

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2021 – 10:07 am BST

PDB ID : 701P

Title : [FeFe]-hydrogenase maturase HydE from T. Maritima (C-ter stretch absent)
Authors : Rohac, R.; Martin, L.; Liu, L.; Basu, D.; Tao, L.; Britt, R.D.; Rauchfuss, T.;

Nicolet, Y.

Deposited on : 2021-03-30

Resolution : 2.58 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 (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.23.1 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)

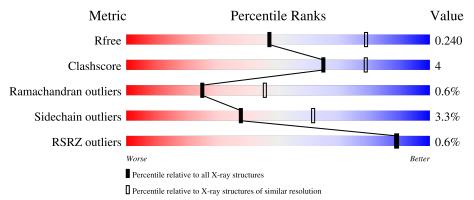
Validation Pipeline (wwPDB-VP) : 2.23.1

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 2.58 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	$egin{array}{l} ext{Whole archive} \ (\# ext{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$		
R_{free}	130704	3676 (2.60-2.56)		
Clashscore	141614	4049 (2.60-2.56)		
Ramachandran outliers	138981	3979 (2.60-2.56)		
Sidechain outliers	138945	3979 (2.60-2.56)		
RSRZ outliers	127900	3614 (2.60-2.56)		

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 <=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					
			<mark>%</mark>					
1	A	347	84%	11% • •				

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	${ m Res}$	Chirality	Geometry	Clashes	Electron density
4	CPS	A	406	-	-	ı	X



2 Entry composition (i)

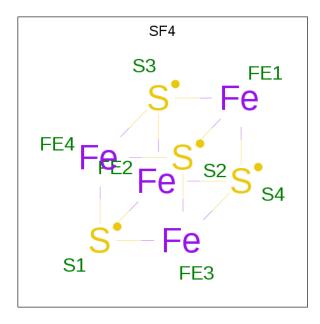
There are 7 unique types of molecules in this entry. The entry contains 2909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 [FeFe] hydrogenase maturase subunit HydE.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	A	332	Total 2666	C 1713	N 450	O 482	S 21	0	15	0

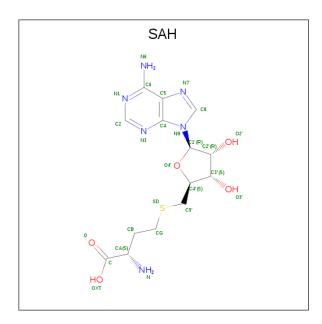
• Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Δ	1	Total	Fe	S	0	0
	A	1	8	4	4		. 0

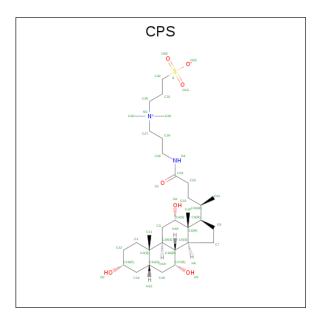
• Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	Α	1	Total	С	N	О	S	0	0
)	A	1	26	14	6	5	1		U

 \bullet Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: $\rm C_{32}H_{58}N_2O_7S).$



Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf		
4	Λ	1	Total	С	N	О	S	0	0
4	A	1	42	32	2	7	1		
4	4 A	A 1	Total	С	N	О	S	0	0
$\frac{4}{}$			42	32	2	7	1	U	

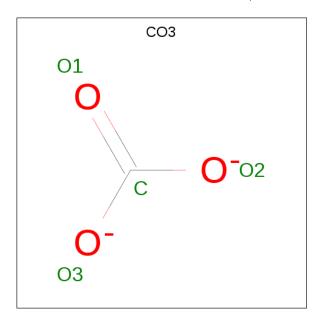
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 29 24 1 4	0	0
4	A	1	Total C N O 29 24 1 4	0	0
4	A	1	Total C O 50 44 6	0	1

 \bullet Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO3).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 4 4	0	1

• Molecule 7 is water.

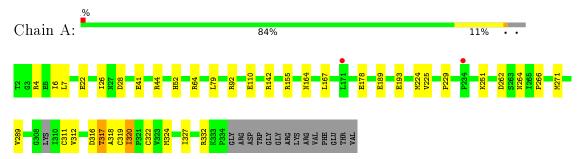
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	9	Total O 9 9	0	0



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: [FeFe] hydrogenase maturase subunit HydE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	52.45Å 79.16Å 85.76Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 2.58	Depositor
resolution (A)	44.75 - 2.58	EDS
% Data completeness	99.5 (40.00-2.58)	Depositor
(in resolution range)	99.7 (44.75-2.58)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.18 \; (at \; 2.58 \text{Å})$	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
D D.	0.179 , 0.240	Depositor
R, R_{free}	0.181 , 0.240	DCC
R_{free} test set	540 reflections $(4.61%)$	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35 \; , 62.3$	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2909	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SAH, SF4, CO3, CPS, CL

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).

Mal	Chain	Bond	lengths	Bond angles		
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.25	0/2771	0.44	0/3751	

There are no bond length outliers.

There are no bond angle outliers.

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	2666	0	2689	19	0
2	A	8	0	0	0	0
3	A	26	0	19	0	0
4	A	192	0	264	5	0
5	A	4	0	0	0	0
6	A	4	0	0	0	0
7	A	9	0	0	2	0
All	All	2909	0	2972	24	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 4.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	Clash overlap (Å)
1:A:311:CYS:SG	7:A:509:HOH:O	2.11	1.07
1:A:92:ARG:HH22	1:A:316:ASP:HB3		
		1.25	0.99
1:A:317:THR:O	1:A:319:CYS:N	2.18	0.76
1:A:92:ARG:NH2	1:A:316:ASP:HB3	2.03	0.73
1:A:142[A]:ARG:NH2	1:A:189:GLU:OE2	2.19	0.70
1:A:79:LEU:O	7:A:501:HOH:O	2.16	0.63
1:A:52:HIS:HB2	1:A:289:VAL:HG22	1.89	0.54
1:A:164:ASN:HB3	1:A:167:LEU:HB3	1.91	0.53
1:A:320:ILE:O	1:A:324[B]:MET:HG2	2.10	0.52
1:A:225:VAL:O	1:A:266[A]:PRO:HD2	2.12	0.50
1:A:224[B]:MET:HG2	1:A:264:ASN:HB2	1.95	0.48
1:A:6:ILE:H	1:A:6:ILE:HD12	1.79	0.48
1:A:26:ILE:O	1:A:251:LYS:NZ	2.48	0.47
1:A:327:ILE:HG23	1:A:332:ARG:HB2	1.97	0.46
4:A:407[B]:CPS:H10B	4:A:407[B]:CPS:H20	1.75	0.45
4:A:407[B]:CPS:H11B	4:A:407[B]:CPS:H3A	1.74	0.45
1:A:64:ARG:HG2	1:A:110:GLU:HB2	1.99	0.45
4:A:405:CPS:H21	4:A:405:CPS:H23A	1.69	0.45
4:A:404:CPS:H31A	4:A:404:CPS:H272	1.43	0.43
1:A:155:ARG:HG2	1:A:193[B]:GLU:HB2	2.01	0.43
4:A:403:CPS:H262	4:A:403:CPS:H30A	1.71	0.43
1:A:4:ARG:HA	1:A:7:LEU:HD12	2.00	0.43
1:A:229:PRO:HD3	1:A:271:MET:SD	2.60	0.41
1:A:142[B]:ARG:NH2	1:A:189:GLU:OE2	2.54	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	A	342/347 (99%)	331 (97%)	9 (3%)	2 (1%)	25 45

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	317	THR
1	A	318	ALA

5.3.2 Protein sidechains (i)

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	Analysed Rotameric O		Percentiles
1	A	$288/303\ (95\%)$	279 (97%)	9 (3%)	40 64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	28	ASP
1	A	41	GLU
1	A	44	ARG
1	A	178	GLU
1	A	262	ASP
1	A	312	VAL
1	A	320	ILE
1	A	322	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	Tuna	Chain	Res	Link	Во	ond leng	ths	В	ond ang	gles
MIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	401	3,1	0,12,12	0.00	-	-		
4	CPS	A	406	-	32,32,45	0.78	0	51,51,70	1.60	7 (13%)
4	CPS	A	404	-	45,45,45	1.42	4 (8%)	69,70,70	1.07	5 (7%)
4	CPS	A	407[B]	-	28,28,45	0.83	1 (3%)	46,46,70	1.68	10 (21%)
4	CPS	A	405	-	32,32,45	0.76	1 (3%)	51,51,70	0.95	1 (1%)
4	CPS	A	407[A]	-	28,28,45	0.80	1 (3%)	46,46,70	1.28	5 (10%)
3	SAH	A	402	2	21,28,28	1.20	2 (9%)	20,40,40	1.75	3 (15%)
4	CPS	A	403	-	45,45,45	1.43	3 (6%)	69,70,70	1.03	4 (5%)
5	CO3	A	408	-	0,3,3	0.00	-	0,3,3	0.00	_

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
4	CPS	A	406	_	-	2/9/74/90	0/4/4/4
2	SF4	A	401	3,1	-	-	0/6/5/5
4	CPS	A	404	-	-	14/25/90/90	0/4/4/4
4	CPS	A	407[B]	-	-	4/4/69/90	0/4/4/4
4	CPS	A	405	-	-	2/9/74/90	0/4/4/4
4	CPS	A	407[A]	_	-	0/4/69/90	0/4/4/4
3	SAH	A	402	2	-	1/7/31/31	0/3/3/3
4	CPS	A	403	-	-	3/25/90/90	0/4/4/4



All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
4	A	404	CPS	C32-S	-7.59	1.66	1.77
4	A	403	CPS	C32-S	-7.59	1.66	1.77
3	A	402	SAH	C2-N3	4.06	1.38	1.32
3	A	402	SAH	C2-N1	2.47	1.38	1.33
4	A	407[B]	CPS	C5-C6	-2.35	1.51	1.55
4	A	403	CPS	C27-N2	-2.33	1.47	1.52
4	A	403	CPS	C30-N2	-2.25	1.47	1.52
4	A	407[A]	CPS	C5-C6	-2.11	1.51	1.55
4	A	404	CPS	C5-C6	-2.11	1.51	1.55
4	A	404	CPS	C30-N2	-2.09	1.47	1.52
4	A	404	CPS	C27-N2	-2.03	1.48	1.52
4	A	405	CPS	C5-C6	-2.03	1.52	1.55

All (35) bond angle outliers are listed below:

3 4 4 4 4	A A A	402 407[B] 406	SAH CPS	N3-C2-N1 C5-C9-C20	-5.44	120.17	128.68
4 4 4	A A	406		C5-C9-C20			120.00
4 4	A		CDC		-5.10	113.40	119.49
4			CPS	C9-C5-C6	-4.80	95.26	100.09
		406	CPS	C6-C5-C4	4.56	111.65	107.40
4	A	406	CPS	C19-C3-C4	-4.21	108.74	114.30
4	A	406	CPS	C19-C18-C6	-4.16	104.00	109.71
4	A	407[B]	CPS	C5-C6-C18	-4.00	109.63	114.74
3	A	402	SAH	C5'-SD-CG	-3.82	90.82	102.27
4	A	407[B]	CPS	C3-C19-C2	-3.26	110.36	113.73
4	A	407[A]	CPS	C5-C6-C18	-3.19	110.66	114.74
4	A	407[A]	CPS	C3-C19-C2	-3.11	110.52	113.73
4	A	407[B]	CPS	C1-C2-C15	3.08	112.33	107.77
4	A	403	CPS	O1S-S-C32	3.07	110.62	106.92
4	A	407[B]	CPS	C19-C2-C15	3.07	112.89	108.58
4	A	406	CPS	C2-C19-C18	3.01	115.05	111.82
4	A	407[A]	CPS	C10-C5-C4	2.95	112.07	109.07
3	A	402	SAH	C3'-C2'-C1'	2.83	105.24	100.98
4	A	407[B]	CPS	C11-C2-C19	-2.71	107.45	111.18
4	A	404	CPS	O2S-S-C32	2.67	110.09	105.77
4	A	407[B]	CPS	C14-C13-C12	-2.65	107.39	110.55
4	A	407[A]	CPS	C9-C5-C6	2.61	102.73	100.09
4	A	407[B]	CPS	C19-C18-C6	-2.60	106.14	109.71
4	A	407[B]	CPS	C9-C5-C6	2.40	102.52	100.09
4	A	406	CPS	C8-C7-C6	-2.31	100.55	105.13
4	A	404	CPS	C31-C32-S	-2.27	109.77	113.25
4	A	407[A]	CPS	C6-C5-C4	-2.25	105.31	107.40

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
4	A	404	CPS	C3-C19-C2	-2.23	111.43	113.73
4	A	403	CPS	C21-C20-C9	2.22	116.33	112.92
4	A	404	CPS	O1S-S-C32	2.21	109.58	106.92
4	A	406	CPS	C1-C2-C15	2.11	110.88	107.77
4	A	404	CPS	C14-C13-C12	-2.09	108.05	110.55
4	A	407[B]	CPS	C7-C6-C5	2.07	105.58	103.55
4	A	403	CPS	C26-C27-N2	-2.07	111.00	115.38
4	A	405	CPS	C5-C9-C20	-2.06	117.04	119.50
4	A	403	CPS	O2S-S-C32	2.04	109.07	105.77

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	CPS	C26-C27-N2-C28
4	A	404	CPS	C26-C27-N2-C30
4	A	404	CPS	N2-C30-C31-C32
4	A	404	CPS	C31-C30-N2-C28
4	A	404	CPS	C31-C30-N2-C29
4	A	404	CPS	C31-C32-S-O2S
4	A	404	CPS	C31-C32-S-O3S
4	A	404	CPS	C31-C32-S-O1S
4	A	404	CPS	C26-C27-N2-C29
4	A	406	CPS	C21-C20-C22-C23
4	A	403	CPS	C9-C20-C22-C23
4	A	404	CPS	N1-C25-C26-C27
4	A	407[B]	CPS	C21-C20-C9-C5
4	A	407[B]	CPS	C22-C20-C9-C5
4	A	404	CPS	O1-C24-N1-C25
4	A	404	CPS	C23-C24-N1-C25
4	A	407[B]	CPS	C21-C20-C9-C8
4	A	407[B]	CPS	C22-C20-C9-C8
4	A	404	CPS	C30-C31-C32-S
4	A	405	CPS	C20-C22-C23-C24
4	A	404	CPS	C31-C30-N2-C27
4	A	406	CPS	C20-C22-C23-C24
4	A	403	CPS	C31-C32-S-O2S
4	A	403	CPS	C31-C32-S-O3S
4	A	405	CPS	C21-C20-C9-C5
3	A	402	SAH	N-CA-CB-CG

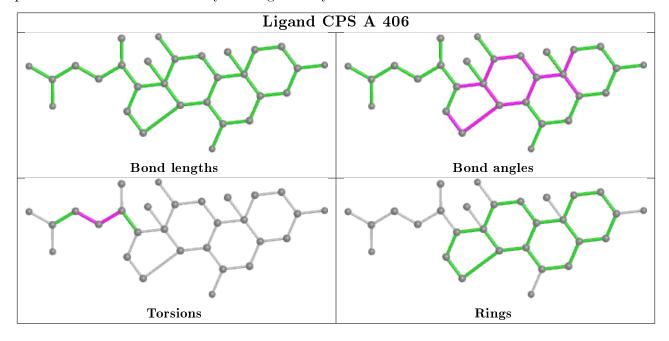
There are no ring outliers.



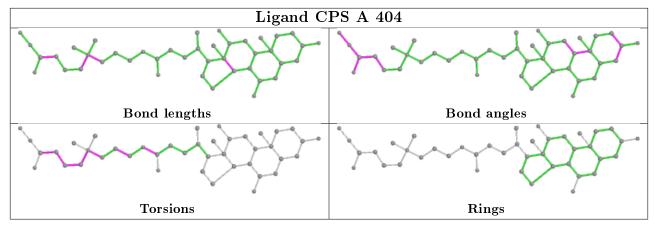
4			•	1 1	•	_	1 /	1 1
4	monomers	are	1nvo	lved	ın	$\mathbf{b} \cdot \mathbf{s}$	hort.	contacts:

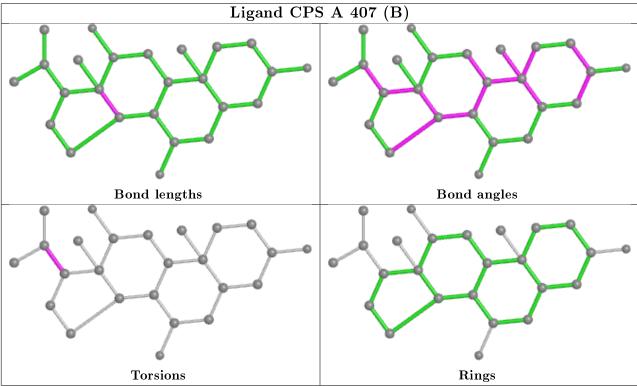
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	CPS	1	0
4	A	407[B]	CPS	2	0
4	A	405	CPS	1	0
4	A	403	CPS	1	0

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.

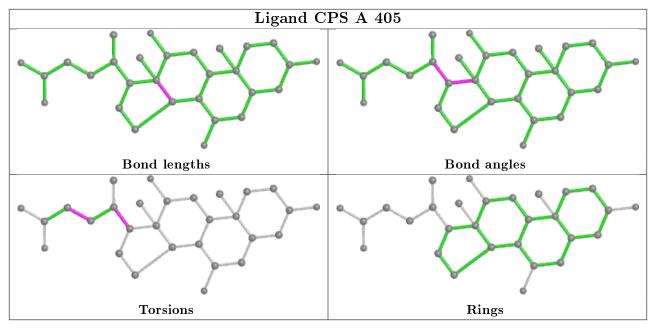


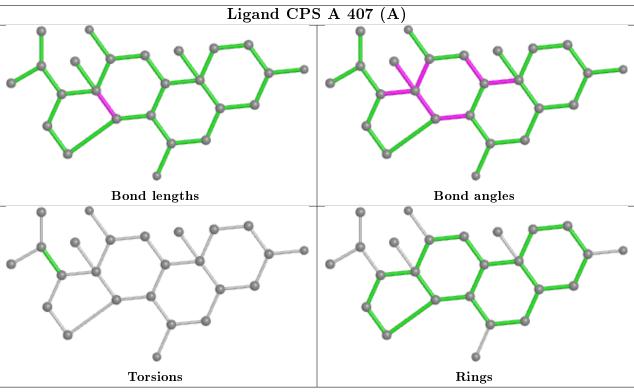




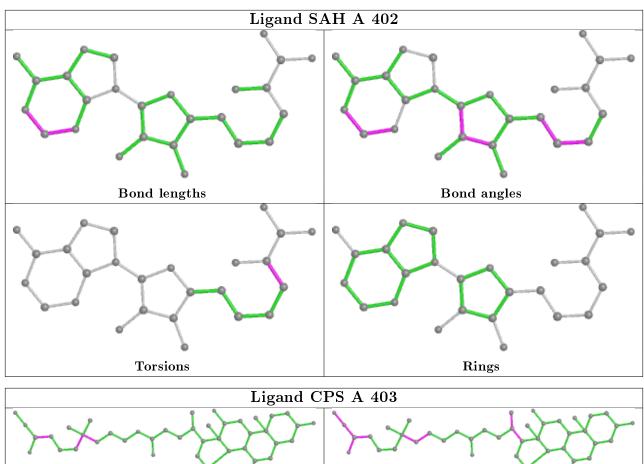


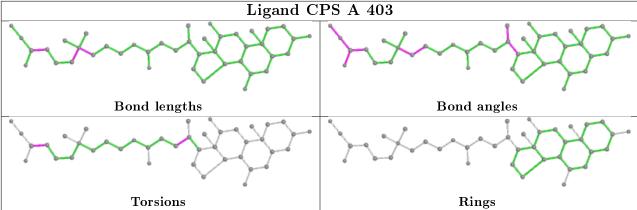












5.7 Other polymers (i)

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, 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$\mathbf{Z}{>}2$ OWAB($\mathbf{\mathring{A}}^2$)	
1	A	332/347 (95%)	0.05	2 (0%) 89 89	46, 70, 102, 122	8 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	PRO	2.9
1	A	171	LEU	2.7

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, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	CPS	A	406	29/42	0.75	0.50	202,204,205,206	0
5	CO3	A	408	4/4	0.82	0.19	104,105,105,106	0
4	CPS	A	404	42/42	0.86	0.36	138,150,207,208	1
4	CPS	A	407[B]	25/42	0.88	0.28	146,147,148,148	25
4	CPS	A	407[A]	25/42	0.88	0.28	66,68,69,71	25

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
6	CL	A	411	1/1	0.90	0.35	62,62,62,62	0
4	CPS	A	405	29/42	0.95	0.20	94,95,98,99	0
4	CPS	A	403	42/42	0.95	0.18	65,68,70,71	5
6	CL	A	409[A]	1/1	0.97	0.32	53,53,53,53	1
6	CL	A	409[B]	1/1	0.97	0.32	52,52,52,52	1
6	CL	A	410	1/1	0.97	0.10	71,71,71,71	0
3	SAH	A	402	26/26	0.97	0.15	58,66,68,69	0
2	SF4	A	401	8/8	0.99	0.09	53,55,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.

