



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 09:52 PM JST

PDB ID : 7WAQ  
Title : SbSOMT in complex with resveratrol  
Authors : Pow, K.C.; Hao, Q.  
Deposited on : 2021-12-14  
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

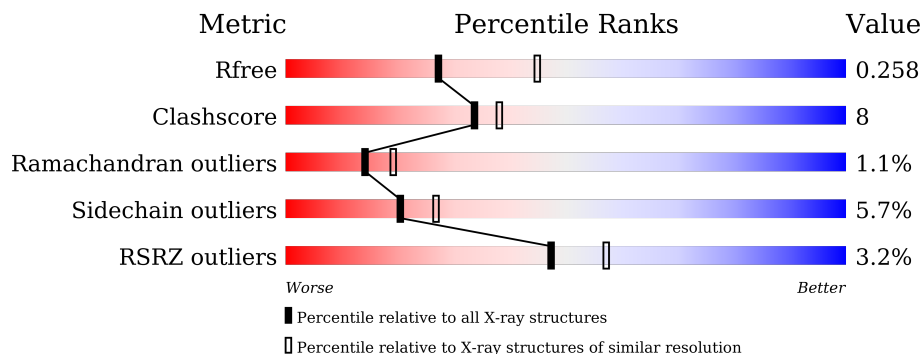
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	376	
1	B	376	
1	C	376	
1	D	376	

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	A	402	-	-	X	-
3	EDO	B	402	-	-	X	-
3	EDO	C	402	-	-	X	-
3	EDO	D	402	-	-	X	-

## 2 Entry composition [i](#)

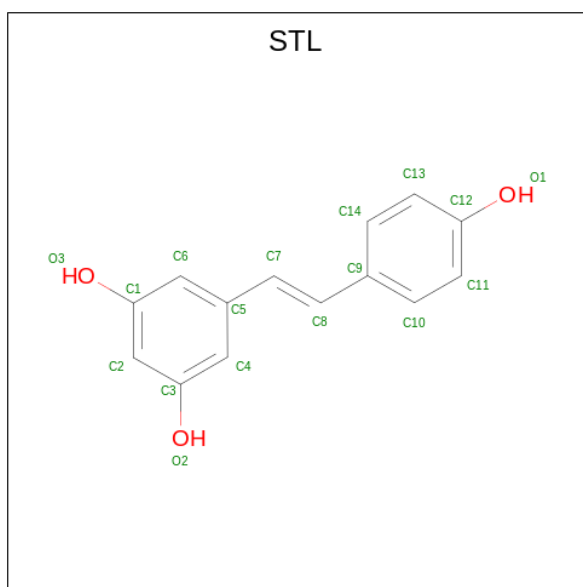
There are 4 unique types of molecules in this entry. The entry contains 11441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 stilbene O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	363	Total 2821	C 1801	N 475	O 522	S 23	0	1	0
1	A	364	Total 2823	C 1801	N 474	O 525	S 23	0	1	0
1	C	364	Total 2817	C 1798	N 473	O 523	S 23	0	0	0
1	D	365	Total 2825	C 1802	N 474	O 526	S 23	0	0	0

- Molecule 2 is RESVERATROL (three-letter code: STL) (formula: C<sub>14</sub>H<sub>12</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



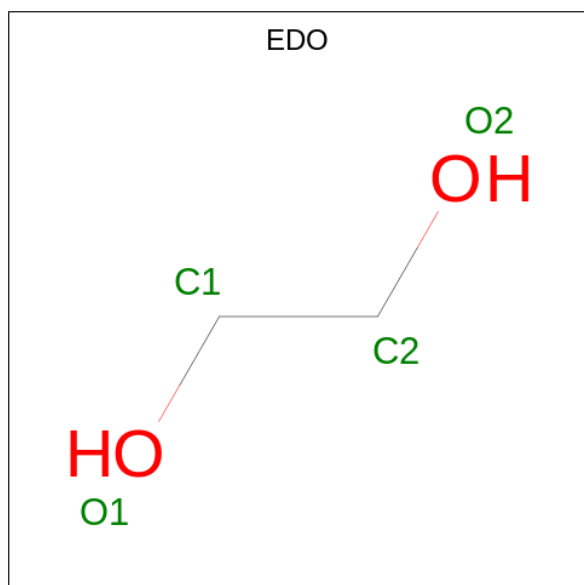
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	Total 17	C 14	O 3	0	0
2	A	1	Total 17	C 14	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			17	14	3		
2	D	1	Total	C	O	0	0
			17	14	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	B	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	19	Total	O	0	0
			19	19		

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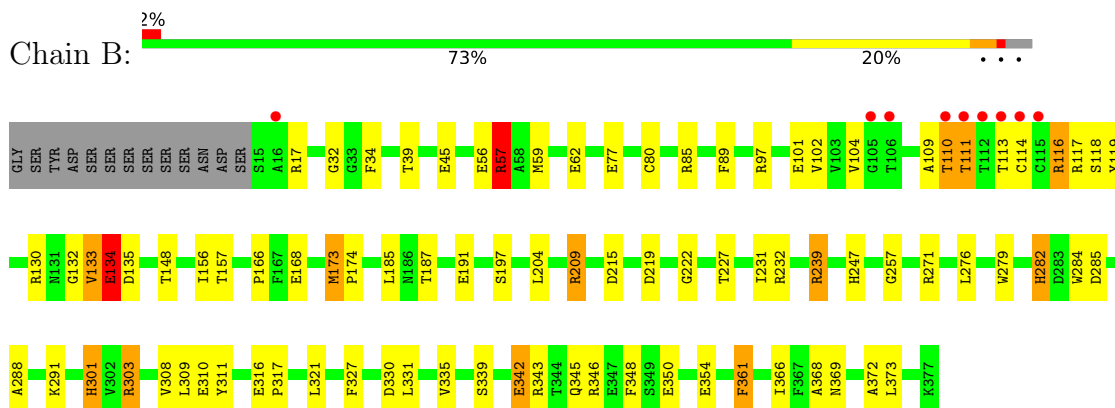
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	18	Total 18	O 18	0	0
4	C	16	Total 16	O 16	0	0
4	D	10	Total 10	O 10	0	0

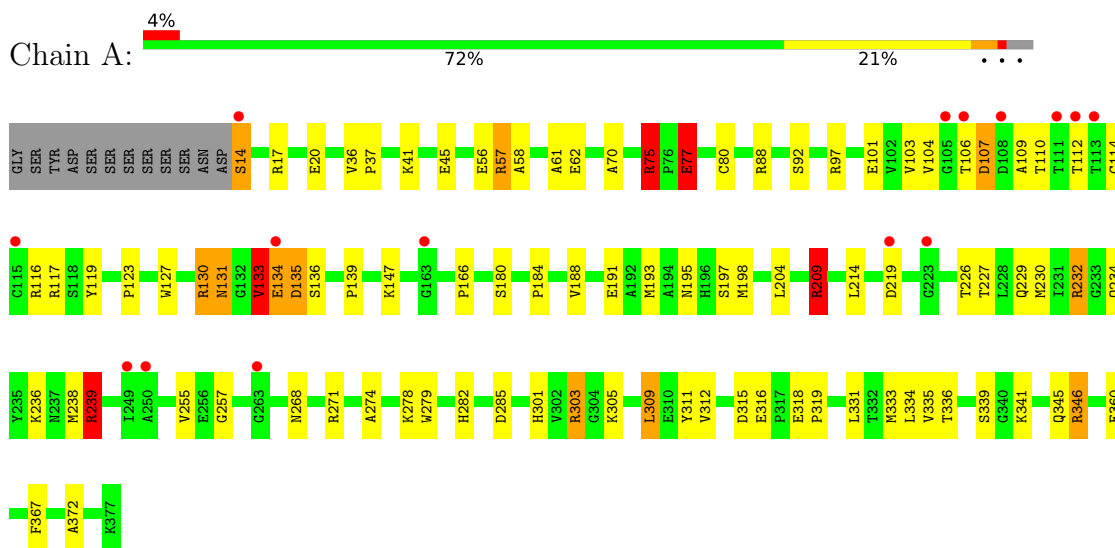
### 3 Residue-property plots

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.

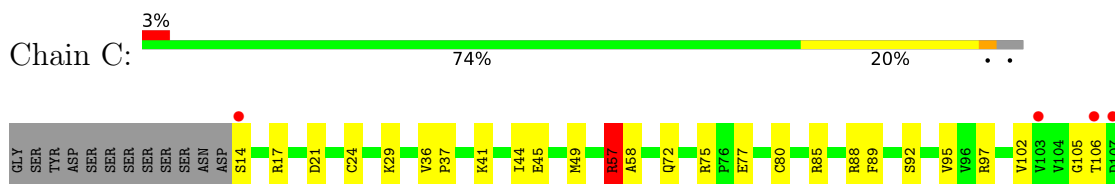
- Molecule 1: stilbene O-methyltransferase

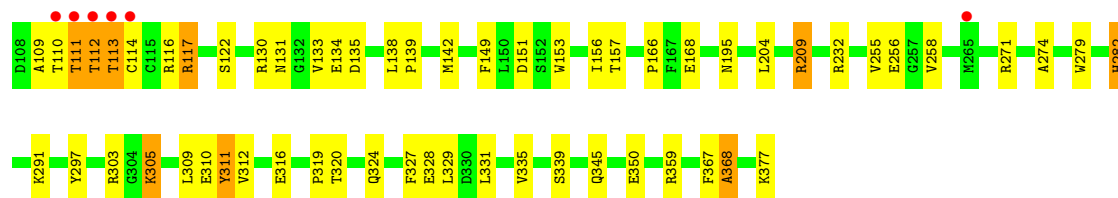


- Molecule 1: stilbene O-methyltransferase

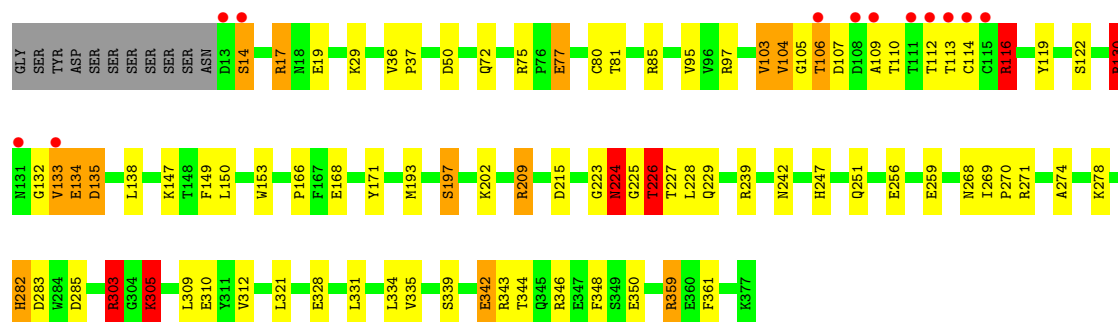
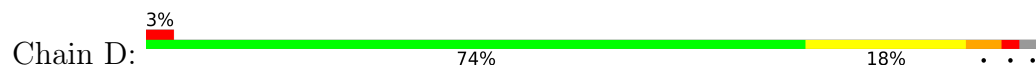


- Molecule 1: stilbene O-methyltransferase





• Molecule 1: stilbene O-methyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.48Å 111.73Å 131.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.56 48.91 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.96-2.56) 100.0 (48.91-2.56)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.186 , 0.257 0.194 , 0.258	Depositor DCC
$R_{free}$ test set	2368 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtrriage
Anisotropy	0.348	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3841e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, STL

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	0.89	8/2881 (0.3%)	1.22	9/3905 (0.2%)
1	B	0.97	16/2880 (0.6%)	1.26	10/3904 (0.3%)
1	C	0.90	6/2875 (0.2%)	1.20	9/3897 (0.2%)
1	D	0.92	8/2883 (0.3%)	1.27	15/3908 (0.4%)
All	All	0.92	38/11519 (0.3%)	1.24	43/15614 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	10
1	C	0	10
1	D	0	10
All	All	0	39

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLU	CD-OE1	10.23	1.36	1.25
1	D	342	GLU	CD-OE1	9.18	1.35	1.25
1	D	168	GLU	CD-OE1	9.15	1.35	1.25
1	D	328	GLU	CD-OE2	8.44	1.34	1.25
1	A	20	GLU	CD-OE2	8.42	1.34	1.25
1	C	339	SER	CA-CB	-8.26	1.40	1.52
1	D	19	GLU	CD-OE1	8.21	1.34	1.25
1	B	350	GLU	CD-OE1	7.72	1.34	1.25
1	A	20	GLU	CD-OE1	7.56	1.33	1.25
1	A	101	GLU	CD-OE2	7.12	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	GLU	CD-OE2	6.98	1.33	1.25
1	B	77	GLU	CD-OE2	6.68	1.32	1.25
1	C	256	GLU	CD-OE1	6.44	1.32	1.25
1	B	173	MET	CG-SD	6.29	1.97	1.81
1	A	77	GLU	CD-OE2	-6.26	1.18	1.25
1	C	168	GLU	CD-OE1	6.23	1.32	1.25
1	C	142	MET	CG-SD	6.13	1.97	1.81
1	D	310	GLU	CD-OE1	-5.96	1.19	1.25
1	C	328	GLU	CD-OE2	5.91	1.32	1.25
1	B	342	GLU	CD-OE2	5.89	1.32	1.25
1	B	350	GLU	CD-OE2	5.87	1.32	1.25
1	B	354	GLU	CD-OE1	5.70	1.31	1.25
1	A	77	GLU	CD-OE1	-5.65	1.19	1.25
1	D	350	GLU	CD-OE2	5.64	1.31	1.25
1	B	101	GLU	CD-OE1	5.63	1.31	1.25
1	B	168	GLU	CD-OE1	5.59	1.31	1.25
1	B	310	GLU	CD-OE2	-5.51	1.19	1.25
1	B	62	GLU	CD-OE1	5.41	1.31	1.25
1	B	45	GLU	CD-OE2	5.40	1.31	1.25
1	A	193	MET	CG-SD	5.31	1.95	1.81
1	B	134	GLU	CD-OE1	5.28	1.31	1.25
1	A	191	GLU	CD-OE2	5.28	1.31	1.25
1	C	350	GLU	CD-OE1	5.26	1.31	1.25
1	D	77	GLU	CD-OE1	5.20	1.31	1.25
1	B	118	SER	CA-CB	-5.20	1.45	1.52
1	B	101	GLU	CD-OE2	5.19	1.31	1.25
1	B	316	GLU	CD-OE1	5.13	1.31	1.25
1	B	342	GLU	CD-OE1	5.10	1.31	1.25

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	303	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	A	17	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	232	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	D	75	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	311	TYR	CB-CG-CD2	-7.54	116.48	121.00
1	A	75	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	311	TYR	CB-CG-CD1	6.99	125.19	121.00
1	C	368	ALA	N-CA-CB	-6.60	100.86	110.10
1	C	345	GLN	CB-CG-CD	6.32	128.02	111.60
1	D	130	ARG	NE-CZ-NH2	-6.29	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	303	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	209	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	D	283	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	224	ASN	CB-CA-C	5.87	122.15	110.40
1	B	303	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	17	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	117	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	359	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	305	LYS	CB-CA-C	-5.63	99.15	110.40
1	D	305	LYS	CB-CA-C	-5.62	99.16	110.40
1	B	187	THR	CA-CB-OG1	-5.62	97.20	109.00
1	D	116	ARG	CB-CG-CD	-5.50	97.31	111.60
1	D	344	THR	CA-CB-OG1	-5.43	97.60	109.00
1	B	311	TYR	CB-CG-CD1	5.42	124.25	121.00
1	B	111	THR	CA-CB-OG1	5.42	120.39	109.00
1	A	318	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	D	283	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	D	215	ASP	CB-CA-C	5.35	121.09	110.40
1	D	328	GLU	CG-CD-OE1	-5.34	107.62	118.30
1	D	17	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	226	THR	CB-CA-C	5.29	125.88	111.60
1	B	110	THR	CA-CB-OG1	5.27	120.06	109.00
1	C	232	ARG	CB-CG-CD	5.26	125.29	111.60
1	C	57	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	311	TYR	CB-CG-CD1	5.23	124.14	121.00
1	A	346	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	209	ARG	CB-CG-CD	5.18	125.08	111.60
1	C	133	VAL	CB-CA-C	5.17	121.23	111.40
1	B	85	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	56	GLU	CB-CA-C	5.09	120.58	110.40
1	A	17	ARG	CB-CG-CD	5.07	124.77	111.60
1	D	171	TYR	CB-CG-CD2	5.05	124.03	121.00

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	CYS	Peptide
1	A	130	ARG	Sidechain
1	A	14	SER	Peptide
1	A	209	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	232	ARG	Sidechain
1	A	239	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	346	ARG	Sidechain
1	B	114	CYS	Peptide
1	B	116	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	17	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	222	GLY	Peptide
1	B	239	ARG	Sidechain
1	B	303	ARG	Sidechain
1	B	346	ARG	Sidechain
1	B	57	ARG	Sidechain
1	C	114	CYS	Peptide
1	C	17	ARG	Sidechain
1	C	209	ARG	Sidechain
1	C	271	ARG	Sidechain
1	C	303	ARG	Sidechain
1	C	359	ARG	Sidechain
1	C	57	ARG	Sidechain
1	C	75	ARG	Sidechain
1	C	88	ARG	Sidechain
1	C	97	ARG	Sidechain
1	D	114	CYS	Peptide
1	D	116	ARG	Sidechain
1	D	130	ARG	Sidechain
1	D	14	SER	Peptide
1	D	17	ARG	Sidechain
1	D	209	ARG	Sidechain
1	D	239	ARG	Sidechain
1	D	303	ARG	Sidechain
1	D	346	ARG	Sidechain
1	D	359	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2823	0	2812	52	0
1	B	2821	0	2809	38	0
1	C	2817	0	2808	49	0
1	D	2825	0	2812	64	0
2	A	17	0	11	2	0
2	B	17	0	12	1	0
2	C	17	0	12	0	0
2	D	17	0	12	0	0
3	A	4	0	6	4	0
3	B	4	0	6	4	0
3	C	8	0	12	6	0
3	D	8	0	12	17	0
4	A	18	0	0	2	0
4	B	19	0	0	0	0
4	C	16	0	0	0	0
4	D	10	0	0	0	0
All	All	11441	0	11324	192	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 8.

All (192) 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:D:226:THR:O	1:D:227:THR:HB	1.49	1.11
1:D:342:GLU:HA	3:D:402:EDO:H22	1.41	0.99
1:C:112:THR:HG22	1:C:113:THR:H	1.32	0.95
1:D:282:HIS:HA	3:D:402:EDO:O1	1.72	0.89
1:C:49:MET:HB3	3:C:402:EDO:H11	1.52	0.89
1:D:103:VAL:HG13	1:D:104:VAL:H	1.40	0.86
1:A:360:GLU:O	4:A:501:HOH:O	1.93	0.85
1:C:44:ILE:HG23	3:C:402:EDO:H12	1.56	0.84
1:D:282:HIS:HB3	3:D:402:EDO:H11	1.58	0.83
1:D:343:ARG:HB2	3:D:402:EDO:H21	1.61	0.83
1:A:61:ALA:HB3	3:A:402:EDO:H11	1.63	0.81
1:D:342:GLU:CA	3:D:402:EDO:H22	2.15	0.76
1:B:271:ARG:HH12	1:B:301[A]:HIS:CD2	2.04	0.75
1:A:110:THR:HG23	1:A:112:THR:O	1.85	0.75
1:D:226:THR:O	1:D:227:THR:CB	2.27	0.73
1:A:184:PRO:O	1:A:188:VAL:HG23	1.89	0.73
1:B:345:GLN:HG3	1:B:361:PHE:CZ	2.25	0.72
1:D:282:HIS:CA	3:D:402:EDO:O1	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LEU:O	1:D:335:VAL:HG23	1.88	0.72
1:A:56:GLU:O	1:D:259:GLU:HG3	1.90	0.70
1:A:134:GLU:HG2	1:A:198:MET:HG2	1.73	0.69
1:D:342:GLU:HA	3:D:402:EDO:C2	2.21	0.68
1:A:57:ARG:NH1	1:A:58:ALA:O	2.27	0.68
1:C:110:THR:OG1	1:C:116:ARG:HG3	1.94	0.68
1:B:133:VAL:O	1:B:135:ASP:N	2.26	0.67
1:D:282:HIS:CB	3:D:402:EDO:H11	2.24	0.67
1:D:282:HIS:HB3	3:D:402:EDO:C1	2.26	0.66
1:C:166:PRO:HG2	1:C:335:VAL:HA	1.78	0.64
1:D:225:GLY:O	1:D:227:THR:N	2.30	0.64
1:A:61:ALA:HB3	3:A:402:EDO:C1	2.27	0.63
1:A:234:GLN:O	1:A:234:GLN:HG2	1.98	0.62
1:D:282:HIS:HA	3:D:402:EDO:HO1	1.64	0.62
1:C:49:MET:CB	3:C:402:EDO:H11	2.29	0.62
1:A:214:LEU:O	1:A:238:MET:HG3	1.99	0.61
1:C:112:THR:HG22	1:C:113:THR:N	2.10	0.61
1:C:49:MET:HB3	3:C:402:EDO:C1	2.30	0.61
1:D:134:GLU:O	1:D:135:ASP:HB2	2.00	0.61
1:C:134:GLU:O	1:C:135:ASP:HB2	2.01	0.60
1:B:282:HIS:HA	3:B:402:EDO:O1	2.02	0.59
1:B:110:THR:HG21	1:B:116:ARG:HA	1.83	0.59
1:A:197:SER:HA	1:A:278:LYS:HE2	1.82	0.59
1:D:226:THR:CG2	1:D:228:LEU:HB2	2.32	0.59
1:D:193:MET:O	1:D:197:SER:HB2	2.02	0.59
1:A:107:ASP:OD2	1:A:110:THR:HG22	2.03	0.58
1:B:271:ARG:HH12	1:B:301[A]:HIS:HD2	1.50	0.58
1:C:311:TYR:CD2	1:C:329:LEU:HD23	2.39	0.58
1:D:133:VAL:HG12	1:D:133:VAL:O	2.04	0.58
1:D:166:PRO:HG2	1:D:335:VAL:HA	1.84	0.57
1:B:166:PRO:HG2	1:B:335:VAL:HA	1.85	0.57
1:A:75:ARG:HB3	1:A:77:GLU:OE1	2.03	0.57
1:B:239:ARG:NH2	1:B:257:GLY:HA2	2.20	0.56
1:D:282:HIS:CB	3:D:402:EDO:C1	2.84	0.56
1:C:255:VAL:HB	1:C:258:VAL:HB	1.87	0.56
1:C:139:PRO:HD2	1:C:195:ASN:OD1	2.06	0.55
1:D:149:PHE:O	1:D:153:TRP:HD1	1.89	0.55
1:B:348:PHE:CZ	3:B:402:EDO:H11	2.42	0.55
1:A:123:PRO:HD2	4:A:518:HOH:O	2.06	0.55
1:A:279:TRP:CH2	2:A:401:STL:H10	2.42	0.55
1:D:282:HIS:CB	3:D:402:EDO:O1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:MET:HB2	1:B:174:PRO:CD	2.37	0.54
1:A:41:LYS:O	1:A:45:GLU:HG3	2.07	0.54
1:A:341:LYS:HA	1:C:85:ARG:NH2	2.23	0.54
1:C:57:ARG:NH1	1:C:58:ALA:O	2.40	0.54
1:D:36:VAL:HB	1:D:37:PRO:HD3	1.90	0.54
1:A:226:THR:O	1:A:230:MET:HG3	2.08	0.53
1:D:223:GLY:O	1:D:224:ASN:HB2	2.09	0.53
1:D:271:ARG:HH22	3:D:403:EDO:H22	1.73	0.53
1:D:106:THR:HG22	1:D:113:THR:HG23	1.90	0.53
1:D:343:ARG:N	3:D:402:EDO:C2	2.72	0.53
1:D:223:GLY:HA3	1:D:242:ASN:HD21	1.72	0.53
1:D:285:ASP:HB3	1:D:339:SER:HB2	1.90	0.52
1:A:309:LEU:HD12	1:A:372:ALA:HA	1.92	0.52
1:A:134:GLU:C	1:A:136:SER:H	2.13	0.51
1:A:116:ARG:HG3	1:A:116:ARG:NH2	2.25	0.51
1:A:80:CYS:HB3	1:A:109:ALA:O	2.10	0.51
1:A:319:PRO:HA	1:C:92:SER:O	2.11	0.51
1:D:226:THR:HG22	1:D:229:GLN:H	1.76	0.51
1:A:285:ASP:HB3	1:A:339:SER:HB2	1.93	0.50
1:D:72:GLN:NE2	1:D:72:GLN:HA	2.26	0.50
1:C:106:THR:CG2	1:C:113:THR:HG23	2.41	0.50
1:C:149:PHE:O	1:C:153:TRP:HD1	1.94	0.50
1:B:148:THR:HG21	1:B:185:LEU:HD22	1.94	0.50
1:D:106:THR:CG2	1:D:113:THR:HG23	2.41	0.50
1:C:106:THR:HG22	1:C:113:THR:HG23	1.93	0.49
1:C:111:THR:HG21	1:C:117:ARG:CZ	2.41	0.49
1:C:130:ARG:HA	1:C:138:LEU:HD23	1.94	0.49
1:A:274:ALA:HA	1:A:305:LYS:O	2.13	0.49
1:D:348:PHE:HZ	3:D:402:EDO:H12	1.78	0.49
1:D:133:VAL:C	1:D:135:ASP:H	2.15	0.49
1:C:297:TYR:CE1	1:C:377:LYS:HG3	2.48	0.49
1:A:116:ARG:HG3	1:A:116:ARG:HH21	1.77	0.49
1:B:343:ARG:HB2	3:B:402:EDO:H11	1.95	0.48
1:C:274:ALA:HA	1:C:305:LYS:O	2.12	0.48
1:C:41:LYS:HE2	1:C:45:GLU:OE1	2.13	0.48
1:A:312:VAL:HG12	1:A:312:VAL:O	2.13	0.48
1:D:226:THR:HG23	1:D:228:LEU:HB2	1.94	0.48
1:C:111:THR:HG23	1:C:116:ARG:HA	1.95	0.48
1:D:36:VAL:HB	1:D:37:PRO:CD	2.44	0.48
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.78	0.48
1:A:133:VAL:HG21	1:D:251:GLN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:HD2	1:A:195:ASN:OD1	2.13	0.48
1:C:367:PHE:CD2	1:C:368:ALA:HB2	2.49	0.48
1:D:223:GLY:HA2	1:D:226:THR:OG1	2.14	0.48
1:A:133:VAL:O	1:A:135:ASP:N	2.46	0.48
1:C:112:THR:CG2	1:C:113:THR:H	2.11	0.48
1:D:130:ARG:HA	1:D:138:LEU:HD23	1.96	0.48
1:B:284:TRP:HB3	1:B:288:ALA:HB3	1.96	0.48
1:B:219:ASP:OD1	1:B:276:LEU:HD23	2.14	0.47
1:D:95:VAL:O	1:D:122:SER:HB2	2.14	0.47
1:D:132:GLY:C	1:D:134:GLU:H	2.18	0.47
1:C:80:CYS:HB3	1:C:109:ALA:O	2.14	0.47
1:B:134:GLU:HG3	1:B:135:ASP:N	2.28	0.47
1:D:110:THR:HG23	1:D:112:THR:O	2.15	0.47
1:B:111:THR:HG22	1:B:117:ARG:NH1	2.29	0.47
1:A:103:VAL:HG11	1:A:107:ASP:HB3	1.95	0.47
1:D:312:VAL:HG12	1:D:312:VAL:O	2.14	0.47
1:D:103:VAL:HG13	1:D:104:VAL:N	2.20	0.47
1:B:271:ARG:NH1	1:B:301[B]:HIS:ND1	2.63	0.46
1:B:330:ASP:HA	1:B:342:GLU:HG2	1.98	0.46
1:A:229:GLN:HB2	1:A:255:VAL:HG11	1.98	0.46
1:D:81:THR:O	1:D:85:ARG:HG3	2.16	0.46
1:A:333:MET:HA	1:A:333:MET:CE	2.46	0.46
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.31	0.46
1:A:97:ARG:HH11	1:A:97:ARG:HG2	1.82	0.46
1:B:227:THR:O	1:B:231:ILE:HG13	2.16	0.45
1:A:104:VAL:HG13	1:A:104:VAL:O	2.16	0.45
1:C:209:ARG:HG2	1:C:209:ARG:HH11	1.82	0.45
1:C:36:VAL:HB	1:C:37:PRO:HD3	1.98	0.45
1:A:336:THR:HG21	2:A:401:STL:O2	2.16	0.45
1:D:348:PHE:CZ	3:D:402:EDO:H12	2.51	0.45
1:B:309:LEU:HD12	1:B:372:ALA:HA	1.99	0.45
1:B:285:ASP:HB3	1:B:339:SER:HB2	1.99	0.45
1:B:368:ALA:O	1:B:369:ASN:HB2	2.17	0.45
1:A:239:ARG:NH2	1:A:257:GLY:HA2	2.32	0.45
1:B:32:GLY:HA2	1:B:34:PHE:CE1	2.52	0.45
1:B:39:THR:HG21	1:B:89:PHE:HD2	1.82	0.44
1:D:103:VAL:HG21	1:D:105:GLY:O	2.16	0.44
1:D:274:ALA:HA	1:D:305:LYS:O	2.18	0.44
1:B:191:GLU:OE2	1:A:70:ALA:HB3	2.17	0.44
1:C:44:ILE:HG23	3:C:402:EDO:C1	2.39	0.44
1:A:334:LEU:HD23	1:A:334:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:O	1:C:324:GLN:HG3	2.17	0.44
1:D:72:GLN:NE2	1:D:72:GLN:CA	2.81	0.44
1:A:61:ALA:CB	3:A:402:EDO:H11	2.40	0.44
1:D:334:LEU:C	1:D:334:LEU:HD23	2.38	0.44
1:C:36:VAL:HB	1:C:37:PRO:CD	2.48	0.44
1:C:110:THR:OG1	1:C:116:ARG:CG	2.64	0.44
1:A:127:TRP:CZ2	1:C:24:CYS:HB2	2.53	0.43
1:A:367:PHE:CE1	1:C:21:ASP:HA	2.53	0.43
1:C:41:LYS:O	1:C:45:GLU:HG3	2.18	0.43
1:B:97:ARG:O	1:B:119:TYR:HA	2.18	0.43
1:A:88:ARG:HD2	1:C:327:PHE:CE1	2.53	0.43
1:B:279:TRP:CH2	2:B:401:STL:H10	2.53	0.43
1:A:331:LEU:HD22	1:C:89:PHE:CD2	2.53	0.43
1:C:282:HIS:HB3	1:C:310:GLU:OE1	2.18	0.43
1:D:133:VAL:O	1:D:135:ASP:N	2.48	0.43
1:C:44:ILE:O	3:C:402:EDO:H21	2.18	0.43
1:A:107:ASP:OD2	1:A:110:THR:CG2	2.66	0.43
1:C:111:THR:HB	1:C:117:ARG:NH1	2.33	0.43
1:B:57:ARG:NH2	1:B:59:MET:HG2	2.34	0.43
1:B:104:VAL:O	1:B:104:VAL:HG13	2.18	0.43
1:A:97:ARG:O	1:A:119:TYR:HA	2.19	0.42
1:A:36:VAL:HB	1:A:37:PRO:CD	2.49	0.42
1:C:95:VAL:O	1:C:122:SER:HB2	2.19	0.42
1:C:130:ARG:HG3	1:C:138:LEU:CD2	2.50	0.42
1:B:80:CYS:HB3	1:B:109:ALA:O	2.20	0.42
1:B:342:GLU:HA	3:B:402:EDO:C2	2.50	0.42
1:B:239:ARG:HH22	1:B:257:GLY:HA2	1.85	0.42
1:D:103:VAL:CG2	1:D:105:GLY:O	2.67	0.42
1:D:223:GLY:HA3	1:D:242:ASN:ND2	2.34	0.41
1:C:156:ILE:O	1:C:157:THR:C	2.58	0.41
1:B:156:ILE:O	1:B:157:THR:C	2.59	0.41
1:C:312:VAL:O	1:C:312:VAL:HG12	2.20	0.41
1:A:166:PRO:HG2	1:A:335:VAL:HA	2.02	0.41
1:C:204:LEU:HD12	1:C:204:LEU:HA	1.94	0.41
1:A:92:SER:O	1:C:319:PRO:HA	2.21	0.41
1:C:279:TRP:CD1	1:C:282:HIS:CE1	3.09	0.41
1:D:223:GLY:O	1:D:224:ASN:CB	2.69	0.41
1:D:50:ASP:OD2	1:D:130:ARG:HB2	2.21	0.41
1:D:80:CYS:HB3	1:D:109:ALA:O	2.21	0.41
1:D:97:ARG:O	1:D:119:TYR:HA	2.20	0.41
1:D:269:ILE:HA	1:D:270:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:HB	1:B:373:LEU:HB2	2.03	0.40
1:A:147:LYS:HE3	1:C:151:ASP:OD1	2.21	0.40
1:B:204:LEU:HD12	1:B:366:ILE:HD12	2.03	0.40
1:D:106:THR:CG2	1:D:113:THR:CG2	2.99	0.40
1:D:343:ARG:H	3:D:402:EDO:C2	2.33	0.40
1:B:317:PRO:HA	1:B:327:PHE:CE2	2.56	0.40
1:A:117:ARG:O	3:A:402:EDO:H21	2.22	0.40
1:A:134:GLU:C	1:A:136:SER:N	2.75	0.40
1:D:150:LEU:HA	1:D:150:LEU:HD23	1.88	0.40
1:D:268:ASN:CG	1:D:269:ILE:N	2.74	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	363/376 (96%)	348 (96%)	11 (3%)	4 (1%)	14 19
1	B	362/376 (96%)	352 (97%)	8 (2%)	2 (1%)	25 33
1	C	362/376 (96%)	348 (96%)	12 (3%)	2 (1%)	25 33
1	D	363/376 (96%)	343 (94%)	12 (3%)	8 (2%)	6 7
All	All	1450/1504 (96%)	1391 (96%)	43 (3%)	16 (1%)	14 19

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	GLY
1	D	14	SER
1	D	103	VAL
1	D	133	VAL
1	D	135	ASP

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Mol	Chain	Res	Type
1	D	224	ASN
1	D	226	THR
1	B	132	GLY
1	B	134	GLU
1	A	131	ASN
1	A	133	VAL
1	D	134	GLU
1	A	135	ASP
1	C	112	THR
1	D	104	VAL
1	A	134	GLU

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/312 (97%)	278 (92%)	24 (8%)	12	15
1	B	301/312 (96%)	287 (95%)	14 (5%)	26	35
1	C	301/312 (96%)	287 (95%)	14 (5%)	26	35
1	D	302/312 (97%)	284 (94%)	18 (6%)	19	24
All	All	1206/1248 (97%)	1136 (94%)	70 (6%)	20	26

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	ARG
1	B	102	VAL
1	B	113	THR
1	B	133	VAL
1	B	197	SER
1	B	215	ASP
1	B	247	HIS
1	B	282	HIS
1	B	291	LYS
1	B	301[A]	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	301[B]	HIS
1	B	321	LEU
1	B	331	LEU
1	B	361	PHE
1	A	14	SER
1	A	57	ARG
1	A	75	ARG
1	A	77	GLU
1	A	106	THR
1	A	107	ASP
1	A	130	ARG
1	A	131	ASN
1	A	133	VAL
1	A	180	SER
1	A	204	LEU
1	A	209	ARG
1	A	227	THR
1	A	232	ARG
1	A	236	LYS
1	A	239	ARG
1	A	268	ASN
1	A	282	HIS
1	A	301	HIS
1	A	303	ARG
1	A	309	LEU
1	A	315	ASP
1	A	316	GLU
1	A	345	GLN
1	C	14	SER
1	C	29	LYS
1	C	57	ARG
1	C	72	GLN
1	C	77	GLU
1	C	102	VAL
1	C	111	THR
1	C	113	THR
1	C	131	ASN
1	C	282	HIS
1	C	291	LYS
1	C	309	LEU
1	C	316	GLU
1	C	331	LEU

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Mol	Chain	Res	Type
1	D	29	LYS
1	D	77	GLU
1	D	106	THR
1	D	107	ASP
1	D	116	ARG
1	D	147	LYS
1	D	197	SER
1	D	202	LYS
1	D	209	ARG
1	D	247	HIS
1	D	256	GLU
1	D	278	LYS
1	D	282	HIS
1	D	303	ARG
1	D	305	LYS
1	D	309	LEU
1	D	321	LEU
1	D	361	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	ASN
1	C	131	ASN
1	C	229	GLN
1	C	268	ASN
1	D	72	GLN
1	D	242	ASN

### 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

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	D	402	-	3,3,3	0.99	0	2,2,2	0.99	0
3	EDO	A	402	-	3,3,3	1.71	1 (33%)	2,2,2	1.67	0
2	STL	A	401	-	18,18,18	0.98	0	24,24,24	1.25	2 (8%)
3	EDO	C	403	-	3,3,3	1.18	0	2,2,2	1.08	0
2	STL	D	401	-	18,18,18	0.80	0	24,24,24	1.94	8 (33%)
3	EDO	B	402	-	3,3,3	1.62	0	2,2,2	1.39	0
3	EDO	D	403	-	3,3,3	0.46	0	2,2,2	0.58	0
3	EDO	C	402	-	3,3,3	1.26	0	2,2,2	1.46	0
2	STL	C	401	-	18,18,18	1.36	2 (11%)	24,24,24	1.88	8 (33%)
2	STL	B	401	-	18,18,18	0.94	1 (5%)	24,24,24	1.01	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	D	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
2	STL	A	401	-	-	0/5/5/5	0/2/2/2
3	EDO	C	403	-	-	0/1/1/1	-
2	STL	D	401	-	-	0/5/5/5	0/2/2/2
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
2	STL	C	401	-	-	0/5/5/5	0/2/2/2
2	STL	B	401	-	-	0/5/5/5	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	STL	O1-C12	3.33	1.44	1.37
2	C	401	STL	C13-C12	2.61	1.43	1.38
2	B	401	STL	O3-C1	2.20	1.42	1.37
3	A	402	EDO	O2-C2	2.17	1.53	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	STL	C5-C6-C1	-4.59	116.19	120.28
2	C	401	STL	O2-C3-C2	3.87	129.90	119.84
2	C	401	STL	C5-C4-C3	3.57	123.46	120.28
2	A	401	STL	O1-C12-C11	-3.37	110.41	120.02
2	C	401	STL	O2-C3-C4	-3.28	111.33	119.84
2	C	401	STL	C6-C5-C7	3.15	129.99	120.60
2	A	401	STL	O1-C12-C13	3.12	128.91	120.02
2	D	401	STL	O1-C12-C11	2.96	128.47	120.02
2	D	401	STL	O1-C12-C13	-2.85	111.90	120.02
2	C	401	STL	C4-C5-C7	-2.75	112.40	120.60
2	D	401	STL	O3-C1-C2	-2.75	112.70	119.84
2	C	401	STL	O1-C12-C13	2.59	127.40	120.02
2	C	401	STL	O1-C12-C11	-2.40	113.17	120.02
2	D	401	STL	C4-C5-C7	-2.32	113.70	120.60
2	C	401	STL	C5-C6-C1	-2.29	118.24	120.28
2	D	401	STL	C4-C3-C2	-2.23	117.34	120.43
2	D	401	STL	O2-C3-C2	2.18	125.51	119.84
2	D	401	STL	C5-C4-C3	2.14	122.19	120.28

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	EDO	O1-C1-C2-O2
3	D	403	EDO	O1-C1-C2-O2
3	D	402	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	EDO	16	0
3	A	402	EDO	4	0
2	A	401	STL	2	0

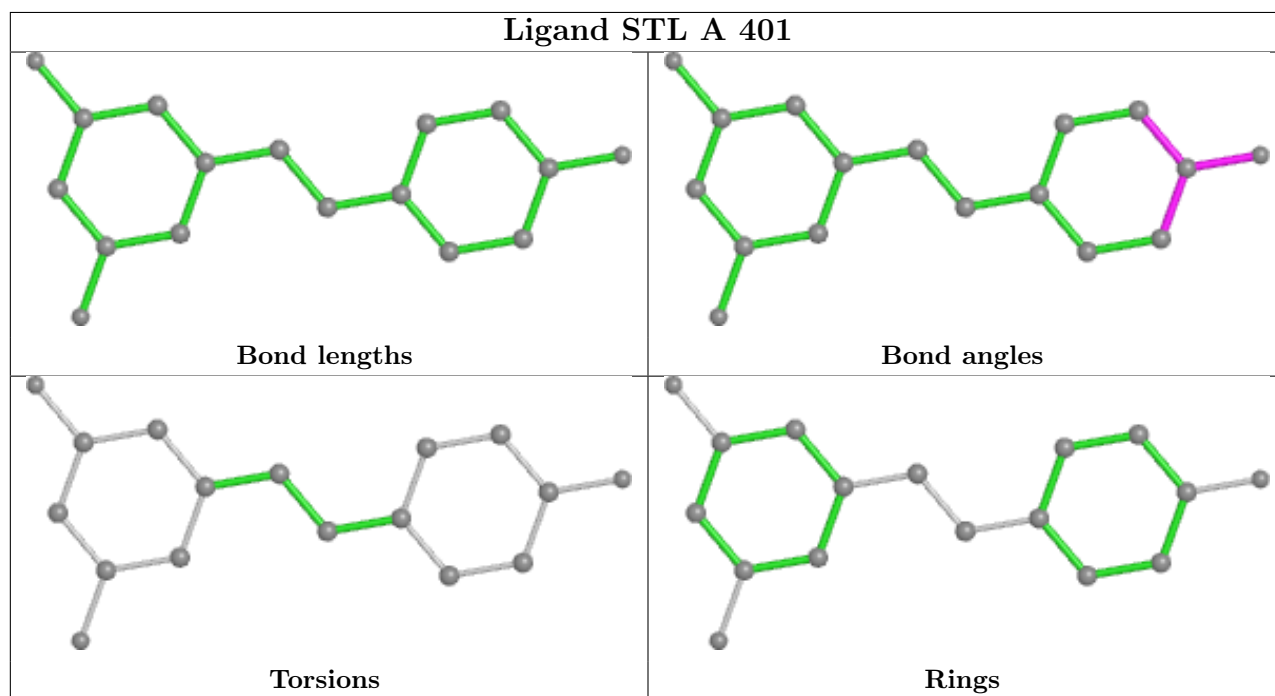
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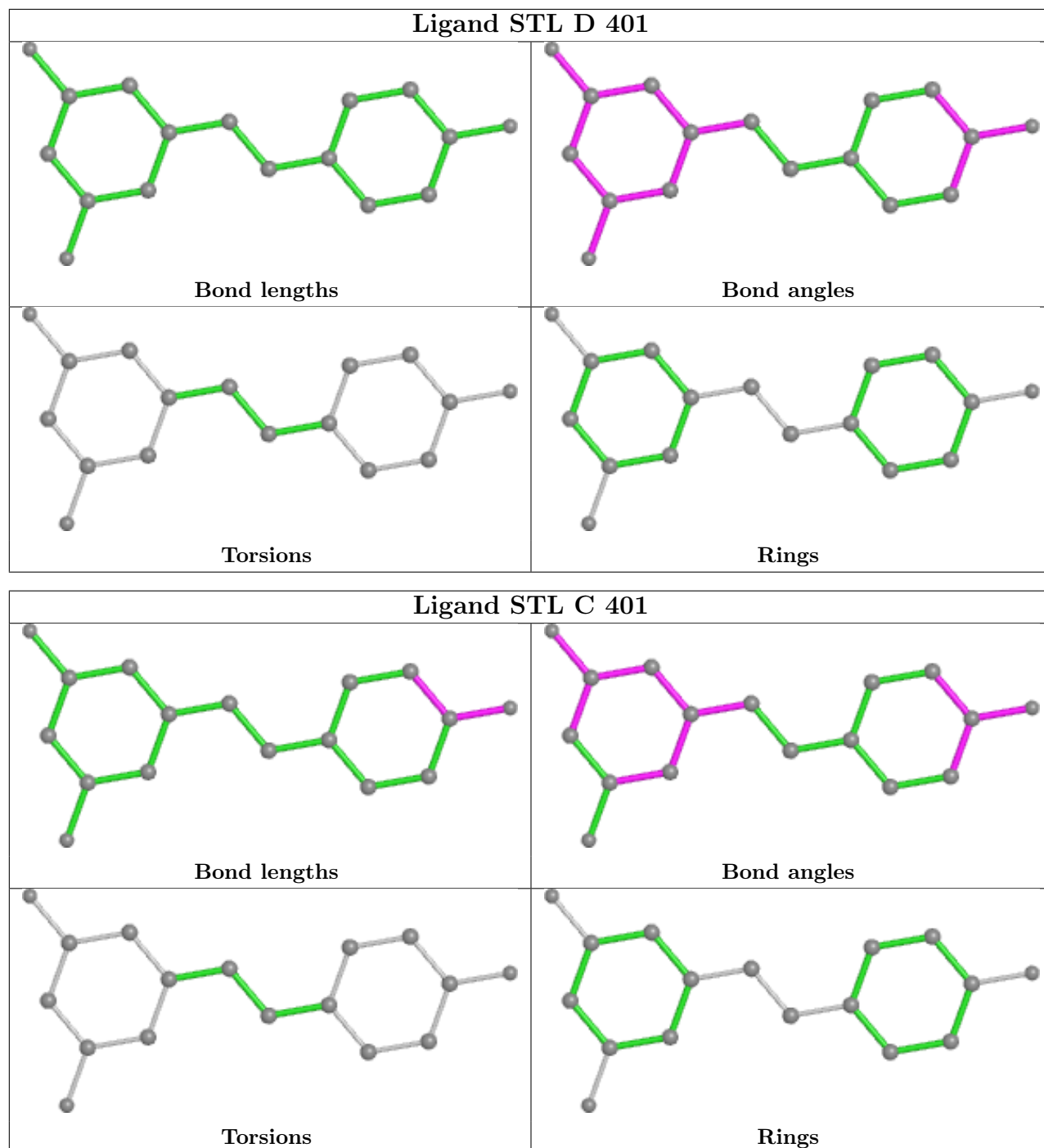


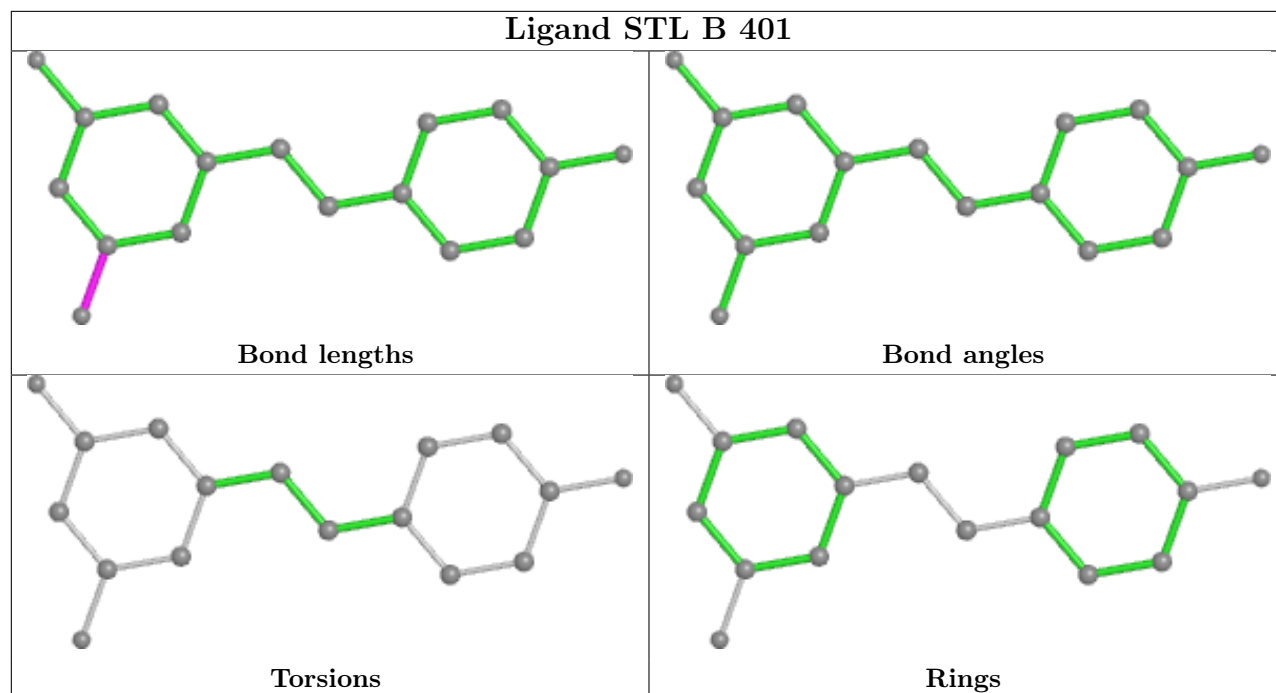
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	EDO	4	0
3	D	403	EDO	1	0
3	C	402	EDO	6	0
2	B	401	STL	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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	364/376 (96%)	0.08	15 (4%) 37 46	37, 74, 127, 166	0
1	B	363/376 (96%)	-0.24	9 (2%) 57 65	35, 54, 105, 166	0
1	C	364/376 (96%)	-0.08	10 (2%) 54 63	34, 59, 105, 187	0
1	D	365/376 (97%)	-0.04	12 (3%) 46 56	33, 64, 114, 148	0
All	All	1456/1504 (96%)	-0.07	46 (3%) 47 57	33, 62, 118, 187	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	THR	9.4
1	C	114	CYS	9.2
1	D	111	THR	9.2
1	C	112	THR	7.6
1	D	112	THR	7.4
1	A	113	THR	7.4
1	A	112	THR	7.3
1	C	113	THR	7.0
1	B	114	CYS	6.1
1	A	106	THR	6.1
1	B	112	THR	5.9
1	C	111	THR	5.7
1	C	107	ASP	5.6
1	B	113	THR	5.5
1	B	106	THR	5.4
1	C	106	THR	5.2
1	A	134	GLU	4.3
1	A	105	GLY	3.9
1	A	250	ALA	3.7
1	D	113	THR	3.2
1	B	16	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	133	VAL	3.1
1	D	108	ASP	3.0
1	D	106	THR	2.9
1	B	105	GLY	2.8
1	D	13	ASP	2.8
1	A	111	THR	2.8
1	D	14	SER	2.8
1	C	14	SER	2.7
1	A	14	SER	2.7
1	C	265	MET	2.6
1	A	263	GLY	2.6
1	A	249	ILE	2.5
1	D	115	CYS	2.5
1	B	115	CYS	2.4
1	C	103	VAL	2.4
1	A	163	GLY	2.3
1	B	110	THR	2.3
1	D	109	ALA	2.3
1	A	115	CYS	2.3
1	A	108	ASP	2.2
1	C	110	THR	2.1
1	D	131	ASN	2.1
1	A	223	GLY	2.1
1	D	114	CYS	2.0
1	A	219	ASP	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](#)

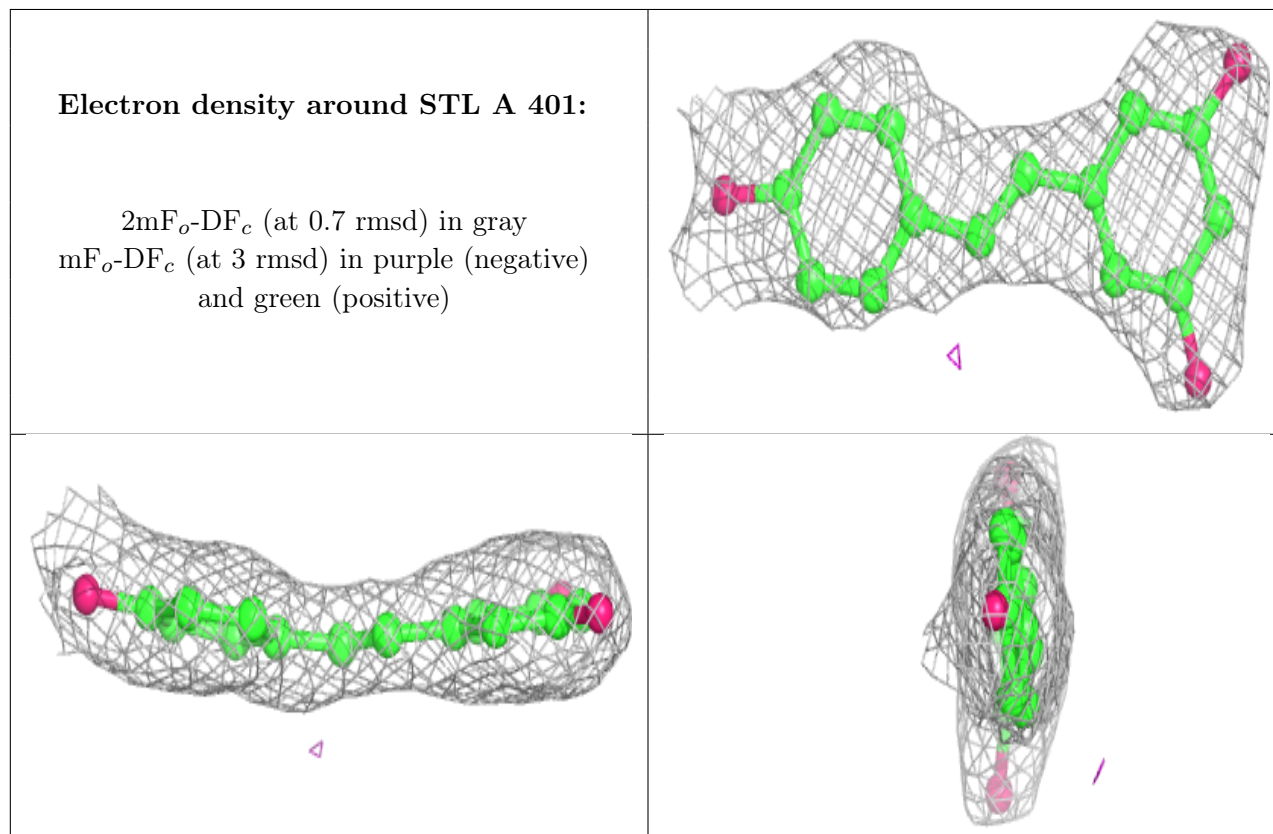
There are no monosaccharides in this entry.

## 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.

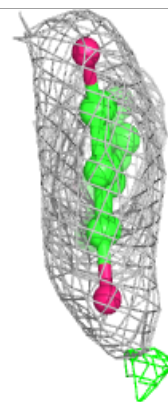
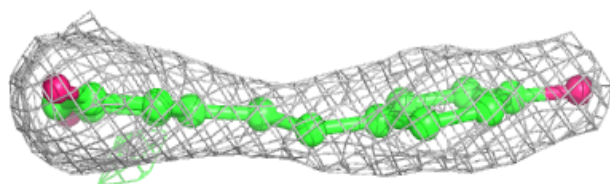
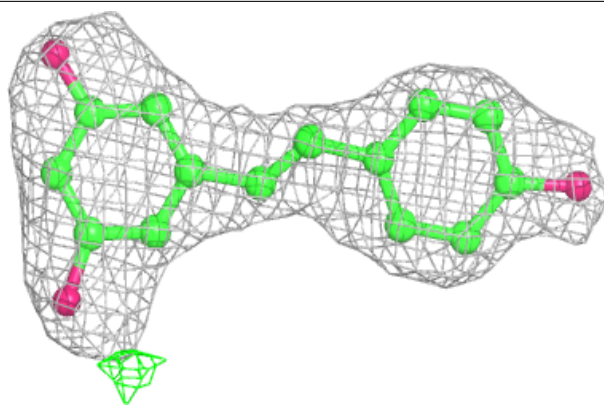
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	D	403	4/4	0.76	0.26	84,85,86,88	0
3	EDO	A	402	4/4	0.81	0.21	62,66,72,79	0
3	EDO	C	403	4/4	0.85	0.33	76,77,81,82	0
3	EDO	C	402	4/4	0.87	0.29	58,71,71,78	0
3	EDO	D	402	4/4	0.93	0.46	59,62,77,85	0
3	EDO	B	402	4/4	0.95	0.28	47,49,54,67	0
2	STL	A	401	17/17	0.95	0.18	50,57,66,68	0
2	STL	C	401	17/17	0.97	0.17	31,49,57,64	0
2	STL	D	401	17/17	0.97	0.19	41,52,58,68	0
2	STL	B	401	17/17	0.98	0.14	34,41,49,52	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.

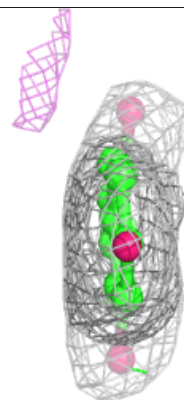
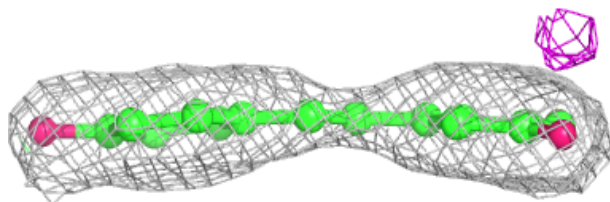
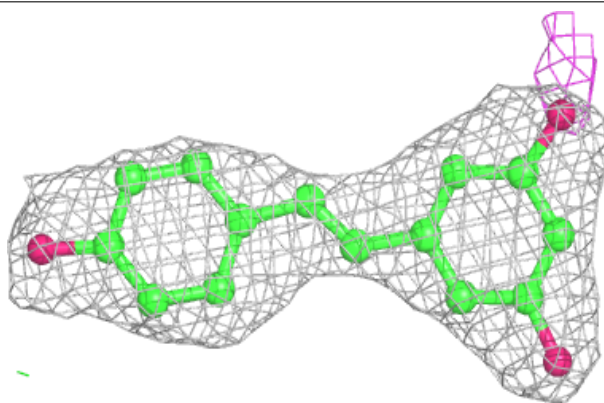


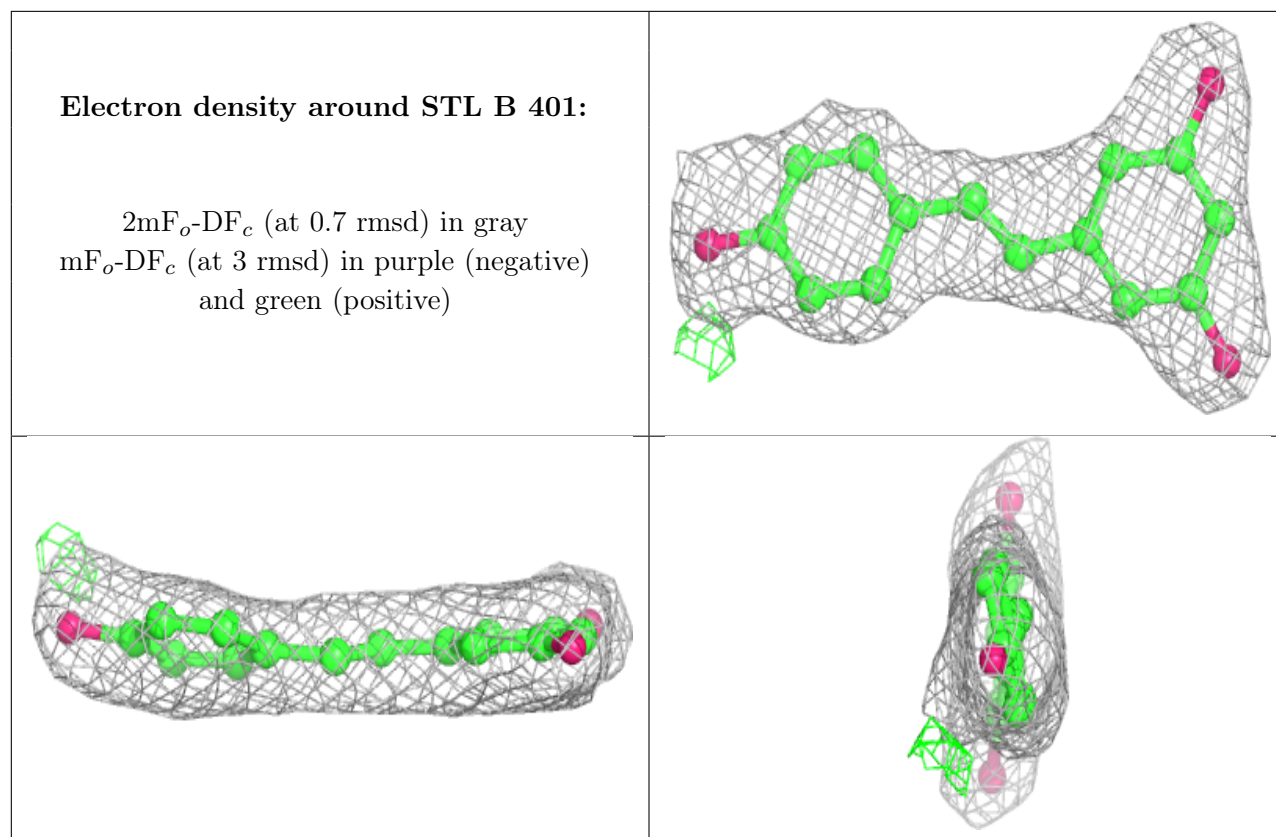
**Electron density around STL C 401:**

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

**Electron density around STL D 401:**

$2mF_o-DF_c$  (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.