Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 08:52 PM EDT

PDB ID	:	1E08
Title	:	Structural model of the [Fe]-Hydrogenase/cytochrome c553 complex combining NMR and soft-docking
Authors	:	Morelli, X.; Czjzek, M.; Hatchikian, C.E.; Bornet, O.; Fontecilla-Camps, J.C.; Palma, N.P.; Moura, J.J.G.; Guerlesquin, F.
Deposited on	:	2000-03-13

This is a Full wwPDB NMR 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/NMRValidationReportHelp
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:

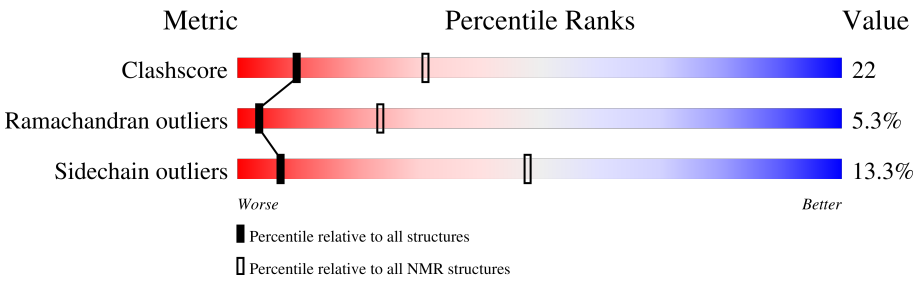
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR, THEORETICAL MODEL

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	371	57% 31% 7% •
2	D	88	55% 24% 16% 6%
3	E	78	67% 27% 5% •

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

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
5	A	PDT	4	-	1

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5058 atoms, of which 882 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called [FE]-HYDROGENASE (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	371	3387	1783	580	465	527	32	0

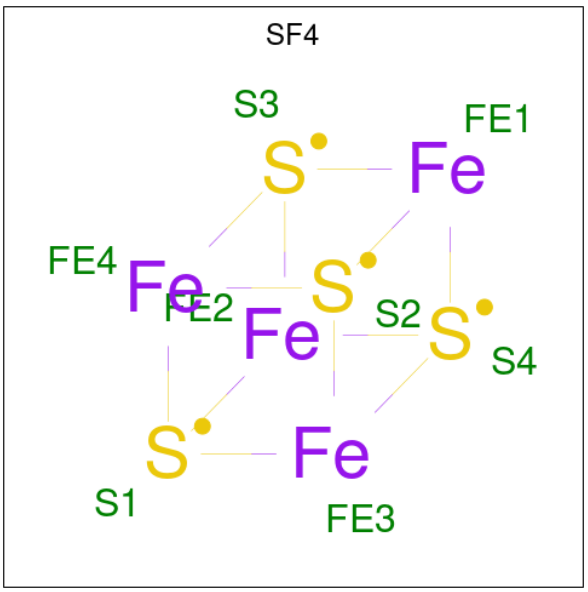
- Molecule 2 is a protein called [FE]-HYDROGENASE (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	D	88	875	457	162	123	132	1	0

- Molecule 3 is a protein called CYTOCHROME C553.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	E	78	710	354	138	97	114	7	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms		
			Total	Fe	S
4	A	1	8	4	4

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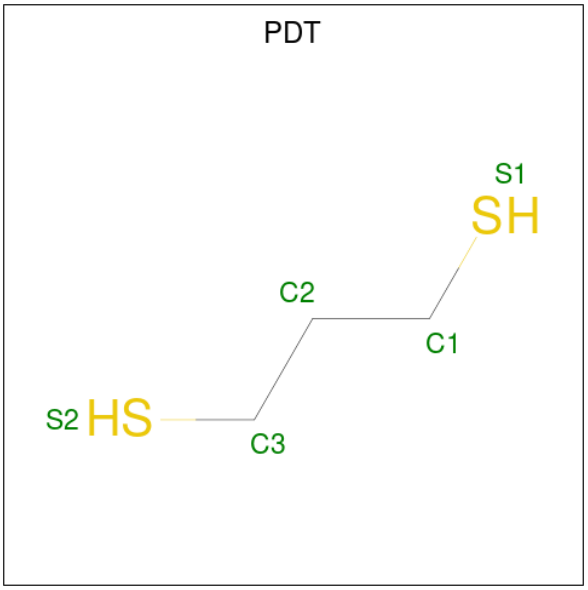
Mol	Chain	Residues	Atoms		
			Total	Fe	S
4	A	1	8	4	4
			Total	Fe	S
4	A	1	8	4	4

- Molecule 5 is 1,3-PROPANEDITHIOL (three-letter code: PDT) (formula: $C_3H_8S_2$).

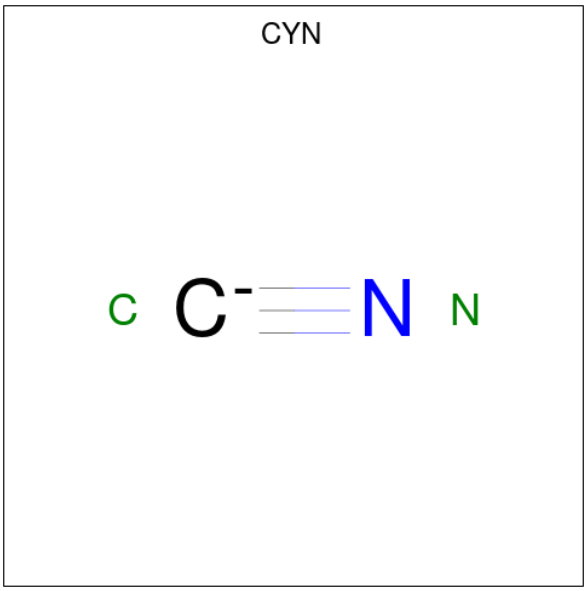


Mol	Chain	Residues	Atoms		
			Total	C	S
5	A	1	5	3	2

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

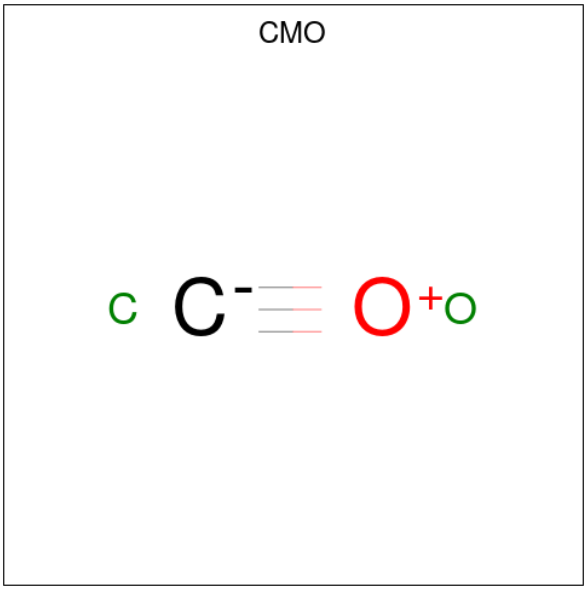
Mol	Chain	Residues	Atoms	
			Total	Fe
6	A	2	2	2

- Molecule 7 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms		
			Total	C	N
7	A	1	2	1	1
			Total	C	N
7	A	1	2	1	1

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).

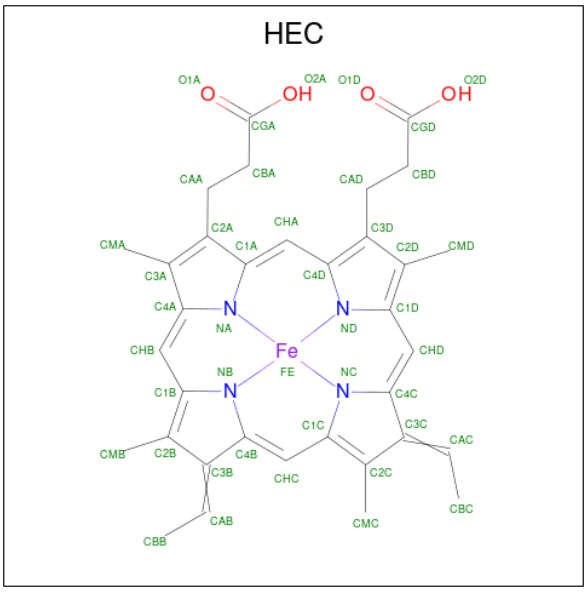


Mol	Chain	Residues	Atoms		
			Total	C	O
8	A	1	2	1	1
			Total	C	O
8	A	1	2	1	1

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
9	D	1	1	1

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms				
			Total	C	Fe	N	O
10	E	1	43	34	1	4	4

- Molecule 11 is water.

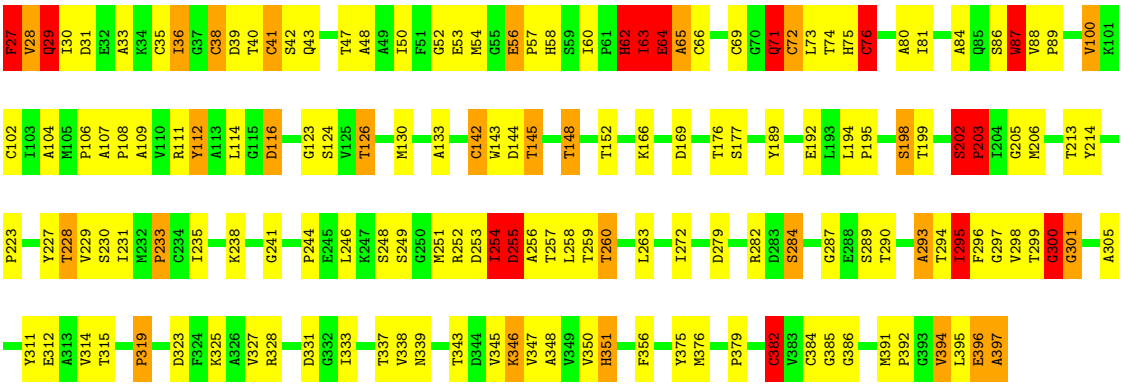
Mol	Chain	Residues	Atoms		
			Total	H	O
11	A	1	3	2	1

4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

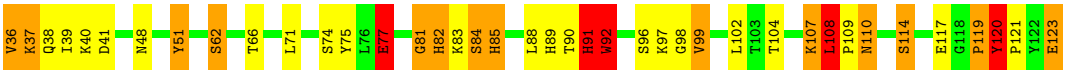
• Molecule 1: [FE]-HYDROGENASE (LARGE SUBUNIT)

Chain A: 57% 31% 7% •



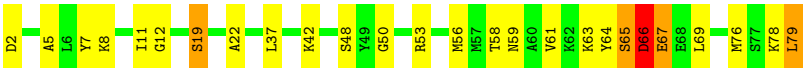
• Molecule 2: [FE]-HYDROGENASE (SMALL SUBUNIT)

Chain D: 55% 24% 16% 6%



• Molecule 3: CYTOCHROME C553

Chain E: 67% 27% 5% •



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *?*.

Of the 1000 calculated structures, 1 were deposited, based on the following criterion: *LEAST SHIFT VARIATION VIOLATION*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.843
UXNMR	structure solution	UXNMR

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, CMO, ZN, CYN, SF4, HEC, PDT

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 (average) 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	1.01	13/2874 (0.5%)	1.65	43/3885 (1.1%)
2	D	1.29	6/733 (0.8%)	1.95	36/988 (3.6%)
3	E	0.75	2/579 (0.3%)	1.17	5/765 (0.7%)
All	All	1.03	21/4186 (0.5%)	1.65	84/5638 (1.5%)

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	Planarity
1	A	7	23
2	D	2	10
3	E	1	3
All	All	10	36

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	CYS	C-N	17.40	1.74	1.34
2	D	77	GLU	C-N	-16.98	0.94	1.34
1	A	65	ALA	C-N	-14.33	1.01	1.34
1	A	27	PHE	C-N	-14.08	1.01	1.34
1	A	203	PRO	N-CD	-10.47	1.33	1.47
2	D	109	PRO	N-CD	-10.19	1.33	1.47
1	A	65	ALA	N-CA	10.06	1.66	1.46
1	A	64	GLU	C-N	8.99	1.54	1.34
1	A	29	GLN	C-N	8.91	1.54	1.34
1	A	202	SER	C-N	-8.46	1.18	1.34
1	A	71	GLN	C-N	-8.01	1.15	1.34
2	D	99	VAL	N-CA	-7.26	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	VAL	N-CA	-6.54	1.33	1.46
2	D	109	PRO	C-O	6.53	1.36	1.23
3	E	67	GLU	N-CA	6.29	1.58	1.46
3	E	64	TYR	C-N	-6.18	1.19	1.34
2	D	110	ASN	C-N	-5.67	1.23	1.34
2	D	39	ILE	N-CA	-5.54	1.35	1.46
1	A	254	ILE	C-N	-5.52	1.21	1.34
1	A	202	SER	C-O	-5.42	1.13	1.23
1	A	203	PRO	CA-CB	-5.19	1.43	1.53

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	GLN	O-C-N	-28.21	77.56	122.70
1	A	29	GLN	CA-C-N	-24.25	63.86	117.20
1	A	63	ILE	O-C-N	16.68	149.38	122.70
1	A	27	PHE	O-C-N	-15.99	97.12	122.70
1	A	64	GLU	O-C-N	15.09	146.84	122.70
1	A	295	ILE	CB-CA-C	-14.75	82.10	111.60
1	A	28	VAL	O-C-N	14.46	145.84	122.70
1	A	346	LYS	O-C-N	14.45	145.82	122.70
1	A	71	GLN	O-C-N	-13.48	101.14	122.70
2	D	120	TYR	O-C-N	12.27	144.41	121.10
2	D	119	PRO	O-C-N	12.07	142.01	122.70
2	D	108	LEU	O-C-N	-11.77	98.74	121.10
1	A	27	PHE	CA-C-N	11.05	141.51	117.20
2	D	39	ILE	CA-CB-CG1	10.94	131.78	111.00
1	A	27	PHE	C-N-CA	10.61	148.22	121.70
1	A	28	VAL	CA-C-N	-10.35	94.43	117.20
1	A	63	ILE	CA-C-N	-10.30	94.55	117.20
2	D	98	GLY	O-C-N	9.41	137.75	122.70
1	A	202	SER	O-C-N	-9.31	103.41	121.10
1	A	346	LYS	CA-C-N	-9.21	96.93	117.20
2	D	108	LEU	N-CA-C	9.10	135.57	111.00
2	D	120	TYR	CA-C-N	-9.05	91.76	117.10
2	D	108	LEU	CA-C-N	8.81	141.76	117.10
2	D	107	LYS	O-C-N	8.67	136.57	122.70
1	A	255	ASP	O-C-N	-8.32	109.38	122.70
1	A	65	ALA	O-C-N	8.31	136.00	122.70
2	D	109	PRO	O-C-N	8.27	135.93	122.70
2	D	107	LYS	C-N-CA	7.97	141.62	121.70
1	A	63	ILE	C-N-CA	7.85	141.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	81	GLY	O-C-N	-7.69	110.39	122.70
2	D	117	GLU	C-N-CA	-7.59	106.37	122.30
1	A	28	VAL	C-N-CA	7.58	140.65	121.70
2	D	39	ILE	N-CA-CB	7.49	128.02	110.80
2	D	109	PRO	CA-C-N	-7.38	100.95	117.20
1	A	203	PRO	CA-C-N	7.37	133.42	117.20
1	A	64	GLU	C-N-CA	7.07	139.36	121.70
2	D	108	LEU	CA-CB-CG	-7.02	99.15	115.30
1	A	397	ALA	N-CA-C	-6.99	92.12	111.00
1	A	64	GLU	CA-C-N	-6.92	101.99	117.20
1	A	64	GLU	N-CA-CB	6.79	122.82	110.60
2	D	123	GLU	N-CA-C	-6.46	93.55	111.00
3	E	79	LEU	N-CA-C	-6.42	93.67	111.00
1	A	87	TRP	CA-CB-CG	6.38	125.81	113.70
1	A	255	ASP	CA-C-N	6.37	131.21	117.20
2	D	107	LYS	CA-C-N	-6.28	103.39	117.20
2	D	98	GLY	CA-C-N	-6.22	103.51	117.20
2	D	99	VAL	CA-CB-CG1	6.16	120.14	110.90
1	A	29	GLN	N-CA-CB	-5.96	99.86	110.60
1	A	64	GLU	CB-CA-C	-5.96	98.49	110.40
3	E	64	TYR	C-N-CA	5.94	136.56	121.70
1	A	65	ALA	CA-C-N	-5.86	104.30	117.20
1	A	253	ASP	O-C-N	5.84	132.05	122.70
1	A	203	PRO	N-CA-C	5.83	127.25	112.10
1	A	65	ALA	CB-CA-C	-5.80	101.40	110.10
3	E	66	ASP	N-CA-CB	-5.75	100.26	110.60
2	D	77	GLU	O-C-N	-5.70	113.58	122.70
2	D	62	SER	N-CA-CB	-5.68	101.97	110.50
2	D	114	SER	N-CA-CB	-5.68	101.98	110.50
1	A	71	GLN	CA-C-N	5.64	129.60	117.20
2	D	91	HIS	N-CA-C	-5.62	95.83	111.00
1	A	300	GLY	N-CA-C	-5.57	99.16	113.10
1	A	62	HIS	O-C-N	5.57	131.61	122.70
1	A	72	CYS	C-N-CA	5.54	135.55	121.70
1	A	279	ASP	N-CA-C	-5.53	96.08	111.00
1	A	396	GLU	N-CA-C	-5.52	96.09	111.00
1	A	382	CYS	CA-CB-SG	-5.51	104.07	114.00
1	A	331	ASP	N-CA-C	-5.51	96.13	111.00
2	D	91	HIS	CA-CB-CG	5.50	122.96	113.60
2	D	77	GLU	CB-CA-C	5.48	121.36	110.40
1	A	100	VAL	N-CA-C	-5.47	96.23	111.00
2	D	36	VAL	N-CA-C	-5.46	96.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	117	GLU	N-CA-C	-5.44	96.31	111.00
2	D	39	ILE	N-CA-C	5.43	125.65	111.00
2	D	92	TRP	N-CA-C	-5.33	96.61	111.00
2	D	39	ILE	CB-CA-C	-5.23	101.14	111.60
3	E	19	SER	N-CA-CB	-5.22	102.67	110.50
3	E	50	GLY	N-CA-C	-5.19	100.12	113.10
2	D	37	LYS	N-CA-C	-5.18	97.01	111.00
2	D	38	GLN	C-N-CA	-5.18	108.75	121.70
2	D	84	SER	N-CA-CB	-5.18	102.73	110.50
1	A	87	TRP	CB-CG-CD1	-5.13	120.33	127.00
2	D	108	LEU	CB-CA-C	-5.08	100.55	110.20
2	D	39	ILE	CA-C-O	-5.07	109.46	120.10
1	A	395	LEU	N-CA-C	-5.01	97.47	111.00

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	54	MET	CA
1	A	60	ILE	CB
1	A	142	CYS	CA
1	A	148	THR	CB
1	A	195	PRO	CA
1	A	206	MET	CA
1	A	319	PRO	CA
2	D	71	LEU	CA
2	D	91	HIS	CA
3	E	9	SER	CA

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	27	PHE	Mainchain,Peptide
1	A	29	GLN	Mainchain
1	A	41	CYS	Mainchain
1	A	76	CYS	Peptide
1	A	80	ALA	Peptide
1	A	84	ALA	Peptide
1	A	112	TYR	Sidechain
1	A	123	GLY	Peptide
1	A	143	TRP	Peptide
1	A	189	TYR	Sidechain
1	A	194	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	198	SER	Peptide
1	A	214	TYR	Sidechain
1	A	233	PRO	Peptide
1	A	255	ASP	Mainchain
1	A	300	GLY	Peptide
1	A	311	TYR	Sidechain
1	A	314	VAL	Peptide
1	A	348	ALA	Mainchain
1	A	356	PHE	Sidechain
1	A	375	TYR	Sidechain
1	A	394	VAL	Peptide
2	D	36	VAL	Peptide
2	D	51	TYR	Sidechain
2	D	77	GLU	Peptide
2	D	81	GLY	Mainchain,Peptide
2	D	82	HIS	Sidechain
2	D	89	HIS	Peptide
2	D	90	THR	Peptide
2	D	108	LEU	Mainchain,Peptide
3	E	7	TYR	Sidechain
3	E	22	ALA	Peptide
3	E	78	LYS	Peptide

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2807	580	2758	153
10	E	43	0	30	1
11	A	1	2	0	6
2	D	713	162	701	36
3	E	572	138	566	16
4	A	24	0	0	1
5	A	5	0	6	15
6	A	2	0	0	2
7	A	4	0	0	14
8	A	4	0	0	9
All	All	4176	882	4061	181

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 22.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:72:CYS:C	1:A:73:LEU:N	1.41	1.74
1:A:295:ILE:CD1	1:A:305:ALA:HB2	1.24	1.62
1:A:62:HIS:HD2	2:D:108:LEU:CD1	1.19	1.47
1:A:71:GLN:HG2	1:A:385:GLY:CA	1.19	1.66
1:A:295:ILE:HD11	1:A:305:ALA:CB	1.17	1.69
1:A:71:GLN:CG	1:A:385:GLY:CA	1.16	2.24
1:A:71:GLN:CD	1:A:385:GLY:HA2	1.15	1.59
1:A:71:GLN:CG	1:A:385:GLY:HA2	1.13	1.72
1:A:203:PRO:HG2	7:A:7:CYN:N	1.13	1.57
1:A:40:THR:OG1	3:E:12:GLY:HA3	1.12	1.43
1:A:62:HIS:CD2	2:D:108:LEU:CD1	1.12	2.31
1:A:71:GLN:OE1	1:A:385:GLY:HA2	1.11	1.44
1:A:62:HIS:CB	2:D:108:LEU:CD2	1.10	2.30
1:A:62:HIS:CD2	2:D:108:LEU:CD2	1.08	2.37
1:A:62:HIS:CD2	2:D:108:LEU:HD13	1.05	1.83
1:A:62:HIS:CD2	2:D:108:LEU:HD22	1.04	1.86
1:A:64:GLU:OE1	2:D:97:LYS:HD3	1.04	1.53
1:A:40:THR:OG1	3:E:12:GLY:CA	1.03	2.05
1:A:62:HIS:CG	2:D:108:LEU:HD22	1.02	1.90
1:A:29:GLN:HG3	1:A:60:ILE:HD11	1.01	1.26
1:A:29:GLN:C	1:A:81:ILE:HG23	0.99	1.78
1:A:62:HIS:CB	2:D:108:LEU:HD22	0.96	1.89
1:A:295:ILE:O	1:A:298:VAL:HG12	0.94	1.60
1:A:203:PRO:CG	7:A:7:CYN:N	0.92	2.32
1:A:62:HIS:CG	2:D:108:LEU:CD2	0.92	2.50
1:A:71:GLN:OE1	1:A:384:CYS:O	0.90	1.89
1:A:62:HIS:HD2	2:D:108:LEU:HD13	0.88	1.13
1:A:40:THR:HG1	3:E:12:GLY:HA3	0.87	1.19
1:A:108:PRO:HD2	8:A:9:CMO:C	0.86	2.00
1:A:62:HIS:HB3	2:D:108:LEU:CD2	0.86	1.96
6:A:5:FE2:FE	11:A:11:HOH:O	0.86	1.27
1:A:295:ILE:HD12	1:A:301:GLY:O	0.85	1.71
1:A:71:GLN:HG2	1:A:385:GLY:C	0.84	1.93
1:A:29:GLN:HG3	1:A:60:ILE:CD1	0.83	2.03
6:A:6:FE2:FE	11:A:11:HOH:O	0.83	1.31
1:A:203:PRO:HG2	7:A:7:CYN:C	0.83	2.03
1:A:71:GLN:OE1	1:A:385:GLY:CA	0.81	2.28
1:A:40:THR:OG1	3:E:12:GLY:N	0.80	2.13
1:A:296:PHE:HB3	5:A:4:PDT:S2	0.78	2.19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:36:ILE:HB	3:E:63:LYS:HE3	0.78	1.53
1:A:62:HIS:HB3	2:D:108:LEU:HD22	0.78	1.50
1:A:109:ALA:N	5:A:4:PDT:S1	0.77	2.58
1:A:29:GLN:CG	1:A:60:ILE:HD11	0.76	2.10
1:A:296:PHE:H	8:A:10:CMO:C	0.76	1.93
1:A:295:ILE:O	1:A:298:VAL:CG1	0.74	2.35
1:A:338:VAL:HB	1:A:345:VAL:HB	0.74	1.58
1:A:241:GLY:HA3	1:A:254:ILE:CG2	0.74	2.12
1:A:71:GLN:CG	1:A:385:GLY:HA3	0.73	2.12
3:E:42:LYS:NZ	3:E:66:ASP:OD1	0.73	2.18
8:A:10:CMO:C	11:A:11:HOH:O	0.71	2.39
8:A:9:CMO:C	11:A:11:HOH:O	0.70	2.39
1:A:62:HIS:CD2	2:D:108:LEU:HD11	0.69	2.19
1:A:109:ALA:HA	1:A:112:TYR:HD2	0.68	1.48
1:A:62:HIS:HD2	2:D:108:LEU:CG	0.68	2.01
1:A:56:GLU:HB3	1:A:57:PRO:HD2	0.68	1.65
1:A:296:PHE:HB3	5:A:4:PDT:C3	0.67	2.19
1:A:294:THR:HA	7:A:8:CYN:N	0.67	2.03
1:A:71:GLN:O	1:A:72:CYS:C	0.67	2.24
1:A:62:HIS:CB	2:D:108:LEU:HD21	0.66	2.20
1:A:104:ALA:HA	1:A:229:VAL:HB	0.66	1.67
5:A:4:PDT:H32	7:A:7:CYN:N	0.64	2.08
1:A:62:HIS:HD2	2:D:108:LEU:CD2	0.63	1.88
1:A:108:PRO:HB2	7:A:8:CYN:N	0.63	2.08
3:E:61:VAL:HA	3:E:69:LEU:HD21	0.63	1.70
1:A:109:ALA:HA	1:A:112:TYR:CD2	0.62	2.29
1:A:241:GLY:CA	1:A:254:ILE:CG2	0.62	2.76
1:A:229:VAL:HA	1:A:256:ALA:HB3	0.62	1.71
1:A:53:GLU:HB2	1:A:56:GLU:HB2	0.62	1.70
1:A:62:HIS:HB2	2:D:108:LEU:CD2	0.62	2.23
1:A:71:GLN:HG2	1:A:385:GLY:O	0.62	1.94
5:A:4:PDT:H32	7:A:7:CYN:C	0.62	2.25
7:A:8:CYN:C	11:A:11:HOH:O	0.62	2.47
1:A:166:LYS:HA	1:A:169:ASP:HB2	0.61	1.73
1:A:295:ILE:CD1	1:A:305:ALA:CB	0.60	2.54
1:A:62:HIS:CG	2:D:108:LEU:HD21	0.59	2.31
1:A:39:ASP:O	1:A:40:THR:HB	0.59	1.96
1:A:64:GLU:OE1	2:D:97:LYS:CD	0.59	2.41
1:A:87:TRP:CD1	1:A:256:ALA:HA	0.59	2.33
1:A:296:PHE:CB	5:A:4:PDT:S2	0.59	2.91
2:D:40:LYS:HD2	2:D:123:GLU:HA	0.58	1.73
1:A:300:GLY:HA2	1:A:327:VAL:HB	0.58	1.75

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
5:A:4:PDT:C3	7:A:7:CYN:C	0.57	2.82
7:A:7:CYN:C	11:A:11:HOH:O	0.57	2.47
1:A:241:GLY:CA	1:A:254:ILE:HG22	0.57	2.28
1:A:52:GLY:HA3	1:A:58:HIS:HA	0.57	1.75
1:A:296:PHE:N	5:A:4:PDT:S2	0.56	2.79
1:A:71:GLN:OE1	1:A:384:CYS:C	0.56	2.43
1:A:295:ILE:H	8:A:10:CMO:C	0.56	2.12
1:A:28:VAL:HG21	1:A:235:ILE:HD13	0.56	1.78
1:A:29:GLN:O	1:A:81:ILE:HA	0.55	2.02
1:A:144:ASP:HB2	1:A:287:GLY:HA3	0.55	1.79
5:A:4:PDT:C1	8:A:9:CMO:C	0.55	2.84
1:A:86:SER:HB3	1:A:258:LEU:HA	0.55	1.78
1:A:100:VAL:HG12	1:A:227:TYR:HB2	0.55	1.78
1:A:202:SER:O	1:A:203:PRO:C	0.55	2.42
1:A:337:THR:HG23	1:A:346:LYS:HE2	0.54	1.78
1:A:76:CYS:HB3	1:A:81:ILE:H	0.54	1.63
1:A:133:ALA:HA	1:A:272:ILE:HD13	0.54	1.78
1:A:203:PRO:CD	7:A:7:CYN:N	0.54	2.71
1:A:43:GLN:OE1	2:D:119:PRO:HD2	0.53	2.02
3:E:76:MET:HA	3:E:79:LEU:HD13	0.53	1.78
1:A:71:GLN:NE2	1:A:75:HIS:NE2	0.53	2.56
1:A:88:VAL:HB	1:A:89:PRO:HD3	0.53	1.79
1:A:62:HIS:CD2	2:D:108:LEU:HD21	0.53	2.30
1:A:241:GLY:C	1:A:254:ILE:CG2	0.52	2.77
1:A:28:VAL:O	1:A:28:VAL:HG13	0.52	2.04
1:A:35:CYS:HA	4:A:1:SF4:S4	0.51	2.46
2:D:74:SER:HA	2:D:77:GLU:OE1	0.51	2.04
1:A:64:GLU:O	1:A:66:CYS:O	0.51	2.28
2:D:82:HIS:HA	2:D:85:HIS:HB3	0.51	1.82
1:A:295:ILE:HD11	1:A:305:ALA:HB2	0.51	0.72
1:A:116:ASP:HB3	1:A:391:MET:HB2	0.51	1.82
1:A:40:THR:HG21	3:E:11:ILE:HG22	0.51	1.83
1:A:325:LYS:HD3	1:A:328:ARG:HD2	0.51	1.82
3:E:65:SER:O	3:E:67:GLU:N	0.51	2.42
1:A:297:GLY:N	5:A:4:PDT:H31	0.50	2.21
1:A:396:GLU:HA	3:E:5:ALA:HB3	0.50	1.80
1:A:106:PRO:HA	1:A:231:ILE:HB	0.50	1.82
1:A:241:GLY:HA3	1:A:254:ILE:CB	0.50	2.37
1:A:130:MET:HB3	1:A:282:ARG:HA	0.49	1.84
1:A:297:GLY:N	5:A:4:PDT:S2	0.49	2.85
1:A:108:PRO:HB2	7:A:8:CYN:C	0.48	2.37
1:A:111:ARG:O	1:A:126:THR:HB	0.48	2.08

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:107:ALA:HB1	5:A:4:PDT:H11	0.48	1.84
1:A:241:GLY:O	1:A:254:ILE:HG22	0.48	2.09
1:A:238:LYS:HG2	1:A:257:THR:HG21	0.48	1.86
1:A:27:PHE:HA	1:A:63:ILE:HG13	0.48	1.85
1:A:233:PRO:HB2	1:A:386:GLY:HA3	0.48	1.86
1:A:62:HIS:HB2	2:D:108:LEU:HD21	0.48	1.84
1:A:29:GLN:CA	1:A:60:ILE:HD11	0.47	2.39
1:A:241:GLY:C	1:A:254:ILE:HG22	0.47	2.30
3:E:53:ARG:HB3	3:E:56:MET:HB2	0.47	1.86
1:A:246:LEU:O	1:A:252:ARG:HA	0.47	2.10
1:A:31:ASP:O	1:A:33:ALA:N	0.47	2.43
1:A:391:MET:HG2	1:A:392:PRO:HA	0.47	1.87
1:A:205:GLY:HA2	1:A:246:LEU:HD11	0.46	1.85
2:D:102:LEU:HB3	2:D:107:LYS:HB2	0.46	1.87
1:A:27:PHE:N	1:A:66:CYS:HB3	0.46	2.26
1:A:63:ILE:CG2	1:A:63:ILE:O	0.46	2.64
1:A:231:ILE:HD13	1:A:263:LEU:HD22	0.46	1.88
1:A:299:THR:HG21	1:A:351:HIS:HB3	0.45	1.88
2:D:120:TYR:H	2:D:121:PRO:HD3	0.45	1.71
1:A:238:LYS:O	1:A:254:ILE:HD13	0.45	2.11
1:A:39:ASP:O	1:A:40:THR:CB	0.45	2.64
1:A:323:ASP:HA	1:A:325:LYS:HE2	0.44	1.87
2:D:74:SER:HA	2:D:77:GLU:CD	0.44	2.33
1:A:114:LEU:HD13	1:A:260:THR:HG22	0.44	1.88
1:A:50:ILE:HG12	1:A:60:ILE:HB	0.44	1.89
1:A:108:PRO:HD2	8:A:9:CMO:O	0.44	2.12
1:A:328:ARG:HA	2:D:51:TYR:HE2	0.44	1.73
1:A:294:THR:CA	7:A:8:CYN:N	0.44	2.80
1:A:298:VAL:HG13	1:A:301:GLY:HA3	0.43	1.90
1:A:392:PRO:HD2	3:E:8:LYS:HZ2	0.43	1.73
2:D:120:TYR:HA	2:D:121:PRO:HD2	0.43	1.60
1:A:397:ALA:O	3:E:2:ASP:N	0.43	2.52
1:A:148:THR:CG2	1:A:203:PRO:HB3	0.43	2.43
1:A:107:ALA:HB1	5:A:4:PDT:C1	0.43	2.44
1:A:233:PRO:HG3	1:A:382:CYS:HB3	0.43	1.90
7:A:7:CYN:C	8:A:10:CMO:C	0.43	2.97
1:A:41:CYS:HA	1:A:75:HIS:ND1	0.43	2.28
1:A:333:ILE:HG12	1:A:350:VAL:HG23	0.43	1.89
1:A:48:ALA:HB3	2:D:110:ASN:HB3	0.43	1.90
1:A:351:HIS:HA	1:A:376:MET:O	0.43	2.13
1:A:312:GLU:HB2	1:A:319:PRO:HG2	0.42	1.89
1:A:223:PRO:HB2	1:A:251:MET:SD	0.42	2.53

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
3:E:37:LEU:HD22	10:E:80:HEC:HMA3	0.42	1.91
2:D:92:TRP:CE3	2:D:92:TRP:HA	0.42	2.50
1:A:71:GLN:HG3	1:A:385:GLY:HA3	0.42	1.90
1:A:241:GLY:HA3	1:A:254:ILE:HB	0.42	1.91
2:D:120:TYR:N	2:D:121:PRO:CD	0.42	2.82
1:A:63:ILE:O	1:A:63:ILE:HG22	0.42	2.15
1:A:244:PRO:HD2	2:D:91:HIS:NE2	0.41	2.30
5:A:4:PDT:H11	8:A:9:CMO:C	0.41	2.45
1:A:290:THR:HB	1:A:293:ALA:HB3	0.41	1.91
1:A:394:VAL:HG22	3:E:8:LYS:HD2	0.41	1.93
1:A:73:LEU:HD23	1:A:81:ILE:HG22	0.41	1.92
1:A:28:VAL:O	1:A:28:VAL:CG1	0.41	2.69
1:A:30:ILE:HG12	1:A:81:ILE:HG12	0.41	1.93
1:A:297:GLY:N	5:A:4:PDT:C3	0.41	2.83
1:A:38:CYS:SG	1:A:39:ASP:O	0.41	2.79
2:D:37:LYS:HB3	2:D:41:ASP:HB2	0.40	1.92

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	369/371 (99%)	297 (80%)	52 (14%)	20 (5%)	3 23
2	D	86/88 (98%)	69 (80%)	10 (12%)	7 (8%)	2 14
3	E	76/78 (97%)	68 (89%)	7 (9%)	1 (1%)	16 63
All	All	531/537 (99%)	434 (82%)	69 (13%)	28 (5%)	3 23

All 28 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	29	GLN
1	A	36	ILE
1	A	54	MET
1	A	56	GLU

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Mol	Chain	Res	Type
1	A	64	GLU
1	A	65	ALA
1	A	71	GLN
1	A	142	CYS
1	A	145	THR
1	A	195	PRO
1	A	202	SER
1	A	203	PRO
1	A	228	THR
1	A	254	ILE
1	A	284	SER
1	A	293	ALA
1	A	295	ILE
1	A	301	GLY
1	A	319	PRO
1	A	379	PRO
2	D	75	TYR
2	D	83	LYS
2	D	85	HIS
2	D	88	LEU
2	D	91	HIS
2	D	108	LEU
2	D	120	TYR
3	E	66	ASP

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	297/297 (100%)	255 (86%)	42 (14%)	6 46
2	D	76/76 (100%)	66 (87%)	10 (13%)	7 48
3	E	55/55 (100%)	50 (91%)	5 (9%)	13 59
All	All	428/428 (100%)	371 (87%)	57 (13%)	7 48

All 57 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	29	GLN
1	A	38	CYS
1	A	42	SER
1	A	47	THR
1	A	62	HIS
1	A	63	ILE
1	A	69	CYS
1	A	74	THR
1	A	76	CYS
1	A	87	TRP
1	A	102	CYS
1	A	116	ASP
1	A	124	SER
1	A	126	THR
1	A	142	CYS
1	A	145	THR
1	A	148	THR
1	A	152	THR
1	A	176	THR
1	A	177	SER
1	A	192	GLU
1	A	198	SER
1	A	199	THR
1	A	202	SER
1	A	206	MET
1	A	213	THR
1	A	228	THR
1	A	230	SER
1	A	248	SER
1	A	249	SER
1	A	254	ILE
1	A	255	ASP
1	A	259	THR
1	A	260	THR
1	A	284	SER
1	A	289	SER
1	A	295	ILE
1	A	315	THR
1	A	339	ASN
1	A	343	THR
1	A	351	HIS
1	A	382	CYS
2	D	48	ASN

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Mol	Chain	Res	Type
2	D	62	SER
2	D	66	THR
2	D	71	LEU
2	D	84	SER
2	D	92	TRP
2	D	96	SER
2	D	99	VAL
2	D	104	THR
2	D	114	SER
3	E	19	SER
3	E	48	SER
3	E	58	THR
3	E	59	ASN
3	E	65	SER

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
7	CYN	A	8	6,8,5	0,1,1	0.00	-
8	CMO	A	10	6,7	0,1,1	0.00	-
4	SF4	A	1	1	0,12,12	0.00	-
8	CMO	A	9	6,7	0,1,1	0.00	-
5	PDT	A	4	6,7	4,4,4	2.80	2 (50%)
4	SF4	A	2	1	0,12,12	0.00	-
7	CYN	A	7	6,8	0,1,1	0.00	-
4	SF4	A	3	1	0,12,12	0.00	-
10	HEC	E	80	3	32,50,50	1.32	2 (6%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
7	CYN	A	8	6,8,5	-	-	-
8	CMO	A	10	6,7	-	-	-
4	SF4	A	1	1	-	-	-
8	CMO	A	9	6,7	-	-	-
5	PDT	A	4	6,7	3,3,3	1.58	0 (0%)
4	SF4	A	2	1	-	-	-
7	CYN	A	7	6,8	-	-	-
4	SF4	A	3	1	-	-	-
10	HEC	E	80	3	24,82,82	1.36	3 (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
4	SF4	A	1	1	-	-	0,6,5,5
5	PDT	A	4	6,7	-	0,2,2,2	-
4	SF4	A	2	1	-	-	0,6,5,5
4	SF4	A	3	1	-	-	0,6,5,5
10	HEC	E	80	3	-	0,10,54,54	-

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4	PDT	C3-S2	4.77	1.97	1.80
10	E	80	HEC	C3C-C2C	4.00	1.36	1.40
10	E	80	HEC	C2B-C3B	3.53	1.37	1.40
5	A	4	PDT	C1-S1	2.91	1.91	1.80

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	80	HEC	C4C-C3C-C2C	2.84	103.28	106.35
10	E	80	HEC	CMC-C2C-C1C	2.20	125.09	128.46
10	E	80	HEC	O1A-CGA-CBA	2.02	116.59	123.08

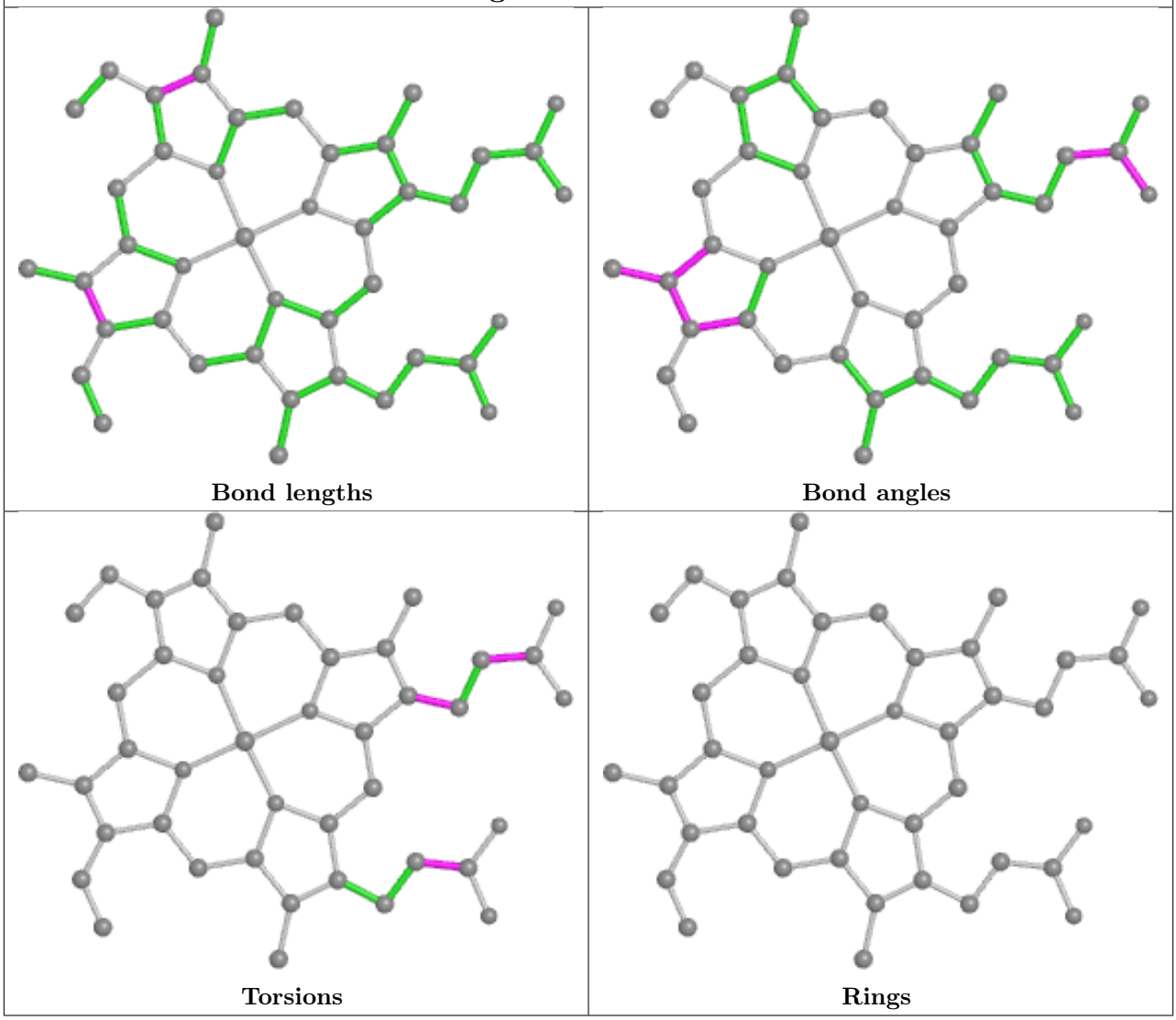
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 HEC E 80



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
3	E	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	72:CYS	C	73:LEU	N	1.74
1	E	64:TYR	C	65:SER	N	1.19
1	A	202:SER	C	203:PRO	N	1.18
1	A	71:GLN	C	72:CYS	N	1.15
1	A	27:PHE	C	28:VAL	N	1.01
1	A	65:ALA	C	66:CYS	N	1.01
1	D	77:GLU	C	78:LYS	N	0.95

7 Chemical shift validation (i)

No chemical shift data were provided