8	EDO	A	1004	-	3,3,3	0.49	0	2,2,2	0.32	0
9	GOL	A	1005	-	5,5,5	0.54	0	5,5,5	2.26	3 (60%)

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
8	EDO	B	1006	-	-	0/1/1/1	-
5	DHT	B	1001	-	-	-	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DHT	A	1001	-	-	-	0/4/4/4
8	EDO	B	1005	-	-	1/1/1/1	-
11	PGE	C	1005	-	-	2/7/7/7	-
8	EDO	D	1005	-	-	0/1/1/1	-
8	EDO	B	1004	-	-	1/1/1/1	-
9	GOL	C	1004	-	-	2/4/4/4	-
5	DHT	C	1001	-	-	-	0/4/4/4
5	DHT	D	1001	-	-	-	0/4/4/4
8	EDO	D	1004	-	-	1/1/1/1	-
8	EDO	D	1007	-	-	0/1/1/1	-
8	EDO	C	1003	-	-	1/1/1/1	-
8	EDO	A	1004	-	-	1/1/1/1	-
9	GOL	A	1005	-	-	4/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	DHT	O17-C17	5.76	1.53	1.43
5	C	1001	DHT	O17-C17	3.93	1.50	1.43
5	B	1001	DHT	O17-C17	3.56	1.49	1.43
5	D	1001	DHT	O17-C17	3.35	1.49	1.43
5	D	1001	DHT	C19-C10	3.17	1.59	1.54
5	A	1001	DHT	O3-C3	2.68	1.26	1.21
5	D	1001	DHT	C10-C9	2.51	1.60	1.56
5	A	1001	DHT	C19-C10	2.32	1.58	1.54
12	D	1006	ACT	CH3-C	2.31	1.51	1.48
5	C	1001	DHT	C10-C5	-2.24	1.51	1.55
5	B	1001	DHT	C19-C10	2.20	1.58	1.54
5	B	1001	DHT	C1-C10	2.02	1.57	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1001	DHT	C2-C3-C4	6.22	125.17	115.89
5	A	1001	DHT	C14-C8-C9	-5.99	101.07	109.09
5	D	1001	DHT	O3-C3-C4	-5.28	115.26	121.96
5	A	1001	DHT	C7-C8-C9	5.14	116.87	110.49
5	A	1001	DHT	C15-C16-C17	5.10	111.11	105.75
5	A	1001	DHT	C10-C9-C8	-4.99	107.18	112.42
5	B	1001	DHT	C2-C3-C4	4.94	123.24	115.89
5	C	1001	DHT	C15-C14-C13	4.44	109.19	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1001	DHT	C18-C13-C12	-4.38	103.67	110.59
5	A	1001	DHT	C15-C14-C13	4.29	109.02	103.84
5	D	1001	DHT	C5-C4-C3	-4.26	105.02	112.73
5	C	1001	DHT	C16-C17-C13	-4.24	101.16	104.53
5	B	1001	DHT	C11-C9-C10	-4.13	109.16	113.91
5	B	1001	DHT	C14-C8-C9	-4.05	103.67	109.09
5	C	1001	DHT	C2-C3-C4	4.04	121.90	115.89
5	C	1001	DHT	C15-C16-C17	3.93	109.88	105.75
5	D	1001	DHT	C6-C7-C8	3.82	118.43	112.14
5	A	1001	DHT	C16-C17-C13	-3.78	101.53	104.53
5	D	1001	DHT	C6-C5-C10	3.75	119.03	112.31
5	C	1001	DHT	C7-C8-C9	3.74	115.13	110.49
5	A	1001	DHT	C2-C3-C4	3.71	121.41	115.89
5	D	1001	DHT	O17-C17-C16	3.68	119.95	111.60
5	A	1001	DHT	C1-C10-C9	-3.67	105.58	111.35
5	D	1001	DHT	C7-C8-C9	3.60	114.96	110.49
5	B	1001	DHT	O3-C3-C4	-3.51	117.51	121.96
5	D	1001	DHT	C19-C10-C9	3.46	115.95	111.18
5	C	1001	DHT	O3-C3-C4	-3.45	117.58	121.96
5	C	1001	DHT	C1-C10-C9	-3.42	105.98	111.35
5	C	1001	DHT	C10-C9-C8	-3.35	108.90	112.42
9	A	1005	GOL	O3-C3-C2	-3.10	95.35	110.20
5	B	1001	DHT	C15-C14-C13	3.03	107.50	103.84
5	B	1001	DHT	C1-C10-C5	3.03	112.25	107.77
5	B	1001	DHT	C5-C4-C3	-2.99	107.33	112.73
5	D	1001	DHT	C1-C10-C5	2.98	112.17	107.77
5	C	1001	DHT	C2-C1-C10	2.98	117.29	113.47
5	C	1001	DHT	C12-C13-C14	2.97	111.87	107.27
5	C	1001	DHT	C16-C15-C14	-2.96	99.26	105.13
5	A	1001	DHT	C1-C10-C5	2.92	112.09	107.77
5	B	1001	DHT	C1-C10-C9	-2.88	106.83	111.35
9	A	1005	GOL	O2-C2-C3	-2.80	96.77	109.12
9	A	1005	GOL	O2-C2-C1	2.72	121.11	109.12
5	A	1001	DHT	C12-C13-C14	2.68	111.43	107.27
5	D	1001	DHT	C6-C5-C4	-2.65	107.37	111.11
5	A	1001	DHT	O3-C3-C4	-2.65	118.60	121.96
5	B	1001	DHT	C18-C13-C17	2.63	113.71	109.54
5	B	1001	DHT	C2-C1-C10	-2.54	110.22	113.47
5	C	1001	DHT	C5-C4-C3	-2.49	108.23	112.73
5	D	1001	DHT	C12-C13-C14	2.43	111.04	107.27
5	A	1001	DHT	C16-C15-C14	-2.43	100.31	105.13
5	D	1001	DHT	O17-C17-C13	-2.40	109.76	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	DHT	C6-C5-C4	-2.37	107.76	111.11
5	A	1001	DHT	C11-C12-C13	-2.35	108.75	112.78
5	A	1001	DHT	C6-C5-C4	-2.33	107.83	111.11
5	C	1001	DHT	C18-C13-C14	2.19	115.79	111.71
5	D	1001	DHT	C19-C10-C1	-2.17	104.76	108.26
5	B	1001	DHT	C10-C9-C8	-2.16	110.15	112.42
5	D	1001	DHT	C15-C14-C8	2.16	122.64	119.08
5	A	1001	DHT	C5-C4-C3	-2.16	108.82	112.73
5	A	1001	DHT	O17-C17-C13	2.15	119.32	114.80
5	C	1001	DHT	C1-C10-C5	2.12	110.90	107.77
5	D	1001	DHT	C15-C14-C13	2.11	106.38	103.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1004	GOL	O1-C1-C2-C3
9	A	1005	GOL	C1-C2-C3-O3
9	A	1005	GOL	O2-C2-C3-O3
9	C	1004	GOL	C1-C2-C3-O3
9	A	1005	GOL	O1-C1-C2-C3
8	D	1004	EDO	O1-C1-C2-O2
11	C	1005	PGE	O1-C1-C2-O2
9	A	1005	GOL	O1-C1-C2-O2
11	C	1005	PGE	C1-C2-O2-C3
8	C	1003	EDO	O1-C1-C2-O2
8	A	1004	EDO	O1-C1-C2-O2
8	B	1005	EDO	O1-C1-C2-O2
8	B	1004	EDO	O1-C1-C2-O2

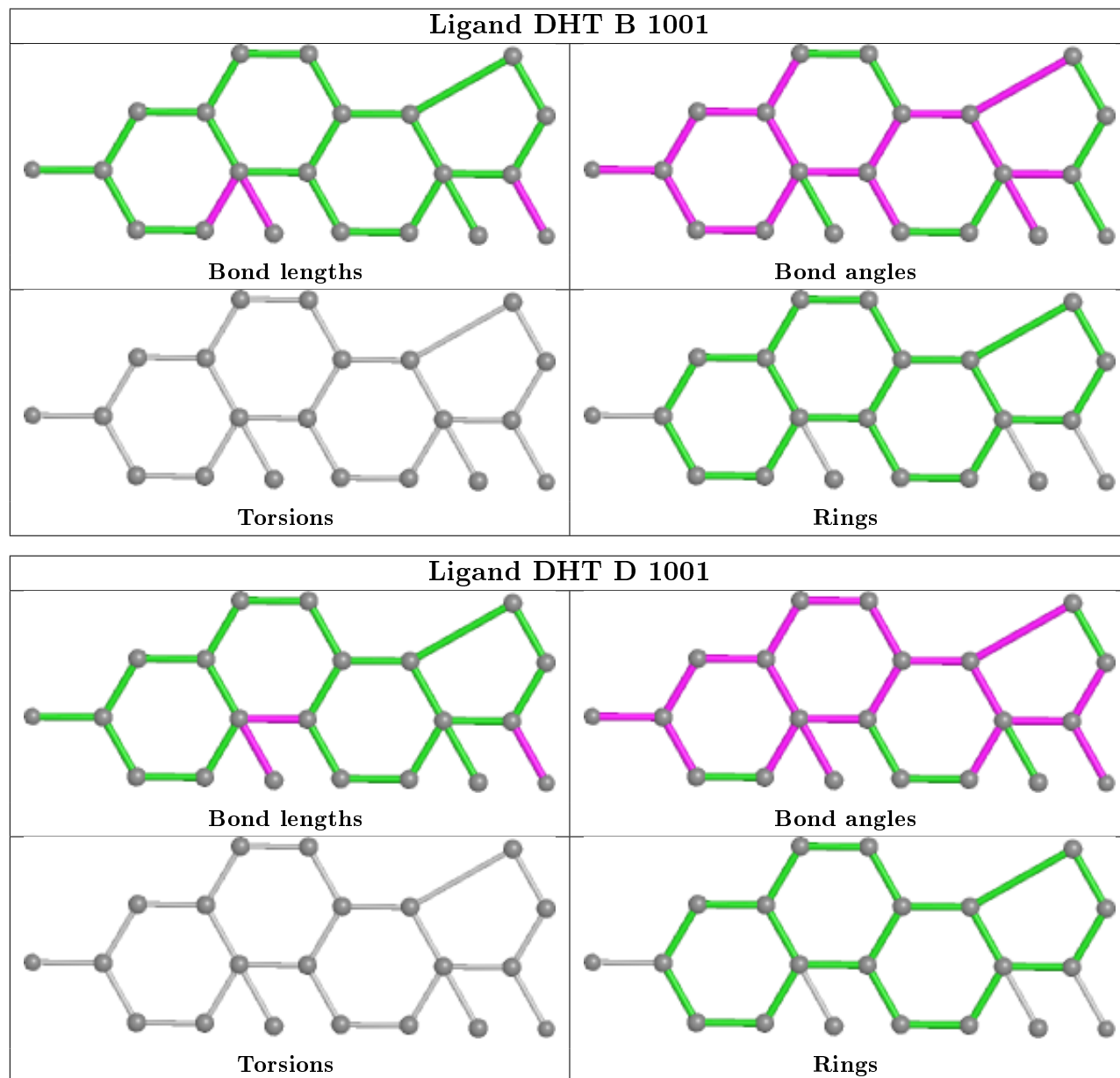
There are no ring outliers.

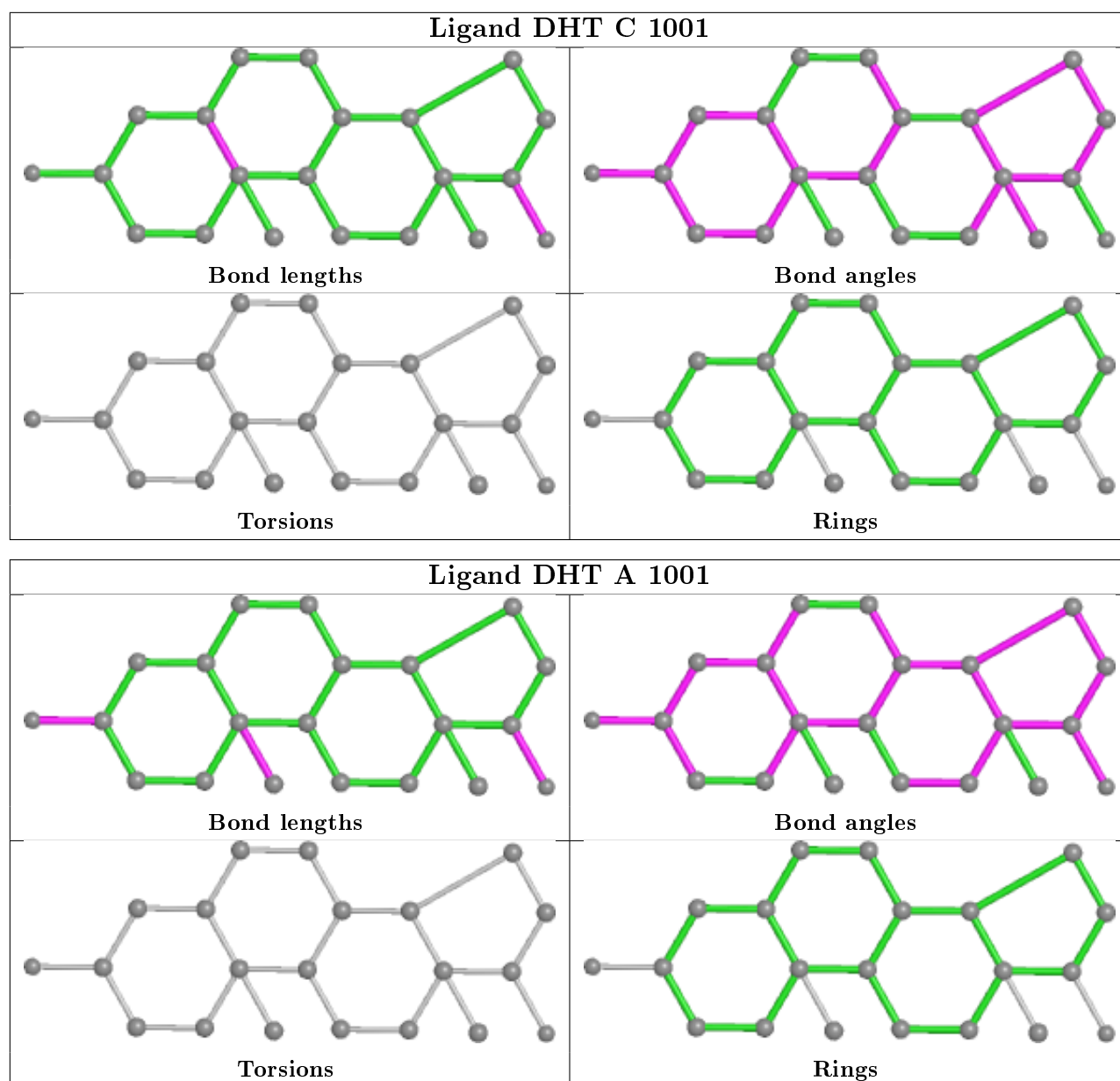
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1005	PGE	1	0
9	C	1004	GOL	1	0
8	A	1004	EDO	2	0
9	A	1005	GOL	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	852:CYS	C	853:SER	N	1.66

## 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	252/252 (100%)	-0.23	0 100 100	24, 37, 59, 83	0
1	C	250/252 (99%)	-0.23	0 100 100	23, 37, 59, 81	0
1	D	249/252 (98%)	-0.23	0 100 100	22, 37, 58, 73	0
2	F	2/3 (66%)	-0.05	0 100 100	56, 56, 56, 69	0
2	K	2/3 (66%)	1.51	1 (50%) 0 0	63, 63, 63, 92	0
2	L	2/3 (66%)	0.75	0 100 100	61, 61, 61, 80	0
2	M	2/3 (66%)	0.55	0 100 100	67, 67, 67, 93	0
3	B	250/252 (99%)	-0.21	0 100 100	24, 38, 59, 76	0
4	G	7/8 (87%)	0.85	1 (14%) 2 3	63, 69, 76, 86	0
4	H	8/8 (100%)	0.52	1 (12%) 3 5	68, 75, 77, 81	0
4	I	8/8 (100%)	0.43	0 100 100	68, 76, 77, 90	0
4	J	8/8 (100%)	0.50	0 100 100	67, 80, 91, 92	0
All	All	1040/1052 (98%)	-0.20	3 (0%) 94 95	22, 37, 66, 93	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	505	ASP	2.8
4	H	66	LEU	2.3
4	G	63	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
3	SNC	B	686	8/9	0.92	0.10	34,39,51,57	2
2	FME	M	503	10/11	0.96	0.12	58,64,66,68	0
2	FME	K	503	10/11	0.97	0.11	56,59,62,65	0
2	FME	F	503	10/11	0.97	0.12	53,55,63,65	0
2	FME	L	503	10/11	0.97	0.10	48,51,58,60	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 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
8	EDO	D	1005	4/4	0.91	0.15	59,64,65,69	0
11	PGE	C	1005	10/10	0.92	0.11	62,69,72,73	0
8	EDO	C	1003	4/4	0.93	0.12	61,64,64,65	0
8	EDO	A	1004	4/4	0.93	0.10	60,65,66,71	0
7	CL	A	1003	1/1	0.95	0.14	72,72,72,72	0
8	EDO	D	1004	4/4	0.96	0.12	53,57,58,64	0
7	CL	D	1003	1/1	0.96	0.08	74,74,74,74	0
5	DHT	D	1001	21/21	0.96	0.11	27,28,29,30	0
8	EDO	B	1005	4/4	0.96	0.13	66,67,70,72	0
8	EDO	D	1007	4/4	0.96	0.13	37,39,44,44	0
8	EDO	B	1006	4/4	0.96	0.16	54,60,60,63	0
5	DHT	A	1001	21/21	0.96	0.13	25,27,30,33	0
10	SO4	A	1006	5/5	0.96	0.13	52,55,59,62	0
9	GOL	A	1005	6/6	0.96	0.12	41,48,50,54	0
8	EDO	B	1004	4/4	0.96	0.12	38,43,43,46	0
10	SO4	C	1007	5/5	0.97	0.07	87,89,91,92	0
7	CL	B	1003	1/1	0.97	0.15	66,66,66,66	0
12	ACT	D	1006	4/4	0.97	0.13	62,63,67,68	0
5	DHT	C	1001	21/21	0.98	0.12	25,26,28,29	0
5	DHT	B	1001	21/21	0.98	0.12	27,29,30,31	0
9	GOL	C	1004	6/6	0.98	0.10	39,46,49,53	0
6	ZN	B	1002	1/1	0.99	0.14	47,47,47,47	0
10	SO4	D	1008	5/5	0.99	0.12	53,56,58,60	0
6	ZN	D	1002	1/1	0.99	0.10	49,49,49,49	0

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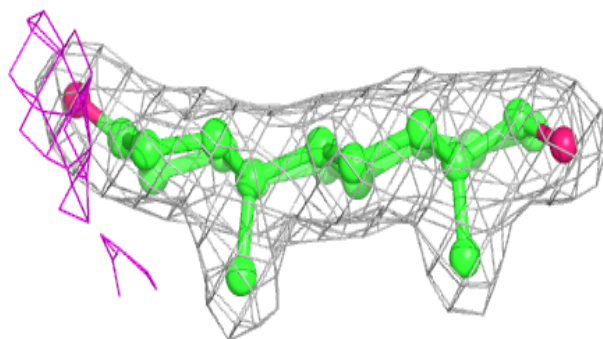
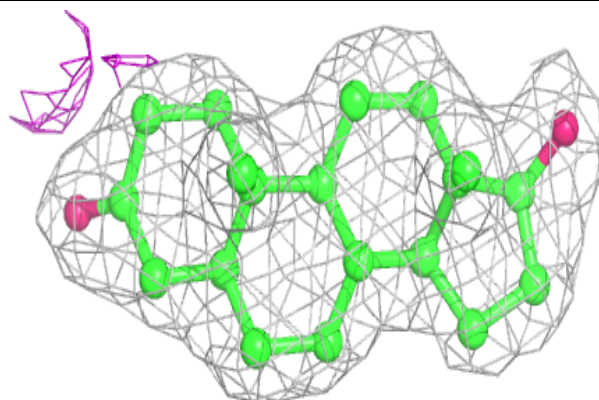
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	SO4	C	1006	5/5	0.99	0.13	47,48,49,49	0
10	SO4	B	1007	5/5	0.99	0.12	50,50,54,56	0
6	ZN	C	1002	1/1	0.99	0.09	53,53,53,53	0
6	ZN	A	1002	1/1	1.00	0.12	51,51,51,51	0

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.

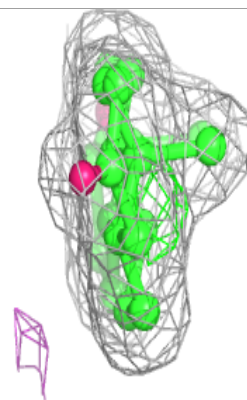
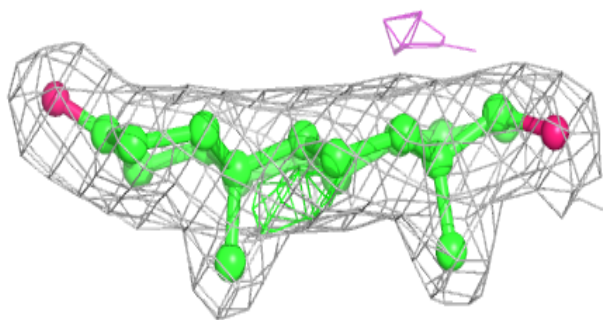
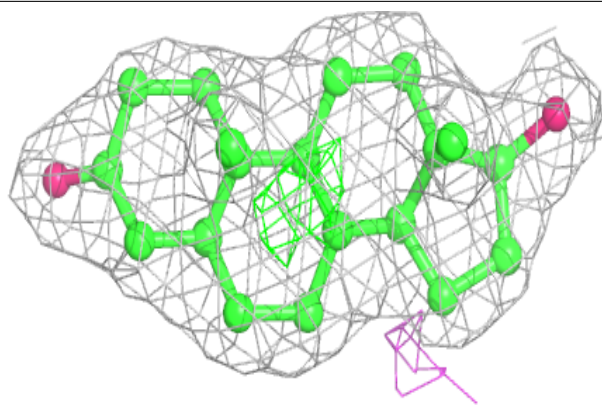
**Electron density around DHT D 1001:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

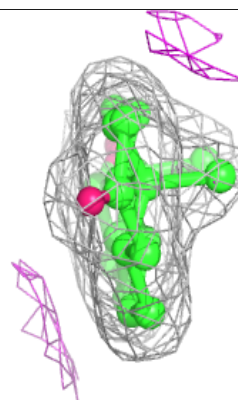
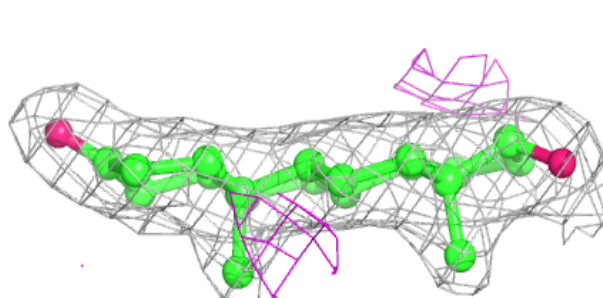
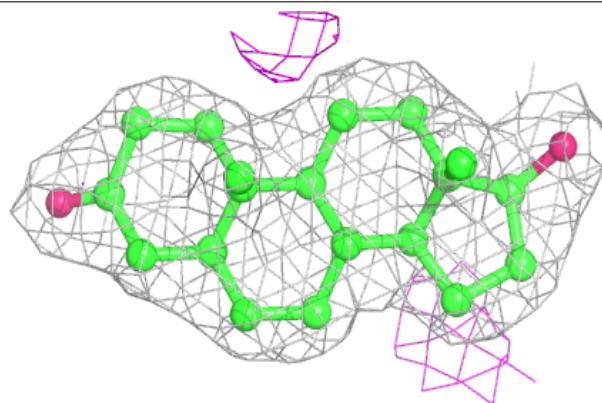


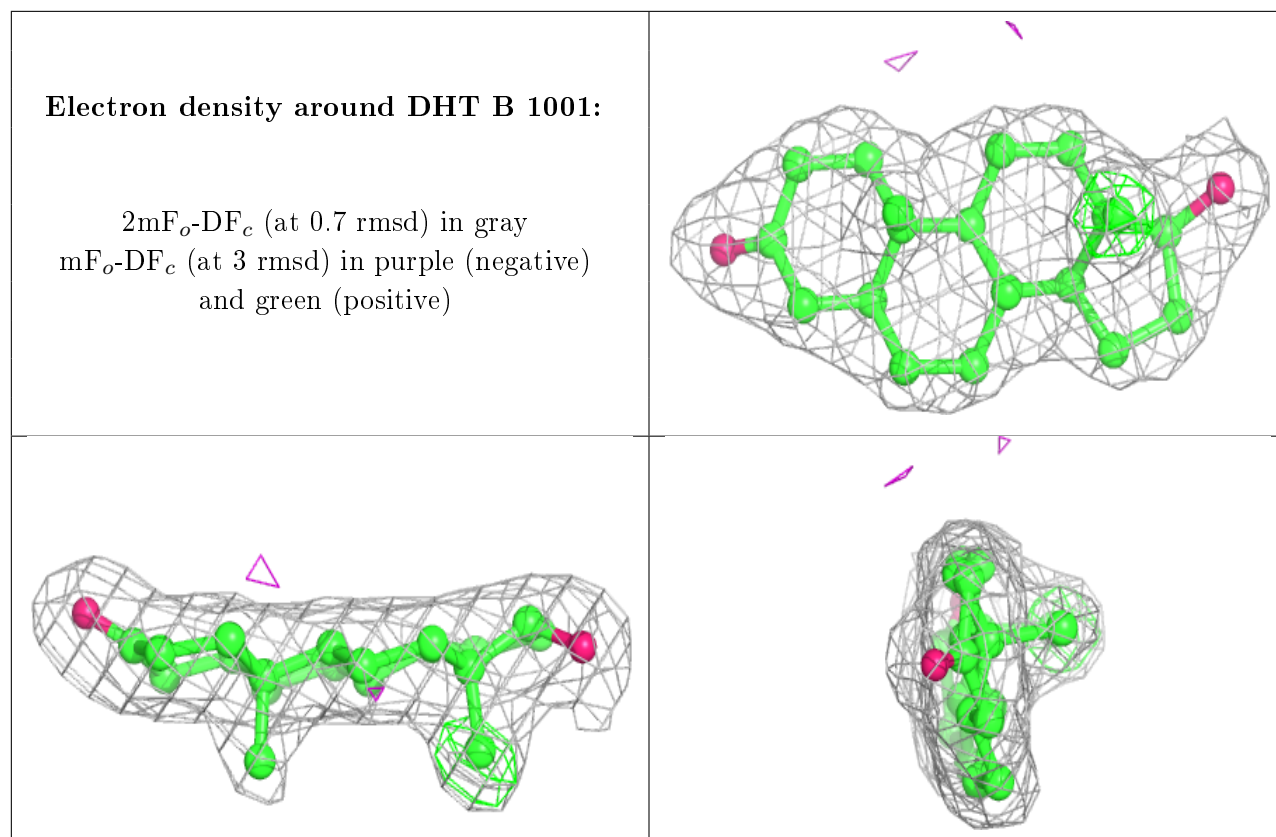
**Electron density around DHT A 1001:**

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

**Electron density around DHT C 1001:**

$2mF_o-DF_c$  (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.