wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 03:39 am BST

PDB ID	:	1MRO
Title	:	METHYL-COENZYME M REDUCTASE
Authors	:	Ermler, U.; Grabarse, W.
Deposited on	:	1997-10-01
Resolution	:	1.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

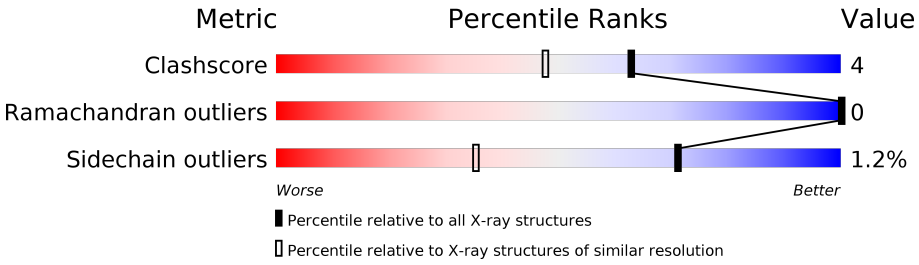
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.16 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	1832 (1.20-1.12)
Ramachandran outliers	138981	1768 (1.20-1.12)
Sidechain outliers	138945	1768 (1.20-1.12)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	89% 10%
1	D	548	90% 10%
2	B	442	91% 9%
2	E	442	93% 7%
3	C	247	91% 8%
3	F	247	91% 8%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21217 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 METHYL-COENZYME M REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	19	15	0
			4293	2717	717	839	20			
1	D	548	Total	C	N	O	S	16	13	0
			4290	2718	716	836	20			

- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	17	13	0
			3352	2123	553	655	21			
2	E	442	Total	C	N	O	S	10	7	0
			3328	2104	552	652	20			

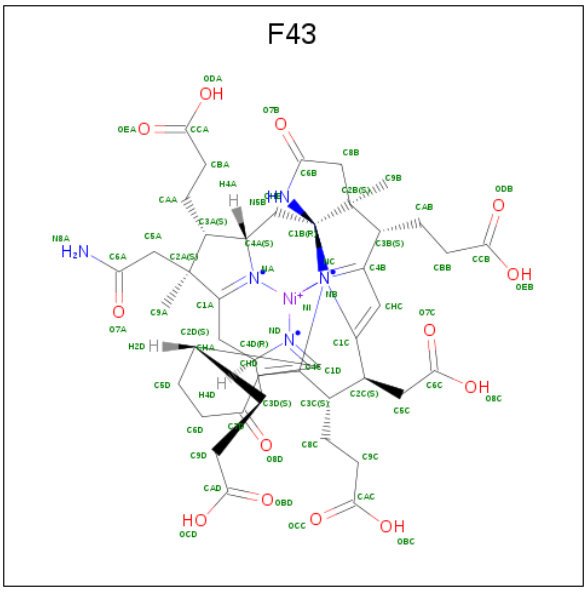
- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	36	6	0
			2021	1253	358	399	11			
3	F	247	Total	C	N	O	S	34	3	0
			2013	1247	357	398	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

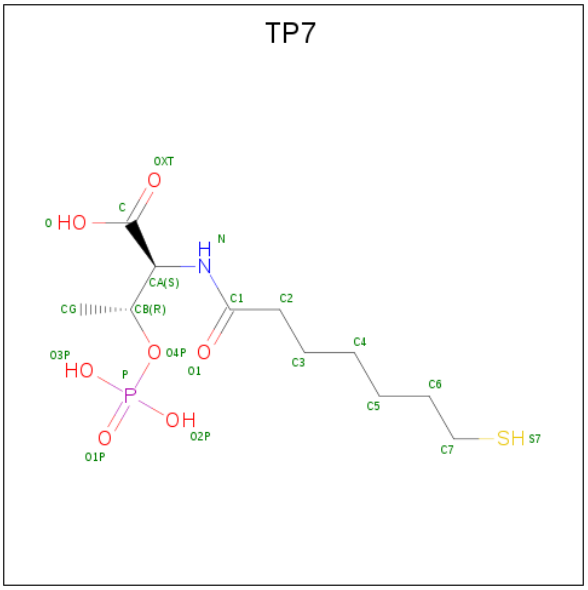
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



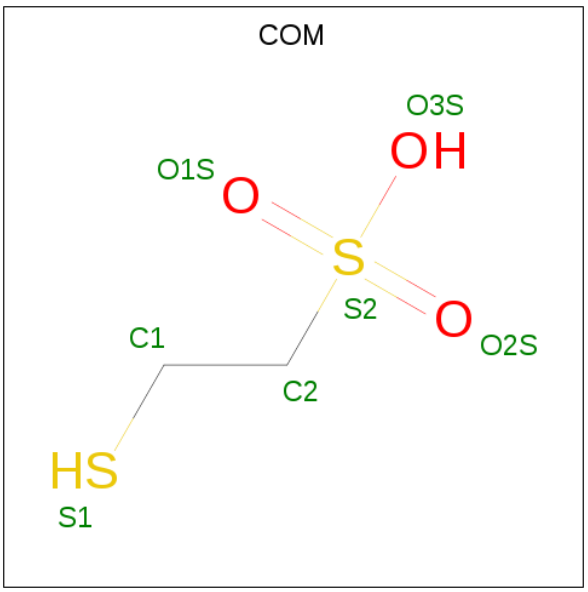
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 6 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



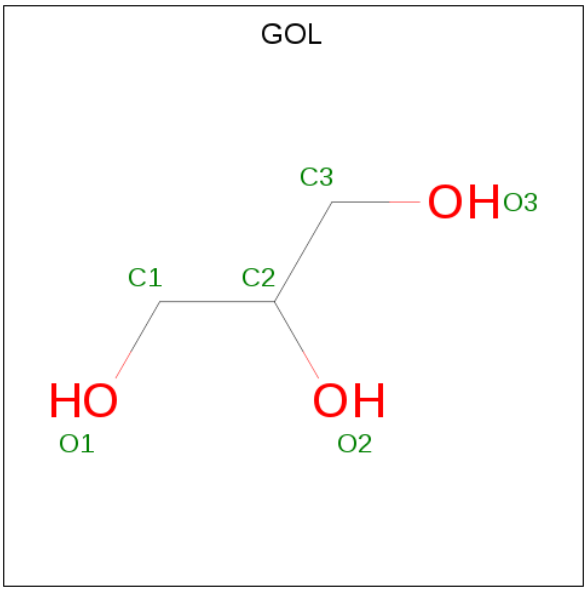
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
6	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0
8	D	1	Total C O 6 3 3	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Na 1 1	0	0
9	F	1	Total Na 1 1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	378	Total O 378 378	0	0
10	B	306	Total O 306 306	0	0
10	C	197	Total O 197 197	0	0
10	D	367	Total O 367 367	0	0
10	E	277	Total O 277 277	0	0
10	F	188	Total O 188 188	0	0

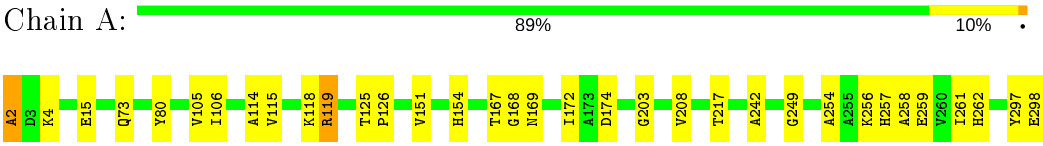
3 Residue-property plots (i)

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.

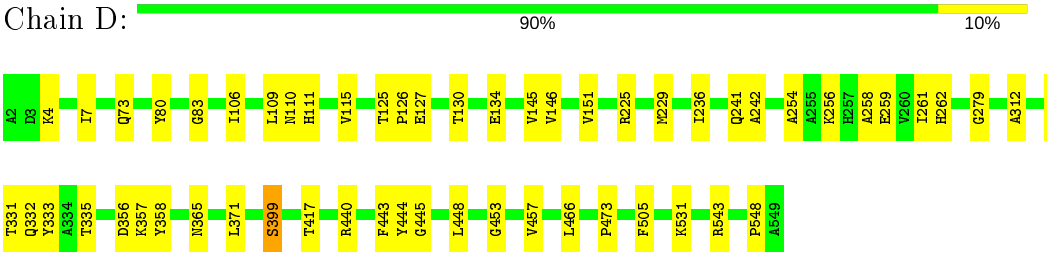
- Molecule 1: METHYL-COENZYME M REDUCTASE

Chain A:



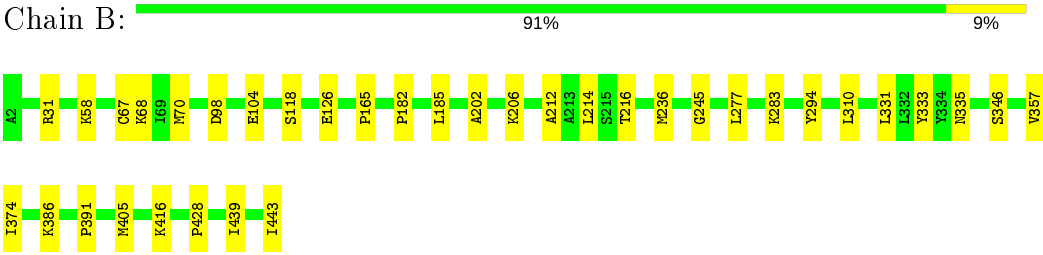
- Molecule 1: METHYL-COENZYME M REDUCTASE

Chain D:



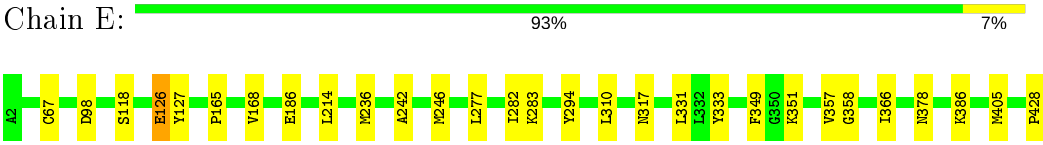
- Molecule 2: METHYL-COENZYME M REDUCTASE

Chain B:



- Molecule 2: METHYL-COENZYME M REDUCTASE

Chain E:

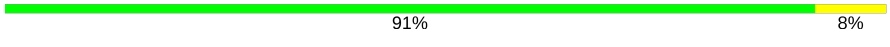


• Molecule 3: METHYL-COENZYME M REDUCTASE

Chain C:

• Molecule 3: METHYL-COENZYME M REDUCTASE

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.72Å 116.88Å 122.58Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	30.00 – 1.16	Depositor
% Data completeness (in resolution range)	92.8 (30.00-1.16)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.197 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21217	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AGM, ZN, NA, MGN, F43, TP7, SMC, GL3, COM, MHS

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	0.36	2/4426 (0.0%)	0.58	6/6006 (0.1%)
1	D	0.32	0/4412	0.48	1/5988 (0.0%)
2	B	0.28	0/3462	0.46	0/4687
2	E	0.29	0/3413	0.45	0/4622
3	C	0.43	2/2083 (0.1%)	0.64	5/2804 (0.2%)
3	F	0.31	0/2061	0.56	4/2775 (0.1%)
All	All	0.33	4/19857 (0.0%)	0.52	16/26882 (0.1%)

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 outliers	#Planarity outliers
1	A	0	3
1	D	0	1
2	B	0	1
2	E	0	1
3	C	0	2
3	F	0	2
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	161	ARG	NE-CZ	-11.34	1.18	1.33
1	A	2	ALA	N-CA	-7.25	1.31	1.46
3	C	161	ARG	CZ-NH1	6.02	1.40	1.33
1	A	2	ALA	CA-C	-5.03	1.39	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	161	ARG	NE-CZ-NH2	16.42	128.51	120.30
1	A	2	ALA	O-C-N	-15.83	97.37	122.70
1	A	2	ALA	CA-C-O	13.59	148.65	120.10
3	C	161	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	D	440	ARG	NE-CZ-NH2	7.47	124.03	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ALA	Mainchain
1	A	257	MHS	Mainchain
1	A	399	SER	Mainchain
2	B	333	TYR	Sidechain
3	C	161	ARG	Sidechain

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	4293	0	4081	43	0
1	D	4290	0	4087	47	0
2	B	3352	0	3352	41	0
2	E	3328	0	3319	26	0
3	C	2021	0	1958	16	0
3	F	2013	0	1947	9	0
4	A	1	0	0	0	0
5	A	62	0	43	2	0
5	D	62	0	43	2	0
6	A	42	0	38	1	0
7	A	7	0	5	1	0
7	D	7	0	5	1	0
8	A	12	0	16	3	0
8	D	12	0	16	3	0
9	C	1	0	0	0	0
9	F	1	0	0	0	0
10	A	378	0	0	7	2
10	B	306	0	0	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	197	0	0	6	1
10	D	367	0	0	14	2
10	E	277	0	0	1	0
10	F	188	0	0	0	0
All	All	21217	0	18910	164	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 4.

The worst 5 of 164 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)
3:C:153[B]:LYS:NZ	3:C:153[B]:LYS:CE	1.68	1.55
1:D:371[B]:LEU:CD2	1:D:371[B]:LEU:CG	1.89	1.50
2:E:236[B]:MET:SD	2:E:236[B]:MET:CG	2.08	1.40
2:E:277[B]:LEU:HD23	2:E:282:ILE:HG13	1.20	1.16
2:B:104[B]:GLU:HG3	10:B:7481:HOH:O	1.45	1.13

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)
10:A:8708:HOH:O	10:D:8435:HOH:O[2_644]	1.87	0.33
10:A:8554:HOH:O	10:D:8672:HOH:O[2_645]	1.98	0.22
10:B:8702:HOH:O	10:C:8682:HOH:O[2_555]	2.19	0.01

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	556/548 (102%)	532 (96%)	24 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	554/548 (101%)	528 (95%)	26 (5%)	0	100	100
2	B	453/442 (102%)	449 (99%)	4 (1%)	0	100	100
2	E	447/442 (101%)	442 (99%)	5 (1%)	0	100	100
3	C	251/247 (102%)	245 (98%)	6 (2%)	0	100	100
3	F	248/247 (100%)	241 (97%)	7 (3%)	0	100	100
All	All	2509/2474 (101%)	2437 (97%)	72 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/433 (104%)	442 (99%)	6 (1%)	69	32
1	D	446/433 (103%)	442 (99%)	4 (1%)	78	48
2	B	354/341 (104%)	351 (99%)	3 (1%)	81	52
2	E	348/341 (102%)	343 (99%)	5 (1%)	67	30
3	C	221/215 (103%)	218 (99%)	3 (1%)	67	30
3	F	218/215 (101%)	214 (98%)	4 (2%)	59	20
All	All	2035/1978 (103%)	2010 (99%)	25 (1%)	71	35

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	248	LEU
1	D	444	TYR
3	F	196	ASP
1	D	127	GLU
1	D	543[A]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	121	GLN
3	F	121	GLN
3	C	238	HIS
1	A	262	HIS
1	D	365	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)

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	MHS	D	257	1	7,11,12	1.59	2 (28%)	6,14,16	1.51	1 (16%)
1	SMC	D	452	1	5,6,7	0.59	0	2,6,8	0.30	0
1	MGN	D	400	1	6,9,10	1.01	1 (16%)	5,12,14	2.02	1 (20%)
1	AGM	D	271	1	10,11,12	0.48	0	6,13,15	0.18	0
1	MGN	A	400	1	6,9,10	1.10	1 (16%)	5,12,14	2.12	1 (20%)
1	SMC	A	452	1	5,6,7	0.49	0	2,6,8	0.34	0
1	AGM	A	271	1	10,11,12	0.44	0	6,13,15	0.24	0
1	MHS	A	257	1	7,11,12	3.57	4 (57%)	6,14,16	2.20	2 (33%)
1	GL3	A	445	1	2,3,4	0.20	0	1,2,4	0.11	0
1	GL3	D	445	1	2,3,4	0.26	0	1,2,4	0.12	0

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
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	D	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	D	271	1	-	1/10/11/13	-
1	MGN	A	400	1	-	0/7/9/12	-
1	SMC	A	452	1	-	1/3/5/7	-
1	AGM	A	271	1	-	2/10/11/13	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	GL3	A	445	1	-	1/1/1/2	-
1	GL3	D	445	1	-	0/1/1/2	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CM-ND1	6.93	1.63	1.47
1	A	257	MHS	CB-CG	5.08	1.58	1.50
1	D	257	MHS	CB-CG	2.80	1.54	1.50
1	D	257	MHS	CD2-NE2	2.71	1.43	1.35
1	A	257	MHS	CE1-NE2	-2.55	1.28	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	MGN	CB2-CA-CB1	-4.55	102.98	111.00
1	D	400	MGN	CB2-CA-CB1	-4.29	103.45	111.00
1	A	257	MHS	CG-CD2-NE2	-3.78	101.77	108.80
1	D	257	MHS	CM-ND1-CG	3.46	129.04	124.44
1	A	257	MHS	CD2-NE2-CE1	2.99	110.45	105.78

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	452	SMC	CA-CB-SG-CS
1	A	452	SMC	CA-CB-SG-CS
1	A	271	AGM	CE2-CD-NE1-CZ
1	A	445	GL3	S-C-CA-N
1	D	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0
1	D	445	GL3	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
5	F43	D	800	1,7	46,71,71	5.28	22 (47%)	48,118,118	3.36	21 (43%)
8	GOL	A	804	-	5,5,5	0.71	0	5,5,5	0.84	0
6	TP7	A	9500	-	16,20,20	2.36	5 (31%)	18,26,26	1.50	3 (16%)
7	COM	A	9800	5	6,6,6	1.48	0	7,8,8	1.39	0
8	GOL	A	807	-	5,5,5	0.73	0	5,5,5	0.84	0
8	GOL	D	805	-	5,5,5	0.72	0	5,5,5	0.84	0
5	F43	A	700	1,7	46,71,71	3.72	18 (39%)	48,118,118	1.97	13 (27%)
6	TP7	A	9000	-	16,20,20	2.28	6 (37%)	18,26,26	1.48	2 (11%)
8	GOL	D	806	-	5,5,5	0.70	0	5,5,5	0.84	0
7	COM	D	9700	5	6,6,6	1.55	2 (33%)	7,8,8	1.41	1 (14%)

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
5	F43	D	800	1,7	-	1/18/185/185	-
8	GOL	A	804	-	-	2/4/4/4	-
6	TP7	A	9500	-	-	3/20/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	COM	A	9800	5	-	0/4/4/4	-
8	GOL	A	807	-	-	2/4/4/4	-
8	GOL	D	805	-	-	2/4/4/4	-
5	F43	A	700	1,7	-	1/18/185/185	-
6	TP7	A	9000	-	-	2/20/24/24	-
8	GOL	D	806	-	-	2/4/4/4	-
7	COM	D	9700	5	-	0/4/4/4	-

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	800	F43	CHB-C1B	-25.06	1.36	1.53
5	D	800	F43	CHD-C1D	15.18	1.63	1.43
5	A	700	F43	NI-NA	13.47	2.18	1.89
5	A	700	F43	NI-NB	12.02	2.15	1.89
5	D	800	F43	NI-NA	8.07	2.06	1.89

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	800	F43	C4D-ND-C1D	-12.08	92.64	108.51
5	D	800	F43	C3D-C4D-ND	8.34	115.32	102.34
5	D	800	F43	C5D-C2D-C1D	7.14	120.06	110.45
5	D	800	F43	C3B-C4B-CHC	-6.38	109.56	123.32
5	D	800	F43	C2D-C1D-CHD	-5.69	114.56	121.85

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	9500	TP7	CB-O4P-P-O2P
6	A	9000	TP7	CB-O4P-P-O2P
5	D	800	F43	C3A-CAA-CBA-CCA
5	A	700	F43	C3A-CAA-CBA-CCA
6	A	9500	TP7	O1-C1-N-CA

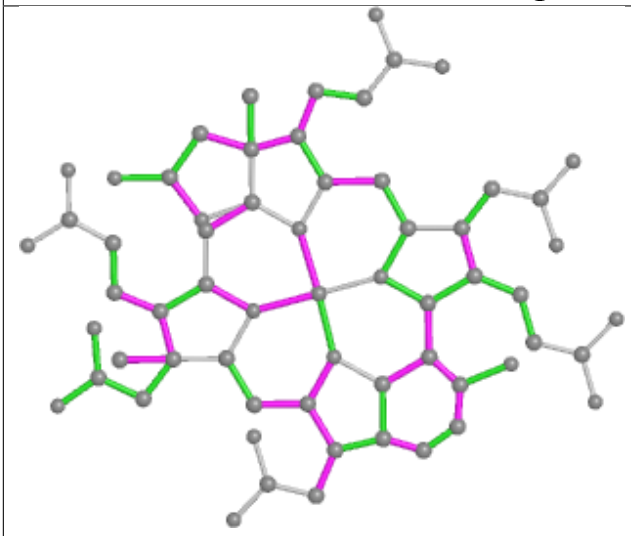
There are no ring outliers.

7 monomers are involved in 13 short contacts:

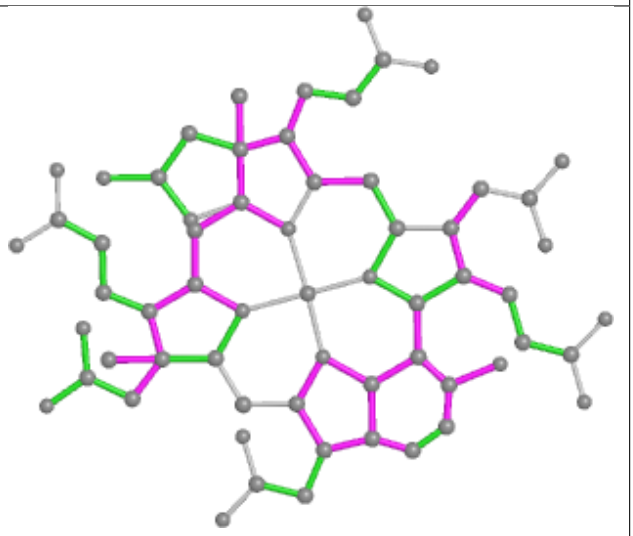
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	800	F43	2	0
8	A	804	GOL	3	0
6	A	9500	TP7	1	0
7	A	9800	COM	1	0
5	A	700	F43	2	0
8	D	806	GOL	3	0
7	D	9700	COM	1	0

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 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.

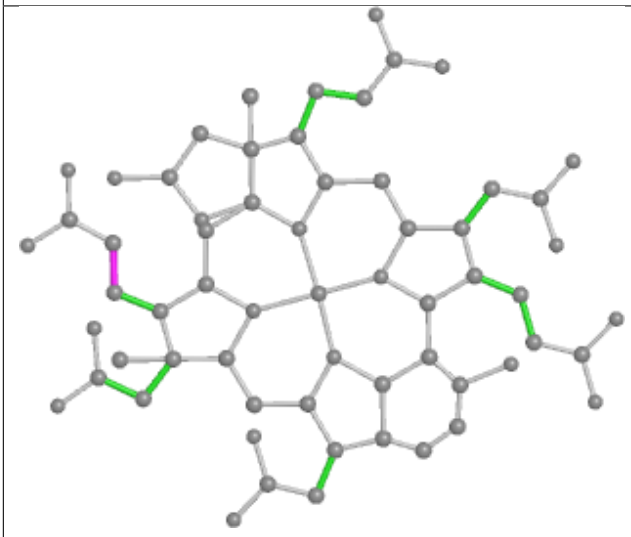
Ligand F43 D 800



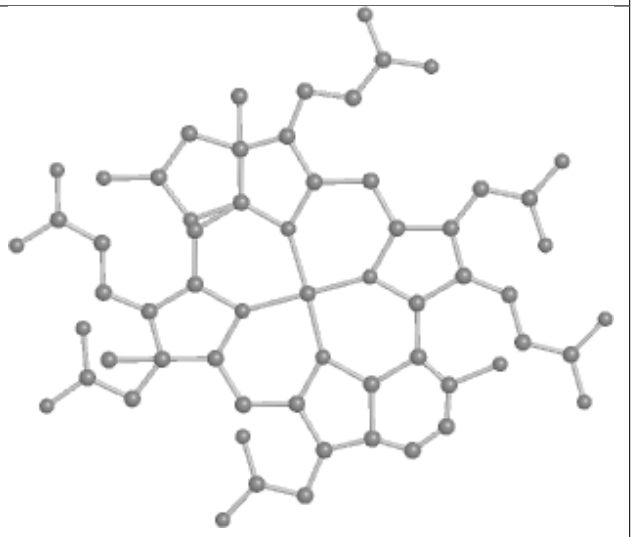
Bond lengths



Bond angles

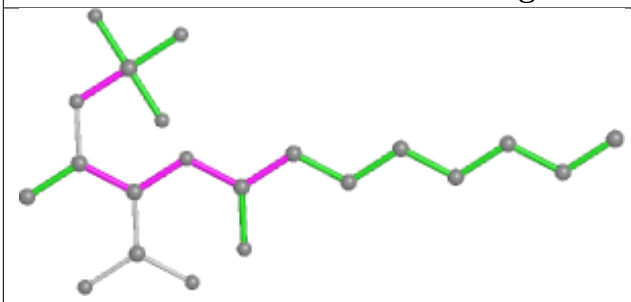


Torsions

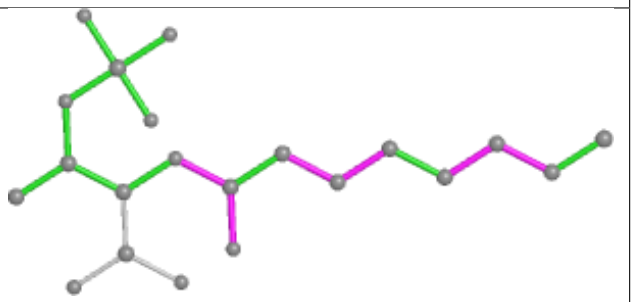


Rings

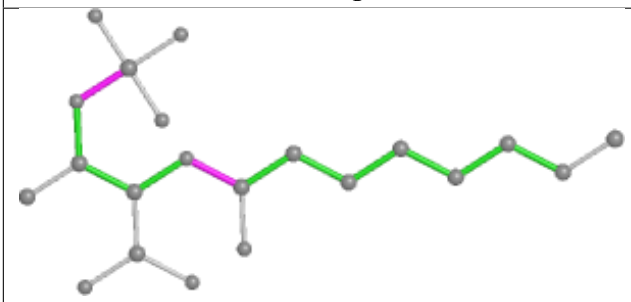
Ligand TP7 A 9500



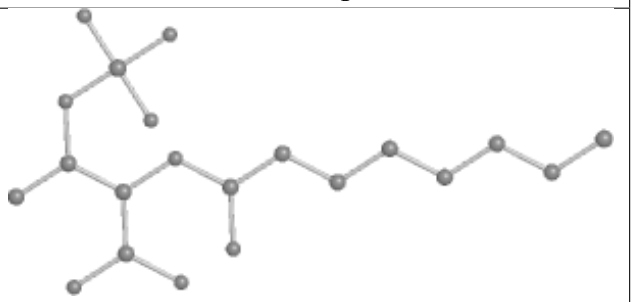
Bond lengths



Bond angles

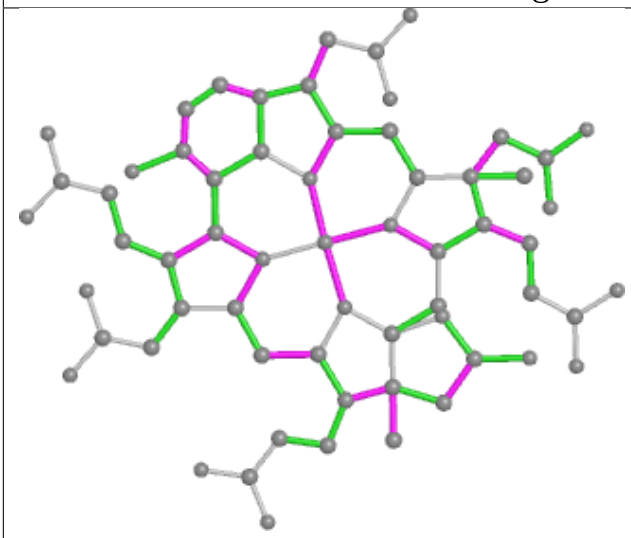


Torsions

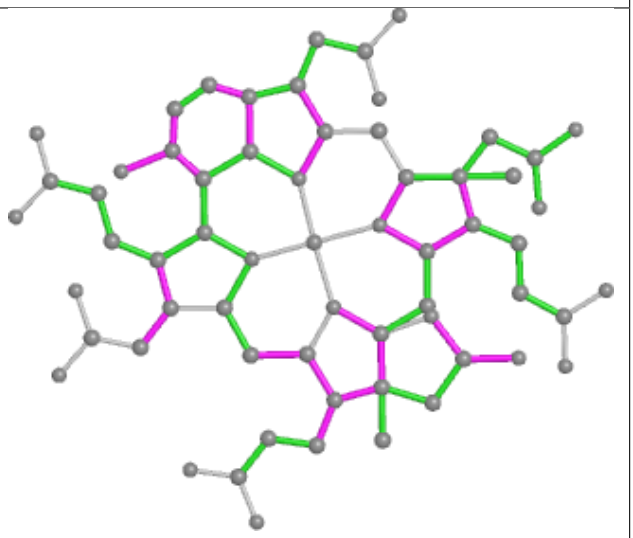


Rings

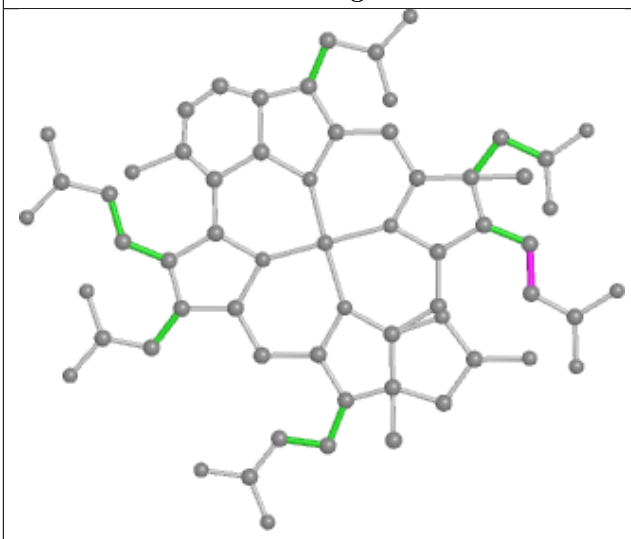
Ligand F43 A 700



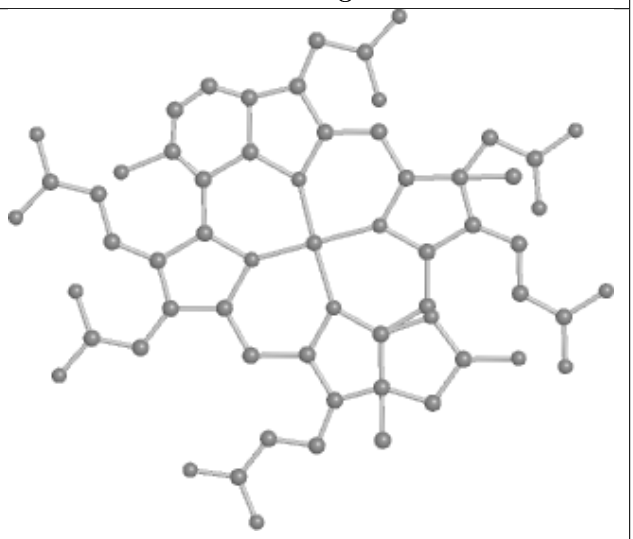
Bond lengths



Bond angles

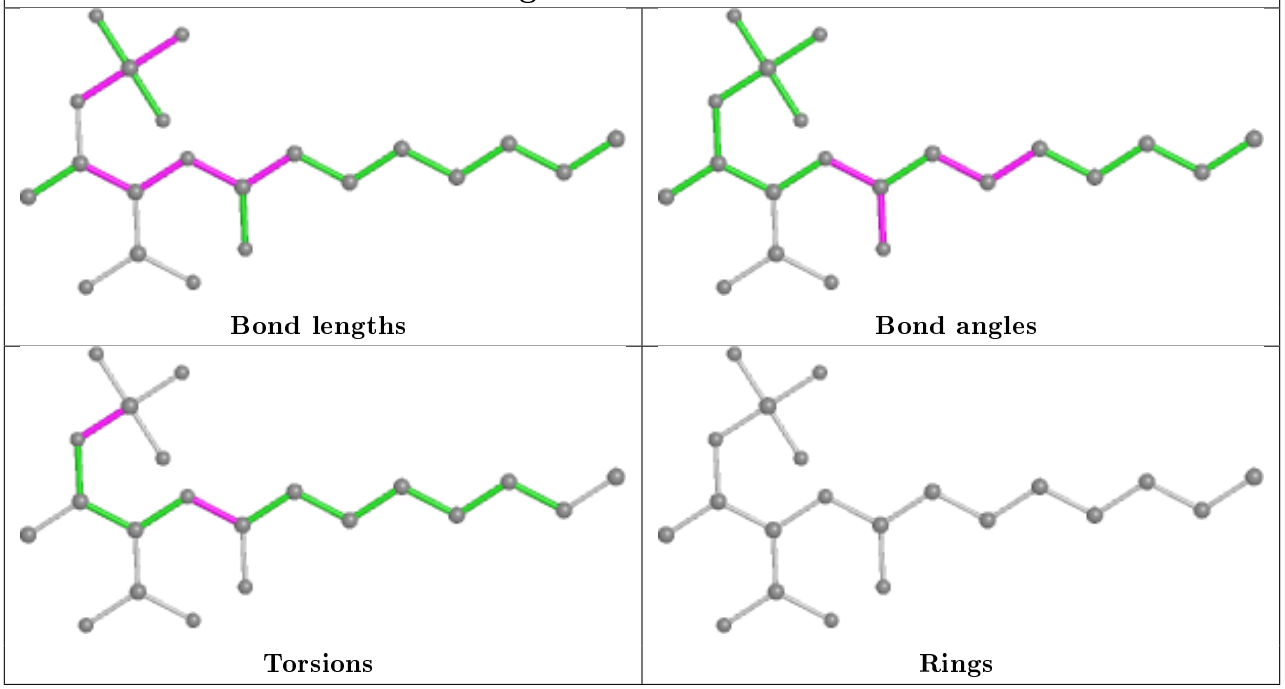


Torsions



Rings

Ligand TP7 A 9000



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	297[B]:TYR	C	298:GLU	N	1.16

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.