



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:08 AM EDT

PDB ID : 1C4C / pdb_00001c4c
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 : 1999-08-16
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

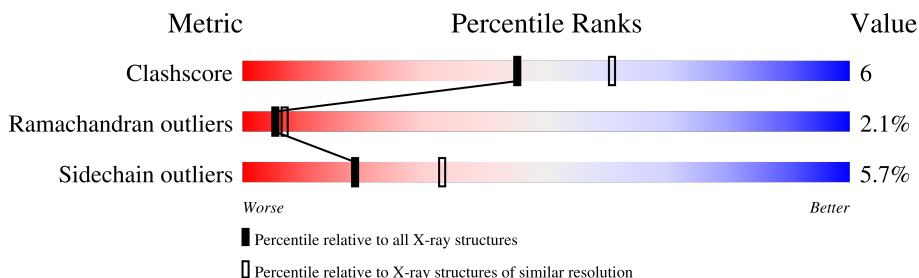
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	574	 76% 20% . .

2 Entry composition [i](#)

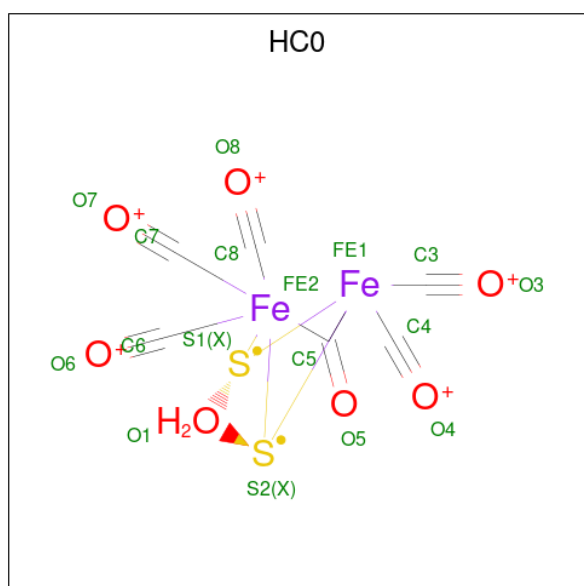
There are 5 unique types of molecules in this entry. The entry contains 4828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	574	Total	C	N	O	S	0	0	0
			4461	2795	767	859	40			

- Molecule 2 is 2 IRON/2 SULFUR/6 CARBONYL/1 WATER INORGANIC CLUSTER (CCD ID: HC0) (formula: $C_6H_2Fe_2O_7S_2$).



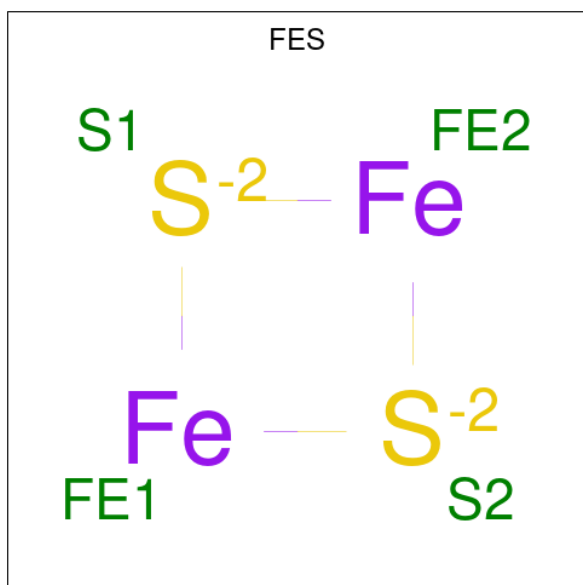
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	O	S	0	0
			17	6	2	7	2		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 5 is water.

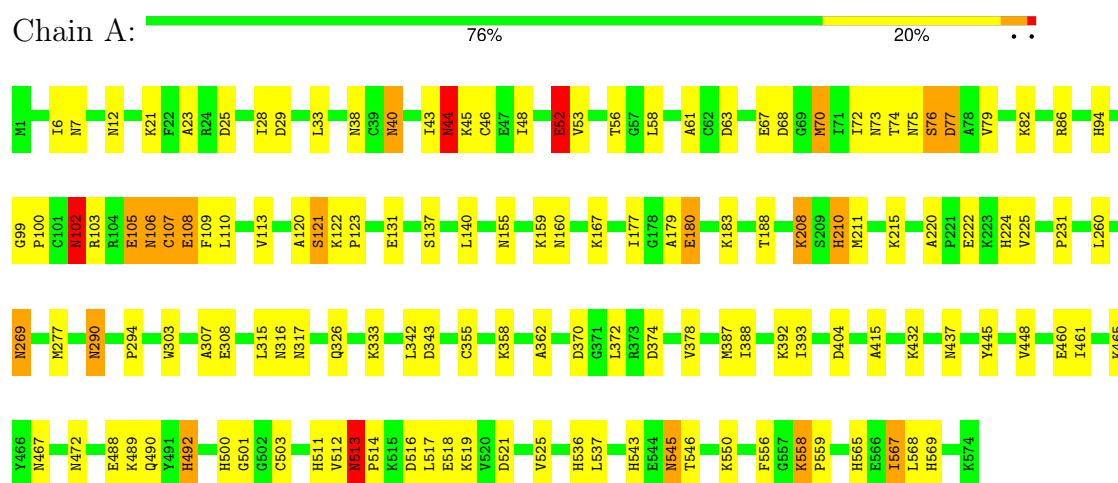
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total	O	0	0
			314	314		

3 Residue-property plots

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)



4 Data and refinement statistics

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	133.50Å 83.80Å 55.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.7 (20.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.857	Depositor
R, R_{free}	0.193 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4828	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: HC0, FES, SF4

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	0.75	11/4534 (0.2%)	1.49	59/6103 (1.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	HIS	CD2-NE2	-7.64	1.29	1.37
1	A	492	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	565	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	210	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	569	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	511	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	536	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	543	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	94	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	500	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	536	HIS	CG-ND1	-5.08	1.32	1.38

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASN	CA-CB-CG	8.63	121.23	112.60
1	A	370	ASP	CA-CB-CG	8.32	120.92	112.60
1	A	545	ASN	CA-CB-CG	8.30	120.90	112.60
1	A	106	ASN	CA-CB-CG	8.01	120.61	112.60
1	A	290	ASN	N-CA-C	7.92	127.68	110.80
1	A	102	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	342	LEU	N-CA-C	6.60	120.81	110.32
1	A	569	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	102	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	A	404	ASP	CA-C-N	6.32	125.54	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ASP	C-N-CA	6.32	125.54	118.97
1	A	160	ASN	N-CA-C	6.30	118.22	111.36
1	A	29	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	374	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	492	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	225	VAL	N-CA-C	6.03	116.49	107.51
1	A	210	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	A	52	GLU	CA-CB-CG	5.88	125.86	114.10
1	A	123	PRO	N-CA-C	5.81	124.44	112.47
1	A	437	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	12	ASN	CA-CB-CG	5.74	118.34	112.60
1	A	25	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	61	ALA	N-CA-C	5.66	118.22	111.71
1	A	343	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	513	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	121	SER	N-CA-C	-5.62	98.83	110.80
1	A	521	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	68	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	40	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	70	MET	N-CA-C	5.50	118.62	110.48
1	A	63	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	220	ALA	CA-C-N	5.45	125.28	119.28
1	A	220	ALA	C-N-CA	5.45	125.28	119.28
1	A	222	GLU	CB-CG-CD	5.45	121.86	112.60
1	A	303	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	A	107	CYS	CA-C-O	-5.39	112.81	120.51
1	A	110	LEU	N-CA-C	-5.35	105.53	111.36
1	A	183	LYS	CB-CG-CD	-5.30	99.10	111.30
1	A	513	ASN	CA-C-N	5.28	125.60	119.47
1	A	513	ASN	C-N-CA	5.28	125.60	119.47
1	A	415	ALA	N-CA-C	5.27	117.77	111.71
1	A	303	TRP	CB-CG-CD1	-5.26	119.01	126.90
1	A	58	LEU	N-CA-C	5.25	116.71	109.15
1	A	105	GLU	CA-CB-CG	5.25	124.59	114.10
1	A	303	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	A	269	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	543	HIS	CB-CG-CD2	-5.15	124.50	131.20
1	A	210	HIS	CB-CG-ND1	5.15	130.43	122.70
1	A	102	ASN	CB-CG-ND2	5.12	124.07	116.40
1	A	567	ILE	N-CA-C	5.08	119.36	113.42
1	A	543	HIS	CA-CB-CG	5.07	118.87	113.80
1	A	558	LYS	CA-C-N	5.07	125.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	LYS	C-N-CA	5.07	125.07	119.90
1	A	40	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	40	ASN	CB-CG-ND2	5.05	123.97	116.40
1	A	545	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	122	LYS	CA-C-N	5.03	126.12	119.84
1	A	122	LYS	C-N-CA	5.03	126.12	119.84
1	A	565	HIS	CB-CG-CD2	-5.02	124.68	131.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4461	0	4430	51	0
2	A	17	0	0	3	0
3	A	32	0	0	1	0
4	A	4	0	0	1	0
5	A	314	0	0	8	0
All	All	4828	0	4430	53	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 6.

All (53) 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	1.27	0.83
1:A:512:VAL:HG11	1:A:517:LEU:HD13	1.71	0.72
1:A:467:ASN:H	1:A:492:HIS:HD2	1.38	0.72
1:A:167:LYS:HE3	1:A:180:GLU:HG2	1.84	0.60
1:A:45:LYS:HB3	4:A:585:FES:S1	2.42	0.59
1:A:43:ILE:HD11	5:A:615:HOH:O	2.05	0.56
1:A:392:LYS:HG3	5:A:620:HOH:O	2.05	0.56
1:A:137:SER:O	1:A:208:LYS:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:LYS:HE2	1:A:460:GLU:O	2.07	0.53
1:A:76:SER:HB3	1:A:79:VAL:HB	1.89	0.53
2:A:580:HC0:S2	2:A:580:HC0:O1	2.66	0.52
2:A:580:HC0:O1	2:A:580:HC0:S1	2.67	0.52
1:A:307:ALA:O	1:A:315:LEU:HD21	2.09	0.52
1:A:52:GLU:HG3	1:A:73:ASN:HB2	1.91	0.52
1:A:6:ILE:HG23	1:A:72:ILE:HB	1.92	0.51
1:A:7:ASN:HD21	1:A:74:THR:H	1.58	0.51
1:A:82:LYS:O	1:A:86:ARG:HG2	2.11	0.51
1:A:67:GLU:HB3	5:A:835:HOH:O	2.11	0.50
1:A:155:ASN:O	1:A:159:LYS:HG2	2.11	0.50
1:A:489:LYS:HG2	5:A:888:HOH:O	2.11	0.50
1:A:488:GLU:HB2	5:A:888:HOH:O	2.12	0.50
1:A:512:VAL:O	1:A:513:ASN:HB3	2.13	0.49
1:A:546:THR:O	1:A:550:LYS:HD3	2.13	0.49
1:A:294:PRO:O	1:A:317:ASN:HB3	2.13	0.49
1:A:472:ASN:ND2	1:A:501:GLY:H	2.02	0.48
1:A:556:PHE:HE1	1:A:567:ILE:HD11	1.77	0.48
1:A:46:CYS:SG	1:A:48:ILE:HG12	2.53	0.48
1:A:102:ASN:HD22	1:A:103:ARG:HG2	1.78	0.48
1:A:210:HIS:HD2	1:A:378:VAL:H	1.63	0.47
1:A:472:ASN:HD21	1:A:501:GLY:N	2.04	0.46
1:A:67:GLU:HB2	1:A:70:MET:HG3	1.98	0.46
1:A:231:PRO:HD3	1:A:269:ASN:ND2	2.31	0.46
1:A:467:ASN:H	1:A:492:HIS:CD2	2.26	0.46
1:A:107:CYS:O	1:A:108:GLU:HB3	2.17	0.45
1:A:355:CYS:HB2	3:A:581:SF4:S3	2.55	0.45
1:A:210:HIS:CD2	1:A:378:VAL:H	2.35	0.45
1:A:445:TYR:O	1:A:448:VAL:HG22	2.16	0.44
1:A:260:LEU:HD13	1:A:387:MET:HE2	1.98	0.44
1:A:179:ALA:HB1	1:A:188:THR:HG21	2.01	0.43
1:A:388:ILE:HG23	1:A:393:ILE:HB	2.00	0.43
1:A:514:PRO:HA	1:A:517:LEU:HB3	2.01	0.43
1:A:23:ALA:HB1	1:A:28:ILE:O	2.18	0.43
1:A:333:LYS:HB2	5:A:657:HOH:O	2.19	0.43
1:A:277:MET:HG3	1:A:559:PRO:HG2	2.00	0.42
1:A:326:GLN:HE22	1:A:362:ALA:HA	1.83	0.42
1:A:503:CYS:CB	2:A:580:HC0:C4	2.97	0.42
1:A:392:LYS:HE2	5:A:620:HOH:O	2.20	0.42
1:A:53:VAL:HG13	1:A:56:THR:OG1	2.20	0.41
1:A:355:CYS:SG	1:A:358:LYS:HG2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:HE2	1:A:38:ASN:HD21	1.86	0.41
1:A:432:LYS:HG3	1:A:461:ILE:HG12	2.02	0.41
1:A:137:SER:HB3	1:A:140:LEU:O	2.21	0.40
1:A:558:LYS:HE3	5:A:634:HOH:O	2.20	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	572/574 (100%)	533 (93%)	27 (5%)	12 (2%)	5 7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	SER
1	A	120	ALA
1	A	121	SER
1	A	44	ASN
1	A	108	GLU
1	A	109	PHE
1	A	308	GLU
1	A	516	ASP
1	A	77	ASP
1	A	290	ASN
1	A	513	ASN
1	A	99	GLY

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	490/490 (100%)	462 (94%)	28 (6%)	18	33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	40	ASN
1	A	44	ASN
1	A	52	GLU
1	A	75	ASN
1	A	77	ASP
1	A	100	PRO
1	A	102	ASN
1	A	105	GLU
1	A	106	ASN
1	A	113	VAL
1	A	131	GLU
1	A	177	ILE
1	A	180	GLU
1	A	208	LYS
1	A	211	MET
1	A	215	LYS
1	A	316	ASN
1	A	372	LEU
1	A	465	LYS
1	A	490	GLN
1	A	513	ASN
1	A	518	GLU
1	A	519	LYS
1	A	525	VAL
1	A	537	LEU
1	A	545	ASN
1	A	568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	ASN
1	A	38	ASN
1	A	40	ASN
1	A	102	ASN
1	A	155	ASN
1	A	170	ASN
1	A	172	ASN
1	A	210	HIS
1	A	219	ASN
1	A	269	ASN
1	A	306	GLN
1	A	316	ASN
1	A	317	ASN
1	A	462	ASN
1	A	472	ASN
1	A	492	HIS
1	A	533	GLN

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 oligosaccharides 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	$\# Z > 2$
3	SF4	A	582	1	0,12,12	-	-	-		
2	HC0	A	580	1	8,19,19	1.49	1 (12%)	0,40,40	-	-
3	SF4	A	583	1	0,12,12	-	-	-		
3	SF4	A	581	1	0,12,12	-	-	-		
4	FES	A	585	1	0,4,4	-	-	-		
3	SF4	A	584	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
3	SF4	A	582	1	-	-	0/6/5/5
2	HC0	A	580	1	-	-	0/5/3/3
3	SF4	A	583	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	584	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	580	HC0	O5-C5	-3.03	1.12	1.17

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

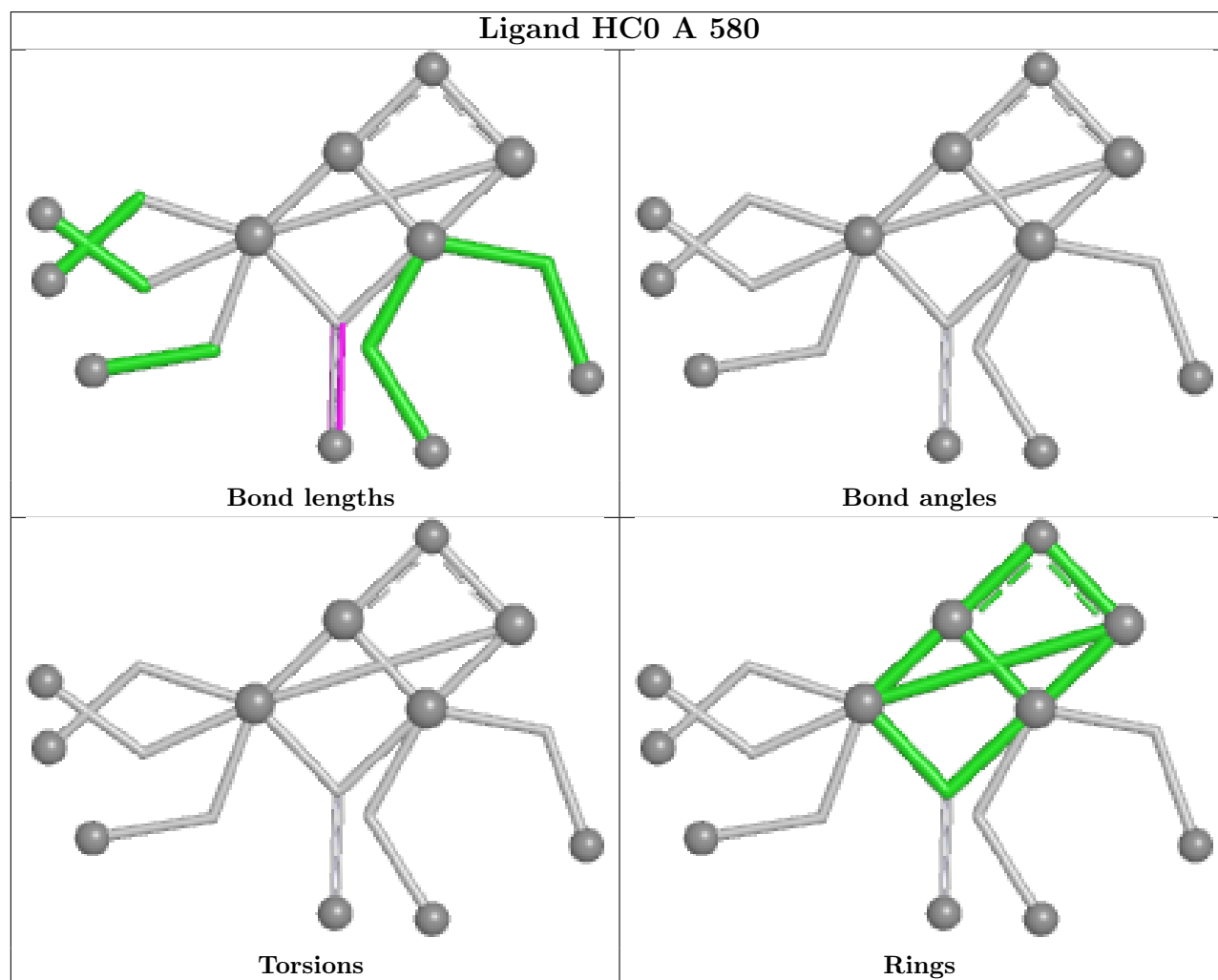
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	580	HC0	3	0
3	A	581	SF4	1	0
4	A	585	FES	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.