



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:41 pm BST

PDB ID : 4OGB  
Title : Crystal structure of the catalytic domain of PDE4D2 with compound 2  
Authors : Feil, S.C.; Parker, M.W.  
Deposited on : 2014-01-15  
Resolution : 2.03 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

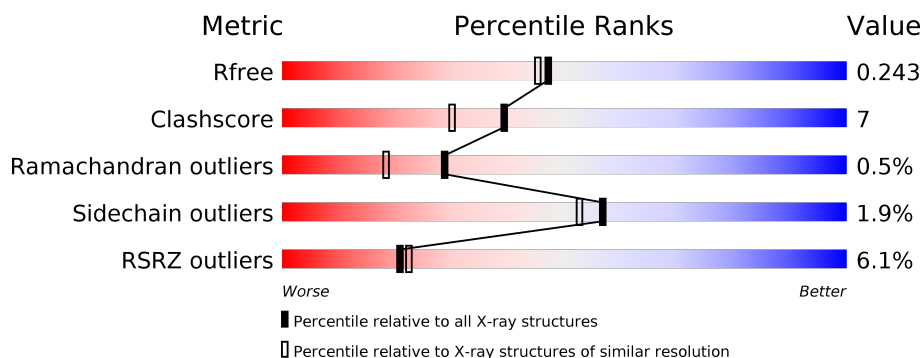
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	361	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>9%</div> </div> </div>
1	B	361	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>11%</div> </div> </div>
1	C	361	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>10%</div> </div> </div>
1	D	361	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	C	512	-	-	X	-
4	PEG	D	515	-	-	-	X
4	PEG	D	516	-	-	X	-
6	DMS	A	513	-	-	X	-

## 2 Entry composition [i](#)

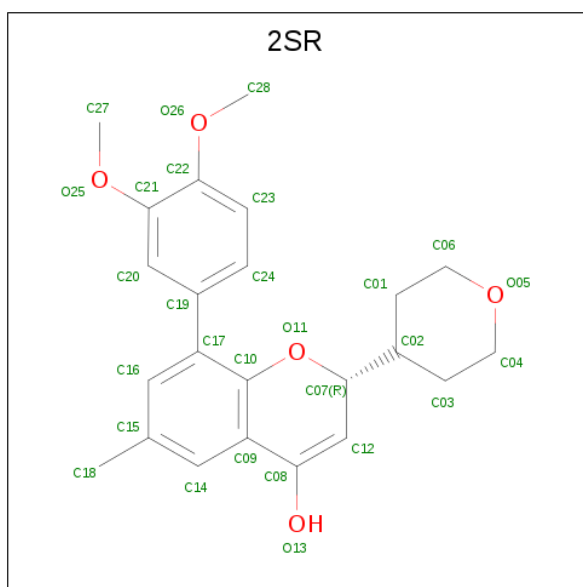
There are 8 unique types of molecules in this entry. The entry contains 11286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2651	1676	453	508	14			
1	B	321	Total	C	N	O	S	0	1	0
			2606	1649	447	496	14			
1	C	325	Total	C	N	O	S	0	1	0
			2642	1669	453	506	14			
1	D	324	Total	C	N	O	S	0	2	0
			2640	1669	452	505	14			

- Molecule 2 is (2R)-8-(3,4-dimethoxyphenyl)-6-methyl-2-(tetrahydro-2H-pyran-4-yl)-2H-chromen-4-ol (three-letter code: 2SR) (formula: C<sub>23</sub>H<sub>26</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	23	5		
2	B	1	Total	C	O	0	0
			28	23	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			28	23	5		
2	D	1	Total	C	O	0	0
			28	23	5		

- 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		
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	B	1	Total	C	O	0	0
			4	2	2		

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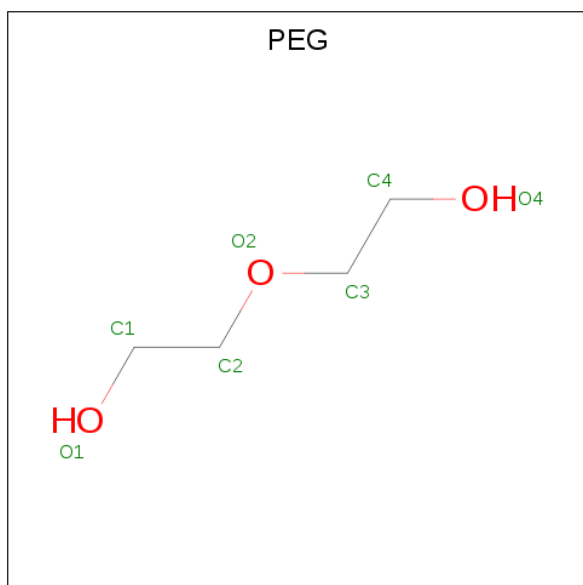
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

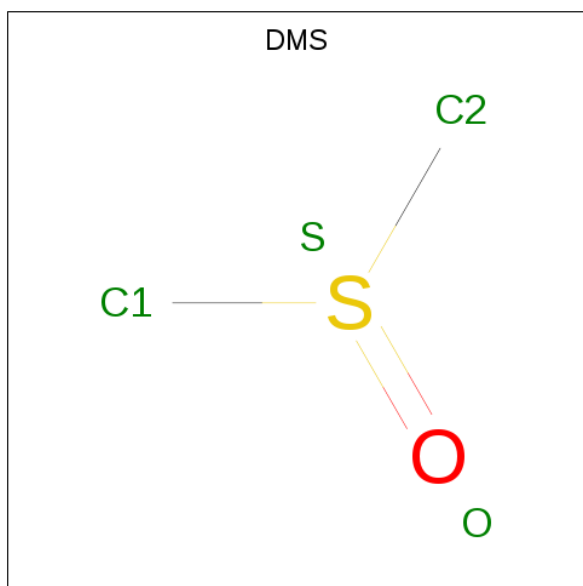
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		
5	A	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Zn	0	0
			2	2		

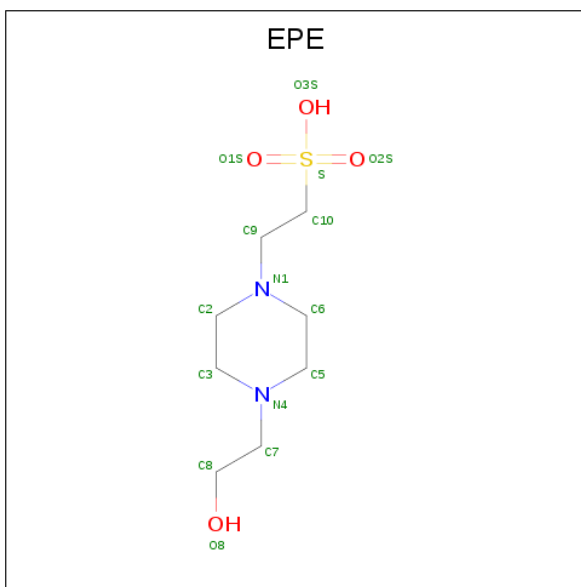
- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

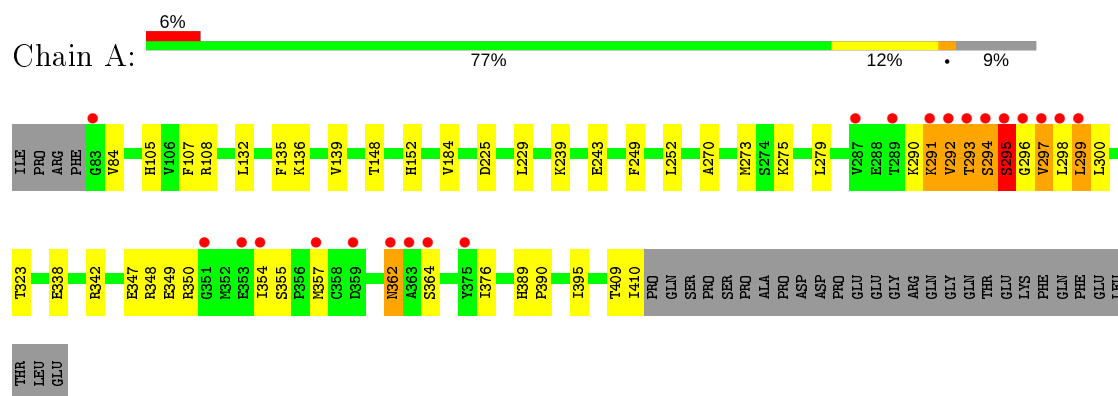
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	120	Total	O	0	0
			120	120		
8	B	104	Total	O	0	0
			104	104		
8	C	77	Total	O	0	0
			77	77		
8	D	131	Total	O	0	0
			131	131		

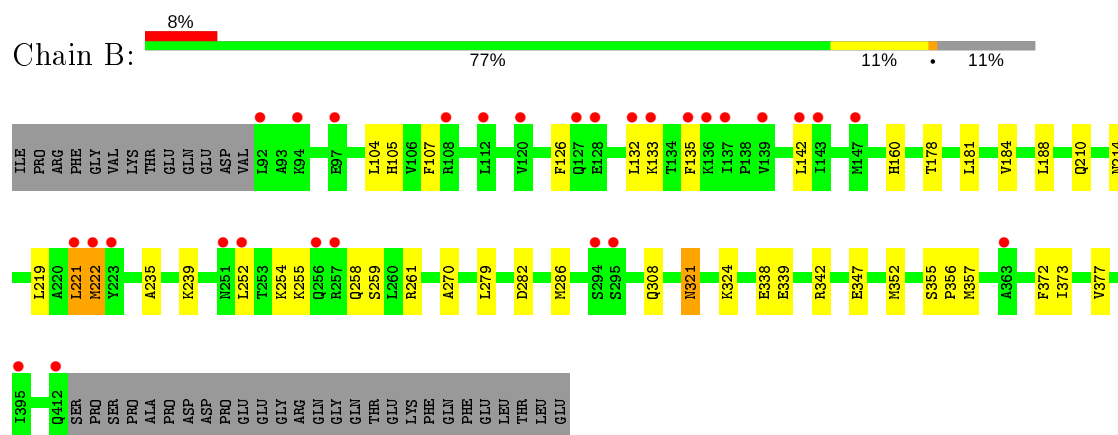
### 3 Residue-property plots

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.

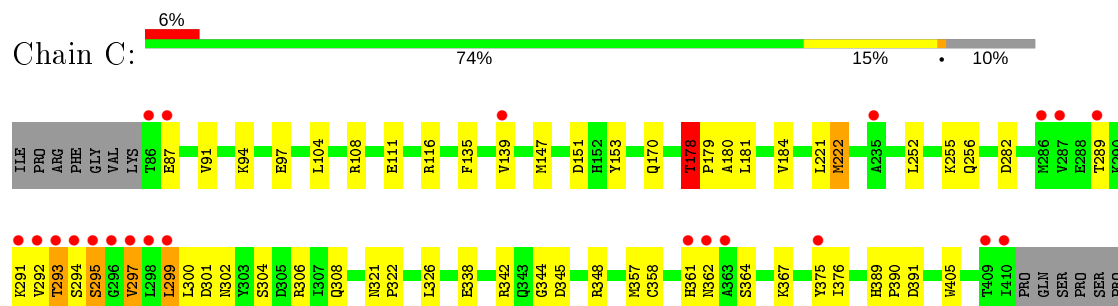
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



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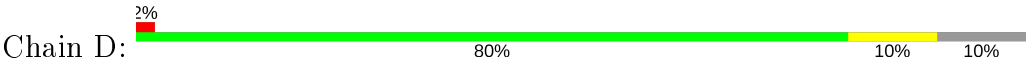


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



ALA  
PRO  
ASP  
ASP  
PRO  
GLU  
GLU  
GLY  
GLY  
ARG  
GLN  
GLY  
GLN  
THR  
GLU  
LYS  
PHE  
GLN  
PHE  
GLU  
LEU  
THR  
LEU  
GLU

● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



ILE  
PRO  
ARG  
PHE  
GLY  
VAL  
LYS  
THR  
GLU  
Q88  
E89  
D90  
W102  
G103  
L104  
H105  
V106  
F107  
V120  
H123  
D140  
Q170  
L219  
A220  
I221  
M222  
V228  
L229  
K262  
A270  
M273  
L279  
M286  
N302  
R306  
I307  
Q308  
N321  
P322  
F340  
F341  
R342  
R348

E349  
R350  
I354  
D359  
K360  
R361  
N362  
A363  
K367  
Y375  
I376  
I410  
F411  
GLN  
SER  
PRO  
SER  
PRO  
PRO  
ALA  
PRO  
ASP  
ASP  
PRO  
GLU  
GLU  
GLY  
ARG  
GLN  
GLY  
GLN  
THR  
GLU  
LYS  
PHE  
GLN  
PHE  
GLU  
LEU  
THR  
LEU  
GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.84Å 111.55Å 160.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 2.03 48.13 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.22-2.03) 99.9 (48.13-2.03)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.03Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.202 , 0.243 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	5713 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: ZN, EPE, EDO, DMS, PEG, 2SR

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	0.51	0/2704	0.55	0/3672
1	B	0.47	0/2660	0.57	1/3615 (0.0%)
1	C	0.57	0/2695	0.57	1/3660 (0.0%)
1	D	0.54	0/2695	0.59	2/3662 (0.1%)
All	All	0.52	0/10754	0.57	4/14609 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	410	ILE	C-N-CD	5.92	140.84	128.40
1	C	178	THR	C-N-CD	5.55	140.06	128.40
1	B	355	SER	C-N-CD	5.36	139.66	128.40
1	D	367	LYS	CB-CA-C	-5.17	100.05	110.40

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	2651	0	2609	47	0
1	B	2606	0	2565	34	0
1	C	2642	0	2596	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2640	0	2587	34	0
2	A	28	0	26	4	0
2	B	28	0	26	2	0
2	C	28	0	26	1	0
2	D	28	0	26	3	0
3	A	32	0	48	6	0
3	B	28	0	42	5	0
3	C	36	0	54	9	0
3	D	32	0	48	2	0
4	A	7	0	10	0	0
4	D	21	0	30	7	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	8	0	12	5	0
6	B	8	0	12	3	0
6	D	8	0	12	0	0
7	C	15	0	17	0	0
8	A	120	0	0	2	0
8	B	104	0	0	5	0
8	C	77	0	0	1	0
8	D	131	0	0	2	0
All	All	11286	0	10746	159	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 7.

All (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:MET:CE	1:D:222:MET:SD	2.25	1.25
1:C:222:MET:HE1	1:D:222:MET:SD	1.80	1.22
1:C:222:MET:HG3	3:C:512:EDO:H21	1.18	1.17
1:C:222:MET:HG3	3:C:512:EDO:C2	1.85	1.05
1:C:222:MET:HE2	1:D:222:MET:SD	2.04	0.98
1:A:290:LYS:O	1:A:291:LYS:HD2	1.70	0.92
1:D:286:MET:CE	1:D:308:GLN:NE2	2.35	0.90
1:C:361:HIS:O	1:C:362:ASN:ND2	2.04	0.89
1:D:286:MET:HE3	1:D:308:GLN:HE22	1.37	0.89
1:C:222:MET:CG	3:C:512:EDO:H21	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:MET:CE	1:D:308:GLN:HE22	1.92	0.83
1:A:290:LYS:C	1:A:291:LYS:HD2	2.01	0.80
1:D:102:TRP:H	4:D:516:PEG:H11	1.48	0.78
1:C:361:HIS:C	1:C:362:ASN:HD22	1.89	0.76
1:A:292:VAL:HG13	1:A:293:THR:N	2.01	0.75
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.71	0.73
1:B:104:LEU:HB3	3:B:509:EDO:H21	1.69	0.73
1:A:292:VAL:HG13	1:A:293:THR:H	1.54	0.70
1:D:286:MET:HE1	1:D:308:GLN:NE2	2.06	0.70
1:A:409:THR:O	1:A:410:ILE:HG22	1.93	0.69
1:C:338:GLU:OE2	1:C:342:ARG:NH2	2.26	0.68
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.27	0.68
1:A:292:VAL:HG22	1:A:297:VAL:H	1.59	0.67
1:C:375:TYR:O	1:C:376:ILE:HD12	1.95	0.67
1:C:180:ALA:C	1:C:297:VAL:HG22	2.16	0.66
1:C:116:ARG:NE	8:C:644:HOH:O	2.28	0.66
1:A:299:LEU:HD12	1:A:299:LEU:C	2.17	0.65
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.78	0.65
1:B:308:GLN:HG3	8:B:605:HOH:O	1.97	0.63
1:B:254:LYS:HE3	1:B:258:GLN:HE22	1.63	0.62
1:A:299:LEU:HD12	1:A:300:LEU:N	2.14	0.61
1:C:180:ALA:O	1:C:297:VAL:HG22	2.00	0.61
1:A:362:ASN:OD1	1:A:362:ASN:N	2.34	0.61
1:C:289:THR:O	1:C:289:THR:HG22	2.00	0.61
1:D:88:GLN:HG3	1:D:90:ASP:H	1.66	0.60
1:B:210:GLN:HE21	1:B:214:ASN:HD21	1.48	0.60
1:A:239:LYS:HZ2	3:A:508:EDO:H22	1.65	0.60
1:A:292:VAL:CG2	1:A:297:VAL:H	2.14	0.60
1:C:292:VAL:O	1:C:292:VAL:HG23	2.00	0.60
1:A:296:GLY:O	1:A:297:VAL:HB	2.02	0.59
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.36	0.59
1:C:302:ASN:O	1:C:306:ARG:HG3	2.03	0.58
1:B:352:MET:HB3	3:B:507:EDO:H22	1.84	0.58
1:C:255:LYS:HG2	3:C:505:EDO:H11	1.85	0.58
1:C:302:ASN:ND2	1:C:302:ASN:H	2.01	0.57
1:A:105:HIS:HB3	6:A:513:DMS:H22	1.87	0.57
1:C:357:MET:SD	2:C:502:2SR:H16	2.45	0.57
1:D:102:TRP:H	4:D:516:PEG:C1	2.18	0.56
1:A:295:SER:OG	1:A:296:GLY:N	2.37	0.56
1:B:135:PHE:HB3	1:B:252:LEU:HD11	1.87	0.56
1:A:338:GLU:OE2	1:A:342:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLY:O	1:A:297:VAL:CB	2.54	0.56
1:C:375:TYR:C	1:C:376:ILE:HD12	2.26	0.56
1:B:356:PRO:O	1:B:357:MET:HB2	2.06	0.56
1:A:249:PHE:CD2	3:A:506:EDO:H22	2.42	0.55
1:D:102:TRP:HB2	4:D:516:PEG:H32	1.88	0.55
1:C:151:ASP:HA	3:C:509:EDO:H21	1.89	0.54
1:D:102:TRP:N	4:D:516:PEG:H11	2.20	0.54
1:C:364:SER:HB2	1:C:367:LYS:HB3	1.89	0.54
1:A:108:ARG:H	6:A:513:DMS:C2	2.20	0.54
1:B:181:LEU:HD23	1:B:184:VAL:HG21	1.89	0.54
1:C:108:ARG:NH1	1:C:111:GLU:OE1	2.40	0.53
1:B:126:PHE:HB3	1:B:132:LEU:HD11	1.91	0.53
1:A:349:GLU:HB3	1:C:147:MET:SD	2.49	0.53
1:B:372:PHE:HE2	6:B:510:DMS:H21	1.74	0.53
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.42	0.53
1:B:357:MET:SD	2:B:501:2SR:H16	2.49	0.53
8:A:627:HOH:O	1:B:222:MET:HG3	2.09	0.52
1:A:107:PHE:HB2	6:A:513:DMS:H23	1.91	0.51
1:C:293:THR:O	1:C:295:SER:N	2.44	0.51
1:D:105[A]:HIS:HE1	1:D:107:PHE:HB2	1.76	0.51
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.93	0.51
1:A:108:ARG:H	6:A:513:DMS:H23	1.75	0.51
1:B:235:ALA:O	1:B:239:LYS:HD3	2.10	0.51
1:C:222:MET:HG3	3:C:512:EDO:C1	2.41	0.51
1:D:220:ALA:HA	1:D:228:VAL:HG21	1.93	0.51
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.75	0.50
1:B:254:LYS:HE3	1:B:258:GLN:NE2	2.26	0.50
1:A:376:ILE:HD13	2:A:501:2SR:H20	1.92	0.50
1:D:123:HIS:HD1	3:D:505:EDO:H11	1.75	0.50
1:A:239:LYS:NZ	3:A:508:EDO:H22	2.27	0.50
1:A:376:ILE:CD1	2:A:501:2SR:H20	2.41	0.50
1:A:323:THR:HB	1:A:395:ILE:HG23	1.92	0.50
1:B:221:LEU:HG	8:B:698:HOH:O	2.12	0.49
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.94	0.49
1:D:105[A]:HIS:CE1	1:D:107:PHE:HB2	2.47	0.49
1:C:178:THR:HG22	1:C:181:LEU:HD12	1.95	0.49
1:D:273:MET:HG3	2:D:502:2SR:H22	1.94	0.49
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.28	0.49
1:A:350:ARG:NH1	8:A:644:HOH:O	2.47	0.47
1:B:321[B]:ASN:HB2	6:B:510:DMS:H22	1.96	0.47
1:B:347:GLU:HG2	3:B:507:EDO:H12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:OD1	3:B:507:EDO:H21	2.14	0.47
1:D:262:LYS:HG3	4:D:507:PEG:H32	1.97	0.47
1:B:178:THR:CG2	1:B:181:LEU:HB2	2.45	0.47
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.72	0.47
1:C:135:PHE:HA	3:C:504:EDO:H21	1.97	0.46
1:C:293:THR:HG23	1:C:299:LEU:HB2	1.98	0.46
1:D:262:LYS:HA	4:D:507:PEG:H41	1.97	0.46
1:D:88:GLN:NE2	8:D:626:HOH:O	2.49	0.46
1:A:348:ARG:HB2	1:A:354:ILE:HD11	1.97	0.46
1:C:304:SER:O	1:C:308:GLN:HB2	2.16	0.46
1:D:342:ARG:HG2	8:D:667:HOH:O	2.16	0.46
1:A:338:GLU:CD	1:A:342:ARG:HH21	2.18	0.45
1:D:348:ARG:HB3	1:D:354:ILE:HD11	1.98	0.45
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.98	0.45
1:A:273:MET:HG3	2:A:501:2SR:H22	1.99	0.45
1:D:350:ARG:HH11	1:D:350:ARG:HG3	1.80	0.45
1:A:148:THR:O	1:A:152:HIS:HD2	2.00	0.45
1:B:282:ASP:HB3	1:B:308:GLN:OE1	2.17	0.45
1:C:252:LEU:HD12	1:C:256:GLN:HB3	1.98	0.44
1:C:344:GLY:HA3	1:C:358:CYS:O	2.17	0.44
1:A:293:THR:O	1:A:294:SER:C	2.56	0.44
1:C:179:PRO:HD2	1:C:391:ASP:OD2	2.17	0.44
2:B:501:2SR:H9	8:B:613:HOH:O	2.18	0.44
1:B:255:LYS:HA	1:B:258:GLN:OE1	2.17	0.44
1:B:252:LEU:HD23	8:B:671:HOH:O	2.18	0.44
1:C:94:LYS:O	1:C:97:GLU:HG2	2.17	0.44
6:B:512:DMS:H13	1:D:140[B]:ASP:OD1	2.17	0.44
1:D:376:ILE:CD1	2:D:502:2SR:H20	2.48	0.44
1:C:222:MET:CB	3:C:512:EDO:H21	2.46	0.43
1:D:359:ASP:HB3	1:D:362:ASN:OD1	2.17	0.43
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.48	0.43
1:B:160:HIS:ND1	1:B:339:GLU:OE2	2.40	0.43
1:C:221:LEU:HD23	1:C:221:LEU:O	2.17	0.43
1:A:299:LEU:CD1	1:A:299:LEU:C	2.85	0.43
1:A:184:VAL:HG11	1:A:300:LEU:HD12	2.01	0.43
1:A:347:GLU:OE2	1:A:355:SER:OG	2.30	0.43
1:C:87:GLU:O	1:C:91:VAL:HG23	2.19	0.43
1:B:373:ILE:HA	1:B:377:VAL:HB	2.01	0.42
1:A:136:LYS:HA	3:A:503:EDO:H21	2.01	0.42
1:A:357:MET:SD	2:A:501:2SR:H16	2.59	0.42
1:A:243:GLU:HG2	3:A:508:EDO:H12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.49	0.42
1:C:321:ASN:HB2	1:C:322:PRO:HD3	2.01	0.42
4:D:507:PEG:H21	4:D:507:PEG:H41	1.89	0.42
1:B:324:LYS:HZ3	3:B:509:EDO:H11	1.84	0.42
1:C:153:TYR:O	3:C:509:EDO:O2	2.28	0.42
1:C:293:THR:C	1:C:295:SER:N	2.72	0.42
1:D:123:HIS:HD1	3:D:505:EDO:C1	2.33	0.42
1:B:188:LEU:HD12	1:B:188:LEU:HA	1.86	0.41
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.55	0.41
1:D:340:PHE:HZ	2:D:502:2SR:H10	1.84	0.41
1:A:389:HIS:HA	1:A:390:PRO:HA	1.77	0.41
1:A:108:ARG:N	6:A:513:DMS:H23	2.34	0.41
1:C:389:HIS:CD2	1:C:390:PRO:HA	2.55	0.41
1:D:321:ASN:HB2	1:D:322:PRO:HD3	2.01	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.88	0.41
1:A:275:LYS:HB3	3:A:507:EDO:H21	2.02	0.41
1:B:133:LYS:HA	1:B:133:LYS:HD3	1.86	0.41
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.02	0.41
1:A:296:GLY:O	1:A:297:VAL:HG23	2.21	0.41
1:B:252:LEU:HB3	8:B:671:HOH:O	2.19	0.41
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.95	0.41
1:C:181:LEU:O	1:C:184:VAL:HG23	2.21	0.40
1:D:270:ALA:HB1	1:D:279:LEU:HD11	2.03	0.40
1:B:132:LEU:HD21	1:B:142:LEU:HD22	2.02	0.40
1:A:135:PHE:HB3	1:A:252:LEU:HD11	2.02	0.40
1:D:302:ASN:O	1:D:306:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/361 (90%)	312 (96%)	10 (3%)	4 (1%)	13	5
1	B	320/361 (89%)	310 (97%)	10 (3%)	0	100	100
1	C	324/361 (90%)	313 (97%)	9 (3%)	2 (1%)	25	15
1	D	324/361 (90%)	318 (98%)	6 (2%)	0	100	100
All	All	1294/1444 (90%)	1253 (97%)	35 (3%)	6 (0%)	29	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	VAL
1	C	294	SER
1	A	295	SER
1	A	292	VAL
1	A	294	SER
1	C	293	THR

### 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	299/329 (91%)	291 (97%)	8 (3%)	44	38
1	B	294/329 (89%)	287 (98%)	7 (2%)	49	42
1	C	298/329 (91%)	290 (97%)	8 (3%)	44	38
1	D	298/329 (91%)	297 (100%)	1 (0%)	92	93
All	All	1189/1316 (90%)	1165 (98%)	24 (2%)	57	50

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	A	291	LYS
1	A	293	THR
1	A	295	SER
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	299	LEU
1	A	362	ASN
1	A	364	SER
1	B	219	LEU
1	B	221	LEU
1	B	222	MET
1	B	259	SER
1	B	286	MET
1	B	321[A]	ASN
1	B	321[B]	ASN
1	C	139	VAL
1	C	178	THR
1	C	222	MET
1	C	291	LYS
1	C	295	SER
1	C	297	VAL
1	C	299	LEU
1	C	301	ASP
1	D	120	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN
1	C	308	GLN
1	C	362	ASN
1	C	389	HIS
1	D	308	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 55 ligands modelled in this entry, 8 are monoatomic - leaving 47 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
3	EDO	B	505	-	3,3,3	0.50	0	2,2,2	0.32	0
7	EPE	C	506	-	15,15,15	0.82	1 (6%)	18,20,20	2.11	6 (33%)
3	EDO	B	511	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	D	511	-	3,3,3	0.52	0	2,2,2	0.26	0
4	PEG	D	515	-	6,6,6	0.31	0	5,5,5	0.33	0
3	EDO	C	512	-	3,3,3	0.53	0	2,2,2	0.26	0
3	EDO	D	514	-	3,3,3	0.57	0	2,2,2	0.12	0
3	EDO	A	505	-	3,3,3	0.42	0	2,2,2	0.50	0
3	EDO	D	503	-	3,3,3	0.35	0	2,2,2	0.42	0
4	PEG	D	516	-	6,6,6	0.34	0	5,5,5	0.57	0
2	2SR	B	501	-	28,31,31	3.09	10 (35%)	36,44,44	1.64	6 (16%)
3	EDO	D	505	-	3,3,3	0.53	0	2,2,2	0.24	0
3	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.36	0
3	EDO	C	503	-	3,3,3	0.41	0	2,2,2	0.52	0
3	EDO	C	508	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.54	0
3	EDO	B	504	-	3,3,3	0.49	0	2,2,2	0.51	0
3	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.58	0
3	EDO	C	509	-	3,3,3	0.49	0	2,2,2	0.41	0
6	DMS	B	512	-	3,3,3	0.62	0	3,3,3	0.50	0
3	EDO	B	509	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.30	0
2	2SR	C	502	-	28,31,31	3.08	11 (39%)	36,44,44	1.78	9 (25%)
3	EDO	B	506	-	3,3,3	0.51	0	2,2,2	0.10	0
6	DMS	A	513	-	3,3,3	0.52	0	3,3,3	0.57	0
3	EDO	D	506	-	3,3,3	0.56	0	2,2,2	0.13	0
3	EDO	B	507	-	3,3,3	0.52	0	2,2,2	0.15	0
3	EDO	C	505	-	3,3,3	0.49	0	2,2,2	0.45	0
3	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.39	0
4	PEG	A	504	-	6,6,6	0.26	0	5,5,5	0.53	0
6	DMS	A	511	-	3,3,3	0.66	0	3,3,3	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	DMS	D	504	-	3,3,3	0.69	0	3,3,3	0.62	0
3	EDO	D	501	-	3,3,3	0.48	0	2,2,2	0.63	0
6	DMS	D	508	-	3,3,3	0.65	0	3,3,3	0.71	0
3	EDO	C	507	-	3,3,3	0.54	0	2,2,2	0.25	0
3	EDO	A	514	-	3,3,3	0.64	0	2,2,2	0.33	0
3	EDO	B	508	-	3,3,3	0.46	0	2,2,2	0.32	0
2	2SR	D	502	-	28,31,31	2.98	11 (39%)	36,44,44	1.75	9 (25%)
3	EDO	A	506	-	3,3,3	0.37	0	2,2,2	0.63	0
4	PEG	D	507	-	6,6,6	0.40	0	5,5,5	0.39	0
6	DMS	B	510	-	3,3,3	0.65	0	3,3,3	0.62	0
3	EDO	C	501	-	3,3,3	0.69	0	2,2,2	0.11	0
3	EDO	D	509	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	D	510	-	3,3,3	0.49	0	2,2,2	0.45	0
3	EDO	C	513	-	3,3,3	0.48	0	2,2,2	0.21	0
2	2SR	A	501	-	28,31,31	3.02	9 (32%)	36,44,44	1.58	5 (13%)
3	EDO	A	507	-	3,3,3	0.54	0	2,2,2	0.25	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	B	505	-	-	1/1/1/1	-
7	EPE	C	506	-	-	6/9/19/19	0/1/1/1
3	EDO	B	511	-	-	0/1/1/1	-
3	EDO	D	511	-	-	0/1/1/1	-
4	PEG	D	515	-	-	2/4/4/4	-
3	EDO	C	512	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
4	PEG	D	516	-	-	3/4/4/4	-
2	2SR	B	501	-	-	8/12/32/32	1/4/4/4
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	C	508	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	C	509	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	509	-	-	1/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
2	2SR	C	502	-	-	7/12/32/32	0/4/4/4
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	D	506	-	-	1/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	C	505	-	-	0/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
4	PEG	A	504	-	-	3/4/4/4	-
3	EDO	D	509	-	-	0/1/1/1	-
3	EDO	D	501	-	-	0/1/1/1	-
3	EDO	C	507	-	-	1/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	B	508	-	-	0/1/1/1	-
2	2SR	D	502	-	-	4/12/32/32	1/4/4/4
3	EDO	A	506	-	-	0/1/1/1	-
4	PEG	D	507	-	-	3/4/4/4	-
3	EDO	C	501	-	-	0/1/1/1	-
3	EDO	D	514	-	-	0/1/1/1	-
3	EDO	D	510	-	-	0/1/1/1	-
3	EDO	C	513	-	-	0/1/1/1	-
2	2SR	A	501	-	-	8/12/32/32	0/4/4/4
3	EDO	A	507	-	-	0/1/1/1	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2SR	O11-C10	11.15	1.54	1.37
2	C	502	2SR	O11-C10	11.13	1.54	1.37
2	B	501	2SR	O11-C10	10.67	1.53	1.37
2	D	502	2SR	O11-C10	10.38	1.53	1.37
2	B	501	2SR	C14-C09	6.65	1.50	1.39
2	D	502	2SR	C14-C09	6.48	1.50	1.39
2	C	502	2SR	C14-C09	6.41	1.49	1.39
2	A	501	2SR	C14-C09	6.28	1.49	1.39
2	C	502	2SR	C17-C10	5.35	1.51	1.41
2	B	501	2SR	C17-C10	5.01	1.50	1.41
2	A	501	2SR	C17-C10	4.98	1.50	1.41
2	D	502	2SR	C17-C10	4.48	1.49	1.41
2	B	501	2SR	O13-C08	4.20	1.41	1.32
2	C	502	2SR	O13-C08	4.14	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	2SR	O13-C08	4.13	1.40	1.32
2	A	501	2SR	O13-C08	4.04	1.40	1.32
2	B	501	2SR	O25-C21	3.76	1.43	1.37
2	C	502	2SR	O25-C21	3.44	1.42	1.37
2	B	501	2SR	C17-C19	3.42	1.55	1.49
2	D	502	2SR	O25-C21	3.16	1.42	1.37
2	D	502	2SR	C17-C19	3.13	1.55	1.49
2	A	501	2SR	C17-C19	3.03	1.54	1.49
2	C	502	2SR	C17-C19	3.01	1.54	1.49
2	A	501	2SR	O25-C21	2.99	1.41	1.37
7	C	506	EPE	C10-S	2.71	1.81	1.77
2	B	501	2SR	C16-C15	2.67	1.43	1.39
2	D	502	2SR	C09-C10	-2.67	1.35	1.40
2	D	502	2SR	C16-C15	2.64	1.43	1.39
2	B	501	2SR	C09-C10	-2.52	1.35	1.40
2	A	501	2SR	C09-C10	-2.43	1.35	1.40
2	A	501	2SR	C16-C15	2.39	1.43	1.39
2	D	502	2SR	C03-C02	-2.37	1.47	1.53
2	D	502	2SR	C14-C15	2.37	1.42	1.39
2	B	501	2SR	C14-C15	2.31	1.42	1.39
2	C	502	2SR	C09-C10	-2.31	1.36	1.40
2	C	502	2SR	C16-C15	2.27	1.42	1.39
2	D	502	2SR	C01-C02	-2.19	1.47	1.53
2	C	502	2SR	C14-C15	2.15	1.42	1.39
2	C	502	2SR	O26-C22	2.11	1.40	1.37
2	B	501	2SR	O26-C22	2.11	1.40	1.37
2	C	502	2SR	C03-C02	-2.06	1.48	1.53
2	A	501	2SR	C03-C02	-2.00	1.48	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	2SR	O25-C21-C22	4.77	122.05	115.41
2	B	501	2SR	O26-C22-C21	4.50	121.68	115.41
7	C	506	EPE	C7-N4-C5	4.30	122.23	111.23
7	C	506	EPE	C5-N4-C3	4.23	118.35	108.83
2	A	501	2SR	O26-C22-C21	4.14	121.18	115.41
2	C	502	2SR	O25-C21-C22	4.10	121.12	115.41
2	D	502	2SR	C06-C01-C02	-4.08	105.07	110.68
2	C	502	2SR	O26-C22-C21	3.98	120.95	115.41
2	D	502	2SR	O26-C22-C21	3.96	120.93	115.41
2	A	501	2SR	O25-C21-C22	3.77	120.66	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	2SR	C04-C03-C02	-3.72	105.56	110.68
2	C	502	2SR	O13-C08-C12	-3.66	118.22	121.73
7	C	506	EPE	O2S-S-C10	3.64	111.30	106.92
2	B	501	2SR	O26-C22-C23	-3.35	118.63	124.37
2	A	501	2SR	O26-C22-C23	-3.26	118.79	124.37
7	C	506	EPE	C7-N4-C3	3.19	119.41	111.23
2	C	502	2SR	C06-C01-C02	3.18	115.05	110.68
2	C	502	2SR	O26-C22-C23	-3.06	119.13	124.37
2	B	501	2SR	O25-C21-C20	-3.03	118.91	124.12
2	D	502	2SR	O26-C22-C23	-2.95	119.31	124.37
2	D	502	2SR	O25-C21-C22	2.89	119.44	115.41
7	C	506	EPE	C6-N1-C2	2.84	115.23	108.83
2	A	501	2SR	O25-C21-C20	-2.79	119.32	124.12
2	C	502	2SR	C04-C03-C02	2.68	114.37	110.68
2	C	502	2SR	O25-C21-C20	-2.64	119.57	124.12
2	D	502	2SR	C27-O25-C21	-2.39	113.92	117.53
2	C	502	2SR	C03-C02-C01	2.38	113.63	109.44
7	C	506	EPE	O3S-S-C10	2.29	109.47	105.77
2	D	502	2SR	O11-C07-C02	-2.21	103.22	107.40
2	D	502	2SR	O25-C21-C20	-2.20	120.34	124.12
2	A	501	2SR	C28-O26-C22	-2.14	114.29	117.53
2	C	502	2SR	C10-C09-C08	2.10	120.16	116.83
2	D	502	2SR	O13-C08-C12	-2.08	119.73	121.73
2	B	501	2SR	C16-C15-C14	2.07	120.56	118.09
2	B	501	2SR	C18-C15-C16	-2.04	117.92	120.94

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	EDO	O1-C1-C2-O2
2	B	501	2SR	C01-C02-C07-O11
2	B	501	2SR	C01-C02-C07-C12
2	B	501	2SR	C03-C02-C07-O11
2	B	501	2SR	C03-C02-C07-C12
3	D	505	EDO	O1-C1-C2-O2
2	C	502	2SR	C01-C02-C07-O11
2	C	502	2SR	C01-C02-C07-C12
2	C	502	2SR	C03-C02-C07-O11
2	C	502	2SR	C03-C02-C07-C12
7	C	506	EPE	C8-C7-N4-C5
7	C	506	EPE	S-C10-C9-N1

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Mol	Chain	Res	Type	Atoms
7	C	506	EPE	C9-C10-S-O1S
7	C	506	EPE	C9-C10-S-O3S
2	A	501	2SR	C01-C02-C07-O11
2	A	501	2SR	C01-C02-C07-C12
2	A	501	2SR	C03-C02-C07-O11
2	A	501	2SR	C03-C02-C07-C12
4	A	504	PEG	C1-C2-O2-C3
2	B	501	2SR	C21-C22-O26-C28
2	B	501	2SR	C23-C22-O26-C28
2	D	502	2SR	C23-C22-O26-C28
4	D	507	PEG	C4-C3-O2-C2
2	A	501	2SR	C21-C22-O26-C28
2	C	502	2SR	C23-C22-O26-C28
2	B	501	2SR	C20-C21-O25-C27
2	D	502	2SR	C21-C22-O26-C28
2	A	501	2SR	C22-C21-O25-C27
2	A	501	2SR	C23-C22-O26-C28
2	D	502	2SR	C22-C21-O25-C27
2	B	501	2SR	C22-C21-O25-C27
3	C	512	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2
3	B	509	EDO	O1-C1-C2-O2
2	C	502	2SR	C21-C22-O26-C28
2	A	501	2SR	C20-C21-O25-C27
4	D	515	PEG	O2-C3-C4-O4
4	A	504	PEG	O1-C1-C2-O2
2	D	502	2SR	C20-C21-O25-C27
4	D	516	PEG	O2-C3-C4-O4
4	D	507	PEG	O1-C1-C2-O2
3	B	505	EDO	O1-C1-C2-O2
4	D	507	PEG	C1-C2-O2-C3
4	D	516	PEG	C1-C2-O2-C3
4	A	504	PEG	C4-C3-O2-C2
3	A	508	EDO	O1-C1-C2-O2
3	C	507	EDO	O1-C1-C2-O2
7	C	506	EPE	C9-C10-S-O2S
4	D	516	PEG	C4-C3-O2-C2
3	D	503	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
7	C	506	EPE	C10-C9-N1-C2
3	A	502	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	502	2SR	C22-C21-O25-C27
4	D	515	PEG	C4-C3-O2-C2
3	D	506	EDO	O1-C1-C2-O2

All (2) ring outliers are listed below:

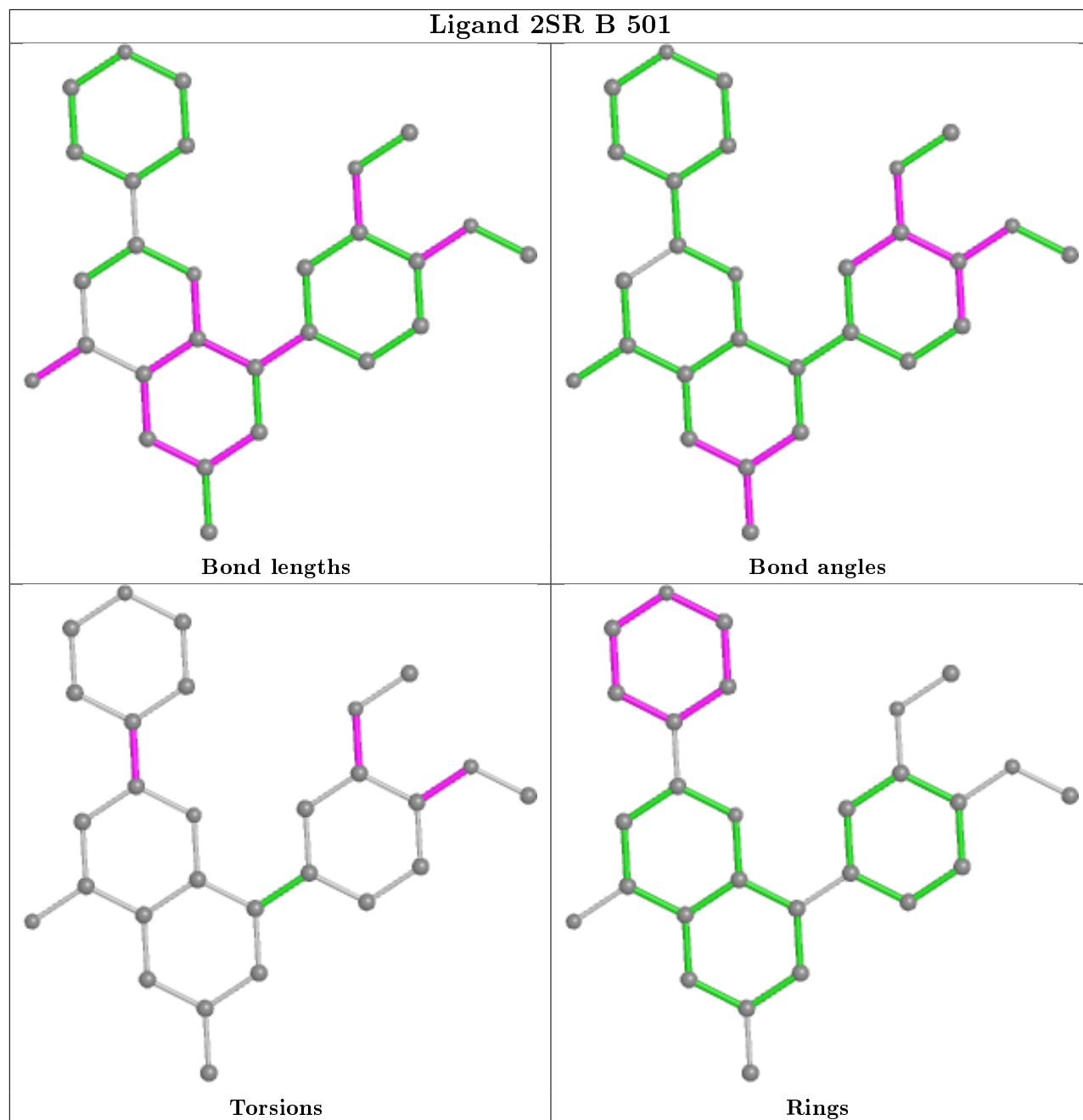
Mol	Chain	Res	Type	Atoms
2	B	501	2SR	C01-C02-C03-C04-C06-O05
2	D	502	2SR	C01-C02-C03-C04-C06-O05

20 monomers are involved in 47 short contacts:

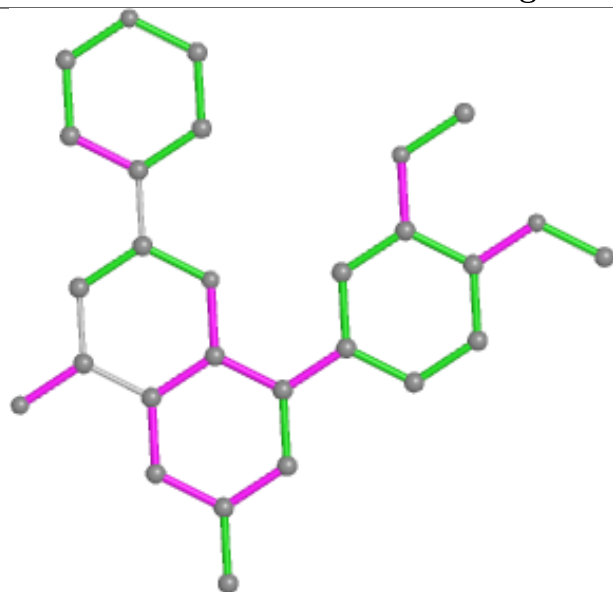
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	512	EDO	5	0
4	D	516	PEG	4	0
2	B	501	2SR	2	0
3	D	505	EDO	2	0
3	A	503	EDO	1	0
3	C	504	EDO	1	0
3	C	509	EDO	2	0
6	B	512	DMS	1	0
3	B	509	EDO	2	0
3	A	508	EDO	3	0
2	C	502	2SR	1	0
6	A	513	DMS	5	0
3	B	507	EDO	3	0
3	C	505	EDO	1	0
2	D	502	2SR	3	0
3	A	506	EDO	1	0
4	D	507	PEG	3	0
6	B	510	DMS	2	0
2	A	501	2SR	4	0
3	A	507	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

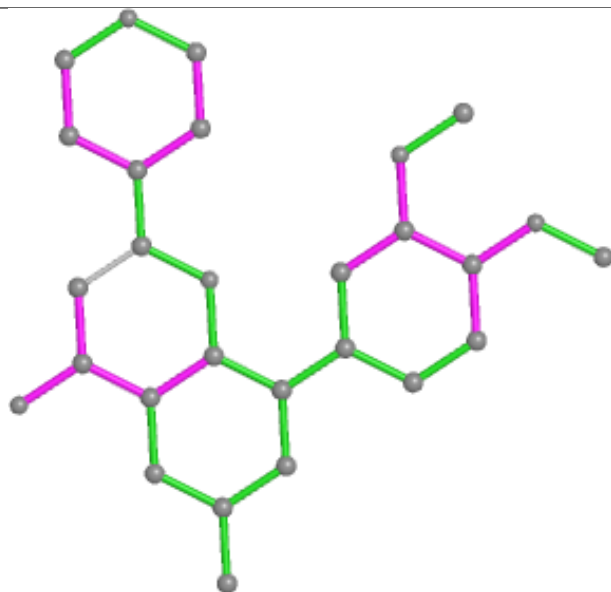
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



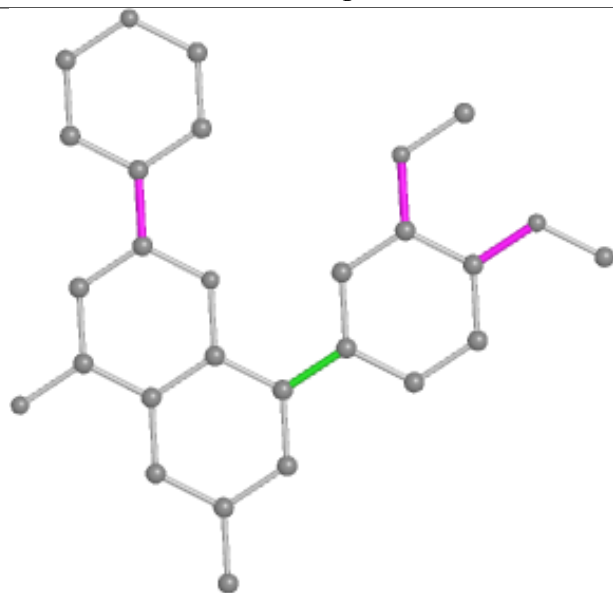
## Ligand 2SR C 502



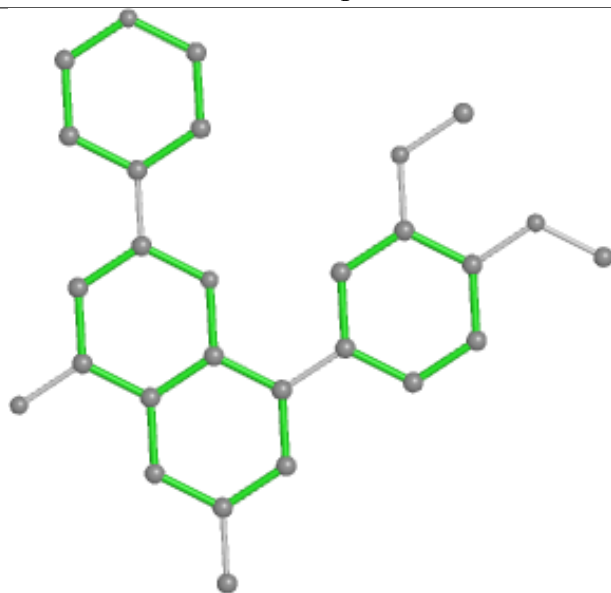
Bond lengths



Bond angles

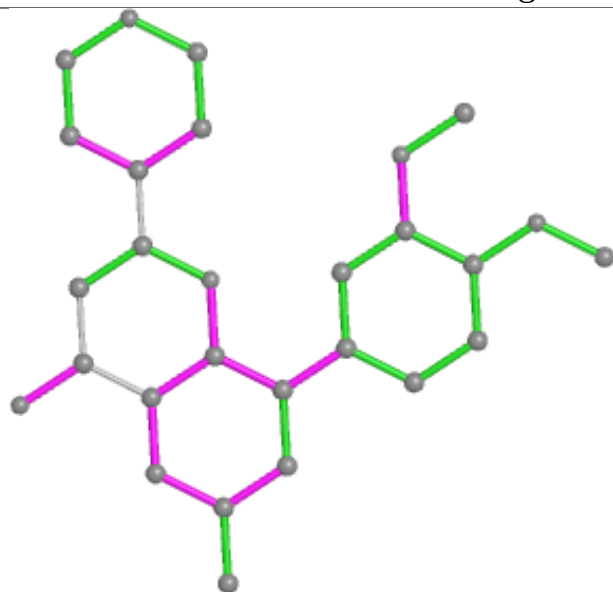


Torsions

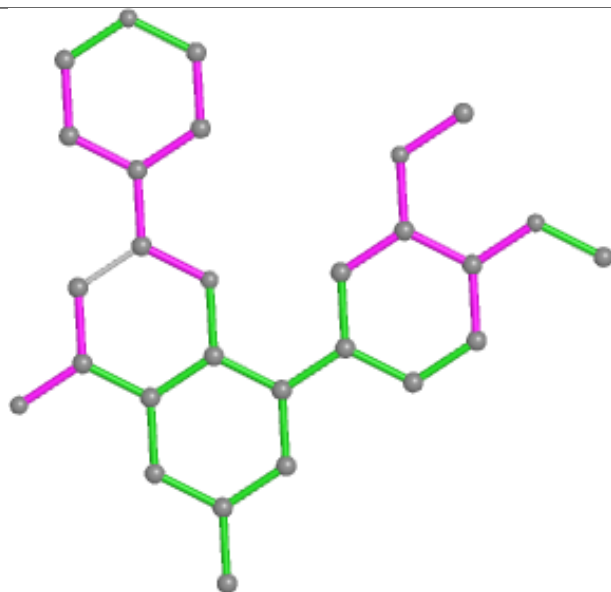


Rings

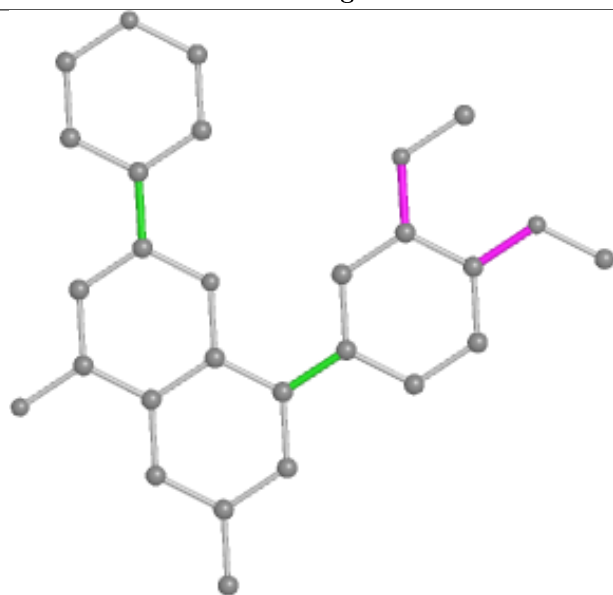
## Ligand 2SR D 502



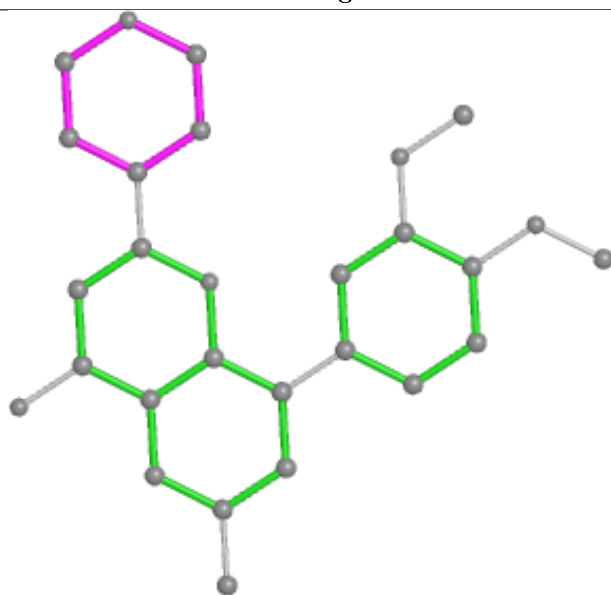
Bond lengths



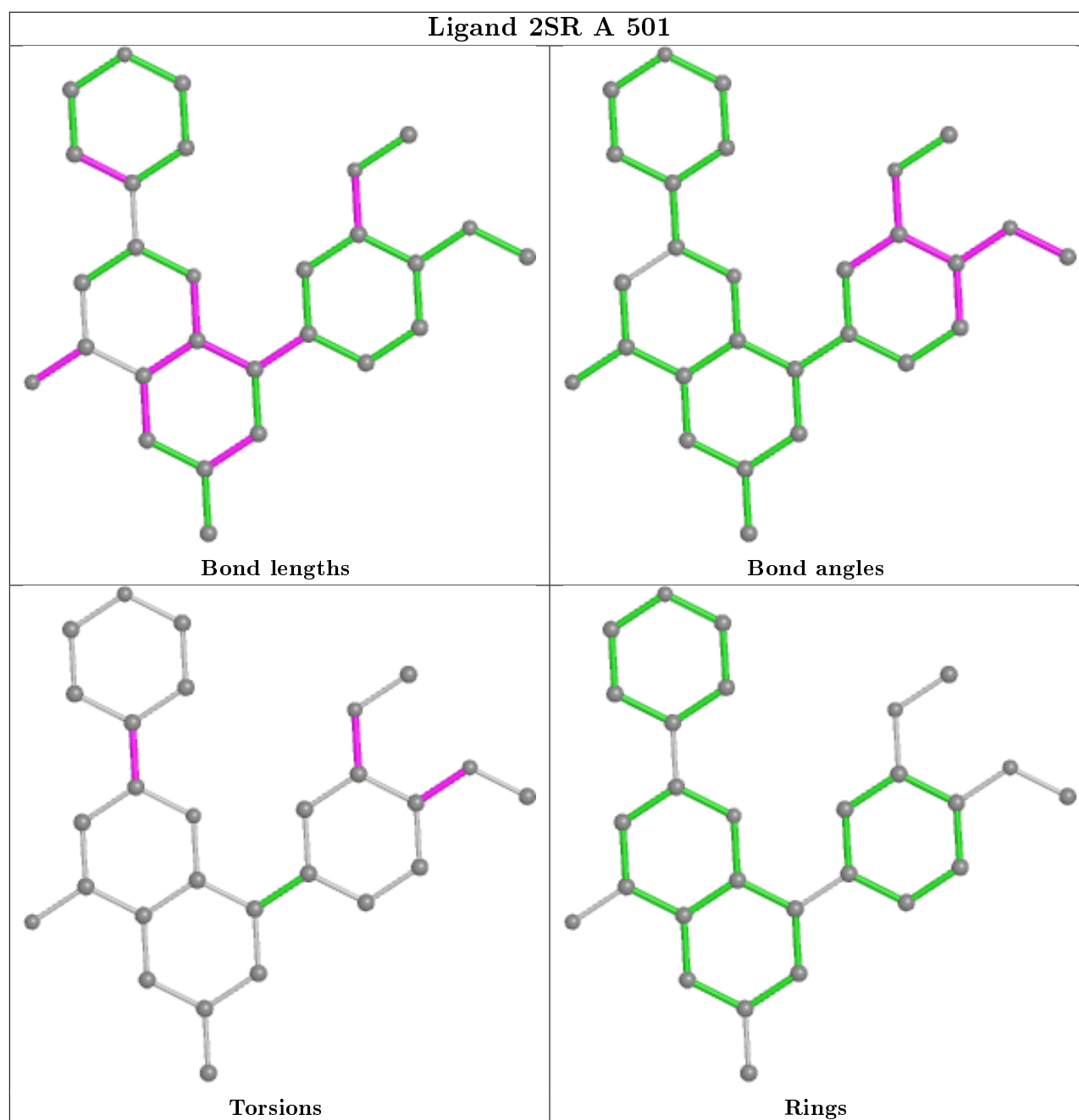
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	328/361 (90%)	0.49	21 (6%) 19 21	17, 32, 59, 115	0
1	B	321/361 (88%)	0.58	29 (9%) 9 10	21, 43, 61, 77	0
1	C	325/361 (90%)	0.48	22 (6%) 17 18	22, 39, 66, 106	0
1	D	324/361 (89%)	0.19	7 (2%) 62 66	16, 29, 56, 75	0
All	All	1298/1444 (89%)	0.44	79 (6%) 21 22	16, 36, 61, 115	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	SER	6.6
1	C	294	SER	6.2
1	A	293	THR	5.9
1	C	292	VAL	5.6
1	A	296	GLY	5.6
1	D	362	ASN	5.5
1	A	294	SER	5.1
1	B	139	VAL	5.1
1	D	363	ALA	5.0
1	C	295	SER	4.8
1	C	293	THR	4.7
1	C	297	VAL	4.7
1	B	94	LYS	4.2
1	A	297	VAL	4.1
1	A	289	THR	4.1
1	C	362	ASN	4.0
1	B	112	LEU	4.0
1	A	83	GLY	3.9
1	A	299	LEU	3.9
1	A	292	VAL	3.8
1	A	298	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	136	LYS	3.6
1	B	132	LEU	3.6
1	C	363	ALA	3.5
1	B	133	LYS	3.4
1	C	409	THR	3.4
1	C	87	GLU	3.3
1	A	362	ASN	3.3
1	B	108	ARG	3.3
1	B	120	VAL	3.3
1	C	296	GLY	3.1
1	D	89	GLU	3.1
1	B	147	MET	3.1
1	A	375	TYR	3.1
1	C	410	ILE	3.1
1	B	257	ARG	3.0
1	A	353	GLU	3.0
1	C	299	LEU	3.0
1	C	289	THR	3.0
1	C	361	HIS	2.9
1	C	291	LYS	2.9
1	B	222	MET	2.9
1	B	92	LEU	2.8
1	C	375	TYR	2.8
1	C	286	MET	2.7
1	A	364	SER	2.6
1	C	287	VAL	2.6
1	B	127	GLN	2.5
1	A	354	ILE	2.5
1	C	139	VAL	2.5
1	B	363	ALA	2.5
1	D	361	HIS	2.4
1	B	97	GLU	2.4
1	A	291	LYS	2.4
1	B	395	ILE	2.4
1	B	135	PHE	2.4
1	B	128	GLU	2.4
1	A	357	MET	2.4
1	B	295	SER	2.4
1	B	412	GLN	2.4
1	D	105[A]	HIS	2.3
1	C	86	THR	2.3
1	B	252	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLY	2.3
1	B	142	LEU	2.3
1	B	223	TYR	2.2
1	A	363	ALA	2.2
1	D	367	LYS	2.2
1	A	359	ASP	2.2
1	B	221	LEU	2.2
1	D	375	TYR	2.1
1	A	287	VAL	2.1
1	B	294	SER	2.1
1	C	298	LEU	2.1
1	C	235	ALA	2.1
1	B	251	ASN	2.0
1	B	256	GLN	2.0
1	B	143	ILE	2.0
1	B	137	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	503	4/4	0.60	0.34	40,40,48,51	0
4	PEG	D	515	7/7	0.65	0.47	53,67,90,105	0
2	2SR	B	501	28/28	0.70	0.27	45,56,68,76	0
3	EDO	B	511	4/4	0.73	0.17	58,58,58,66	0
3	EDO	C	512	4/4	0.74	0.35	43,45,52,54	0
3	EDO	C	508	4/4	0.76	0.22	57,57,60,60	0
3	EDO	A	507	4/4	0.76	0.21	46,49,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2SR	A	501	28/28	0.77	0.35	51,62,70,72	0
2	2SR	C	502	28/28	0.78	0.26	46,58,63,67	0
3	EDO	D	505	4/4	0.80	0.16	41,50,51,52	0
2	2SR	D	502	28/28	0.81	0.23	47,54,58,59	0
3	EDO	D	506	4/4	0.84	0.22	41,42,43,48	0
3	EDO	C	509	4/4	0.84	0.18	34,41,43,47	0
3	EDO	C	507	4/4	0.84	0.29	45,46,47,48	0
3	EDO	B	509	4/4	0.84	0.40	40,46,48,54	0
3	EDO	B	505	4/4	0.84	0.33	45,46,49,54	0
3	EDO	D	509	4/4	0.85	0.18	38,47,49,52	0
3	EDO	D	511	4/4	0.85	0.18	49,49,50,55	0
4	PEG	D	516	7/7	0.86	0.27	36,44,59,69	0
3	EDO	A	514	4/4	0.86	0.23	27,38,38,45	0
4	PEG	D	507	7/7	0.87	0.18	29,33,37,42	0
6	DMS	A	513	4/4	0.88	0.19	29,46,51,55	0
6	DMS	D	508	4/4	0.89	0.19	38,42,53,61	0
3	EDO	C	501	4/4	0.89	0.16	35,38,41,43	0
4	PEG	A	504	7/7	0.89	0.20	33,36,46,51	0
3	EDO	C	503	4/4	0.89	0.24	39,41,44,55	0
3	EDO	A	502	4/4	0.90	0.29	52,52,53,54	0
3	EDO	B	507	4/4	0.90	0.32	30,30,38,41	0
6	DMS	A	511	4/4	0.90	0.23	45,59,63,71	0
3	EDO	A	505	4/4	0.91	0.14	27,32,36,39	0
3	EDO	A	512	4/4	0.91	0.20	28,30,30,31	0
3	EDO	C	513	4/4	0.91	0.12	41,53,55,58	0
3	EDO	C	504	4/4	0.91	0.29	45,45,50,53	0
3	EDO	A	508	4/4	0.91	0.21	30,31,36,51	0
6	DMS	D	504	4/4	0.92	0.29	41,42,55,63	0
3	EDO	C	505	4/4	0.92	0.12	44,44,52,54	0
3	EDO	D	510	4/4	0.92	0.24	38,40,45,52	0
3	EDO	B	504	4/4	0.92	0.13	35,40,40,50	0
6	DMS	B	512	4/4	0.92	0.29	33,45,52,66	0
3	EDO	A	506	4/4	0.94	0.18	31,31,32,34	0
3	EDO	B	506	4/4	0.94	0.11	40,41,42,43	0
3	EDO	B	508	4/4	0.94	0.14	55,57,63,64	0
3	EDO	D	503	4/4	0.94	0.16	34,35,36,43	0
6	DMS	B	510	4/4	0.95	0.38	59,64,73,74	0
7	EPE	C	506	15/15	0.96	0.24	41,52,71,74	0
3	EDO	D	501	4/4	0.97	0.12	30,31,33,37	0
3	EDO	D	514	4/4	0.97	0.12	25,28,29,30	0
5	ZN	B	503	1/1	0.98	0.08	35,35,35,35	1
5	ZN	A	509	1/1	0.99	0.14	28,28,28,28	0

*Continued on next page...*

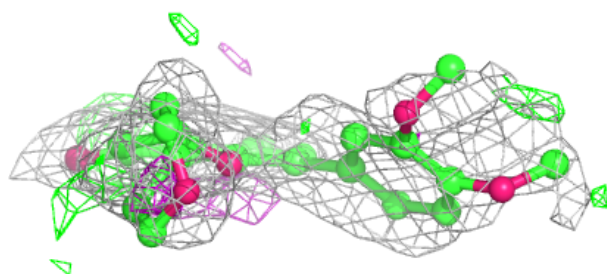
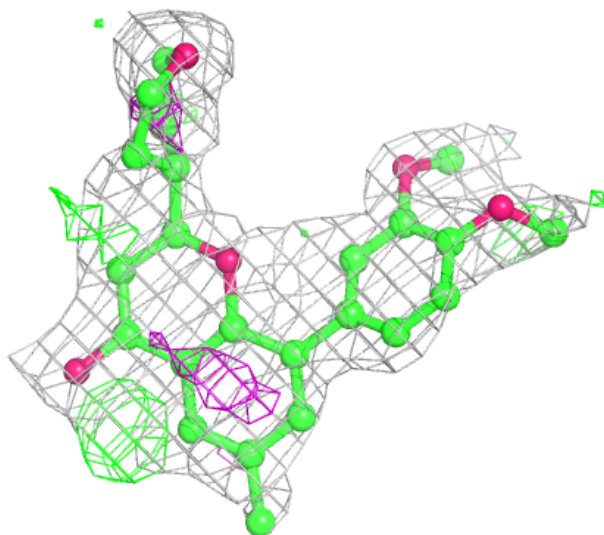
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	C	511	1/1	0.99	0.10	32,32,32,32	1
5	ZN	D	513	1/1	0.99	0.10	33,33,33,33	1
5	ZN	A	510	1/1	0.99	0.10	30,30,30,30	1
5	ZN	C	510	1/1	0.99	0.12	33,33,33,33	0
5	ZN	B	502	1/1	0.99	0.08	34,34,34,34	0
5	ZN	D	512	1/1	1.00	0.12	27,27,27,27	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.

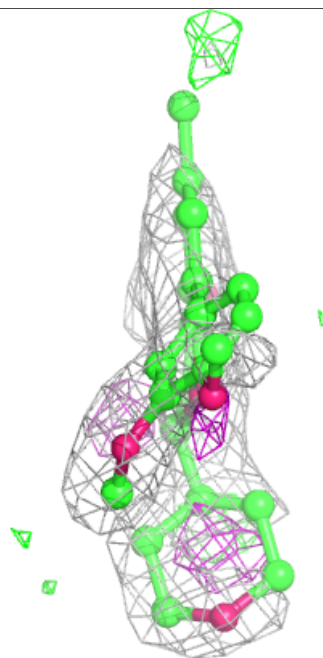
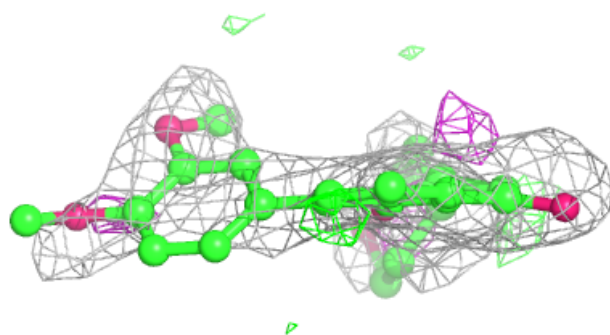
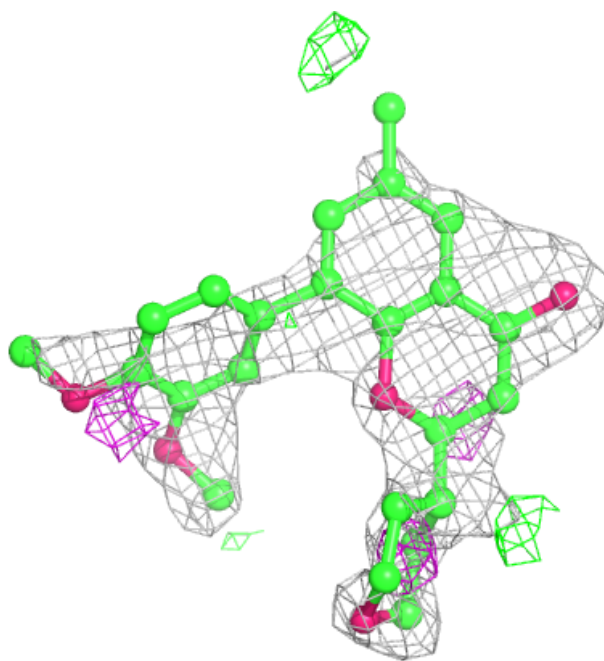
**Electron density around 2SR B 501:**

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)



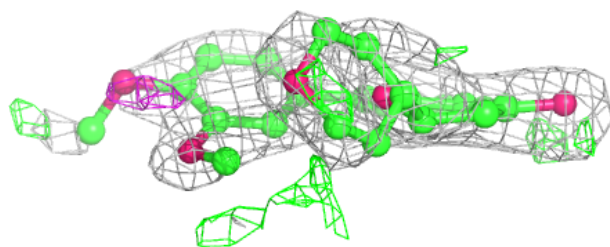
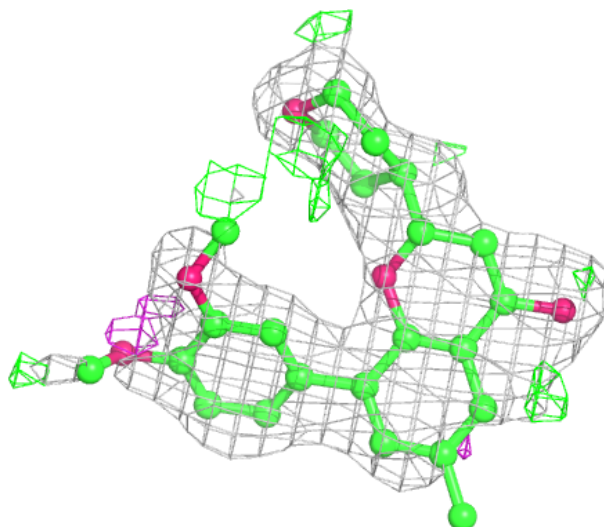
**Electron density around 2SR A 501:**

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



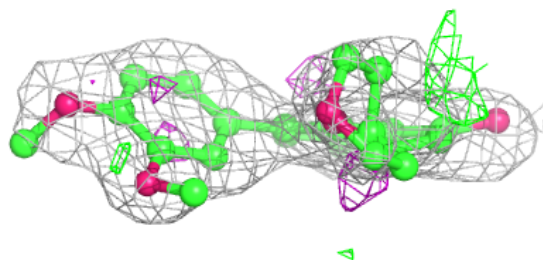
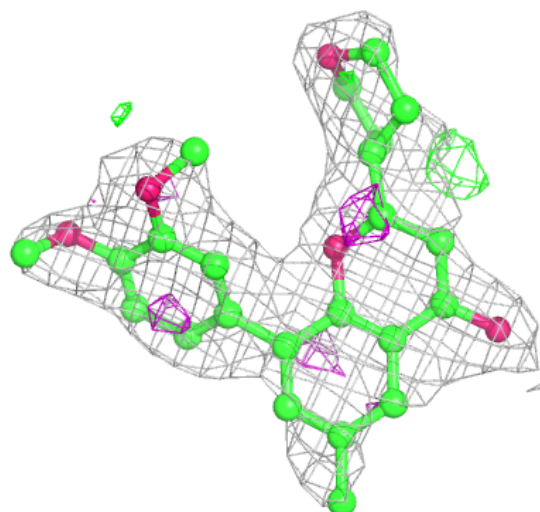
**Electron density around 2SR C 502:**

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



**Electron density around 2SR D 502:**

$2mF_o-DF_c$  (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.