



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:42 PM UTC

PDB ID : 5VPW / pdb_00005vpw
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

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>.

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

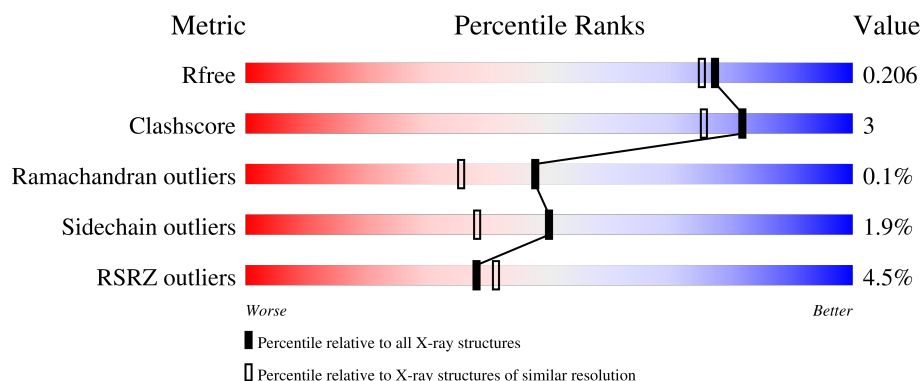
1 Overall quality at a glance

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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	3% 94% 5% ..
1	C	520	8% 86% 9% • 5%
2	B	458	3% 94% 6%
2	D	458	3% 95% 5%

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.

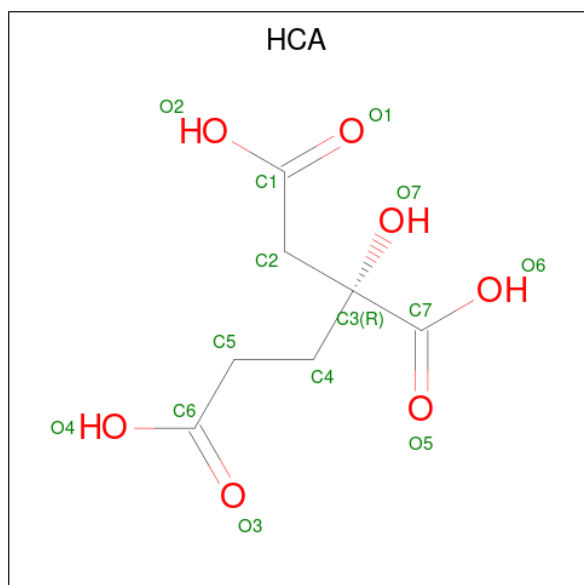
- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein alpha chain.

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.

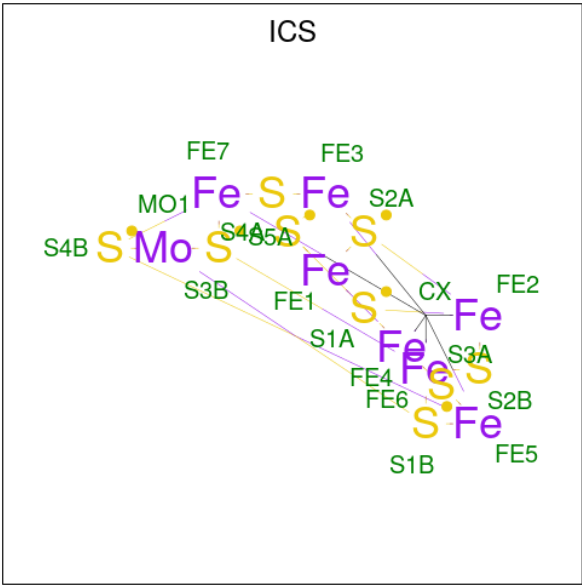
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	458	Total	C	N	O	S	0	1	0
			3525	2239	581	684	21			
2	D	458	Total	C	N	O	S	0	0	0
			3519	2236	580	682	21			

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



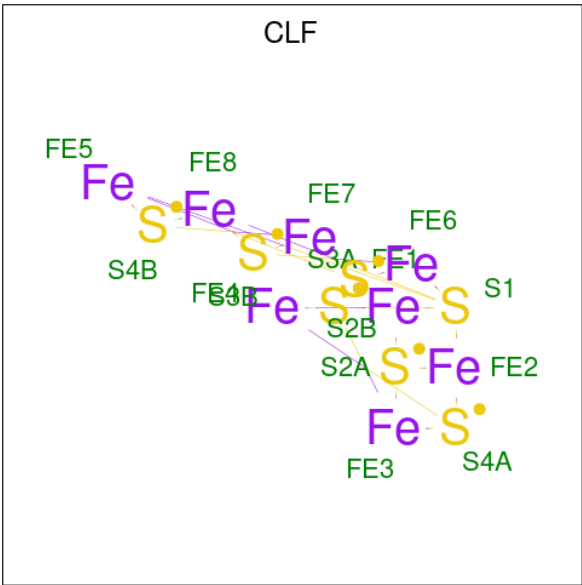
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe₇MoS₉).



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 (CCD ID: CLF) (formula: Fe₈S₇).



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 (CCD ID: FE2) (formula: Fe).

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

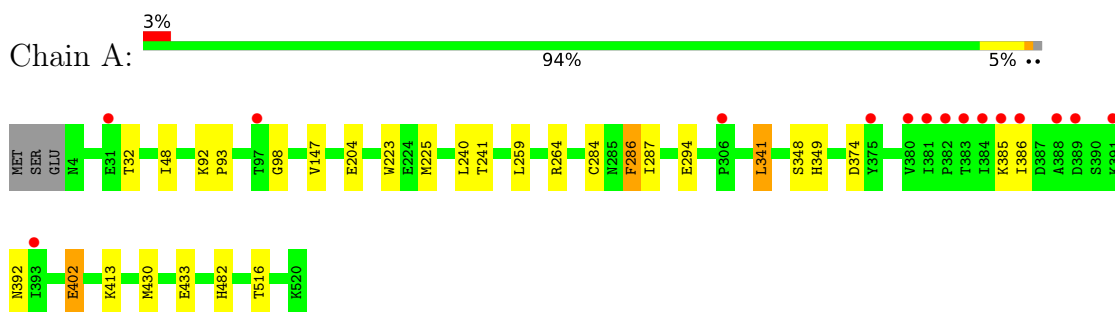
- Molecule 7 is water.

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		

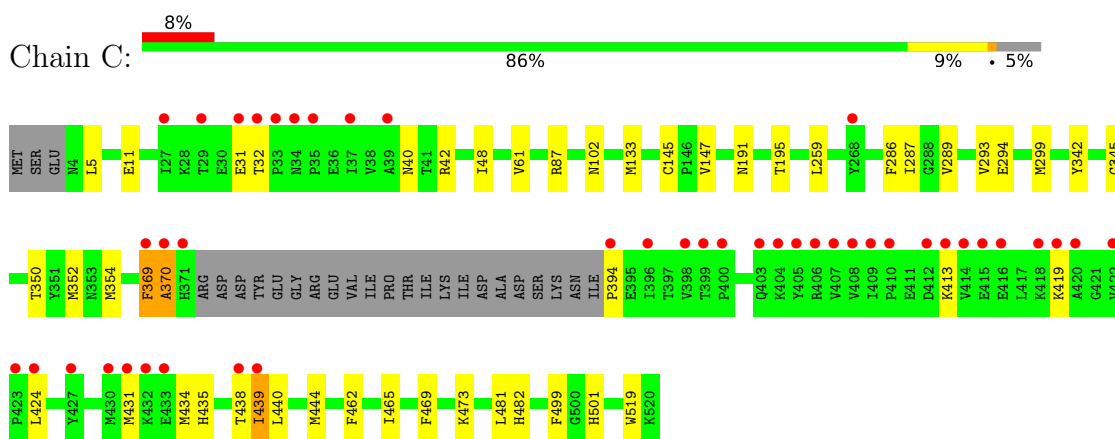
3 Residue-property plots [i](#)

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.

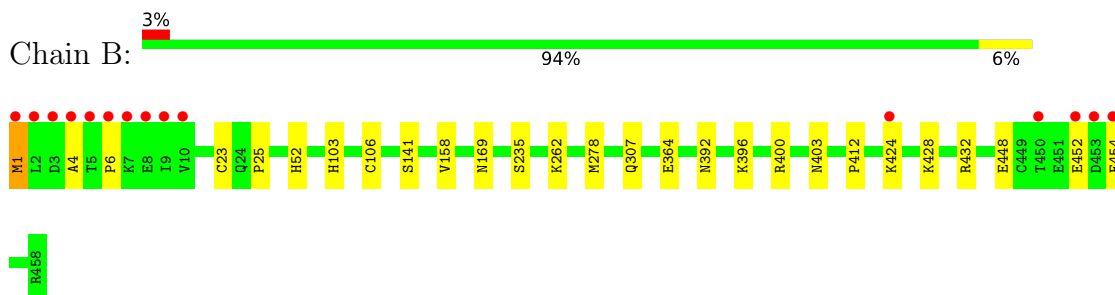
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



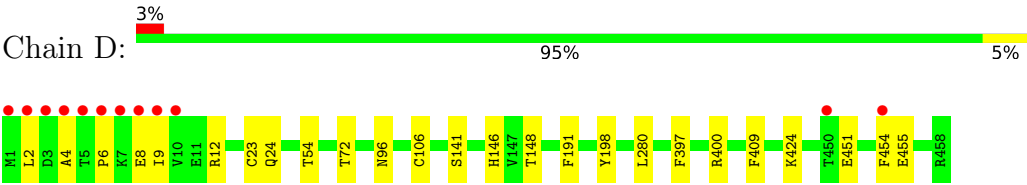
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	9638 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, FE2, HCA

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	0.80	0/4131	0.88	3/5582 (0.1%)
1	C	0.80	3/3942 (0.1%)	0.89	5/5325 (0.1%)
2	B	0.81	0/3596	0.92	0/4863
2	D	0.81	1/3590 (0.0%)	0.92	1/4855 (0.0%)
All	All	0.80	4/15259 (0.0%)	0.90	9/20625 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	96	ASN	C-O	-7.36	1.20	1.23
1	C	370	ALA	CA-C	6.06	1.60	1.52
1	C	369	PHE	C-O	5.52	1.28	1.23
1	C	370	ALA	C-O	-5.44	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	ILE	N-CA-C	9.79	122.36	108.36
1	A	147	VAL	N-CA-C	7.00	117.14	110.42
1	C	369	PHE	N-CA-C	6.39	122.15	113.21
1	A	516	THR	CA-C-N	-5.22	115.00	120.38
1	A	516	THR	C-N-CA	-5.22	115.00	120.38
1	C	11	GLU	N-CA-C	5.10	117.23	111.11
1	C	145	CYS	CA-C-N	-5.07	114.57	120.04
1	C	145	CYS	C-N-CA	-5.07	114.57	120.04
1	C	147	VAL	N-CA-C	5.05	115.27	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4042	0	3988	14	1
1	C	3856	0	3805	30	0
2	B	3525	0	3512	19	0
2	D	3519	0	3508	20	1
3	A	14	0	6	4	0
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	76	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 3.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:MET:HA	2:B:278:MET:HE2	1.35	1.02
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	0.70
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
1:C:431:MET:HE2	1:C:440:LEU:HD22	1.80	0.61
1:A:430:MET:CE	7:A:851:HOH:O	2.50	0.60
1:C:369:PHE:CD1	1:C:369:PHE:C	2.81	0.59
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
2:D:23:CYS:HB2	2:D:141:SER:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ALA:O	2:B:6:PRO:HD3	2.06	0.56
2:B:278:MET:HE1	1:C:519:TRP:HB3	1.86	0.55
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: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
1:C:133:MET:HE1	2:D:12:ARG:HD3	1.93	0.51
2:B:1:MET:HE1	2:D:454:PHE:CG	2.46	0.50
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
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:C:354:MET:HE3	1:C:499:PHE:CD2	2.49	0.47
1:A:259:LEU:HB3	1:A:284:CYS:HB2	1.96	0.47
1:A:93:PRO:HB3	1:A:98:GLY:O	2.15	0.47
3:A:601:HCA:O2	3:A:601:HCA:O7	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	2.52	0.45
1:C:465:ILE:HG21	2:D:54:THR:HG23	1.98	0.45
2:D:4:ALA:O	2:D:6:PRO:HD3	2.15	0.45
1:A:348:SER:H	1:A:430:MET:HE1	1.82	0.45
2:B:392:ASN:HB2	2:B:412:PRO:O	2.17	0.44
1:C:342:TYR:CG	1:C:444:MET:HE2	2.52	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
2:B:278:MET:HE2	2:B:278:MET:CA	2.26	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:482:HIS:HB3	3:C:601:HCA:O5	2.19	0.43
1:C:369:PHE:O	1:C:369:PHE:HD1	2.02	0.43
3:C:601:HCA:O1	3:C:601:HCA:O7	2.37	0.43
2:B:396:LYS:NZ	2:D:455:GLU:O	2.49	0.42
2:B:400:ARG:HD3	2:D:454:PHE:CZ	2.55	0.42
1:C:352:MET:SD	1:C:434:MET:HE3	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HA	1:C:87:ARG:NH1	2.34	0.42
1:C:191:ASN:ND2	1:C:394:PRO:O	2.50	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:CD1	1:C:369:PHE:O	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
1:C:287:ILE:HB	1:C:350:THR:HB	2.03	0.41
1:C:352:MET:HE1	1:C:434:MET:HE3	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
2:D:198:TYR:CD2	2:D:198:TYR:C	2.99	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

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	516/520 (99%)	497 (96%)	18 (4%)	1 (0%)	43	31
1	C	491/520 (94%)	471 (96%)	19 (4%)	1 (0%)	43	31
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%)	48	35

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%)	425 (98%)	10 (2%)	44	30
1	C	414/437 (95%)	403 (97%)	11 (3%)	39	24
2	B	385/384 (100%)	377 (98%)	8 (2%)	47	33
2	D	384/384 (100%)	382 (100%)	2 (0%)	81	77
All	All	1618/1642 (98%)	1587 (98%)	31 (2%)	50	38

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	204	GLU
1	A	286	PHE
1	A	294	GLU
1	A	341	LEU
1	A	385	LYS
1	A	386	ILE
1	A	392	ASN
1	A	402	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	LYS
2	B	1	MET
2	B	158	VAL
2	B	262	LYS
2	B	307	GLN
2	B	364	GLU
2	B	424	LYS
2	B	432	ARG
2	B	452	GLU
1	C	31	GLU
1	C	32	THR
1	C	40	ASN
1	C	42	ARG
1	C	102	ASN
1	C	286	PHE
1	C	294	GLU
1	C	413	LYS
1	C	419	LYS
1	C	424	LEU
1	C	439	ILE
2	D	8	GLU
2	D	148	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	205	GLN
1	A	211	ASN
1	A	237	ASN
1	A	349	HIS
1	A	353	ASN
1	A	403	GLN
1	A	487	ASN
1	A	501	HIS
2	B	422	ASN
1	C	263	HIS
1	C	349	HIS
1	C	501	HIS
2	D	90	ASN
2	D	138	ASN
2	D	307	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	CLF	A	603	2,1	0,24,24	-	-	-		
3	HCA	A	601	-	13,13,13	1.08	0	15,18,18	1.71	4 (26%)
5	CLF	C	603	2,1	0,24,24	-	-	-		
3	HCA	C	601	-	13,13,13	0.96	0	15,18,18	1.36	2 (13%)
4	ICS	A	602	1	6,30,30	2.07	3 (50%)	-		
4	ICS	C	602	1	6,30,30	1.39	1 (16%)	-		

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HCA	C	601	-	-	2/17/17/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ICS	S5A-FE3	3.12	2.32	2.24
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	S2B-FE6	-2.30	2.19	2.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HCA	O6-C7-C3	3.98	120.78	113.14
3	C	601	HCA	O6-C7-C3	2.77	118.46	113.14
3	C	601	HCA	C4-C5-C6	2.59	118.77	112.77
3	A	601	HCA	O4-C6-C5	2.27	121.18	114.00
3	A	601	HCA	C4-C5-C6	2.20	117.88	112.77
3	A	601	HCA	O3-C6-C5	-2.11	116.40	123.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	HCA	C1-C2-C3-C4
3	C	601	HCA	C1-C2-C3-C7
3	A	601	HCA	O2-C1-C2-C3
3	A	601	HCA	C4-C3-C7-O6
3	A	601	HCA	O1-C1-C2-C3

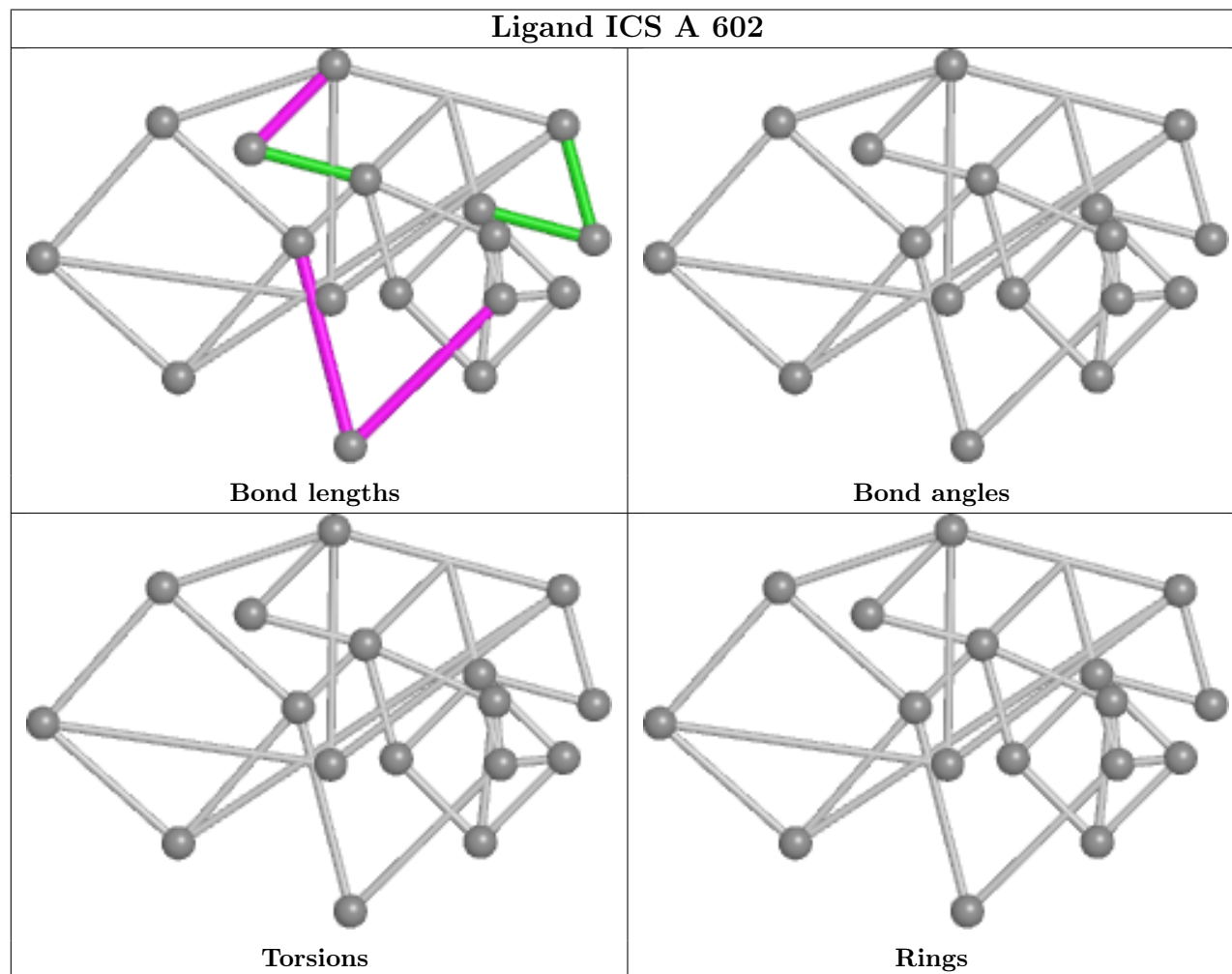
There are no ring outliers.

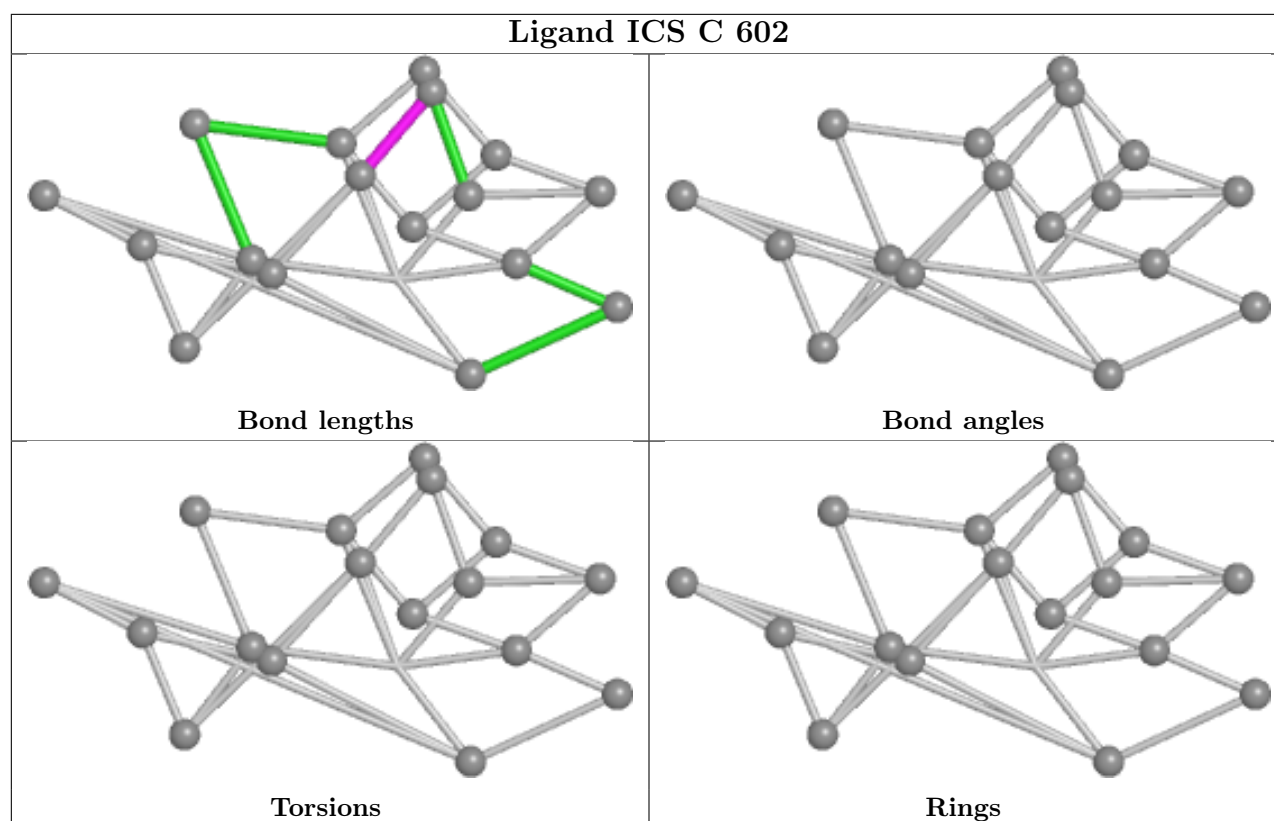
2 monomers are involved in 7 short contacts:

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.





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, 95th 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 ²)	Q<0.9
1	A	517/520 (99%)	-0.09	15 (2%) 53 57	13, 24, 53, 88	1 (0%)
1	C	495/520 (95%)	0.23	44 (8%) 15 15	16, 26, 80, 125	0
2	B	458/458 (100%)	-0.11	15 (3%) 49 53	10, 23, 50, 96	1 (0%)
2	D	458/458 (100%)	-0.17	12 (2%) 57 61	15, 23, 47, 98	0
All	All	1928/1956 (98%)	-0.03	86 (4%) 38 41	10, 24, 58, 125	2 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	454	PHE	7.6
2	D	454	PHE	6.3
1	A	386	ILE	6.2
2	D	9	ILE	6.1
2	B	6	PRO	5.8
1	C	396	ILE	5.8
2	D	1	MET	5.7
2	D	2	LEU	5.5
1	C	394	PRO	5.3
1	C	370	ALA	5.1
2	B	1	MET	5.1
1	C	371	HIS	5.0
1	C	409	ILE	4.8
2	B	2	LEU	4.8
1	C	408	VAL	4.7
2	B	5	THR	4.7
1	C	407	VAL	4.7
2	B	10	VAL	4.4
1	A	382	PRO	4.4
1	C	29	THR	4.2
2	D	10	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	32	THR	4.0
2	D	5	THR	4.0
1	A	381	ILE	3.9
1	C	414	VAL	3.9
2	B	9	ILE	3.8
1	C	398	VAL	3.8
2	B	4	ALA	3.7
1	C	404	LYS	3.7
2	D	8	GLU	3.7
1	C	430	MET	3.7
1	A	384	ILE	3.7
1	C	27	ILE	3.6
1	C	400	PRO	3.5
2	B	7	LYS	3.4
1	C	33	PRO	3.4
2	B	3	ASP	3.4
1	A	388	ALA	3.4
1	C	37	ILE	3.3
1	A	306	PRO	3.3
2	D	4	ALA	3.3
2	D	6	PRO	3.2
1	C	424	LEU	3.2
1	A	380	VAL	3.1
2	D	3	ASP	3.0
1	C	399	THR	3.0
1	C	405	TYR	3.0
1	C	35	PRO	2.8
1	A	385	LYS	2.7
1	C	412	ASP	2.7
1	C	439	ILE	2.7
1	C	423	PRO	2.6
2	B	8	GLU	2.6
1	C	427	TYR	2.6
2	D	7	LYS	2.6
1	C	268	TYR	2.5
1	C	31	GLU	2.5
2	B	452	GLU	2.5
1	C	420	ALA	2.5
1	A	389	ASP	2.5
1	C	419	LYS	2.5
1	A	383	THR	2.5
2	B	453	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	369	PHE	2.4
1	C	431	MET	2.4
1	C	432	LYS	2.4
1	C	438	THR	2.3
2	B	450	THR	2.3
1	C	410	PRO	2.3
1	A	97	THR	2.3
1	C	34	ASN	2.3
1	A	393	ILE	2.3
1	C	413	LYS	2.3
1	C	415	GLU	2.2
1	A	391	LYS	2.2
1	C	418	LYS	2.2
1	A	31	GLU	2.2
1	C	433	GLU	2.2
1	C	403	GLN	2.2
1	C	39	ALA	2.2
2	B	424	LYS	2.2
1	C	406	ARG	2.2
2	D	450	THR	2.1
1	C	422	VAL	2.1
1	C	416	GLU	2.1
1	A	375	TYR	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, 95th 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.

Continued on next page...

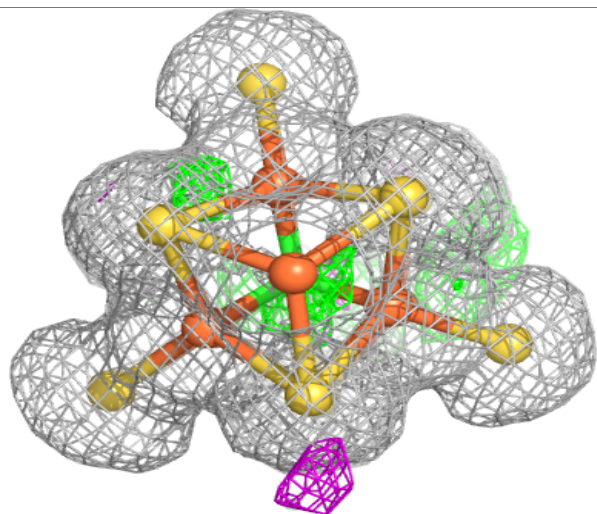
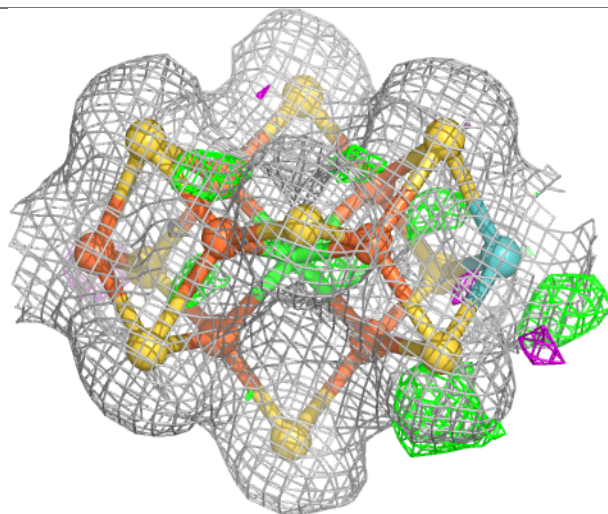
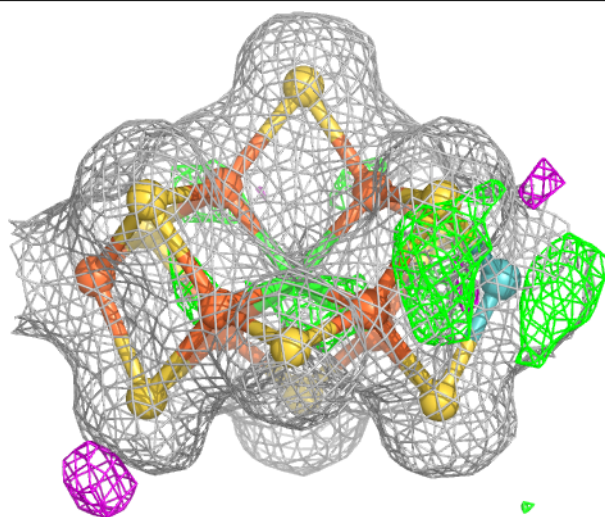
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HCA	A	601	14/14	0.97	0.05	14,17,20,24	0
3	HCA	C	601	14/14	0.97	0.05	16,18,24,24	0
4	ICS	C	602	18/18	0.99	0.03	18,20,21,21	0
6	FE2	B	502	1/1	0.99	0.02	16,16,16,16	1
5	CLF	A	603	15/15	1.00	0.02	15,16,18,20	0
5	CLF	C	603	15/15	1.00	0.02	17,18,20,21	0
6	FE2	B	501	1/1	1.00	0.02	16,16,16,16	1
4	ICS	A	602	18/18	1.00	0.02	15,16,18,18	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.

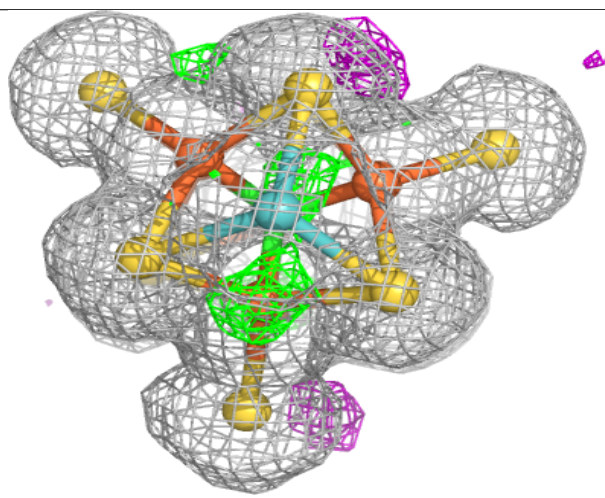
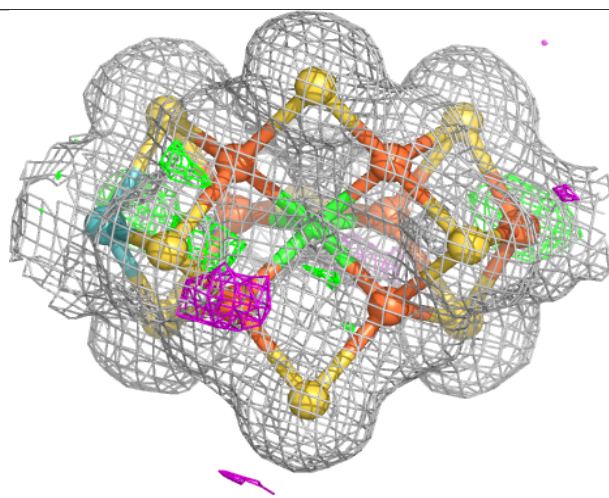
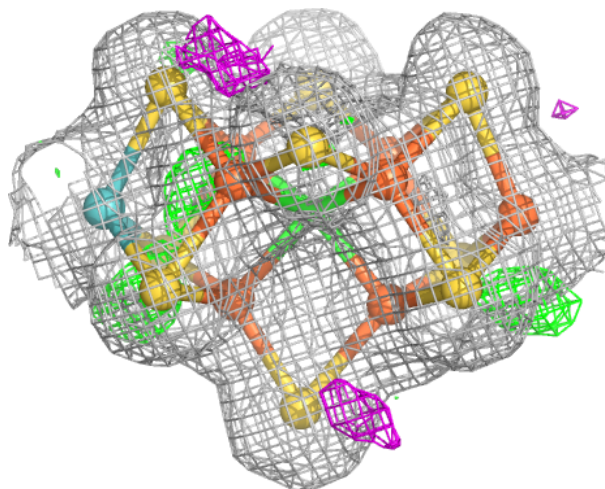
Electron density around ICS C 602:

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



Electron density around ICS A 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.