



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:45 pm BST

PDB ID : 5VPW  
Title : Nitrogenase Cp1 at pH 5  
Authors : Morrison, C.N.; Spatzal, T.; Rees, D.C.  
Deposited on : 2017-05-05  
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

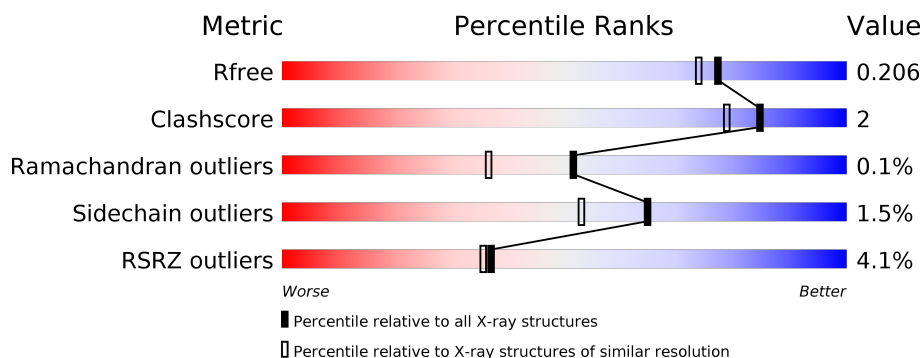
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	520	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>8%</div> <div>5%</div> </div> <div>• •</div> </div>
1	C	520	<div> <div>8%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>5%</div> </div> <div></div> </div>
2	B	458	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> <div></div> </div>
2	D	458	<div> <div>3%</div> <div> <div></div> <div>96%</div> </div> <div>•</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15565 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.

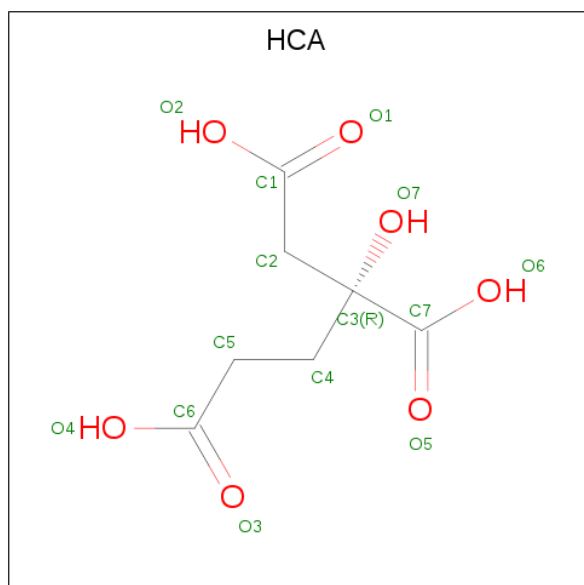
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	1	0
			4042	2570	676	768	28			
1	C	495	Total	C	N	O	S	0	0	0
			3856	2456	644	729	27			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

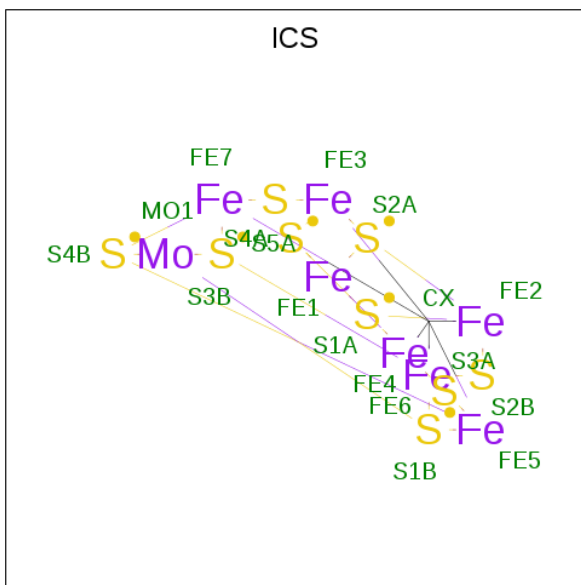
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	458	Total	C	N	O	S	0	1	0
			3525	2239	581	684	21			
2	D	458	Total	C	N	O	S	0	0	0
			3519	2236	580	682	21			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula:  $C_7H_{10}O_7$ ).



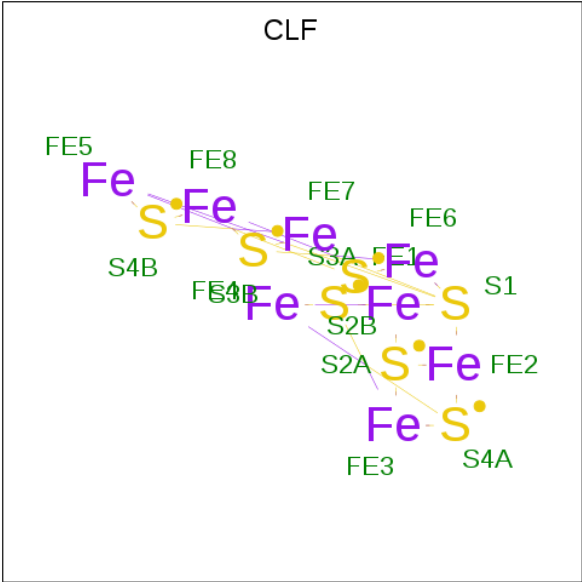
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula:  $\text{CFe}_7\text{MoS}_9$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		
4	C	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

- Molecule 5 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula:  $\text{Fe}_8\text{S}_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			15	8	7		
5	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Fe	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	163	Total	O	0	0
			163	163		
7	B	116	Total	O	0	0
			116	116		
7	C	115	Total	O	0	0
			115	115		
7	D	133	Total	O	0	0
			133	133		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.62Å 146.28Å 116.74Å 90.00° 103.55° 90.00°	Depositor
Resolution (Å)	39.20 – 1.85 39.20 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.20-1.85) 98.4 (39.20-1.85)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.167 , 0.201 0.177 , 0.206	Depositor DCC
$R_{free}$ test set	9635 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: ICS, CLF, HCA, FE2

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	0.58	0/4131	0.69	1/5582 (0.0%)
1	C	0.58	0/3942	0.69	0/5325
2	B	0.59	0/3596	0.70	1/4863 (0.0%)
2	D	0.60	0/3590	0.71	0/4855
All	All	0.59	0/15259	0.70	2/20625 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LEU	CA-CB-CG	6.14	129.43	115.30
2	B	58	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4042	0	3988	13	1
1	C	3856	0	3805	29	0
2	B	3525	0	3512	16	0
2	D	3519	0	3508	17	1
3	A	14	0	6	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	6	3	0
4	A	18	0	0	0	0
4	C	18	0	0	0	0
5	A	15	0	0	0	0
5	C	15	0	0	0	0
6	B	2	0	0	0	0
7	A	163	0	0	2	0
7	B	116	0	0	1	0
7	C	115	0	0	1	0
7	D	133	0	0	0	0
All	All	15565	0	14825	70	1

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 2.

All (70) 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:5:LEU:HD23	1:C:439:ILE:HD13	1.69	0.73
2:B:278:MET:HA	2:B:278:MET:CE	2.19	0.72
2:B:278:MET:HE1	1:C:519:TRP:HB3	1.72	0.71
1:C:435:HIS:NE2	1:C:438:THR:HG22	2.09	0.68
1:C:431:MET:CE	1:C:440:LEU:HD22	2.29	0.62
2:B:278:MET:HA	2:B:278:MET:HE2	1.81	0.61
1:A:430:MET:CE	7:A:851:HOH:O	2.50	0.60
1:A:287:ILE:HD12	7:A:806:HOH:O	2.02	0.59
1:A:349:HIS:CE1	1:A:433:GLU:HB3	2.37	0.57
2:B:106:CYS:HB3	2:B:141[A]:SER:OG	2.03	0.57
1:C:431:MET:HE2	1:C:440:LEU:HD22	1.86	0.56
2:D:23:CYS:HB2	2:D:141:SER:HB2	1.87	0.56
2:B:4:ALA:O	2:B:6:PRO:HD3	2.06	0.56
1:C:501:HIS:HD2	7:C:809:HOH:O	1.89	0.55
2:D:106:CYS:HB3	2:D:141:SER:OG	2.06	0.55
1:C:369:PHE:C	1:C:369:PHE:CD1	2.81	0.54
1:A:264:ARG:HD2	1:A:374:ASP:OD2	2.08	0.54
1:C:435:HIS:O	1:C:438:THR:HG23	2.09	0.53
1:A:225[B]:MET:HG2	1:A:286:PHE:CD2	2.44	0.53
2:B:403:ASN:ND2	2:B:448:GLU:OE1	2.35	0.50
2:D:409:PHE:CE1	2:D:424:LYS:CD	2.96	0.49
1:A:482:HIS:HB3	3:A:601:HCA:O6	2.13	0.49
2:B:454:PHE:CE1	2:D:400:ARG:HD3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:409:PHE:CE1	2:D:424:LYS:HD3	2.48	0.48
1:C:469:PHE:O	1:C:473:LYS:HG2	2.14	0.47
2:D:24:GLN:HA	2:D:146:HIS:HA	1.96	0.47
2:B:454:PHE:CZ	2:D:400:ARG:HD3	2.50	0.47
1:A:259:LEU:HB3	1:A:284:CYS:HB2	1.96	0.47
1:C:133:MET:HE1	2:D:12:ARG:HD3	1.95	0.47
1:A:93:PRO:HB3	1:A:98:GLY:O	2.15	0.47
3:A:601:HCA:O7	3:A:601:HCA:O2	2.34	0.46
2:B:400:ARG:HD3	2:D:454:PHE:CE1	2.51	0.46
2:B:103:HIS:ND1	7:B:601:HOH:O	1.75	0.45
1:C:342:TYR:CD2	1:C:444:MET:HE2	2.51	0.45
1:C:465:ILE:HG21	2:D:54:THR:HG23	1.98	0.45
1:C:431:MET:HE3	1:C:440:LEU:HD22	1.98	0.45
2:D:4:ALA:O	2:D:6:PRO:HD3	2.15	0.45
2:B:392:ASN:HB2	2:B:412:PRO:O	2.17	0.44
1:A:341:LEU:HD12	1:A:341:LEU:N	2.32	0.44
1:A:482:HIS:CG	3:A:601:HCA:H52	2.52	0.44
2:B:25:PRO:HB2	2:B:52:HIS:CE1	2.53	0.44
1:C:434:MET:HE2	1:C:434:MET:HB3	1.91	0.44
1:C:462:PHE:HB3	1:C:481:LEU:HG	2.00	0.44
1:C:342:TYR:CD2	1:C:444:MET:CE	3.00	0.44
1:C:342:TYR:CG	1:C:444:MET:HE2	2.53	0.43
1:C:482:HIS:HB3	3:C:601:HCA:O5	2.19	0.43
1:C:369:PHE:HD1	1:C:369:PHE:O	2.02	0.43
3:C:601:HCA:O1	3:C:601:HCA:O7	2.37	0.43
2:B:400:ARG:HD3	2:D:454:PHE:CZ	2.55	0.42
1:C:191:ASN:ND2	1:C:394:PRO:O	2.50	0.42
1:C:61:VAL:HA	1:C:87:ARG:NH1	2.34	0.42
1:C:191:ASN:O	1:C:195:THR:HG23	2.19	0.42
1:C:259:LEU:HD21	1:C:299:MET:HG2	2.02	0.42
1:C:482:HIS:CG	3:C:601:HCA:H52	2.55	0.42
2:D:2:LEU:HD11	2:D:397:PHE:HB3	2.01	0.42
2:D:409:PHE:CE1	2:D:424:LYS:HD2	2.55	0.42
1:C:289:VAL:O	1:C:293:VAL:HG13	2.20	0.42
1:A:482:HIS:ND1	3:A:601:HCA:H52	2.35	0.41
2:D:451:GLU:O	2:D:454:PHE:HB2	2.21	0.41
1:C:345:GLY:O	1:C:370:ALA:HB2	2.21	0.41
1:C:369:PHE:O	1:C:369:PHE:CD1	2.74	0.41
1:A:92:LYS:HG2	1:A:223:TRP:CZ2	2.56	0.41
2:B:23:CYS:HB2	2:B:141[A]:SER:HB2	2.03	0.41
1:C:435:HIS:CD2	1:C:438:THR:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ILE:HB	1:C:350:THR:HB	2.03	0.41
2:B:428:LYS:HE2	2:B:428:LYS:HB3	1.90	0.40
2:D:191:PHE:CZ	2:D:280:LEU:HD21	2.56	0.40
1:A:240:LEU:HA	1:A:241:THR:HA	1.74	0.40
2:B:169:ASN:OD1	2:B:235:SER:HA	2.22	0.40
2:D:23:CYS:CB	2:D:141:SER:HB2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:OE2	2:D:72:THR:OG1[1_556]	1.85	0.35

## 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	516/520 (99%)	497 (96%)	18 (4%)	1 (0%)	47	33
1	C	491/520 (94%)	471 (96%)	19 (4%)	1 (0%)	47	33
2	B	457/458 (100%)	448 (98%)	9 (2%)	0	100	100
2	D	456/458 (100%)	450 (99%)	6 (1%)	0	100	100
All	All	1920/1956 (98%)	1866 (97%)	52 (3%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	C	48	ILE

### 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	435/437 (100%)	424 (98%)	11 (2%)	47	31
1	C	414/437 (95%)	406 (98%)	8 (2%)	57	43
2	B	385/384 (100%)	380 (99%)	5 (1%)	69	58
2	D	384/384 (100%)	383 (100%)	1 (0%)	92	91
All	All	1618/1642 (98%)	1593 (98%)	25 (2%)	65	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	92	LYS
1	A	204	GLU
1	A	286	PHE
1	A	294	GLU
1	A	341	LEU
1	A	386	ILE
1	A	392	ASN
1	A	402	GLU
1	A	413	LYS
1	A	461	PHE
2	B	262	LYS
2	B	307	GLN
2	B	364	GLU
2	B	424	LYS
2	B	454	PHE
1	C	31	GLU
1	C	40	ASN
1	C	42	ARG
1	C	286	PHE
1	C	294	GLU
1	C	413	LYS
1	C	439	ILE
1	C	461	PHE
2	D	8	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	205	GLN
1	A	349	HIS
1	A	353	ASN
1	A	403	GLN
1	A	501	HIS
2	B	422	ASN
1	C	4	ASN
1	C	501	HIS
2	D	307	GLN
2	D	308	GLN
2	D	422	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HCA	A	601	-	4,13,13	0.65	0	4,18,18	2.96	3 (75%)
4	ICS	A	602	1	18,30,30	2.44	10 (55%)	-		
4	ICS	C	602	1	18,30,30	2.69	9 (50%)	-		
5	CLF	C	603	1,2	0,24,24	0.00	-	-		
5	CLF	A	603	1,2	0,24,24	0.00	-	-		
3	HCA	C	601	-	4,13,13	1.12	0	4,18,18	2.66	1 (25%)

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
5	CLF	C	603	1,2	-	-	0/12/10/10
3	HCA	A	601	-	-	1/7/17/17	-
5	CLF	A	603	1,2	-	-	0/12/10/10
3	HCA	C	601	-	-	2/7/17/17	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ICS	S1B-FE6	-5.93	2.17	2.32
4	A	602	ICS	S1B-FE6	-4.66	2.20	2.32
4	C	602	ICS	S4B-FE7	-4.39	2.21	2.32
4	C	602	ICS	S2A-FE2	-4.38	2.21	2.32
4	A	602	ICS	S4A-FE3	-3.84	2.22	2.32
4	C	602	ICS	S3B-FE6	-3.53	2.23	2.32
4	A	602	ICS	S5A-FE3	3.12	2.32	2.24
4	A	602	ICS	S2A-FE2	-2.96	2.25	2.32
4	C	602	ICS	S1B-FE5	-2.81	2.25	2.32
4	C	602	ICS	S3B-FE7	-2.71	2.25	2.32
4	C	602	ICS	S2B-FE6	-2.63	2.18	2.24
4	A	602	ICS	S5A-FE7	-2.54	2.18	2.24
4	A	602	ICS	S4B-FE7	-2.54	2.26	2.32
4	A	602	ICS	S4B-FE5	-2.52	2.26	2.32
4	A	602	ICS	S3B-FE6	-2.48	2.26	2.32
4	C	602	ICS	S1A-FE4	-2.46	2.26	2.32
4	C	602	ICS	S1A-FE2	-2.38	2.26	2.32
4	A	602	ICS	S2B-FE6	-2.30	2.19	2.24
4	A	602	ICS	S2A-FE3	-2.06	2.27	2.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	HCA	C4-C5-C6	4.88	118.77	111.39
3	A	601	HCA	C4-C5-C6	4.28	117.88	111.39
3	A	601	HCA	C4-C3-C7	-3.10	106.06	111.52
3	A	601	HCA	C3-C2-C1	-2.34	111.23	114.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	HCA	C1-C2-C3-C4
3	A	601	HCA	C1-C2-C3-C4
3	C	601	HCA	C2-C3-C4-C5

There are no ring outliers.

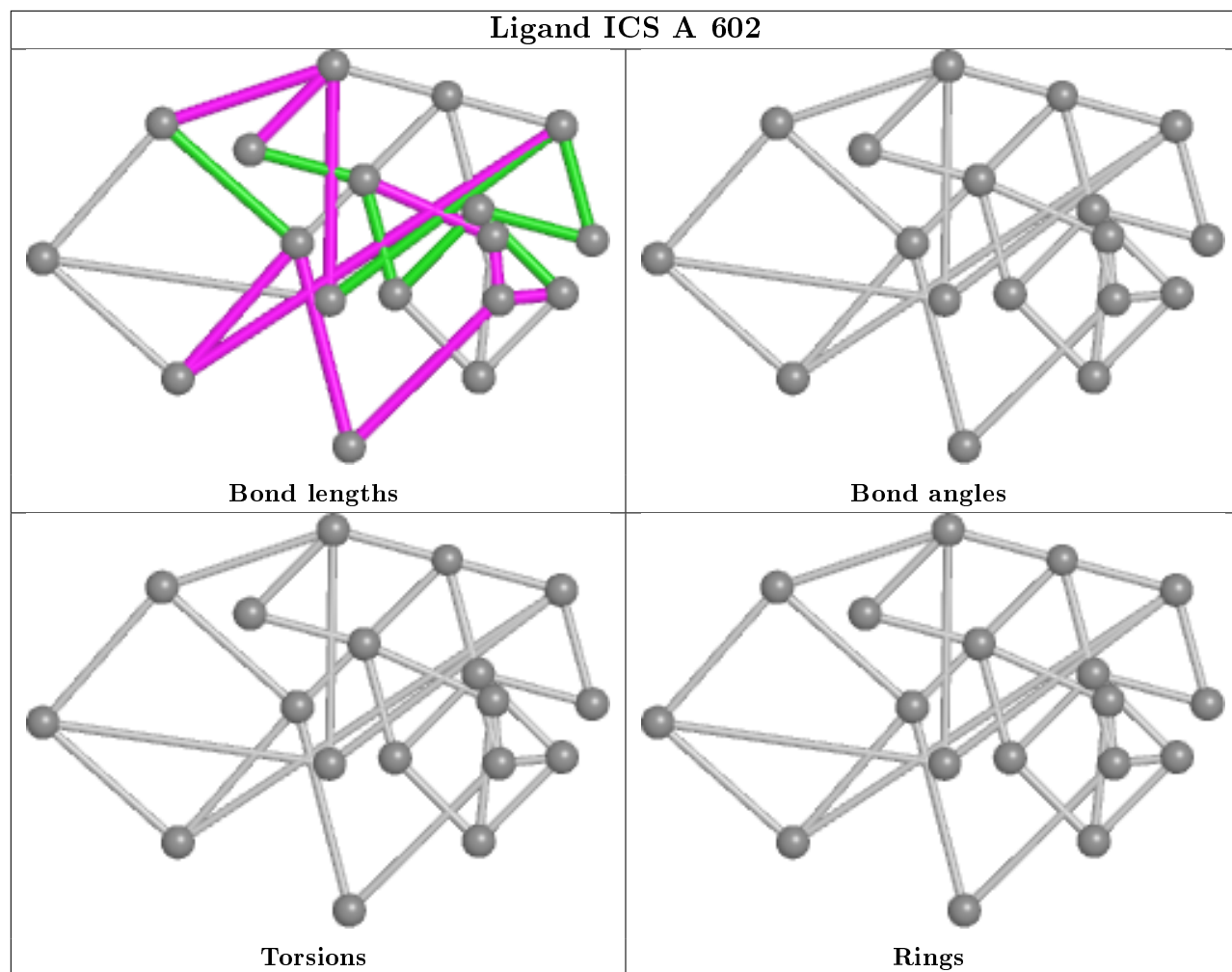
2 monomers are involved in 7 short contacts:

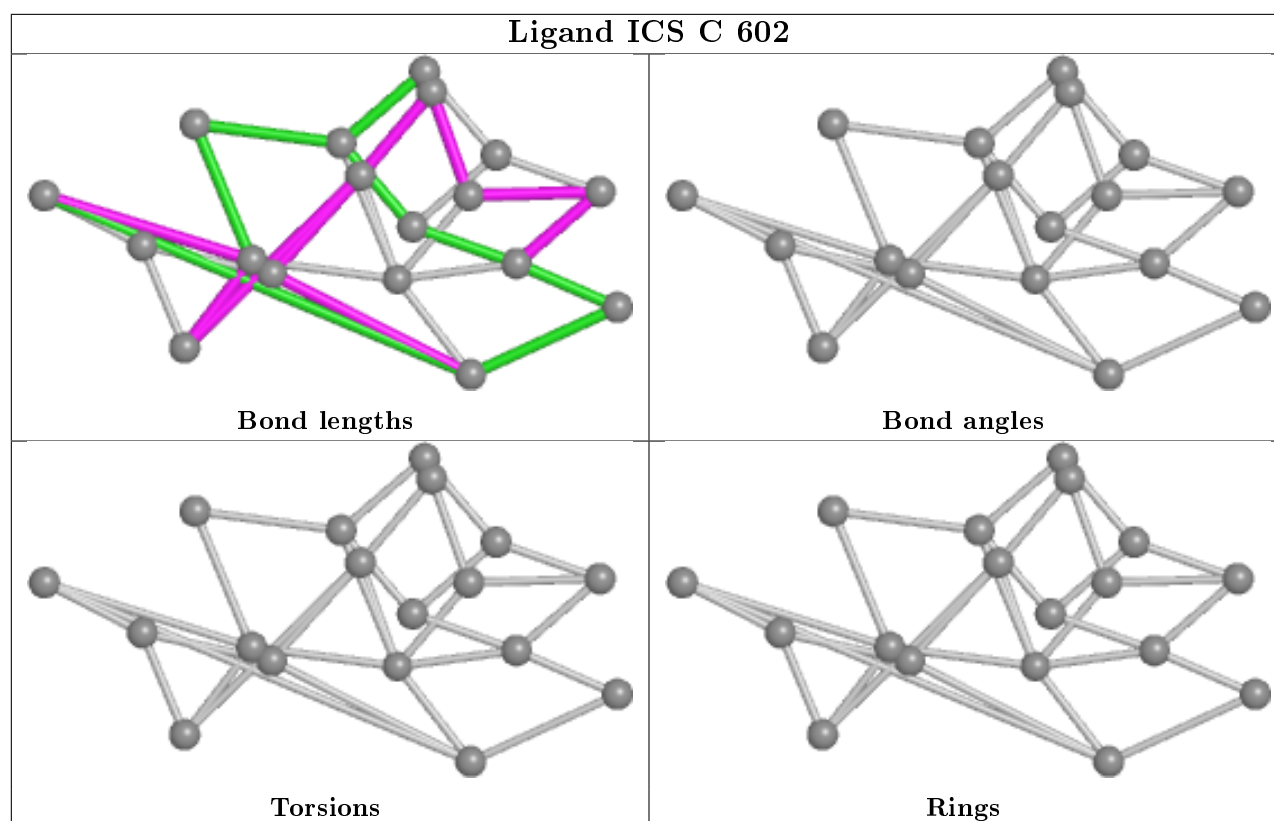
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HCA	4	0
3	C	601	HCA	3	0

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 ICS A 602





## 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	517/520 (99%)	-0.33	12 (2%) 60 59	15, 24, 53, 88	0
1	C	495/520 (95%)	-0.02	43 (8%) 10 9	16, 26, 80, 125	0
2	B	458/458 (100%)	-0.28	12 (2%) 56 54	15, 23, 50, 96	0
2	D	458/458 (100%)	-0.32	12 (2%) 56 54	15, 23, 47, 98	0
All	All	1928/1956 (98%)	-0.24	79 (4%) 37 35	15, 24, 58, 125	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	GLU	6.7
1	C	32	THR	6.2
1	C	402	GLU	6.0
2	B	8	GLU	5.8
2	D	8	GLU	5.8
1	C	407	VAL	5.6
2	B	3	ASP	5.4
1	C	403	GLN	5.2
1	C	412	ASP	5.1
1	A	382	PRO	5.1
1	A	386	ILE	5.0
1	C	30	GLU	4.9
1	C	420	ALA	4.9
1	C	29	THR	4.8
2	B	9	ILE	4.8
1	C	36	GLU	4.8
1	C	399	THR	4.7
1	C	415	GLU	4.6
2	D	5	THR	4.5
2	D	9	ILE	4.4
2	B	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	1	MET	4.4
2	D	2	LEU	4.4
1	C	408	VAL	4.3
1	C	400	PRO	4.2
1	C	405	TYR	4.1
1	C	411	GLU	4.0
1	C	35	PRO	4.0
1	C	432	LYS	4.0
1	C	404	LYS	3.9
1	C	410	PRO	3.9
1	C	419	LYS	3.9
2	B	2	LEU	3.7
2	B	7	LYS	3.7
2	B	5	THR	3.7
2	D	3	ASP	3.7
1	C	396	ILE	3.6
1	C	421	GLY	3.6
1	C	414	VAL	3.6
2	B	4	ALA	3.5
1	C	397	THR	3.4
2	B	454	PHE	3.4
2	D	6	PRO	3.4
1	A	381	ILE	3.4
1	A	383	THR	3.3
1	C	398	VAL	3.3
1	C	409	ILE	3.3
1	C	34	ASN	3.2
1	C	416	GLU	3.2
1	C	370	ALA	3.1
1	C	401	ASP	3.1
1	C	433	GLU	3.0
1	A	385	LYS	3.0
1	C	436	ASP	2.9
1	C	418	LYS	2.9
1	C	413	LYS	2.8
2	B	6	PRO	2.8
2	D	10	VAL	2.8
1	C	33	PRO	2.8
1	C	406	ARG	2.8
1	A	306	PRO	2.7
2	D	454	PHE	2.7
1	C	423	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	465	ILE	2.4
1	A	30	GLU	2.4
1	A	388	ALA	2.3
1	A	384	ILE	2.2
1	C	27	ILE	2.2
2	B	26	VAL	2.1
2	D	7	LYS	2.1
1	A	415	GLU	2.1
1	C	427	TYR	2.1
2	D	287	GLU	2.1
1	A	97	THR	2.0
2	D	4	ALA	2.0
1	A	31	GLU	2.0
1	C	431	MET	2.0
2	B	55	VAL	2.0
1	C	395	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å <sup>2</sup> )	Q<0.9
3	HCA	A	601	14/14	0.97	0.14	14,17,20,24	0
3	HCA	C	601	14/14	0.98	0.14	16,18,24,24	0
6	FE2	B	501	1/1	0.99	0.09	16,16,16,16	1
4	ICS	A	602	18/18	1.00	0.09	15,16,18,18	0
5	CLF	C	603	15/15	1.00	0.07	17,18,20,21	0
6	FE2	B	502	1/1	1.00	0.11	16,16,16,16	1
5	CLF	A	603	15/15	1.00	0.08	15,16,18,20	0

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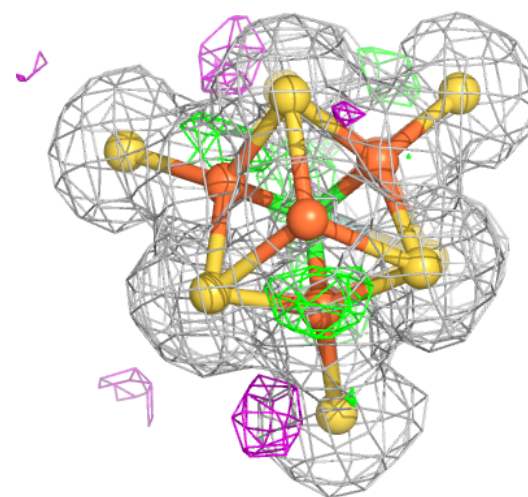
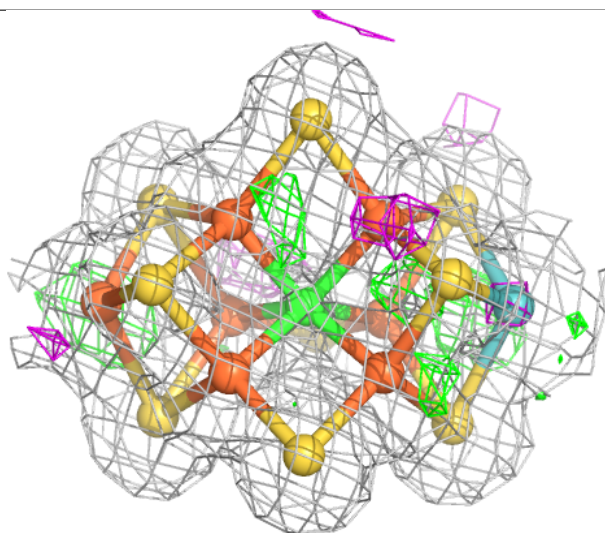
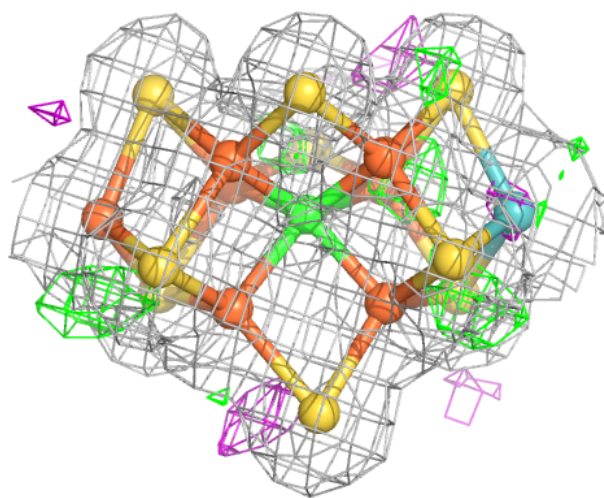
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ICS	C	602	18/18	1.00	0.09	18,20,21,21	0

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.

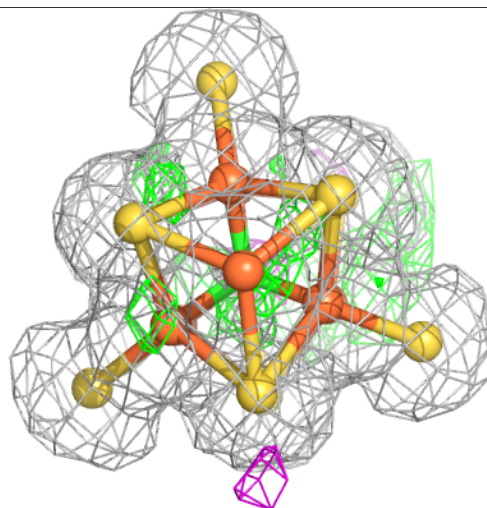
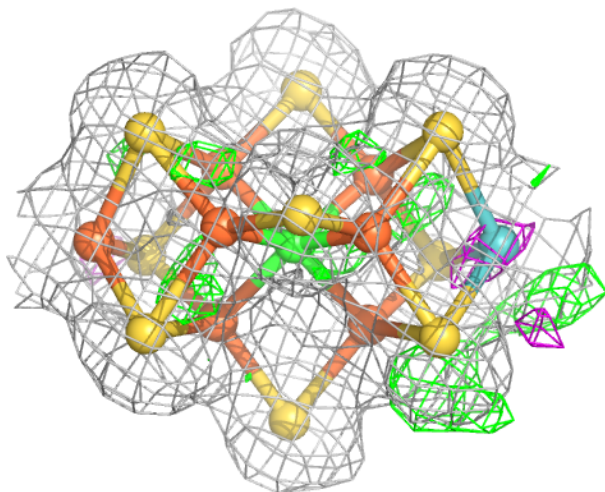
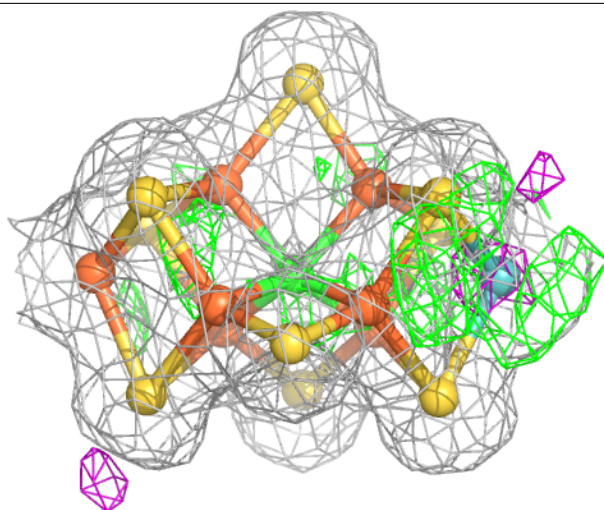
**Electron density around ICS A 602:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ICS C 602:**

$2mF_o-DF_c$  (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.