



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 02:44 pm GMT

PDB ID : 9ER9
Title : Hydrogenase-1 Ni-R state
Authors : Carr, S.B.; Li, W.; Wong, K.l.; Ash, P.A.; Vincent, K.A.
Deposited on : 2024-03-22
Resolution : 1.40 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

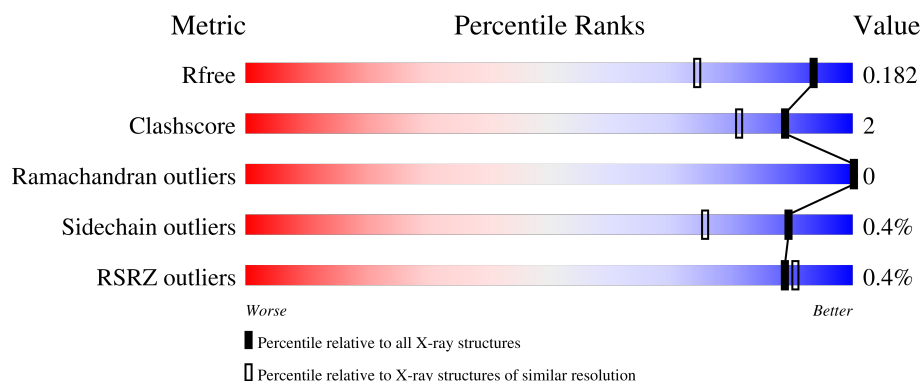
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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	S	279	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % 86% 8% • 6% </div> </div>
1	T	279	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 90% • 6% </div> </div>
2	L	582	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 95% • </div> </div>
2	M	582	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 95% • </div> </div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 15022 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 Hydrogenase-1 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	263	Total	C	N	O	S	0	6	0
			2066	1310	353	382	21			
1	T	263	Total	C	N	O	S	0	5	0
			2056	1308	351	376	21			

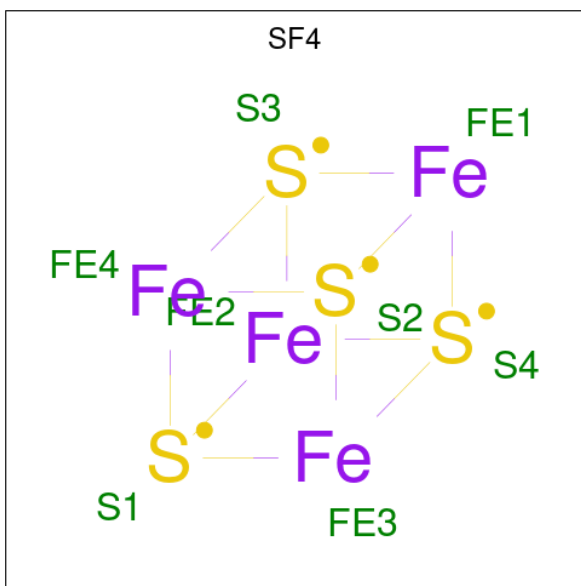
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	272	ARG	-	expression tag	UNP P69739
S	273	SER	-	expression tag	UNP P69739
S	274	HIS	-	expression tag	UNP P69739
S	275	HIS	-	expression tag	UNP P69739
S	276	HIS	-	expression tag	UNP P69739
S	277	HIS	-	expression tag	UNP P69739
S	278	HIS	-	expression tag	UNP P69739
S	279	HIS	-	expression tag	UNP P69739
T	272	ARG	-	expression tag	UNP P69739
T	273	SER	-	expression tag	UNP P69739
T	274	HIS	-	expression tag	UNP P69739
T	275	HIS	-	expression tag	UNP P69739
T	276	HIS	-	expression tag	UNP P69739
T	277	HIS	-	expression tag	UNP P69739
T	278	HIS	-	expression tag	UNP P69739
T	279	HIS	-	expression tag	UNP P69739

- Molecule 2 is a protein called Hydrogenase-1 large chain.

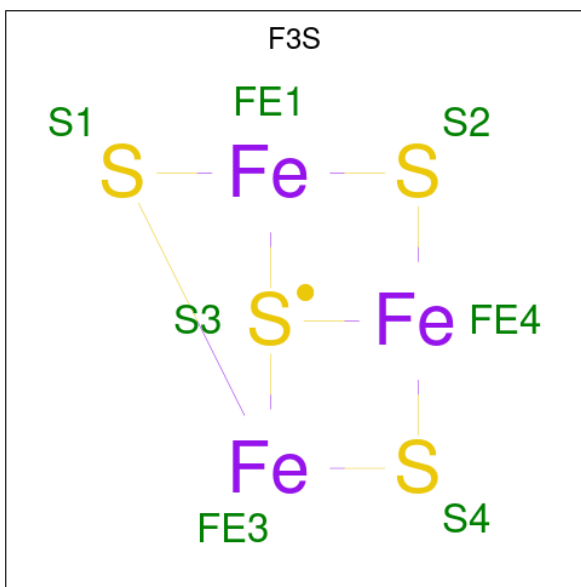
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	14	0
			4630	2938	816	849	27			
2	M	581	Total	C	N	O	S	0	13	0
			4621	2937	810	847	27			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



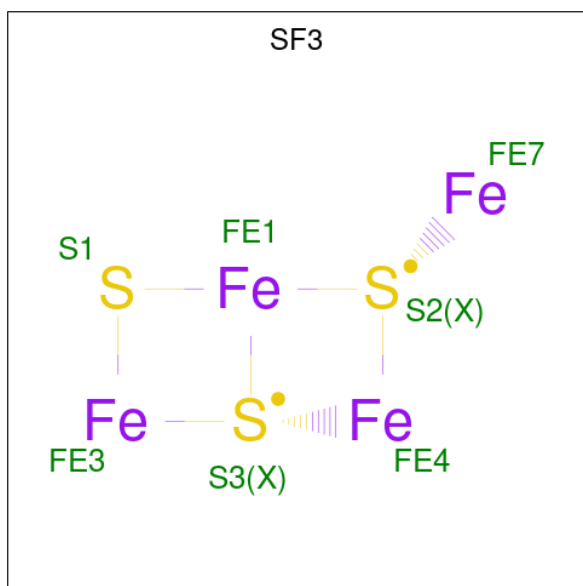
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: SF3) (formula: Fe_4S_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	0
			7	4	3		
5	T	1	Total	Fe	S	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

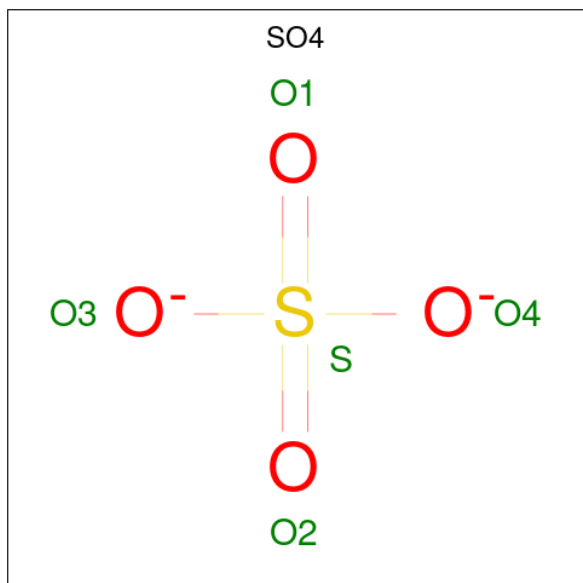
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total	Cl	0	0
			1	1		
6	L	1	Total	Cl	0	0
			1	1		
6	T	2	Total	Cl	0	0
			2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



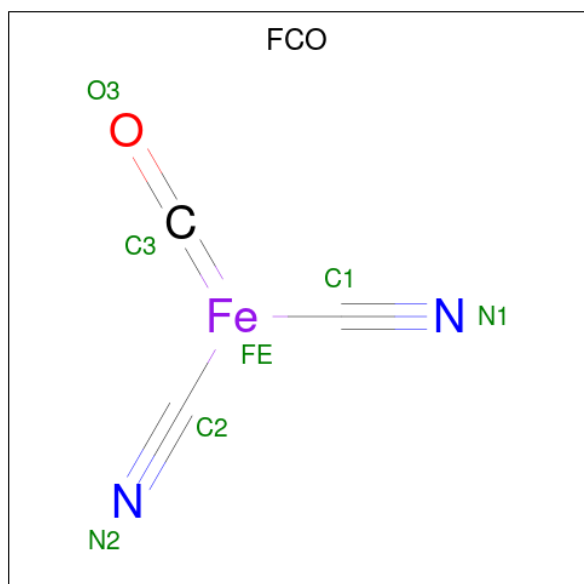
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	S	1	Total	C	O	0	0
			6	3	3		
7	S	1	Total	C	O	0	0
			6	3	3		
7	T	1	Total	C	O	0	0
			6	3	3		
7	T	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
9	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	1	Total	Ni	0	0
			1	1		
10	M	1	Total	Ni	0	0
			1	1		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

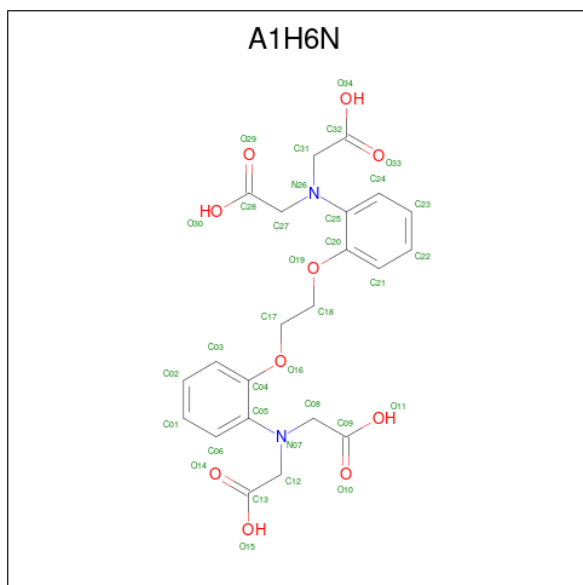
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Mg	0	0
			1	1		

- Molecule 12 is 2-[[2-[2-[bis(2-hydroxy-2-oxoethyl)amino]phenoxy]ethoxy]phenyl]-(2-hydroxy-2-oxoethyl)amino]ethanoic acid (three-letter code: A1H6N) (formula: C₂₂H₂₄N₂O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			34	22	2	10		
12	M	1	Total	C	N	O	0	0
			34	22	2	10		

- Molecule 13 is EUROPIUM ION (three-letter code: EU) (formula: Eu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total	Eu	0	0
			1	1		
13	M	1	Total	Eu	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	S	232	Total	O	0	0
			232	232		

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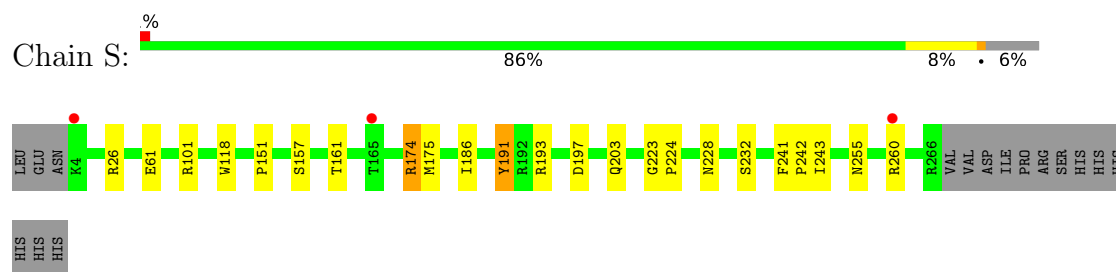
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	488	Total 488	O 488	0	0
14	T	220	Total 220	O 220	0	0
14	M	544	Total 544	O 544	0	0

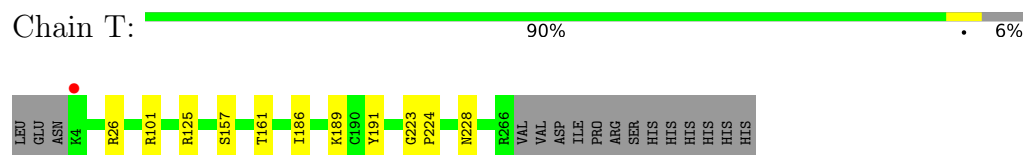
3 Residue-property plots [i](#)

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.

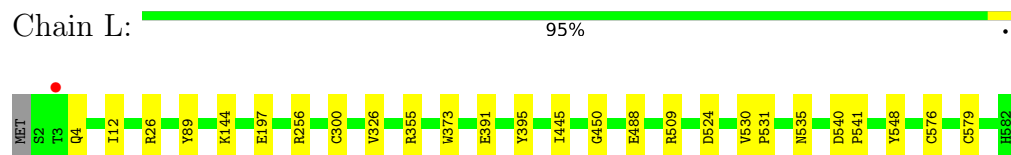
- Molecule 1: Hydrogenase-1 small chain



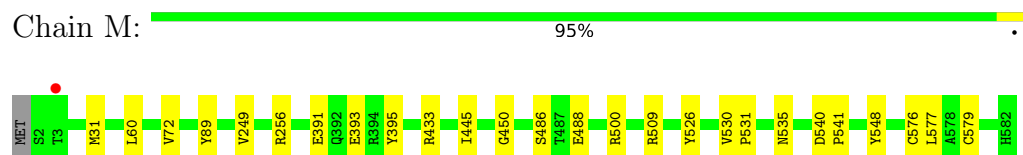
- Molecule 1: Hydrogenase-1 small chain



- Molecule 2: Hydrogenase-1 large chain



- Molecule 2: Hydrogenase-1 large chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.57Å 97.06Å 182.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.88 – 1.40 85.88 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.88-1.40) 99.9 (85.88-1.40)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.164 , 0.179 0.167 , 0.182	Depositor DCC
R_{free} test set	16285 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15022	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H6N, MG, CL, SF3, SO4, EU, SF4, F3S, GOL, NI, FCO

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	S	0.51	0/2133	0.80	1/2896 (0.0%)
1	T	0.54	0/2126	0.79	0/2885
2	L	0.50	0/4791	0.79	3/6515 (0.0%)
2	M	0.53	1/4777 (0.0%)	0.78	2/6497 (0.0%)
All	All	0.52	1/13827 (0.0%)	0.79	6/18793 (0.0%)

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	S	0	2
1	T	0	2
2	L	0	2
2	M	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	393	GLU	CD-OE1	7.29	1.33	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	89	TYR	CB-CG-CD1	7.34	125.40	121.00
2	L	26	ARG	NE-CZ-NH1	6.81	123.70	120.30
2	M	89	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	S	193	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	89	TYR	CB-CG-CD2	-5.51	117.69	121.00
2	L	89	TYR	CB-CG-CD1	5.37	124.22	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	256[A]	ARG	Sidechain
2	L	256[B]	ARG	Sidechain
2	M	256[A]	ARG	Sidechain
2	M	256[B]	ARG	Sidechain
1	S	174	ARG	Sidechain
1	S	26	ARG	Sidechain
1	T	125	ARG	Sidechain
1	T	26	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	S	2066	0	2003	15	0
1	T	2056	0	2010	5	0
2	L	4630	0	4546	13	0
2	M	4621	0	4536	15	0
3	S	8	0	0	0	0
3	T	8	0	0	0	0
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
6	L	1	0	0	0	0
6	S	1	0	0	0	0
6	T	2	0	0	0	0
7	S	12	0	16	0	0
7	T	12	0	16	0	0
8	L	5	0	0	0	0
9	L	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	7	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
12	L	34	0	0	0	0
12	M	34	0	0	1	0
13	L	1	0	0	0	0
13	M	1	0	0	0	0
14	L	488	0	0	1	0
14	M	544	0	0	2	0
14	S	232	0	0	4	0
14	T	220	0	0	1	0
All	All	15022	0	13127	47	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 2.

All (47) 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:S:197:ASP:HB2	14:T:616:HOH:O	1.96	0.66
12:M:604:A1H6N:C05	12:M:604:A1H6N:O11	2.47	0.62
2:L:530:VAL:CG1	2:L:531:PRO:HD2	2.35	0.56
2:M:60[B]:LEU:HD13	2:M:526:TYR:CG	2.41	0.55
1:S:260:ARG:HG3	14:S:515:HOH:O	2.05	0.55
1:S:61:GLU:OE1	1:S:101:ARG:NH1	2.33	0.55
1:S:101:ARG:HH21	1:S:101:ARG:HG3	1.71	0.54
1:S:161[A]:THR:HG22	14:S:562:HOH:O	2.09	0.53
2:L:144:LYS:HB3	2:L:197[A]:GLU:HG2	1.89	0.53
1:S:161[A]:THR:CG2	14:S:562:HOH:O	2.57	0.53
2:M:530:VAL:CG1	2:M:531:PRO:HD2	2.39	0.53
2:M:486[A]:SER:OG	2:M:488[A]:GLU:OE1	2.24	0.52
2:M:60[B]:LEU:HD11	2:M:72:VAL:CG1	2.40	0.52
2:L:488:GLU:HB2	14:L:751:HOH:O	2.09	0.51
1:S:186:ILE:HD11	1:S:228:ASN:HB3	1.93	0.51
2:L:4:GLN:HA	2:L:12:ILE:O	2.11	0.49
1:S:157:SER:O	1:S:161[A]:THR:HG23	2.12	0.49
2:M:31:MET:HB2	2:M:577:LEU:HG	1.94	0.48
1:T:186:ILE:HD11	1:T:228:ASN:HB3	1.96	0.47
2:L:355[A]:ARG:HG3	2:L:373:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:174:ARG:NH2	1:S:175[A]:MET:HE2	2.30	0.47
1:T:101:ARG:HH11	1:T:101:ARG:HG3	1.81	0.46
2:L:530:VAL:HG12	2:L:531:PRO:HD2	1.97	0.46
2:L:445:ILE:O	2:L:450:GLY:HA3	2.16	0.46
2:L:540:ASP:HB2	2:L:541:PRO:CD	2.46	0.45
2:L:300:CYS:HA	2:L:326:VAL:O	2.16	0.45
2:M:433:ARG:HD2	14:M:1201:HOH:O	2.17	0.45
2:M:500[B]:ARG:NH2	14:M:706:HOH:O	2.49	0.45
2:M:540:ASP:HB2	2:M:541:PRO:CD	2.47	0.44
1:S:223:GLY:N	1:S:224:PRO:CD	2.81	0.43
2:M:530:VAL:HG13	2:M:531:PRO:HD2	2.00	0.43
2:M:445:ILE:O	2:M:450:GLY:HA3	2.18	0.43
1:T:223:GLY:N	1:T:224:PRO:CD	2.83	0.42
1:S:232[B]:SER:OG	2:M:249:VAL:HB	2.19	0.42
2:M:535:ASN:HB3	2:M:548:TYR:CE1	2.55	0.42
2:L:509:ARG:CD	2:L:576:CYS:HB2	2.50	0.42
1:S:203[B]:GLN:NE2	14:S:506:HOH:O	2.52	0.41
2:L:530:VAL:HG11	2:L:579:CYS:HB3	2.02	0.41
2:M:530:VAL:HG11	2:M:579:CYS:HB3	2.02	0.41
1:T:157:SER:O	1:T:161:THR:HG23	2.20	0.41
2:M:509:ARG:CD	2:M:576:CYS:HB2	2.50	0.41
2:M:391:GLU:HA	2:M:395:TYR:CD2	2.55	0.41
2:L:391:GLU:HA	2:L:395:TYR:CD2	2.56	0.41
1:S:191:TYR:HB2	1:T:189:LYS:O	2.20	0.41
1:S:241:PHE:CE2	1:S:243:ILE:HB	2.56	0.41
1:S:118:TRP:CD2	1:S:255:ASN:HB2	2.55	0.40
2:L:535:ASN:HB3	2:L:548:TYR:CE1	2.56	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	S	267/279 (96%)	255 (96%)	12 (4%)	0	100	100
1	T	266/279 (95%)	258 (97%)	8 (3%)	0	100	100
2	L	593/582 (102%)	579 (98%)	14 (2%)	0	100	100
2	M	592/582 (102%)	577 (98%)	15 (2%)	0	100	100
All	All	1718/1722 (100%)	1669 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	S	222/232 (96%)	219 (99%)	3 (1%)	62	35
1	T	221/232 (95%)	220 (100%)	1 (0%)	86	71
2	L	494/481 (103%)	493 (100%)	1 (0%)	92	79
2	M	493/481 (102%)	493 (100%)	0	100	100
All	All	1430/1426 (100%)	1425 (100%)	5 (0%)	89	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	151	PRO
1	S	191	TYR
1	S	242	PRO
2	L	524	ASP
1	T	191	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	61	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 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	$\# Z > 2$
8	SO4	L	601	-	4,4,4	0.38	0	6,6,6	0.22	0
7	GOL	T	405	-	5,5,5	0.33	0	5,5,5	0.35	0
4	F3S	S	402	1	0,9,9	-	-	-		
12	A1H6N	L	605	13	35,35,35	1.12	2 (5%)	46,46,46	1.18	6 (13%)
12	A1H6N	M	604	13	35,35,35	1.43	5 (14%)	46,46,46	1.35	7 (15%)
7	GOL	T	406	-	5,5,5	0.35	0	5,5,5	0.41	0
7	GOL	S	406	-	5,5,5	0.46	0	5,5,5	0.45	0
3	SF4	T	401	1	0,12,12	-	-	-		
5	SF3	T	403	1	0,8,8	-	-	-		
4	F3S	T	402	1	0,9,9	-	-	-		
9	FCO	L	602	2	0,6,6	-	-	-		
5	SF3	S	403	1	0,8,8	-	-	-		
3	SF4	S	401	1	0,12,12	-	-	-		
9	FCO	M	601	2	0,6,6	-	-	-		
7	GOL	S	405	-	5,5,5	0.31	0	5,5,5	0.45	0

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	T	405	-	-	0/4/4/4	-
4	F3S	S	402	1	-	-	0/3/3/3
12	A1H6N	L	605	13	-	10/31/31/31	0/2/2/2
12	A1H6N	M	604	13	-	12/31/31/31	0/2/2/2
7	GOL	T	406	-	-	0/4/4/4	-
7	GOL	S	406	-	-	0/4/4/4	-
3	SF4	T	401	1	-	-	0/6/5/5
5	SF3	T	403	1	-	-	0/2/2/2
4	F3S	T	402	1	-	-	0/3/3/3
5	SF3	S	403	1	-	-	0/2/2/2
3	SF4	S	401	1	-	-	0/6/5/5
7	GOL	S	405	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	604	A1H6N	C05-N07	4.55	1.51	1.41
12	L	605	A1H6N	C25-N26	3.19	1.48	1.41
12	L	605	A1H6N	C05-N07	2.38	1.46	1.41
12	M	604	A1H6N	O34-C32	-2.38	1.22	1.30
12	M	604	A1H6N	C25-N26	2.05	1.45	1.41
12	M	604	A1H6N	C25-C20	-2.02	1.36	1.40
12	M	604	A1H6N	C12-C13	2.01	1.55	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	604	A1H6N	C09-C08-N07	-3.62	105.27	114.37
12	M	604	A1H6N	O15-C13-C12	2.77	124.35	113.45
12	M	604	A1H6N	C31-N26-C25	2.75	126.45	118.87
12	M	604	A1H6N	O15-C13-O14	-2.67	116.64	123.30
12	L	605	A1H6N	O15-C13-C12	2.62	123.79	113.45
12	M	604	A1H6N	C17-O16-C04	2.60	124.06	117.69
12	L	605	A1H6N	C12-N07-C05	2.51	125.78	118.87
12	M	604	A1H6N	C06-C05-N07	-2.42	118.45	122.30
12	L	605	A1H6N	C24-C25-N26	-2.39	118.49	122.30
12	L	605	A1H6N	C06-C05-N07	-2.26	118.70	122.30
12	L	605	A1H6N	O11-C09-C08	2.24	122.28	113.45
12	L	605	A1H6N	O15-C13-O14	-2.24	117.72	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	604	A1H6N	C04-C05-N07	2.22	123.48	119.33

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	605	A1H6N	C13-C12-N07-C05
12	L	605	A1H6N	C13-C12-N07-C08
12	L	605	A1H6N	C28-C27-N26-C25
12	L	605	A1H6N	C28-C27-N26-C31
12	M	604	A1H6N	C09-C08-N07-C05
12	M	604	A1H6N	C09-C08-N07-C12
12	M	604	A1H6N	C32-C31-N26-C25
12	M	604	A1H6N	C32-C31-N26-C27
12	M	604	A1H6N	N26-C31-C32-O33
12	M	604	A1H6N	N26-C31-C32-O34
12	L	605	A1H6N	N26-C27-C28-O29
12	L	605	A1H6N	N26-C27-C28-O30
12	M	604	A1H6N	C28-C27-N26-C31
12	L	605	A1H6N	N07-C12-C13-O14
12	L	605	A1H6N	N07-C12-C13-O15
12	M	604	A1H6N	C04-C05-N07-C08
12	M	604	A1H6N	C20-C25-N26-C31
12	M	604	A1H6N	N07-C08-C09-O10
12	L	605	A1H6N	C24-C25-N26-C27
12	M	604	A1H6N	C06-C05-N07-C08
12	M	604	A1H6N	C28-C27-N26-C25
12	L	605	A1H6N	C20-C25-N26-C27

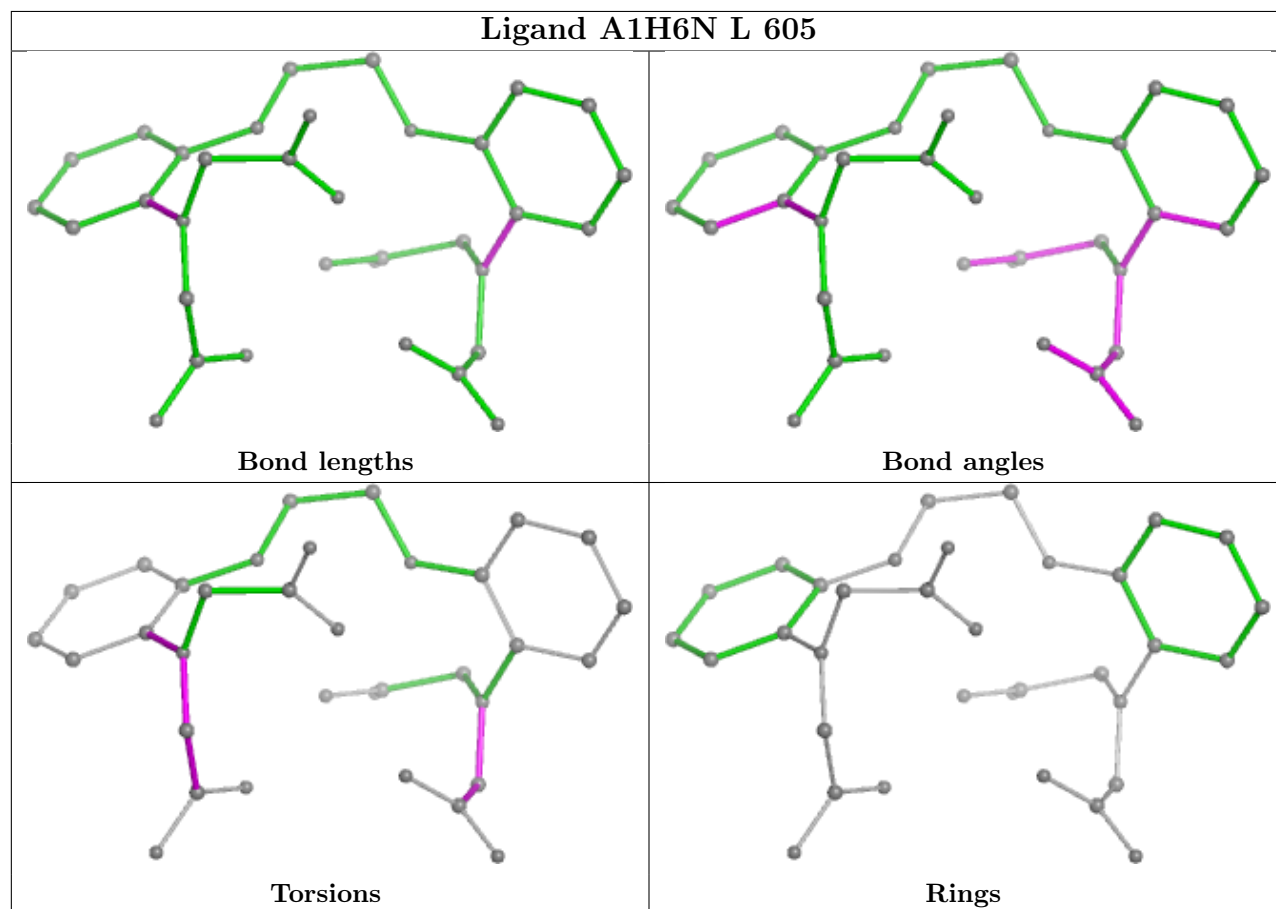
There are no ring outliers.

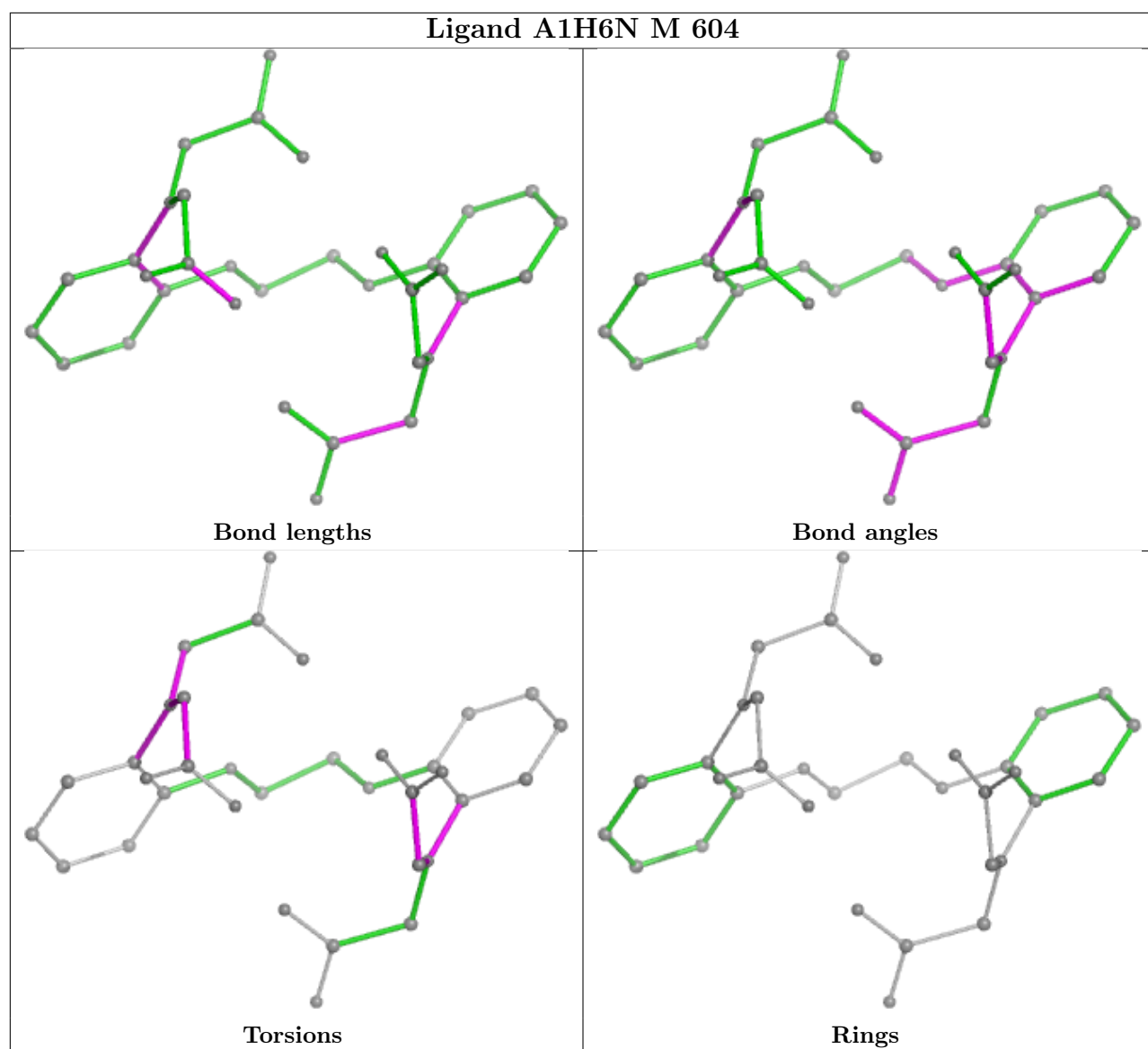
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	604	A1H6N	1	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 [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, 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	S	263/279 (94%)	-0.43	3 (1%) 77 79	4, 11, 23, 57	6 (2%)
1	T	263/279 (94%)	-0.29	1 (0%) 89 90	7, 12, 25, 60	5 (1%)
2	L	581/582 (99%)	-0.32	1 (0%) 92 92	5, 13, 25, 56	14 (2%)
2	M	581/582 (99%)	-0.36	1 (0%) 92 92	5, 12, 22, 38	13 (2%)
All	All	1688/1722 (98%)	-0.34	6 (0%) 89 90	4, 12, 24, 60	38 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	4	LYS	4.0
1	S	4	LYS	3.0
1	S	260	ARG	2.2
2	M	3	THR	2.1
1	S	165	THR	2.1
2	L	3	THR	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 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,

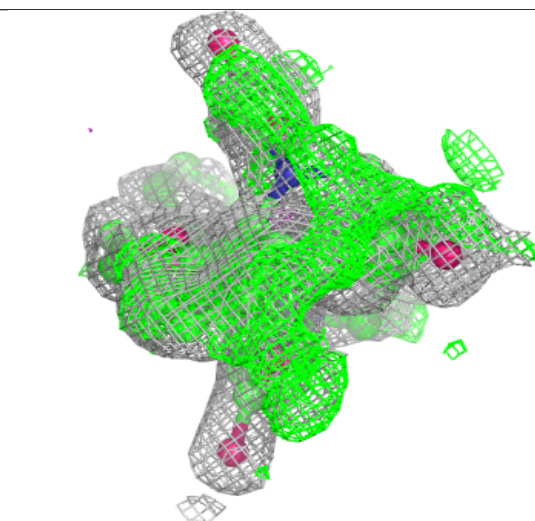
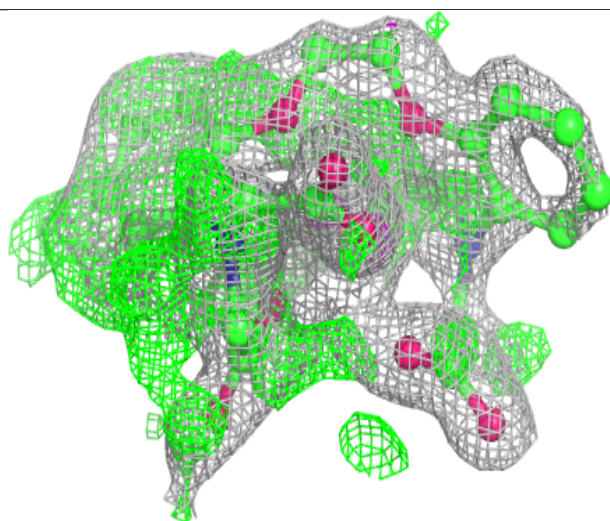
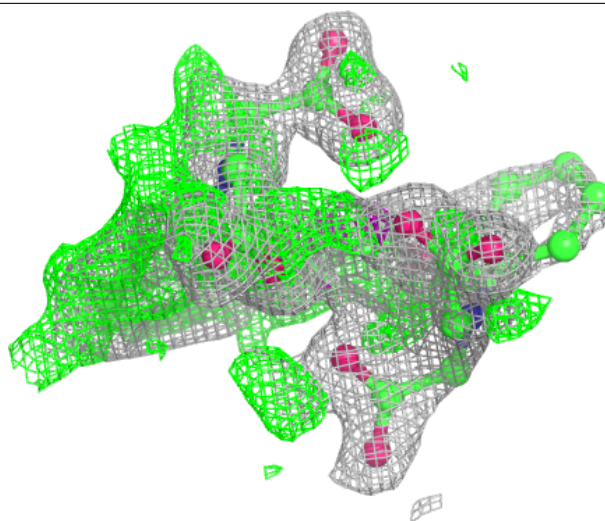
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	A1H6N	M	604	34/34	0.85	0.18	11,17,21,22	34
7	GOL	T	406	6/6	0.88	0.12	14,20,20,23	0
6	CL	L	606	1/1	0.88	0.13	38,38,38,38	0
12	A1H6N	L	605	34/34	0.89	0.13	13,16,19,20	34
7	GOL	S	406	6/6	0.90	0.12	12,19,20,21	0
6	CL	T	407	1/1	0.91	0.11	36,36,36,36	0
7	GOL	T	405	6/6	0.92	0.09	18,19,22,23	0
7	GOL	S	405	6/6	0.93	0.09	17,18,21,22	0
8	SO4	L	601	5/5	0.95	0.07	19,23,24,24	5
13	EU	L	607	1/1	0.96	0.12	31,31,31,31	1
13	EU	M	605	1/1	0.97	0.11	30,30,30,30	1
6	CL	T	404	1/1	0.99	0.05	15,15,15,15	0
11	MG	L	604	1/1	0.99	0.02	8,8,8,8	0
6	CL	S	404	1/1	0.99	0.05	15,15,15,15	0
4	F3S	S	402	7/7	1.00	0.01	8,9,9,9	0
9	FCO	L	602	7/7	1.00	0.03	9,9,10,10	0
9	FCO	M	601	7/7	1.00	0.03	9,10,11,11	0
10	NI	L	603	1/1	1.00	0.03	14,14,14,14	0
10	NI	M	602	1/1	1.00	0.03	14,14,14,14	0
4	F3S	T	402	7/7	1.00	0.01	9,9,9,10	0
11	MG	M	603	1/1	1.00	0.02	8,8,8,8	0
5	SF3	S	403	7/7	1.00	0.01	9,9,9,9	0
5	SF3	T	403	7/7	1.00	0.02	10,10,10,10	0
3	SF4	S	401	8/8	1.00	0.02	9,9,10,10	0
3	SF4	T	401	8/8	1.00	0.02	9,10,10,10	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.

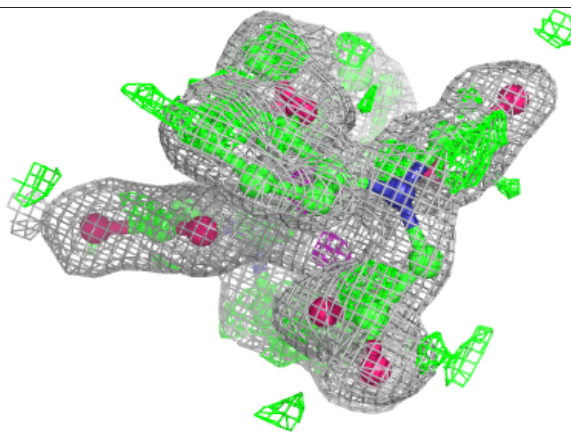
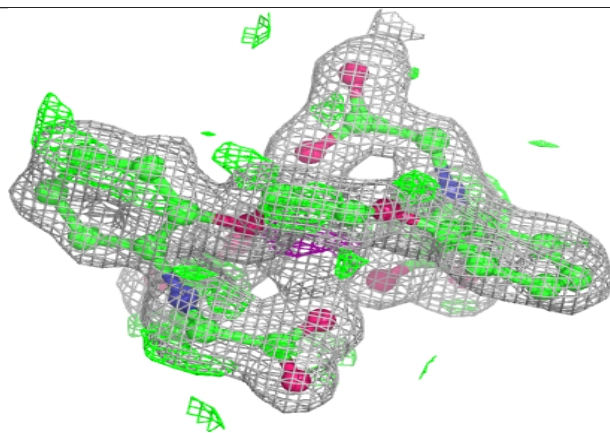
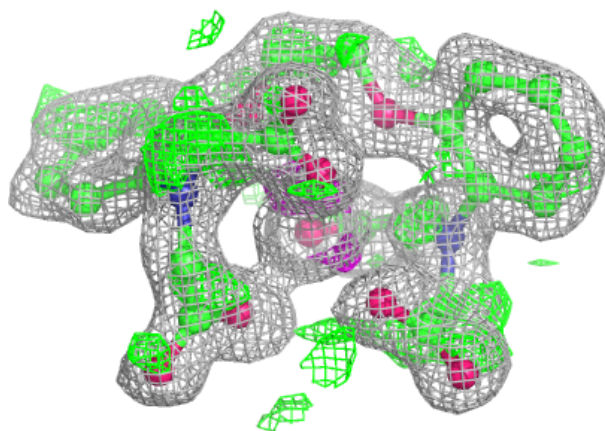
Electron density around A1H6N M 604:

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



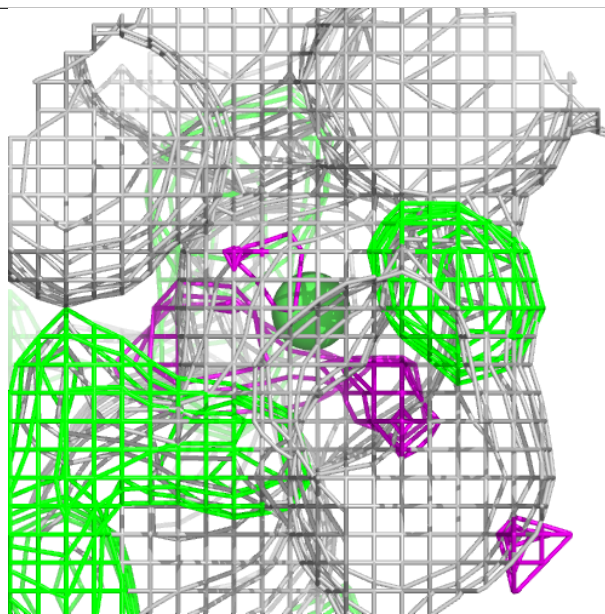
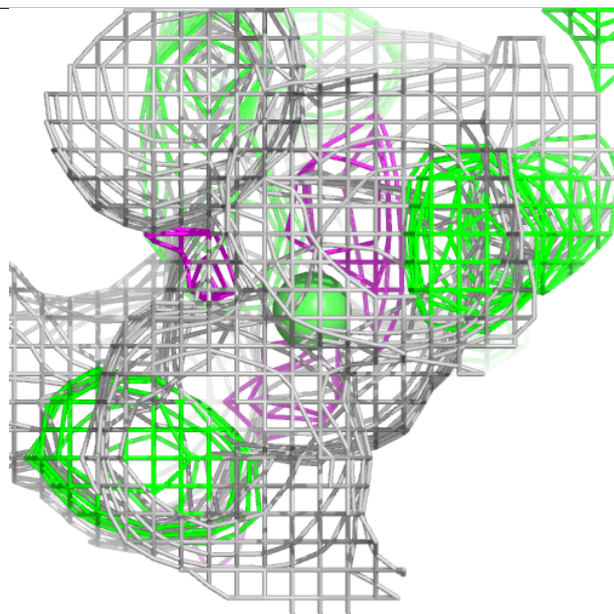
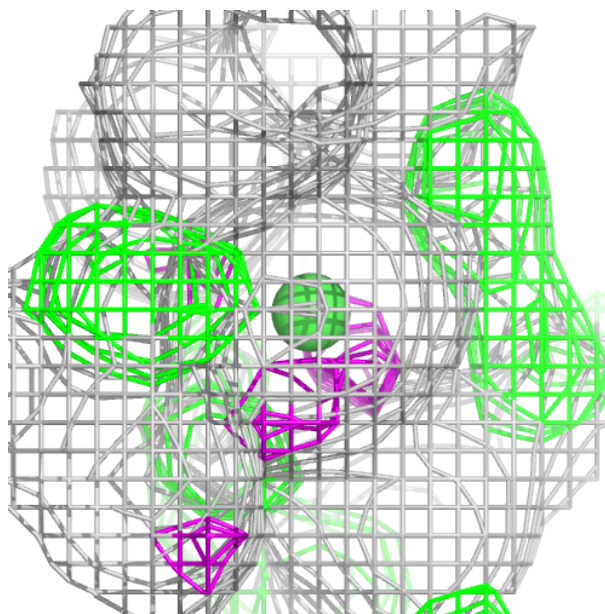
Electron density around A1H6N L 605:

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



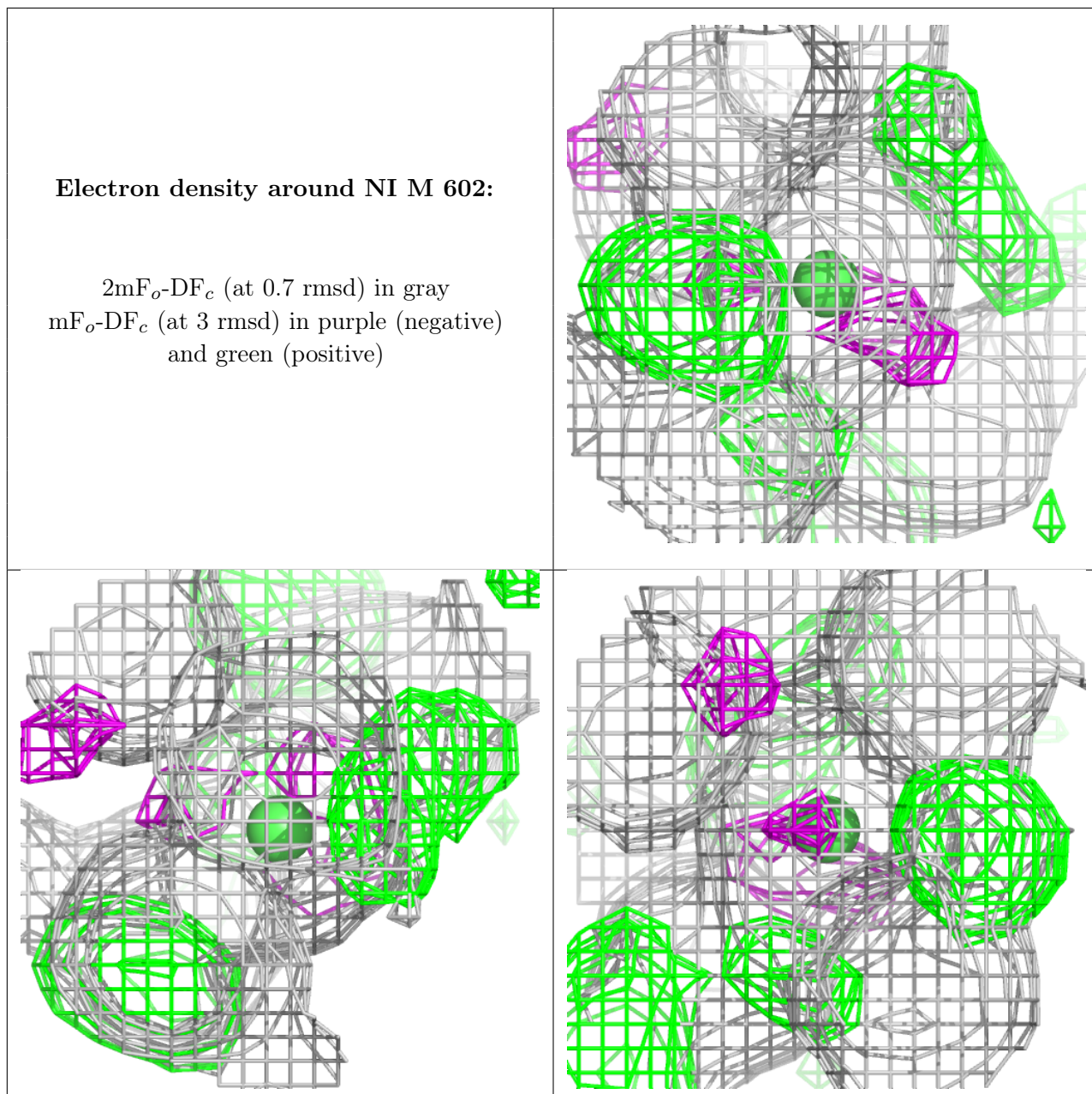
Electron density around NI L 603:

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



Electron density around NI M 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 ⓘ

There are no such residues in this entry.