



## Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 09:54 AM EST

PDB ID : 4IYO  
Title : Crystal structure of cystathionine gamma lyase from *Xanthomonas oryzae* pv. *oryzae* (XometC) in complex with E-site serine, A-site serine, A-site external aldimine structure with aminoacrylate and A-site iminopropionate intermediates  
Authors : Ngo, H.P.T.; Kim, J.K.; Kang, L.W.  
Deposited on : 2013-01-29  
Resolution : 1.80 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

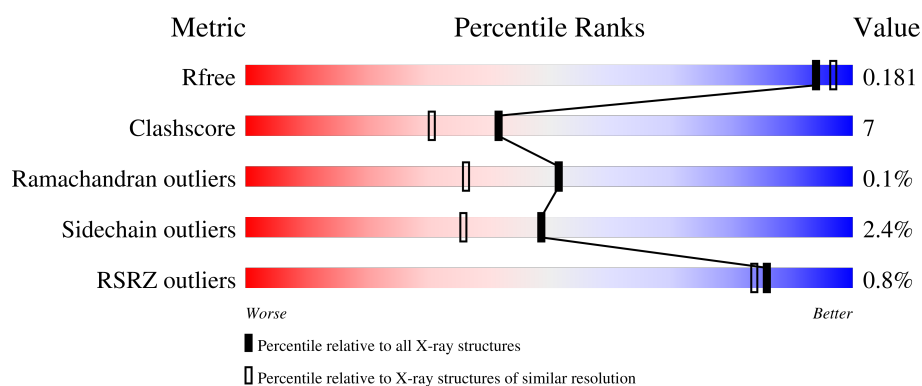
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	397	 79% 15% . .
2	B	397	 82% 12% . .
2	C	397	 2% 82% 12% . .
2	D	397	 % 84% 10% . .

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
3	SER	D	402	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13006 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.

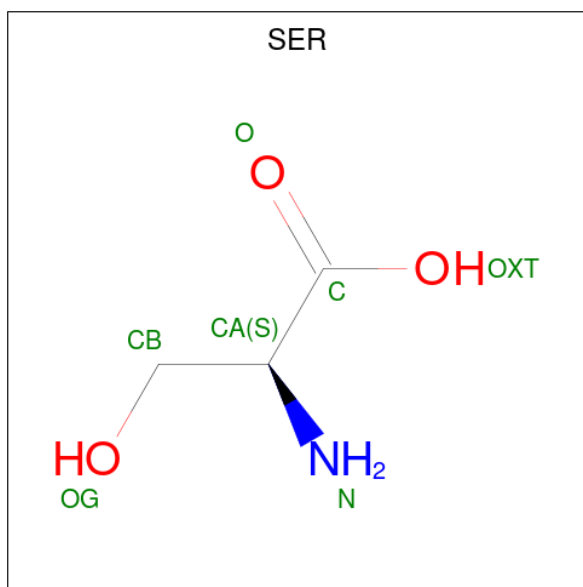
- Molecule 1 is a protein called Cystathionine gamma-lyase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2881	1825	506	535	15	0	5	0

- Molecule 2 is a protein called Cystathionine gamma-lyase-like protein, LYS201A modified.

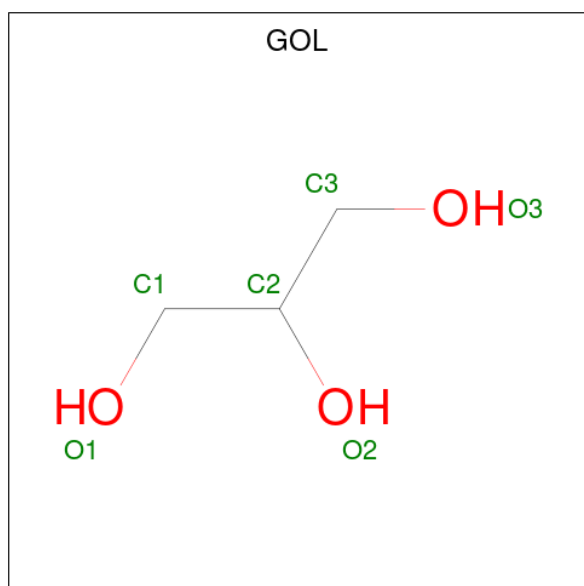
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	381	2890	1828	506	540	1	15	0	4	0
2	C	381	2890	1828	506	540	1	15	0	4	0
2	D	384	2924	1846	515	547	1	15	0	5	0

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			7	3	1	3		
3	B	1	Total	C	N	O	0	0
			7	3	1	3		
3	C	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



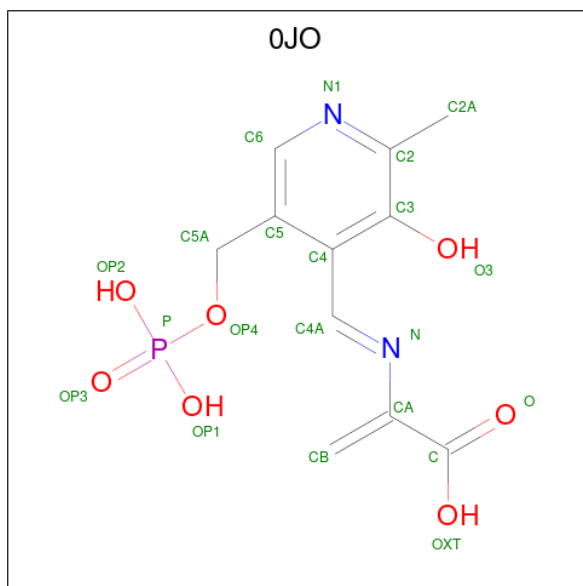
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



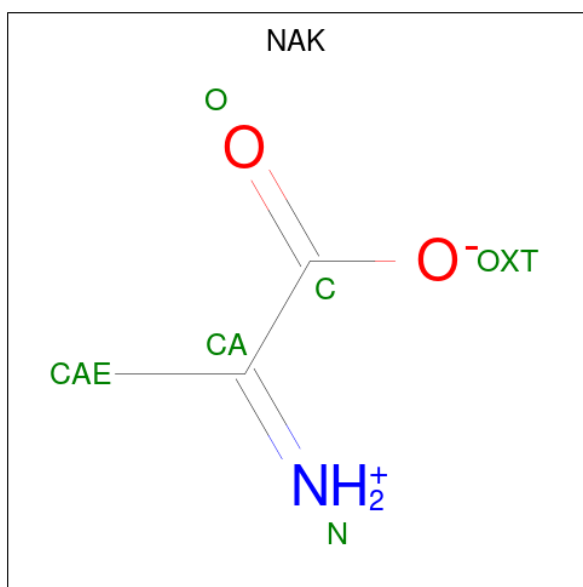
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	O	S			
			5	4	1	0	0	

- Molecule 6 is 2-[(E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (three-letter code: 0JO) (formula:  $C_{11}H_{13}N_2O_7P$ ).



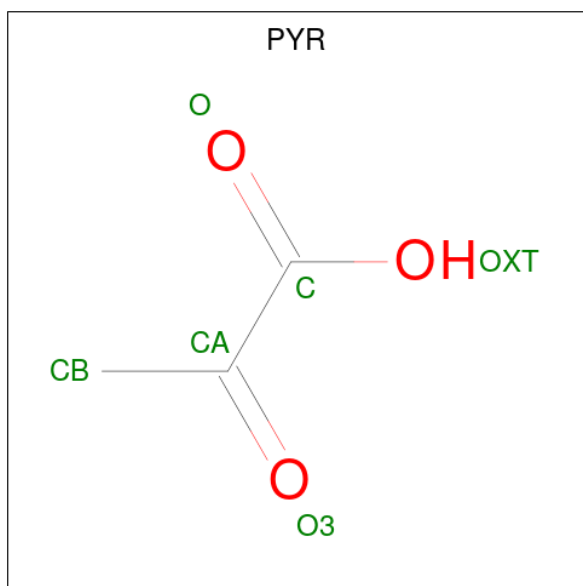
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P		
			21	11	2	7	1	0	

- Molecule 7 is AMINO-ACRYLATE (three-letter code: NAK) (formula:  $C_3H_5NO_2$ ).



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

- Molecule 8 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



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

- Molecule 9 is water.

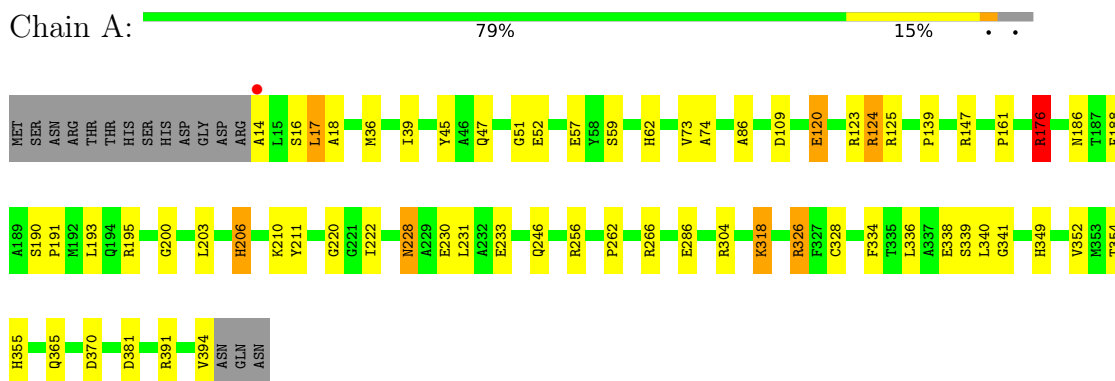


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	324	Total 324	O 324	0	0
9	B	365	Total 365	O 365	0	0
9	C	300	Total 300	O 300	0	0
9	D	335	Total 335	O 335	0	0

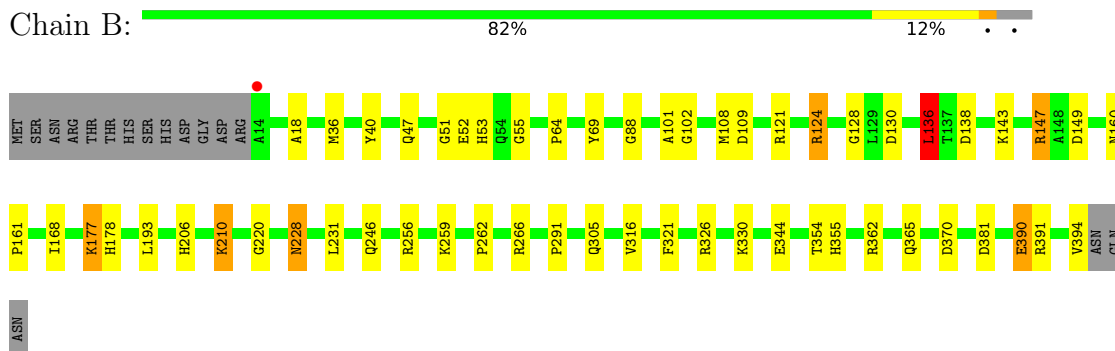
### 3 Residue-property plots [i](#)

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

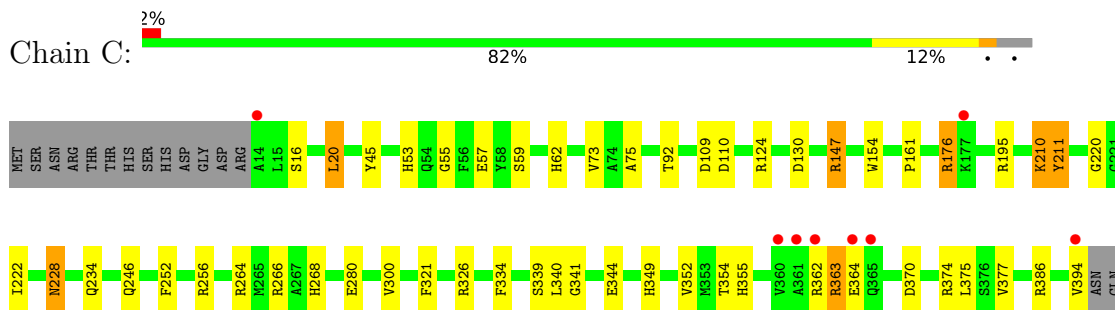
- Molecule 1: Cystathionine gamma-lyase-like protein



- Molecule 2: Cystathionine gamma-lyase-like protein, LYS201A modified




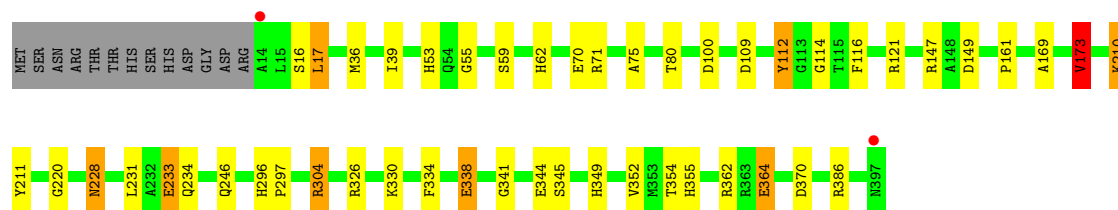
- Molecule 2: Cystathionine gamma-lyase-like protein, LYS201A modified



ASN

- Molecule 2: Cystathionine gamma-lyase-like protein, LYS201A modified

Chain D:  %



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.32Å 86.34Å 226.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.82 – 1.80 33.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.82-1.80) 100.0 (33.82-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.136 , 0.180 0.137 , 0.181	Depositor DCC
$R_{free}$ test set	6971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAK, LLP, SO4, GOL, PYR, OJO

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	1.32	12/2954 (0.4%)	1.15	16/4007 (0.4%)
2	B	1.32	7/2935 (0.2%)	1.07	8/3982 (0.2%)
2	C	1.34	10/2935 (0.3%)	1.09	13/3982 (0.3%)
2	D	1.29	10/2972 (0.3%)	1.09	11/4031 (0.3%)
All	All	1.32	39/11796 (0.3%)	1.10	48/16002 (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
2	B	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	233	GLU	CG-CD	7.50	1.63	1.51
2	D	364	GLU	CD-OE2	6.79	1.33	1.25
2	D	70	GLU	CB-CG	6.50	1.64	1.52
2	B	69	TYR	CD2-CE2	6.46	1.49	1.39
2	C	344	GLU	CG-CD	6.38	1.61	1.51
2	C	176	ARG	CZ-NH1	6.13	1.41	1.33
1	A	120	GLU	CG-CD	6.12	1.61	1.51
2	D	116	PHE	CD1-CE1	6.00	1.51	1.39
2	D	112	TYR	CD1-CE1	5.80	1.48	1.39
2	B	344	GLU	CG-CD	5.77	1.60	1.51
2	C	252	PHE	CE2-CZ	5.77	1.48	1.37
1	A	233	GLU	CG-CD	5.71	1.60	1.51
2	D	338	GLU	CD-OE1	-5.71	1.19	1.25
2	C	280	GLU	CB-CG	-5.66	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	316	VAL	CB-CG2	-5.62	1.41	1.52
2	C	211	TYR	CD1-CE1	5.60	1.47	1.39
2	C	394	VAL	CB-CG1	5.55	1.64	1.52
1	A	45	TYR	CD1-CE1	5.48	1.47	1.39
1	A	328	CYS	CB-SG	-5.40	1.73	1.81
1	A	74	ALA	CA-CB	5.34	1.63	1.52
2	C	45	TYR	CD1-CE1	5.33	1.47	1.39
1	A	334	PHE	CD2-CE2	5.27	1.49	1.39
2	D	75	ALA	CA-CB	5.23	1.63	1.52
2	D	80	THR	CB-CG2	5.23	1.69	1.52
2	D	338	GLU	CG-CD	5.22	1.59	1.51
1	A	394	VAL	CB-CG1	5.21	1.63	1.52
2	C	75	ALA	CA-CB	5.20	1.63	1.52
2	C	364	GLU	CG-CD	5.18	1.59	1.51
1	A	334	PHE	CE1-CZ	5.16	1.47	1.37
2	B	101	ALA	CA-CB	5.14	1.63	1.52
1	A	57	GLU	CD-OE2	-5.13	1.20	1.25
2	B	390	GLU	CG-CD	5.13	1.59	1.51
2	D	344	GLU	CG-CD	5.08	1.59	1.51
1	A	334	PHE	CD1-CE1	5.08	1.49	1.39
2	B	88	GLY	N-CA	5.08	1.53	1.46
2	B	69	TYR	CD1-CE1	5.04	1.47	1.39
1	A	188	PHE	CE1-CZ	5.04	1.47	1.37
2	C	334	PHE	CD1-CE1	5.02	1.49	1.39
1	A	86	ALA	CA-CB	5.01	1.62	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	-12.59	114.00	120.30
2	B	121	ARG	NE-CZ-NH2	-10.16	115.22	120.30
2	C	363	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	176	ARG	NE-CZ-NH2	9.94	125.27	120.30
2	C	176	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	C	176	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	304	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	D	109	ASP	CB-CG-OD1	8.31	125.78	118.30
2	C	363	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	109	ASP	CB-CG-OD1	7.71	125.24	118.30
2	D	100	ASP	CB-CG-OD1	7.46	125.02	118.30
2	D	362	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	304	ARG	NE-CZ-NH2	-7.27	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	LEU	CB-CG-CD1	7.26	123.33	111.00
1	A	193	LEU	CB-CG-CD2	7.16	123.18	111.00
1	A	147	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	D	121	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	17	LEU	CB-CG-CD1	6.93	122.78	111.00
2	D	304	ARG	NE-CZ-NH2	-6.89	116.85	120.30
2	C	374	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	125	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	318	LYS	CD-CE-NZ	-6.70	96.30	111.70
2	D	149	ASP	CB-CG-OD1	6.67	124.30	118.30
2	C	20	LEU	CB-CG-CD1	6.56	122.15	111.00
2	D	304	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	256	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	D	17	LEU	CB-CG-CD1	6.36	121.82	111.00
2	C	109	ASP	CB-CG-OD1	6.28	123.95	118.30
2	C	266	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	123	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	C	264	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	B	193	LEU	CB-CG-CD2	5.90	121.02	111.00
2	B	109	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	391	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	C	264	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	C	256	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	336	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	A	256	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	391	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	D	121	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	B	256	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	D	147	ARG	CB-CG-CD	-5.16	98.18	111.60
1	A	206	HIS	CB-CA-C	-5.11	100.19	110.40
2	B	362	ARG	NE-CZ-NH1	-5.11	117.75	120.30
2	B	138	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	D	173	VAL	CG1-CB-CG2	5.04	118.97	110.90
2	C	375	LEU	CB-CG-CD1	-5.03	102.45	111.00
2	C	110	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	206	HIS	Peptide

## 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	2881	0	2906	48	0
2	B	2890	0	2896	45	0
2	C	2890	0	2897	31	0
2	D	2924	0	2929	38	0
3	A	7	0	4	2	0
3	B	7	0	4	0	0
3	C	7	0	4	0	0
3	D	14	0	8	9	0
4	A	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	3	0
5	A	5	0	0	0	0
6	A	21	0	9	4	0
7	B	6	0	0	2	0
7	C	6	0	0	2	0
8	B	6	0	0	0	0
9	A	324	0	0	11	0
9	B	365	0	0	7	0
9	C	300	0	0	15	0
9	D	335	0	0	15	0
All	All	13006	0	11681	163	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 (163) 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:A:124:ARG:NH1	1:A:124:ARG:HB3	1.30	1.38
1:A:370:ASP:HB2	9:A:775:HOH:O	1.19	1.36
1:A:124:ARG:HH11	1:A:124:ARG:CB	1.38	1.36
2:D:210:LLP:C4'	3:D:402:SER:N	1.96	1.28
2:C:210:LLP:C4'	7:C:402:NAK:N	2.02	1.21
2:B:210:LLP:C4'	7:B:402:NAK:N	2.15	1.09
2:C:210:LLP:H4'1	7:C:402:NAK:N	1.70	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:364:GLU:OE1	9:D:738:HOH:O	1.80	0.98
2:D:210:LLP:H4'1	3:D:402:SER:N	1.78	0.96
2:C:53:HIS:HD2	2:C:55:GLY:H	1.15	0.94
2:B:210:LLP:H4'1	7:B:402:NAK:N	1.83	0.93
2:B:52:GLU:HG3	9:B:730:HOH:O	1.69	0.92
2:D:53:HIS:HD2	2:D:55:GLY:H	1.17	0.91
1:A:124:ARG:HB3	1:A:124:ARG:HH11	0.74	0.90
2:B:124:ARG:HB2	2:B:124:ARG:HH21	1.37	0.90
2:D:210:LLP:HE3	3:D:402:SER:HA	1.53	0.90
2:B:53:HIS:HD2	2:B:55:GLY:H	1.10	0.89
1:A:52:GLU:HG2	9:A:670:HOH:O	1.72	0.89
2:C:362:ARG:HD3	9:C:526:HOH:O	1.73	0.87
1:A:124:ARG:HH11	1:A:124:ARG:CG	1.87	0.87
2:B:266:ARG:NH1	9:B:847:HOH:O	2.07	0.87
2:B:168:ILE:H	2:B:305:GLN:HE22	1.24	0.86
2:B:143:LYS:HE3	2:B:178:HIS:HE1	1.40	0.84
2:C:386:ARG:HD3	9:C:646:HOH:O	1.77	0.83
2:B:326:ARG:HE	2:B:330:LYS:HD2	1.47	0.80
2:D:220:GLY:HA3	2:D:246:GLN:HE22	1.46	0.80
2:C:124:ARG:HD2	9:C:627:HOH:O	1.79	0.80
4:D:403:GOL:H32	9:D:522:HOH:O	1.81	0.80
1:A:326:ARG:HH11	1:A:326:ARG:HG3	1.47	0.78
1:A:36:MET:HE1	9:A:816:HOH:O	1.82	0.78
1:A:338:GLU:OE1	3:A:401:SER:HB3	1.84	0.77
2:D:210:LLP:CE	3:D:402:SER:HA	2.15	0.77
2:B:147:ARG:NH1	2:B:149:ASP:OD2	2.18	0.77
4:D:403:GOL:H2	9:D:749:HOH:O	1.85	0.76
1:A:124:ARG:NH1	1:A:124:ARG:CB	2.15	0.76
4:C:403:GOL:H12	9:C:568:HOH:O	1.85	0.76
1:A:210[B]:LYS:HZ1	6:A:404:OJO:C4A	2.01	0.74
1:A:370:ASP:OD1	9:A:743:HOH:O	2.05	0.74
2:C:220:GLY:HA3	2:C:246:GLN:HE22	1.53	0.73
1:A:220:GLY:HA3	1:A:246:GLN:HE22	1.54	0.72
2:B:124:ARG:HH21	2:B:124:ARG:CB	2.01	0.72
1:A:36:MET:HE1	9:C:676:HOH:O	1.90	0.71
1:A:266:ARG:NH1	9:A:675:HOH:O	2.24	0.71
2:B:220:GLY:HA3	2:B:246:GLN:HE22	1.57	0.70
2:C:363:ARG:NH2	9:C:723:HOH:O	2.24	0.69
2:B:143:LYS:HE3	2:B:178:HIS:CE1	2.26	0.68
2:B:266:ARG:NH2	9:B:829:HOH:O	2.19	0.67
2:B:53:HIS:CD2	2:B:55:GLY:H	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:NH1	9:B:865:HOH:O	2.27	0.67
1:A:210[B]:LYS:HZ1	6:A:404:OJO:CA	2.08	0.66
1:A:210[B]:LYS:NZ	6:A:404:OJO:C4A	2.58	0.66
2:D:354:THR:OG1	2:D:355:HIS:HD2	1.78	0.66
2:B:36:MET:HE1	9:D:719:HOH:O	1.95	0.66
2:B:259:LYS:HE3	9:D:569:HOH:O	1.94	0.66
1:A:354:THR:OG1	1:A:355:HIS:HD2	1.80	0.63
2:D:210:LLP:C4'	3:D:402:SER:CA	2.77	0.63
2:C:268:HIS:HE1	9:C:560:HOH:O	1.81	0.63
1:A:52:GLU:CG	9:A:670:HOH:O	2.38	0.62
2:B:47:GLN:HE22	2:B:51:GLY:H	1.48	0.61
1:A:14:ALA:N	9:A:821:HOH:O	2.31	0.61
2:B:354:THR:OG1	2:B:355:HIS:HD2	1.84	0.61
2:B:381:ASP:HB2	2:D:16[A]:SER:OG	2.00	0.61
2:B:326:ARG:HD2	9:B:693:HOH:O	2.01	0.60
9:B:760:HOH:O	2:D:36:MET:HE3	2.00	0.60
2:B:47:GLN:NE2	2:B:51:GLY:H	1.99	0.59
2:D:53:HIS:CD2	2:D:55:GLY:H	2.09	0.58
1:A:266:ARG:NH2	9:A:813:HOH:O	2.21	0.58
2:D:36:MET:HE3	9:D:812:HOH:O	2.04	0.58
2:B:147:ARG:HH12	2:B:149:ASP:CG	2.08	0.57
2:D:71:ARG:HG3	4:D:403:GOL:H31	1.86	0.57
2:C:354:THR:OG1	2:C:355:HIS:HD2	1.87	0.57
2:D:36:MET:CE	9:D:812:HOH:O	2.52	0.57
2:C:234:GLN:NE2	9:C:734:HOH:O	2.38	0.57
1:A:36:MET:CE	9:C:676:HOH:O	2.48	0.57
1:A:349:HIS:HD2	1:A:352:VAL:H	1.52	0.57
2:D:210:LLP:H4'1	3:D:402:SER:CA	2.34	0.57
2:D:53:HIS:HD2	2:D:55:GLY:N	1.97	0.57
2:B:391:ARG:O	2:B:394:VAL:HG22	2.05	0.56
2:D:210:LLP:C4	3:D:402:SER:N	2.67	0.56
2:C:53:HIS:CD2	2:C:55:GLY:H	2.08	0.55
2:C:268:HIS:HD2	2:C:377:VAL:O	1.89	0.55
2:D:364:GLU:HG3	9:D:733:HOH:O	2.06	0.55
2:B:124:ARG:HB2	2:B:124:ARG:NH2	2.16	0.55
1:A:349:HIS:HE1	1:A:370:ASP:O	1.89	0.54
2:C:228:ASN:C	2:C:228:ASN:HD22	2.10	0.54
2:C:349:HIS:HE1	2:C:370:ASP:O	1.89	0.54
2:C:362:ARG:NH1	9:C:738:HOH:O	2.39	0.54
9:C:771:HOH:O	2:D:234:GLN:HG2	2.06	0.54
1:A:161:PRO:HD3	1:A:355:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:GLU:CG	9:B:730:HOH:O	2.42	0.54
1:A:228:ASN:C	1:A:228:ASN:HD22	2.11	0.53
2:C:386:ARG:CD	9:C:646:HOH:O	2.45	0.53
2:B:228:ASN:ND2	2:B:231:LEU:H	2.07	0.52
2:D:349:HIS:HE1	2:D:370:ASP:O	1.92	0.51
2:D:228:ASN:HD22	2:D:228:ASN:C	2.14	0.51
1:A:338:GLU:OE1	3:A:401:SER:CB	2.57	0.51
2:B:108:MET:SD	2:B:136:LEU:HB2	2.49	0.51
1:A:326:ARG:HH11	1:A:326:ARG:CG	2.19	0.51
1:A:52:GLU:CD	9:A:670:HOH:O	2.50	0.50
1:A:230:GLU:HG3	9:A:594:HOH:O	2.11	0.49
2:C:363:ARG:HD2	9:C:562:HOH:O	2.13	0.49
2:B:53:HIS:HD2	2:B:55:GLY:N	1.93	0.49
2:B:228:ASN:C	2:B:228:ASN:HD22	2.16	0.49
1:A:211:TYR:CE1	1:A:341:GLY:HA2	2.48	0.48
1:A:210[B]:LYS:NZ	6:A:404:OJO:N	2.56	0.48
2:B:147:ARG:NH1	2:B:149:ASP:CG	2.66	0.48
2:D:330:LYS:HE2	9:D:789:HOH:O	2.14	0.48
1:A:120:GLU:HA	1:A:124:ARG:HD3	1.95	0.48
2:C:130:ASP:OD2	2:C:147:ARG:NH2	2.47	0.47
2:C:161:PRO:HD3	2:C:355:HIS:CE1	2.49	0.47
2:D:233:GLU:HG2	9:D:635:HOH:O	2.13	0.47
2:D:349:HIS:HD2	2:D:352:VAL:H	1.63	0.47
2:D:304:ARG:NE	9:D:775:HOH:O	2.00	0.46
1:A:18:ALA:HA	1:A:262:PRO:HG2	1.98	0.46
1:A:73:VAL:HG11	1:A:222:ILE:HG21	1.97	0.46
2:B:177:LYS:N	2:B:177:LYS:HD3	2.30	0.46
2:D:169:ALA:O	2:D:173:VAL:HG13	2.15	0.46
2:B:36:MET:HE1	9:D:569:HOH:O	2.16	0.46
2:D:304:ARG:NH2	9:D:775:HOH:O	2.48	0.46
2:C:57:GLU:CD	9:C:745:HOH:O	2.54	0.46
2:B:147:ARG:HH11	2:B:147:ARG:HG3	1.80	0.45
2:D:211:TYR:CE1	2:D:341:GLY:HA2	2.52	0.45
1:A:228:ASN:ND2	1:A:231:LEU:H	2.14	0.45
1:A:286:GLU:OE1	1:A:318:LYS:HE3	2.16	0.45
1:A:176:ARG:NH1	1:A:200:GLY:O	2.45	0.45
1:A:36:MET:CE	9:A:816:HOH:O	2.54	0.45
1:A:39:ILE:HB	2:D:39:ILE:HB	1.99	0.45
1:A:381:ASP:HB2	2:C:16[A]:SER:OG	2.17	0.45
2:B:130:ASP:OD2	2:B:147:ARG:NH2	2.42	0.45
2:C:59[A]:SER:HA	2:C:62:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:HE22	1:A:51:GLY:H	1.63	0.44
2:B:161:PRO:HD3	2:B:355:HIS:CE1	2.52	0.44
2:C:234:GLN:HB3	9:D:815:HOH:O	2.17	0.44
2:D:59:SER:HA	2:D:62:HIS:O	2.17	0.44
2:B:160:ASN:O	2:B:355:HIS:HE1	2.00	0.44
2:C:300:VAL:HG13	9:C:606:HOH:O	2.17	0.43
1:A:47:GLN:NE2	1:A:51:GLY:H	2.17	0.43
2:B:143:LYS:CE	2:B:178:HIS:HE1	2.21	0.43
2:C:211:TYR:CE1	2:C:341:GLY:HA2	2.53	0.43
1:A:59:SER:HA	1:A:62:HIS:O	2.18	0.43
2:C:321:PHE:HB2	2:C:370:ASP:HB3	2.01	0.43
2:C:53:HIS:HD2	2:C:55:GLY:N	1.98	0.42
2:D:326:ARG:NE	2:D:330:LYS:HD2	2.34	0.42
1:A:354:THR:OG1	1:A:355:HIS:CD2	2.68	0.42
2:D:161:PRO:HD3	2:D:355:HIS:CE1	2.55	0.42
2:C:92:THR:HG23	2:C:154:TRP:CH2	2.56	0.41
2:D:112:TYR:CE2	2:D:114:GLY:HA3	2.55	0.41
1:A:186:ASN:HB3	1:A:206:HIS:CE1	2.56	0.41
2:B:18:ALA:HA	2:B:262:PRO:HG2	2.01	0.41
2:D:228:ASN:ND2	2:D:231:LEU:H	2.19	0.41
1:A:190:SER:HB2	1:A:191:PRO:HD2	2.02	0.41
2:B:102:GLY:HA2	2:B:128:GLY:O	2.21	0.41
2:C:73:VAL:HG11	2:C:222:ILE:HG21	2.03	0.41
3:D:401:SER:N	9:D:835:HOH:O	2.54	0.41
2:B:390:GLU:O	2:B:394:VAL:HG13	2.20	0.41
2:D:338:GLU:OE1	3:D:401:SER:HB3	2.20	0.41
2:B:40:TYR:CD1	2:B:64:PRO:HB2	2.56	0.40
2:B:160:ASN:O	2:B:355:HIS:CE1	2.75	0.40
2:B:321:PHE:HB2	2:B:370:ASP:HB3	2.02	0.40
2:C:349:HIS:HD2	2:C:352:VAL:H	1.70	0.40
2:D:334:PHE:CD2	2:D:345:SER:HB3	2.57	0.40
2:D:296:HIS:HA	2:D:297:PRO:HD3	1.98	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	384/397 (97%)	373 (97%)	10 (3%)	1 (0%)	41	27
2	B	382/397 (96%)	374 (98%)	8 (2%)	0	100	100
2	C	382/397 (96%)	374 (98%)	7 (2%)	1 (0%)	41	27
2	D	386/397 (97%)	380 (98%)	6 (2%)	0	100	100
All	All	1534/1588 (97%)	1501 (98%)	31 (2%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	339	SER
1	A	339	SER

### 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	303/313 (97%)	291 (96%)	12 (4%)	31	16
2	B	301/312 (96%)	294 (98%)	7 (2%)	50	37
2	C	301/312 (96%)	294 (98%)	7 (2%)	50	37
2	D	305/312 (98%)	301 (99%)	4 (1%)	69	62
All	All	1210/1249 (97%)	1180 (98%)	30 (2%)	49	34

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	SER
1	A	16[B]	SER
1	A	17	LEU
1	A	124	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	139	PRO
1	A	176	ARG
1	A	195	ARG
1	A	203	LEU
1	A	228	ASN
1	A	326	ARG
1	A	340	LEU
1	A	365	GLN
2	B	124	ARG
2	B	136	LEU
2	B	147	ARG
2	B	177	LYS
2	B	228	ASN
2	B	291	PRO
2	B	365	GLN
2	C	20	LEU
2	C	147	ARG
2	C	176	ARG
2	C	195	ARG
2	C	228	ASN
2	C	326	ARG
2	C	340	LEU
2	D	17	LEU
2	D	173	VAL
2	D	228	ASN
2	D	386	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	47	GLN
1	A	228	ASN
1	A	240	ASN
1	A	246	GLN
1	A	271	ASN
1	A	349	HIS
1	A	355	HIS
2	B	47	GLN
2	B	53	HIS
2	B	178	HIS
2	B	228	ASN
2	B	240	ASN

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Mol	Chain	Res	Type
2	B	246	GLN
2	B	271	ASN
2	B	305	GLN
2	B	355	HIS
2	B	365	GLN
2	C	53	HIS
2	C	228	ASN
2	C	234	GLN
2	C	240	ASN
2	C	246	GLN
2	C	268	HIS
2	C	271	ASN
2	C	349	HIS
2	C	355	HIS
2	C	365	GLN
2	D	53	HIS
2	D	228	ASN
2	D	240	ASN
2	D	246	GLN
2	D	271	ASN
2	D	349	HIS
2	D	355	HIS
2	D	396	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
2	LLP	C	210	2	23,24,25	2.62	9 (39%)	25,32,34	2.18	7 (28%)
2	LLP	B	210	2	23,24,25	2.74	11 (47%)	25,32,34	2.16	9 (36%)
2	LLP	D	210	2	23,24,25	2.35	8 (34%)	25,32,34	1.97	8 (32%)

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	LLP	C	210	2	-	6/16/17/19	0/1/1/1
2	LLP	B	210	2	-	4/16/17/19	0/1/1/1
2	LLP	D	210	2	-	7/16/17/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	LLP	C3-C2	7.67	1.48	1.40
2	C	210	LLP	C3-C2	6.67	1.47	1.40
2	C	210	LLP	C4-C5	5.44	1.48	1.42
2	B	210	LLP	C4-C5	5.33	1.48	1.42
2	D	210	LLP	C3-C2	5.26	1.46	1.40
2	D	210	LLP	C4-C5	5.16	1.48	1.42
2	B	210	LLP	C4-C3	4.30	1.47	1.40
2	D	210	LLP	C4-C3	3.87	1.46	1.40
2	C	210	LLP	P-OP3	-3.71	1.40	1.54
2	C	210	LLP	P-OP2	-3.71	1.40	1.54
2	B	210	LLP	P-OP3	-3.66	1.40	1.54
2	D	210	LLP	P-OP3	-3.55	1.41	1.54
2	D	210	LLP	P-OP2	-3.48	1.41	1.54
2	C	210	LLP	OP4-C5'	-3.48	1.32	1.45
2	C	210	LLP	C4-C3	3.43	1.46	1.40
2	B	210	LLP	OP4-C5'	-3.13	1.33	1.45
2	D	210	LLP	C4'-NZ	3.01	1.37	1.27
2	D	210	LLP	OP4-C5'	-2.99	1.33	1.45
2	B	210	LLP	P-OP2	-2.96	1.43	1.54
2	C	210	LLP	P-OP1	-2.95	1.41	1.50
2	B	210	LLP	P-OP1	-2.89	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	LLP	CD-CE	2.55	1.60	1.51
2	B	210	LLP	CB-CA	-2.34	1.50	1.53
2	C	210	LLP	C4'-NZ	2.33	1.35	1.27
2	B	210	LLP	C4'-NZ	2.23	1.34	1.27
2	C	210	LLP	CB-CA	2.13	1.56	1.53
2	D	210	LLP	P-OP4	-2.11	1.53	1.60
2	B	210	LLP	CE-NZ	2.08	1.51	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	LLP	OP4-C5'-C5	6.14	121.05	109.35
2	C	210	LLP	OP4-C5'-C5	5.33	119.50	109.35
2	C	210	LLP	C3-C4-C5	-4.53	114.78	118.26
2	D	210	LLP	CE-NZ-C4'	4.32	132.16	118.90
2	B	210	LLP	OP2-P-OP4	-4.24	95.46	106.73
2	D	210	LLP	C2'-C2-C3	-4.03	115.92	120.89
2	C	210	LLP	CE-NZ-C4'	4.00	131.18	118.90
2	B	210	LLP	CE-NZ-C4'	3.76	130.43	118.90
2	C	210	LLP	C2'-C2-N1	3.07	123.66	117.67
2	D	210	LLP	C5-C4-C4'	3.05	126.58	121.56
2	B	210	LLP	OP3-P-OP2	2.94	118.88	107.64
2	D	210	LLP	C2'-C2-N1	2.92	123.37	117.67
2	C	210	LLP	OP2-P-OP4	-2.73	99.46	106.73
2	D	210	LLP	OP4-C5'-C5	2.66	114.41	109.35
2	D	210	LLP	CD-CE-NZ	2.54	117.16	110.93
2	C	210	LLP	C2'-C2-C3	-2.48	117.83	120.89
2	D	210	LLP	C3-C4-C5	-2.43	116.39	118.26
2	B	210	LLP	C4-C3-C2	-2.37	118.72	120.19
2	C	210	LLP	C4-C3-C2	2.35	121.64	120.19
2	B	210	LLP	C3-C4-C5	-2.27	116.52	118.26
2	B	210	LLP	C4-C4'-NZ	-2.26	113.94	124.31
2	D	210	LLP	OP3-P-OP2	2.25	116.24	107.64
2	B	210	LLP	C6-N1-C2	2.02	122.91	119.17
2	B	210	LLP	O3-C3-C2	2.02	121.89	117.49

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	210	LLP	O-C-CA-CB
2	C	210	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	D	210	LLP	O-C-CA-CB
2	B	210	LLP	CG-CD-CE-NZ
2	C	210	LLP	CG-CD-CE-NZ
2	D	210	LLP	CG-CD-CE-NZ
2	C	210	LLP	CA-CB-CG-CD
2	D	210	LLP	C3-C4-C4'-NZ
2	B	210	LLP	CD-CE-NZ-C4'
2	D	210	LLP	CD-CE-NZ-C4'
2	D	210	LLP	C5-C4-C4'-NZ
2	B	210	LLP	C3-C4-C4'-NZ
2	C	210	LLP	C3-C4-C4'-NZ
2	D	210	LLP	C-CA-CB-CG
2	C	210	LLP	C5-C4-C4'-NZ
2	C	210	LLP	CD-CE-NZ-C4'
2	D	210	LLP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	210	LLP	2	0
2	B	210	LLP	2	0
2	D	210	LLP	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
4	GOL	D	403	-	5,5,5	0.41	0	5,5,5	0.82	0
3	SER	B	401	-	5,6,6	0.99	0	5,7,7	1.57	1 (20%)
3	SER	D	402	-	5,6,6	1.55	1 (20%)	5,7,7	0.72	0
7	NAK	C	402	-	4,5,5	1.23	1 (25%)	4,6,6	3.69	2 (50%)
8	PYR	B	403	-	5,5,5	2.74	2 (40%)	3,6,6	2.20	2 (66%)
6	OJO	A	404	-	20,21,21	2.72	7 (35%)	23,30,30	2.00	6 (26%)
3	SER	C	401	-	5,6,6	1.10	1 (20%)	5,7,7	1.97	2 (40%)
4	GOL	C	403	-	5,5,5	0.45	0	5,5,5	1.21	0
3	SER	D	401	-	5,6,6	0.77	0	5,7,7	1.24	1 (20%)
5	SO4	A	403	-	4,4,4	0.43	0	6,6,6	0.35	0
4	GOL	A	402	-	5,5,5	0.66	0	5,5,5	0.25	0
3	SER	A	401	-	5,6,6	1.07	1 (20%)	5,7,7	1.23	1 (20%)
7	NAK	B	402	-	4,5,5	1.05	0	4,6,6	3.07	3 (75%)

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
4	GOL	D	403	-	-	4/4/4/4	-
3	SER	B	401	-	-	0/6/6/6	-
3	SER	D	402	-	-	2/6/6/6	-
7	NAK	C	402	-	-	2/2/4/4	-
8	PYR	B	403	-	-	0/4/4/4	-
6	OJO	A	404	-	-	0/10/15/15	0/1/1/1
3	SER	C	401	-	-	0/6/6/6	-
4	GOL	C	403	-	-	2/4/4/4	-
3	SER	D	401	-	-	1/6/6/6	-
4	GOL	A	402	-	-	0/4/4/4	-
3	SER	A	401	-	-	2/6/6/6	-
7	NAK	B	402	-	-	2/2/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	404	OJO	C4-C3	6.70	1.50	1.40
6	A	404	OJO	C3-C2	5.87	1.46	1.40
6	A	404	OJO	C4A-N	4.85	1.34	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	PYR	O-C	4.65	1.35	1.22
6	A	404	OJO	C2A-C2	3.52	1.56	1.50
8	B	403	PYR	CA-C	-3.40	1.42	1.54
6	A	404	OJO	C4-C5	3.07	1.45	1.42
3	D	402	SER	OXT-C	-2.95	1.20	1.30
6	A	404	OJO	C4-C4A	2.46	1.51	1.46
6	A	404	OJO	OXT-C	-2.35	1.23	1.30
7	C	402	NAK	OXT-C	-2.15	1.24	1.30
3	A	401	SER	OXT-C	-2.12	1.23	1.30
3	C	401	SER	OXT-C	-2.03	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	402	NAK	CAE-CA-C	6.35	124.34	118.17
6	A	404	OJO	C3-C4-C5	-5.73	113.86	118.26
7	B	402	NAK	CAE-CA-C	4.50	122.54	118.17
3	C	401	SER	OXT-C-O	-3.63	115.85	124.09
7	C	402	NAK	O-C-CA	-3.53	116.87	121.38
7	B	402	NAK	O-C-CA	-3.51	116.89	121.38
6	A	404	OJO	C4-C3-C2	-3.44	118.06	120.19
8	B	403	PYR	OXT-C-O	-3.04	116.64	123.61
6	A	404	OJO	C4-C4A-N	-2.87	116.21	123.19
6	A	404	OJO	C2A-C2-C3	-2.60	117.67	120.89
6	A	404	OJO	C5-C4-C4A	2.57	125.79	121.56
3	B	401	SER	OXT-C-CA	2.46	121.75	113.38
6	A	404	OJO	C6-C5-C4	2.37	122.52	118.15
3	C	401	SER	OXT-C-CA	2.37	121.47	113.38
3	D	401	SER	OXT-C-O	-2.35	118.76	124.09
7	B	402	NAK	OXT-C-CA	2.17	121.05	116.35
3	A	401	SER	OXT-C-O	-2.13	119.25	124.09
8	B	403	PYR	O3-CA-CB	-2.09	115.10	119.73

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	402	SER	N-CA-CB-OG
4	C	403	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-C3
7	B	402	NAK	OXT-C-CA-CAE
7	B	402	NAK	O-C-CA-CAE

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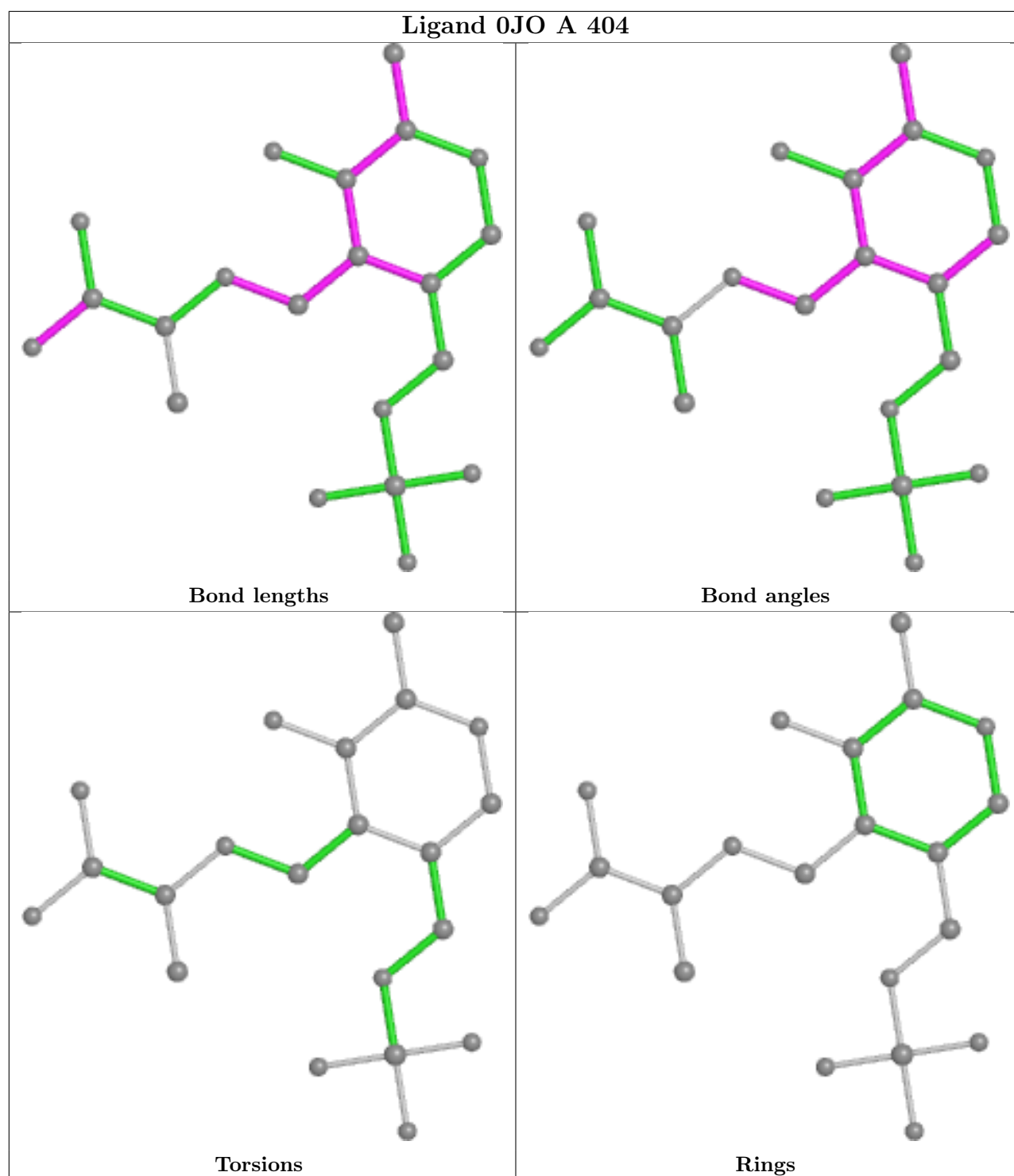
Mol	Chain	Res	Type	Atoms
7	C	402	NAK	O-C-CA-CAE
4	D	403	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-O2
3	A	401	SER	O-C-CA-CB
4	C	403	GOL	O2-C2-C3-O3
3	D	402	SER	C-CA-CB-OG
7	C	402	NAK	OXT-C-CA-CAE
4	D	403	GOL	O2-C2-C3-O3
3	A	401	SER	OXT-C-CA-CB
3	D	401	SER	OXT-C-CA-CB

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	GOL	3	0
3	D	402	SER	7	0
7	C	402	NAK	2	0
6	A	404	OJO	4	0
4	C	403	GOL	1	0
3	D	401	SER	2	0
3	A	401	SER	2	0
7	B	402	NAK	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 [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%)	-0.63	1 (0%) 94 92	9, 14, 26, 37	0
2	B	380/397 (95%)	-0.66	1 (0%) 94 92	9, 14, 25, 39	0
2	C	380/397 (95%)	-0.33	8 (2%) 63 59	10, 17, 34, 49	0
2	D	383/397 (96%)	-0.57	2 (0%) 91 89	10, 15, 26, 55	0
All	All	1524/1588 (95%)	-0.55	12 (0%) 86 84	9, 15, 29, 55	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ALA	4.7
2	B	14	ALA	4.4
2	C	361	ALA	3.7
2	C	394	VAL	3.5
2	C	365	GLN	3.2
2	C	362	ARG	3.0
2	C	360	VAL	3.0
2	D	397	ASN	2.8
2	D	14	ALA	2.4
2	C	177	LYS	2.3
2	C	364	GLU	2.2
2	C	14	ALA	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( $\text{\AA}^2$ )	Q<0.9
2	LLP	D	210	24/25	0.96	0.12	10,16,28,30	0
2	LLP	C	210	24/25	0.97	0.13	11,17,26,27	0
2	LLP	B	210	24/25	0.97	0.12	9,17,24,25	0

### 6.3 Carbohydrates [i](#)

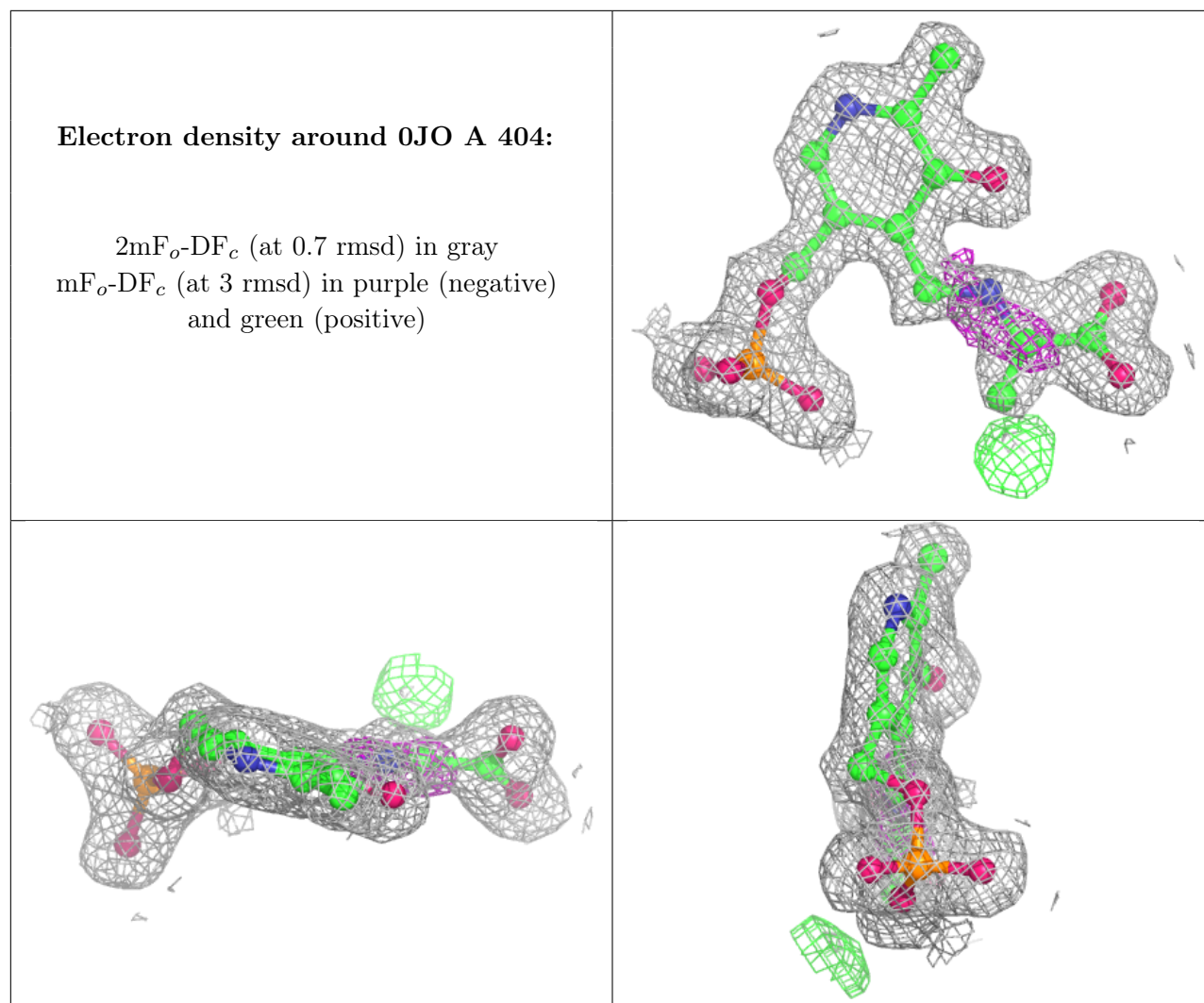
There are no monosaccharides in this entry.

### 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
4	GOL	D	403	6/6	0.92	0.25	17,41,41,44	0
4	GOL	C	403	6/6	0.93	0.33	26,34,41,53	0
3	SER	A	401	7/7	0.93	0.10	26,30,30,31	0
7	NAK	C	402	6/6	0.93	0.18	27,33,38,38	0
8	PYR	B	403	6/6	0.94	0.11	18,23,30,34	0
3	SER	C	401	7/7	0.95	0.08	30,31,32,33	0
3	SER	D	401	7/7	0.95	0.08	21,23,26,27	0
3	SER	D	402	7/7	0.96	0.11	18,21,24,30	0
4	GOL	A	402	6/6	0.96	0.06	17,18,20,20	0
3	SER	B	401	7/7	0.96	0.08	19,20,23,26	0
7	NAK	B	402	6/6	0.97	0.13	20,24,31,32	0
6	OJO	A	404	21/21	0.98	0.09	11,19,25,26	0
5	SO4	A	403	5/5	0.99	0.14	32,37,41,41	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.