wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2020 – 07:54 AM BST

PDB ID	:	7ADY
Title	:	CO-removed state of the active site of vanadium nitrogenase VFe protein
Authors	:	Rohde, M.; Grunau, K.; Einsle, O.
Deposited on	:	2020-09-16
Resolution	:	1.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

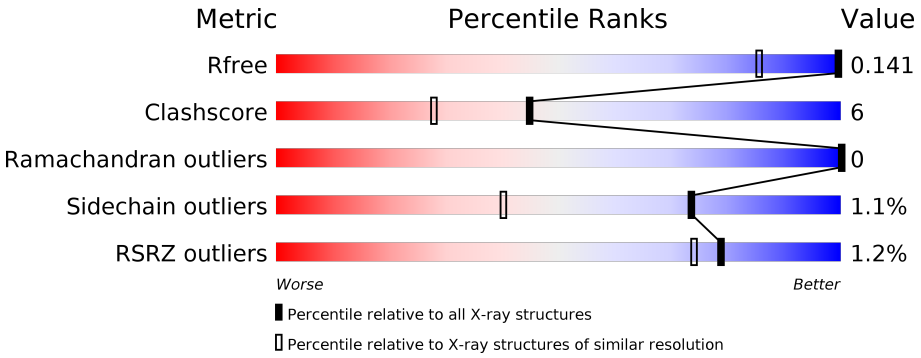
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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 >=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 <=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	474	91% 7%
1	D	474	87% 12%
2	B	475	90% 6%
2	E	475	88% 9%
3	C	113	84% 14%
3	F	113	7% 84% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	EDO	E	505	-	X	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 20082 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 vanadium-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	10	0
			3865	2463	662	711	29			
1	D	473	Total	C	N	O	S	0	13	0
			3879	2473	661	716	29			

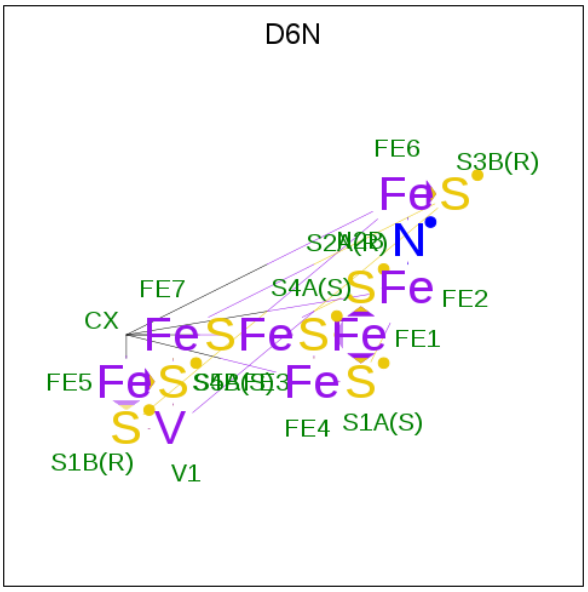
- Molecule 2 is a protein called Nitrogenase vanadium-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	0	12	0
			3725	2370	637	694	24			
2	E	466	Total	C	N	O	S	0	23	0
			3824	2431	657	711	25			

- Molecule 3 is a protein called Nitrogenase vanadium-iron protein delta chain.

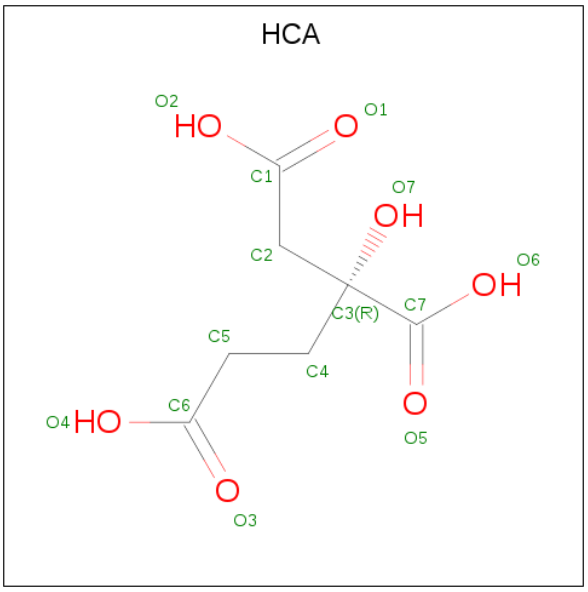
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	113	Total	C	N	O	S	0	2	0
			964	604	175	182	3			
3	F	111	Total	C	N	O	S	0	4	0
			969	606	180	181	2			

- Molecule 4 is FeV (three-letter code: D6N) (formula: CFe_7NS_7V) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Fe S V 16 1 7 7 1	0	0
4	D	1	Total C Fe S V 16 1 7 7 1	0	0

- Molecule 5 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



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

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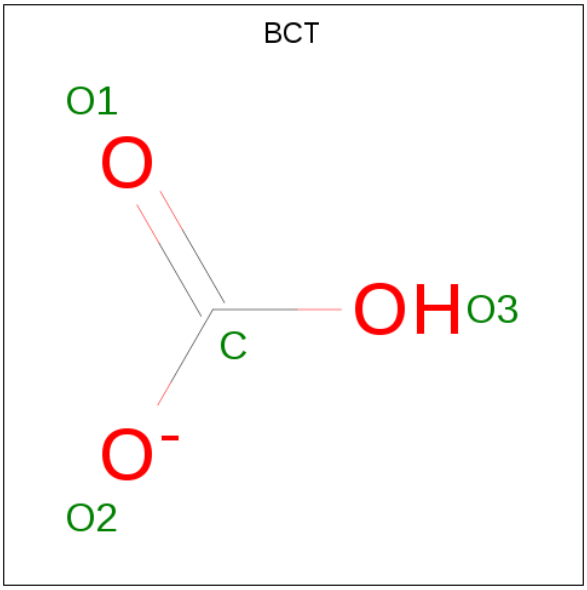
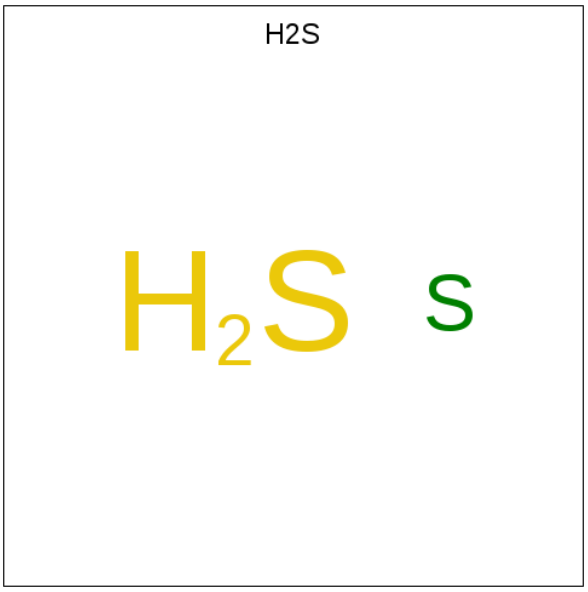
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 14 7 7	0	0

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



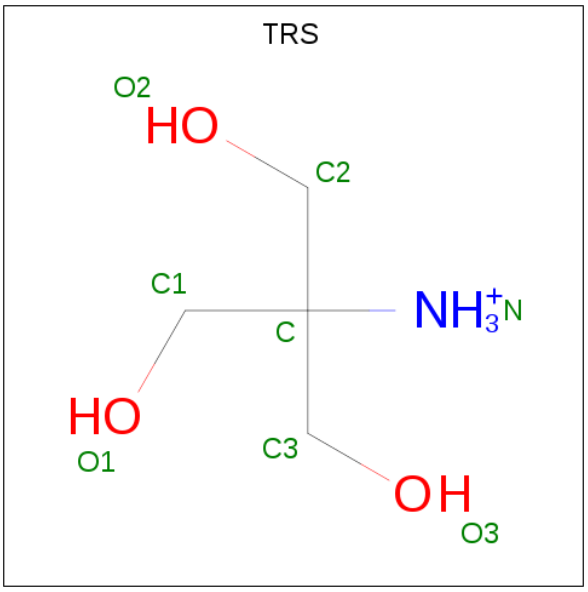
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 1 3	0	0
6	D	1	Total C O 4 1 3	0	0

- Molecule 7 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total S 1 1	0	0
7	D	1	Total S 1 1	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 8 4 1 3	0	0

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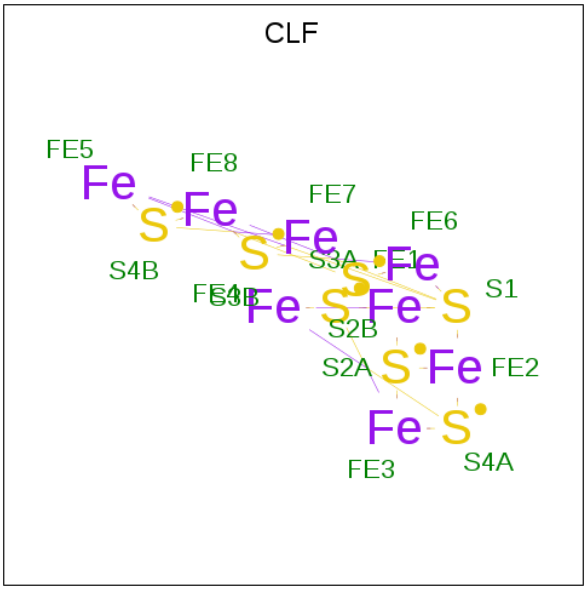
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 8 4 1 3	0	0
8	D	1	Total C N O 8 4 1 3	0	0

- Molecule 9 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).

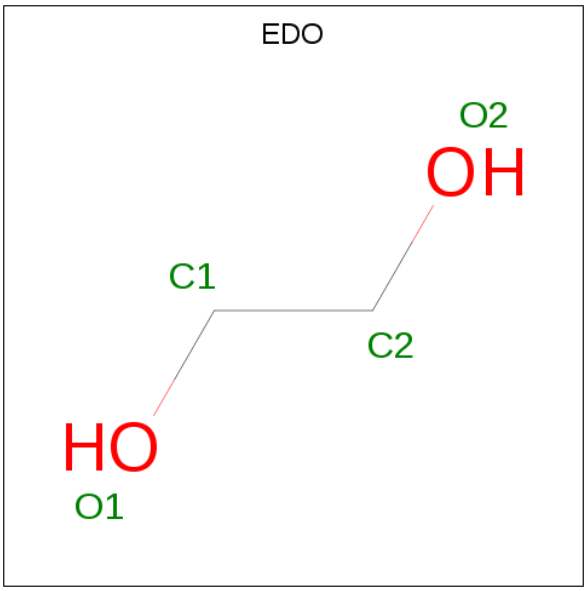


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 16 9 7	0	1
9	E	1	Total Fe S 16 9 7	0	1

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Mg 2 2	0	0
10	C	1	Total Mg 1 1	0	0
10	F	1	Total Mg 1 1	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 8 4 4	0	1
11	B	1	Total C O 4 2 2	0	0
11	B	1	Total C O 8 4 4	0	1
11	C	1	Total C O 4 2 2	0	0
11	E	1	Total C O 4 2 2	0	0
11	E	1	Total C O 8 4 4	0	1
11	E	1	Total C O 4 2 2	0	0
11	E	1	Total C O 4 2 2	0	0
11	F	1	Total C O 4 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	546	Total O 569 569	0	22
12	B	543	Total O 569 569	0	25
12	C	170	Total O 173 173	0	4

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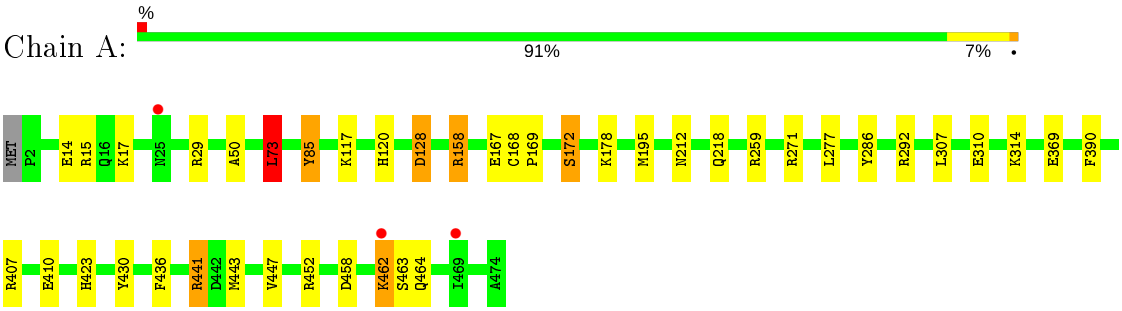
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	565	Total O 592 592	0	26
12	E	593	Total O 631 631	0	34
12	F	140	Total O 144 144	0	4

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.

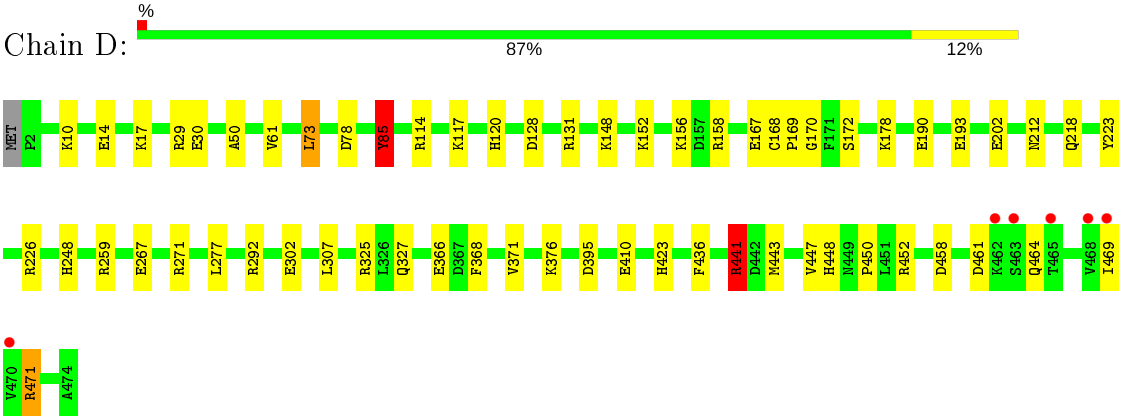
- Molecule 1: Nitrogenase vanadium-iron protein alpha chain

Chain A:



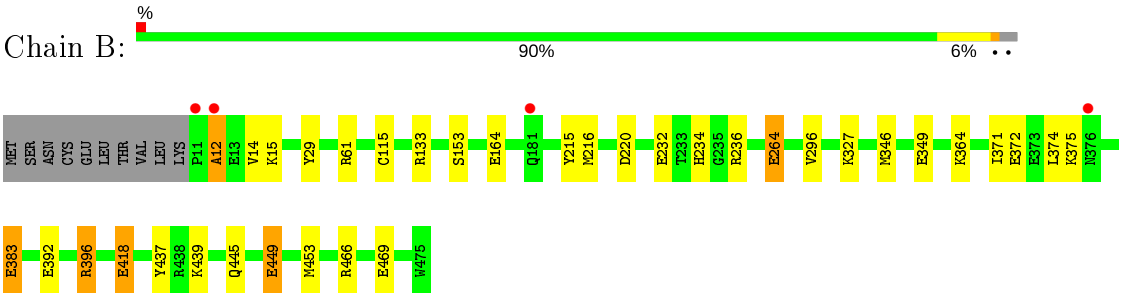
- Molecule 1: Nitrogenase vanadium-iron protein alpha chain

Chain D:



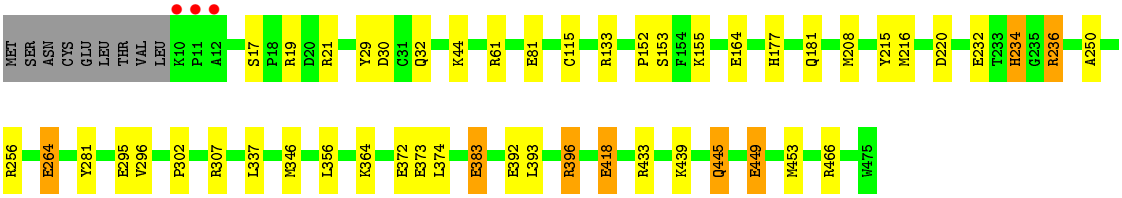
- Molecule 2: Nitrogenase vanadium-iron protein beta chain

Chain B:

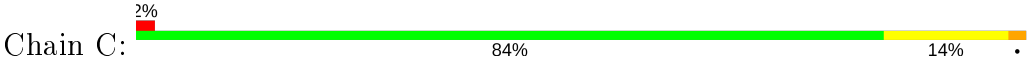


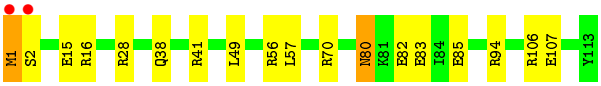
- Molecule 2: Nitrogenase vanadium-iron protein beta chain

Chain E:

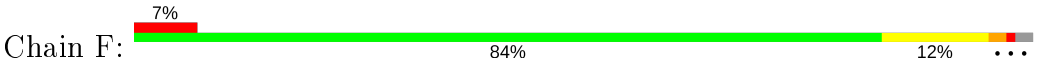


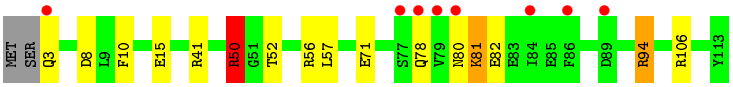
- Molecule 3: Nitrogenase vanadium-iron protein delta chain





- Molecule 3: Nitrogenase vanadium-iron protein delta chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.58Å 80.03Å 107.20Å 83.99° 72.48° 75.03°	Depositor
Resolution (Å)	46.66 – 1.05 46.62 – 1.05	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.66-1.05) 94.1 (46.62-1.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.121 , 0.141 0.121 , 0.141	Depositor DCC
R_{free} test set	5039 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	10.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	20082	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 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, D6N, CLF, EDO, H2S, HCA, BCT, TRS

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	0.86	6/3966 (0.2%)	0.99	14/5357 (0.3%)
1	D	0.86	7/3986 (0.2%)	1.00	17/5384 (0.3%)
2	B	0.91	11/3811 (0.3%)	1.00	11/5156 (0.2%)
2	E	0.92	13/3919 (0.3%)	1.00	14/5299 (0.3%)
3	C	1.11	5/984 (0.5%)	1.08	7/1329 (0.5%)
3	F	0.98	4/989 (0.4%)	1.09	2/1335 (0.1%)
All	All	0.91	46/17655 (0.3%)	1.01	65/23860 (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	1
1	D	0	1
2	B	0	1
2	E	0	2
3	F	0	1
All	All	0	6

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	449[A]	GLU	CD-OE2	-11.88	1.12	1.25
2	E	449[B]	GLU	CD-OE2	-11.88	1.12	1.25
1	D	172	SER	CB-OG	-11.64	1.27	1.42
2	B	383	GLU	CD-OE1	10.21	1.36	1.25
3	C	2	SER	CB-OG	10.20	1.55	1.42

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	396	ARG	NE-CZ-NH1	-12.50	114.05	120.30
2	E	466	ARG	NE-CZ-NH2	-11.24	114.68	120.30
2	B	466	ARG	NE-CZ-NH2	-11.07	114.76	120.30
2	B	466	ARG	NE-CZ-NH1	10.33	125.47	120.30
2	E	256	ARG	NE-CZ-NH1	-10.22	115.19	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	441	ARG	Sidechain
2	B	445	GLN	Sidechain
1	D	441	ARG	Sidechain
2	E	234[B]	HIS	Peptide
2	E	445	GLN	Sidechain

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	3865	0	3778	35	0
1	D	3879	0	3800	53	0
2	B	3725	0	3710	35	0
2	E	3824	0	3814	68	0
3	C	964	0	928	15	2
3	F	969	0	933	21	0
4	A	16	0	0	0	0
4	D	16	0	0	0	0
5	A	14	0	6	1	0
5	D	14	0	6	1	0
6	A	4	0	0	0	0
6	D	4	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	16	0	24	1	0
8	D	8	0	12	1	0
9	B	16	0	0	0	0
9	E	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	2	0	0	0	0
10	C	1	0	0	0	0
10	F	1	0	0	0	0
11	B	20	0	29	0	0
11	C	4	0	6	0	0
11	E	20	0	28	3	0
11	F	4	0	6	0	0
12	A	569	0	0	11	0
12	B	569	0	0	23	1
12	C	173	0	0	11	0
12	D	592	0	0	30	3
12	E	631	0	0	30	0
12	F	144	0	0	4	0
All	All	20082	0	17080	224	3

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.

The worst 5 of 224 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)
12:D:668:HOH:O	2:E:418[A]:GLU:HG3	1.23	1.36
2:E:392[B]:GLU:OE2	2:E:396:ARG:NH1	1.61	1.31
1:A:172:SER:CB	12:A:601:HOH:O	1.65	1.27
3:C:38[A]:GLN:NE2	12:C:301:HOH:O	1.71	1.21
1:A:172:SER:HB2	12:A:601:HOH:O	1.22	1.18

All (3) 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)
3:C:82:GLU:OE1	12:D:1156:HOH:O[1_644]	1.26	0.94
3:C:82:GLU:CD	12:D:1156:HOH:O[1_644]	1.47	0.73
12:B:993:HOH:O	12:D:1097:HOH:O[1_554]	2.06	0.14

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	480/474 (101%)	465 (97%)	15 (3%)	0	100	100
1	D	485/474 (102%)	471 (97%)	14 (3%)	0	100	100
2	B	474/475 (100%)	465 (98%)	9 (2%)	0	100	100
2	E	487/475 (102%)	479 (98%)	8 (2%)	0	100	100
3	C	113/113 (100%)	108 (96%)	5 (4%)	0	100	100
3	F	113/113 (100%)	111 (98%)	2 (2%)	0	100	100
All	All	2152/2124 (101%)	2099 (98%)	53 (2%)	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	A	414/404 (102%)	406 (98%)	8 (2%)	57	19
1	D	417/404 (103%)	409 (98%)	8 (2%)	57	19
2	B	400/398 (100%)	400 (100%)	0	100	100
2	E	412/398 (104%)	412 (100%)	0	100	100
3	C	104/102 (102%)	102 (98%)	2 (2%)	57	19
3	F	104/102 (102%)	100 (96%)	4 (4%)	33	4
All	All	1851/1808 (102%)	1829 (99%)	22 (1%)	73	37

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	80	ASN
1	D	73	LEU
3	F	94[A]	ARG
1	D	10	LYS
1	D	29	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	78	GLN
3	C	80	ASN
1	D	448	HIS
3	C	46	GLN
1	D	218	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 25 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	$\#\|Z\|>2$
11	EDO	E	504	-	3,3,3	0.59	0	2,2,2	0.25	0
11	EDO	E	505	-	3,3,3	1.87	1 (33%)	2,2,2	1.89	1 (50%)
8	TRS	A	505	-	7,7,7	0.29	0	9,9,9	0.27	0
11	EDO	B	506[A]	-	3,3,3	0.46	0	2,2,2	0.66	0
5	HCA	A	502	4	4,13,13	1.07	0	4,18,18	1.30	1 (25%)
11	EDO	B	506[B]	-	3,3,3	0.27	0	2,2,2	0.41	0
4	D6N	A	501	1,12,5,6	6,26,28	1.14	0	-		
9	CLF	E	501[A]	2	0,24,24	0.00	-	-		
9	CLF	E	501[B]	2	0,24,24	0.00	-	-		
11	EDO	F	202	-	3,3,3	0.71	0	2,2,2	0.38	0
6	BCT	A	503	4	0,3,3	0.00	-	0,3,3	0.00	-
5	HCA	D	502	4	4,13,13	0.62	0	4,18,18	1.69	1 (25%)
8	TRS	A	506	-	7,7,7	0.38	0	9,9,9	0.56	0
6	BCT	D	503	4	0,3,3	0.00	-	0,3,3	0.00	-
9	CLF	B	501[B]	2	0,24,24	0.00	-	-		
9	CLF	B	501[A]	2	0,24,24	0.00	-	-		
11	EDO	B	504[B]	-	3,3,3	0.36	0	2,2,2	0.45	0
11	EDO	B	504[A]	-	3,3,3	0.20	0	2,2,2	0.59	0
11	EDO	C	202	-	3,3,3	1.46	1 (33%)	2,2,2	0.02	0
11	EDO	E	503[B]	-	3,3,3	0.26	0	2,2,2	0.54	0
11	EDO	B	505	-	3,3,3	0.84	0	2,2,2	0.33	0
11	EDO	E	503[A]	-	3,3,3	0.35	0	2,2,2	0.42	0
8	TRS	D	505	-	7,7,7	0.43	0	9,9,9	0.57	0
4	D6N	D	501	1,12,5,6	6,26,28	1.34	1 (16%)	-		
11	EDO	E	502	-	3,3,3	0.81	0	2,2,2	0.27	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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TRS	A	506	-	-	2/9/9/9	-
11	EDO	B	505	-	-	0/1/1/1	-
11	EDO	E	505	-	-	1/1/1/1	-
11	EDO	E	503[A]	-	-	0/1/1/1	-
9	CLF	B	501[A]	2	-	-	0/12/10/10
11	EDO	E	503[B]	-	-	1/1/1/1	-
11	EDO	E	504	-	-	0/1/1/1	-
9	CLF	B	501[B]	2	-	-	0/12/10/10
8	TRS	D	505	-	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TRS	A	505	-	-	0/9/9/9	-
9	CLF	E	501[A]	2	-	-	0/12/10/10
9	CLF	E	501[B]	2	-	-	0/12/10/10
11	EDO	B	506[A]	-	-	0/1/1/1	-
5	HCA	A	502	4	-	0/7/17/17	-
11	EDO	F	202	-	-	0/1/1/1	-
11	EDO	B	504[B]	-	-	1/1/1/1	-
11	EDO	E	502	-	-	0/1/1/1	-
11	EDO	B	506[B]	-	-	0/1/1/1	-
11	EDO	B	504[A]	-	-	0/1/1/1	-
11	EDO	C	202	-	-	0/1/1/1	-
5	HCA	D	502	4	-	0/7/17/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	D6N	S4B-FE7	-2.45	2.23	2.31
11	C	202	EDO	O2-C2	2.20	1.53	1.42
11	E	505	EDO	O2-C2	2.09	1.52	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	502	HCA	C3-C2-C1	-2.94	110.28	114.98
11	E	505	EDO	O1-C1-C2	2.45	129.50	111.91
5	A	502	HCA	C3-C2-C1	-2.24	111.39	114.98

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	506	TRS	C2-C-C3-O3
8	A	506	TRS	N-C-C3-O3
11	E	505	EDO	O1-C1-C2-O2
11	E	503[B]	EDO	O1-C1-C2-O2
8	D	505	TRS	C3-C-C1-O1

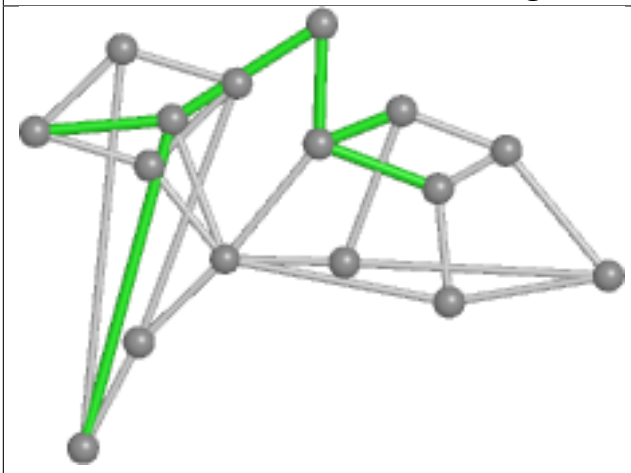
There are no ring outliers.

5 monomers are involved in 7 short contacts:

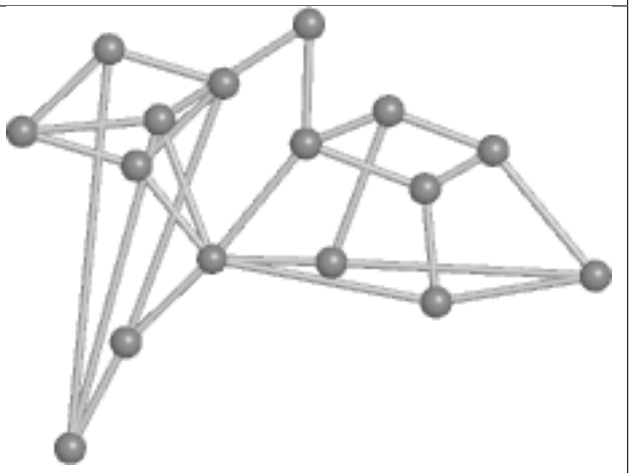
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	505	EDO	3	0
5	A	502	HCA	1	0
5	D	502	HCA	1	0
8	A	506	TRS	1	0
8	D	505	TRS	1	0

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 then 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.

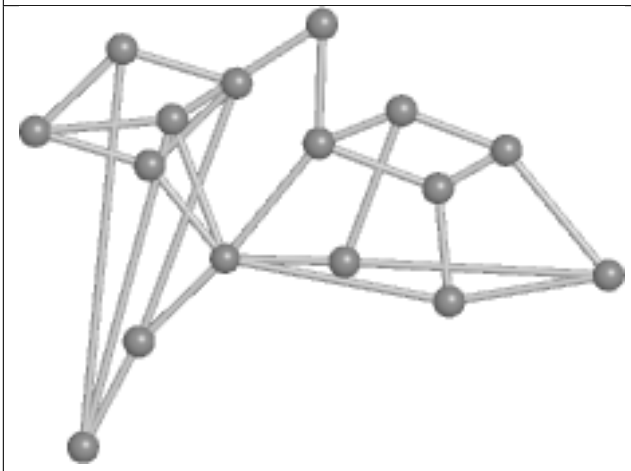
Ligand D6N A 501



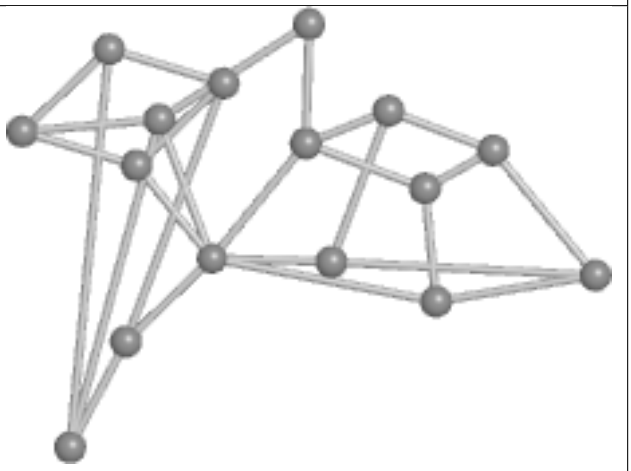
Bond lengths



Bond angles

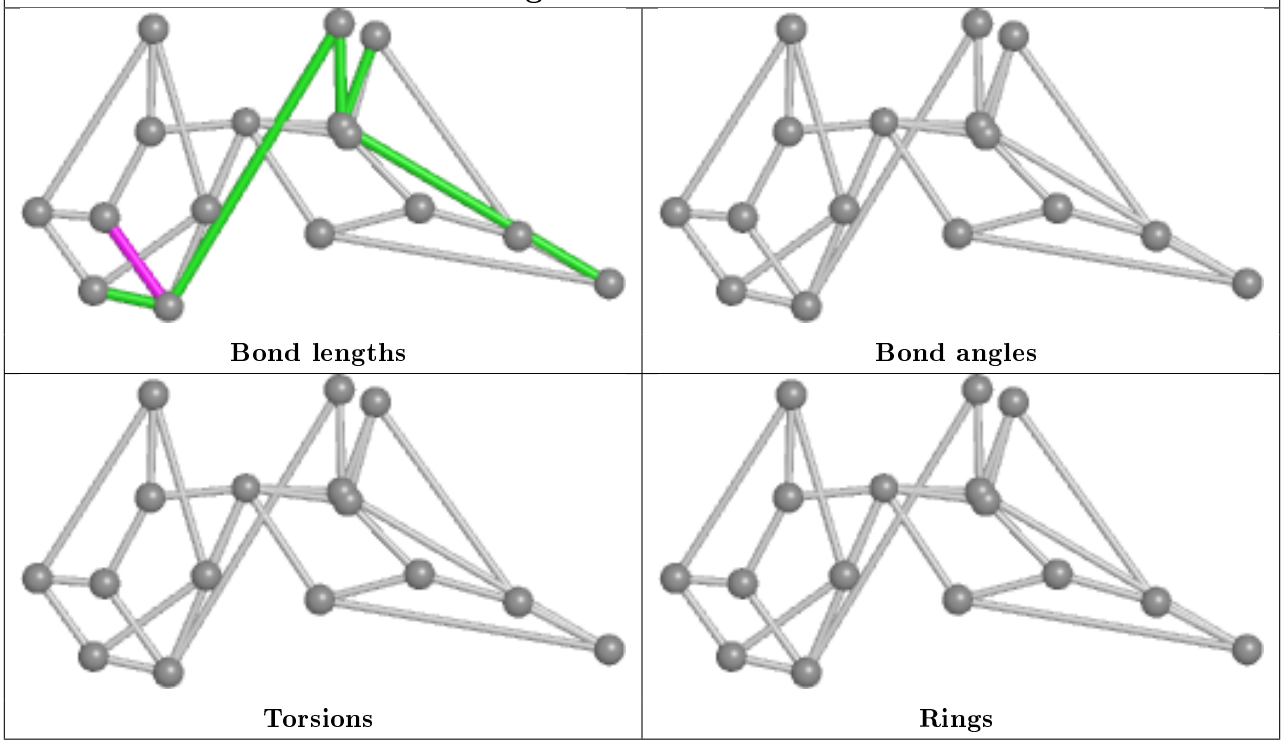


Torsions



Rings

Ligand D6N D 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	462:LYS	C	463:SER	N	2.27

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^{th} 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	473/474 (99%)	-0.54	3 (0%)	89	86	8, 11, 21, 44	0
1	D	473/474 (99%)	-0.55	6 (1%)	77	71	6, 11, 22, 39	0
2	B	465/475 (97%)	-0.53	4 (0%)	84	80	7, 11, 23, 76	0
2	E	466/475 (98%)	-0.57	3 (0%)	89	86	6, 10, 21, 72	0
3	C	113/113 (100%)	-0.37	2 (1%)	68	62	11, 16, 29, 51	0
3	F	111/113 (98%)	-0.06	8 (7%)	15	16	9, 17, 39, 53	0
All	All	2101/2124 (98%)	-0.51	26 (1%)	79	74	6, 11, 24, 76	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	12	ALA	5.9
2	E	10	LYS	5.8
3	C	1	MET	4.5
3	F	84	ILE	4.3
2	B	11[A]	PRO	3.8

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

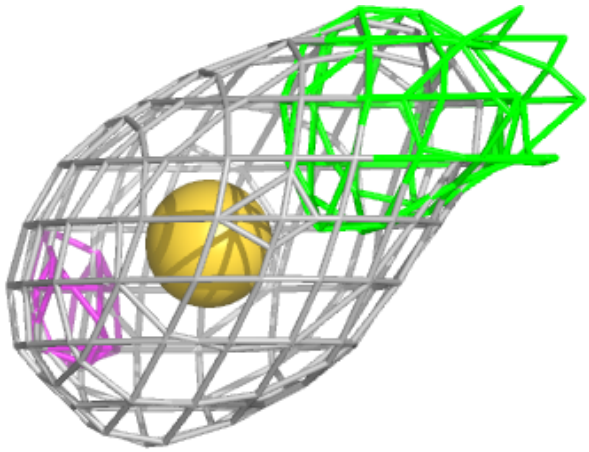
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

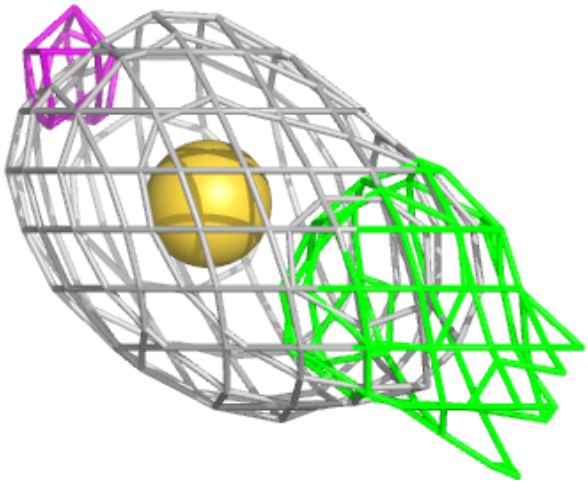
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	C	202	4/4	0.83	0.14	23,23,23,25	0
8	TRS	D	505	8/8	0.85	0.17	22,26,27,34	0
8	TRS	A	506	8/8	0.86	0.23	28,32,41,44	0
11	EDO	B	506[A]	4/4	0.92	0.14	12,20,21,24	4
11	EDO	B	506[B]	4/4	0.92	0.14	16,20,22,24	4
11	EDO	F	202	4/4	0.92	0.09	16,16,18,21	4
8	TRS	A	505	8/8	0.94	0.08	17,20,25,25	0
11	EDO	B	504[B]	4/4	0.96	0.10	19,20,20,21	4
11	EDO	B	505	4/4	0.96	0.12	22,25,25,27	0
11	EDO	B	504[A]	4/4	0.96	0.10	11,12,12,13	4
11	EDO	E	505	4/4	0.97	0.19	16,17,20,24	0
11	EDO	E	504	4/4	0.98	0.08	14,18,18,19	0
11	EDO	E	503[A]	4/4	0.98	0.07	8,8,9,9	4
11	EDO	E	503[B]	4/4	0.98	0.07	21,22,22,27	4
11	EDO	E	502	4/4	0.98	0.06	16,18,18,19	0
7	H2S	A	504	1/1	0.99	0.04	15,15,15,15	0
10	MG	F	201	1/1	0.99	0.11	16,16,16,16	0
5	HCA	D	502	14/14	0.99	0.07	6,6,11,11	0
5	HCA	A	502	14/14	0.99	0.06	7,8,11,12	0
10	MG	B	503	1/1	1.00	0.03	8,8,8,8	0
9	CLF	E	501[B]	15/15	1.00	0.04	6,6,7,12	1
6	BCT	A	503	4/4	1.00	0.07	8,8,9,9	0
4	D6N	A	501	16/17	1.00	0.04	7,8,8,8	0
10	MG	B	502	1/1	1.00	0.04	9,9,9,9	0
9	CLF	E	501[A]	15/15	1.00	0.04	4,6,6,7	1
6	BCT	D	503	4/4	1.00	0.06	6,7,7,7	0
9	CLF	B	501[B]	15/15	1.00	0.03	8,8,9,15	1
7	H2S	D	504	1/1	1.00	0.02	14,14,14,14	0
4	D6N	D	501	16/17	1.00	0.04	6,7,7,7	0
9	CLF	B	501[A]	15/15	1.00	0.03	6,8,8,9	1
10	MG	C	201	1/1	1.00	0.07	15,15,15,15	0

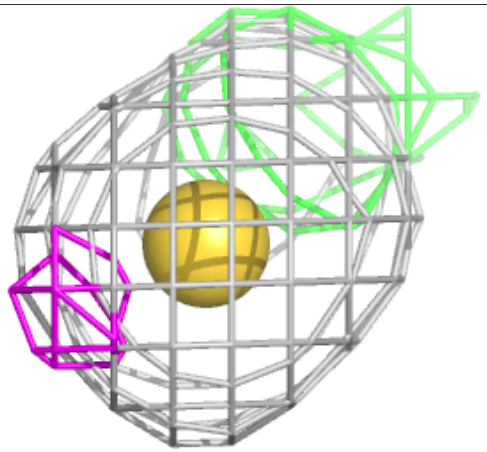
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around H2S A 504:

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

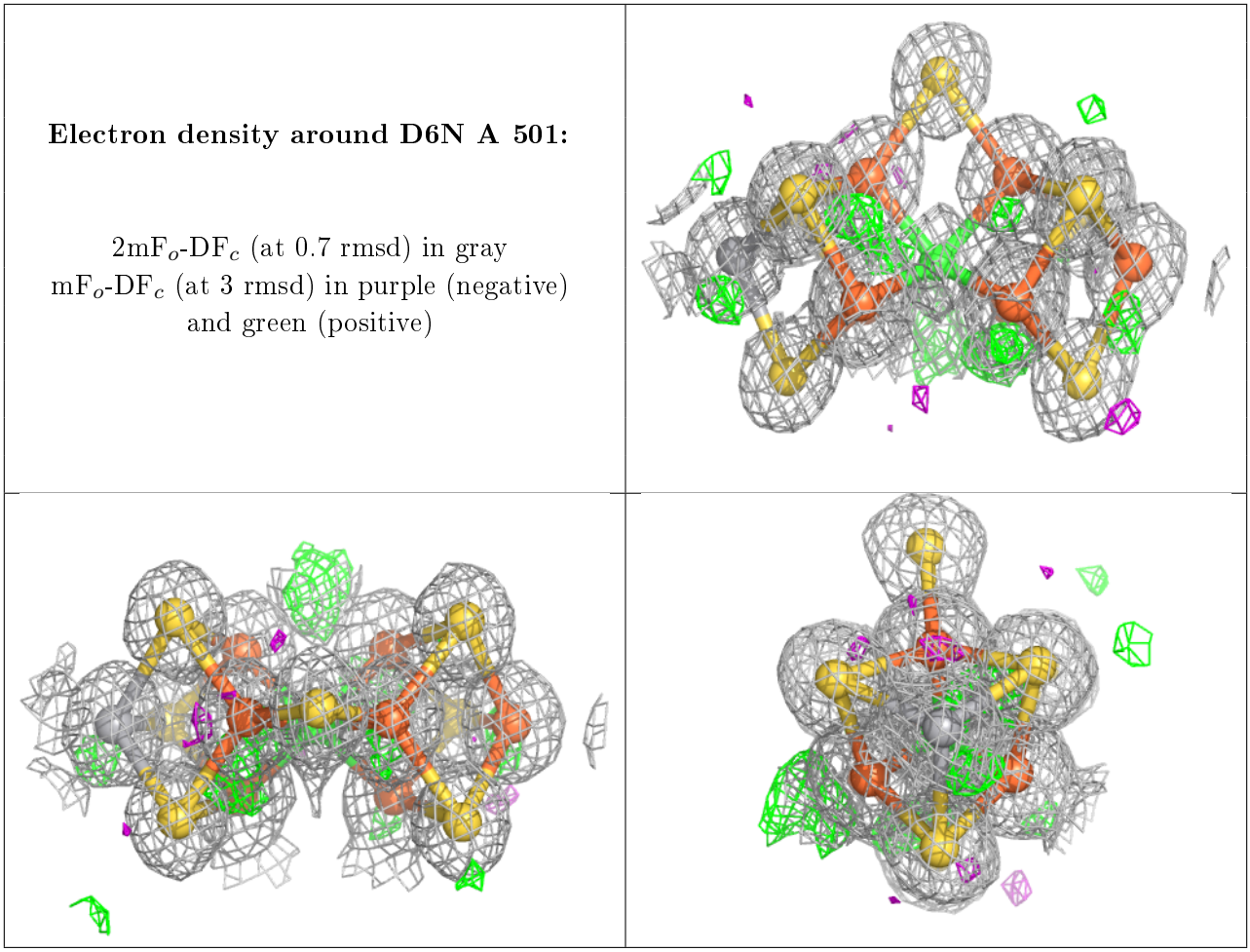






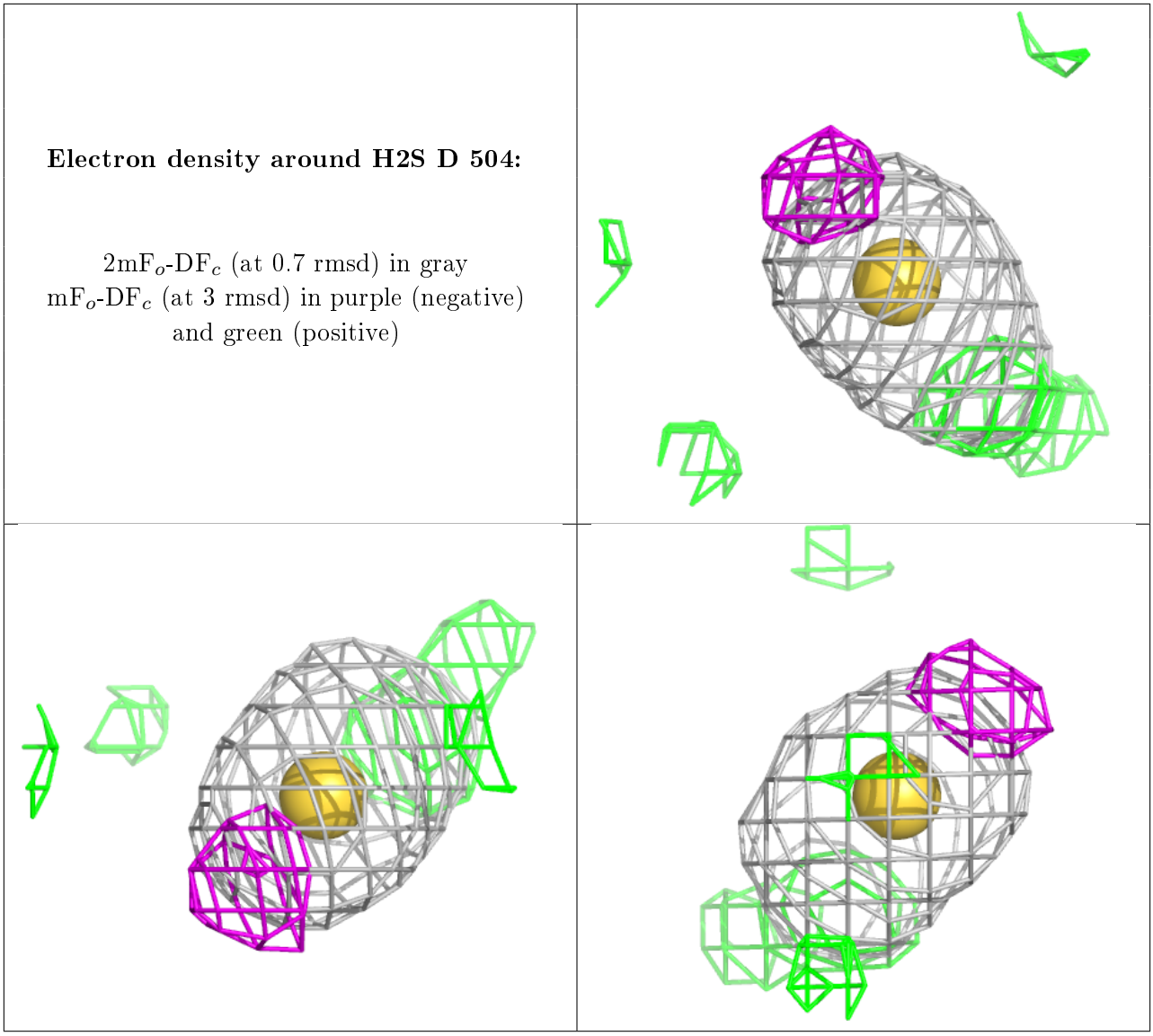
Electron density around D6N A 501:

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



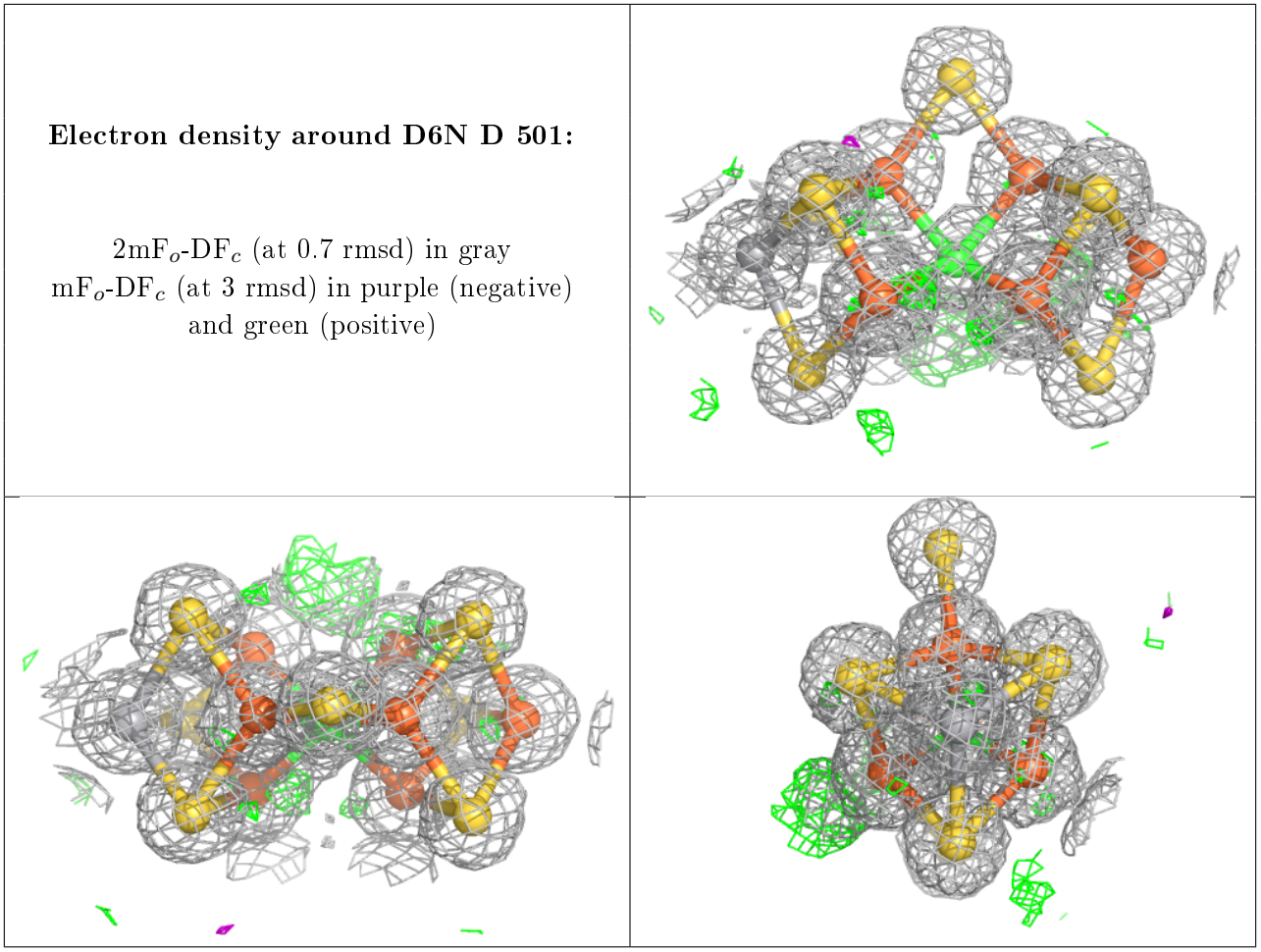
Electron density around H2S D 504:

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



Electron density around D6N D 501:

$2mF_o$-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.