Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 10:14 AM EDT

PDB ID	:	1C4A
Title	:	BINDING OF EXOGENOUSLY ADDED CARBON MONOXIDE AT THE ACTIVE SITE OF THE FE-ONLY HYDROGENASE (CPI) FROM CLOSTRIDIUM PASTEURIANUM
Authors	:	Lemon, B.J.; Peters, J.W.
Deposited on	:	1999-08-13
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

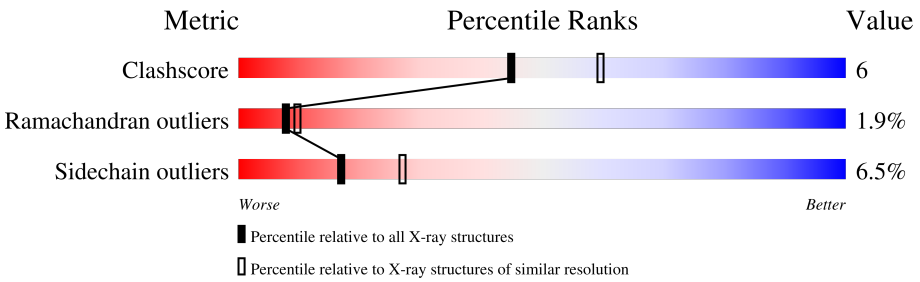
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	574	79% 18% •

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
3	SF4	A	581	-	-	X	-
3	SF4	A	583	-	-	X	-

2 Entry composition (i)

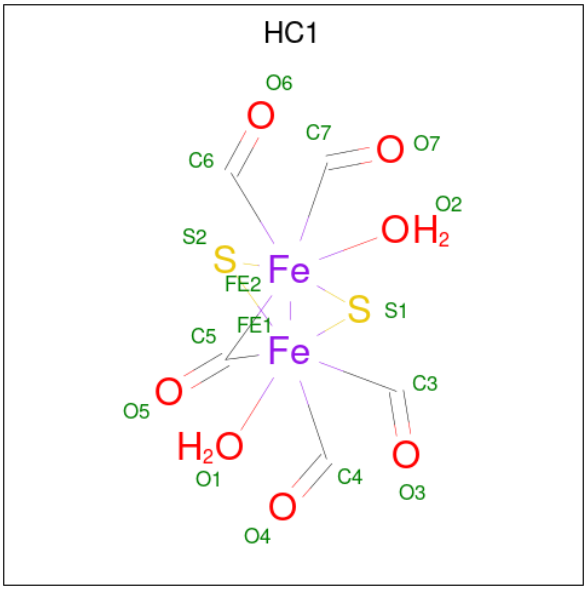
There are 5 unique types of molecules in this entry. The entry contains 4840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (FE-ONLY HYDROGENASE).

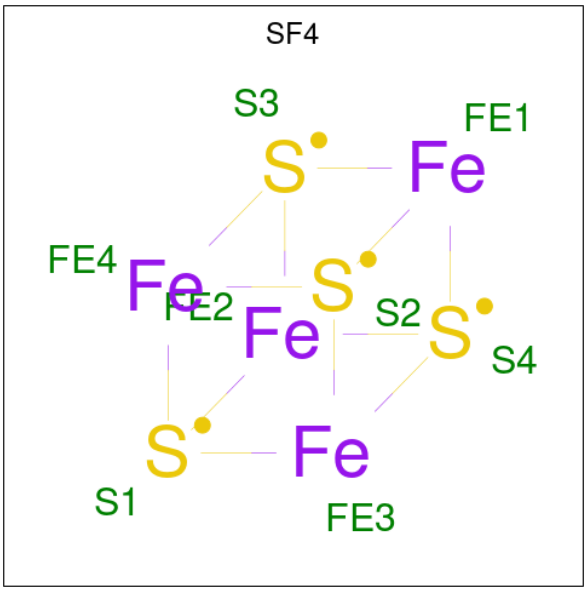
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	574	4461	2795	767	859	40	0	0	0

- Molecule 2 is 2 IRON/2 SULFUR/5 CARBONYL/2 WATER INORGANIC CLUSTER (three-letter code: HC1) (formula: $C_5H_8Fe_2O_7S_2$).



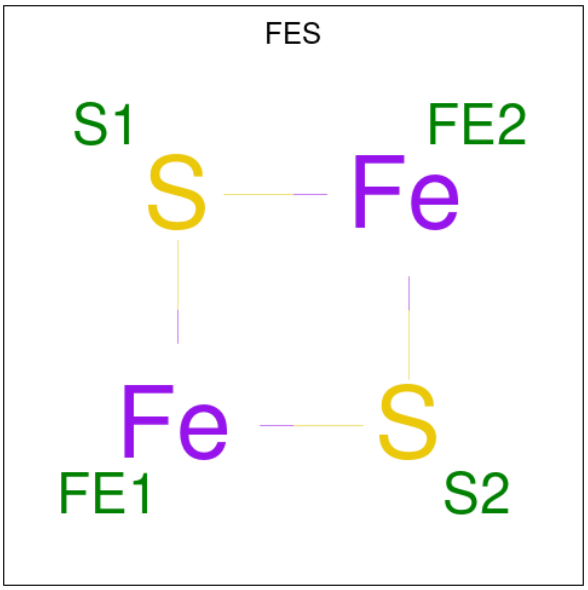
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	O	S		
2	A	1	16	5	2	7	2	0	0

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



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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	4	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	327	327	327	0	0

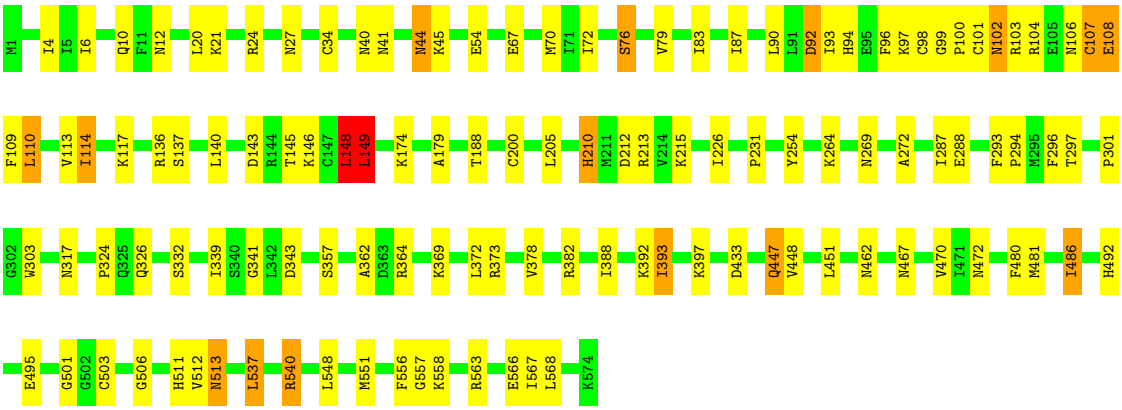
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (FE-ONLY HYDROGENASE)

Chain A: 79% 18% •



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.70Å 84.00Å 55.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	90.4 (20.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.857	Depositor
R, R_{free}	0.199 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4840	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

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: SF4, FES, HC1

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	0.64	1/4534 (0.0%)	1.20	27/6103 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	HIS	CD2-NE2	-5.00	1.26	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	551	MET	CA-CB-CG	9.68	129.76	113.30
1	A	148	LEU	CA-CB-CG	9.21	136.49	115.30
1	A	96	PHE	CB-CG-CD1	-7.88	115.29	120.80
1	A	303	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	303	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	A	548	LEU	CA-CB-CG	7.16	131.77	115.30
1	A	96	PHE	CB-CG-CD2	6.81	125.57	120.80
1	A	551	MET	CB-CA-C	-6.76	96.88	110.40
1	A	254	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	A	136	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	96	PHE	CA-CB-CG	5.90	128.07	113.90
1	A	540	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	303	TRP	CG-CD2-CE3	5.89	139.20	133.90
1	A	551	MET	N-CA-CB	5.87	121.16	110.60
1	A	303	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	A	213	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	288	GLU	CA-C-N	-5.54	105.00	117.20
1	A	343	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	382	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	373	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	LYS	CA-C-N	-5.24	105.67	117.20
1	A	303	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	A	373	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	364	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	339	ILE	CA-C-N	5.13	128.48	117.20
1	A	364	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	99	GLY	N-CA-C	-5.03	100.53	113.10

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	4461	0	4430	56	0
2	A	16	0	0	3	0
3	A	32	0	0	5	0
4	A	4	0	0	1	0
5	A	327	0	0	7	1
All	All	4840	0	4430	58	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 6.

All (58) 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:A:472:ASN:HD21	1:A:501:GLY:H	1.37	0.71
1:A:467:ASN:H	1:A:492:HIS:HD2	1.44	0.64
1:A:45:LYS:HB3	4:A:585:FES:S1	2.37	0.64
1:A:537:LEU:HD11	5:A:677:HOH:O	1.99	0.62
1:A:481:MET:SD	1:A:486:ILE:HG13	2.40	0.61
1:A:447:GLN:HE21	1:A:447:GLN:H	1.51	0.57
1:A:226:ILE:HD12	1:A:264:LYS:HB2	1.87	0.56
1:A:76:SER:HB3	1:A:79:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD22	1:A:148:LEU:HB2	1.88	0.54
1:A:4:ILE:HG22	1:A:70:MET:HB2	1.90	0.54
1:A:472:ASN:ND2	1:A:501:GLY:H	2.05	0.54
1:A:231:PRO:HD3	1:A:269:ASN:ND2	2.24	0.53
2:A:580:HC1:S1	2:A:580:HC1:O1	2.67	0.53
1:A:149:LEU:HA	3:A:583:SF4:S1	2.49	0.53
2:A:580:HC1:O1	2:A:580:HC1:S2	2.67	0.52
1:A:512:VAL:O	1:A:513:ASN:HB3	2.09	0.52
1:A:388:ILE:HG23	1:A:393:ILE:HG13	1.92	0.51
1:A:98:CYS:O	1:A:104:ARG:HB3	2.12	0.49
1:A:107:CYS:O	1:A:108:GLU:HB2	2.13	0.49
1:A:137:SER:HB3	1:A:140:LEU:O	2.11	0.49
1:A:97:LYS:O	1:A:101:CYS:HB2	2.13	0.48
1:A:563:ARG:HA	1:A:566:GLU:HG2	1.95	0.48
1:A:556:PHE:HE2	1:A:567:ILE:HD11	1.79	0.48
1:A:205:LEU:HG	3:A:583:SF4:S2	2.54	0.48
1:A:174:LYS:HE2	5:A:592:HOH:O	2.14	0.47
1:A:102:ASN:HD22	1:A:103:ARG:HG2	1.80	0.47
1:A:109:PHE:O	1:A:113:VAL:HG23	2.15	0.46
1:A:179:ALA:HB1	1:A:188:THR:HG21	1.98	0.46
1:A:212:ASP:HB2	5:A:753:HOH:O	2.15	0.46
1:A:448:VAL:HB	1:A:470:VAL:HG21	1.97	0.46
1:A:70:MET:HA	5:A:589:HOH:O	2.15	0.45
1:A:110:LEU:O	1:A:114:ILE:HG23	2.16	0.45
1:A:210:HIS:HD2	1:A:378:VAL:H	1.64	0.45
1:A:294:PRO:HG2	1:A:296:PHE:CE1	2.52	0.45
1:A:41:ASN:O	1:A:45:LYS:HG2	2.17	0.44
1:A:287:ILE:HA	1:A:293:PHE:HZ	1.83	0.44
1:A:294:PRO:O	1:A:317:ASN:HB3	2.18	0.43
1:A:369:LYS:HG2	5:A:804:HOH:O	2.17	0.43
1:A:143:ASP:OD1	1:A:145:THR:HB	2.19	0.43
1:A:503:CYS:CB	2:A:580:HC1:C4	2.97	0.43
1:A:272:ALA:HA	1:A:324:PRO:HG3	2.01	0.43
1:A:6:ILE:HG12	1:A:72:ILE:HD12	2.01	0.43
1:A:480:PHE:CE2	1:A:486:ILE:HG12	2.54	0.42
1:A:326:GLN:HE22	1:A:362:ALA:HA	1.84	0.42
1:A:145:THR:HG22	1:A:146:LYS:HD2	2.01	0.42
1:A:388:ILE:HG23	1:A:393:ILE:CG1	2.49	0.42
1:A:83:ILE:HB	5:A:762:HOH:O	2.19	0.42
1:A:34:CYS:SG	1:A:40:ASN:HB2	2.60	0.42
1:A:90:LEU:HD13	1:A:148:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASN:ND2	1:A:103:ARG:HG2	2.36	0.41
1:A:200:CYS:HA	3:A:583:SF4:S3	2.60	0.41
1:A:210:HIS:CD2	1:A:378:VAL:H	2.38	0.41
1:A:20:LEU:O	1:A:24:ARG:HB2	2.21	0.41
1:A:297:THR:HG23	1:A:495:GLU:HA	2.02	0.41
1:A:301:PRO:HD2	3:A:581:SF4:S2	2.61	0.41
1:A:511:HIS:HD2	5:A:801:HOH:O	2.03	0.41
1:A:506:GLY:HA3	3:A:581:SF4:S3	2.61	0.40
1:A:566:GLU:HG3	1:A:567:ILE:HG23	2.04	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)
5:A:608:HOH:O	5:A:618:HOH:O[4_456]	2.18	0.02

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	572/574 (100%)	537 (94%)	24 (4%)	11 (2%)	8 10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	92	ASP
1	A	149	LEU
1	A	558	LYS
1	A	76	SER
1	A	108	GLU
1	A	557	GLY

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Mol	Chain	Res	Type
1	A	44	ASN
1	A	107	CYS
1	A	513	ASN
1	A	341	GLY

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	Rotameric	Outliers	Percentiles
1	A	490/490 (100%)	458 (94%)	32 (6%)	17 27

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	12	ASN
1	A	21	LYS
1	A	44	ASN
1	A	54	GLU
1	A	67	GLU
1	A	87	ILE
1	A	92	ASP
1	A	93	ILE
1	A	100	PRO
1	A	102	ASN
1	A	106	ASN
1	A	110	LEU
1	A	114	ILE
1	A	148	LEU
1	A	149	LEU
1	A	210	HIS
1	A	215	LYS
1	A	332	SER
1	A	357	SER
1	A	372	LEU
1	A	392	LYS

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Mol	Chain	Res	Type
1	A	393	ILE
1	A	397	LYS
1	A	433	ASP
1	A	447	GLN
1	A	451	LEU
1	A	462	ASN
1	A	486	ILE
1	A	537	LEU
1	A	540	ARG
1	A	568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	12	ASN
1	A	89	GLN
1	A	102	ASN
1	A	189	ASN
1	A	195	GLN
1	A	210	HIS
1	A	259	GLN
1	A	269	ASN
1	A	306	GLN
1	A	325	GLN
1	A	326	GLN
1	A	447	GLN
1	A	462	ASN
1	A	472	ASN
1	A	492	HIS
1	A	511	HIS

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)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	HC1	A	580	1	1,18,18	0.82	0	-		
3	SF4	A	584	1	0,12,12	-	-	-		
3	SF4	A	582	1	0,12,12	-	-	-		
3	SF4	A	581	1	0,12,12	-	-	-		
4	FES	A	585	1	0,4,4	-	-	-		
3	SF4	A	583	1	0,12,12	-	-	-		

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
2	HC1	A	580	1	-	-	0/3/3/3
3	SF4	A	584	1	-	-	0/6/5/5
3	SF4	A	582	1	-	-	0/6/5/5
3	SF4	A	581	1	-	-	0/6/5/5
4	FES	A	585	1	-	-	0/1/1/1
3	SF4	A	583	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	580	HC1	3	0
3	A	581	SF4	2	0
4	A	585	FES	1	0
3	A	583	SF4	3	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.