



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:01 AM UTC

PDB ID : 1E08 / pdb_00001e08
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 ⓘ 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)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

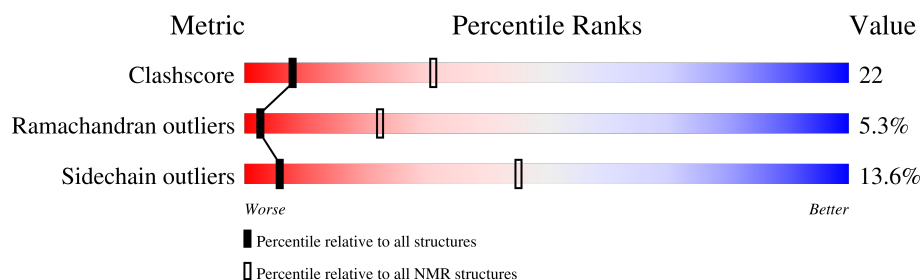
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	371	50% 35% 10% 6%
2	D	88	41% 35% 16% 8%
3	E	78	58% 31% 10% .

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 ⓘ

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
1	A	371	Total	C	H	N	O	S	0
			3387	1783	580	465	527	32	

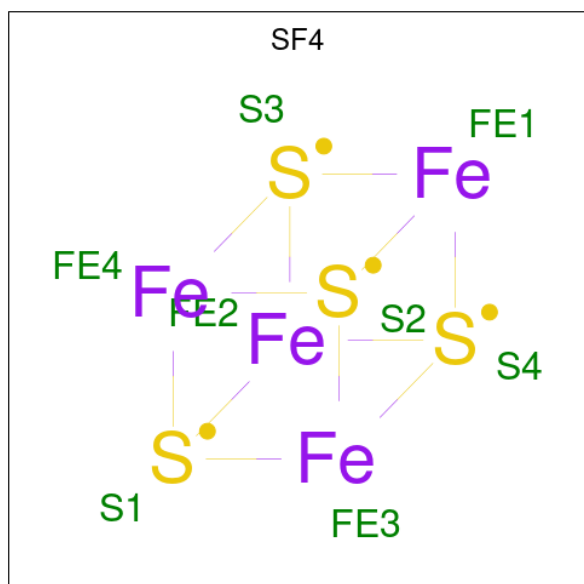
- Molecule 2 is a protein called [FE]-HYDROGENASE (SMALL SUBUNIT).

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

- Molecule 3 is a protein called CYTOCHROME C553.

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

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



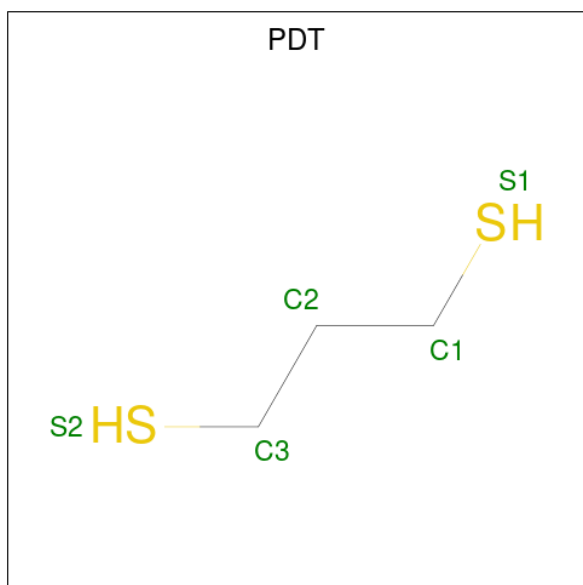
Mol	Chain	Residues	Atoms		
4	A	1	Total	Fe	S
			8	4	4

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 1,3-PROPANEDITHIOL (CCD ID: PDT) (formula: $C_3H_8S_2$).

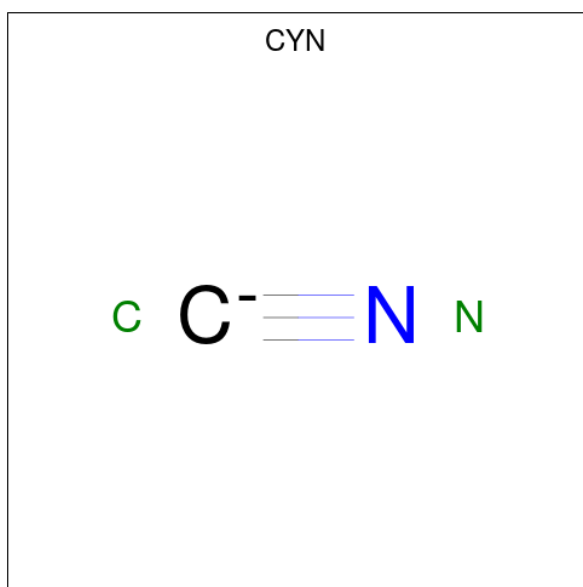


Mol	Chain	Residues	Atoms		
5	A	1	Total	C	S
			5	3	2

- Molecule 6 is FE (II) ION (CCD ID: FE2) (formula: Fe).

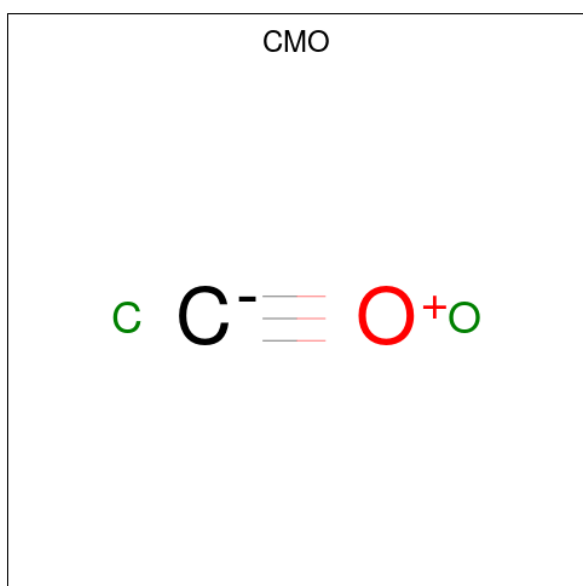
Mol	Chain	Residues	Atoms	
6	A	2	Total	Fe
			2	2

- Molecule 7 is CYANIDE ION (CCD ID: CYN) (formula: CN).



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

- Molecule 8 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).

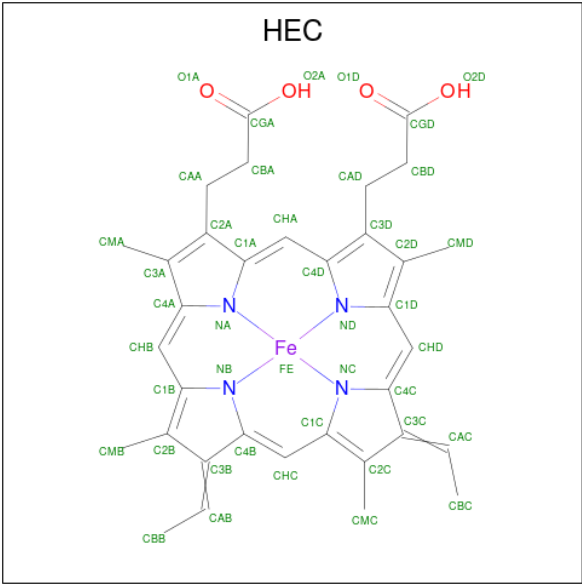


Mol	Chain	Residues	Atoms		
8	A	1	Total	C	O
			2	1	1
8	A	1	Total	C	O
			2	1	1

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
9	D	1	Total	Zn
			1	1

- Molecule 10 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

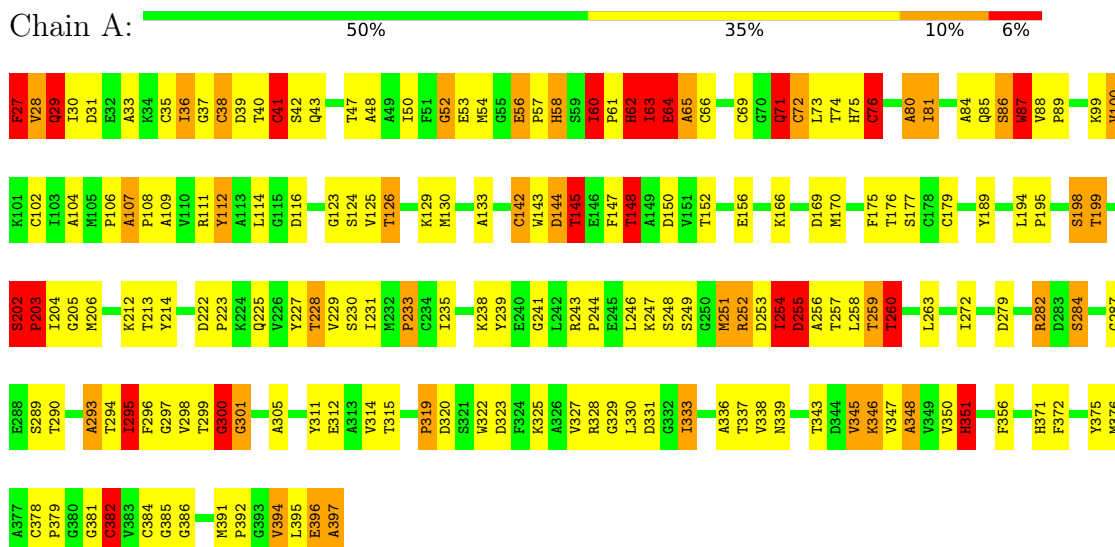
- Molecule 11 is water.

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

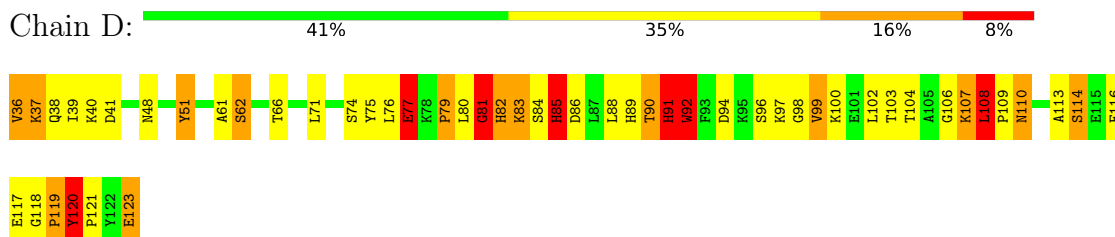
4 Residue-property plots

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.

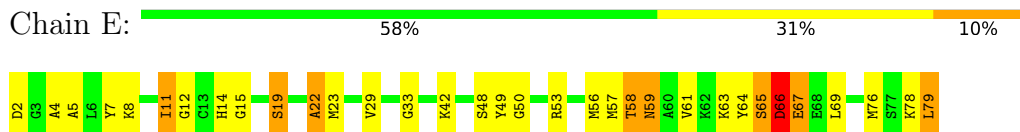
• Molecule 1: [FE]-HYDROGENASE (LARGE SUBUNIT)



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



• Molecule 3: CYTOCHROME C553



5 Refinement protocol and experimental data overview

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: CYN, SF4, HEC, CMO, ZN, PDT, FE2

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	1.47	27/2874 (0.9%)	2.22	114/3885 (2.9%)
2	D	2.23	15/733 (2.0%)	2.75	68/988 (6.9%)
3	E	1.01	4/579 (0.7%)	1.80	21/765 (2.7%)
All	All	1.58	46/4186 (1.1%)	2.27	203/5638 (3.6%)

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)
2	D	77	GLU	C-N	-44.94	0.94	1.33
1	A	72	CYS	C-N	32.13	1.74	1.33
1	A	27	PHE	C-N	-26.00	1.01	1.33
1	A	65	ALA	C-N	-23.52	1.01	1.33
1	A	65	ALA	N-CA	15.72	1.66	1.46
1	A	29	GLN	C-N	15.03	1.54	1.33
1	A	64	GLU	C-N	15.03	1.54	1.33
1	A	71	GLN	C-N	-13.56	1.15	1.33
2	D	99	VAL	N-CA	-12.60	1.31	1.46
1	A	347	VAL	N-CA	-10.46	1.33	1.46
1	A	203	PRO	N-CD	-10.40	1.33	1.47
2	D	109	PRO	N-CD	-10.12	1.33	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	64	TYR	C-N	-9.89	1.19	1.33
3	E	66	ASP	CA-C	9.65	1.65	1.52
3	E	67	GLU	N-CA	9.50	1.58	1.46
2	D	109	PRO	C-O	9.50	1.36	1.24
1	A	41	CYS	C-N	9.49	1.44	1.33
2	D	39	ILE	N-CA	-9.45	1.35	1.46
1	A	254	ILE	C-N	-8.82	1.21	1.33
2	D	110	ASN	C-N	-8.77	1.23	1.33
1	A	202	SER	C-O	-8.73	1.13	1.24
1	A	252	ARG	C-N	-7.97	1.23	1.33
1	A	63	ILE	C-O	7.62	1.31	1.24
2	D	38	GLN	C-N	7.54	1.43	1.33
1	A	203	PRO	CA-CB	-7.47	1.43	1.53
2	D	109	PRO	CA-C	6.96	1.62	1.52
1	A	64	GLU	C-O	6.71	1.32	1.24
1	A	202	SER	C-N	-6.69	1.18	1.33
1	A	295	ILE	C-N	-6.53	1.25	1.33
2	D	107	LYS	CA-C	6.44	1.60	1.52
1	A	64	GLU	N-CA	6.31	1.54	1.46
1	A	61	PRO	C-N	6.29	1.41	1.33
3	E	66	ASP	C-N	6.13	1.44	1.33
1	A	204	ILE	N-CA	5.90	1.54	1.46
2	D	99	VAL	C-O	-5.89	1.17	1.24
1	A	63	ILE	C-N	5.81	1.41	1.33
1	A	346	LYS	CA-C	-5.78	1.45	1.52
1	A	346	LYS	C-O	5.71	1.30	1.23
1	A	347	VAL	CA-CB	-5.65	1.46	1.54
2	D	100	LYS	N-CA	5.47	1.53	1.46
2	D	108	LEU	CA-CB	-5.36	1.45	1.53
2	D	119	PRO	C-O	5.28	1.30	1.24
1	A	28	VAL	C-N	-5.26	1.26	1.33
2	D	81	GLY	CA-C	5.15	1.56	1.51
2	D	119	PRO	CA-C	-5.11	1.45	1.52
1	A	28	VAL	C-O	5.09	1.29	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLN	O-C-N	-33.85	77.56	122.59
1	A	28	VAL	O-C-N	25.41	145.84	122.97
1	A	63	ILE	O-C-N	23.71	149.38	122.83
2	D	81	GLY	O-C-N	-20.57	110.39	123.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	120	TYR	O-C-N	20.08	144.41	121.32
2	D	108	LEU	O-C-N	-19.63	98.74	121.32
1	A	346	LYS	O-C-N	19.44	145.82	123.27
1	A	64	GLU	O-C-N	18.24	146.84	122.59
1	A	295	ILE	CB-CA-C	-17.80	82.10	111.29
1	A	27	PHE	CA-C-N	16.92	148.22	122.84
1	A	27	PHE	C-N-CA	16.92	148.22	122.84
1	A	27	PHE	O-C-N	-16.18	97.12	123.00
1	A	71	GLN	O-C-N	-16.13	101.14	122.59
1	A	202	SER	O-C-N	-15.57	103.41	121.32
2	D	39	ILE	N-CA-C	14.73	125.65	110.62
2	D	119	PRO	O-C-N	14.35	142.01	122.64
2	D	39	ILE	N-CA-CB	12.85	128.02	110.54
2	D	39	ILE	CA-CB-CG1	12.57	131.78	110.40
2	D	107	LYS	O-C-N	11.71	136.57	123.10
2	D	108	LEU	N-CA-C	11.66	135.57	109.81
2	D	98	GLY	O-C-N	11.58	137.75	122.70
1	A	72	CYS	CA-C-N	11.12	135.55	120.54
1	A	72	CYS	C-N-CA	11.12	135.55	120.54
2	D	39	ILE	CA-C-O	-11.05	109.46	120.95
1	A	63	ILE	CA-C-N	10.36	141.33	121.54
1	A	63	ILE	C-N-CA	10.36	141.33	121.54
1	A	65	ALA	O-C-N	10.08	136.00	122.59
1	A	28	VAL	CA-C-N	10.01	140.65	121.54
1	A	28	VAL	C-N-CA	10.01	140.65	121.54
1	A	255	ASP	O-C-N	-9.93	109.38	122.59
2	D	117	GLU	CA-C-N	-9.88	106.37	121.87
2	D	117	GLU	C-N-CA	-9.88	106.37	121.87
2	D	109	PRO	O-C-N	9.84	135.93	122.64
1	A	170	MET	N-CA-C	-9.62	99.47	108.13
1	A	64	GLU	CA-C-N	9.33	139.36	121.54
1	A	64	GLU	C-N-CA	9.33	139.36	121.54
1	A	395	LEU	N-CA-C	-9.31	97.47	111.34
2	D	91	HIS	CA-CB-CG	9.16	122.96	113.80
1	A	345	VAL	O-C-N	9.12	129.62	121.96
1	A	107	ALA	CA-C-N	9.07	128.67	119.24
1	A	107	ALA	C-N-CA	9.07	128.67	119.24
1	A	253	ASP	O-C-N	8.57	132.05	122.11
2	D	38	GLN	CA-C-N	-8.54	108.75	120.46
2	D	38	GLN	C-N-CA	-8.54	108.75	120.46
1	A	331	ASP	N-CA-C	-8.52	96.13	109.07
2	D	117	GLU	N-CA-C	-8.42	96.31	108.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLU	N-CA-C	-8.30	96.09	108.79
2	D	39	ILE	CB-CA-C	-8.15	101.14	112.14
2	D	37	LYS	N-CA-C	-8.14	97.01	109.14
1	A	255	ASP	CA-CB-CG	-8.14	104.46	112.60
2	D	107	LYS	CA-C-N	8.12	141.62	121.80
2	D	107	LYS	C-N-CA	8.12	141.62	121.80
1	A	100	VAL	N-CA-C	-7.89	96.23	107.75
3	E	64	TYR	CA-C-N	7.86	136.56	121.54
3	E	64	TYR	C-N-CA	7.86	136.56	121.54
2	D	85	HIS	CA-CB-CG	7.85	121.65	113.80
1	A	61	PRO	CA-C-N	-7.83	112.40	123.20
1	A	61	PRO	C-N-CA	-7.83	112.40	123.20
2	D	106	GLY	CA-C-N	-7.63	109.66	122.64
2	D	106	GLY	C-N-CA	-7.63	109.66	122.64
1	A	41	CYS	N-CA-C	-7.62	104.49	114.31
1	A	279	ASP	N-CA-C	-7.54	96.08	108.07
2	D	90	THR	N-CA-C	-7.51	98.88	109.69
1	A	29	GLN	CA-C-N	-7.50	112.71	123.06
1	A	29	GLN	C-N-CA	-7.50	112.71	123.06
1	A	85	GLN	N-CA-C	-7.39	97.82	109.50
1	A	64	GLU	N-CA-CB	7.30	122.82	110.49
1	A	329	GLY	N-CA-C	-7.29	100.63	111.19
1	A	203	PRO	N-CA-C	7.17	127.25	112.47
1	A	247	LYS	CA-C-N	7.04	129.72	120.28
1	A	247	LYS	C-N-CA	7.04	129.72	120.28
2	D	91	HIS	N-CA-C	-7.03	95.83	110.80
3	E	49	TYR	N-CA-C	-7.00	98.43	109.07
1	A	58	HIS	CA-CB-CG	6.97	120.77	113.80
2	D	77	GLU	CA-C-O	6.95	127.21	119.78
2	D	116	PHE	CA-C-N	6.89	133.59	121.80
2	D	116	PHE	C-N-CA	6.89	133.59	121.80
1	A	330	LEU	N-CA-C	-6.88	98.62	109.50
1	A	351	HIS	CA-CB-CG	6.85	120.65	113.80
2	D	103	THR	CA-C-N	6.85	130.14	120.28
2	D	103	THR	C-N-CA	6.85	130.14	120.28
1	A	397	ALA	N-CA-C	-6.74	92.12	111.00
1	A	52	GLY	N-CA-C	-6.67	101.78	110.45
1	A	179	CYS	CB-CA-C	6.67	116.77	110.17
1	A	348	ALA	O-C-N	-6.64	114.76	123.13
1	A	243	ARG	CA-C-N	6.58	126.28	119.56
1	A	243	ARG	C-N-CA	6.58	126.28	119.56
1	A	320	ASP	N-CA-C	-6.56	105.28	113.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	GLU	CA-C-O	-6.53	111.17	120.51
1	A	62	HIS	O-C-N	6.50	131.61	122.83
3	E	50	GLY	N-CA-C	-6.45	100.12	110.18
1	A	87	TRP	CA-CB-CG	6.43	125.81	113.60
2	D	83	LYS	CA-C-N	6.35	129.96	120.31
2	D	83	LYS	C-N-CA	6.35	129.96	120.31
2	D	109	PRO	CA-C-N	6.32	132.94	120.94
2	D	109	PRO	C-N-CA	6.32	132.94	120.94
1	A	29	GLN	N-CA-CB	-6.29	99.86	110.49
3	E	57	MET	CA-C-N	6.24	128.64	120.28
3	E	57	MET	C-N-CA	6.24	128.64	120.28
2	D	123	GLU	N-CA-C	-6.23	93.55	111.00
2	D	77	GLU	CB-CA-C	6.21	121.36	111.23
3	E	79	LEU	N-CA-C	-6.19	93.67	111.00
1	A	203	PRO	CA-C-O	-6.12	109.46	120.60
3	E	14	HIS	CA-CB-CG	6.12	119.92	113.80
1	A	71	GLN	CA-C-O	6.12	129.26	120.51
1	A	381	GLY	CA-C-N	6.10	129.06	120.28
1	A	381	GLY	C-N-CA	6.10	129.06	120.28
1	A	63	ILE	N-CA-C	6.09	117.55	108.54
1	A	87	TRP	CA-C-N	6.09	126.27	120.43
1	A	87	TRP	C-N-CA	6.09	126.27	120.43
1	A	295	ILE	N-CA-CB	6.07	121.25	111.23
2	D	61	ALA	CA-C-N	6.07	129.02	120.28
2	D	61	ALA	C-N-CA	6.07	129.02	120.28
3	E	66	ASP	N-CA-CB	-6.05	100.26	110.49
1	A	37	GLY	CA-C-N	6.05	133.09	121.54
1	A	37	GLY	C-N-CA	6.05	133.09	121.54
2	D	77	GLU	O-C-N	-6.04	113.58	122.04
1	A	144	ASP	CA-C-N	6.03	133.05	121.54
1	A	144	ASP	C-N-CA	6.03	133.05	121.54
1	A	282	ARG	N-CA-C	-6.02	100.34	109.85
1	A	99	LYS	N-CA-C	-6.00	106.28	113.97
1	A	64	GLU	CB-CA-C	-6.00	98.49	110.42
1	A	347	VAL	N-CA-CB	-5.98	101.36	111.23
1	A	71	GLN	CA-C-N	-5.98	111.04	120.60
1	A	71	GLN	C-N-CA	-5.98	111.04	120.60
2	D	86	ASP	N-CA-C	-5.95	98.13	110.80
1	A	202	SER	CA-C-O	5.95	128.31	120.16
1	A	300	GLY	N-CA-C	-5.91	99.16	113.18
1	A	81	ILE	N-CA-C	-5.90	99.21	108.23
1	A	41	CYS	O-C-N	-5.80	115.95	122.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	TRP	N-CA-C	-5.80	104.60	112.26
2	D	117	GLU	O-C-N	5.78	129.33	123.26
2	D	80	LEU	N-CA-CB	-5.76	103.97	112.78
2	D	99	VAL	CA-CB-CG1	5.73	120.14	110.40
2	D	85	HIS	CA-C-N	5.71	132.46	121.54
2	D	85	HIS	C-N-CA	5.71	132.46	121.54
3	E	22	ALA	CA-C-N	5.67	128.15	120.38
3	E	22	ALA	C-N-CA	5.67	128.15	120.38
2	D	76	LEU	O-C-N	5.64	128.66	122.11
2	D	109	PRO	N-CA-C	-5.64	100.85	112.47
1	A	175	PHE	CA-CB-CG	5.63	119.43	113.80
1	A	259	THR	CA-C-N	5.62	127.82	120.28
1	A	259	THR	C-N-CA	5.62	127.82	120.28
1	A	222	ASP	N-CA-C	-5.62	102.99	110.07
3	E	29	VAL	N-CA-C	-5.61	105.38	110.82
3	E	66	ASP	O-C-N	-5.59	115.16	122.59
1	A	254	ILE	O-C-N	5.59	129.56	122.57
2	D	39	ILE	CA-CB-CG2	-5.58	101.01	110.50
2	D	77	GLU	CA-CB-CG	-5.57	102.97	114.10
1	A	199	THR	N-CA-CB	-5.56	103.45	110.45
1	A	86	SER	N-CA-C	-5.52	100.40	109.40
2	D	118	GLY	CA-C-N	5.48	126.69	119.84
2	D	118	GLY	C-N-CA	5.48	126.69	119.84
3	E	15	GLY	N-CA-C	-5.45	106.18	112.29
1	A	225	GLN	N-CA-C	-5.45	105.94	112.59
1	A	378	CYS	CA-C-N	5.44	126.64	119.84
1	A	378	CYS	C-N-CA	5.44	126.64	119.84
3	E	59	ASN	CA-CB-CG	5.44	118.04	112.60
2	D	77	GLU	N-CA-CB	-5.44	104.46	112.78
1	A	150	ASP	N-CA-C	-5.42	105.45	111.36
1	A	382	CYS	N-CA-CB	-5.36	101.97	110.22
1	A	60	ILE	CA-CB-CG1	5.36	119.51	110.40
2	D	62	SER	N-CA-CB	-5.36	101.97	110.22
1	A	336	ALA	N-CA-C	-5.35	100.68	109.40
1	A	239	TYR	CA-C-N	5.33	128.17	120.38
1	A	239	TYR	C-N-CA	5.33	128.17	120.38
2	D	48	ASN	CA-CB-CG	5.33	117.93	112.60
2	D	94	ASP	N-CA-C	-5.32	100.02	109.06
2	D	79	PRO	O-C-N	5.30	129.47	123.00
3	E	19	SER	N-CA-CB	-5.28	102.67	110.53
2	D	99	VAL	CA-C-O	-5.27	115.58	121.17
2	D	109	PRO	CB-CA-C	5.27	120.26	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	ALA	N-CA-C	-5.27	105.18	111.03
1	A	251	MET	N-CA-C	-5.26	100.52	108.52
2	D	36	VAL	N-CA-C	-5.26	96.26	111.00
1	A	371	HIS	N-CA-C	-5.24	107.26	113.97
2	D	113	ALA	CA-C-N	5.23	131.54	121.54
2	D	113	ALA	C-N-CA	5.23	131.54	121.54
1	A	148	THR	N-CA-CB	-5.21	102.20	110.22
1	A	156	GLU	CA-C-N	5.21	125.61	119.94
1	A	156	GLU	C-N-CA	5.21	125.61	119.94
2	D	98	GLY	CA-C-N	5.19	127.10	120.56
2	D	98	GLY	C-N-CA	5.19	127.10	120.56
1	A	125	VAL	CA-C-N	5.17	127.73	120.28
1	A	125	VAL	C-N-CA	5.17	127.73	120.28
1	A	333	ILE	N-CA-C	-5.17	100.20	107.75
1	A	129	LYS	N-CA-C	-5.17	106.29	112.59
2	D	119	PRO	CA-C-O	-5.17	111.20	120.60
1	A	260	THR	N-CA-CB	-5.15	102.56	110.12
2	D	92	TRP	N-CA-C	-5.14	96.61	111.00
3	E	33	GLY	CA-C-N	5.10	131.28	121.54
3	E	33	GLY	C-N-CA	5.10	131.28	121.54
1	A	212	LYS	CA-C-N	5.09	127.37	120.44
1	A	212	LYS	C-N-CA	5.09	127.37	120.44
1	A	372	PHE	N-CA-C	-5.07	101.48	109.50
3	E	66	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	295	ILE	N-CA-C	5.04	119.82	109.34
1	A	80	ALA	N-CA-C	-5.04	107.27	113.41
2	D	114	SER	N-CA-CB	-5.04	101.98	110.49
1	A	145	THR	N-CA-CB	-5.03	101.99	110.49
3	E	58	THR	N-CA-CB	-5.02	102.75	110.12
1	A	147	PHE	CA-C-N	5.00	127.48	120.28
1	A	147	PHE	C-N-CA	5.00	127.48	120.28

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	Peptide,Mainchain
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
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	Peptide,Mainchain
2	D	82	HIS	Sidechain
2	D	89	HIS	Peptide
2	D	90	THR	Peptide
2	D	108	LEU	Peptide,Mainchain
3	E	7	TYR	Sidechain
3	E	22	ALA	Peptide
3	E	78	LYS	Peptide

6.2 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 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	2761	154
11	A	1	2	0	6
2	D	713	162	701	39
3	E	572	138	566	17
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	4064	184

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	1.46	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:CD	1:A:385:GLY:HA2	1.19	1.59
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: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:29:GLN:C	1:A:81:ILE:HG23	1.04	1.78
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:29:GLN:HG3	1:A:60:ILE:HD11	1.01	1.26
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:71:GLN:HG2	1:A:385:GLY:C	0.89	1.93
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: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
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
2:D:119:PRO:CG	3:E:23:MET:HE2	0.69	2.18
2:D:119:PRO:HG3	3:E:23:MET:HE2	0.69	1.66
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:62:HIS:CB	2:D:108:LEU:HD21	0.66	2.20
1:A:71:GLN:O	1:A:72:CYS:C	0.66	2.24
1:A:104:ALA:HA	1:A:229:VAL:HB	0.66	1.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:392:PRO:HD2	3:E:8:LYS:HZ1	0.62	1.55
1:A:166:LYS:HA	1:A:169:ASP:HB2	0.61	1.73
1:A:71:GLN:OE1	1:A:384:CYS:C	0.61	2.43
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:202:SER:O	1:A:203:PRO:C	0.59	2.42
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
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:241:GLY:C	1:A:254:ILE:CG2	0.57	2.77
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:HG22	0.52	2.30
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
2:D:74:SER:HA	2:D:77:GLU:CD	0.49	2.33
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
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
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
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
2:D:79:PRO:C	2:D:81:GLY:H	0.43	2.21
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
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:241:GLY:C	1:A:254:ILE:HG21	0.41	2.40
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

6.3.1 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 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%)	2	22
2	D	86/88 (98%)	69 (80%)	10 (12%)	7 (8%)	1	13
3	E	76/78 (97%)	68 (89%)	7 (9%)	1 (1%)	12	60
All	All	531/537 (99%)	434 (82%)	69 (13%)	28 (5%)	2	22

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	5	44
2	D	76/76 (100%)	66 (87%)	10 (13%)	6	46
3	E	55/55 (100%)	49 (89%)	6 (11%)	8	52
All	All	428/428 (100%)	370 (86%)	58 (14%)	6	45

All 58 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	60	ILE
1	A	62	HIS
1	A	63	ILE
1	A	69	CYS
1	A	71	GLN
1	A	74	THR
1	A	76	CYS
1	A	87	TRP
1	A	102	CYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	SER
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	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	108	LEU
2	D	114	SER
3	E	11	ILE
3	E	19	SER
3	E	48	SER
3	E	58	THR
3	E	59	ASN
3	E	65	SER

6.3.3 RNA ⓘ

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 oligosaccharides 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
4	SF4	A	3	1	0,12,12	0.00	-
4	SF4	A	2	1	0,12,12	0.00	-
8	CMO	A	10	6,7	0,1,1	0.00	-
7	CYN	A	7	8,6	1,1,1	0.53	0 (0%)
8	CMO	A	9	6,7	0,1,1	0.00	-
5	PDT	A	4	6,7	4,4,4	2.50	2 (50%)
10	HEC	E	80	3	46,50,50	1.48	2 (4%)
7	CYN	A	8	5,8,6	1,1,1	0.86	0 (0%)
4	SF4	A	1	1	0,12,12	0.00	-

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
4	SF4	A	3	1	-	-	-
4	SF4	A	2	1	-	-	-

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
8	CMO	A	10	6,7	-	-	-
7	CYN	A	7	8,6	-	-	-
8	CMO	A	9	6,7	-	-	-
5	PDT	A	4	6,7	3,3,3	1.65	0 (0%)
10	HEC	E	80	3	58,82,82	1.62	3 (5%)
7	CYN	A	8	5,8,6	-	-	-
4	SF4	A	1	1	-	-	-

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	3	1	-	-	0,6,5,5
4	SF4	A	2	1	-	-	0,6,5,5
5	PDT	A	4	6,7	-	0,2,2,2	-
10	HEC	E	80	3	-	0,14,54,54	-
4	SF4	A	1	1	-	-	0,6,5,5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	80	HEC	CAC-C3C	5.84	1.54	1.35
10	E	80	HEC	CAB-C3B	5.80	1.53	1.35
5	A	4	PDT	C3-S2	4.22	1.97	1.80
5	A	4	PDT	C1-S1	2.61	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(°)	Ideal(°)
10	E	80	HEC	CBC-CAC-C3C	8.30	110.84	127.43
10	E	80	HEC	CBB-CAB-C3B	6.88	113.69	127.43
10	E	80	HEC	O1A-CGA-CBA	2.05	116.59	123.09

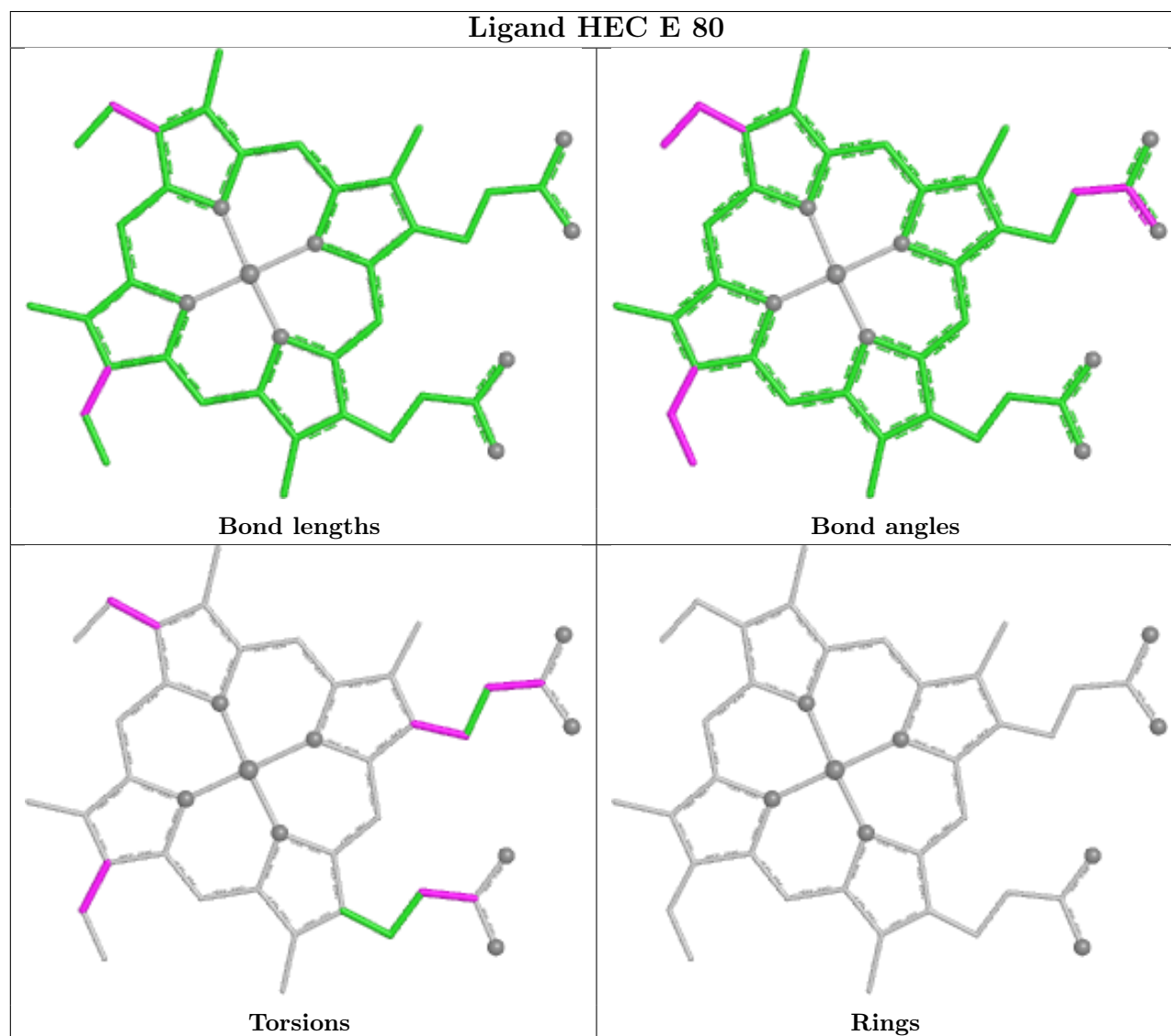
There are no chirality outliers.

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 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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues

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

No chemical shift data were provided