



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 05:02 PM BST

PDB ID : 4IY7  
Title : crystal structure of cystathionine gamma lyase (XometC) from Xanthomonas oryzae pv. oryzae in complex with E-site serine, A-site external aldimine structure with serine and A-site external aldimine structure with aminoacrylate intermediates  
Authors : Ngo, H.P.T.; Kim, J.K.; Kang, L.W.  
Deposited on : 2013-01-28  
Resolution : 1.70 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

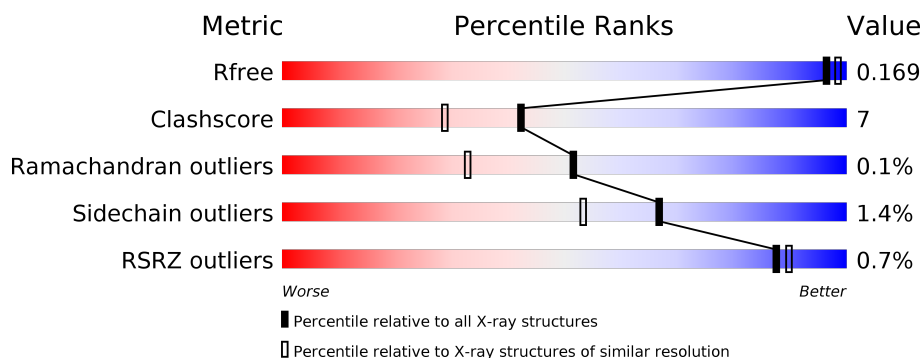
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	397	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	397	<div> <div></div> <div>82%</div> <div>13%</div> <div>••</div> </div>
1	C	397	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>
1	D	397	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</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
6	PYR	B	402	-	-	X	-
7	KOU	B	403	-	-	X	-
7	KOU	C	402	-	-	X	-
7	KOU	D	403	-	-	X	-

## 2 Entry composition [i](#)

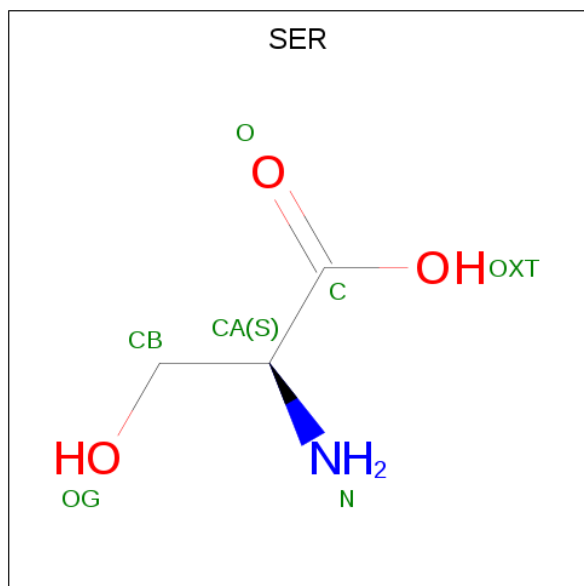
There are 8 unique types of molecules in this entry. The entry contains 13157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cystathionine gamma-lyase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	6	0
			2889	1830	509	535	15			
1	B	381	Total	C	N	O	S	0	7	0
			2892	1832	509	536	15			
1	C	381	Total	C	N	O	S	0	5	0
			2886	1828	509	534	15			
1	D	383	Total	C	N	O	S	0	8	0
			2918	1849	515	539	15			

- Molecule 2 is SERINE (three-letter code: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	3	1	3		
2	B	1	Total	C	N	O	0	0
			7	3	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			7	3	1	3		
2	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



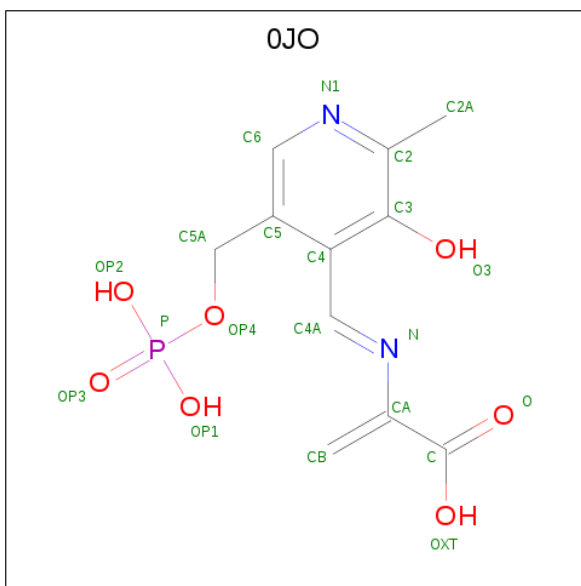
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



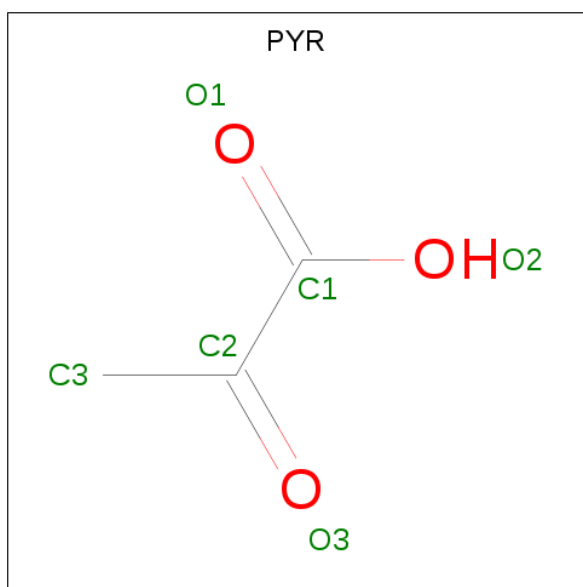
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (three-letter code: 0JO) (formula:  $C_{11}H_{13}N_2O_7P$ ).



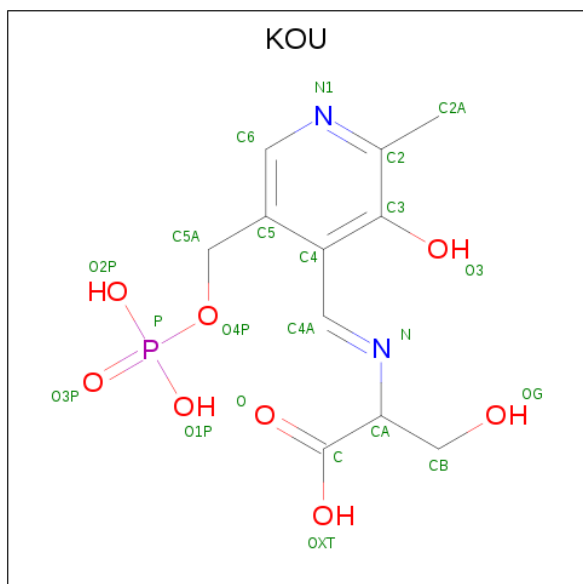
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



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

- Molecule 7 is (E)-N-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene)-L-serine (three-letter code: KOU) (formula:  $C_{11}H_{15}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
7	D	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 8 is water.

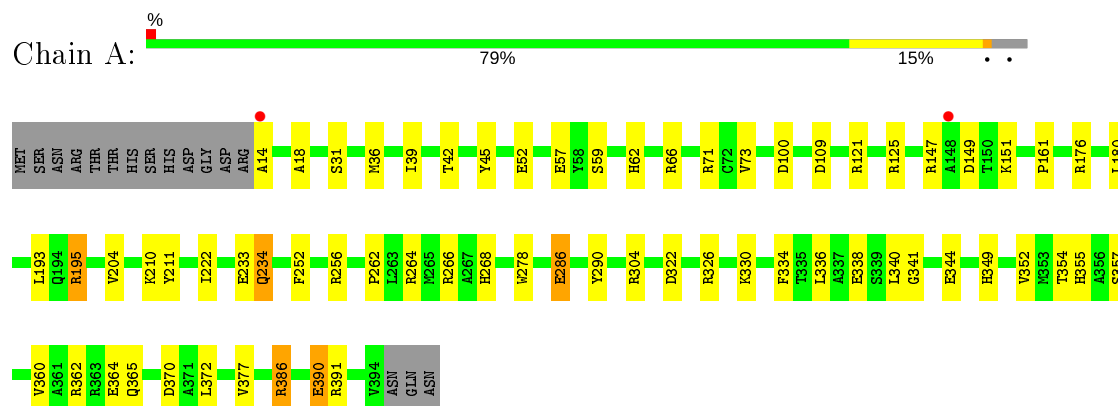
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	346	Total	O	0	0
			346	346		
8	B	389	Total	O	0	0
			389	389		
8	C	332	Total	O	0	0
			332	332		
8	D	361	Total	O	0	0
			361	361		



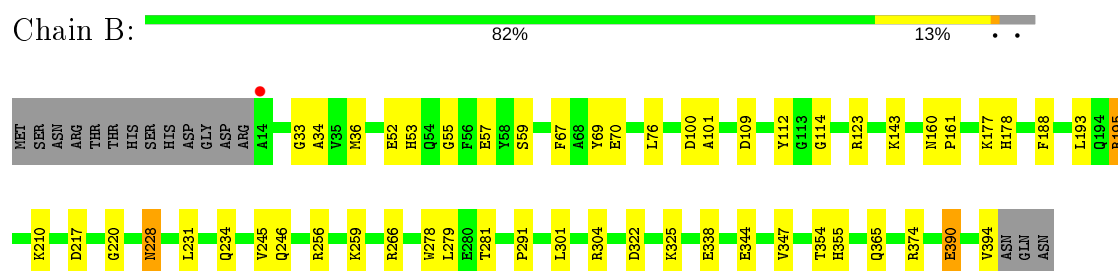
### 3 Residue-property plots

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.

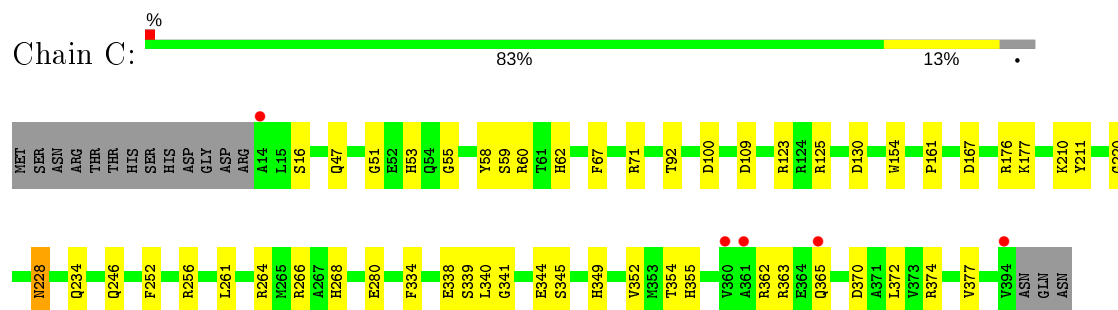
- Molecule 1: Cystathionine gamma-lyase-like protein



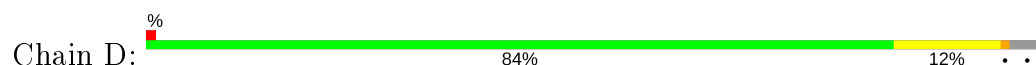
- Molecule 1: Cystathionine gamma-lyase-like protein

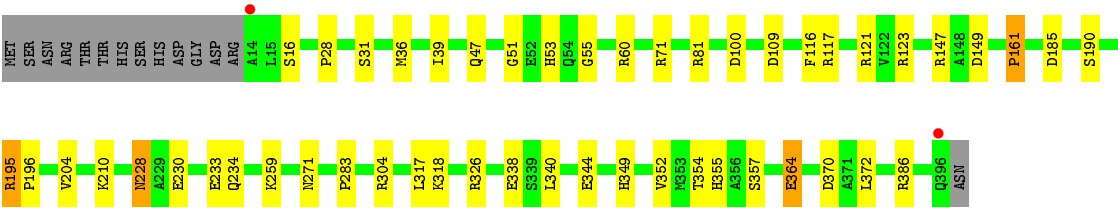


- Molecule 1: Cystathionine gamma-lyase-like protein



- Molecule 1: Cystathionine gamma-lyase-like protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.22Å 86.07Å 226.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.23 – 1.70 30.23 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.23-1.70) 100.0 (30.23-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.134 , 0.169 0.134 , 0.169	Depositor DCC
$R_{free}$ test set	8207 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.7	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	0.97	EDS
Total number of atoms	13157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, OJO, KOU, PYR, SO4

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	1.41	16/2965 (0.5%)	1.26	26/4022 (0.6%)
1	B	1.41	13/2971 (0.4%)	1.21	19/4030 (0.5%)
1	C	1.39	5/2959 (0.2%)	1.17	19/4014 (0.5%)
1	D	1.39	9/3000 (0.3%)	1.20	16/4067 (0.4%)
All	All	1.40	43/11895 (0.4%)	1.21	80/16133 (0.5%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	GLU	CD-OE2	-11.75	1.12	1.25
1	A	233	GLU	CG-CD	9.78	1.66	1.51
1	D	338	GLU	CD-OE1	-8.94	1.15	1.25
1	A	57	GLU	CD-OE1	8.39	1.34	1.25
1	A	344	GLU	CG-CD	7.68	1.63	1.51
1	D	233	GLU	CG-CD	7.39	1.63	1.51
1	C	252	PHE	CE2-CZ	7.15	1.50	1.37
1	A	338	GLU	CD-OE1	-6.91	1.18	1.25
1	A	390	GLU	CG-CD	6.78	1.62	1.51
1	B	390	GLU	CG-CD	6.74	1.62	1.51
1	B	123	ARG	CZ-NH1	6.58	1.41	1.33
1	A	286	GLU	CG-CD	-6.53	1.42	1.51
1	A	57	GLU	CD-OE2	-6.50	1.18	1.25
1	C	338	GLU	CD-OE1	-6.18	1.18	1.25
1	B	188	PHE	CE2-CZ	6.15	1.49	1.37
1	B	347	VAL	CB-CG2	5.89	1.65	1.52
1	A	357	SER	CB-OG	5.79	1.49	1.42
1	D	116	PHE	CD1-CE1	5.77	1.50	1.39
1	B	67	PHE	CD1-CE1	5.77	1.50	1.39
1	B	101	ALA	CA-CB	5.74	1.64	1.52
1	B	259	LYS	CE-NZ	-5.71	1.34	1.49
1	A	290	TYR	CG-CD1	5.68	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	GLU	CD-OE1	5.68	1.31	1.25
1	B	245	VAL	CB-CG2	5.66	1.64	1.52
1	D	233	GLU	CD-OE2	5.63	1.31	1.25
1	A	233	GLU	CB-CG	5.63	1.62	1.52
1	A	233	GLU	CD-OE1	5.59	1.31	1.25
1	D	233	GLU	CD-OE1	5.54	1.31	1.25
1	A	252	PHE	CE2-CZ	5.49	1.47	1.37
1	A	334	PHE	CE1-CZ	5.33	1.47	1.37
1	B	59	SER	CA-CB	5.30	1.60	1.52
1	B	344	GLU	CG-CD	5.26	1.59	1.51
1	B	69	TYR	CD2-CE2	5.23	1.47	1.39
1	C	344	GLU	CD-OE2	5.22	1.31	1.25
1	D	344	GLU	CG-CD	5.18	1.59	1.51
1	C	280	GLU	CB-CG	-5.18	1.42	1.52
1	D	190	SER	CB-OG	5.17	1.49	1.42
1	A	45	TYR	CE2-CZ	5.17	1.45	1.38
1	D	357	SER	CB-OG	5.15	1.49	1.42
1	C	58	TYR	CG-CD2	5.14	1.45	1.39
1	D	364	GLU	CD-OE2	5.13	1.31	1.25
1	A	204	VAL	CB-CG2	5.08	1.63	1.52
1	A	45	TYR	CD2-CE2	5.01	1.46	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	A	66	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	109	ASP	CB-CG-OD1	9.90	127.21	118.30
1	A	121	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	C	109	ASP	CB-CG-OD1	9.54	126.89	118.30
1	D	121	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	A	256	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	193	LEU	CB-CG-CD2	8.80	125.97	111.00
1	A	304	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	C	176	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	B	109	ASP	CB-CG-OD1	8.28	125.75	118.30
1	A	391	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	121	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	B	195[A]	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	195[B]	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	195[A]	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	195[B]	ARG	NE-CZ-NH1	7.79	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	193	LEU	CB-CG-CD2	7.36	123.52	111.00
1	C	264	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	C	374	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	123	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	C	266	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	386	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	C	176	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	372	LEU	CA-CB-CG	6.80	130.93	115.30
1	B	67	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	A	149	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	71	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	B	304	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	176	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	A	176	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	125	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	D	117	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	147	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	286	GLU	OE1-CD-OE2	6.43	131.02	123.30
1	D	60	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	C	67	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	B	374	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	322	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	B	100	ASP	CB-CG-OD1	6.14	123.82	118.30
1	B	325	LYS	CD-CE-NZ	-6.13	97.61	111.70
1	C	123	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	304	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	100	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	167	ASP	CB-CG-OD1	5.91	123.61	118.30
1	C	372	LEU	CB-CG-CD2	-5.85	101.05	111.00
1	B	59	SER	N-CA-CB	5.77	119.16	110.50
1	D	364	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	D	109	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	301	LEU	CB-CG-CD1	5.73	120.75	111.00
1	C	60	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	256	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	256	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	279	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	C	363	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	195[A]	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	195[B]	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	264	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	C	125	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	149	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	176	ARG	CD-NE-CZ	5.32	131.04	123.60
1	A	256	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	121	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	100	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	195[A]	ARG	CD-NE-CZ	5.25	130.95	123.60
1	D	195[B]	ARG	CD-NE-CZ	5.25	130.95	123.60
1	D	81	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	130	ASP	CB-CG-OD1	5.22	123.00	118.30
1	D	71	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	71	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	57	GLU	CG-CD-OE2	-5.08	108.13	118.30
1	C	374	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	261	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	C	100	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	362	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	B	100	ASP	CB-CG-OD2	-5.02	113.79	118.30
1	A	336	LEU	CB-CG-CD2	-5.01	102.49	111.00
1	D	60	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2889	0	2919	40	0
1	B	2892	0	2924	52	0
1	C	2886	0	2914	33	0
1	D	2918	0	2959	38	0
2	A	7	0	4	0	0
2	B	7	0	4	0	0
2	C	7	0	4	0	0
2	D	7	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	16	0	0
4	A	5	0	0	0	0
5	A	21	0	9	3	0
6	B	6	0	3	5	0
6	D	6	0	3	3	0
7	B	22	0	11	11	0
7	C	22	0	11	12	0
7	D	22	0	12	13	0
8	A	346	0	0	14	0
8	B	389	0	0	13	0
8	C	332	0	0	8	0
8	D	361	0	0	12	0
All	All	13157	0	11797	162	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 (162) 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:B:210[A]:LYS:NZ	7:B:403:KOU:C4A	2.20	1.05
1:C:210[A]:LYS:HZ1	7:C:402:KOU:C4A	1.75	0.98
1:C:210[B]:LYS:HZ1	7:C:402:KOU:HA	1.29	0.97
1:D:304:ARG:NH1	8:D:794:HOH:O	1.98	0.95
1:B:53:HIS:HD2	1:B:55:GLY:H	1.11	0.95
1:B:52:GLU:HG3	8:B:799:HOH:O	1.66	0.94
1:B:281:THR:HA	8:B:839:HOH:O	1.67	0.93
1:B:281:THR:HG22	8:B:839:HOH:O	1.67	0.92
6:D:402:PYR:H31	8:D:565:HOH:O	1.68	0.92
1:B:210[A]:LYS:HZ1	7:B:403:KOU:C4A	1.81	0.92
1:D:53:HIS:HD2	1:D:55:GLY:H	1.13	0.91
1:C:53:HIS:HD2	1:C:55:GLY:H	1.16	0.89
1:C:210[A]:LYS:NZ	7:C:402:KOU:C4A	2.35	0.89
1:D:210[A]:LYS:HZ1	7:D:403:KOU:C4A	1.86	0.88
1:A:266:ARG:NH1	8:A:686:HOH:O	2.07	0.88
1:B:210[A]:LYS:HZ1	7:B:403:KOU:H4A	1.36	0.88
1:A:210[B]:LYS:HZ1	5:A:405:OJO:C4A	1.88	0.85
1:B:36:MET:CE	8:D:817:HOH:O	2.24	0.85
1:D:210[A]:LYS:NZ	7:D:403:KOU:C4A	2.40	0.84
1:B:210[A]:LYS:HZ3	7:B:403:KOU:C4A	1.91	0.81
1:A:36:MET:CE	8:C:746:HOH:O	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLY:HA3	1:C:246:GLN:HE22	1.46	0.78
1:B:234:GLN:HA	6:B:402:PYR:H31	1.65	0.76
1:B:195[A]:ARG:CZ	8:B:540:HOH:O	2.34	0.76
1:D:259[B]:LYS:HE2	8:D:682:HOH:O	1.86	0.75
1:B:281:THR:CA	8:B:839:HOH:O	2.26	0.75
1:A:370:ASP:OD1	8:A:716:HOH:O	2.03	0.74
1:C:210[A]:LYS:HZ1	7:C:402:KOU:CA	1.99	0.74
1:A:210[B]:LYS:NZ	5:A:405:OJO:C4A	2.50	0.74
1:C:210[A]:LYS:NZ	7:C:402:KOU:N	2.34	0.72
1:B:394:VAL:HG23	1:B:394:VAL:O	1.88	0.71
1:B:220:GLY:HA3	1:B:246:GLN:HE22	1.56	0.70
1:C:210[B]:LYS:NZ	7:C:402:KOU:HA	2.05	0.70
1:A:14:ALA:N	8:A:845:HOH:O	2.25	0.70
1:B:76:LEU:O	1:B:195[B]:ARG:HD2	1.93	0.69
1:C:71:ARG:NH2	8:C:790:HOH:O	2.21	0.68
1:D:210[A]:LYS:HZ3	7:D:403:KOU:HA	1.59	0.67
1:A:326:ARG:HD3	8:A:784:HOH:O	1.93	0.67
1:B:195[A]:ARG:NE	8:B:540:HOH:O	2.28	0.67
1:B:210[B]:LYS:HE3	7:B:403:KOU:HA	1.78	0.66
1:B:143:LYS:HE3	1:B:178:HIS:HE1	1.60	0.66
1:B:53:HIS:CD2	1:B:55:GLY:H	2.03	0.66
1:D:354:THR:OG1	1:D:355:HIS:HD2	1.80	0.65
1:D:210[A]:LYS:NZ	7:D:403:KOU:HA	2.13	0.64
1:B:354:THR:OG1	1:B:355:HIS:HD2	1.80	0.64
1:B:266:ARG:NH2	8:B:815:HOH:O	2.29	0.63
1:A:268:HIS:HD2	1:A:377:VAL:O	1.80	0.63
1:C:234:GLN:NE2	8:C:763:HOH:O	2.31	0.63
1:C:354:THR:OG1	1:C:355:HIS:HD2	1.81	0.63
1:A:234:GLN:HA	1:A:234:GLN:HE21	1.64	0.62
1:A:354:THR:OG1	1:A:355:HIS:HD2	1.81	0.62
1:D:386:ARG:HD3	8:D:790:HOH:O	2.00	0.60
1:C:349:HIS:HE1	1:C:370:ASP:O	1.84	0.60
1:A:349:HIS:HD2	1:A:352:VAL:H	1.47	0.60
1:A:268:HIS:HE1	8:A:551:HOH:O	1.85	0.60
1:B:36:MET:HE3	8:D:817:HOH:O	1.92	0.60
1:D:53:HIS:HD2	1:D:55:GLY:N	1.94	0.60
1:B:36:MET:HE1	8:D:817:HOH:O	1.94	0.60
1:B:52:GLU:CG	8:B:799:HOH:O	2.38	0.59
1:C:268:HIS:HE1	8:C:536:HOH:O	1.84	0.59
1:C:349:HIS:HD2	1:C:352:VAL:H	1.51	0.59
1:B:234:GLN:HA	6:B:402:PYR:C3	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLN:HE22	1:C:51:GLY:H	1.51	0.58
1:A:36:MET:HE1	8:C:746:HOH:O	1.98	0.58
1:D:349:HIS:HE1	1:D:370:ASP:O	1.86	0.58
1:D:271:ASN:ND2	6:D:402:PYR:O1	2.29	0.58
1:C:210[A]:LYS:HE2	7:C:402:KOU:HA	1.85	0.58
1:A:36:MET:HE3	8:C:746:HOH:O	1.98	0.58
1:A:326:ARG:HG2	8:A:777:HOH:O	2.04	0.57
1:A:266:ARG:NH2	8:A:734:HOH:O	2.35	0.56
1:B:234:GLN:CA	6:B:402:PYR:H31	2.36	0.56
1:B:143:LYS:HE3	1:B:178:HIS:CE1	2.41	0.56
1:D:53:HIS:CD2	1:D:55:GLY:H	2.06	0.56
1:A:362:ARG:HA	1:A:365:GLN:HG2	1.88	0.56
1:B:210[A]:LYS:HE2	7:B:403:KOU:HA	1.88	0.56
1:C:210[A]:LYS:HZ1	7:C:402:KOU:HA	1.71	0.54
1:D:210[A]:LYS:HZ3	7:D:403:KOU:CA	2.20	0.54
1:B:228:ASN:C	1:B:228:ASN:HD22	2.11	0.54
1:D:210[B]:LYS:CE	7:D:403:KOU:HA	2.38	0.53
1:D:210[B]:LYS:HZ1	7:D:403:KOU:HA	1.74	0.53
1:B:210[B]:LYS:CE	7:B:403:KOU:HA	2.39	0.52
1:B:394:VAL:CG2	1:B:394:VAL:O	2.57	0.52
6:D:402:PYR:H33	8:D:610:HOH:O	2.09	0.52
1:D:364:GLU:HG3	8:D:757:HOH:O	2.09	0.51
1:A:52:GLU:HG2	8:A:713:HOH:O	2.11	0.51
1:A:73:VAL:HG11	1:A:222:ILE:HG21	1.93	0.51
1:C:210[A]:LYS:CE	7:C:402:KOU:HA	2.41	0.50
1:D:210[A]:LYS:HZ1	7:D:403:KOU:H4A	1.72	0.50
1:B:278:TRP:HZ2	1:B:390:GLU:HG2	1.76	0.50
1:A:349:HIS:HE1	1:A:370:ASP:O	1.94	0.50
1:B:195[A]:ARG:NH2	8:B:540:HOH:O	2.44	0.50
1:B:234:GLN:CB	6:B:402:PYR:H31	2.42	0.49
1:D:47:GLN:HE22	1:D:51:GLY:H	1.60	0.49
1:A:278:TRP:HZ2	1:A:390:GLU:HG2	1.77	0.49
1:A:386:ARG:NH1	8:A:507:HOH:O	2.27	0.49
1:B:281:THR:CG2	8:B:839:HOH:O	2.38	0.49
1:A:52:GLU:CG	8:A:713:HOH:O	2.61	0.49
1:B:228:ASN:ND2	1:B:231:LEU:H	2.10	0.48
1:C:47:GLN:NE2	1:C:51:GLY:H	2.11	0.48
1:C:268:HIS:HD2	1:C:377:VAL:O	1.95	0.48
1:C:210[A]:LYS:HZ2	7:C:402:KOU:C4A	2.23	0.48
1:D:228:ASN:C	1:D:228:ASN:HD22	2.17	0.48
1:D:210[B]:LYS:HE3	7:D:403:KOU:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210[A]:LYS:CE	7:B:403:KOU:HA	2.43	0.48
1:A:161:PRO:HD3	1:A:355:HIS:CE1	2.49	0.48
1:D:47:GLN:NE2	1:D:51:GLY:H	2.12	0.47
1:B:210[A]:LYS:NZ	7:B:403:KOU:HA	2.29	0.47
8:B:666:HOH:O	1:D:28:PRO:HG3	2.15	0.47
1:D:196:PRO:HB2	1:D:204:VAL:HG22	1.97	0.47
1:D:234:GLN:NE2	8:D:796:HOH:O	2.47	0.47
1:C:59:SER:HA	1:C:62:HIS:O	2.15	0.46
1:B:234:GLN:HG2	6:B:402:PYR:H31	1.97	0.46
1:C:210[B]:LYS:CE	7:C:402:KOU:HA	2.45	0.46
1:A:326:ARG:NE	8:A:841:HOH:O	2.37	0.46
1:A:211:TYR:CE1	1:A:341:GLY:HA2	2.51	0.46
1:A:326:ARG:NH2	1:A:330:LYS:HD2	2.31	0.46
1:B:210[A]:LYS:HZ3	7:B:403:KOU:HA	1.81	0.46
1:C:53:HIS:HD2	1:C:55:GLY:N	1.98	0.46
1:B:112:TYR:CE2	1:B:114:GLY:HA3	2.50	0.45
1:D:326:ARG:NH2	8:D:766:HOH:O	2.48	0.45
1:D:210[A]:LYS:NZ	7:D:403:KOU:N	2.57	0.45
1:A:151:LYS:HE3	8:A:702:HOH:O	2.15	0.45
1:D:283:PRO:O	1:D:318[A]:LYS:HE2	2.16	0.45
1:C:334:PHE:CD2	1:C:345:SER:HB3	2.52	0.45
1:A:42:THR:HA	1:B:217:ASP:HA	1.99	0.45
1:D:195[B]:ARG:NH2	8:D:699:HOH:O	2.32	0.45
1:A:18:ALA:HA	1:A:262:PRO:HG2	1.99	0.45
1:B:161:PRO:HD3	1:B:355:HIS:CE1	2.52	0.45
1:C:210[A]:LYS:NZ	7:C:402:KOU:HA	2.32	0.45
1:B:281:THR:CB	8:B:839:HOH:O	2.54	0.44
1:B:57:GLU:CD	8:B:818:HOH:O	2.55	0.44
1:A:31[B]:SER:HG	1:D:31[B]:SER:HG	1.60	0.44
1:C:228:ASN:C	1:C:228:ASN:HD22	2.19	0.44
1:A:195[B]:ARG:NH2	8:A:796:HOH:O	2.50	0.44
1:B:53:HIS:HD2	1:B:55:GLY:N	1.95	0.43
1:C:53:HIS:CD2	1:C:55:GLY:H	2.09	0.43
1:B:33:GLY:O	1:B:34:ALA:C	2.56	0.43
1:D:210[B]:LYS:NZ	7:D:403:KOU:HA	2.33	0.43
1:B:278:TRP:CZ2	1:B:390:GLU:HG2	2.54	0.43
1:D:349:HIS:HD2	1:D:352:VAL:H	1.67	0.43
1:C:177:LYS:HD3	8:C:713:HOH:O	2.19	0.43
1:B:278:TRP:CZ2	1:B:390:GLU:CG	3.02	0.42
1:A:349:HIS:CD2	1:A:352:VAL:H	2.34	0.42
1:C:161:PRO:HD3	1:C:355:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:O	1:A:364:GLU:HG2	2.20	0.42
1:B:160:ASN:O	1:B:355:HIS:HE1	2.02	0.42
1:D:36:MET:SD	1:D:259[B]:LYS:HE3	2.59	0.42
1:A:39:ILE:HB	1:D:39:ILE:HB	2.02	0.42
1:D:161:PRO:HD3	1:D:355:HIS:CE1	2.55	0.41
1:B:210[A]:LYS:HZ3	7:B:403:KOU:CA	2.33	0.41
1:A:52:GLU:CD	8:A:713:HOH:O	2.58	0.41
1:B:143:LYS:NZ	1:B:177:LYS:HD3	2.36	0.41
1:D:185:ASP:OD2	7:D:403:KOU:N1	2.53	0.41
1:A:210[B]:LYS:HZ1	5:A:405:OJO:CA	2.33	0.41
1:A:59:SER:HA	1:A:62:HIS:O	2.20	0.41
1:C:92:THR:HG23	1:C:154:TRP:CH2	2.56	0.41
1:A:354:THR:OG1	1:A:355:HIS:CD2	2.69	0.41
1:C:16[A]:SER:OG	8:C:503:HOH:O	2.22	0.41
1:D:210[A]:LYS:CE	7:D:403:KOU:HA	2.51	0.40
1:D:230:GLU:O	1:D:234:GLN:HG3	2.21	0.40
1:C:211:TYR:CE1	1:C:341:GLY:HA2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/397 (97%)	376 (98%)	9 (2%)	0	100	100
1	B	386/397 (97%)	376 (97%)	10 (3%)	0	100	100
1	C	384/397 (97%)	373 (97%)	10 (3%)	1 (0%)	41	24
1	D	389/397 (98%)	380 (98%)	9 (2%)	0	100	100
All	All	1544/1588 (97%)	1505 (98%)	38 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	339	SER

### 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	304/313 (97%)	298 (98%)	6 (2%)	55	38
1	B	305/313 (97%)	302 (99%)	3 (1%)	76	67
1	C	303/313 (97%)	300 (99%)	3 (1%)	76	67
1	D	308/313 (98%)	302 (98%)	6 (2%)	57	41
All	All	1220/1252 (97%)	1202 (98%)	18 (2%)	67	51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	234	GLN
1	A	286	GLU
1	A	322	ASP
1	A	340	LEU
1	A	372	LEU
1	B	228	ASN
1	B	291	PRO
1	B	365	GLN
1	C	228	ASN
1	C	340	LEU
1	C	365	GLN
1	D	16[A]	SER
1	D	16[B]	SER
1	D	161	PRO
1	D	228	ASN
1	D	317	LEU
1	D	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
1	A	239	GLN
1	A	240	ASN
1	A	268	HIS
1	A	271	ASN
1	A	349	HIS
1	A	355	HIS
1	B	53	HIS
1	B	178	HIS
1	B	228	ASN
1	B	240	ASN
1	B	246	GLN
1	B	271	ASN
1	B	355	HIS
1	B	365	GLN
1	C	47	GLN
1	C	53	HIS
1	C	228	ASN
1	C	239	GLN
1	C	240	ASN
1	C	246	GLN
1	C	268	HIS
1	C	271	ASN
1	C	349	HIS
1	C	355	HIS
1	D	47	GLN
1	D	53	HIS
1	D	228	ASN
1	D	234	GLN
1	D	240	ASN
1	D	349	HIS
1	D	355	HIS
1	D	396	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

13 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
7	KOU	D	403	-	19,22,22	2.64	6 (31%)	23,31,31	2.42	7 (30%)
6	PYR	B	402	-	2,5,5	3.40	2 (100%)	2,6,6	2.42	1 (50%)
3	GOL	A	402	-	5,5,5	0.78	0	5,5,5	0.40	0
5	0JO	A	405	-	18,21,21	2.74	5 (27%)	21,30,30	1.66	4 (19%)
6	PYR	D	402	-	2,5,5	1.95	1 (50%)	2,6,6	1.14	0
2	SER	C	401	-	3,6,6	1.12	0	1,7,7	0.69	0
4	SO4	A	404	-	4,4,4	0.25	0	6,6,6	0.50	0
2	SER	A	401	-	3,6,6	1.30	0	1,7,7	0.99	0
2	SER	B	401	-	3,6,6	0.80	0	1,7,7	0.15	0
7	KOU	C	402	-	19,22,22	2.62	8 (42%)	23,31,31	2.39	6 (26%)
2	SER	D	401	-	3,6,6	1.14	0	1,7,7	0.93	0
7	KOU	B	403	-	19,22,22	2.50	5 (26%)	23,31,31	1.77	5 (21%)
3	GOL	A	403	-	5,5,5	0.91	0	5,5,5	1.85	1 (20%)

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	KOU	D	403	-	-	4/13/17/17	0/1/1/1
6	PYR	B	402	-	-	0/0/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
5	0JO	A	405	-	-	0/9/15/15	0/1/1/1
6	PYR	D	402	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SER	C	401	-	-	0/2/6/6	-
2	SER	A	401	-	-	0/2/6/6	-
2	SER	B	401	-	-	0/2/6/6	-
7	KOU	C	402	-	-	4/13/17/17	0/1/1/1
2	SER	D	401	-	-	0/2/6/6	-
7	KOU	B	403	-	-	5/13/17/17	0/1/1/1
3	GOL	A	403	-	-	3/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	403	KOU	C3-C2	6.70	1.47	1.40
5	A	405	OJO	C3-C2	5.78	1.46	1.40
5	A	405	OJO	C4-C5	5.75	1.49	1.42
7	C	402	KOU	C3-C2	5.74	1.46	1.40
7	B	403	KOU	C4-C3	5.55	1.49	1.40
7	C	402	KOU	C4-C3	5.47	1.49	1.40
5	A	405	OJO	C4A-N	5.42	1.35	1.28
7	B	403	KOU	C4-C5	5.06	1.48	1.42
7	D	403	KOU	C4-C3	5.03	1.48	1.40
7	B	403	KOU	C4A-N	4.86	1.36	1.27
7	D	403	KOU	C4A-N	4.56	1.35	1.27
7	B	403	KOU	C3-C2	4.49	1.45	1.40
5	A	405	OJO	C4-C3	4.45	1.47	1.40
7	C	402	KOU	C4-C5	4.32	1.47	1.42
6	B	402	PYR	O3-C2	4.22	1.35	1.22
7	C	402	KOU	C4A-N	3.89	1.34	1.27
7	D	403	KOU	C4-C5	3.65	1.46	1.42
7	D	403	KOU	C4-C4A	3.15	1.52	1.46
5	A	405	OJO	C4-C4A	2.91	1.52	1.46
7	C	402	KOU	CA-N	2.76	1.49	1.46
6	D	402	PYR	O3-C2	2.76	1.31	1.22
7	D	403	KOU	C2A-C2	2.33	1.54	1.50
6	B	402	PYR	C3-C2	-2.31	1.42	1.49
7	C	402	KOU	P-O2P	-2.20	1.46	1.54
7	C	402	KOU	C2A-C2	2.19	1.54	1.50
7	C	402	KOU	C5A-C5	2.16	1.56	1.50
7	B	403	KOU	C4-C4A	2.01	1.50	1.46

All (24) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	402	KOU	CA-N-C4A	8.08	128.36	117.40
7	D	403	KOU	C3-C4-C5	-6.29	113.43	118.26
7	B	403	KOU	C3-C4-C5	-5.44	114.09	118.26
7	D	403	KOU	C2A-C2-C3	-5.11	114.58	120.89
5	A	405	OJO	C3-C4-C5	-4.69	114.66	118.26
7	D	403	KOU	C5-C4-C4A	4.54	129.03	121.56
7	D	403	KOU	CA-N-C4A	3.97	122.78	117.40
3	A	403	GOL	C3-C2-C1	-3.87	96.66	111.70
7	C	402	KOU	C3-C4-C5	-3.45	115.61	118.26
7	B	403	KOU	C5-C4-C4A	3.34	127.06	121.56
7	B	403	KOU	C4-C4A-N	-3.16	115.99	123.01
7	D	403	KOU	C2A-C2-N1	3.09	123.71	117.67
6	B	402	PYR	O3-C2-C3	-2.97	113.48	120.17
7	C	402	KOU	O4P-C5A-C5	-2.80	104.01	109.35
7	C	402	KOU	O1P-P-O4P	-2.67	99.64	106.73
5	A	405	OJO	C4-C4A-N	-2.52	117.08	123.19
7	B	403	KOU	OG-CB-CA	-2.36	99.40	111.09
7	C	402	KOU	C6-N1-C2	2.27	123.37	119.17
5	A	405	OJO	OP4-P-OP3	-2.21	100.28	106.47
5	A	405	OJO	C4-C3-C2	-2.17	118.84	120.19
7	D	403	KOU	OG-CB-CA	-2.14	100.50	111.09
7	D	403	KOU	C6-C5-C4	2.11	122.04	118.15
7	B	403	KOU	O1P-P-O4P	-2.03	101.33	106.73
7	C	402	KOU	C5-C6-N1	-2.02	120.46	123.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	403	KOU	C-CA-N-C4A
7	D	403	KOU	CB-CA-N-C4A
7	D	403	KOU	N-CA-CB-OG
7	C	402	KOU	C-CA-N-C4A
7	C	402	KOU	CB-CA-N-C4A
7	C	402	KOU	C-CA-CB-OG
7	C	402	KOU	N-CA-CB-OG
7	B	403	KOU	CB-CA-N-C4A
7	B	403	KOU	C-CA-CB-OG
7	B	403	KOU	N-CA-CB-OG
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-O2
7	B	403	KOU	C-CA-N-C4A
7	D	403	KOU	C-CA-CB-OG

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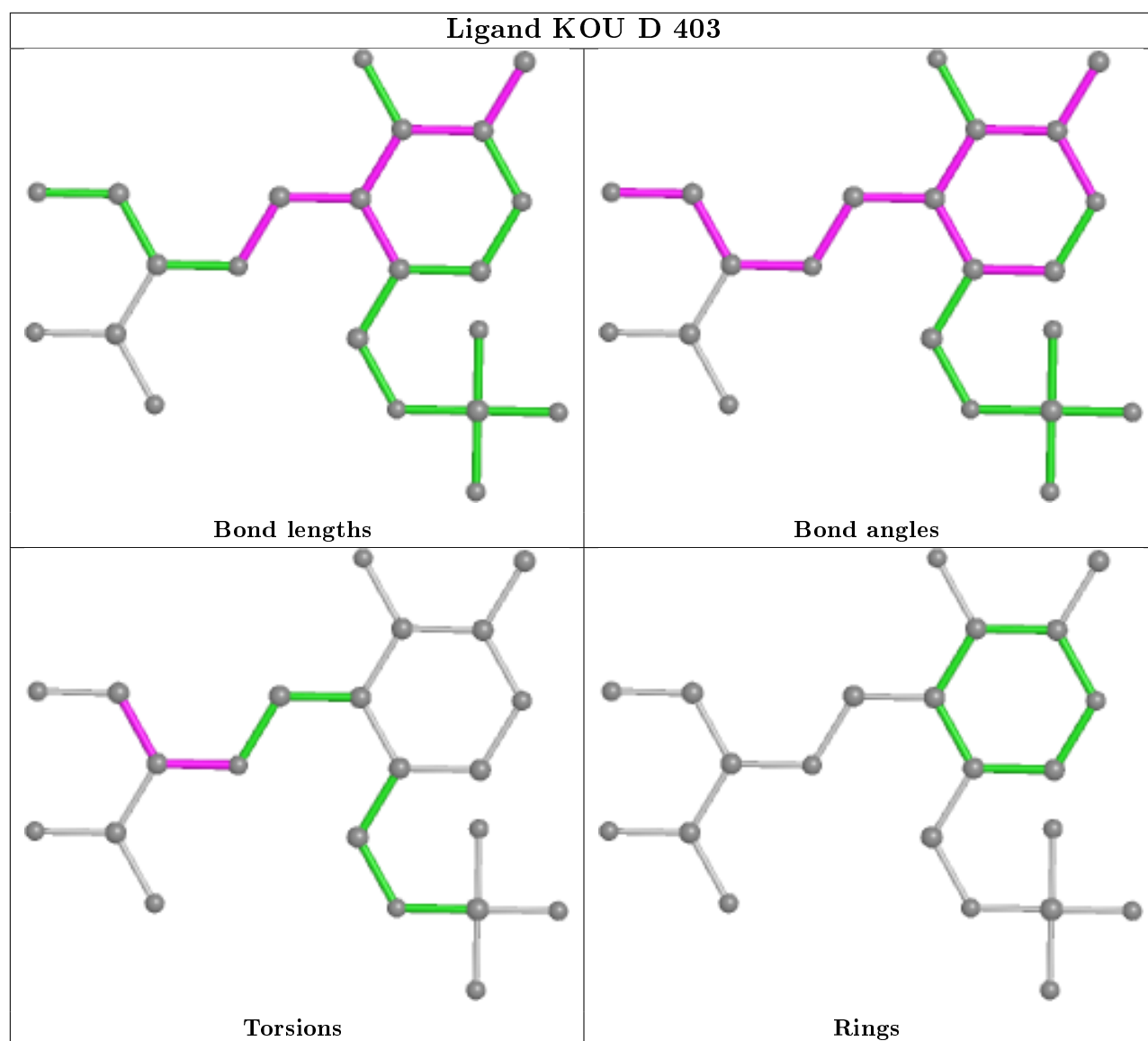
Mol	Chain	Res	Type	Atoms
3	A	403	GOL	C1-C2-C3-O3
7	B	403	KOU	C3-C4-C4A-N

There are no ring outliers.

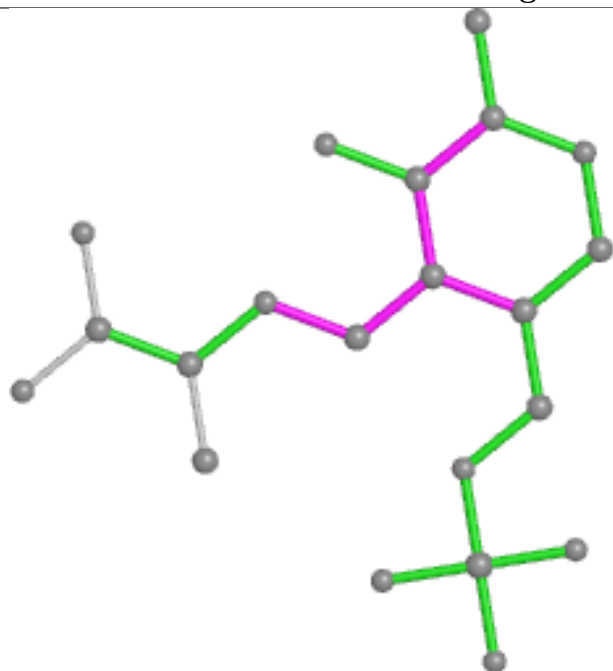
6 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	403	KOU	13	0
6	B	402	PYR	5	0
5	A	405	OJO	3	0
6	D	402	PYR	3	0
7	C	402	KOU	12	0
7	B	403	KOU	11	0

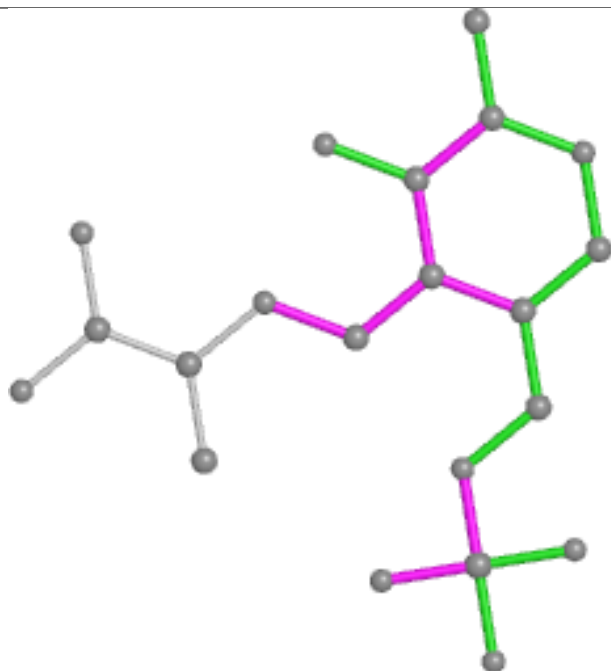
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



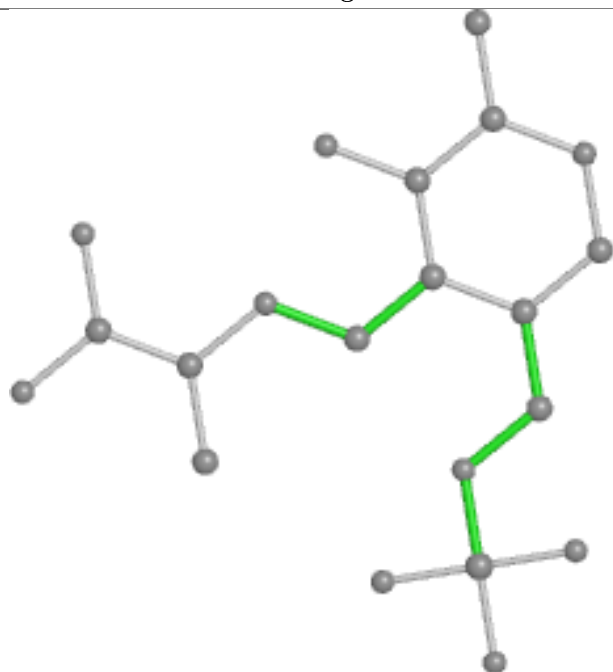
## Ligand 0JO A 405



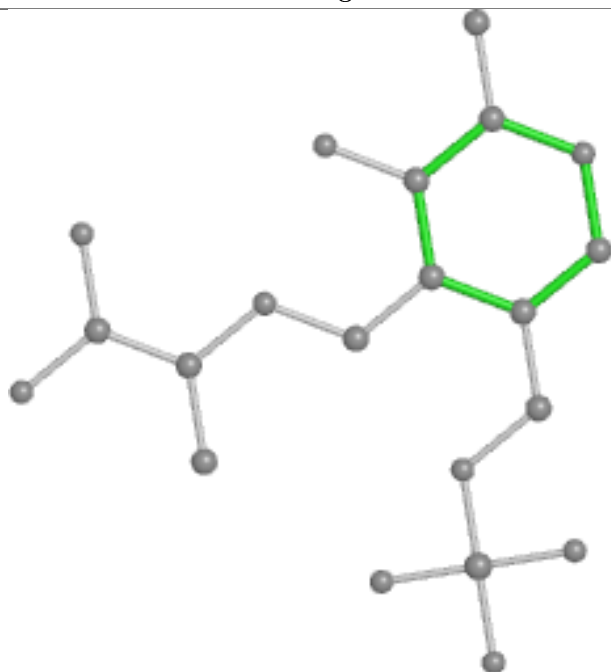
Bond lengths



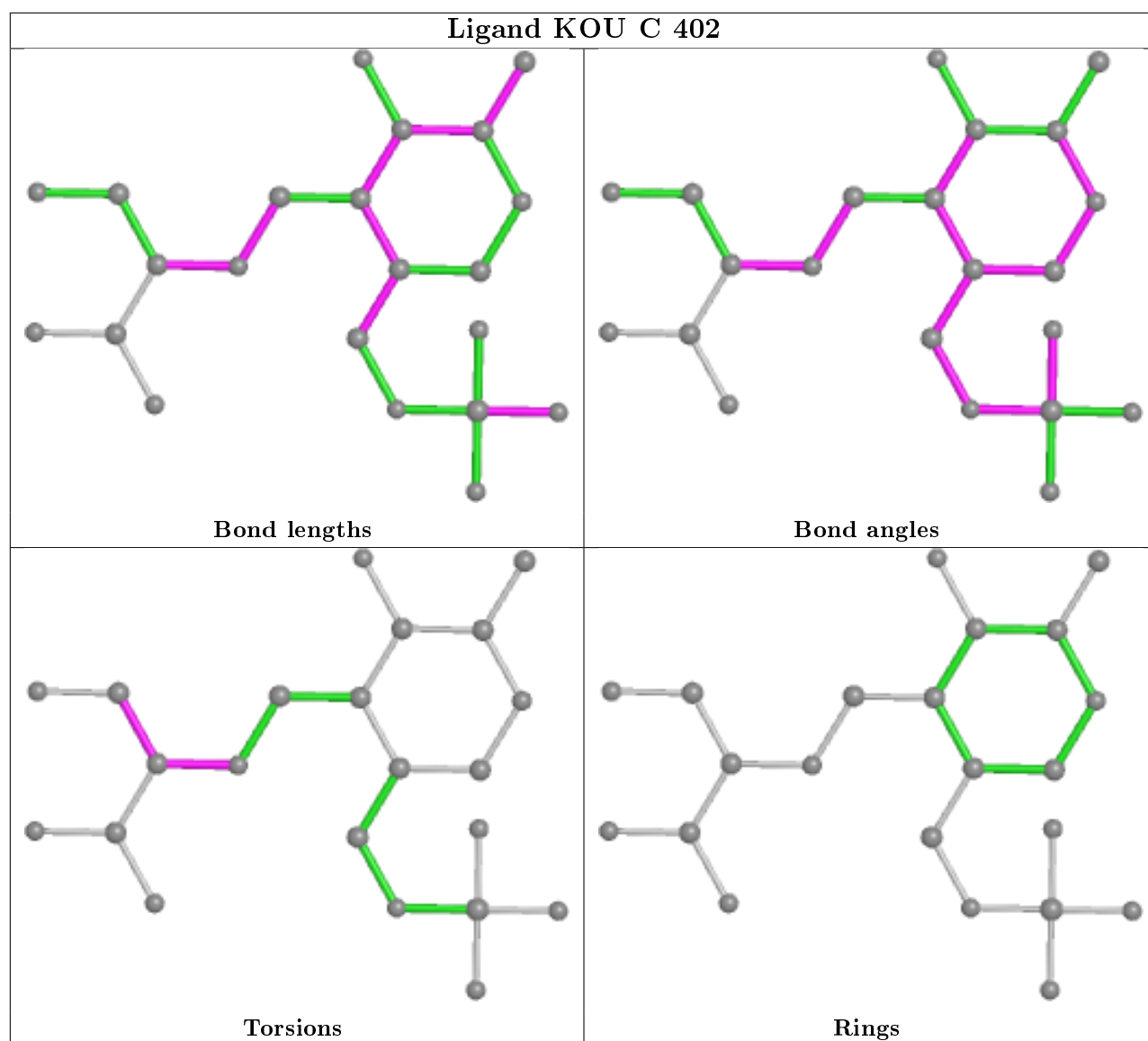
Bond angles

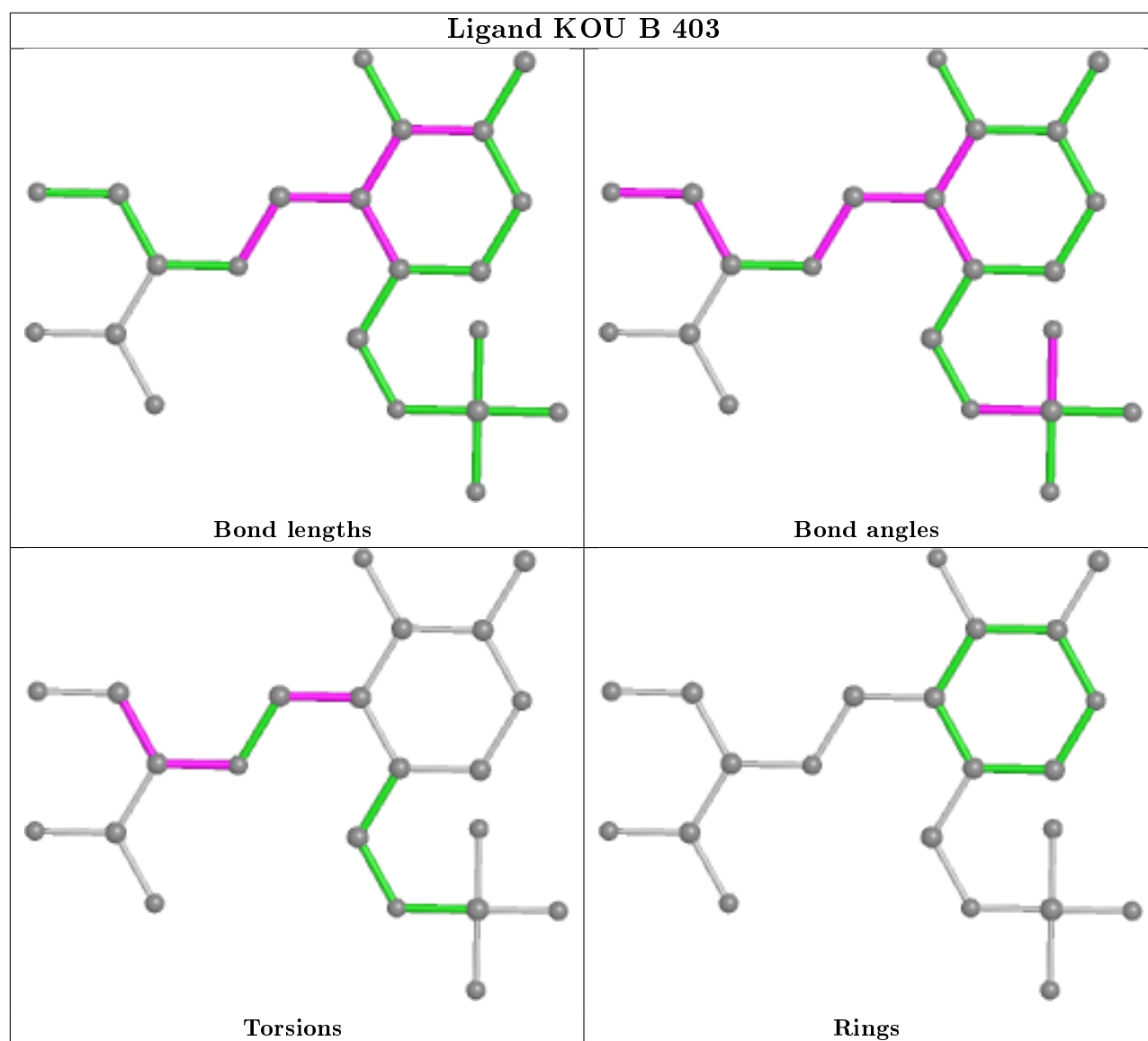


Torsions



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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	381/397 (95%)	-0.52	2 (0%) 91 92	7, 12, 24, 35	0
1	B	381/397 (95%)	-0.58	1 (0%) 94 94	7, 11, 22, 33	0
1	C	381/397 (95%)	-0.32	5 (1%) 77 81	7, 14, 28, 36	0
1	D	383/397 (96%)	-0.50	2 (0%) 91 92	8, 12, 23, 39	0
All	All	1526/1588 (96%)	-0.48	10 (0%) 87 90	7, 12, 25, 39	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	ALA	5.3
1	A	14	ALA	4.4
1	C	394	VAL	4.2
1	D	14	ALA	4.0
1	C	14	ALA	3.4
1	D	396	GLN	3.3
1	C	361	ALA	2.5
1	C	360	VAL	2.5
1	A	148	ALA	2.3
1	C	365	GLN	2.2

### 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

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.

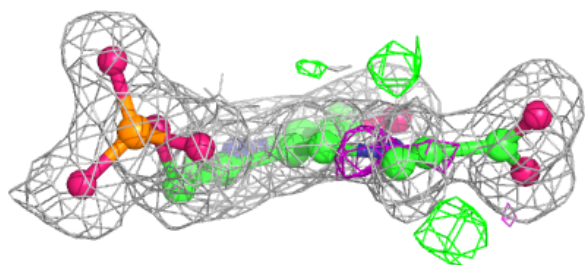
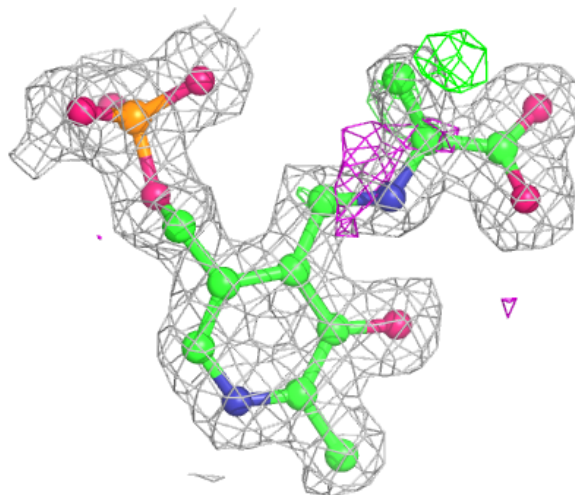
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PYR	D	402	6/6	0.85	0.21	25,28,32,34	0
3	GOL	A	403	6/6	0.85	0.11	28,33,35,39	0
6	PYR	B	402	6/6	0.90	0.15	13,25,31,35	0
2	SER	A	401	7/7	0.95	0.09	19,22,23,26	0
2	SER	C	401	7/7	0.95	0.07	18,20,21,24	0
2	SER	B	401	7/7	0.97	0.05	14,16,17,21	0
2	SER	D	401	7/7	0.97	0.06	17,19,21,21	0
3	GOL	A	402	6/6	0.97	0.06	13,14,17,17	0
5	OJO	A	405	21/21	0.98	0.07	7,12,18,20	0
7	KOU	C	402	22/22	0.98	0.10	8,17,25,33	0
4	SO4	A	404	5/5	0.98	0.17	30,38,42,46	0
7	KOU	B	403	22/22	0.98	0.08	9,13,20,29	0
7	KOU	D	403	22/22	0.98	0.09	9,14,19,29	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.



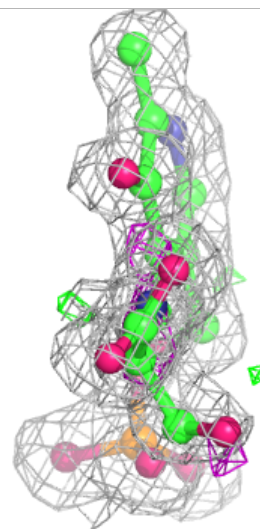
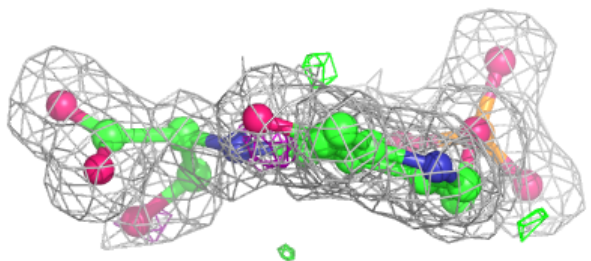
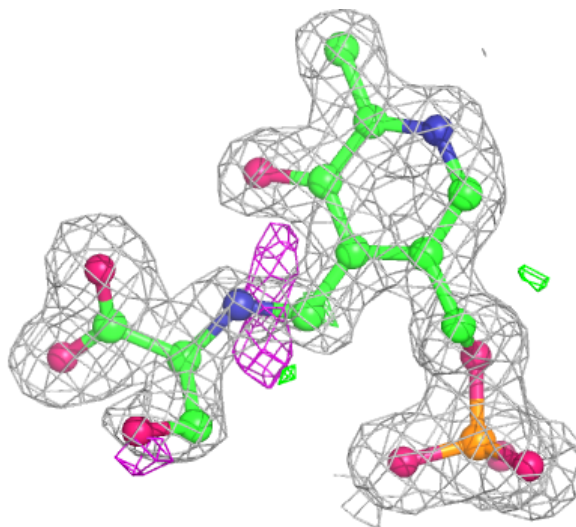
**Electron density around 0JO A 405:**

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



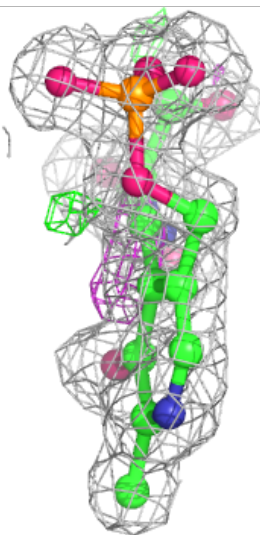
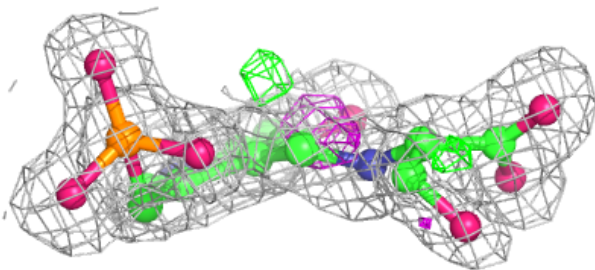
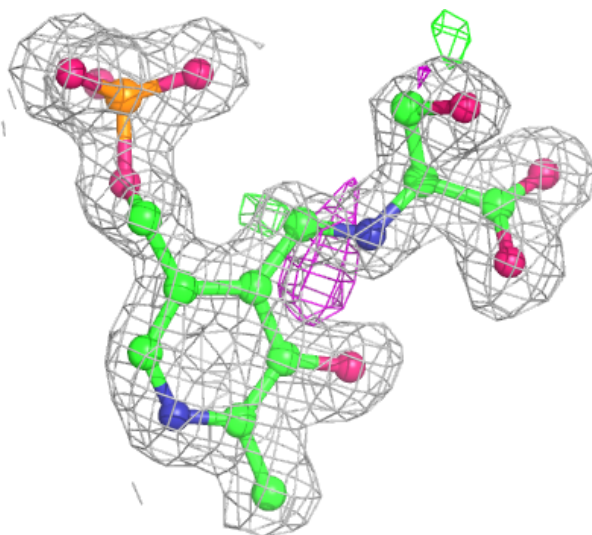
**Electron density around KOU C 402:**

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



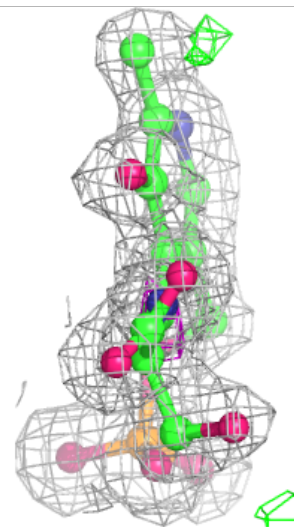
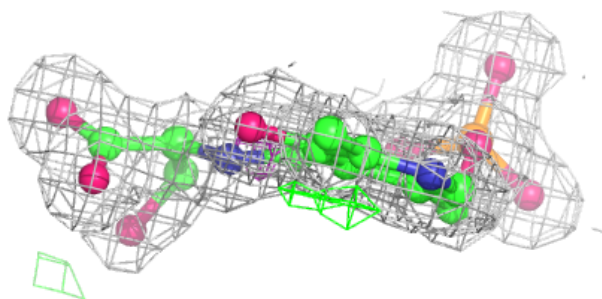
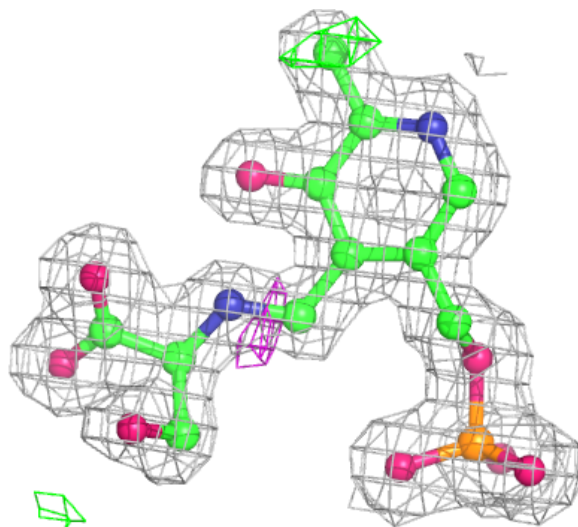
**Electron density around KOU B 403:**

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



**Electron density around KOU D 403:**

$2mF_o-DF_c$  (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.