



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2017 – 11:36 PM EST

PDB ID : 1MMO
Title : CRYSTAL STRUCTURE OF A BACTERIAL NON-HAEM IRON HYDROXYLASE THAT CATALYSES THE BIOLOGICAL OXIDATION OF METHANE
Authors : Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.; Nordlund, P.
Deposited on : unknown
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

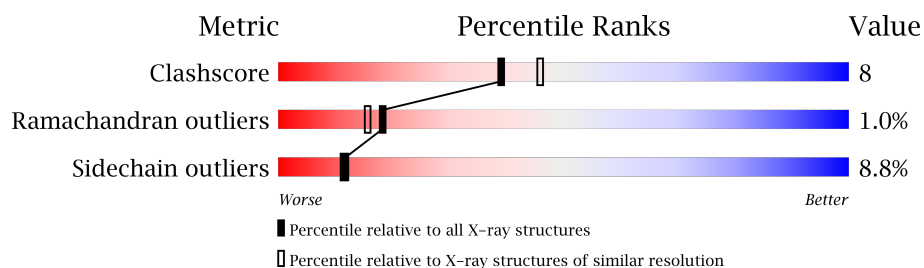
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	384	
1	C	384	
2	D	512	
2	E	512	
3	G	162	
3	H	162	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23859 atoms, of which 5642 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 METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	384	Total	C	H	N	O	S	0	0	0
			3855	2024	705	544	574	8			
1	C	384	Total	C	H	N	O	S	0	0	0
			3855	2024	705	544	574	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	142	THR	ASP	CONFLICT	UNP P18798
B	143	SER	GLU	CONFLICT	UNP P18798
B	144	SER	PHE	CONFLICT	UNP P18798
B	145	CYS	ILE	CONFLICT	UNP P18798
C	142	THR	ASP	CONFLICT	UNP P18798
C	143	SER	GLU	CONFLICT	UNP P18798
C	144	SER	PHE	CONFLICT	UNP P18798
C	145	CYS	ILE	CONFLICT	UNP P18798

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	512	Total	C	H	N	O	S	0	0	0
			5122	2680	936	721	767	18			
2	E	512	Total	C	H	N	O	S	0	0	0
			5122	2680	936	721	767	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	306	ASP	ASN	CONFLICT	UNP P22869
D	444	GLU	GLN	CONFLICT	UNP P22869

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Chain	Residue	Modelled	Actual	Comment	Reference
E	306	ASP	ASN	CONFLICT	UNP P22869
E	444	GLU	GLN	CONFLICT	UNP P22869

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			
3	H	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	38	ASP	HIS	CONFLICT	UNP P11987
G	80	LYS	ASN	CONFLICT	UNP P11987
H	38	ASP	HIS	CONFLICT	UNP P11987
H	80	LYS	ASN	CONFLICT	UNP P11987

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Fe	0	0
			2	2		
4	E	2	Total	Fe	0	0
			2	2		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

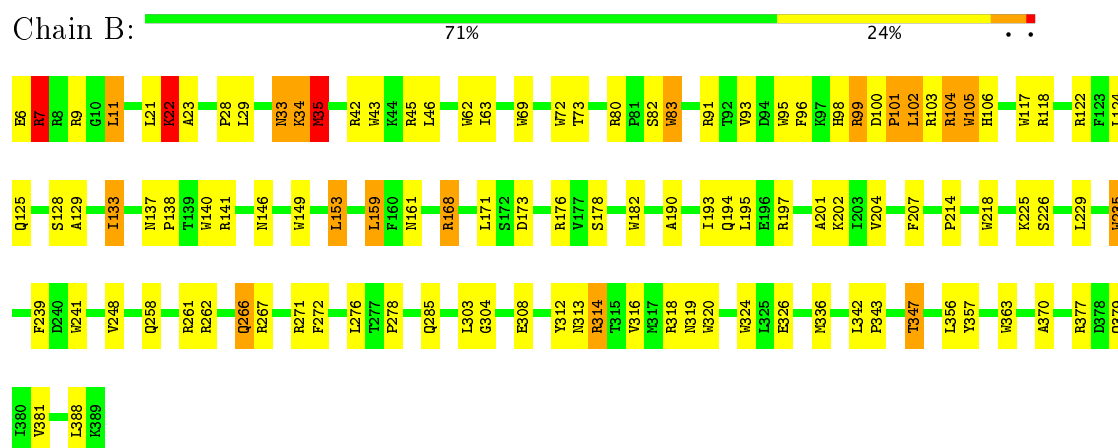
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	164	Total	H	O	0	0
			492	328	164		
6	C	142	Total	H	O	0	0
			426	284	142		
6	D	194	Total	H	O	0	0
			582	388	194		
6	E	199	Total	H	O	0	0
			597	398	199		
6	G	74	Total	H	O	0	0
			222	148	74		
6	H	86	Total	H	O	0	0
			258	172	86		

3 Residue-property plots

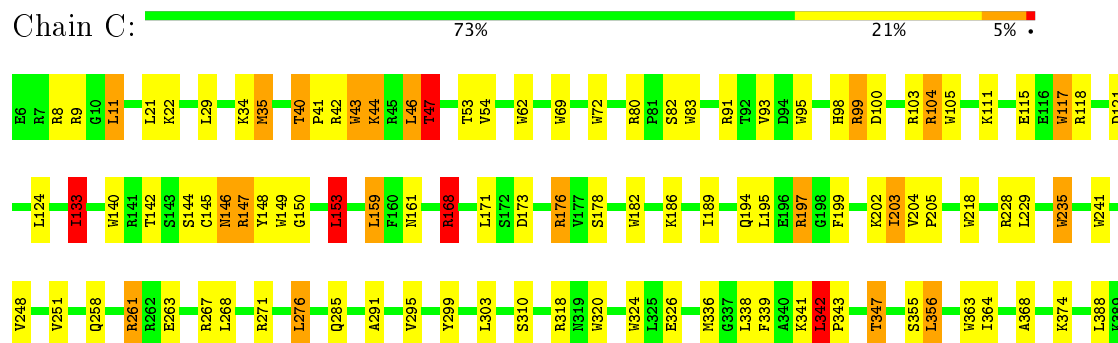
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

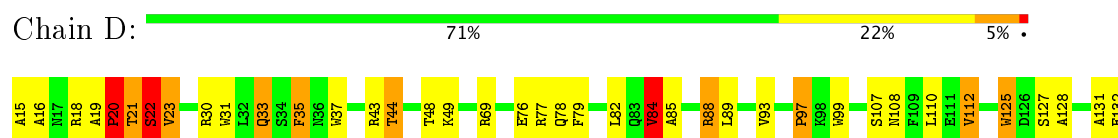
• Molecule 1: METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN)

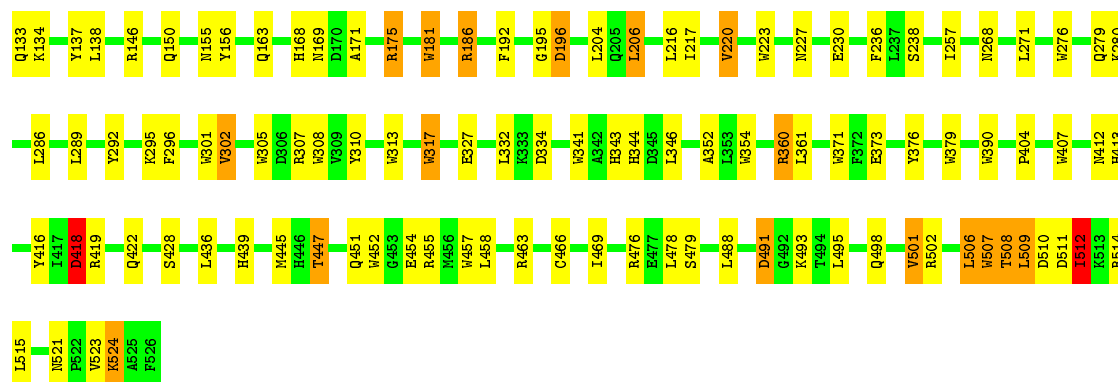


• Molecule 1: METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN)



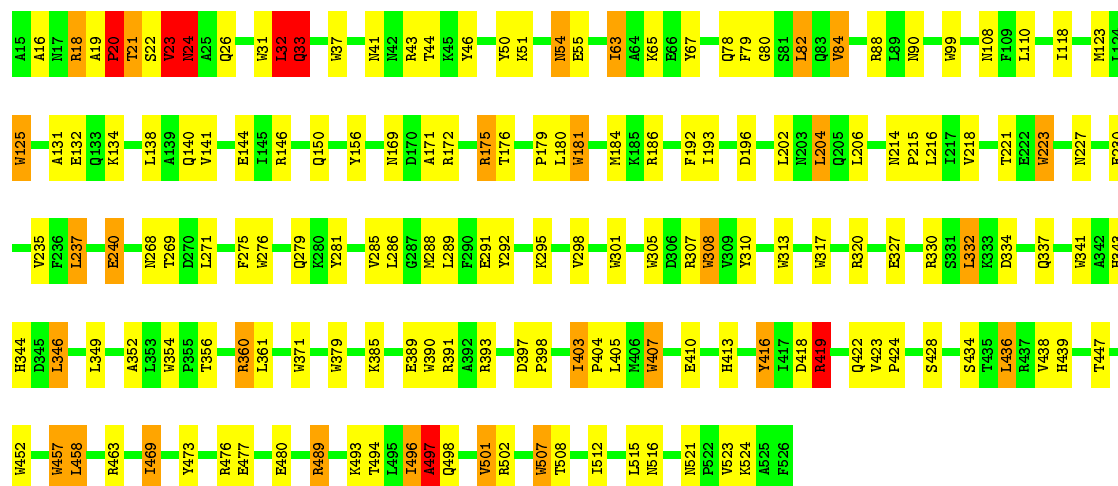
• Molecule 2: METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN)





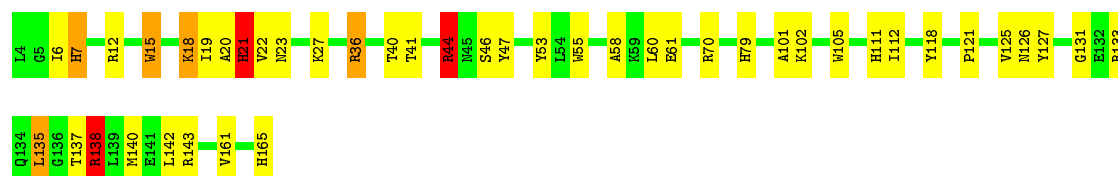
• Molecule 2: METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN)

Chain E: 68% 25% 5% .



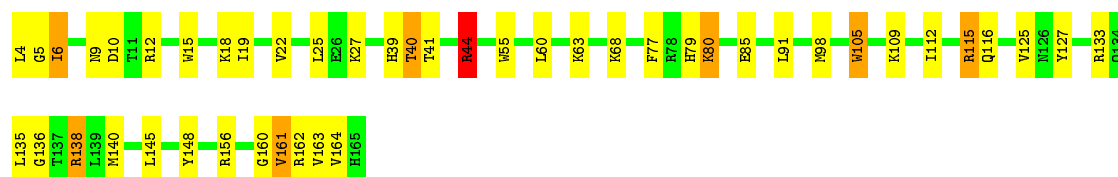
• Molecule 3: METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN)

Chain G: 73% 22% . .



• Molecule 3: METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN)

Chain H: 72% 23% . .



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, α , β , γ	62.60 Å 110.10 Å 333.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23859	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: ACY, FE

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	B	0.83	0/3245	1.68	95/4407 (2.2%)
1	C	0.84	0/3245	1.72	89/4407 (2.0%)
2	D	0.85	0/4311	1.70	129/5855 (2.2%)
2	E	0.85	0/4311	1.67	119/5855 (2.0%)
3	G	0.85	0/1366	1.58	28/1840 (1.5%)
3	H	0.82	0/1366	1.52	22/1840 (1.2%)
All	All	0.84	0/17844	1.67	482/24204 (2.0%)

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	C	0	1
2	D	0	2
2	E	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 482 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	ARG	NE-CZ-NH2	-23.56	108.52	120.30
1	C	168	ARG	NE-CZ-NH1	21.25	130.92	120.30
1	C	118	ARG	NE-CZ-NH1	15.50	128.05	120.30
2	E	360	ARG	NE-CZ-NH1	14.50	127.55	120.30
2	D	175	ARG	NE-CZ-NH2	-14.04	113.28	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	TYR	Sidechain
2	D	19	ALA	Peptide
2	D	22	SER	Mainchain
2	E	19	ALA	Peptide
2	E	24	ASN	Mainchain

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	B	3150	705	2998	57	0
1	C	3150	705	2998	50	0
2	D	4186	936	3990	74	0
2	E	4186	936	3990	92	0
3	G	1337	321	1323	24	0
3	H	1337	321	1323	28	1
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	D	4	0	3	0	0
5	E	4	0	3	0	0
6	B	164	328	0	19	1
6	C	142	284	0	5	0
6	D	194	388	0	10	1
6	E	199	398	0	25	1
6	G	74	148	0	4	0
6	H	86	172	0	15	2
All	All	18217	5642	16628	288	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 8.

The worst 5 of 288 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)
2:D:171:ALA:O	2:D:175:ARG:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:44:THR:HB	6:E:640:HOH:O	1.84	0.78
2:E:507:TRP:HB3	6:E:700:HOH:O	1.83	0.77
1:C:267:ARG:HH22	1:C:347:THR:HG21	1.50	0.77
2:D:44:THR:HG23	2:D:127:SER:HA	1.68	0.75

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)
3:H:27:LYS:HZ1	6:H:249:HOH:H1[4_465]	1.28	0.32
6:B:521:HOH:O	6:H:169:HOH:H1[1_545]	1.52	0.08
6:D:672:HOH:O	6:E:673:HOH:H2[3_645]	1.60	0.00

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	B	382/384 (100%)	359 (94%)	19 (5%)	4 (1%)	18	16
1	C	382/384 (100%)	368 (96%)	10 (3%)	4 (1%)	18	16
2	D	510/512 (100%)	481 (94%)	22 (4%)	7 (1%)	13	10
2	E	510/512 (100%)	482 (94%)	23 (4%)	5 (1%)	18	16
3	G	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	28	29
3	H	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	28	29
All	All	2104/2116 (99%)	2002 (95%)	80 (4%)	22 (1%)	18	16

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	MET
1	C	46	LEU

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Mol	Chain	Res	Type
1	C	47	THR
2	D	22	SER
2	D	196	ASP

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	B	318/318 (100%)	293 (92%)	25 (8%)	14	14
1	C	318/318 (100%)	288 (91%)	30 (9%)	10	10
2	D	432/432 (100%)	389 (90%)	43 (10%)	9	8
2	E	432/432 (100%)	392 (91%)	40 (9%)	10	10
3	G	140/140 (100%)	128 (91%)	12 (9%)	12	12
3	H	140/140 (100%)	133 (95%)	7 (5%)	28	34
All	All	1780/1780 (100%)	1623 (91%)	157 (9%)	12	11

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	206	LEU
2	D	458	LEU
3	G	125	VAL
2	D	271	LEU
2	D	310	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	252	GLN
2	D	344	HIS
3	H	7	HIS
2	D	278	GLN
2	D	439	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ACY	D	1	4	1,3,3	2.29	1 (100%)	0,3,3	0.00	-
5	ACY	E	527	4	1,3,3	1.74	0	0,3,3	0.00	-

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	ACY	D	1	4	-	0/0/0/0	0/0/0/0
5	ACY	E	527	4	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	ACY	CH3-C	2.29	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.