



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2021 – 02:14 PM JST

PDB ID : 7CIP  
Title : Microbial Hormone-sensitive lipase E53 wild type  
Authors : Yang, X.; Li, Z.; Xu, X.; Li, J.  
Deposited on : 2020-07-08  
Resolution : 1.75 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 : 2.22  
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) : 2.22

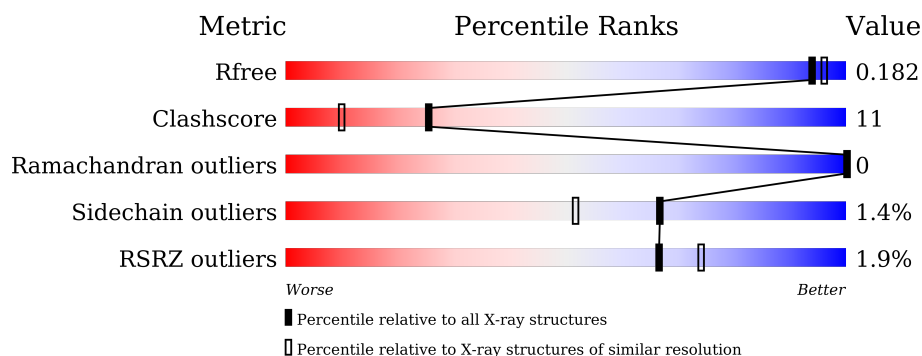
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	314	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> <div style="width: 3%;"></div> <div style="width: 0%;"></div> </div> 91% 6% ..
1	B	314	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> <div style="width: 0%;"></div> </div> 90% 9% .
1	C	314	<div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> <div style="width: 0%;"></div> </div> 92% 7% .
1	D	314	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> </div> 90% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	809	-	-	X	-
3	EDO	B	624	-	-	X	-
4	6NA	D	1412	-	-	-	X
4	6NA	D	1418	-	-	X	-
5	DMS	A	406	-	-	X	-
5	DMS	A	407	-	-	-	X
5	DMS	A	414	-	-	X	X
5	DMS	C	820	-	-	X	-
6	CCN	A	408	-	-	X	-
6	CCN	A	409	-	-	X	-
6	CCN	B	607	-	-	X	-
6	CCN	B	614	-	-	X	-
6	CCN	B	618	-	-	X	-
6	CCN	C	807	-	-	X	X
6	CCN	D	1403	-	-	X	-
6	CCN	D	1408	-	-	X	-
6	CCN	D	1411	-	-	-	X
6	CCN	D	1415	-	-	X	-
6	CCN	D	1419	-	-	X	-
7	D8F	A	416	-	-	X	-
7	D8F	B	623	-	X	X	-
7	D8F	C	817	-	-	X	-
7	D8F	D	1423	-	-	X	-

## 2 Entry composition [i](#)

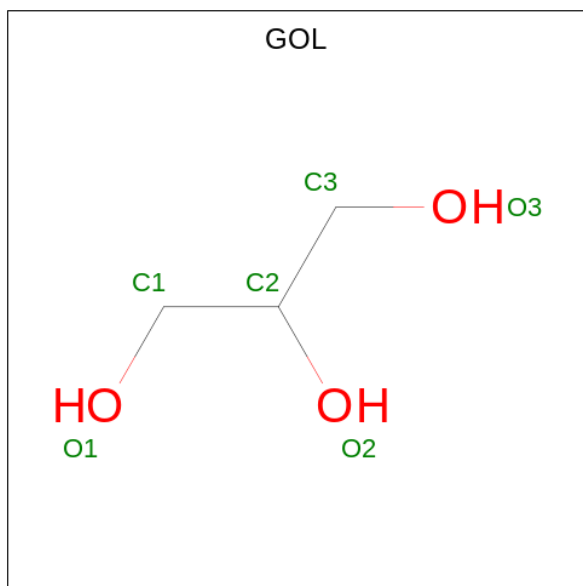
There are 13 unique types of molecules in this entry. The entry contains 11012 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2277	1444	391	430	12			
1	B	309	Total	C	N	O	S	0	0	0
			2289	1450	391	436	12			
1	C	309	Total	C	N	O	S	0	0	0
			2285	1448	391	434	12			
1	D	309	Total	C	N	O	S	0	0	0
			2289	1450	391	436	12			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



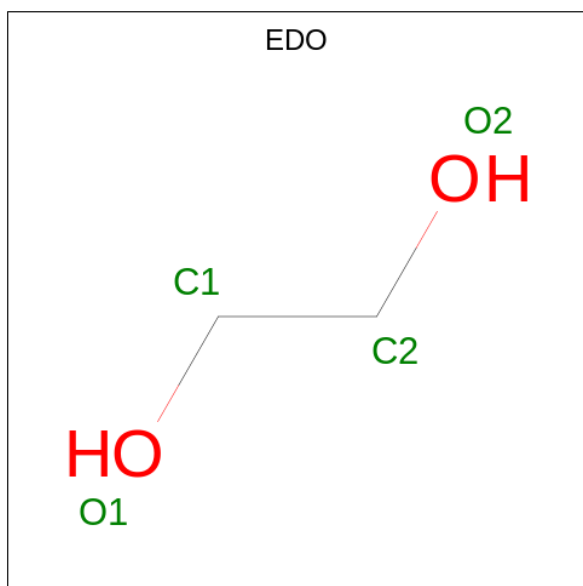
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



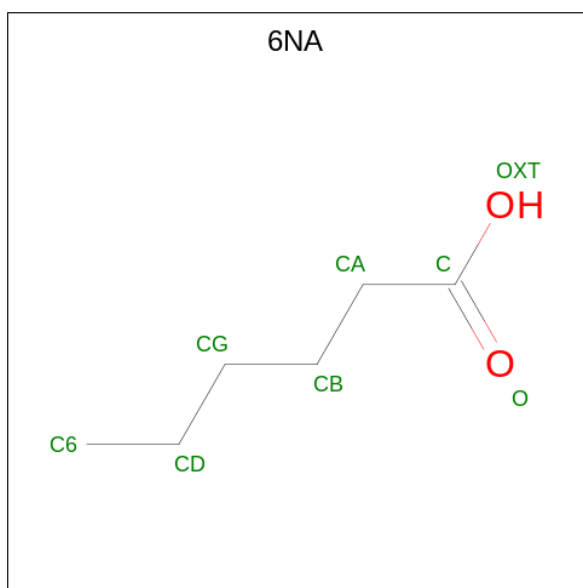
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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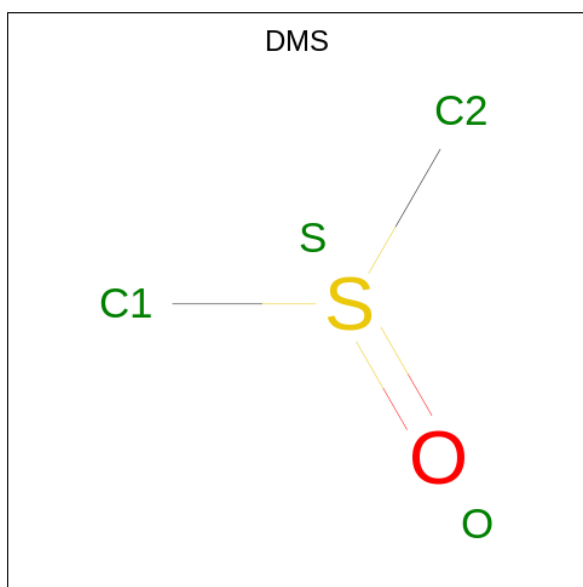
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0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

- Molecule 4 is HEXANOIC ACID (three-letter code: 6NA) (formula:  $C_6H_{12}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

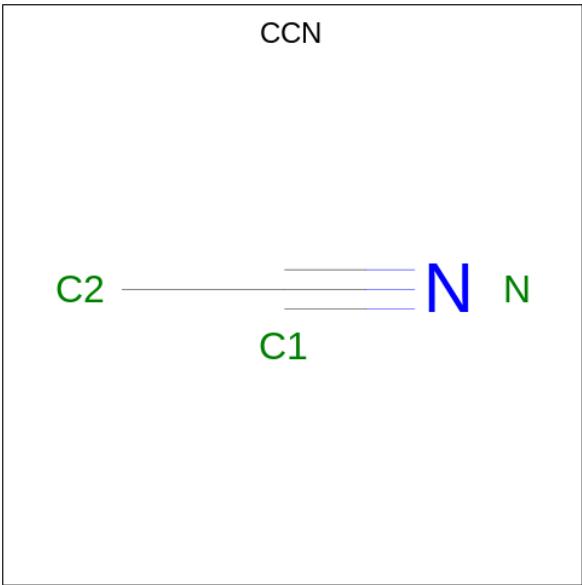
- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 6 is ACETONITRILE (three-letter code: CCN) (formula: C<sub>2</sub>H<sub>3</sub>N).





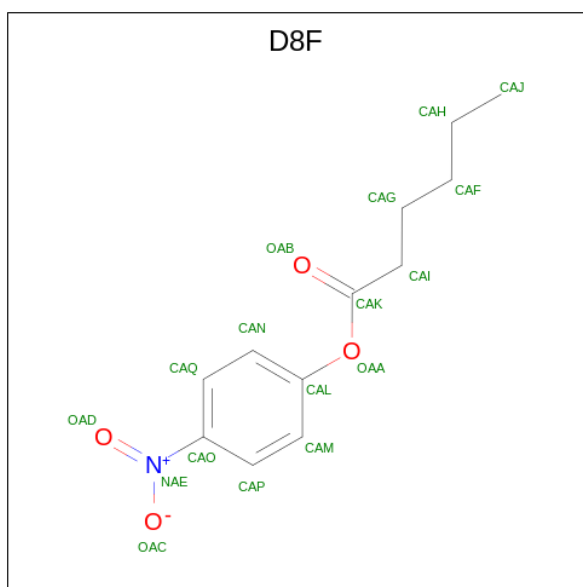
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			3	2	1		
6	A	1	Total	C	N	0	0
			3	2	1		
6	A	1	Total	C	N	0	0
			3	2	1		
6	A	1	Total	C	N	0	0
			3	2	1		
6	A	1	Total	C	N	0	0
			3	2	1		
6	A	1	Total	C	N	0	0
			3	2	1		
6	B	1	Total	C	N	0	0
			3	2	1		
6	B	1	Total	C	N	0	0
			3	2	1		
6	B	1	Total	C	N	0	0
			3	2	1		
6	B	1	Total	C	N	0	0
			3	2	1		
6	B	1	Total	C	N	0	0
			3	2	1		
6	C	1	Total	C	N	0	0
			3	2	1		
6	C	1	Total	C	N	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		
6	D	1	Total	C	N	0	0
			3	2	1		

- Molecule 7 is (4-nitrophenyl) hexanoate (three-letter code: D8F) (formula:  $C_{12}H_{15}NO_4$ ) (labeled as "Ligand of Interest" by depositor).



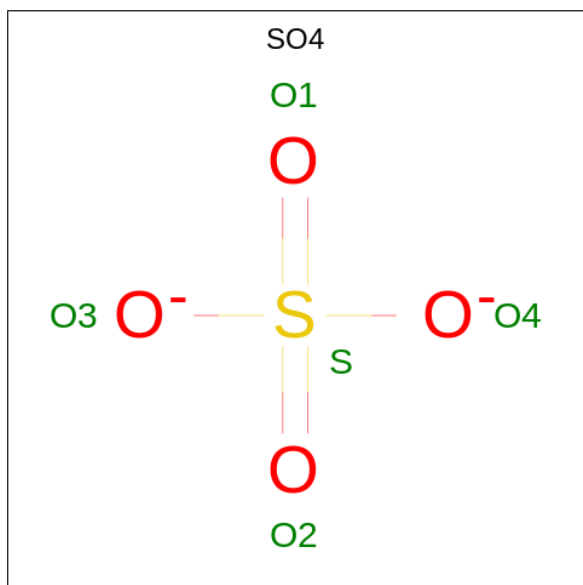
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			17	12	1	4		

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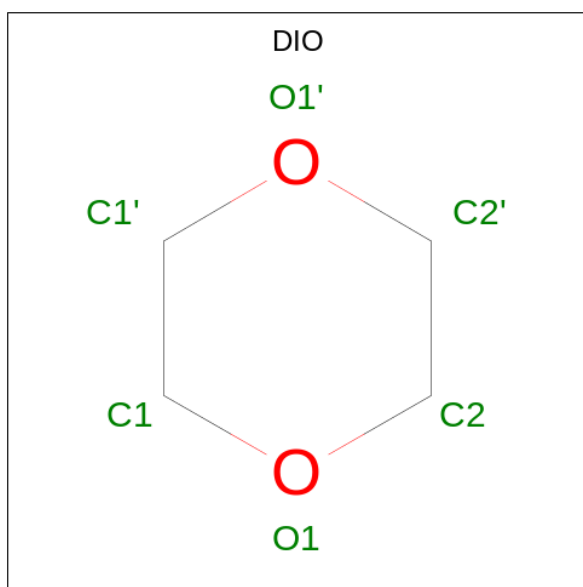
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			17	12	1	4		
7	C	1	Total	C	N	O	0	0
			17	12	1	4		
7	D	1	Total	C	N	O	0	0
			17	12	1	4		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



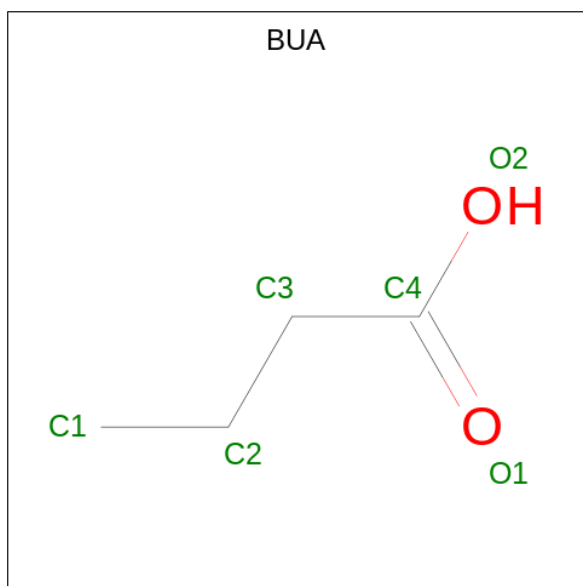
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



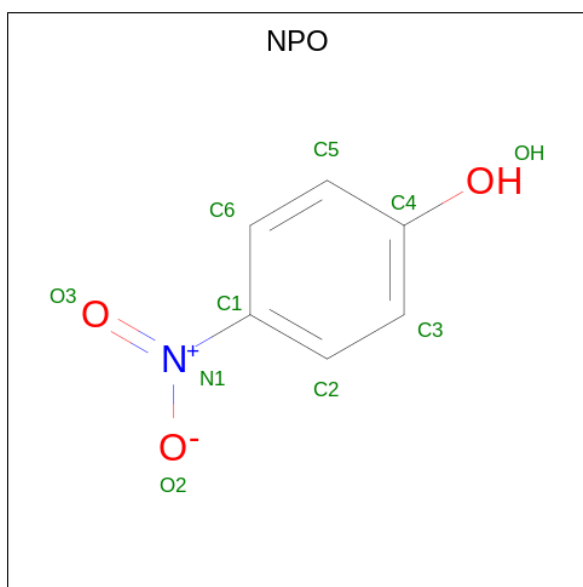
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 10 is butanoic acid (three-letter code: BUA) (formula:  $C_4H_8O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 11 is P-NITROPHENOL (three-letter code: NPO) (formula:  $C_6H_5NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			10	6	1	3		
11	B	1	Total	C	N	O	0	0
			10	6	1	3		
11	D	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	Na	0	0
			1	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	401	Total	O	0	0
			401	401		
13	B	325	Total	O	0	0
			325	325		
13	C	396	Total	O	0	0
			396	396		
13	D	311	Total	O	0	0
			311	311		

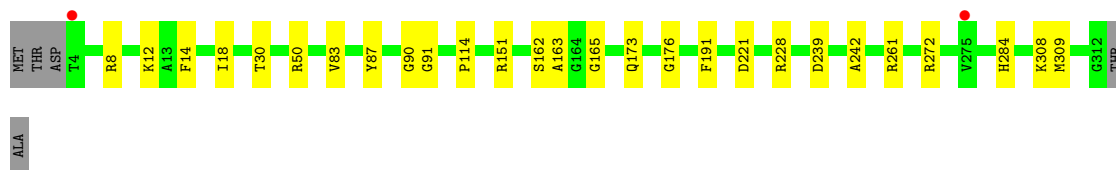
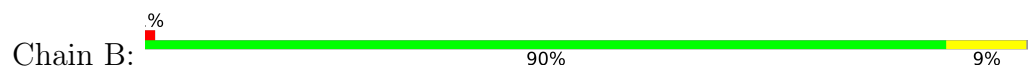
### 3 Residue-property plots [i](#)

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

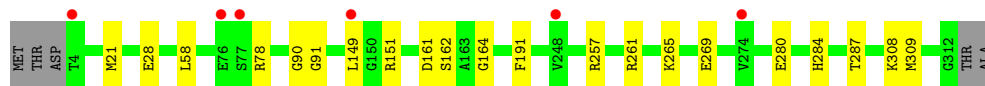
- Molecule 1: Lipase



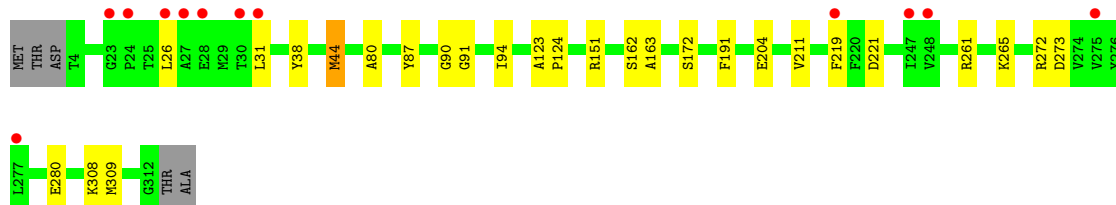
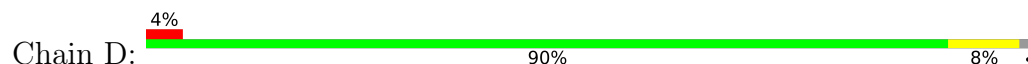
- Molecule 1: Lipase



- Molecule 1: Lipase



- Molecule 1: Lipase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.58Å 129.84Å 221.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 1.75 48.71 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.71-1.75) 99.9 (48.71-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.176 , 0.181 0.177 , 0.182	Depositor DCC
$R_{free}$ test set	2000 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	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	0.97	EDS
Total number of atoms	11012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.07% 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: DMS, BUA, EDO, 6NA, NA, CCN, SO4, D8F, DIO, NPO, GOL

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	0.50	0/2328	0.70	2/3178 (0.1%)
1	B	0.46	0/2340	0.63	0/3193
1	C	0.51	0/2336	0.68	1/3188 (0.0%)
1	D	0.48	0/2340	0.64	0/3193
All	All	0.49	0/9344	0.66	3/12752 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	78	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	47	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	2277	0	2257	46	0
1	B	2289	0	2269	38	0
1	C	2285	0	2265	45	0
1	D	2289	0	2269	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	30	0	38	9	0
2	D	12	0	15	2	0
3	A	16	0	24	4	0
3	B	28	0	42	9	0
3	C	32	0	48	2	0
3	D	24	0	36	2	0
4	A	16	0	22	3	0
4	C	8	0	11	0	0
4	D	16	0	22	21	0
5	A	16	0	24	16	0
5	B	20	0	30	1	0
5	C	8	0	12	7	0
5	D	8	0	12	0	0
6	A	18	0	18	6	0
6	B	18	0	18	11	0
6	C	9	0	9	4	0
6	D	27	0	27	11	0
7	A	17	0	0	7	0
7	B	17	0	0	14	0
7	C	17	0	0	11	0
7	D	17	0	0	10	0
8	A	10	0	0	0	0
9	B	6	0	8	0	0
10	B	6	0	7	2	0
11	B	20	0	8	1	0
11	D	10	0	4	2	0
12	C	1	0	0	0	0
13	A	401	0	0	22	0
13	B	325	0	0	13	0
13	C	396	0	0	9	0
13	D	311	0	0	18	0
All	All	11012	0	9511	202	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 11.

All (202) 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)
5:A:414:DMS:O	13:A:501:HOH:O	1.72	1.04
1:C:280:GLU:HG3	4:D:1418:6NA:C6	1.87	1.03
1:C:280:GLU:OE1	13:C:901:HOH:O	1.75	1.02
1:A:47:ARG:HH22	5:A:414:DMS:C2	1.77	0.98
5:C:819:DMS:S	4:D:1418:6NA:H6C3	2.06	0.95
1:A:56:ARG:NH1	1:A:58:LEU:HD21	1.81	0.94
1:C:280:GLU:CG	4:D:1418:6NA:H6C1	1.97	0.94
1:C:280:GLU:CG	4:D:1418:6NA:C6	2.48	0.92
2:C:809:GOL:H31	13:D:1537:HOH:O	1.74	0.86
1:A:47:ARG:HH22	5:A:414:DMS:H21	1.39	0.86
1:A:151:ARG:HH12	5:A:406:DMS:H12	1.42	0.84
6:A:408:CCN:H23	13:A:642:HOH:O	1.78	0.82
1:C:280:GLU:HG3	4:D:1418:6NA:H6C2	1.61	0.82
3:A:412:EDO:O1	13:A:502:HOH:O	1.97	0.81
1:C:91:GLY:H	7:C:817:D8F:CAN	1.93	0.81
1:A:91:GLY:H	7:A:416:D8F:CAN	1.95	0.79
1:C:261:ARG:HH12	2:C:809:GOL:H32	1.47	0.79
1:C:58:LEU:HB2	6:C:807:CCN:H22	1.65	0.76
1:C:269:GLU:OE2	6:D:1408:CCN:H23	1.86	0.75
1:D:90:GLY:H	7:D:1423:D8F:CAN	2.01	0.74
1:D:80:ALA:O	6:D:1407:CCN:H22	1.86	0.74
5:C:819:DMS:O	4:D:1418:6NA:H6C3	1.88	0.73
1:A:47:ARG:NH2	5:A:414:DMS:C2	2.51	0.72
6:A:408:CCN:H22	13:A:606:HOH:O	1.88	0.72
11:B:620:NPO:O2	13:B:701:HOH:O	2.06	0.72
6:B:609:CCN:N	13:B:703:HOH:O	2.23	0.72
3:A:405:EDO:O1	13:A:503:HOH:O	2.04	0.72
13:C:1173:HOH:O	6:D:1403:CCN:H22	1.90	0.71
1:A:159:ILE:HB	13:A:836:HOH:O	1.90	0.70
1:D:272:ARG:HB3	4:D:1418:6NA:OXT	1.91	0.69
1:A:47:ARG:HH22	5:A:414:DMS:H22	1.55	0.69
2:C:809:GOL:C3	13:D:1537:HOH:O	2.38	0.69
1:A:309:MET:SD	13:B:930:HOH:O	2.49	0.69
1:D:204:GLU:HG2	13:D:1616:HOH:O	1.94	0.67
1:A:47:ARG:NH2	5:A:414:DMS:H22	2.09	0.67
1:A:159:ILE:CD1	13:A:836:HOH:O	2.42	0.67
1:D:308:LYS:NZ	13:D:1504:HOH:O	2.27	0.66
5:C:820:DMS:H11	13:C:1192:HOH:O	1.95	0.66
6:D:1419:CCN:H22	13:D:1635:HOH:O	1.95	0.64
1:A:151:ARG:O	13:A:504:HOH:O	2.15	0.64
1:B:221:ASP:OD1	1:B:228:ARG:NH1	2.30	0.64
1:C:309:MET:SD	13:D:1726:HOH:O	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:605:EDO:O2	13:B:702:HOH:O	2.14	0.64
2:C:809:GOL:H11	13:D:1566:HOH:O	1.96	0.64
1:B:12:LYS:NZ	3:B:608:EDO:O2	2.32	0.63
1:B:163:ALA:H	7:B:623:D8F:CAQ	2.12	0.63
1:A:257:ARG:HH12	4:A:403:6NA:HBC1	1.64	0.63
1:A:56:ARG:NH1	1:A:58:LEU:CD2	2.61	0.62
1:A:151:ARG:HH12	5:A:406:DMS:C1	2.11	0.62
1:B:50:ARG:NH1	13:B:704:HOH:O	2.33	0.62
1:B:30:THR:OG1	6:B:607:CCN:H23	2.00	0.62
1:A:91:GLY:N	7:A:416:D8F:CAN	2.63	0.61
1:D:162:SER:OG	7:D:1423:D8F:CAL	2.48	0.61
10:B:615:BUA:H12	13:B:1004:HOH:O	2.00	0.61
1:A:309:MET:CE	1:B:309:MET:HE2	2.30	0.61
1:A:151:ARG:HH22	5:A:406:DMS:H11	1.65	0.61
1:D:162:SER:OG	7:D:1423:D8F:CAQ	2.49	0.61
1:C:162:SER:HG	7:C:817:D8F:CAM	2.13	0.60
1:A:159:ILE:CB	13:A:836:HOH:O	2.45	0.60
6:A:408:CCN:H21	13:A:804:HOH:O	2.00	0.60
1:C:91:GLY:N	7:C:817:D8F:CAN	2.63	0.60
6:D:1411:CCN:H22	13:D:1782:HOH:O	2.02	0.60
1:A:309:MET:HE2	1:B:309:MET:HE2	1.83	0.60
1:C:280:GLU:CG	4:D:1418:6NA:H6C2	2.25	0.60
1:C:261:ARG:HH22	2:C:809:GOL:H12	1.65	0.60
1:D:280:GLU:OE1	13:D:1501:HOH:O	2.16	0.59
1:C:149:LEU:HD23	13:C:931:HOH:O	2.03	0.59
6:A:409:CCN:H22	13:A:529:HOH:O	2.02	0.59
5:C:820:DMS:O	13:C:902:HOH:O	2.16	0.59
1:A:151:ARG:HH22	5:A:406:DMS:C1	2.17	0.58
1:C:28:GLU:HG3	6:C:808:CCN:H22	1.85	0.58
1:C:21:MET:HE1	2:C:813:GOL:H31	1.85	0.57
1:B:90:GLY:H	7:B:623:D8F:CAN	2.17	0.57
1:B:91:GLY:H	7:B:623:D8F:CAN	2.18	0.57
5:C:820:DMS:H12	13:D:1731:HOH:O	2.04	0.57
1:C:90:GLY:H	7:C:817:D8F:CAN	2.18	0.57
1:B:91:GLY:H	7:B:623:D8F:CAQ	2.18	0.56
1:C:162:SER:OG	7:C:817:D8F:CAL	2.52	0.56
1:C:309:MET:CE	1:D:309:MET:HE3	2.36	0.56
1:D:31:LEU:HD13	4:D:1412:6NA:HGC2	1.87	0.56
1:D:162:SER:OG	7:D:1423:D8F:CAN	2.54	0.56
1:C:280:GLU:CD	4:D:1418:6NA:H6C1	2.26	0.56
1:D:219:PHE:CZ	4:D:1412:6NA:H6C3	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:EDO:H22	13:B:720:HOH:O	2.06	0.55
1:A:162:SER:HG	7:A:416:D8F:CAM	2.20	0.55
1:C:21:MET:HE1	2:C:813:GOL:C3	2.36	0.54
5:C:820:DMS:H22	13:C:1192:HOH:O	2.08	0.54
1:D:265:LYS:NZ	6:D:1403:CCN:H21	2.23	0.54
1:A:91:GLY:HA2	7:A:416:D8F:CAQ	2.37	0.54
1:B:176:GLY:HA3	6:B:618:CCN:H23	1.89	0.54
1:D:261:ARG:HH22	3:D:1414:EDO:C1	2.19	0.54
1:C:162:SER:OG	7:C:817:D8F:CAM	2.56	0.54
1:D:273:ASP:HB2	4:D:1418:6NA:HAC2	1.90	0.54
1:D:44:MET:HB2	6:D:1415:CCN:C1	2.38	0.53
1:C:280:GLU:HG2	4:D:1418:6NA:H6C1	1.85	0.53
1:A:159:ILE:HG21	13:A:836:HOH:O	2.07	0.53
1:A:159:ILE:CG2	13:A:836:HOH:O	2.55	0.53
1:C:161:ASP:O	1:C:164:GLY:N	2.42	0.53
5:A:414:DMS:H23	13:A:512:HOH:O	2.09	0.53
1:C:309:MET:HE2	1:D:309:MET:HE3	1.91	0.52
1:A:151:ARG:C	13:A:504:HOH:O	2.48	0.52
1:B:162:SER:HG	7:B:623:D8F:CAM	2.22	0.52
6:D:1419:CCN:H21	13:D:1686:HOH:O	2.08	0.52
1:A:302:ARG:HE	3:A:404:EDO:C2	2.23	0.51
1:B:162:SER:OG	7:B:623:D8F:CAL	2.58	0.51
1:C:269:GLU:OE1	1:D:265:LYS:NZ	2.42	0.51
1:C:91:GLY:H	7:C:817:D8F:CAQ	2.23	0.51
1:D:172:SER:HB2	13:D:1603:HOH:O	2.11	0.51
1:D:273:ASP:H	4:D:1418:6NA:CA	2.24	0.51
1:A:197:ALA:H	5:A:415:DMS:C1	2.23	0.51
1:C:308:LYS:HE3	13:C:1172:HOH:O	2.11	0.51
1:D:91:GLY:H	7:D:1423:D8F:CAN	2.24	0.51
1:C:21:MET:CE	2:C:813:GOL:H12	2.42	0.50
1:A:23:GLY:HA3	13:A:679:HOH:O	2.12	0.50
1:C:280:GLU:HG2	4:D:1418:6NA:C6	2.36	0.50
1:B:242:ALA:HB3	6:B:618:CCN:H22	1.93	0.50
6:B:607:CCN:H22	13:B:939:HOH:O	2.12	0.49
6:A:410:CCN:H23	13:A:780:HOH:O	2.11	0.49
1:B:162:SER:O	1:B:165:GLY:N	2.44	0.49
1:D:44:MET:CE	11:D:1421:NPO:O2	2.60	0.49
1:D:221:ASP:HB2	2:D:1410:GOL:H32	1.93	0.49
1:B:162:SER:OG	7:B:623:D8F:CAN	2.60	0.49
1:A:159:ILE:HD12	13:A:836:HOH:O	2.11	0.48
1:B:8:ARG:HB3	3:B:605:EDO:H22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:GLU:OE2	4:D:1418:6NA:H6C1	2.13	0.48
1:D:162:SER:OG	7:D:1423:D8F:CAM	2.61	0.48
1:B:272:ARG:HH12	5:B:612:DMS:C1	2.26	0.48
1:B:308:LYS:O	10:B:615:BUA:H13	2.13	0.48
1:C:58:LEU:HB2	6:C:807:CCN:C2	2.41	0.48
1:A:162:SER:HG	1:A:284:HIS:CE1	2.32	0.48
3:B:602:EDO:C2	13:B:720:HOH:O	2.61	0.48
1:A:162:SER:OG	7:A:416:D8F:CAL	2.62	0.47
1:A:297:GLN:HG2	5:A:414:DMS:H22	1.96	0.47
1:A:162:SER:OG	7:A:416:D8F:CAM	2.63	0.47
6:B:618:CCN:C2	13:B:812:HOH:O	2.63	0.46
1:D:123:ALA:HB1	1:D:124:PRO:HA	1.98	0.46
1:C:91:GLY:HA2	7:C:817:D8F:CAQ	2.45	0.46
1:B:83:VAL:HG22	1:B:114:PRO:HG2	1.97	0.46
1:A:197:ALA:H	5:A:415:DMS:H12	1.80	0.46
1:D:261:ARG:HH11	6:D:1408:CCN:H22	1.79	0.46
1:A:26:LEU:HA	1:A:29:MET:HE3	1.98	0.46
1:D:31:LEU:HD21	1:D:124:PRO:HD2	1.98	0.46
1:A:265:LYS:HZ1	4:A:417:6NA:HBC1	1.80	0.46
6:D:1408:CCN:H21	13:D:1515:HOH:O	2.14	0.45
1:B:162:SER:HG	7:B:623:D8F:CAL	2.29	0.45
1:A:76:GLU:O	5:A:406:DMS:H13	2.17	0.45
1:D:162:SER:OG	7:D:1423:D8F:CAO	2.65	0.45
1:A:90:GLY:H	7:A:416:D8F:CAN	2.29	0.45
1:A:159:ILE:HD13	13:A:836:HOH:O	2.14	0.45
1:B:91:GLY:HA2	7:B:623:D8F:CAQ	2.47	0.45
1:C:261:ARG:HH22	2:C:809:GOL:C1	2.30	0.45
1:B:162:SER:HB3	7:B:623:D8F:CAN	2.47	0.45
1:B:173:GLN:HB3	6:B:614:CCN:H23	1.99	0.45
3:B:624:EDO:H11	13:B:885:HOH:O	2.16	0.45
4:D:1418:6NA:HDC2	13:D:1604:HOH:O	2.15	0.45
1:C:287:THR:HA	13:C:917:HOH:O	2.17	0.45
1:A:193:LEU:HD11	5:A:415:DMS:H13	1.99	0.44
3:B:624:EDO:C1	13:B:885:HOH:O	2.64	0.44
4:D:1418:6NA:CD	13:D:1604:HOH:O	2.64	0.44
1:C:162:SER:OG	7:C:817:D8F:CAN	2.65	0.44
1:D:261:ARG:HH22	3:D:1414:EDO:H11	1.82	0.44
1:C:162:SER:HG	1:C:284:HIS:CE1	2.36	0.44
1:C:309:MET:CE	1:D:309:MET:CE	2.95	0.44
5:C:819:DMS:H21	13:D:1590:HOH:O	2.17	0.44
1:D:44:MET:HB2	6:D:1415:CCN:C2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:MET:HE3	1:D:309:MET:CE	2.48	0.43
1:C:257:ARG:HH22	3:C:805:EDO:H21	1.83	0.43
1:A:76:GLU:CB	13:A:833:HOH:O	2.66	0.43
1:B:162:SER:HG	1:B:284:HIS:CE1	2.35	0.43
1:C:162:SER:HG	7:C:817:D8F:CAL	2.31	0.43
1:C:265:LYS:HE3	3:C:818:EDO:H12	2.01	0.43
1:A:309:MET:HE3	1:B:309:MET:HE2	2.01	0.43
1:B:163:ALA:HB2	7:B:623:D8F:CAQ	2.49	0.43
1:B:239:ASP:H	6:B:614:CCN:H22	1.84	0.43
1:D:44:MET:HE2	11:D:1421:NPO:O2	2.19	0.43
1:B:14:PHE:CE2	1:B:18:ILE:HD11	2.54	0.42
1:B:91:GLY:N	7:B:623:D8F:CAQ	2.82	0.42
1:D:162:SER:OG	7:D:1423:D8F:CAP	2.68	0.42
4:D:1418:6NA:HDC1	4:D:1418:6NA:HAC1	1.83	0.42
3:A:405:EDO:H12	13:A:777:HOH:O	2.19	0.42
1:D:38:TYR:HB2	1:D:94:ILE:HD12	2.02	0.42
1:B:239:ASP:H	6:B:614:CCN:C2	2.33	0.42
6:C:807:CCN:H21	13:C:1078:HOH:O	2.20	0.42
1:A:309:MET:CE	1:B:309:MET:CE	2.96	0.41
1:B:261:ARG:HH12	3:B:624:EDO:H22	1.85	0.41
1:A:162:SER:O	1:A:165:GLY:N	2.49	0.41
1:A:257:ARG:NH1	4:A:403:6NA:HBC1	2.33	0.41
1:B:162:SER:CB	7:B:623:D8F:CAN	2.98	0.41
1:B:239:ASP:N	6:B:614:CCN:H22	2.35	0.41
6:B:618:CCN:H21	13:B:812:HOH:O	2.19	0.41
1:C:309:MET:HE3	1:D:309:MET:HE3	2.02	0.41
1:B:162:SER:O	1:B:163:ALA:C	2.57	0.41
1:D:163:ALA:H	7:D:1423:D8F:CAQ	2.34	0.41
6:A:409:CCN:C2	13:A:529:HOH:O	2.65	0.41
1:D:272:ARG:NE	4:D:1418:6NA:OXT	2.54	0.41
1:D:26:LEU:O	4:D:1412:6NA:H6C1	2.21	0.41
1:D:91:GLY:H	7:D:1423:D8F:CAQ	2.33	0.40
2:D:1401:GOL:H12	13:D:1619:HOH:O	2.20	0.40
1:B:162:SER:OG	7:B:623:D8F:CAM	2.69	0.40
1:B:261:ARG:HH12	3:B:624:EDO:C2	2.34	0.40
1:D:204:GLU:HB3	13:D:1762:HOH:O	2.21	0.40
1:C:91:GLY:N	7:C:817:D8F:CAQ	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
1	B	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	C	307/314 (98%)	298 (97%)	9 (3%)	0	100	100
1	D	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
All	All	1228/1256 (98%)	1196 (97%)	32 (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	232/240 (97%)	229 (99%)	3 (1%)	69	54
1	B	235/240 (98%)	232 (99%)	3 (1%)	69	54
1	C	234/240 (98%)	232 (99%)	2 (1%)	78	67
1	D	235/240 (98%)	230 (98%)	5 (2%)	53	31
All	All	936/960 (98%)	923 (99%)	13 (1%)	67	52

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	151	ARG

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Mol	Chain	Res	Type
1	A	178	LYS
1	B	87	TYR
1	B	151	ARG
1	B	191	PHE
1	C	151	ARG
1	C	191	PHE
1	D	44	MET
1	D	87	TYR
1	D	151	ARG
1	D	191	PHE
1	D	211	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 1 is monoatomic - leaving 87 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
5	DMS	B	617	-	3,3,3	0.67	0	3,3,3	0.68	0
6	CCN	A	413	-	2,2,2	0.91	0	1,1,1	0.03	0
6	CCN	A	411	-	2,2,2	0.91	0	1,1,1	0.38	0
5	DMS	D	1413	-	3,3,3	0.71	0	3,3,3	0.84	0
2	GOL	C	809	-	5,5,5	0.78	0	5,5,5	1.17	0
4	6NA	A	403	-	4,7,7	0.35	0	3,7,7	0.42	0
3	EDO	D	1422	-	3,3,3	0.40	0	2,2,2	0.27	0
3	EDO	C	812	-	3,3,3	0.58	0	2,2,2	0.21	0
2	GOL	C	813	-	5,5,5	1.37	1 (20%)	5,5,5	0.63	0
5	DMS	B	611	-	3,3,3	0.68	0	3,3,3	0.83	0
6	CCN	B	618	-	2,2,2	0.88	0	1,1,1	0.21	0
3	EDO	C	815	-	3,3,3	0.45	0	2,2,2	0.38	0
6	CCN	D	1420	-	2,2,2	0.94	0	1,1,1	0.27	0
4	6NA	D	1418	-	4,7,7	0.12	0	3,7,7	0.41	0
3	EDO	C	806	-	3,3,3	0.47	0	2,2,2	0.65	0
3	EDO	C	805	-	3,3,3	0.46	0	2,2,2	0.41	0
5	DMS	B	612	-	3,3,3	0.66	0	3,3,3	0.93	0
3	EDO	A	412	-	3,3,3	0.33	0	2,2,2	0.40	0
3	EDO	B	602	-	3,3,3	0.26	0	2,2,2	0.78	0
7	D8F	B	623	-	16,17,17	2.86	7 (43%)	19,21,21	3.96	7 (36%)
3	EDO	B	606	-	3,3,3	0.48	0	2,2,2	0.31	0
6	CCN	A	409	-	2,2,2	0.92	0	1,1,1	0.39	0
6	CCN	C	808	-	2,2,2	0.84	0	1,1,1	0.24	0
5	DMS	B	616	-	3,3,3	0.71	0	3,3,3	0.72	0
7	D8F	D	1423	-	16,17,17	2.60	6 (37%)	19,21,21	3.71	7 (36%)
5	DMS	D	1409	-	3,3,3	0.70	0	3,3,3	0.61	0
6	CCN	B	609	-	2,2,2	0.90	0	1,1,1	0.23	0
2	GOL	B	619	-	5,5,5	1.24	1 (20%)	5,5,5	0.88	0
5	DMS	C	820	-	3,3,3	0.70	0	3,3,3	0.97	0
8	SO4	A	419	-	4,4,4	0.12	0	6,6,6	0.08	0
7	D8F	C	817	-	16,17,17	1.29	3 (18%)	19,21,21	1.48	4 (21%)
5	DMS	B	622	-	3,3,3	0.83	0	3,3,3	0.78	0
6	CCN	C	807	-	2,2,2	0.94	0	1,1,1	0.21	0
4	6NA	D	1412	-	4,7,7	0.39	0	3,7,7	0.90	0
3	EDO	D	1414	-	3,3,3	0.45	0	2,2,2	0.92	0
5	DMS	A	415	-	3,3,3	0.49	0	3,3,3	1.09	0
3	EDO	D	1404	-	3,3,3	0.45	0	2,2,2	0.32	0
6	CCN	B	614	-	2,2,2	0.91	0	1,1,1	0.35	0
6	CCN	D	1415	-	2,2,2	0.96	0	1,1,1	0.25	0
7	D8F	A	416	-	16,17,17	1.25	3 (18%)	19,21,21	1.37	3 (15%)
3	EDO	B	624	-	3,3,3	0.38	0	2,2,2	0.18	0
5	DMS	A	414	-	3,3,3	0.70	0	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	DIO	B	604	-	6,6,6	0.69	0	6,6,6	1.10	1 (16%)
6	CCN	C	811	-	2,2,2	0.90	0	1,1,1	0.30	0
11	NPO	D	1421	-	9,10,10	2.02	4 (44%)	11,13,13	1.11	1 (9%)
2	GOL	C	816	-	5,5,5	0.81	0	5,5,5	1.24	1 (20%)
3	EDO	B	603	-	3,3,3	0.35	0	2,2,2	0.86	0
6	CCN	A	410	-	2,2,2	0.90	0	1,1,1	0.24	0
6	CCN	D	1411	-	2,2,2	0.94	0	1,1,1	0.44	0
3	EDO	A	405	-	3,3,3	0.46	0	2,2,2	0.15	0
11	NPO	B	620	-	9,10,10	1.28	1 (11%)	11,13,13	2.32	4 (36%)
6	CCN	D	1416	-	2,2,2	0.97	0	1,1,1	0.37	0
3	EDO	C	804	-	3,3,3	0.43	0	2,2,2	0.71	0
6	CCN	D	1419	-	2,2,2	0.98	0	1,1,1	0.24	0
3	EDO	C	803	-	3,3,3	0.45	0	2,2,2	0.31	0
6	CCN	B	610	-	2,2,2	0.91	0	1,1,1	0.36	0
6	CCN	D	1407	-	2,2,2	0.86	0	1,1,1	0.15	0
4	6NA	C	810	-	4,7,7	0.40	0	3,7,7	0.73	0
3	EDO	C	801	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	C	818	-	3,3,3	0.59	0	2,2,2	0.43	0
2	GOL	C	802	-	5,5,5	1.30	0	5,5,5	1.40	1 (20%)
6	CCN	B	613	-	2,2,2	0.90	0	1,1,1	0.51	0
3	EDO	B	608	-	3,3,3	0.50	0	2,2,2	0.47	0
3	EDO	D	1402	-	3,3,3	0.51	0	2,2,2	0.25	0
5	DMS	A	407	-	3,3,3	0.63	0	3,3,3	0.42	0
3	EDO	B	605	-	3,3,3	0.41	0	2,2,2	0.54	0
3	EDO	D	1405	-	3,3,3	0.40	0	2,2,2	0.59	0
6	CCN	D	1408	-	2,2,2	1.03	0	1,1,1	0.25	0
5	DMS	C	819	-	3,3,3	0.69	0	3,3,3	0.85	0
4	6NA	A	417	-	4,7,7	0.44	0	3,7,7	0.31	0
6	CCN	B	607	-	2,2,2	0.88	0	1,1,1	0.42	0
6	CCN	A	408	-	2,2,2	0.91	0	1,1,1	0.20	0
8	SO4	A	420	-	4,4,4	0.16	0	6,6,6	0.20	0
11	NPO	B	621	-	9,10,10	1.28	2 (22%)	11,13,13	0.78	0
2	GOL	A	401	-	5,5,5	1.28	1 (20%)	5,5,5	0.72	0
6	CCN	D	1403	-	2,2,2	0.89	0	1,1,1	0.37	0
2	GOL	D	1410	-	5,5,5	0.85	0	5,5,5	1.01	0
6	CCN	D	1417	-	2,2,2	0.98	0	1,1,1	0.43	0
2	GOL	C	814	-	5,5,5	0.81	0	5,5,5	0.85	0
6	CCN	A	418	-	2,2,2	0.92	0	1,1,1	0.26	0
3	EDO	D	1406	-	3,3,3	0.54	0	2,2,2	0.21	0
2	GOL	D	1401	-	5,5,5	0.83	0	5,5,5	1.51	1 (20%)
3	EDO	A	404	-	3,3,3	0.56	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	A	406	-	3,3,3	0.76	0	3,3,3	1.48	1 (33%)
10	BUA	B	615	-	2,5,5	0.54	0	2,5,5	0.31	0
3	EDO	B	601	-	3,3,3	0.56	0	2,2,2	0.08	0
3	EDO	A	402	-	3,3,3	0.30	0	2,2,2	0.56	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	EDO	A	412	-	-	0/1/1/1	-
3	EDO	B	608	-	-	0/1/1/1	-
3	EDO	D	1404	-	-	1/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
3	EDO	D	1402	-	-	1/1/1/1	-
3	EDO	B	605	-	-	1/1/1/1	-
7	D8F	B	623	-	-	9/11/13/13	0/1/1/1
7	D8F	A	416	-	-	8/11/13/13	0/1/1/1
3	EDO	D	1405	-	-	0/1/1/1	-
3	EDO	B	606	-	-	1/1/1/1	-
3	EDO	B	624	-	-	1/1/1/1	-
2	GOL	C	809	-	-	4/4/4/4	-
4	6NA	A	403	-	-	3/3/5/5	-
9	DIO	B	604	-	-	-	0/1/1/1
3	EDO	D	1422	-	-	1/1/1/1	-
4	6NA	A	417	-	-	1/3/5/5	-
3	EDO	C	812	-	-	1/1/1/1	-
11	NPO	D	1421	-	-	0/2/4/4	0/1/1/1
7	D8F	D	1423	-	-	4/11/13/13	0/1/1/1
2	GOL	C	813	-	-	2/4/4/4	-
2	GOL	C	816	-	-	2/4/4/4	-
11	NPO	B	621	-	-	0/2/4/4	0/1/1/1
2	GOL	B	619	-	-	4/4/4/4	-
2	GOL	A	401	-	-	1/4/4/4	-
3	EDO	B	603	-	-	0/1/1/1	-
2	GOL	D	1410	-	-	4/4/4/4	-
3	EDO	C	815	-	-	1/1/1/1	-
3	EDO	A	405	-	-	1/1/1/1	-
11	NPO	B	620	-	-	1/2/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	814	-	-	2/4/4/4	-
3	EDO	C	804	-	-	0/1/1/1	-
3	EDO	D	1406	-	-	1/1/1/1	-
2	GOL	D	1401	-	-	2/4/4/4	-
3	EDO	A	404	-	-	1/1/1/1	-
7	D8F	C	817	-	-	5/11/13/13	0/1/1/1
3	EDO	C	803	-	-	0/1/1/1	-
10	BUA	B	615	-	-	1/1/3/3	-
4	6NA	D	1418	-	-	2/3/5/5	-
3	EDO	C	806	-	-	1/1/1/1	-
4	6NA	C	810	-	-	2/3/5/5	-
4	6NA	D	1412	-	-	2/3/5/5	-
3	EDO	C	801	-	-	0/1/1/1	-
3	EDO	B	601	-	-	1/1/1/1	-
3	EDO	C	805	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
2	GOL	C	802	-	-	2/4/4/4	-
3	EDO	C	818	-	-	1/1/1/1	-
3	EDO	D	1414	-	-	1/1/1/1	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	623	D8F	CAP-CAO	5.94	1.50	1.38
7	B	623	D8F	CAQ-CAO	5.91	1.50	1.38
7	D	1423	D8F	CAQ-CAO	5.54	1.49	1.38
7	D	1423	D8F	CAQ-CAN	4.87	1.47	1.38
7	D	1423	D8F	CAM-CAL	4.38	1.47	1.38
7	B	623	D8F	CAQ-CAN	4.24	1.46	1.38
7	B	623	D8F	CAN-CAL	4.12	1.46	1.38
7	B	623	D8F	OAA-CAK	3.66	1.46	1.35
7	D	1423	D8F	CAN-CAL	3.53	1.45	1.38
7	D	1423	D8F	OAA-CAK	3.38	1.45	1.35
11	D	1421	NPO	C3-C4	-3.31	1.32	1.38
7	A	416	D8F	OAA-CAK	3.27	1.45	1.35
11	D	1421	NPO	C6-C1	-3.24	1.32	1.38
7	C	817	D8F	OAA-CAK	3.10	1.44	1.35
11	B	620	NPO	C1-N1	-2.97	1.38	1.45
7	C	817	D8F	CAO-NAE	-2.88	1.38	1.45
11	B	621	NPO	C1-N1	-2.72	1.38	1.45
11	D	1421	NPO	C1-N1	-2.65	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	416	D8F	OAA-CAL	-2.53	1.35	1.41
7	C	817	D8F	OAA-CAL	-2.44	1.35	1.41
7	A	416	D8F	CAO-NAE	-2.41	1.39	1.45
7	D	1423	D8F	CAO-NAE	-2.39	1.39	1.45
11	B	621	NPO	O3-N1	-2.35	1.18	1.22
7	B	623	D8F	CAO-NAE	-2.29	1.39	1.45
11	D	1421	NPO	O3-N1	2.22	1.26	1.22
7	B	623	D8F	OAA-CAL	-2.19	1.36	1.41
2	A	401	GOL	C1-C2	2.13	1.60	1.51
2	C	813	GOL	C3-C2	2.08	1.60	1.51
2	B	619	GOL	C1-C2	2.06	1.60	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	623	D8F	CAN-CAQ-CAO	-10.56	105.38	120.08
7	D	1423	D8F	CAQ-CAN-CAL	-10.23	107.23	119.73
7	D	1423	D8F	CAQ-CAO-NAE	7.92	125.34	119.38
7	B	623	D8F	CAP-CAO-NAE	-7.21	113.95	119.38
7	B	623	D8F	CAQ-CAN-CAL	6.33	127.47	119.73
7	B	623	D8F	CAQ-CAO-CAP	6.22	130.12	119.86
7	D	1423	D8F	CAN-CAQ-CAO	5.99	128.42	120.08
11	B	620	NPO	C2-C1-N1	-5.25	115.42	119.38
7	D	1423	D8F	CAN-CAL-CAM	4.81	127.58	120.18
7	B	623	D8F	CAQ-CAO-NAE	-4.58	115.93	119.38
7	A	416	D8F	OAA-CAK-CAI	3.93	122.03	110.67
7	B	623	D8F	OAA-CAK-CAI	3.83	121.74	110.67
7	D	1423	D8F	OAA-CAK-CAI	3.77	121.55	110.67
7	C	817	D8F	CAQ-CAO-NAE	3.58	122.07	119.38
11	B	620	NPO	C6-C1-N1	3.42	121.95	119.38
7	B	623	D8F	CAM-CAP-CAO	-3.38	115.37	120.08
7	C	817	D8F	OAA-CAK-CAI	3.14	119.74	110.67
7	A	416	D8F	OAA-CAK-OAB	-3.11	116.89	122.84
11	D	1421	NPO	C2-C1-N1	2.88	121.54	119.38
7	C	817	D8F	CAP-CAO-NAE	-2.77	117.29	119.38
11	B	620	NPO	O3-N1-C1	2.71	122.64	118.80
7	D	1423	D8F	OAA-CAK-OAB	-2.62	117.82	122.84
7	C	817	D8F	OAA-CAK-OAB	-2.62	117.84	122.84
5	A	406	DMS	O-S-C1	2.55	119.53	106.54
2	D	1401	GOL	C3-C2-C1	-2.47	102.12	111.70
7	D	1423	D8F	CAQ-CAO-CAP	-2.24	116.16	119.86
2	C	802	GOL	O3-C3-C2	-2.14	99.92	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	416	D8F	CAQ-CAO-NAE	2.06	120.93	119.38
2	C	816	GOL	O2-C2-C3	2.05	118.13	109.12
9	B	604	DIO	C2'-O1'-C1'	2.03	116.68	109.89
11	B	620	NPO	C5-C6-C1	-2.03	117.26	120.08

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	619	GOL	O1-C1-C2-O2
2	B	619	GOL	O1-C1-C2-C3
2	B	619	GOL	C1-C2-C3-O3
2	C	802	GOL	C1-C2-C3-O3
2	C	802	GOL	O2-C2-C3-O3
2	C	809	GOL	O1-C1-C2-C3
2	C	809	GOL	C1-C2-C3-O3
2	C	813	GOL	C1-C2-C3-O3
2	C	814	GOL	C1-C2-C3-O3
2	C	814	GOL	O2-C2-C3-O3
2	C	816	GOL	O1-C1-C2-C3
7	A	416	D8F	CAI-CAK-OAA-CAL
7	A	416	D8F	OAB-CAK-OAA-CAL
7	B	623	D8F	CAI-CAK-OAA-CAL
7	B	623	D8F	OAB-CAK-OAA-CAL
7	C	817	D8F	CAI-CAK-OAA-CAL
7	C	817	D8F	OAB-CAK-OAA-CAL
7	C	817	D8F	CAP-CAO-NAE-OAD
7	C	817	D8F	CAQ-CAO-NAE-OAD
7	D	1423	D8F	CAI-CAK-OAA-CAL
7	D	1423	D8F	OAB-CAK-OAA-CAL
4	D	1418	6NA	CA-CB-CG-CD
2	C	809	GOL	O1-C1-C2-O2
2	C	809	GOL	O2-C2-C3-O3
4	C	810	6NA	CA-CB-CG-CD
2	A	401	GOL	O1-C1-C2-C3
2	D	1401	GOL	C1-C2-C3-O3
2	D	1410	GOL	O1-C1-C2-C3
2	D	1410	GOL	C1-C2-C3-O3
4	A	403	6NA	CA-CB-CG-CD
2	C	813	GOL	O2-C2-C3-O3
2	D	1401	GOL	O2-C2-C3-O3
2	D	1410	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	1410	GOL	O2-C2-C3-O3
3	A	405	EDO	O1-C1-C2-O2
3	B	601	EDO	O1-C1-C2-O2
3	B	605	EDO	O1-C1-C2-O2
3	B	606	EDO	O1-C1-C2-O2
3	D	1402	EDO	O1-C1-C2-O2
3	D	1422	EDO	O1-C1-C2-O2
7	B	623	D8F	CAF-CAG-CAI-CAK
4	C	810	6NA	C6-CD-CG-CB
2	B	619	GOL	O2-C2-C3-O3
3	B	624	EDO	O1-C1-C2-O2
3	C	812	EDO	O1-C1-C2-O2
3	C	818	EDO	O1-C1-C2-O2
7	D	1423	D8F	CAH-CAF-CAG-CAI
7	A	416	D8F	CAH-CAF-CAG-CAI
4	A	417	6NA	CA-CB-CG-CD
4	D	1412	6NA	C6-CD-CG-CB
7	B	623	D8F	CAG-CAF-CAH-CAJ
7	A	416	D8F	CAQ-CAO-NAE-OAD
7	B	623	D8F	CAP-CAO-NAE-OAD
7	B	623	D8F	CAQ-CAO-NAE-OAD
3	A	404	EDO	O1-C1-C2-O2
3	C	805	EDO	O1-C1-C2-O2
3	D	1404	EDO	O1-C1-C2-O2
7	A	416	D8F	CAM-CAL-OAA-CAK
4	A	403	6NA	C-CA-CB-CG
4	D	1418	6NA	C-CA-CB-CG
3	D	1406	EDO	O1-C1-C2-O2
7	B	623	D8F	CAM-CAL-OAA-CAK
7	A	416	D8F	CAG-CAF-CAH-CAJ
7	A	416	D8F	CAN-CAL-OAA-CAK
2	C	816	GOL	O1-C1-C2-O2
7	A	416	D8F	CAP-CAO-NAE-OAD
7	B	623	D8F	CAH-CAF-CAG-CAI
3	C	815	EDO	O1-C1-C2-O2
7	C	817	D8F	CAH-CAF-CAG-CAI
10	B	615	BUA	C1-C2-C3-C4
7	B	623	D8F	CAN-CAL-OAA-CAK
4	D	1412	6NA	CA-CB-CG-CD
4	A	403	6NA	C6-CD-CG-CB
3	D	1414	EDO	O1-C1-C2-O2
7	D	1423	D8F	CAF-CAG-CAI-CAK

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Mol	Chain	Res	Type	Atoms
3	C	806	EDO	O1-C1-C2-O2
11	B	620	NPO	C6-C1-N1-O3

There are no ring outliers.

46 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	809	GOL	6	0
4	A	403	6NA	2	0
2	C	813	GOL	3	0
6	B	618	CCN	4	0
4	D	1418	6NA	18	0
3	C	805	EDO	1	0
5	B	612	DMS	1	0
3	A	412	EDO	1	0
3	B	602	EDO	2	0
7	B	623	D8F	14	0
6	A	409	CCN	2	0
6	C	808	CCN	1	0
7	D	1423	D8F	10	0
6	B	609	CCN	1	0
5	C	820	DMS	4	0
7	C	817	D8F	11	0
6	C	807	CCN	3	0
4	D	1412	6NA	3	0
3	D	1414	EDO	2	0
5	A	415	DMS	3	0
6	B	614	CCN	4	0
6	D	1415	CCN	2	0
7	A	416	D8F	7	0
3	B	624	EDO	4	0
5	A	414	DMS	8	0
11	D	1421	NPO	2	0
6	A	410	CCN	1	0
6	D	1411	CCN	1	0
3	A	405	EDO	2	0
11	B	620	NPO	1	0
6	D	1419	CCN	2	0
6	D	1407	CCN	1	0
3	C	818	EDO	1	0
3	B	608	EDO	1	0
3	B	605	EDO	2	0

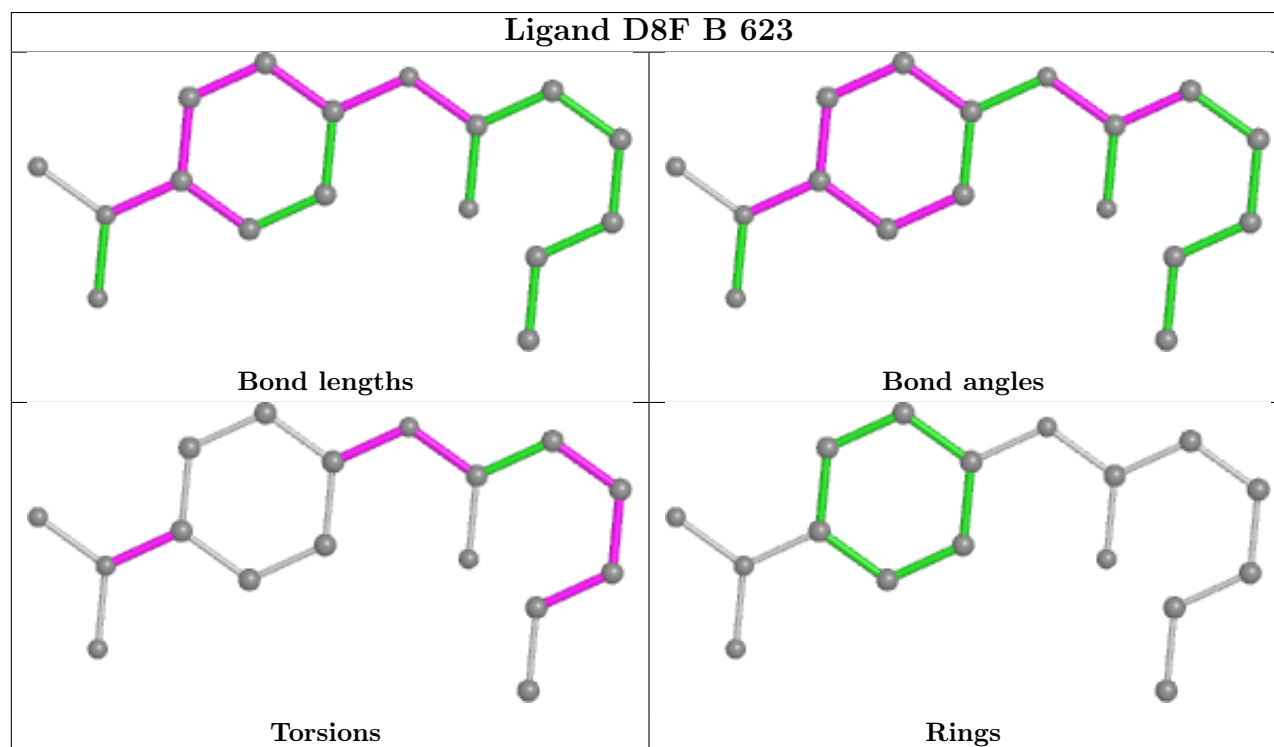
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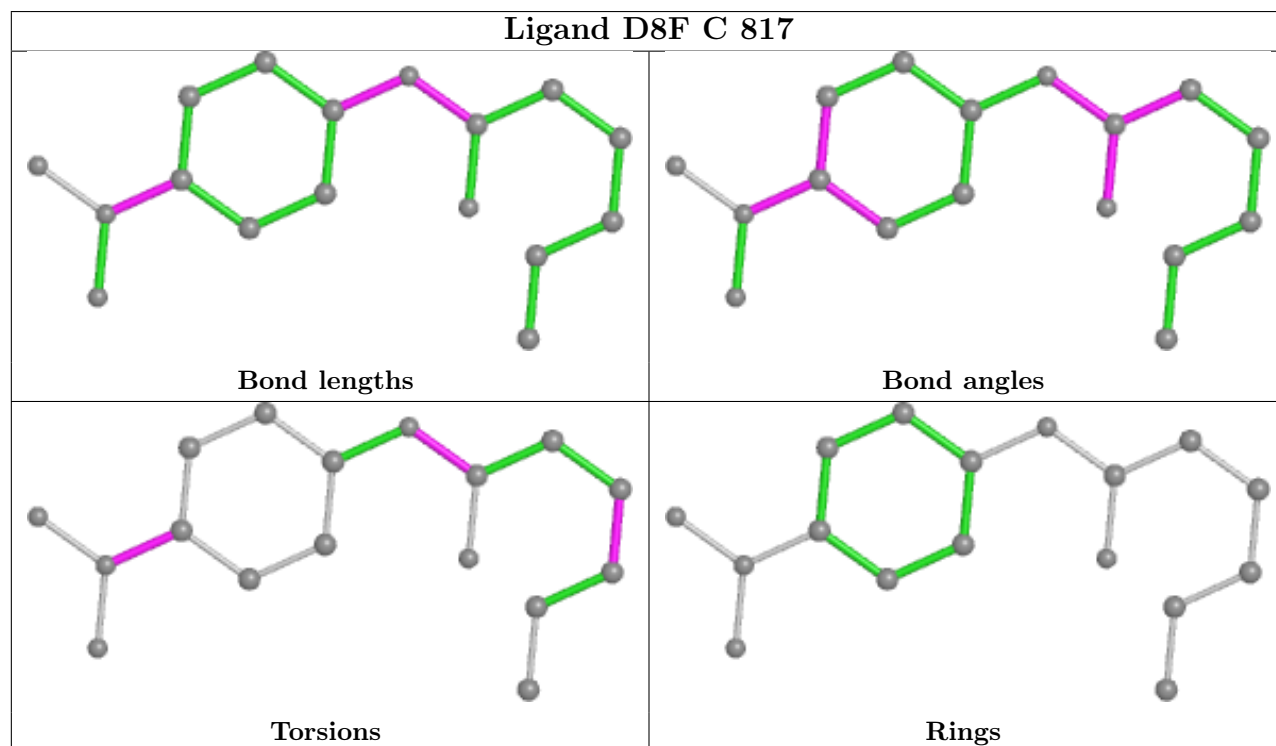
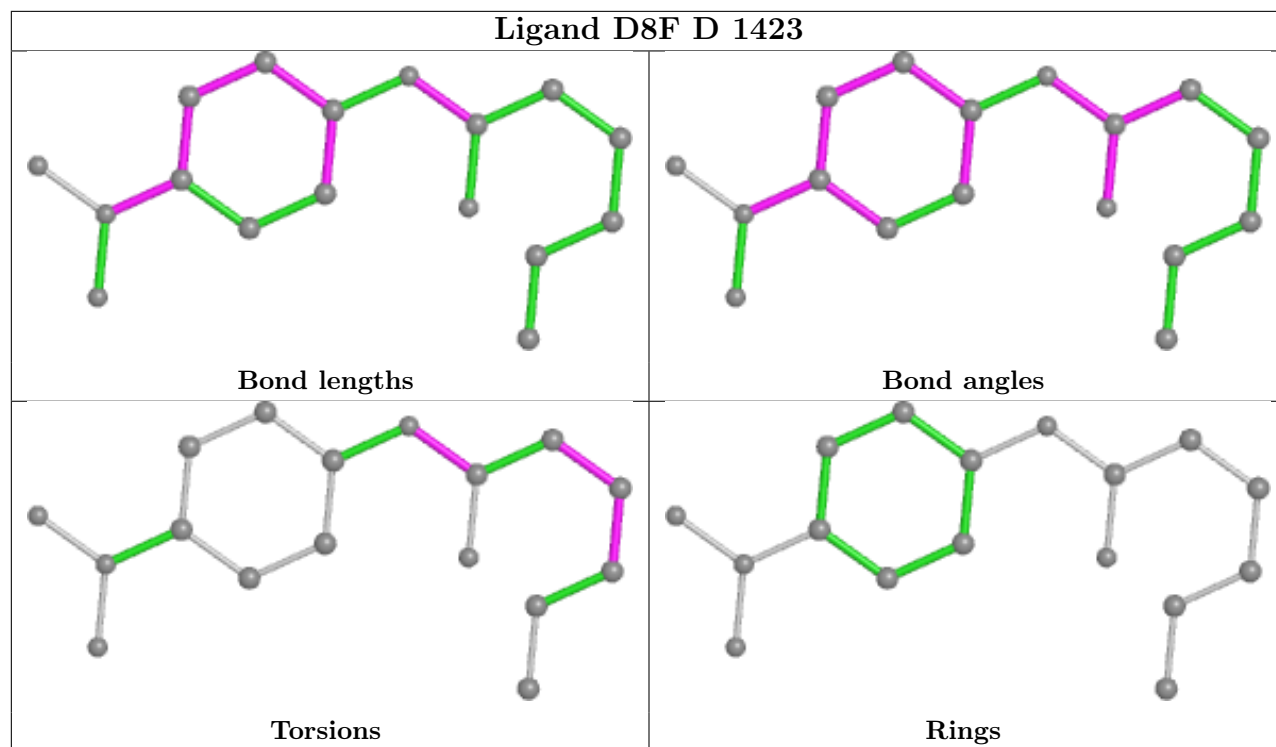


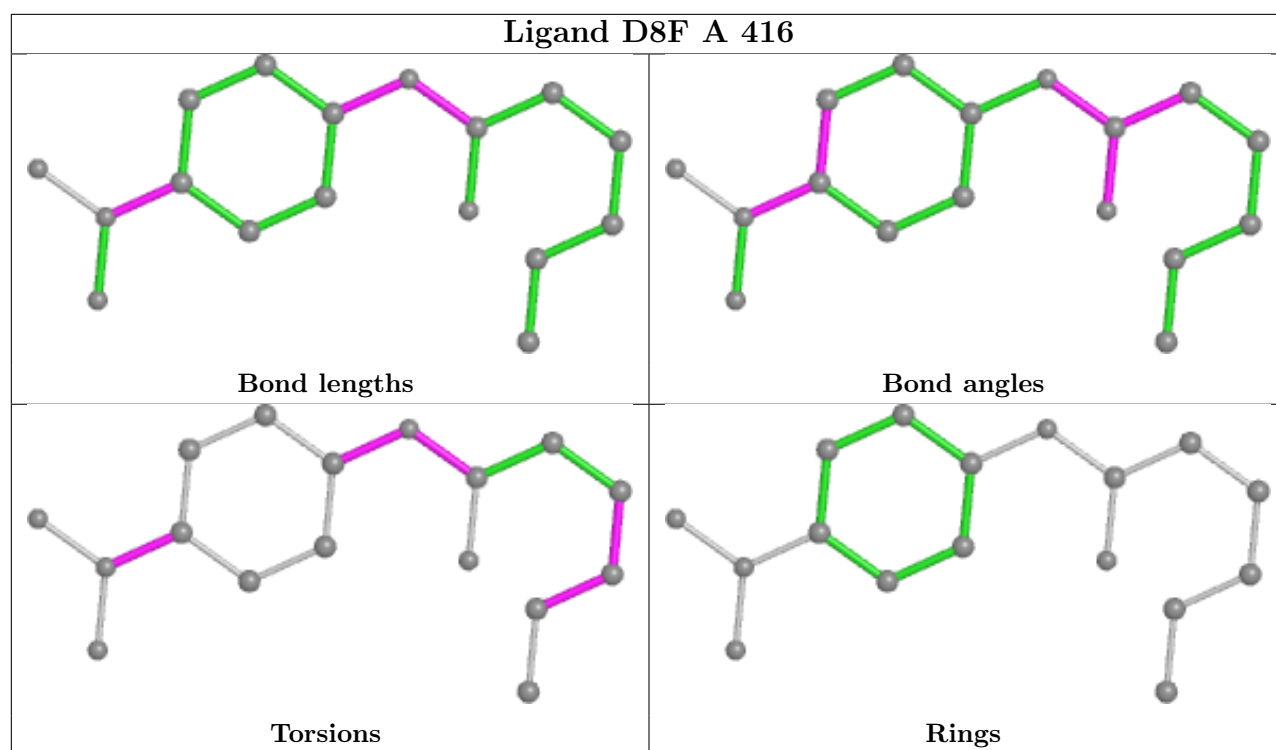
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1408	CCN	3	0
5	C	819	DMS	3	0
4	A	417	6NA	1	0
6	B	607	CCN	2	0
6	A	408	CCN	3	0
6	D	1403	CCN	2	0
2	D	1410	GOL	1	0
2	D	1401	GOL	1	0
3	A	404	EDO	1	0
5	A	406	DMS	5	0
10	B	615	BUA	2	0

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







## 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	309/314 (98%)	-0.13	3 (0%) 82 87	19, 25, 40, 49	0
1	B	309/314 (98%)	-0.12	2 (0%) 89 92	22, 28, 45, 59	0
1	C	309/314 (98%)	-0.05	6 (1%) 66 74	19, 25, 40, 50	0
1	D	309/314 (98%)	0.09	12 (3%) 39 45	21, 29, 49, 62	0
All	All	1236/1256 (98%)	-0.05	23 (1%) 66 74	19, 27, 45, 62	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	30	THR	3.7
1	C	4	THR	3.5
1	D	31	LEU	3.2
1	D	27	ALA	3.1
1	C	77	SER	3.0
1	D	247	ILE	2.8
1	D	28	GLU	2.6
1	A	77	SER	2.6
1	C	149	LEU	2.4
1	D	24	PRO	2.3
1	D	219	PHE	2.3
1	A	147	SER	2.3
1	D	275	VAL	2.3
1	C	274	VAL	2.3
1	C	76	GLU	2.3
1	C	248	VAL	2.2
1	B	4	THR	2.2
1	D	248	VAL	2.1
1	A	4	THR	2.1
1	B	275	VAL	2.1
1	D	277	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	26	LEU	2.0
1	D	23	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [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
5	DMS	A	414	4/4	0.20	0.41	54,61,62,72	4
5	DMS	A	415	4/4	0.40	0.26	21,30,62,66	4
11	NPO	B	621	10/10	0.47	0.23	147,176,183,186	10
2	GOL	C	813	6/6	0.52	0.25	47,57,58,61	0
4	6NA	D	1412	8/8	0.53	0.50	55,68,75,77	0
10	BUA	B	615	6/6	0.56	0.17	33,52,58,61	0
11	NPO	D	1421	10/10	0.56	0.27	66,79,114,114	10
6	CCN	D	1411	3/3	0.57	0.45	47,47,55,56	0
6	CCN	A	413	3/3	0.57	0.26	39,39,46,48	0
11	NPO	B	620	10/10	0.59	0.26	168,176,183,184	10
4	6NA	C	810	8/8	0.60	0.23	46,57,65,68	0
5	DMS	D	1413	4/4	0.62	0.27	73,83,92,102	0
6	CCN	A	411	3/3	0.64	0.23	46,46,51,53	0
5	DMS	A	407	4/4	0.66	0.40	77,77,84,94	0
6	CCN	B	607	3/3	0.67	0.24	50,50,52,59	0
6	CCN	D	1407	3/3	0.68	0.26	41,41,48,54	0
3	EDO	B	608	4/4	0.69	0.13	57,60,61,65	0
6	CCN	D	1408	3/3	0.70	0.23	26,26,40,41	0
6	CCN	C	811	3/3	0.70	0.27	34,34,43,44	0
3	EDO	A	412	4/4	0.72	0.27	51,54,57,57	0
6	CCN	A	409	3/3	0.74	0.18	44,44,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CCN	D	1415	3/3	0.74	0.16	39,39,40,51	0
5	DMS	A	406	4/4	0.75	0.34	66,67,71,89	0
7	D8F	A	416	17/17	0.75	0.21	28,42,54,56	0
6	CCN	C	807	3/3	0.75	0.45	43,43,50,52	0
3	EDO	B	605	4/4	0.76	0.37	38,48,48,59	0
3	EDO	C	806	4/4	0.76	0.29	55,58,59,63	0
6	CCN	A	408	3/3	0.77	0.26	36,36,45,46	0
7	D8F	B	623	17/17	0.77	0.22	36,44,56,58	0
6	CCN	B	613	3/3	0.77	0.27	44,44,54,54	0
4	6NA	D	1418	8/8	0.78	0.32	29,37,44,46	8
6	CCN	A	410	3/3	0.78	0.33	42,42,43,49	0
6	CCN	D	1416	3/3	0.78	0.22	35,35,38,40	0
4	6NA	A	417	8/8	0.79	0.25	55,61,63,66	0
7	D8F	D	1423	17/17	0.79	0.18	33,45,54,55	0
3	EDO	C	812	4/4	0.80	0.22	53,57,63,68	0
5	DMS	B	622	4/4	0.80	0.31	58,65,66,75	0
2	GOL	D	1410	6/6	0.80	0.27	48,49,58,63	0
6	CCN	D	1420	3/3	0.81	0.13	47,47,50,52	0
2	GOL	B	619	6/6	0.81	0.23	46,55,60,67	0
6	CCN	B	614	3/3	0.81	0.45	39,39,46,58	0
6	CCN	B	609	3/3	0.81	0.20	47,47,48,51	0
12	NA	C	821	1/1	0.81	0.25	77,77,77,77	0
3	EDO	A	405	4/4	0.82	0.24	41,50,52,58	0
6	CCN	B	610	3/3	0.83	0.12	46,46,52,54	0
2	GOL	C	816	6/6	0.83	0.23	53,59,66,73	0
6	CCN	D	1419	3/3	0.83	0.21	39,39,43,49	0
4	6NA	A	403	8/8	0.84	0.16	36,42,47,48	0
3	EDO	B	624	4/4	0.84	0.13	38,39,41,42	0
7	D8F	C	817	17/17	0.84	0.19	26,39,51,51	0
5	DMS	B	616	4/4	0.84	0.35	57,79,82,85	0
3	EDO	A	404	4/4	0.84	0.15	42,45,46,59	0
3	EDO	B	601	4/4	0.84	0.14	38,40,49,61	0
3	EDO	C	815	4/4	0.84	0.17	49,50,65,65	0
3	EDO	D	1402	4/4	0.84	0.19	40,43,50,56	0
3	EDO	D	1422	4/4	0.84	0.17	39,46,48,51	0
6	CCN	D	1417	3/3	0.85	0.23	40,40,50,51	0
5	DMS	D	1409	4/4	0.85	0.36	74,80,90,94	0
6	CCN	A	418	3/3	0.85	0.19	32,32,41,49	0
6	CCN	C	808	3/3	0.86	0.48	49,49,50,50	0
3	EDO	B	606	4/4	0.86	0.44	51,55,56,62	0
6	CCN	D	1403	3/3	0.86	0.15	43,43,50,52	0
3	EDO	C	805	4/4	0.86	0.23	40,40,51,57	0

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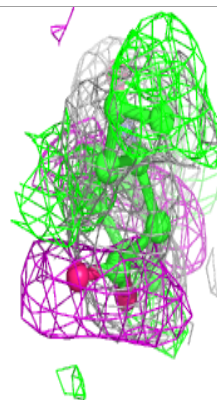
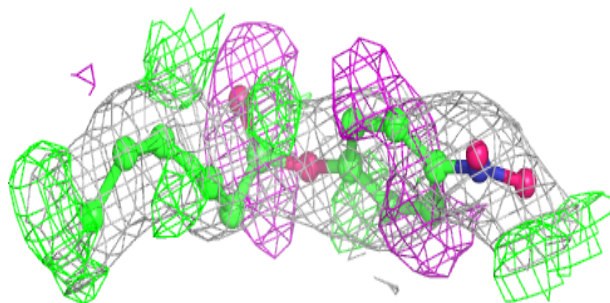
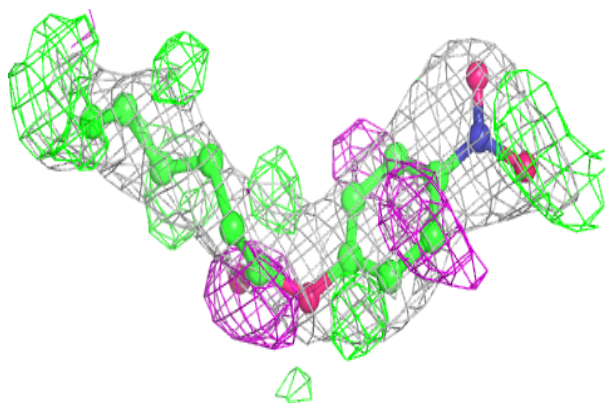
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	818	4/4	0.87	0.28	41,42,44,56	0
5	DMS	C	820	4/4	0.87	0.21	63,65,74,79	0
2	GOL	C	814	6/6	0.87	0.11	42,42,52,56	0
3	EDO	D	1406	4/4	0.87	0.14	37,40,54,63	0
3	EDO	D	1414	4/4	0.87	0.10	35,40,42,43	0
3	EDO	C	803	4/4	0.87	0.19	52,54,61,67	0
2	GOL	C	802	6/6	0.88	0.13	29,36,39,43	0
5	DMS	B	617	4/4	0.89	0.19	59,63,64,70	0
5	DMS	C	819	4/4	0.90	0.19	64,66,73,79	0
3	EDO	D	1405	4/4	0.90	0.16	38,43,45,46	0
2	GOL	C	809	6/6	0.90	0.15	31,40,46,46	6
5	DMS	B	611	4/4	0.91	0.24	67,75,78,85	0
2	GOL	D	1401	6/6	0.91	0.20	35,45,46,60	0
3	EDO	C	804	4/4	0.91	0.16	35,37,46,50	0
2	GOL	A	401	6/6	0.91	0.12	30,33,40,40	0
3	EDO	D	1404	4/4	0.93	0.13	34,43,43,59	0
3	EDO	B	603	4/4	0.93	0.24	37,45,46,47	0
3	EDO	C	801	4/4	0.94	0.09	39,42,47,48	0
3	EDO	A	402	4/4	0.94	0.11	36,40,42,44	0
6	CCN	B	618	3/3	0.94	0.44	35,35,38,39	0
3	EDO	B	602	4/4	0.95	0.13	31,37,41,45	0
9	DIO	B	604	6/6	0.96	0.08	36,36,37,43	0
5	DMS	B	612	4/4	0.96	0.13	48,52,58,59	0
8	SO4	A	420	5/5	0.96	0.31	56,56,70,84	0
8	SO4	A	419	5/5	0.97	0.18	55,58,69,69	0

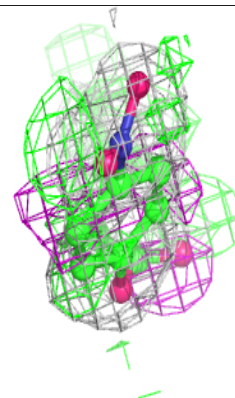
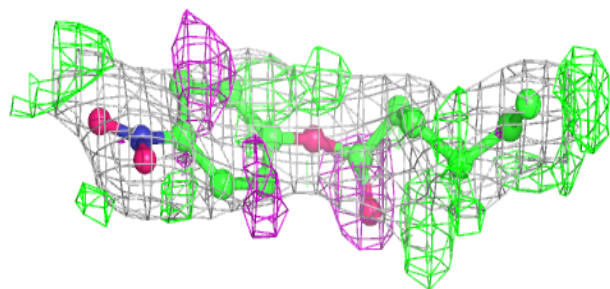
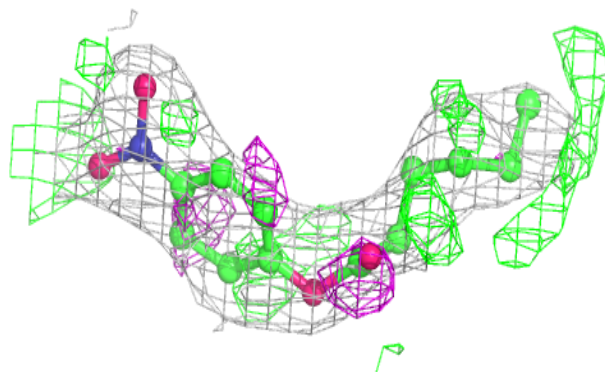
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around D8F A 416:**

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

**Electron density around D8F B 623:**

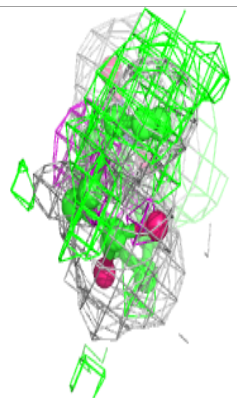
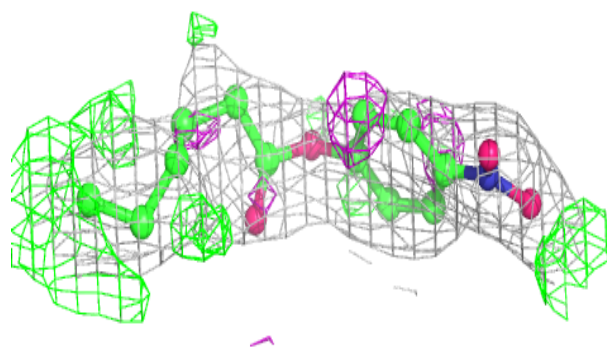
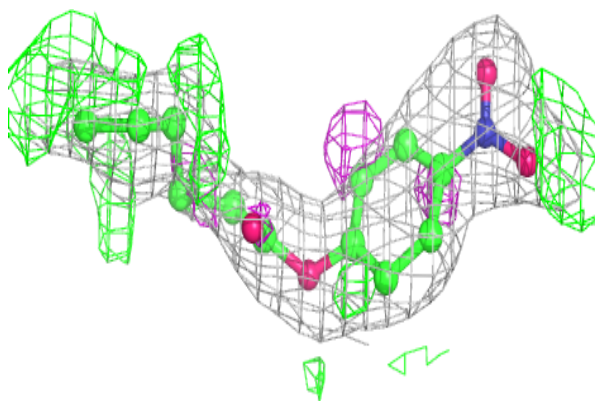
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



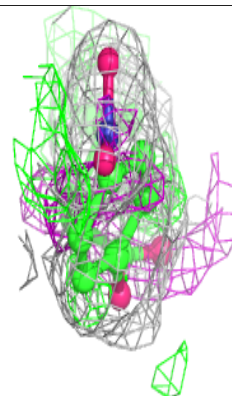
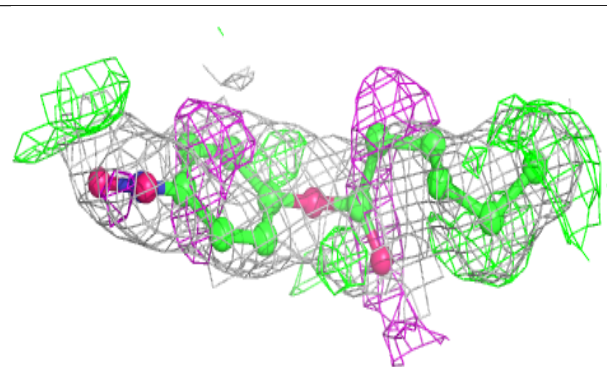
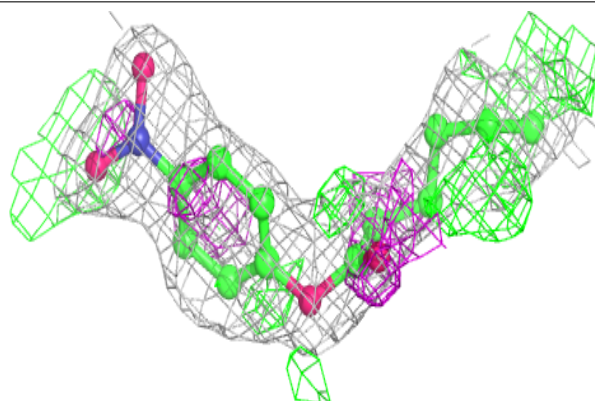


**Electron density around D8F D 1423:**

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

**Electron density around D8F C 817:**

$2mF_o-DF_c$  (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.