



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:00 am BST

PDB ID : 6FBA  
Title : Crystal Structure of truncated aspartate transcarbamoylase from Plasmodium falciparum with bound inhibitor 2,3-naphthalenediol  
Authors : Lunev, S.; Bosch, S.S.; Batista, F.A.; Wang, C.; Wrenger, C.; Groves, M.R.  
Deposited on : 2017-12-18  
Resolution : 2.00 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

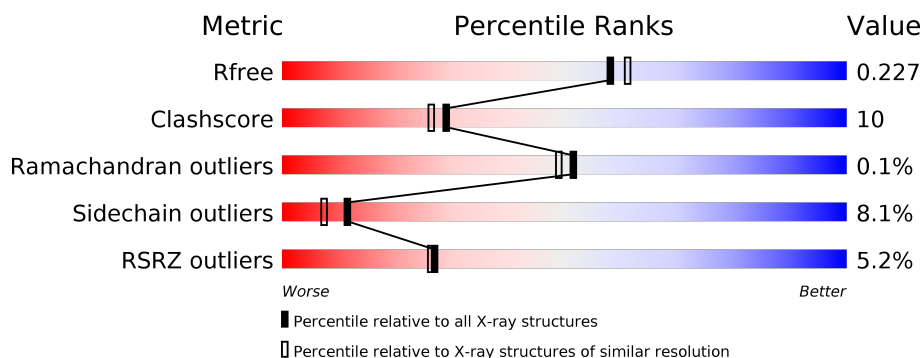
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	349	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>• • 8%</div> </div> </div>
1	B	349	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>5% 9%</div> </div> </div>
2	C	349	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• • 6%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MLI	A	405	-	-	X	X
6	MLI	C	404	-	-	-	X
9	PEG	B	404	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 8085 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 Aspartate transcarbamoylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2601	1660	430	503	8			
1	B	317	Total	C	N	O	S	0	1	0
			2577	1646	426	497	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	-	expression tag	UNP O15804
A	377	ALA	-	expression tag	UNP O15804
A	378	TRP	-	expression tag	UNP O15804
A	379	SER	-	expression tag	UNP O15804
A	380	HIS	-	expression tag	UNP O15804
A	381	PRO	-	expression tag	UNP O15804
A	382	GLN	-	expression tag	UNP O15804
A	383	PHE	-	expression tag	UNP O15804
A	384	GLU	-	expression tag	UNP O15804
A	385	LYS	-	expression tag	UNP O15804
B	376	SER	-	expression tag	UNP O15804
B	377	ALA	-	expression tag	UNP O15804
B	378	TRP	-	expression tag	UNP O15804
B	379	SER	-	expression tag	UNP O15804
B	380	HIS	-	expression tag	UNP O15804
B	381	PRO	-	expression tag	UNP O15804
B	382	GLN	-	expression tag	UNP O15804
B	383	PHE	-	expression tag	UNP O15804
B	384	GLU	-	expression tag	UNP O15804
B	385	LYS	-	expression tag	UNP O15804

- Molecule 2 is a protein called Aspartate transcarbamoylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	328	Total	C	N	O	S	0	0	0
			2659	1695	437	519	8			

There are 10 discrepancies between the modelled and reference sequences:

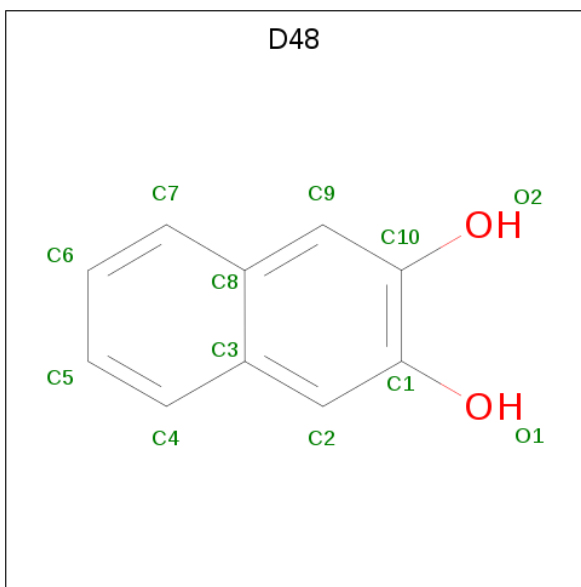
Chain	Residue	Modelled	Actual	Comment	Reference
C	376	SER	-	expression tag	UNP O15804
C	377	ALA	-	expression tag	UNP O15804
C	378	TRP	-	expression tag	UNP O15804
C	379	SER	-	expression tag	UNP O15804
C	380	HIS	-	expression tag	UNP O15804
C	381	PRO	-	expression tag	UNP O15804
C	382	GLN	-	expression tag	UNP O15804
C	383	PHE	-	expression tag	UNP O15804
C	384	GLU	-	expression tag	UNP O15804
C	385	LYS	-	expression tag	UNP O15804

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



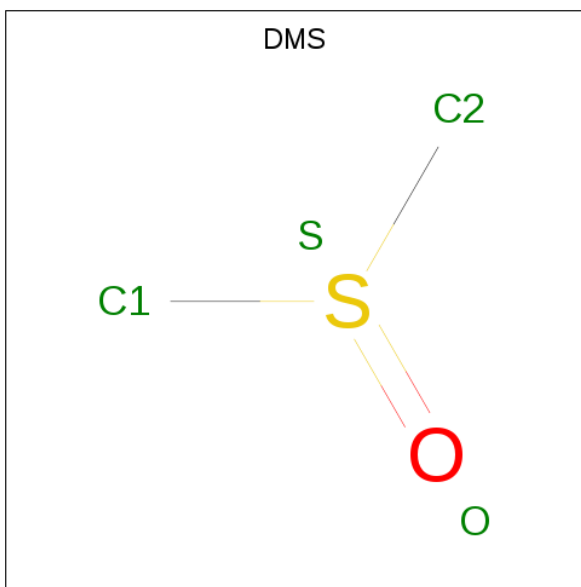
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is naphthalene-2,3-diol (three-letter code: D48) (formula: C<sub>10</sub>H<sub>8</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	10	2		
4	B	1	Total	C	O	0	0
			12	10	2		
4	C	1	Total	C	O	0	0
			12	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



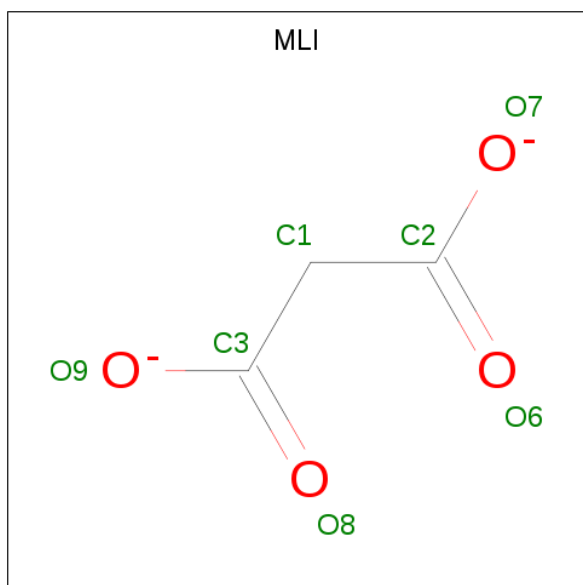
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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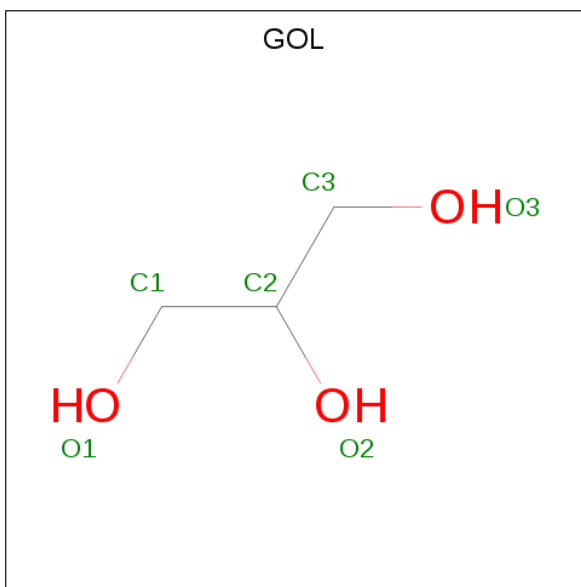
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula:  $\text{C}_3\text{H}_2\text{O}_4$ ).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).

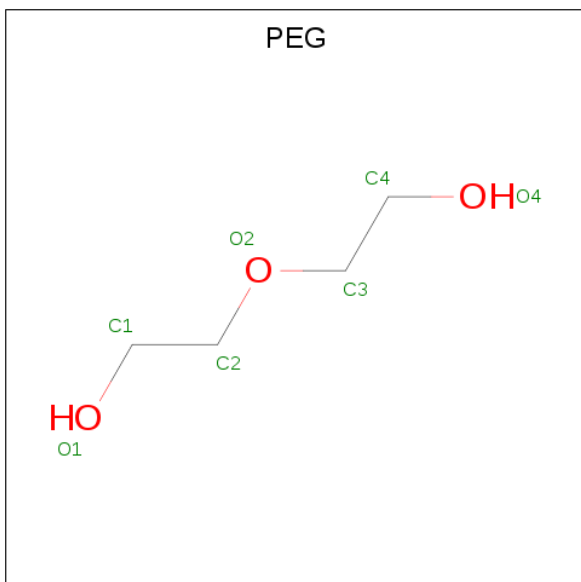


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 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
9	B	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		

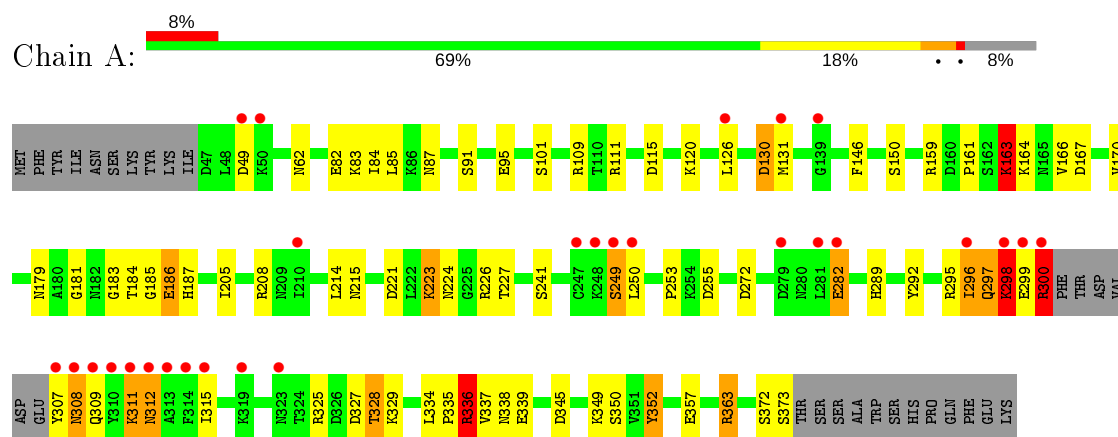
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	33	Total	O	0	0
			33	33		
10	B	50	Total	O	0	0
			50	50		
10	C	59	Total	O	0	0
			59	59		

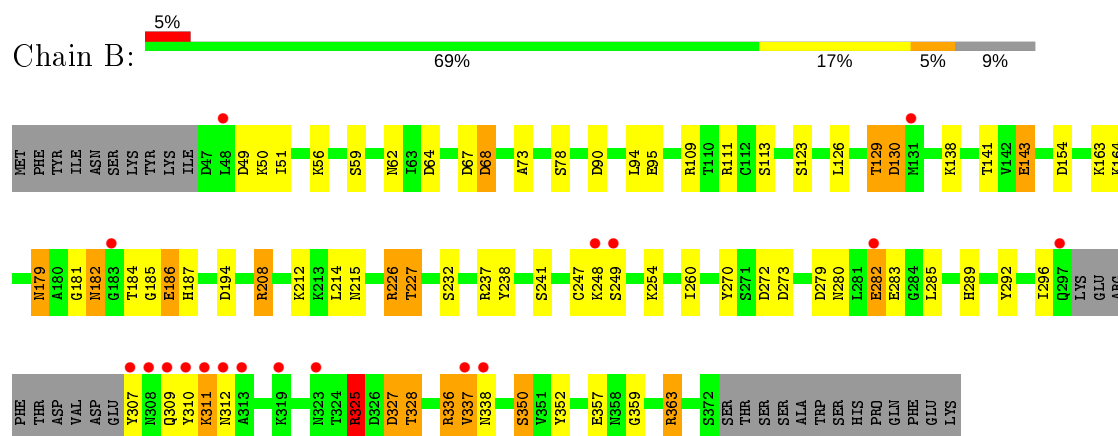
### 3 Residue-property plots [i](#)

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

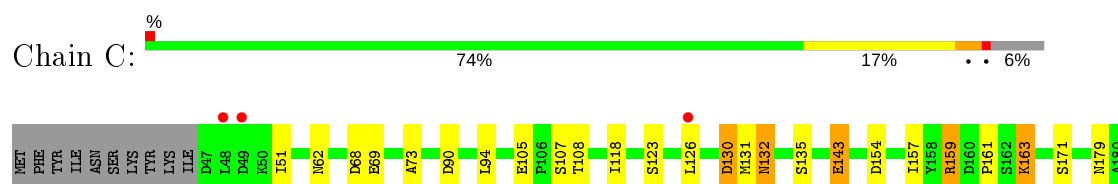
- Molecule 1: Aspartate transcarbamoylase

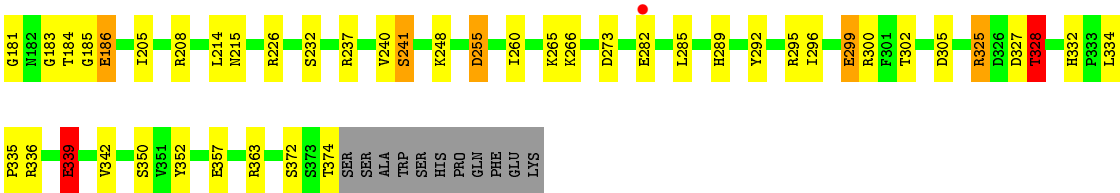


- Molecule 1: Aspartate transcarbamoylase



- Molecule 2: Aspartate transcarbamoylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.76Å 86.76Å 138.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.13 – 2.00 43.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (75.13-2.00) 99.7 (43.38-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.184 , 0.225 0.189 , 0.227	Depositor DCC
$R_{free}$ test set	3991 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.049 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, DMS, NA, MLI, D48, SO4, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.19	4/2647 (0.2%)	1.24	20/3573 (0.6%)
1	B	1.28	14/2623 (0.5%)	1.29	26/3542 (0.7%)
2	C	1.34	11/2699 (0.4%)	1.31	23/3645 (0.6%)
All	All	1.27	29/7969 (0.4%)	1.28	69/10760 (0.6%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CD-OE1	10.76	1.37	1.25
1	B	357	GLU	CD-OE1	-9.53	1.15	1.25
2	C	186	GLU	CD-OE1	9.16	1.35	1.25
1	A	363	ARG	CZ-NH2	8.76	1.44	1.33
2	C	363	ARG	CZ-NH2	8.62	1.44	1.33
2	C	372	SER	CB-OG	-8.19	1.31	1.42
2	C	241	SER	CB-OG	-7.29	1.32	1.42
1	B	241	SER	CB-OG	-6.63	1.33	1.42
1	A	357	GLU	CD-OE1	-6.58	1.18	1.25
2	C	357	GLU	CD-OE1	-6.58	1.18	1.25
1	B	279	ASP	CB-CG	-6.56	1.38	1.51
2	C	107	SER	CB-OG	6.39	1.50	1.42
1	B	238	TYR	CE1-CZ	6.36	1.46	1.38
2	C	69	GLU	CD-OE1	6.29	1.32	1.25
1	B	78	SER	CB-OG	-6.28	1.34	1.42
2	C	328	THR	CB-CG2	-6.16	1.32	1.52
1	A	372	SER	CB-OG	-6.11	1.34	1.42
1	B	350	SER	CB-OG	-6.07	1.34	1.42
1	B	186	GLU	CG-CD	6.00	1.60	1.51
1	B	208	ARG	CZ-NH2	-5.78	1.25	1.33
1	B	270	TYR	CE1-CZ	-5.78	1.31	1.38
1	B	90	ASP	CB-CG	5.75	1.63	1.51
2	C	339	GLU	CD-OE2	-5.74	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	186	GLU	CG-CD	5.71	1.60	1.51
1	B	363	ARG	CZ-NH2	5.55	1.40	1.33
1	B	59	SER	CB-OG	-5.38	1.35	1.42
1	B	241	SER	CA-CB	5.35	1.60	1.52
2	C	292	TYR	CG-CD1	5.26	1.46	1.39
1	B	64	ASP	CB-CG	5.17	1.62	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	363	ARG	NE-CZ-NH1	-17.64	111.48	120.30
1	B	363	ARG	NE-CZ-NH1	-16.71	111.95	120.30
1	A	363	ARG	NE-CZ-NH1	-13.33	113.63	120.30
2	C	363	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	A	336	ARG	NE-CZ-NH1	-12.89	113.85	120.30
1	A	208	ARG	NE-CZ-NH1	12.01	126.31	120.30
2	C	237	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	363	ARG	NE-CZ-NH2	11.05	125.83	120.30
1	A	208	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	B	208	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	167	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	B	90	ASP	CB-CG-OD2	9.42	126.78	118.30
2	C	68	ASP	CB-CG-OD1	9.23	126.60	118.30
1	B	325	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	336	ARG	NE-CZ-NH2	-9.03	115.79	120.30
2	C	208	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	B	111	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	C	305	ASP	CB-CG-OD2	8.78	126.21	118.30
1	A	272	ASP	CB-CG-OD1	8.77	126.19	118.30
1	B	111	ARG	NE-CZ-NH2	-8.55	116.02	120.30
2	C	208	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	159	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	B	67	ASP	CB-CG-OD1	8.40	125.86	118.30
1	B	130	ASP	CB-CG-OD1	-8.20	110.92	118.30
1	B	154	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	111	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	C	90	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	237	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	B	194	ASP	CB-CG-OD2	7.40	124.96	118.30
2	C	68	ASP	CB-CG-OD2	-7.01	111.99	118.30
2	C	325	ARG	NE-CZ-NH2	7.00	123.80	120.30
2	C	131	MET	CG-SD-CE	6.96	111.33	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	208	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	363	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	A	159	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	B	272	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	68	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	130	ASP	CB-CG-OD2	6.61	124.25	118.30
2	C	159	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	A	167	ASP	CB-CG-OD1	6.37	124.03	118.30
2	C	130	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	336	ARG	NE-CZ-NH2	6.26	123.43	120.30
2	C	90	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	212	LYS	CD-CE-NZ	-6.05	97.77	111.70
2	C	255	ASP	CB-CG-OD1	-6.04	112.86	118.30
2	C	130	ASP	CB-CG-OD1	-6.02	112.88	118.30
2	C	300	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	327	ASP	CB-CG-OD1	5.95	123.65	118.30
2	C	265	LYS	CD-CE-NZ	-5.83	98.29	111.70
2	C	154	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	143	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	B	95	GLU	N-CA-C	5.68	126.34	111.00
1	B	64	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	130	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	111	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	298	LYS	CB-CG-CD	5.43	125.73	111.60
2	C	273	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	163	LYS	CA-CB-CG	5.31	125.08	113.40
1	A	300	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	82	GLU	OE1-CD-OE2	5.30	129.66	123.30
2	C	295	ARG	CG-CD-NE	-5.26	100.75	111.80
1	B	336	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	C	325	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	C	295	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	208	ARG	CD-NE-CZ	5.12	130.76	123.60
1	B	138	LYS	CD-CE-NZ	5.04	123.30	111.70
1	A	95	GLU	N-CA-C	5.02	124.55	111.00
1	B	67	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	2601	0	2613	63	0
1	B	2577	0	2588	53	0
2	C	2659	0	2660	35	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	0	1	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
6	A	14	0	4	4	0
6	C	7	0	2	0	0
7	A	6	0	8	0	0
7	C	6	0	8	1	0
8	A	1	0	0	0	0
9	B	7	0	10	6	0
9	C	7	0	10	2	0
10	A	33	0	0	9	0
10	B	50	0	0	2	0
10	C	59	0	0	1	0
All	All	8085	0	7921	152	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 10.

All (152) 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)
2:C:62:ASN:HD22	2:C:186:GLU:HG3	1.05	1.13
1:A:163:LYS:HB2	1:A:184:THR:HG23	1.33	1.04
1:A:163:LYS:CB	1:A:184:THR:HG23	1.91	1.00
1:B:307:TYR:CE2	1:B:311:LYS:HD2	1.98	0.97
1:A:62:ASN:HD22	1:A:186:GLU:HG3	1.39	0.88
2:C:62:ASN:ND2	2:C:186:GLU:HG3	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:CYS:HB3	1:B:310:TYR:HE1	1.35	0.88
1:B:247:CYS:CB	1:B:310:TYR:HE1	1.89	0.84
1:A:163:LYS:HB2	1:A:184:THR:CG2	2.08	0.81
1:B:62:ASN:HA	1:B:186:GLU:CG	2.11	0.80
1:A:227:THR:CG2	1:A:292:TYR:OH	2.30	0.80
1:B:62:ASN:HA	1:B:186:GLU:HG2	1.62	0.80
1:B:226[B]:ARG:HH11	1:B:226[B]:ARG:CG	1.95	0.77
1:B:141:THR:HG23	9:B:404:PEG:H12	1.68	0.76
1:A:62:ASN:ND2	1:A:186:GLU:HG3	2.04	0.73
1:A:308:ASN:ND2	1:A:308:ASN:H	1.85	0.72
2:C:132:ASN:ND2	2:C:135:SER:OG	2.22	0.72
1:B:141:THR:HG21	9:B:404:PEG:H42	1.70	0.71
1:A:337:VAL:HG21	10:A:502:HOH:O	1.91	0.71
1:B:226[B]:ARG:HH11	1:B:226[B]:ARG:HG2	1.54	0.70
1:A:337:VAL:HG23	1:A:338:ASN:H	1.56	0.69
2:C:332:HIS:NE2	2:C:339:GLU:OE2	2.23	0.69
1:B:325:ARG:HD3	1:B:327:ASP:OD1	1.93	0.69
1:A:62:ASN:HD22	1:A:186:GLU:CG	2.04	0.68
1:B:247:CYS:HB3	1:B:310:TYR:CE1	2.25	0.67
1:B:141:THR:CG2	9:B:404:PEG:H42	2.25	0.67
1:A:223:LYS:CD	1:A:249:SER:O	2.43	0.67
2:C:163:LYS:H	2:C:163:LYS:HD3	1.60	0.67
9:B:404:PEG:H32	2:C:342:VAL:CG2	2.25	0.67
1:A:223:LYS:HD2	1:A:250:LEU:HA	1.77	0.66
1:B:249:SER:OG	1:B:310:TYR:CZ	2.49	0.65
1:A:312:ASN:OD1	1:A:315:ILE:HD11	1.97	0.65
1:A:298:LYS:HG3	1:A:307:TYR:CE2	2.32	0.65
1:B:226[B]:ARG:CG	1:B:226[B]:ARG:NH1	2.57	0.64
1:A:185:GLY:HA2	1:A:226:ARG:HG2	1.79	0.63
1:B:247:CYS:CB	1:B:310:TYR:CE1	2.77	0.63
2:C:215:ASN:H	2:C:289:HIS:HD2	1.44	0.63
1:A:336:ARG:NH1	1:A:345:ASP:OD1	2.27	0.63
2:C:185:GLY:HA2	2:C:226:ARG:HG3	1.80	0.63
1:A:163:LYS:HB3	1:A:184:THR:HG23	1.80	0.62
1:A:337:VAL:CG2	10:A:502:HOH:O	2.47	0.62
1:A:227:THR:HG21	1:A:292:TYR:OH	1.99	0.62
2:C:325:ARG:HB2	2:C:328:THR:HG22	1.81	0.61
1:A:296:ILE:O	10:A:502:HOH:O	2.16	0.61
1:B:185:GLY:HA3	1:B:226[B]:ARG:HB3	1.82	0.61
1:B:226[A]:ARG:HG2	1:B:227:THR:N	2.15	0.60
1:A:311:LYS:CE	10:A:502:HOH:O	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:GLU:HG3	9:C:403:PEG:C3	2.31	0.60
1:A:325:ARG:O	1:A:328:THR:HG23	2.02	0.60
1:B:182:ASN:ND2	10:B:502:HOH:O	2.35	0.59
1:B:350:SER:HB2	1:B:352:TYR:CE2	2.38	0.59
1:A:296:ILE:HD12	1:A:296:ILE:C	2.23	0.58
1:A:223:LYS:HD3	1:A:249:SER:O	2.02	0.58
9:B:404:PEG:H32	2:C:342:VAL:HG23	1.85	0.57
1:B:129:THR:O	1:B:129:THR:HG23	2.03	0.57
2:C:132:ASN:ND2	2:C:135:SER:H	2.01	0.57
1:A:307:TYR:OH	1:A:311:LYS:NZ	2.37	0.56
1:A:221:ASP:OD2	1:A:224:ASN:HB2	2.05	0.56
2:C:296:ILE:HD11	10:C:553:HOH:O	2.06	0.56
2:C:325:ARG:HD3	2:C:327:ASP:OD1	2.05	0.56
2:C:325:ARG:O	2:C:328:THR:HG23	2.05	0.55
2:C:62:ASN:HD22	2:C:186:GLU:CG	1.98	0.55
1:A:109:ARG:H	6:A:405:MLI:C1	2.20	0.55
1:A:363:ARG:NH1	10:A:501:HOH:O	2.08	0.55
2:C:163:LYS:N	2:C:163:LYS:HD3	2.21	0.55
2:C:179:ASN:ND2	2:C:181:GLY:H	2.03	0.55
1:A:325:ARG:HD3	1:A:327:ASP:OD1	2.07	0.54
1:A:350:SER:HB2	1:A:352:TYR:CE1	2.42	0.54
2:C:350:SER:HB2	2:C:352:TYR:CE2	2.42	0.54
2:C:143:GLU:HG3	9:C:403:PEG:H32	1.89	0.54
1:B:62:ASN:HD22	1:B:186:GLU:HG2	1.72	0.54
2:C:132:ASN:C	2:C:132:ASN:HD22	2.10	0.53
1:A:179:ASN:ND2	1:A:181:GLY:H	2.06	0.53
1:A:91:SER:OG	1:A:120:LYS:HE3	2.08	0.53
1:B:325:ARG:HB2	1:B:328:THR:HG22	1.91	0.53
1:A:185:GLY:HA2	1:A:226:ARG:CG	2.39	0.53
1:B:227:THR:CG2	1:B:292:TYR:OH	2.58	0.52
1:A:337:VAL:HG23	1:A:338:ASN:N	2.24	0.52
1:B:325:ARG:HB2	1:B:328:THR:CG2	2.39	0.52
1:B:280:ASN:HD22	1:B:282:GLU:HG2	1.75	0.52
1:B:337:VAL:HG23	1:B:338:ASN:H	1.75	0.52
1:B:185:GLY:HA2	1:B:226[A]:ARG:HG3	1.92	0.52
1:B:179:ASN:ND2	1:B:181:GLY:H	2.08	0.51
2:C:325:ARG:HB3	7:C:405:GOL:H12	1.90	0.51
1:B:215:ASN:H	1:B:289:HIS:HD2	1.58	0.51
1:B:185:GLY:CA	1:B:226[B]:ARG:HB3	2.40	0.51
2:C:215:ASN:H	2:C:289:HIS:CD2	2.27	0.51
1:B:94:LEU:O	1:B:123:SER:OG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:325:ARG:HB2	2:C:328:THR:CG2	2.41	0.50
1:A:227:THR:HG23	1:A:292:TYR:OH	2.10	0.50
1:A:299:GLU:OE2	1:A:299:GLU:N	2.34	0.50
2:C:94:LEU:O	2:C:123:SER:OG	2.26	0.50
1:B:51:ILE:HG21	1:B:73:ALA:HB2	1.94	0.49
1:A:253:PRO:HB2	1:A:255:ASP:OD1	2.12	0.49
1:B:215:ASN:H	1:B:289:HIS:CD2	2.30	0.49
1:B:141:THR:HG21	9:B:404:PEG:C4	2.42	0.49
1:A:187:HIS:HB2	1:A:226:ARG:HD2	1.94	0.49
1:B:359:GLY:O	1:B:363:ARG:HG3	2.13	0.48
1:B:182:ASN:HD22	1:B:184:THR:H	1.61	0.48
1:B:307:TYR:CE2	1:B:311:LYS:CD	2.87	0.48
1:A:109:ARG:H	6:A:405:MLI:H12	1.78	0.48
1:A:311:LYS:HE2	1:A:337:VAL:HG23	1.95	0.48
1:A:296:ILE:HG23	1:A:311:LYS:HE3	1.96	0.48
1:A:166:VAL:O	1:A:170:VAL:HG23	2.14	0.47
2:C:161:PRO:O	2:C:183:GLY:HA3	2.14	0.47
1:A:297:GLN:HG3	1:A:300:ARG:HE	1.79	0.47
2:C:51:ILE:HG21	2:C:73:ALA:HB2	1.96	0.47
1:B:226[B]:ARG:HG3	1:B:226[B]:ARG:NH1	2.30	0.47
2:C:105:GLU:OE1	2:C:159:ARG:HD3	2.14	0.47
1:B:185:GLY:HA2	1:B:226[A]:ARG:CG	2.44	0.47
2:C:299:GLU:H	2:C:299:GLU:CD	2.18	0.47
1:B:62:ASN:HA	1:B:186:GLU:HG3	1.94	0.46
1:A:336:ARG:HH12	1:A:345:ASP:CG	2.18	0.46
1:B:187:HIS:HB3	10:B:521:HOH:O	2.15	0.46
2:C:185:GLY:CA	2:C:226:ARG:HG3	2.46	0.46
1:A:215:ASN:H	1:A:289:HIS:HD2	1.64	0.46
1:A:298:LYS:HG3	1:A:307:TYR:CD2	2.50	0.46
1:B:227:THR:HG23	1:B:292:TYR:OH	2.15	0.46
2:C:232:SER:HB3	2:C:260:ILE:HD11	1.98	0.46
1:A:115:ASP:OD1	10:A:503:HOH:O	2.21	0.45
1:B:182:ASN:C	1:B:182:ASN:HD22	2.20	0.45
1:A:311:LYS:HD3	1:A:311:LYS:O	2.16	0.45
2:C:205:ILE:HD11	2:C:240:VAL:CG2	2.47	0.45
1:B:307:TYR:CD2	1:B:311:LYS:HD2	2.50	0.45
1:B:232:SER:HB3	1:B:260:ILE:HD11	1.99	0.44
1:A:109:ARG:H	6:A:405:MLI:H11	1.82	0.44
6:A:404:MLI:H12	10:A:505:HOH:O	2.16	0.44
1:A:163:LYS:CB	1:A:184:THR:CG2	2.79	0.44
1:A:255:ASP:N	1:A:255:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:NH1	1:A:327:ASP:OD2	2.51	0.44
1:A:334:LEU:HB3	1:A:335:PRO:HA	1.99	0.44
1:A:296:ILE:HG22	1:A:339:GLU:CG	2.49	0.43
1:B:325:ARG:O	1:B:328:THR:HG23	2.19	0.43
1:A:282:GLU:HG2	1:A:282:GLU:H	1.60	0.42
1:A:84:ILE:HG22	1:A:85:LEU:HD12	2.02	0.42
1:B:182:ASN:ND2	1:B:184:THR:H	2.17	0.42
1:A:363:ARG:NE	10:A:501:HOH:O	2.36	0.42
1:A:311:LYS:HE3	10:A:502:HOH:O	2.18	0.42
2:C:118:ILE:HD11	2:C:157:ILE:CD1	2.50	0.41
2:C:334:LEU:HB3	2:C:335:PRO:HA	2.02	0.41
1:A:329:LYS:HA	1:A:349:LYS:O	2.20	0.41
1:A:146:PHE:O	1:A:150:SER:OG	2.28	0.41
1:A:296:ILE:HG12	1:A:311:LYS:HA	2.03	0.41
1:B:185:GLY:CA	1:B:226[A]:ARG:HG3	2.50	0.41
4:A:402:D48:C8	1:B:109:ARG:HG2	2.51	0.41
1:B:185:GLY:HA3	1:B:226[B]:ARG:HG2	2.02	0.41
1:B:68:ASP:OD2	1:B:208:ARG:NH2	2.50	0.41
1:A:83:LYS:O	1:A:87:ASN:ND2	2.43	0.40
1:B:62:ASN:CA	1:B:186:GLU:HG2	2.43	0.40
1:A:161:PRO:O	1:A:183:GLY:HA3	2.22	0.40
1:B:280:ASN:ND2	1:B:283:GLU:H	2.19	0.40
2:C:185:GLY:HA2	2:C:226:ARG:CG	2.49	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	317/349 (91%)	301 (95%)	16 (5%)	0	100	100
1	B	314/349 (90%)	307 (98%)	6 (2%)	1 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	325/349 (93%)	316 (97%)	9 (3%)	0	100	100
All	All	956/1047 (91%)	924 (97%)	31 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	337	VAL

### 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	301/328 (92%)	276 (92%)	25 (8%)	11	7
1	B	298/328 (91%)	270 (91%)	28 (9%)	8	5
2	C	307/327 (94%)	286 (93%)	21 (7%)	16	11
All	All	906/983 (92%)	832 (92%)	74 (8%)	11	7

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	101	SER
1	A	126	LEU
1	A	130	ASP
1	A	131	MET
1	A	163	LYS
1	A	164	LYS
1	A	205	ILE
1	A	214	LEU
1	A	223	LYS
1	A	241	SER
1	A	249	SER
1	A	282	GLU
1	A	296	ILE

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Mol	Chain	Res	Type
1	A	297	GLN
1	A	298	LYS
1	A	300	ARG
1	A	308	ASN
1	A	309	GLN
1	A	311	LYS
1	A	312	ASN
1	A	328	THR
1	A	336	ARG
1	A	352	TYR
1	A	373	SER
1	B	49	ASP
1	B	50	LYS
1	B	56	LYS
1	B	113	SER
1	B	126	LEU
1	B	129	THR
1	B	130	ASP
1	B	143	GLU
1	B	163	LYS
1	B	164	LYS
1	B	179	ASN
1	B	182	ASN
1	B	214	LEU
1	B	226[A]	ARG
1	B	226[B]	ARG
1	B	227	THR
1	B	248	LYS
1	B	254	LYS
1	B	273	ASP
1	B	282	GLU
1	B	285	LEU
1	B	296	ILE
1	B	309	GLN
1	B	311	LYS
1	B	312	ASN
1	B	325	ARG
1	B	328	THR
1	B	336	ARG
2	C	108	THR
2	C	126	LEU
2	C	130	ASP

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Mol	Chain	Res	Type
2	C	132	ASN
2	C	143	GLU
2	C	163	LYS
2	C	171	SER
2	C	184	THR
2	C	214	LEU
2	C	241	SER
2	C	248	LYS
2	C	255	ASP
2	C	266	LYS
2	C	282	GLU
2	C	285	LEU
2	C	299	GLU
2	C	302	THR
2	C	328	THR
2	C	336	ARG
2	C	339	GLU
2	C	374	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	127	ASN
1	A	165	ASN
1	A	179	ASN
1	A	243	ASN
1	A	289	HIS
1	A	297	GLN
1	A	308	ASN
1	A	309	GLN
1	B	62	ASN
1	B	87	ASN
1	B	165	ASN
1	B	179	ASN
1	B	182	ASN
1	B	243	ASN
1	B	280	ASN
1	B	289	HIS
1	B	338	ASN
2	C	62	ASN
2	C	127	ASN

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Mol	Chain	Res	Type
2	C	132	ASN
2	C	165	ASN
2	C	179	ASN
2	C	243	ASN
2	C	289	HIS
2	C	308	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CSO	C	247	2	3,6,7	1.24	0	0,6,8	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	C	247	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	SO4	B	401	-	4,4,4	0.51	0	6,6,6	0.81	0
9	PEG	B	404	-	6,6,6	0.82	0	5,5,5	2.12	1 (20%)
7	GOL	C	405	-	5,5,5	0.54	0	5,5,5	0.75	0
4	D48	A	402	-	13,13,13	0.56	0	18,18,18	0.71	0
4	D48	C	401	-	13,13,13	0.55	0	18,18,18	0.58	0
6	MLI	A	405	-	0,6,6	0.00	-	0,7,7	0.00	-
7	GOL	A	406	-	5,5,5	0.70	0	5,5,5	0.77	0
5	DMS	C	402	-	3,3,3	0.57	0	3,3,3	1.13	0
4	D48	B	402	-	13,13,13	0.58	0	18,18,18	0.39	0
3	SO4	A	401	-	4,4,4	0.57	0	6,6,6	0.35	0
6	MLI	A	404	-	0,6,6	0.00	-	0,7,7	0.00	-
9	PEG	C	403	-	6,6,6	0.91	0	5,5,5	1.34	1 (20%)
5	DMS	A	403	-	3,3,3	0.52	0	3,3,3	0.65	0
5	DMS	B	403	-	3,3,3	0.60	0	3,3,3	0.41	0
6	MLI	C	404	-	0,6,6	0.00	-	0,7,7	0.00	-

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
7	GOL	A	406	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	B	404	-	-	2/4/4/4	-
7	GOL	C	405	-	-	4/4/4/4	-
4	D48	A	402	-	-	-	0/2/2/2
4	D48	C	401	-	-	-	0/2/2/2
6	MLI	A	405	-	-	0/0/4/4	-
9	PEG	C	403	-	-	4/4/4/4	-
6	MLI	A	404	-	-	0/0/4/4	-
4	D48	B	402	-	-	-	0/2/2/2
6	MLI	C	404	-	-	0/0/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	404	PEG	O2-C2-C1	3.61	125.92	110.07
9	C	403	PEG	O2-C3-C4	2.67	121.78	110.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

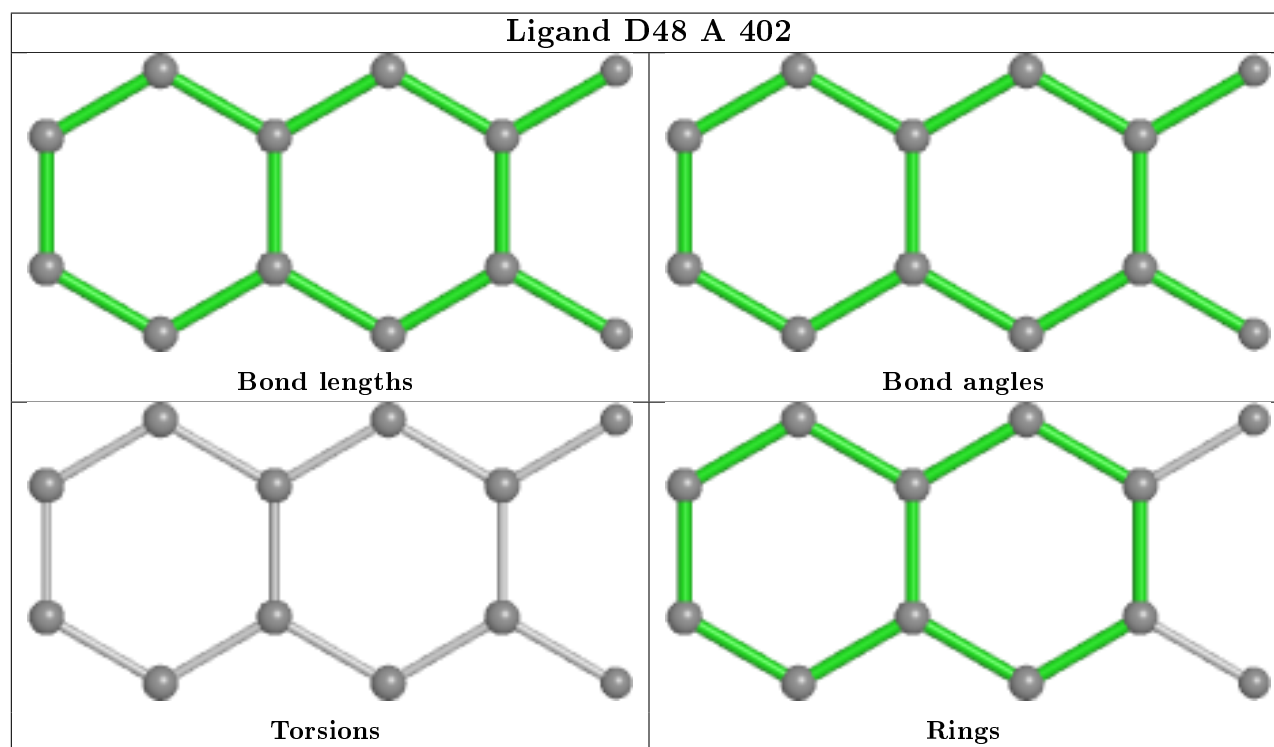
Mol	Chain	Res	Type	Atoms
7	C	405	GOL	O1-C1-C2-C3
7	C	405	GOL	C1-C2-C3-O3
7	A	406	GOL	O1-C1-C2-C3
7	A	406	GOL	C1-C2-C3-O3
7	A	406	GOL	O2-C2-C3-O3
7	C	405	GOL	O2-C2-C3-O3
7	A	406	GOL	O1-C1-C2-O2
9	B	404	PEG	O2-C3-C4-O4
7	C	405	GOL	O1-C1-C2-O2
9	C	403	PEG	O2-C3-C4-O4
9	B	404	PEG	C4-C3-O2-C2
9	C	403	PEG	C4-C3-O2-C2
9	C	403	PEG	O1-C1-C2-O2
9	C	403	PEG	C1-C2-O2-C3

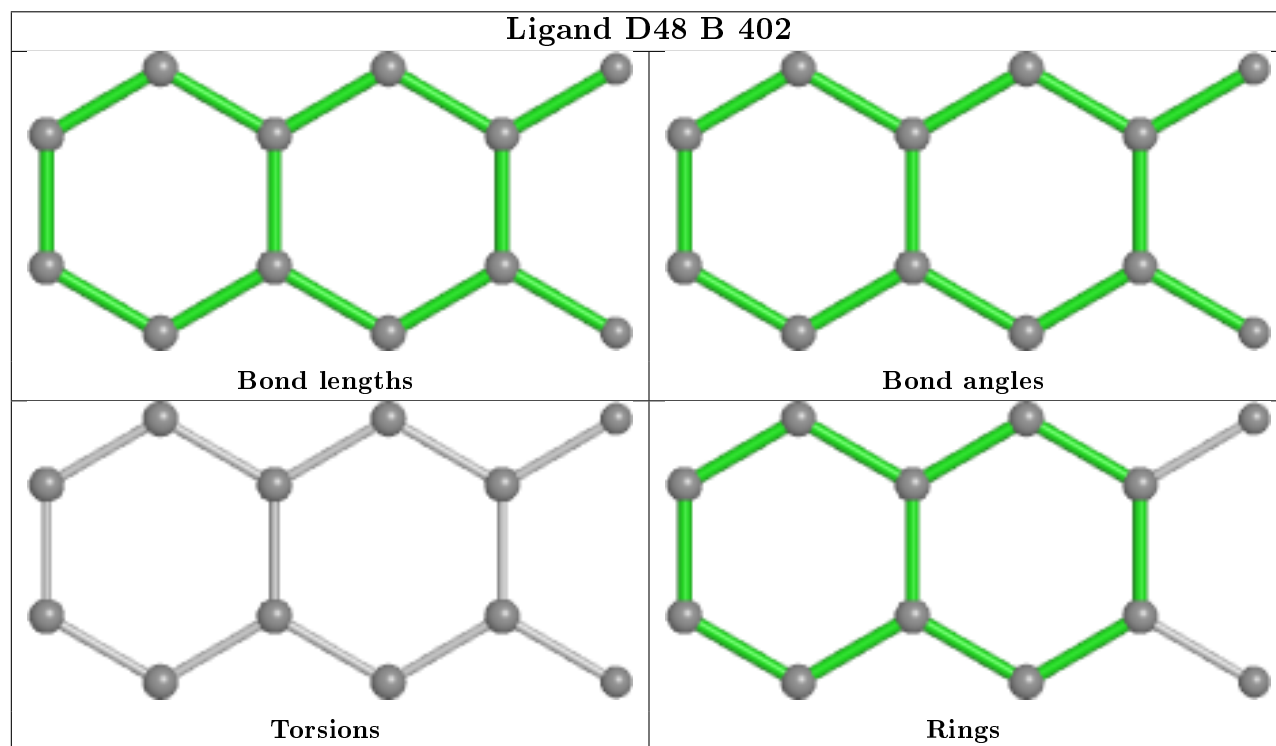
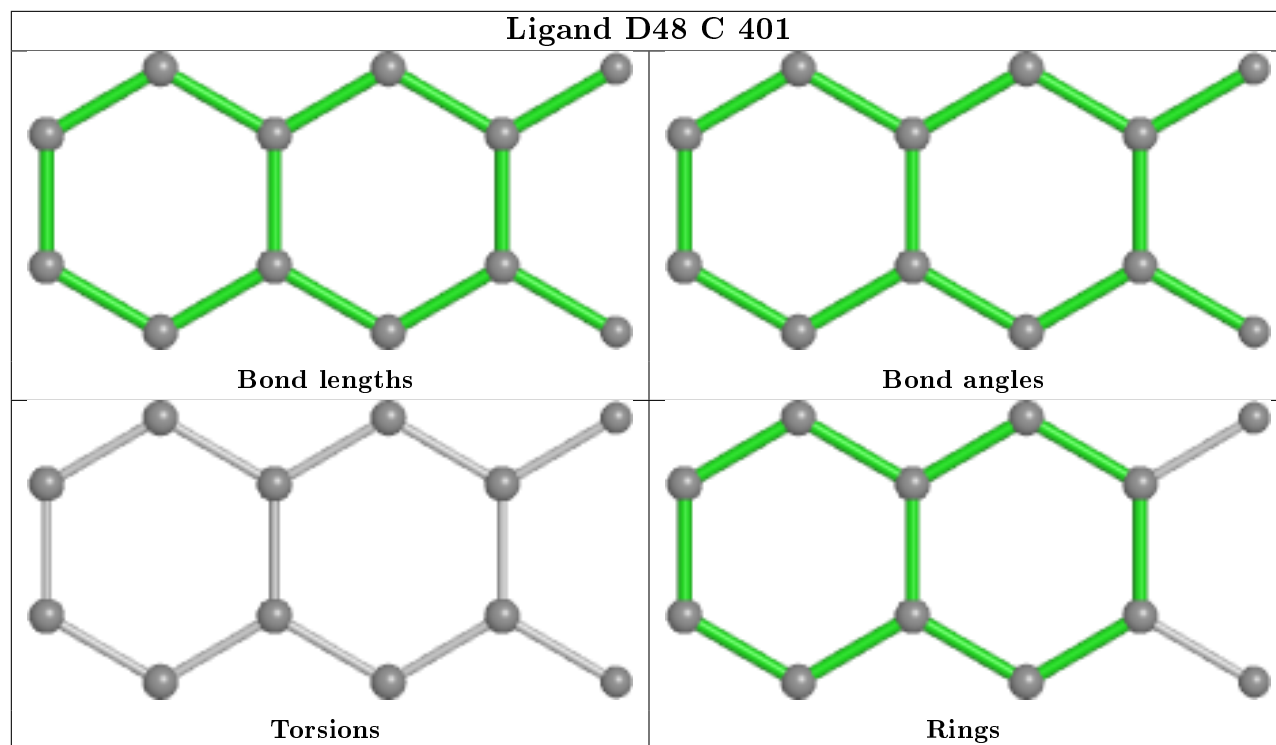
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	404	PEG	6	0
7	C	405	GOL	1	0
4	A	402	D48	1	0
6	A	405	MLI	3	0
6	A	404	MLI	1	0
9	C	403	PEG	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 ⓘ

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	321/349 (91%)	0.27	28 (8%) 10 9	27, 47, 81, 120	0
1	B	317/349 (90%)	-0.01	18 (5%) 23 23	26, 40, 75, 111	0
2	C	327/349 (93%)	-0.28	4 (1%) 79 78	25, 37, 60, 78	0
All	All	965/1047 (92%)	-0.01	50 (5%) 27 26	25, 41, 74, 120	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	TYR	7.9
1	A	307	TYR	7.1
1	A	310	TYR	6.3
1	A	309	GLN	6.0
1	B	308	ASN	5.9
1	A	313	ALA	5.9
1	B	309	GLN	5.8
1	A	298	LYS	4.3
1	A	314	PHE	3.9
1	A	131	MET	3.9
1	B	131	MET	3.7
1	A	248	LYS	3.7
1	A	308	ASN	3.7
1	A	249	SER	3.7
1	B	48	LEU	3.6
1	A	311	LYS	3.5
1	B	311	LYS	3.5
1	A	312	ASN	3.4
1	B	338	ASN	3.4
1	A	299	GLU	3.3
1	A	250	LEU	3.3
1	A	296	ILE	3.1
1	B	307	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	48	LEU	3.0
1	A	315	ILE	2.9
1	A	210	ILE	2.8
1	A	300	ARG	2.8
1	B	313	ALA	2.8
1	A	139	GLY	2.7
1	A	319	LYS	2.7
1	B	312	ASN	2.7
1	A	281	LEU	2.7
1	A	50	LYS	2.7
1	B	319	LYS	2.6
1	A	49	ASP	2.6
1	B	248	LYS	2.5
1	A	247	CYS	2.5
1	B	337	VAL	2.4
1	B	323	ASN	2.4
1	B	282	GLU	2.3
1	B	183	GLY	2.3
1	A	126	LEU	2.2
1	A	282	GLU	2.2
1	B	297	GLN	2.2
1	B	249	SER	2.2
1	A	279	ASP	2.1
2	C	49	ASP	2.1
1	A	323	ASN	2.0
2	C	126	LEU	2.0
2	C	282	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	CSO	C	247	7/8	0.96	0.07	39,42,43,46	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

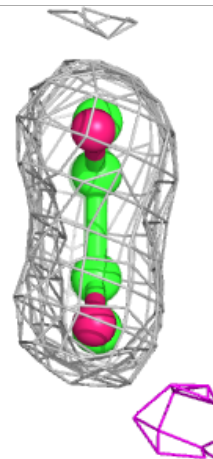
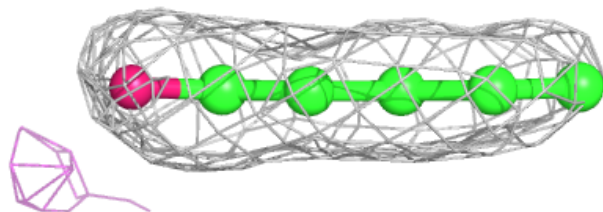
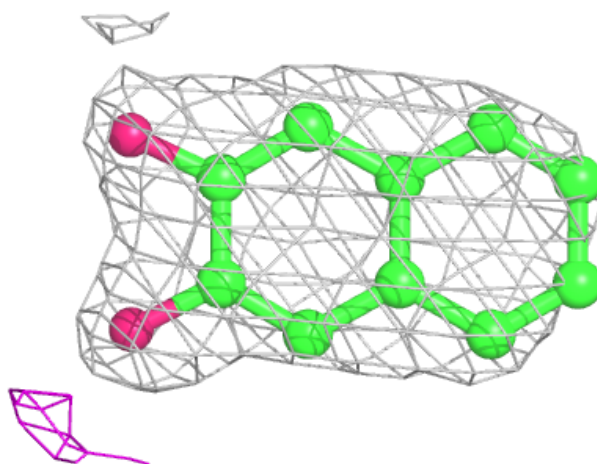
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MLI	A	405	7/7	0.74	0.45	27,36,40,51	7
9	PEG	C	403	7/7	0.76	0.23	51,59,66,67	0
5	DMS	C	402	4/4	0.77	0.19	66,79,82,85	0
7	GOL	C	405	6/6	0.78	0.19	62,65,72,80	0
6	MLI	C	404	7/7	0.80	0.51	29,35,42,44	7
7	GOL	A	406	6/6	0.83	0.21	51,61,66,69	0
4	D48	A	402	12/12	0.90	0.16	39,44,48,49	12
9	PEG	B	404	7/7	0.91	0.25	34,40,46,49	0
6	MLI	A	404	7/7	0.92	0.13	47,59,65,69	0
4	D48	B	402	12/12	0.95	0.10	42,44,48,50	0
8	NA	A	407	1/1	0.96	0.14	39,39,39,39	0
5	DMS	B	403	4/4	0.97	0.10	63,63,70,75	0
4	D48	C	401	12/12	0.97	0.09	36,39,42,44	0
3	SO4	A	401	5/5	0.99	0.08	36,36,41,42	0
5	DMS	A	403	4/4	0.99	0.10	65,69,71,72	0
3	SO4	B	401	5/5	1.00	0.10	30,31,43,46	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.



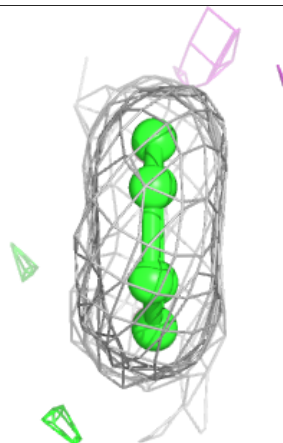
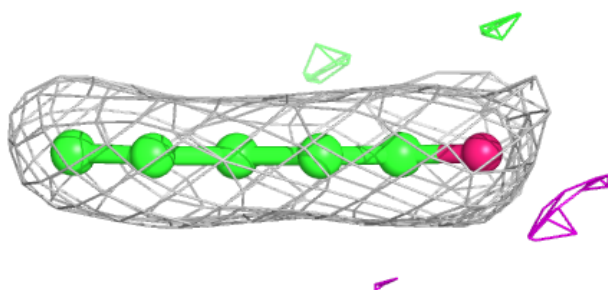
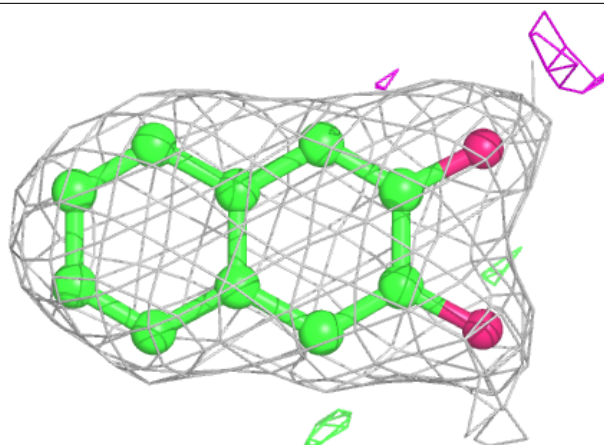
**Electron density around D48 A 402:**

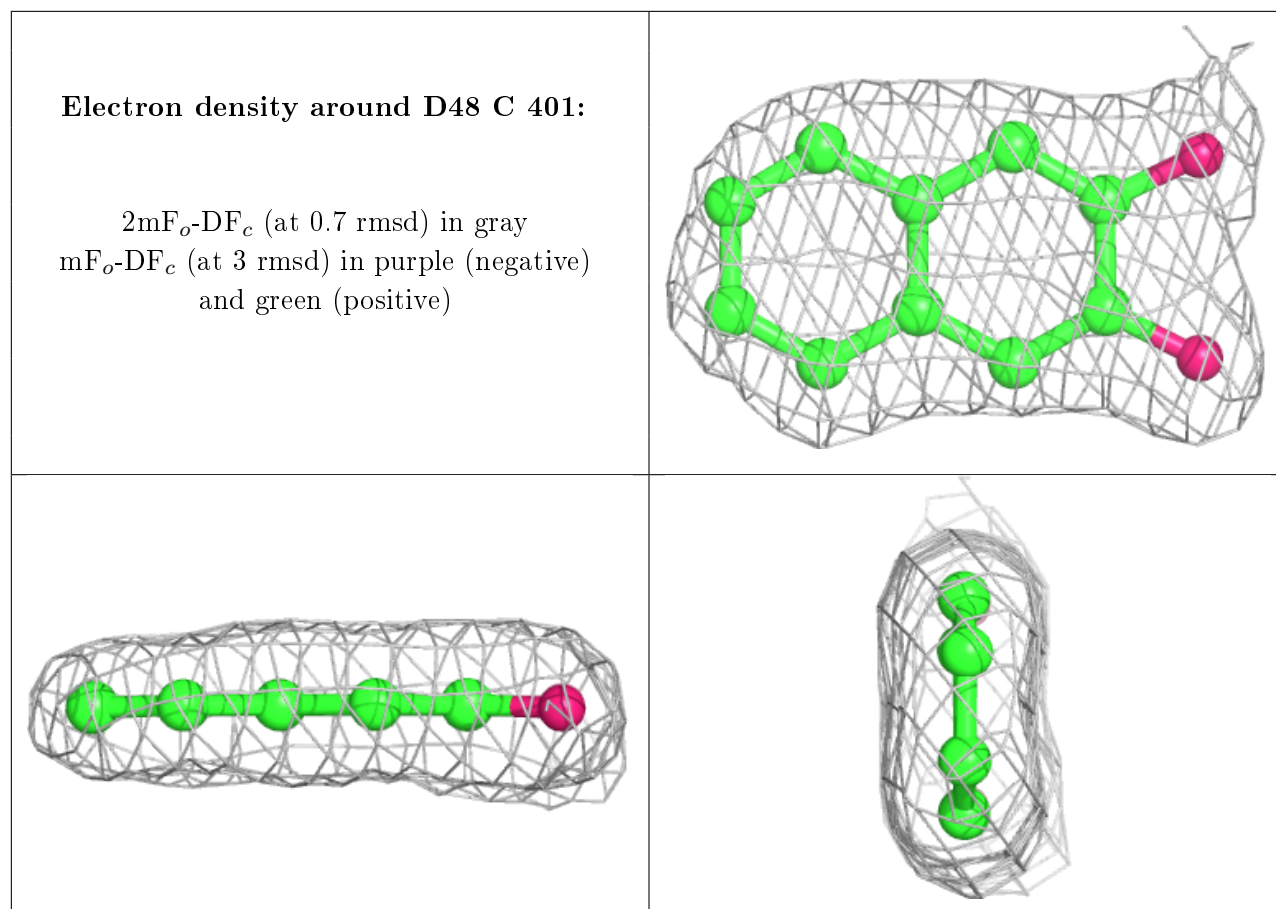
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around D48 B 402:**

$2mF_o - DF_c$  (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.