



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:34 am BST

PDB ID : 4GEP  
Title : SULFITE REDUCTASE HEMOPROTEIN CYANIDE COMPLEX REDUCED WITH CRII EDTA  
Authors : Crane, B.R.; Getzoff, E.D.  
Deposited on : 1997-07-10  
Resolution : 2.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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**  
buster-report : 1.1.7 (2018)  
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) : 2.11

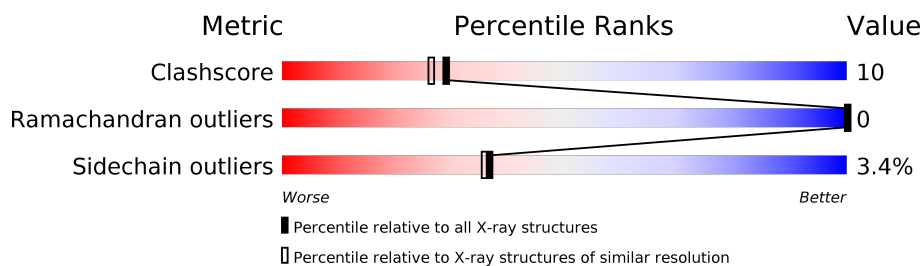
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	497	 73%      17%      • 8%

## 2 Entry composition [i](#)

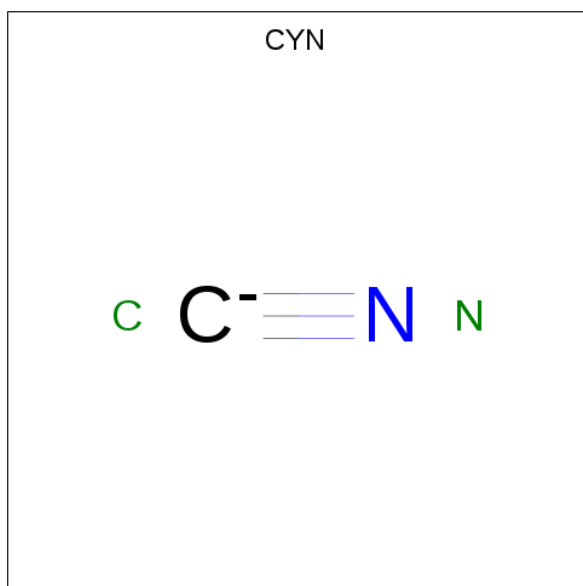
There are 6 unique types of molecules in this entry. The entry contains 4035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SULFITE REDUCTASE HEMOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3590	2271	647	656	16			

- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).

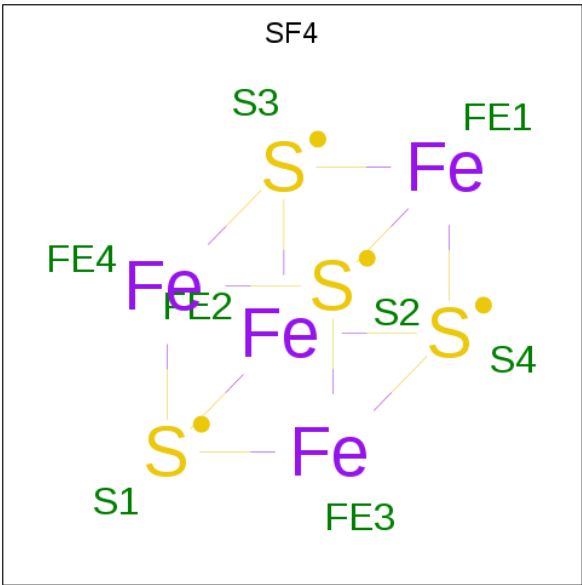


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			2	1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

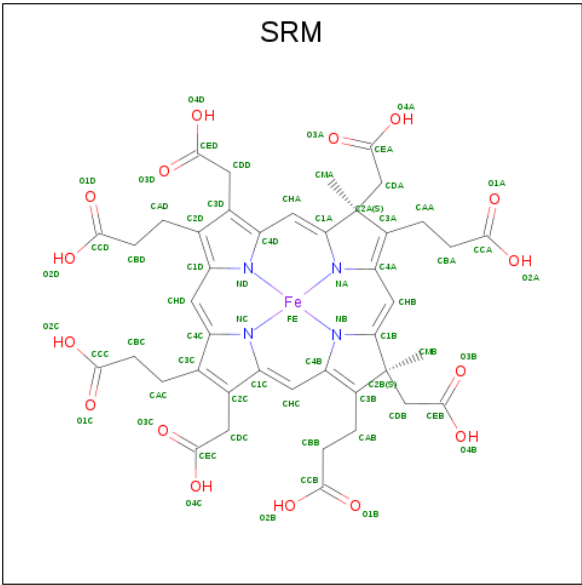
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 5 is SIROHEME (three-letter code: SRM) (formula:  $C_{42}H_{42}FeN_4O_{16}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0
			63	42	1	4	16	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	371	Total 371	O 371	0	0

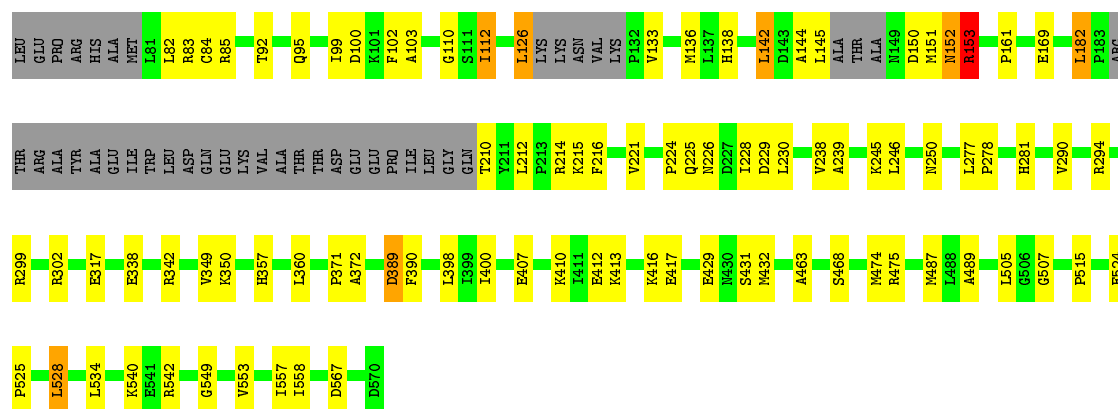
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: SULFITE REDUCTASE HEMOPROTEIN

Chain A: 



## 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 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.80 Å 77.40 Å 87.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.7 (10.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: K, SRM, SF4, CYN

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	0.49	0/3664	0.74	3/4952 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	153	ARG	O-C-N	-6.41	112.44	122.70
1	A	505	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	112	ILE	N-CA-C	-5.28	96.73	111.00

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	3590	0	3595	70	1
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
5	A	63	0	34	1	0
6	A	371	0	0	22	3
All	All	4035	0	3629	70	3



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 10.

All (70) 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:133:VAL:HB	6:A:880:HOH:O	1.25	1.30
1:A:558:ILE:HG23	6:A:928:HOH:O	1.52	1.07
1:A:210:THR:HB	1:A:294:ARG:HD3	1.55	0.87
1:A:145:LEU:N	6:A:948:HOH:O	2.08	0.86
1:A:161:PRO:HA	1:A:225:GLN:HE22	1.40	0.85
1:A:102:PHE:CZ	1:A:133:VAL:HG12	2.16	0.80
1:A:214:ARG:NH1	6:A:847:HOH:O	2.17	0.78
1:A:558:ILE:CG2	6:A:928:HOH:O	2.19	0.77
1:A:553:VAL:HG22	6:A:928:HOH:O	1.89	0.72
1:A:299:ARG:HE	1:A:299:ARG:HA	1.55	0.69
1:A:145:LEU:HD21	1:A:182:LEU:HD11	1.74	0.68
1:A:161:PRO:HA	1:A:225:GLN:NE2	2.08	0.68
1:A:350:LYS:HG3	6:A:767:HOH:O	1.96	0.65
1:A:567:ASP:OD2	6:A:854:HOH:O	2.15	0.64
1:A:151:MET:HB2	1:A:212:LEU:HD12	1.79	0.64
1:A:145:LEU:HD13	1:A:152:ASN:O	1.97	0.64
1:A:212:LEU:HD13	1:A:216:PHE:HB2	1.81	0.63
1:A:144:ALA:CA	6:A:948:HOH:O	2.47	0.62
1:A:84:CYS:SG	1:A:142:LEU:HG	2.40	0.61
1:A:350:LYS:HE3	6:A:767:HOH:O	2.00	0.61
1:A:317:GLU:HG2	6:A:668:HOH:O	2.00	0.61
1:A:82:LEU:CD2	6:A:880:HOH:O	2.48	0.60
1:A:553:VAL:CG2	6:A:928:HOH:O	2.49	0.60
1:A:138:HIS:O	6:A:946:HOH:O	2.17	0.60
1:A:151:MET:HB3	1:A:215:LYS:HA	1.83	0.59
1:A:95:GLN:O	1:A:99:ILE:HG23	2.04	0.58
1:A:429:GLU:OE2	6:A:843:HOH:O	2.16	0.58
1:A:83:ARG:HD3	5:A:580:SRM:O1B	2.04	0.58
1:A:214:ARG:HA	6:A:781:HOH:O	2.05	0.56
1:A:534:LEU:HD22	1:A:557:ILE:HD13	1.89	0.55
1:A:540:LYS:HE2	6:A:855:HOH:O	2.06	0.54
1:A:145:LEU:CD2	1:A:182:LEU:HD11	2.37	0.53
1:A:212:LEU:HD21	1:A:290:VAL:HG13	1.89	0.53
1:A:144:ALA:HA	6:A:948:HOH:O	2.09	0.53
1:A:475:ARG:HD2	1:A:489:ALA:HB2	1.92	0.51
1:A:210:THR:HG22	1:A:294:ARG:HH11	1.74	0.51
1:A:524:GLU:HB3	1:A:525:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:MET:HG3	1:A:212:LEU:HB2	1.92	0.50
1:A:542:ARG:NH2	6:A:954:HOH:O	2.07	0.50
1:A:92:THR:HA	1:A:389:ASP:HB3	1.94	0.50
1:A:413:LYS:O	1:A:417:GLU:HG2	2.11	0.49
1:A:100:ASP:HA	1:A:112:ILE:HD11	1.94	0.49
1:A:169:GLU:HG3	6:A:829:HOH:O	2.11	0.48
1:A:360:LEU:HD11	1:A:400:ILE:HD11	1.95	0.48
1:A:153:ARG:HD2	1:A:153:ARG:HA	1.50	0.47
1:A:214:ARG:CA	6:A:781:HOH:O	2.61	0.47
1:A:221:VAL:HG22	1:A:228:ILE:HD11	1.98	0.46
1:A:103:ALA:O	1:A:110:GLY:HA2	2.16	0.46
1:A:390:PHE:HB3	1:A:398:LEU:HD11	1.98	0.46
1:A:431:SER:HA	1:A:474:MET:O	2.16	0.46
1:A:238:VAL:HB	1:A:250:ASN:HB2	1.98	0.45
1:A:224:PRO:HB3	6:A:778:HOH:O	2.17	0.45
1:A:463:ALA:HA	1:A:468:SER:OG	2.16	0.45
1:A:412:GLU:O	1:A:416:LYS:HB2	2.18	0.44
1:A:226:ASN:O	1:A:342:ARG:HG2	2.17	0.43
1:A:85:ARG:HB2	1:A:145:LEU:HG	2.00	0.43
1:A:407:GLU:OE1	1:A:410:LYS:HD2	2.18	0.43
1:A:524:GLU:HG2	1:A:528:LEU:HD22	2.01	0.43
1:A:239:ALA:HB1	1:A:246:LEU:HD11	1.99	0.43
1:A:487:MET:O	1:A:515:PRO:HD2	2.18	0.43
1:A:136:MET:C	1:A:136:MET:SD	2.98	0.42
1:A:142:LEU:HA	1:A:142:LEU:HD12	1.89	0.42
1:A:278:PRO:HD2	1:A:281:HIS:HD2	1.85	0.42
1:A:85:ARG:HD3	1:A:145:LEU:HD21	2.01	0.42
1:A:507:GLY:O	1:A:549:GLY:HA3	2.20	0.41
1:A:145:LEU:HD22	1:A:150:ASP:OD2	2.19	0.41
1:A:371:PRO:O	1:A:372:ALA:HB3	2.21	0.41
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.90	0.40
1:A:349:VAL:HG22	1:A:357:HIS:HB2	2.03	0.40
1:A:432:MET:O	1:A:475:ARG:HA	2.21	0.40

All (3) 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)
1:A:126:LEU:CD2	6:A:935:HOH:O[2_564]	1.89	0.31
6:A:724:HOH:O	6:A:955:HOH:O[2_564]	2.05	0.15
6:A:887:HOH:O	6:A:941:HOH:O[2_564]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 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 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	448/497 (90%)	435 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	379/413 (92%)	366 (97%)	13 (3%)	37	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	142	LEU
1	A	152	ASN
1	A	153	ARG
1	A	182	LEU
1	A	229	ASP
1	A	230	LEU
1	A	245	LYS
1	A	277	LEU
1	A	302	ARG
1	A	338	GLU
1	A	389	ASP
1	A	528	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	281	HIS
1	A	355	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SF4	A	575	1	0,12,12	0.00	-	-		
2	CYN	A	585	5	0,1,1	0.00	-	-		
5	SRM	A	580	1,2	34,70,70	1.43	6 (17%)	38,112,112	2.99	12 (31%)

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	575	1	-	-	0/6/5/5
5	SRM	A	580	1,2	-	6/22/126/126	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	580	SRM	C1C-C2C	4.11	1.51	1.42
5	A	580	SRM	CAA-C3A	-3.09	1.46	1.51
5	A	580	SRM	FE-NA	3.06	2.07	1.95
5	A	580	SRM	C4C-C3C	3.03	1.49	1.42
5	A	580	SRM	C4A-NA	-2.50	1.34	1.39
5	A	580	SRM	FE-NB	2.30	2.04	1.95

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	580	SRM	CAB-C3B-C2B	-10.67	111.46	123.52
5	A	580	SRM	CAA-C3A-C2A	-8.48	113.94	123.52
5	A	580	SRM	C4B-NB-C1B	6.44	109.94	106.28
5	A	580	SRM	CMA-C2A-CDA	4.13	115.78	109.96
5	A	580	SRM	CDD-C3D-C4D	-3.99	121.31	127.36
5	A	580	SRM	C3B-C4B-NB	-3.65	106.06	110.14
5	A	580	SRM	CDD-C3D-C2D	3.01	131.87	126.49
5	A	580	SRM	CMB-C2B-CDB	2.87	114.00	109.96
5	A	580	SRM	C4A-NA-C1A	2.82	107.88	106.28
5	A	580	SRM	CBA-CAA-C3A	-2.64	107.18	113.40
5	A	580	SRM	CBB-CAB-C3B	-2.31	107.96	113.40
5	A	580	SRM	CBC-CAC-C3C	2.23	116.58	112.48

There are no chirality outliers.

All (6) torsion outliers are listed below:

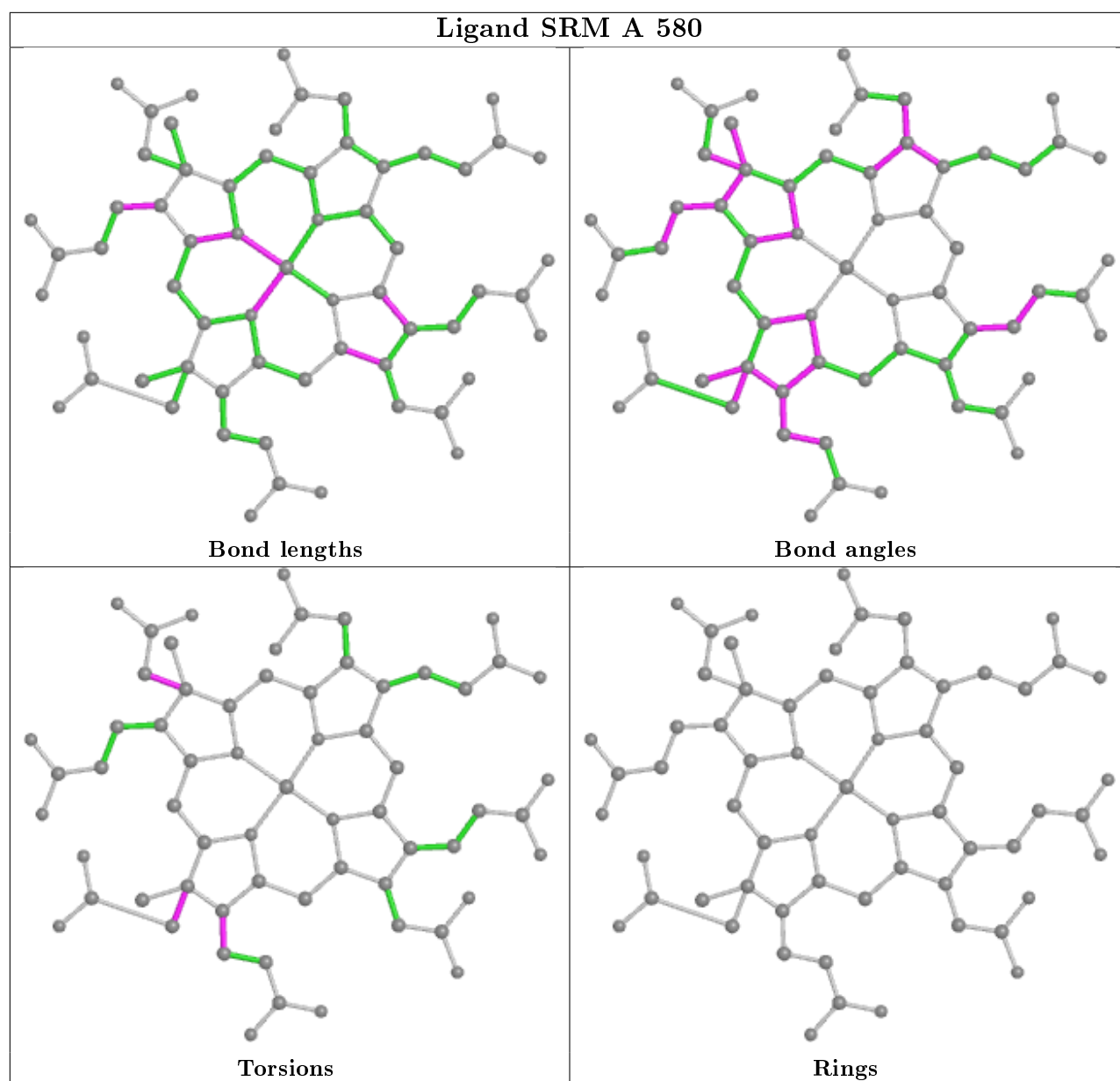
Mol	Chain	Res	Type	Atoms
5	A	580	SRM	C1A-C2A-CDA-CEA
5	A	580	SRM	CMA-C2A-CDA-CEA
5	A	580	SRM	CMB-C2B-CDB-CEB
5	A	580	SRM	C3B-C2B-CDB-CEB
5	A	580	SRM	C3A-C2A-CDA-CEA
5	A	580	SRM	C2B-C3B-CAB-CBB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	580	SRM	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 [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

### 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.