



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 06:09 pm GMT

PDB ID : 9HT5 / pdb\_00009ht5  
Title : Structure of YIUA from Yersinia ruckeri with Iron and nitrilotriacetic acid  
Authors : Thompson, S.; Thomsen, E.; Duhme-Klair, A.; Butler, A.; Grogan, G.  
Deposited on : 2024-12-19  
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

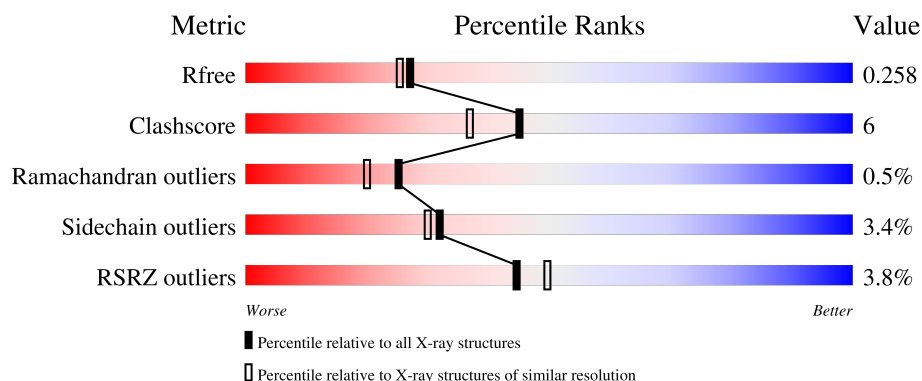
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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))
$R_{free}$	164625	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (2.16-2.12)

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	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 85%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>85%</span> <span>11%</span> <span>..</span> </div> </div>
1	B	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 12%, green 85%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>85%</span> <span>12%</span> <span>...</span> </div> </div>
1	C	347	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 1%, yellow 12%, green 79%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>79%</span> <span>12%</span> <span>• 8%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7790 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.

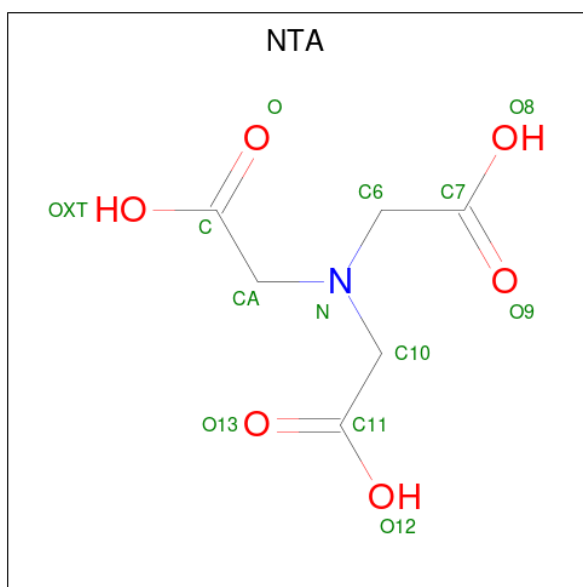
- Molecule 1 is a protein called Periplasmic substrate-binding transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	2	0
			2565	1644	428	486	7			
1	B	344	Total	C	N	O	S	0	0	0
			2579	1644	433	495	7			
1	C	318	Total	C	N	O	S	0	0	0
			2366	1518	397	444	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	ALA	conflict	UNP A0A085U4N5
A	12	VAL	ALA	conflict	UNP A0A085U4N5
A	233	THR	ALA	conflict	UNP A0A085U4N5
A	262	GLU	ALA	conflict	UNP A0A085U4N5
A	315	GLN	GLU	conflict	UNP A0A085U4N5
A	324	ASN	LYS	conflict	UNP A0A085U4N5
B	0	SER	ALA	conflict	UNP A0A085U4N5
B	12	VAL	ALA	conflict	UNP A0A085U4N5
B	233	THR	ALA	conflict	UNP A0A085U4N5
B	262	GLU	ALA	conflict	UNP A0A085U4N5
B	315	GLN	GLU	conflict	UNP A0A085U4N5
B	324	ASN	LYS	conflict	UNP A0A085U4N5
C	0	SER	ALA	conflict	UNP A0A085U4N5
C	12	VAL	ALA	conflict	UNP A0A085U4N5
C	233	THR	ALA	conflict	UNP A0A085U4N5
C	262	GLU	ALA	conflict	UNP A0A085U4N5
C	315	GLN	GLU	conflict	UNP A0A085U4N5
C	324	ASN	LYS	conflict	UNP A0A085U4N5

- Molecule 2 is NITRILOTRIACETIC ACID (CCD ID: NTA) (formula:  $C_6H_9NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	6	1	6		
2	B	1	Total	C	N	O	0	0
			13	6	1	6		
2	C	1	Total	C	N	O	0	0
			13	6	1	6		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

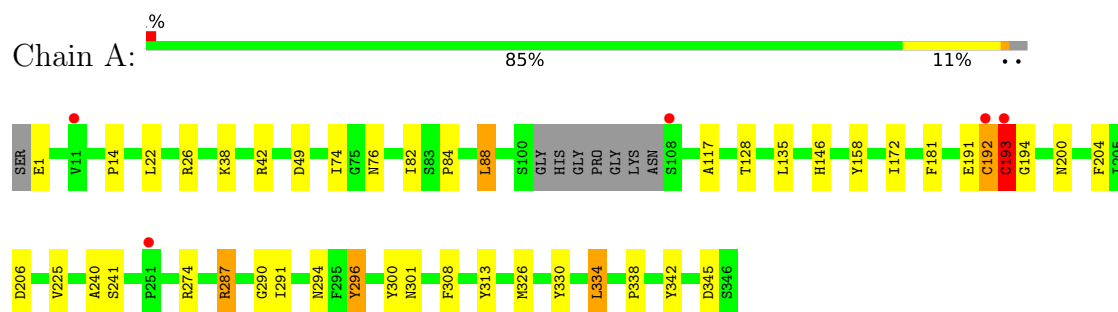
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	99	Total	O	0	0
			99	99		
4	C	49	Total	O	0	0
			49	49		

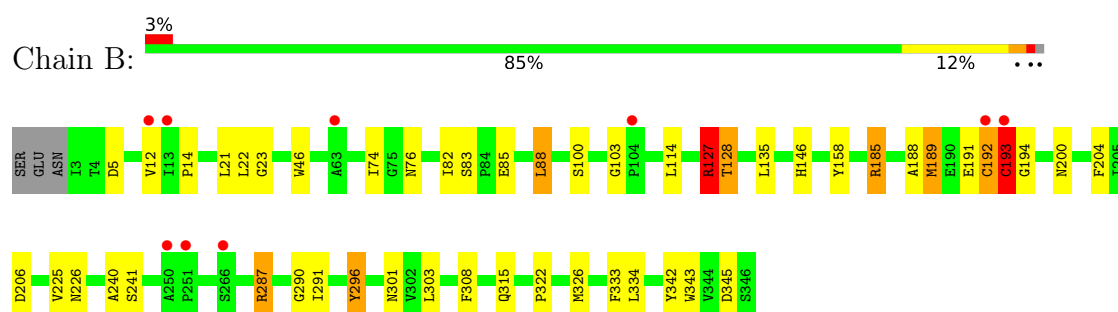
### 3 Residue-property plots

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.

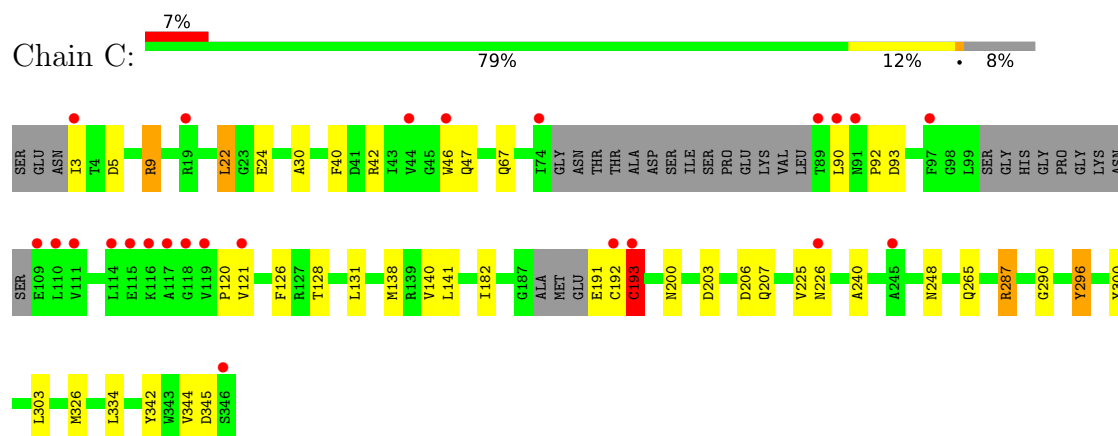
- Molecule 1: Periplasmic substrate-binding transport protein



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.15Å 59.39Å 101.17Å 101.36° 94.49° 100.54°	Depositor
Resolution (Å)	54.78 – 2.14 54.78 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.9 (54.78-2.14) 98.9 (54.78-2.14)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.205 , 0.253 0.214 , 0.258	Depositor DCC
$R_{free}$ test set	2330 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.54% 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: NTA, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.70	2/2625 (0.1%)	1.16	13/3573 (0.4%)
1	B	0.65	0/2636	1.16	12/3596 (0.3%)
1	C	0.63	0/2417	1.13	6/3295 (0.2%)
All	All	0.66	2/7678 (0.0%)	1.15	31/10464 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49[A]	ASP	C-O	8.86	1.34	1.24
1	A	49[B]	ASP	C-O	8.86	1.34	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49[A]	ASP	CA-C-O	10.19	131.61	120.10
1	A	49[B]	ASP	CA-C-O	10.19	131.61	120.10
1	A	193	CYS	CB-CA-C	8.68	127.69	110.42
1	C	193	CYS	CB-CA-C	8.17	126.69	110.42
1	B	193	CYS	CB-CA-C	7.77	125.89	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49[A]	ASP	O-C-N	-7.28	114.40	122.12
1	A	49[B]	ASP	O-C-N	-7.28	114.40	122.12
1	B	333	PHE	N-CA-CB	-7.02	101.72	110.98
1	C	40	PHE	N-CA-CB	-6.66	100.55	110.61
1	B	315	GLN	N-CA-CB	6.24	119.49	110.20
1	B	308	PHE	CA-CB-CG	6.21	120.01	113.80
1	C	67	GLN	CB-CA-C	-6.20	98.43	110.46
1	B	192	CYS	N-CA-C	6.14	118.74	109.23
1	A	192	CYS	N-CA-C	6.06	119.07	109.50
1	C	206	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	181	PHE	N-CA-CB	5.65	119.64	110.77
1	C	192	CYS	N-CA-C	5.52	118.46	109.24
1	A	206	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	345	ASP	CB-CA-C	-5.50	100.20	109.50
1	C	345	ASP	CB-CA-C	-5.47	100.77	109.80
1	B	185	ARG	CG-CD-NE	5.47	124.03	112.00
1	A	308	PHE	CA-CB-CG	5.43	119.23	113.80
1	B	206	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	191	GLU	CA-C-N	-5.28	113.59	122.29
1	B	191	GLU	C-N-CA	-5.28	113.59	122.29
1	B	192	CYS	CB-CA-C	-5.18	98.06	109.56
1	A	194	GLY	N-CA-C	-5.17	103.53	111.64
1	B	345	ASP	CB-CA-C	-5.13	100.83	109.50
1	A	191	GLU	CA-C-N	-5.09	114.68	122.62
1	A	191	GLU	C-N-CA	-5.09	114.68	122.62
1	B	194	GLY	N-CA-C	-5.06	104.65	111.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	ARG	Sidechain
1	A	42	ARG	Sidechain
1	B	127	ARG	Sidechain
1	C	42	ARG	Sidechain
1	C	9	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2565	0	2499	24	0
1	B	2579	0	2478	32	0
1	C	2366	0	2244	30	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
2	C	13	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	90	0	0	1	0
4	B	99	0	0	3	0
4	C	49	0	0	2	0
All	All	7790	0	7221	85	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 6.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:MET:HA	1:C:138:MET:HE2	1.41	0.99
1:B:192:CYS:HG	1:B:193:CYS:HG	1.12	0.89
1:A:88:LEU:HD21	1:A:117:ALA:HB2	1.56	0.87
1:C:138:MET:HE1	1:C:141:LEU:HD12	1.62	0.81
1:C:90:LEU:O	1:C:92:PRO:HD3	1.81	0.80
1:B:326:MET:HE1	1:B:342:TYR:CD2	2.18	0.79
1:A:88:LEU:HD11	1:A:117:ALA:CB	2.17	0.74
1:C:226:ASN:HB2	4:C:542:HOH:O	1.87	0.73
1:C:138:MET:HE2	1:C:138:MET:CA	2.17	0.73
1:B:193:CYS:HB2	1:B:225:VAL:O	1.89	0.73
1:C:287:ARG:HG2	1:C:287:ARG:HH11	1.58	0.68
1:A:26:ARG:HH11	1:A:294:ASN:HD21	1.42	0.68
1:A:287:ARG:HH11	1:A:287:ARG:HG2	1.58	0.68
1:A:26:ARG:HH11	1:A:294:ASN:ND2	1.94	0.65
1:C:126:PHE:CZ	1:C:138:MET:HE3	2.32	0.65
1:C:138:MET:CE	1:C:141:LEU:HD12	2.27	0.65
1:B:287:ARG:HG2	1:B:287:ARG:HH11	1.61	0.65
1:C:138:MET:HA	1:C:138:MET:CE	2.22	0.64
1:C:126:PHE:HZ	1:C:138:MET:HE3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:O	1:B:189:MET:CB	2.46	0.63
1:C:30:ALA:HB1	1:C:138:MET:HE1	1.80	0.62
1:A:193:CYS:HB2	1:A:225:VAL:O	2.00	0.62
1:B:76:ASN:HD21	1:B:83:SER:HB2	1.67	0.60
1:B:14:PRO:O	1:B:146:HIS:HE1	1.85	0.58
1:B:88:LEU:CD1	1:B:114:LEU:HD23	2.33	0.58
1:C:193:CYS:HB2	1:C:225:VAL:O	2.03	0.57
1:C:90:LEU:C	1:C:92:PRO:HD3	2.29	0.57
1:B:226:ASN:HB2	4:B:571:HOH:O	2.04	0.56
1:A:338:PRO:HG2	1:C:248:ASN:ND2	2.19	0.56
1:B:21:LEU:HD11	1:B:74:ILE:HD11	1.88	0.56
1:A:76:ASN:HD21	1:A:84:PRO:HD2	1.70	0.56
1:C:303:LEU:HD13	1:C:326:MET:HE3	1.89	0.55
1:C:326:MET:HE2	4:C:501:HOH:O	2.08	0.54
1:A:326:MET:HE1	1:A:342:TYR:CD2	2.43	0.54
1:B:127:ARG:HD2	1:B:296:TYR:CE2	2.43	0.54
1:A:88:LEU:HD11	1:A:117:ALA:HB3	1.89	0.52
1:C:287:ARG:HH11	1:C:287:ARG:CG	2.22	0.51
1:B:303:LEU:HD13	1:B:326:MET:HE3	1.93	0.51
1:A:287:ARG:HH11	1:A:287:ARG:CG	2.22	0.51
1:C:93:ASP:O	1:C:120:PRO:HD2	2.11	0.50
1:B:88:LEU:HD11	1:B:114:LEU:HD23	1.93	0.50
1:A:14:PRO:O	1:A:146:HIS:HE1	1.95	0.49
1:C:22:LEU:O	1:C:46:TRP:HA	2.12	0.49
1:B:287:ARG:HH11	1:B:287:ARG:CG	2.23	0.49
1:C:90:LEU:O	1:C:92:PRO:CD	2.59	0.47
1:B:85:GLU:H	1:B:85:GLU:CD	2.24	0.46
1:C:326:MET:HE1	1:C:342:TYR:CD1	2.51	0.46
1:C:131:LEU:HB2	1:C:203:ASP:HB3	1.98	0.46
1:B:241:SER:HA	1:B:291:ILE:O	2.17	0.45
1:A:241:SER:HA	1:A:291:ILE:O	2.17	0.45
1:A:172:ILE:HD13	1:A:313:TYR:CE1	2.52	0.45
1:A:76:ASN:ND2	1:A:84:PRO:HD2	2.32	0.45
1:A:14:PRO:O	1:A:146:HIS:CE1	2.70	0.44
1:B:88:LEU:HD13	1:B:114:LEU:HD23	2.00	0.44
1:A:74:ILE:HA	1:A:82:ILE:O	2.17	0.44
1:B:14:PRO:O	1:B:146:HIS:CE1	2.69	0.44
1:B:200:ASN:HD21	1:B:296:TYR:HB2	1.81	0.44
1:A:240:ALA:O	1:A:290:GLY:HA2	2.18	0.44
1:B:240:ALA:O	1:B:290:GLY:HA2	2.18	0.44
1:A:135:LEU:HD21	1:A:158:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:HD21	1:A:296:TYR:HB2	1.82	0.43
1:C:131:LEU:HD13	1:C:207:GLN:CD	2.44	0.43
1:B:5:ASP:OD1	1:B:5:ASP:C	2.61	0.43
1:A:192:CYS:SG	1:A:193:CYS:N	2.92	0.43
1:B:192:CYS:CB	1:B:193:CYS:HG	2.30	0.43
1:C:240:ALA:O	1:C:290:GLY:HA2	2.19	0.42
1:A:38:LYS:HG3	4:A:584:HOH:O	2.18	0.42
1:C:200:ASN:HD21	1:C:296:TYR:HB2	1.84	0.42
1:C:126:PHE:HZ	1:C:138:MET:CE	2.30	0.42
1:B:135:LEU:HD21	1:B:158:TYR:CD1	2.54	0.42
1:B:100:SER:HB3	1:B:128:THR:CG2	2.50	0.42
1:B:322:PRO:HB2	1:B:343:TRP:CZ2	2.55	0.41
1:A:330:TYR:HA	1:A:334:LEU:HB2	2.01	0.41
1:B:128:THR:HG22	4:B:594:HOH:O	2.20	0.41
1:B:192:CYS:SG	1:B:193:CYS:N	2.94	0.41
1:B:22:LEU:O	1:B:46:TRP:HA	2.20	0.41
1:B:76:ASN:ND2	1:B:83:SER:HB2	2.34	0.41
1:C:3:ILE:HG12	1:C:140:VAL:HG22	2.03	0.41
1:C:5:ASP:OD1	1:C:5:ASP:C	2.63	0.41
1:C:265:GLN:HG2	1:C:344:VAL:CG2	2.50	0.41
1:B:74:ILE:HA	1:B:82:ILE:O	2.21	0.41
1:B:204:PHE:CZ	1:B:301:ASN:HB2	2.56	0.41
1:C:9:ARG:NH1	1:C:121:VAL:O	2.54	0.41
1:A:204:PHE:CZ	1:A:301:ASN:HB2	2.57	0.40
1:B:103:GLY:HA3	4:B:569:HOH:O	2.20	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	337/347 (97%)	327 (97%)	9 (3%)	1 (0%)	37	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	342/347 (99%)	330 (96%)	9 (3%)	3 (1%)	14	8
1	C	310/347 (89%)	302 (97%)	7 (2%)	1 (0%)	37	33
All	All	989/1041 (95%)	959 (97%)	25 (2%)	5 (0%)	25	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	CYS
1	B	189	MET
1	B	193	CYS
1	B	23	GLY
1	C	193	CYS

### 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	264/291 (91%)	256 (97%)	8 (3%)	36	35
1	B	266/291 (91%)	258 (97%)	8 (3%)	36	35
1	C	235/291 (81%)	225 (96%)	10 (4%)	25	21
All	All	765/873 (88%)	739 (97%)	26 (3%)	32	30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	22	LEU
1	A	88	LEU
1	A	128	THR
1	A	287	ARG
1	A	296	TYR
1	A	300	TYR
1	A	334	LEU
1	B	12	VAL

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Mol	Chain	Res	Type
1	B	88	LEU
1	B	127	ARG
1	B	128	THR
1	B	185	ARG
1	B	287	ARG
1	B	296	TYR
1	B	334	LEU
1	C	22	LEU
1	C	24	GLU
1	C	47	GLN
1	C	128	THR
1	C	182	ILE
1	C	191	GLU
1	C	287	ARG
1	C	296	TYR
1	C	300	TYR
1	C	334	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	76	ASN
1	A	146	HIS
1	A	200	ASN
1	A	216	ASN
1	A	258	GLN
1	A	294	ASN
1	A	323	ASN
1	B	37	GLN
1	B	76	ASN
1	B	113	GLN
1	B	146	HIS
1	B	200	ASN
1	B	207	GLN
1	B	216	ASN
1	B	306	GLN
1	C	200	ASN
1	C	207	GLN
1	C	216	ASN
1	C	306	GLN
1	C	323	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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$
2	NTA	B	401	3	12,12,12	1.11	1 (8%)	15,15,15	1.40	2 (13%)
2	NTA	C	401	3	12,12,12	1.17	1 (8%)	15,15,15	1.22	1 (6%)
2	NTA	A	401	3	12,12,12	1.31	1 (8%)	15,15,15	1.17	1 (6%)

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	NTA	B	401	3	-	3/12/12/12	-
2	NTA	C	401	3	-	3/12/12/12	-
2	NTA	A	401	3	-	3/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NTA	O12-C11	-2.57	1.22	1.30
2	B	401	NTA	O8-C7	-2.32	1.22	1.30
2	C	401	NTA	O12-C11	-2.10	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NTA	CA-N-C10	2.68	117.61	111.54
2	B	401	NTA	CA-N-C10	2.57	117.35	111.54
2	A	401	NTA	CA-N-C10	2.56	117.32	111.54
2	B	401	NTA	CA-N-C6	2.39	116.95	111.54

There are no chirality outliers.

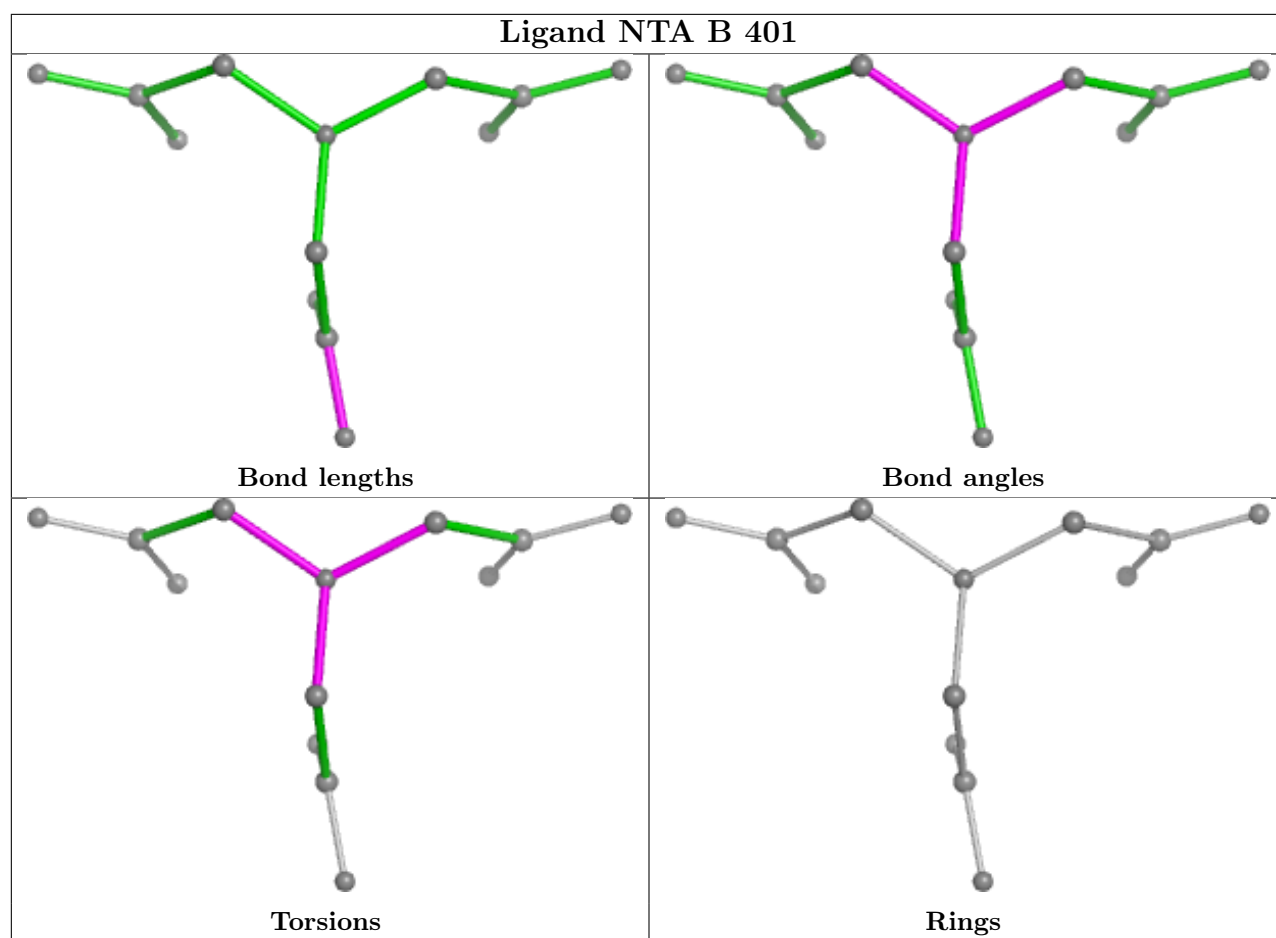
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NTA	C7-C6-N-C10
2	C	401	NTA	C-CA-N-C10
2	A	401	NTA	C-CA-N-C10
2	B	401	NTA	C7-C6-N-C10
2	B	401	NTA	C-CA-N-C10
2	C	401	NTA	C7-C6-N-C10
2	C	401	NTA	C11-C10-N-CA
2	A	401	NTA	C11-C10-N-CA
2	B	401	NTA	C11-C10-N-CA

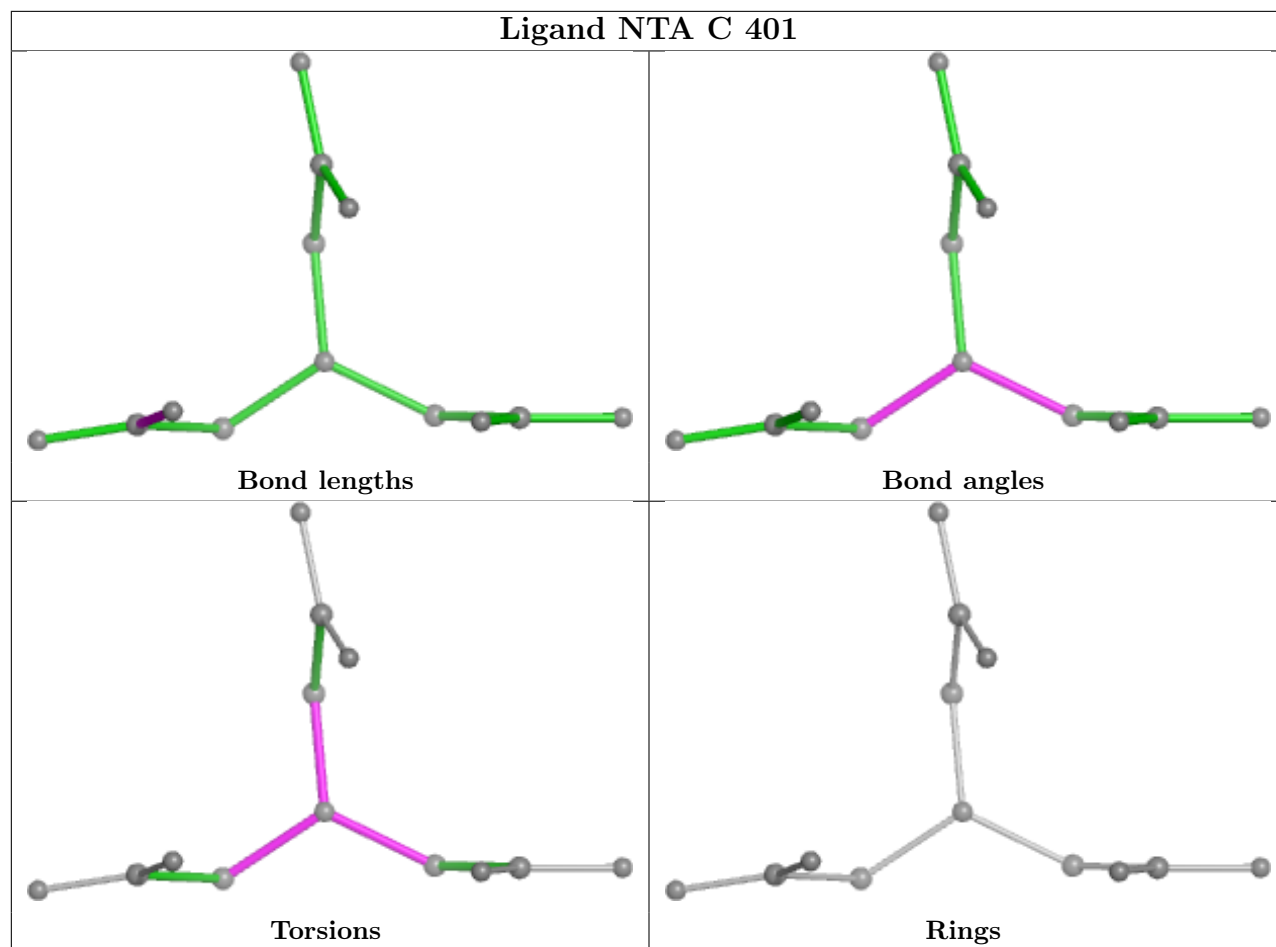
There are no ring outliers.

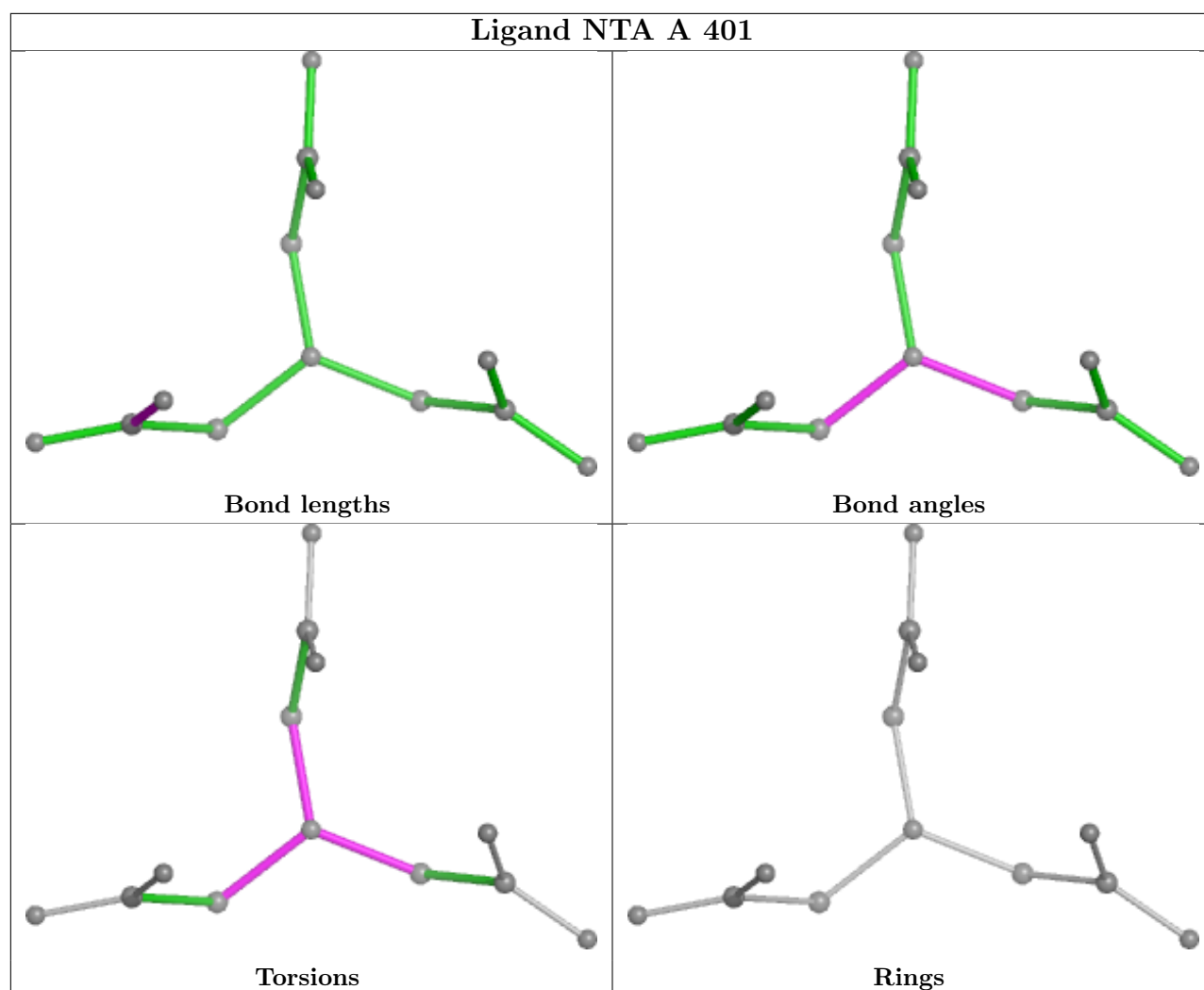
No monomer is involved in short contacts.

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	339/347 (97%)	0.13	5 (1%) 71 75	14, 30, 49, 88	2 (0%)
1	B	344/347 (99%)	0.15	9 (2%) 57 61	19, 30, 50, 91	0
1	C	318/347 (91%)	0.65	24 (7%) 22 26	21, 39, 65, 118	0
All	All	1001/1041 (96%)	0.30	38 (3%) 44 50	14, 33, 58, 118	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	PRO	4.6
1	C	111	VAL	4.1
1	C	117	ALA	4.1
1	C	89	THR	3.8
1	C	118	GLY	3.7
1	C	121	VAL	3.6
1	C	192	CYS	3.6
1	A	192	CYS	3.4
1	B	192	CYS	3.3
1	B	250	ALA	3.3
1	C	110	LEU	3.2
1	B	12	VAL	3.1
1	C	116	LYS	3.1
1	C	19	ARG	3.0
1	B	63	ALA	3.0
1	A	193	CYS	3.0
1	A	251	PRO	2.9
1	C	109	GLU	2.9
1	C	44	VAL	2.8
1	C	74	ILE	2.8
1	C	119	VAL	2.8
1	B	193	CYS	2.8
1	A	108	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	193	CYS	2.7
1	C	114	LEU	2.6
1	A	11	VAL	2.5
1	C	91	ASN	2.3
1	C	245	ALA	2.3
1	C	226	ASN	2.3
1	C	3	ILE	2.2
1	C	90	LEU	2.2
1	C	97	PHE	2.2
1	B	251	PRO	2.2
1	B	13	ILE	2.2
1	B	266	SER	2.1
1	C	46	TRP	2.1
1	C	115	GLU	2.1
1	C	346	SER	2.1

## 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 oligosaccharides in this entry.

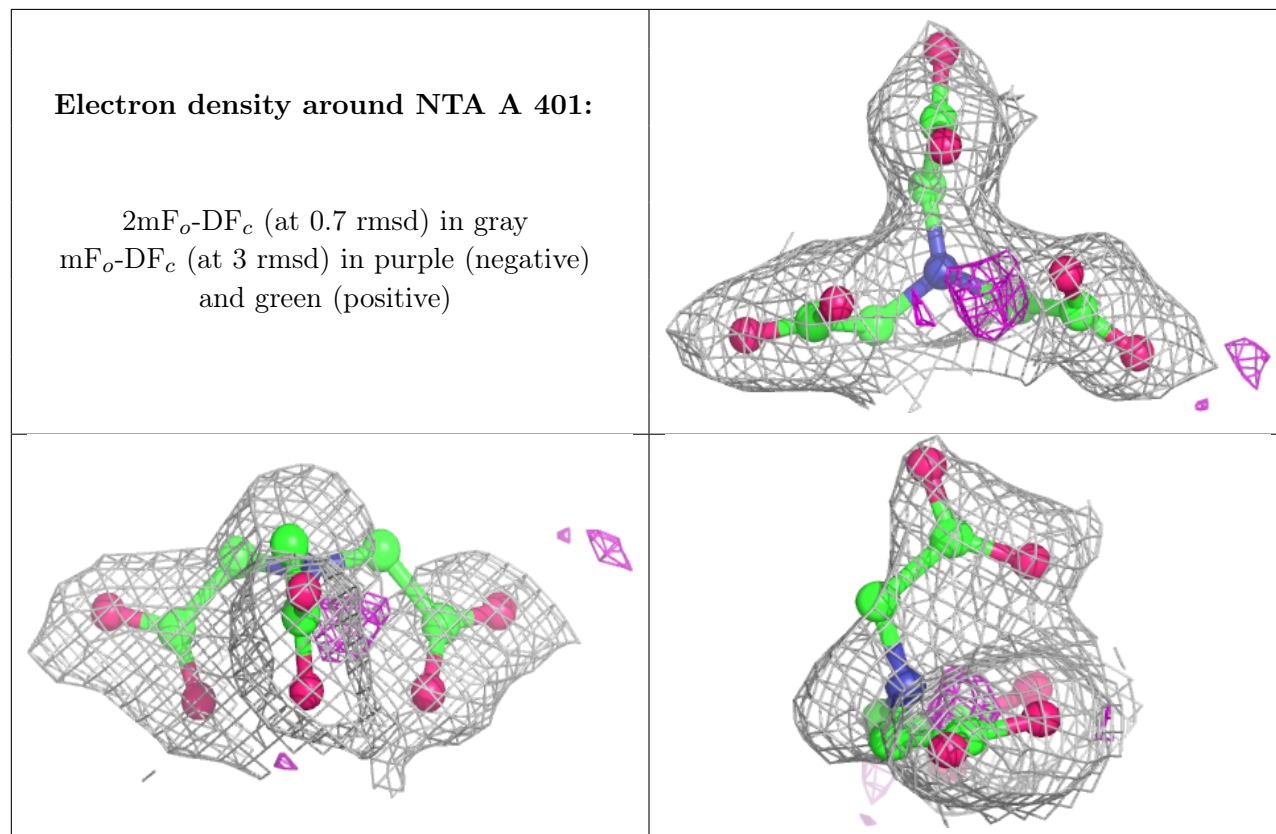
## 6.4 Ligands [i](#)

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
2	NTA	A	401	13/13	0.89	0.10	32,51,56,65	0
2	NTA	C	401	13/13	0.92	0.09	30,43,51,58	0
2	NTA	B	401	13/13	0.95	0.07	30,35,37,37	0
3	FE	A	402	1/1	0.98	0.08	44,44,44,44	0
3	FE	C	402	1/1	0.99	0.04	38,38,38,38	0
3	FE	B	402	1/1	1.00	0.02	30,30,30,30	0

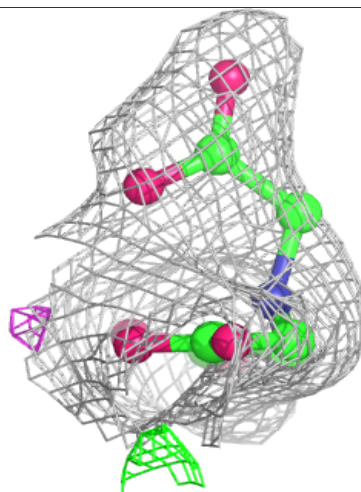
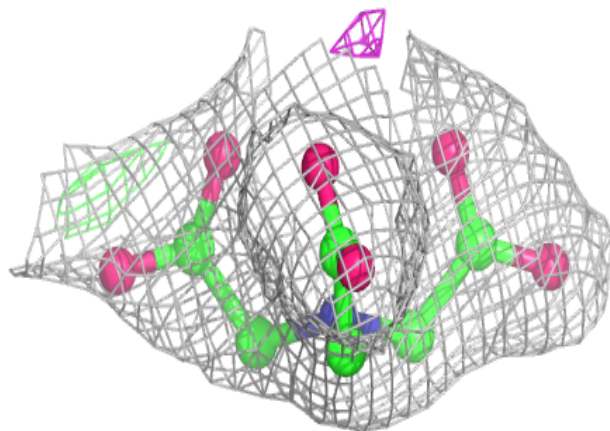
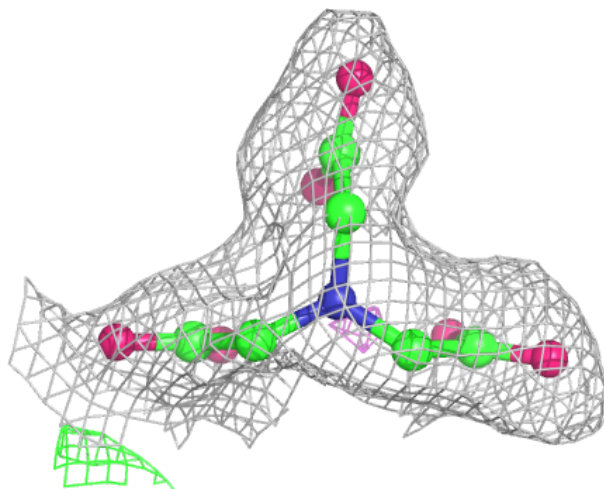
The following is a graphical depiction of the model fit to experimental electron density of all

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.



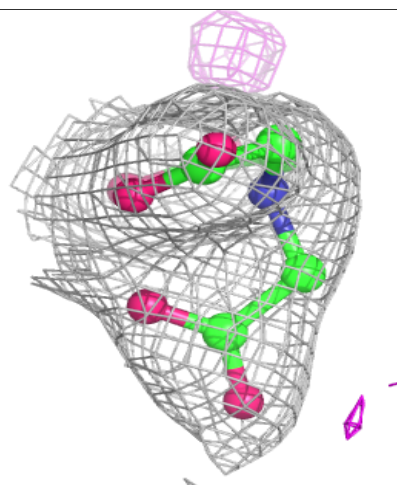
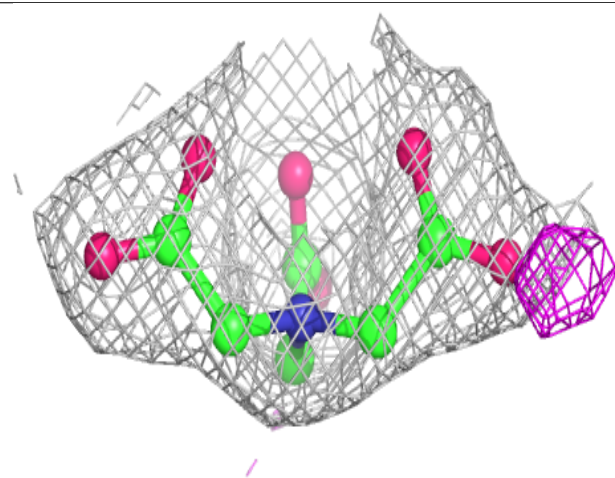
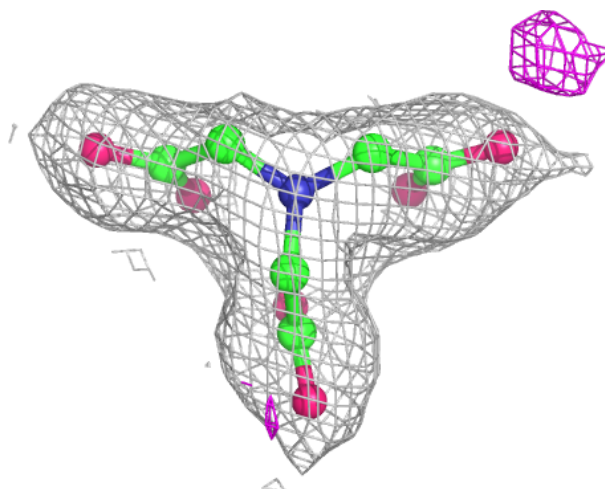
**Electron density around NTA C 401:**

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



**Electron density around NTA B 401:**

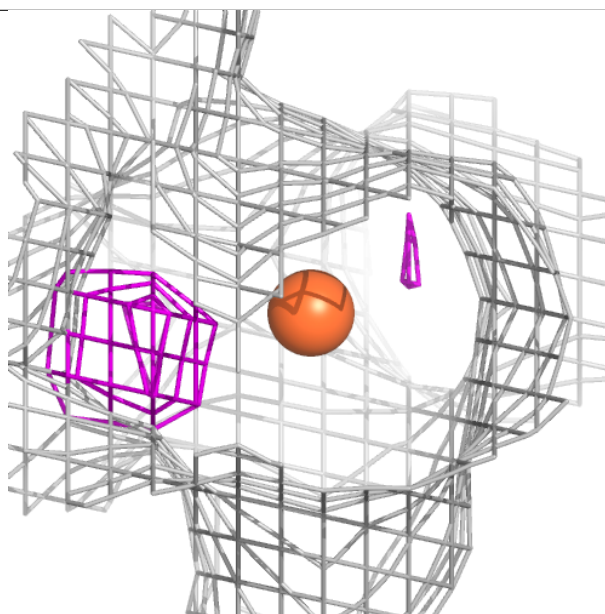
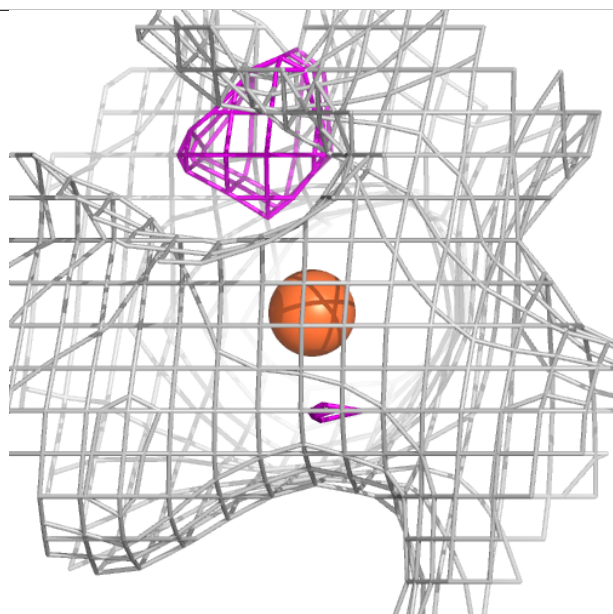
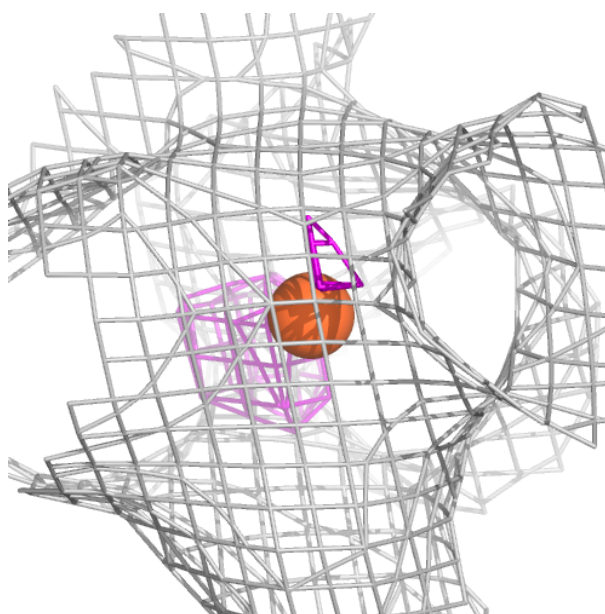
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FE A 402:**

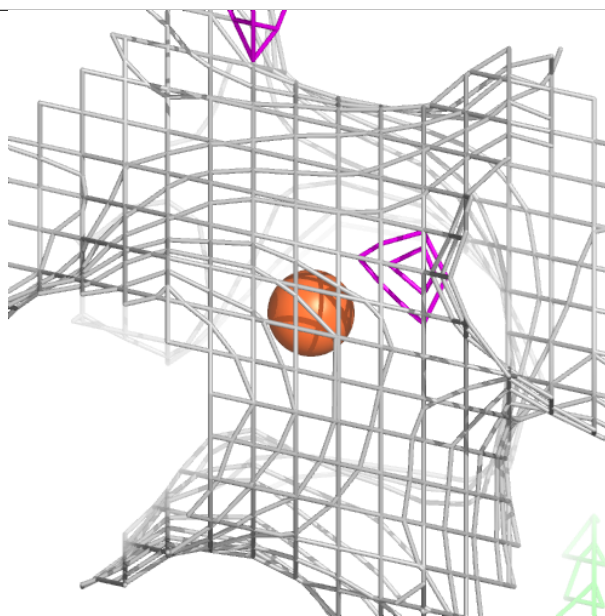
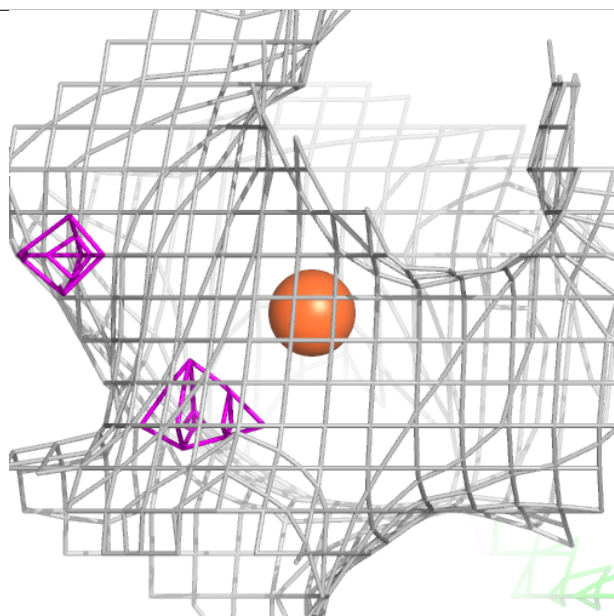
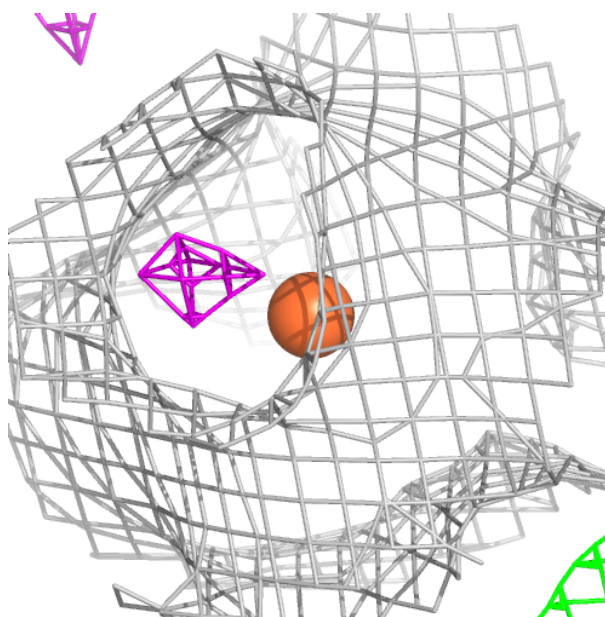
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





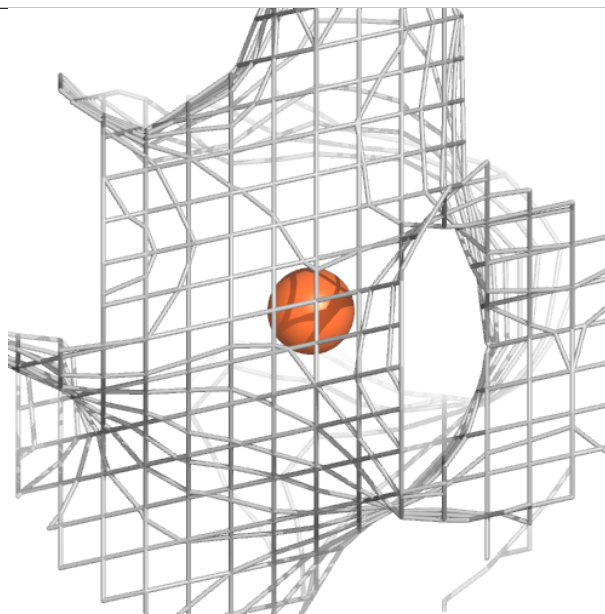
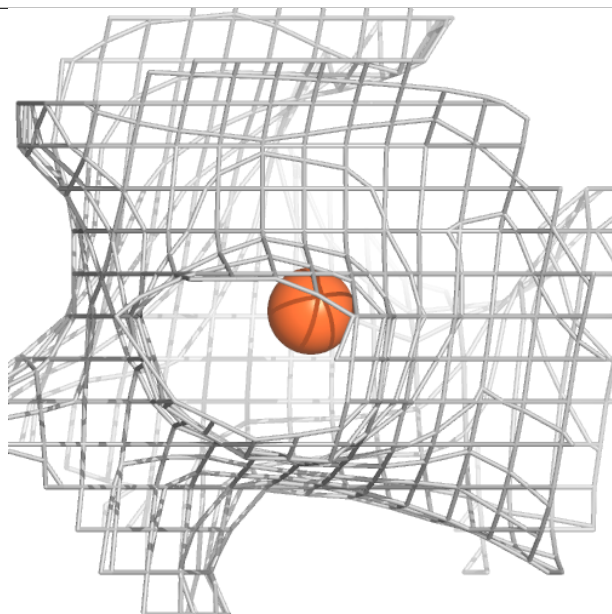
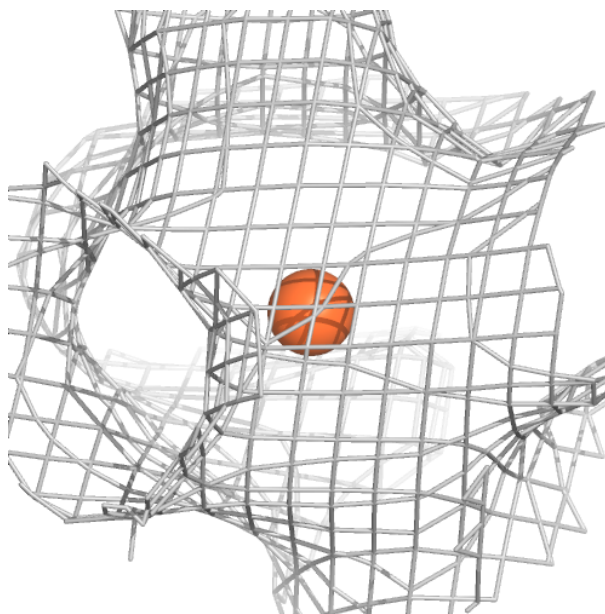
**Electron density around FE C 402:**

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



**Electron density around FE 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.