WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2021 – 05:39 AM EDT

PDB ID : 1FP4

Title : CRYSTAL STRUCTURE OF THE ALPHA-H195Q MUTANT OF NITRO-GENASE

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Deposited on : 2000-08-30

Resolution : 2.50 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
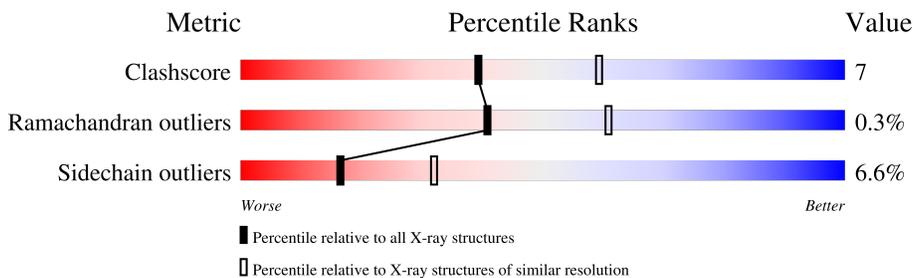with specific help available everywhere you see the (i) symbol.

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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 2.50 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		6.6%

Worse — *Better*

▮ Percentile relative to all X-ray structures
◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of 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	492	69% 22% • 5%
1	C	492	71% 21% • 5%
2	B	523	76% 21% •
2	D	523	77% 20% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFM	A	496	-	-	X	-
4	CFM	C	497	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 16295 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3708	2360	629	695	24			
1	C	468	Total	C	N	O	S	0	0	0
			3712	2363	630	695	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLN	HIS	engineered mutation	UNP P07328
C	195	GLN	HIS	engineered mutation	UNP P07328

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).
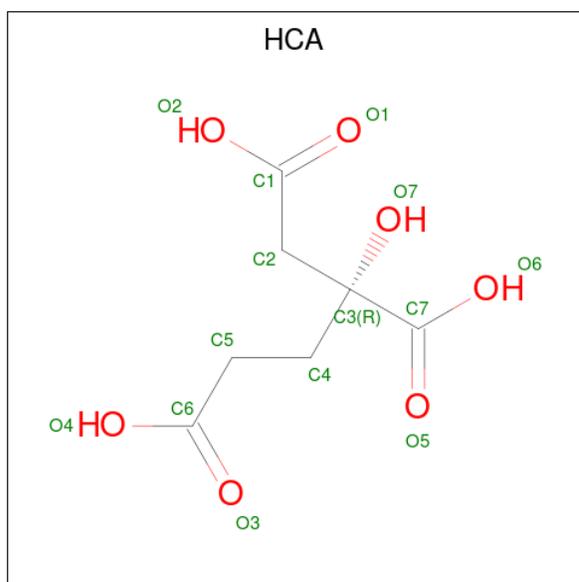
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 14	C 7	O 7	0	0
3	C	1	Total 14	C 7	O 7	0	0

- Molecule 4 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).
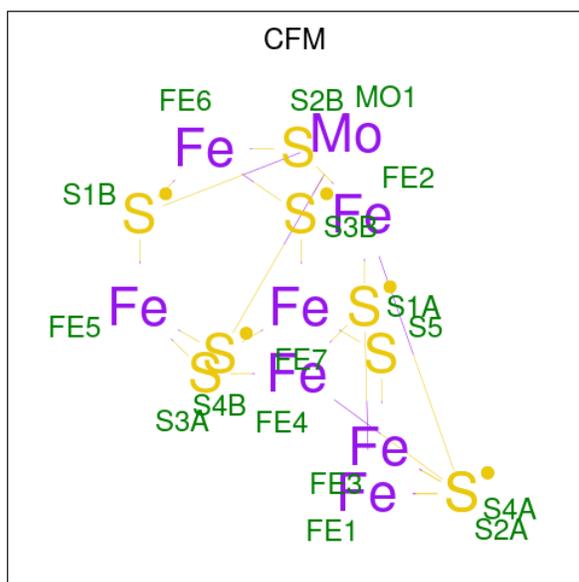
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 17	Fe 7	Mo 1	S 9	0	0
4	C	1	Total 17	Fe 7	Mo 1	S 9	0	0

- Molecule 5 is FE-S CLUSTER (three-letter code: CLP) (formula: Fe_8S_8).
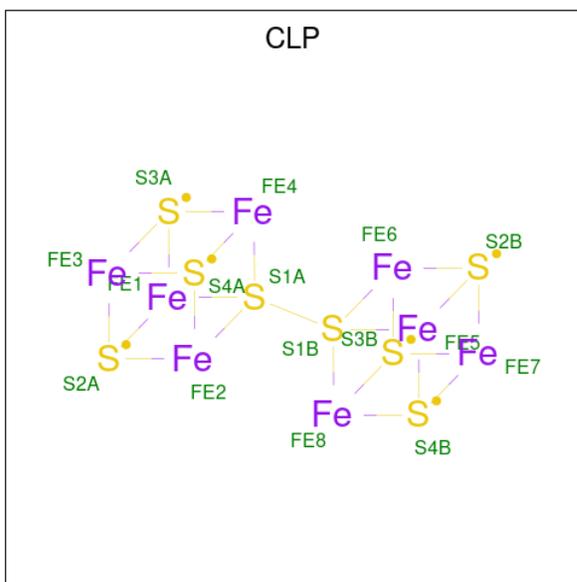
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 15	Fe 8	S 7	0	0
5	C	1	Total 15	Fe 8	S 7	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Ca 1	0	0
6	D	1	Total 1	Ca 1	0	0

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	102	Total 102	O 102	0	0
7	B	114	Total 114	O 114	0	0
7	C	74	Total 74	O 74	0	0
7	D	143	Total 143	O 143	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

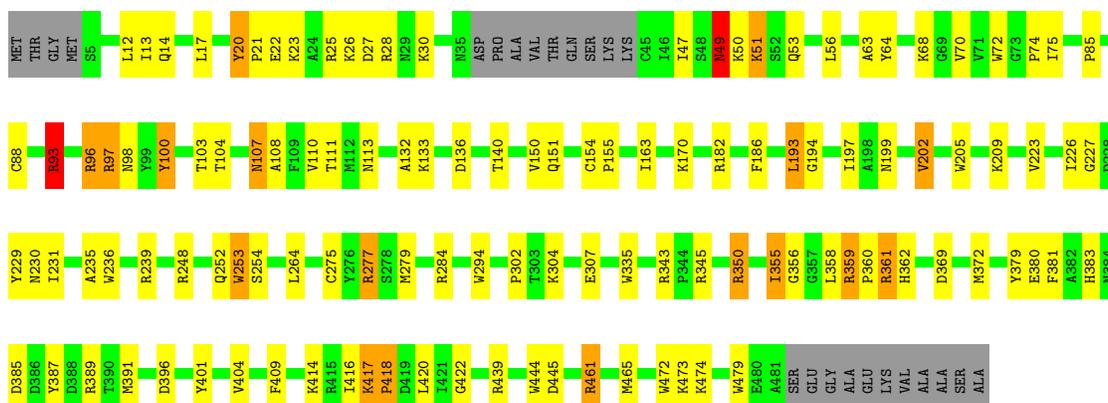Note EDS was not executed.

- Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN
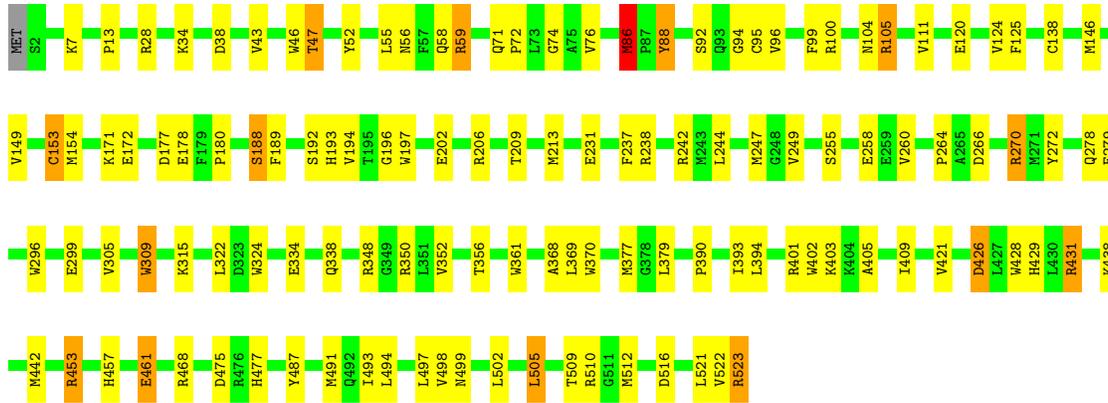
Chain A:
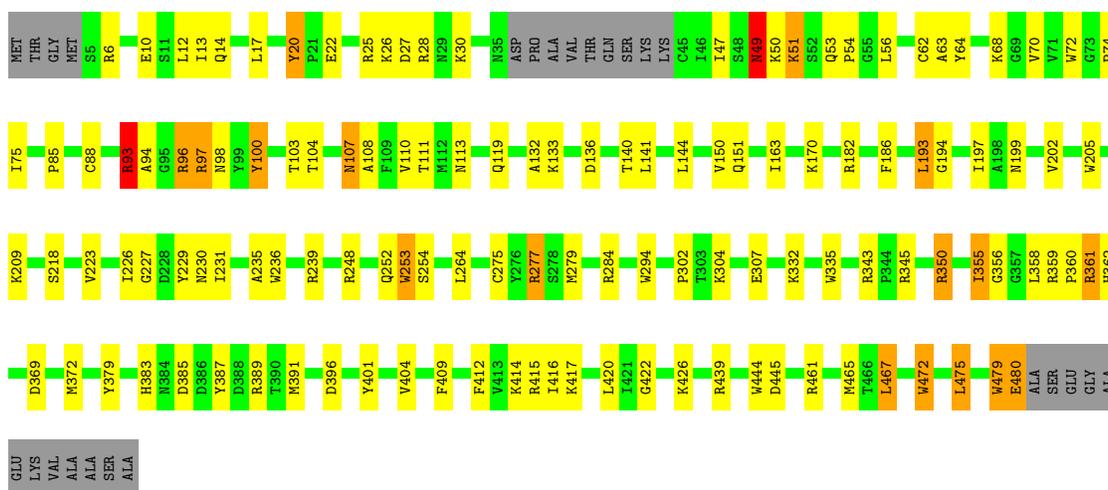
- Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

Chain C:

- Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain B:

MET S2 K7 P13 R28 K34 D38 V43 W46 T47 Y52 L55 N56 F57 Q58 R59 Q71 P72 L73 G74 A75 V76 M86 P87 Y88 S92 Q93 G94 C95 V96 F99 R100 N104 R105 V111 E120 V124 F125 C138 M146

V149 C153 M154 K171 E172 D177 E178 F179 P180 S188 F189 S192 H193 V194 T195 G196 W197 E202 R206 T209 M213 E231 F237 R238 R242 M243 L244 M247 G248 V249 S255 E258 E259 V260 P264 A265 D266 R270 M271 Y272 Q278 E279

W296 E299 V305 W309 K315 L322 D323 W324 E334 Q338 R348 G349 R350 L351 V352 T356 W361 A368 L369 W370 M377 G378 L379 P390 I393 L394 R401 W402 K403 K404 A405 I409 V421 D426 L427 W428 H429 L430 R431 K438

M442 R453 H457 E461 R468 D475 R476 H477 Y487 M491 Q492 I493 L494 L497 V498 N499 L502 L505 T509 R510 G511 M512 D516 L521 V522 R523

• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain D:　　　77%　　　20%　　　•

MET S2 Q3 Q4 K7 P13 K21 R28 K34 D38 W46 T47 Y52 L55 N56 F57 Q58 R59 Q71 P72 V76 M86 P87 Y88 S92 C95 F99 R100 R105 V111 E120 V124 F125 C138 M146 V149 C153

M154 K171 E172 D177 E178 F179 P180 S188 S192 H193 V194 T195 G196 W197 E202 R206 T209 M213 N221 E231 F237 R238 R242 M243 L244 M247 G248 V249 S255 E258 E259 V260 P264 R270 M271 Y272 Q278 E279 A287 W296

E299 V305 W309 V313 P314 K315 W324 Q338 R348 G349 R350 L351 V352 T356 W361 L362 K365 A368 L369 W370 M377 G378 L379 P390 I393 L394 R401 W402 K403 K404 A405 I409 V421 D426 L427 W428 H429 L430 R431 K438

M442 R453 E461 R468 D475 R476 H477 Y487 M491 Q492 I493 L494 L497 V498 N499 L502 L505 T509 R510 G511 M512 D516 L521 V522 R523

4 Data and refinement statistics ⓘ

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	107.20Å 130.20Å 80.40Å 90.00° 111.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16295	wwPDB-VP
Average B, all atoms (Å²)	28.0	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: CA, CLP, HCA, CFM

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	0.74	0/3793	1.41	49/5114 (1.0%)
1	C	0.85	1/3797 (0.0%)	1.44	56/5120 (1.1%)
2	B	0.72	0/4280	1.31	55/5786 (1.0%)
2	D	0.72	0/4280	1.30	56/5786 (1.0%)
All	All	0.76	1/16150 (0.0%)	1.36	216/21806 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	418	PRO	N-CD	-26.97	1.10	1.47

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	ASN	CB-CA-C	-14.28	81.84	110.40
1	C	49	ASN	CB-CA-C	-13.93	82.54	110.40
1	C	418	PRO	CA-N-CD	13.66	130.82	111.70
1	C	418	PRO	N-CA-CB	-10.43	90.78	103.30
1	C	50	LYS	N-CA-CB	-10.30	92.05	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3708	0	3638	70	0
1	C	3712	0	3640	61	0
2	B	4174	0	4087	67	0
2	D	4174	0	4087	59	0
3	A	14	0	6	0	0
3	C	14	0	6	0	0
4	A	17	0	0	5	0
4	C	17	0	0	6	0
5	A	15	0	0	3	0
5	C	15	0	0	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	102	0	0	7	0
7	B	114	0	0	2	0
7	C	74	0	0	2	0
7	D	143	0	0	2	0
All	All	16295	0	15464	232	0

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 7.

The worst 5 of 232 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:B:146:MET:HG3	2:B:180:PRO:HB2	1.62	0.82
2:D:390:PRO:HB2	2:D:393:ILE:HD11	1.63	0.81
2:B:390:PRO:HB2	2:B:393:ILE:HD11	1.64	0.80
1:C:350:ARG:NH1	1:C:416:ILE:O	2.17	0.77
2:D:146:MET:HG3	2:D:180:PRO:HB2	1.66	0.77

There are no symmetry-related clashes.

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	463/492 (94%)	433 (94%)	28 (6%)	2 (0%)	34	54
1	C	464/492 (94%)	437 (94%)	26 (6%)	1 (0%)	47	68
2	B	520/523 (99%)	508 (98%)	11 (2%)	1 (0%)	47	68
2	D	520/523 (99%)	507 (98%)	12 (2%)	1 (0%)	47	68
All	All	1967/2030 (97%)	1885 (96%)	77 (4%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
2	B	255	SER
2	D	255	SER
1	A	355	ILE
1	C	355	ILE

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	397/415 (96%)	367 (92%)	30 (8%)	13	25
1	C	396/415 (95%)	369 (93%)	27 (7%)	16	30
2	B	454/455 (100%)	426 (94%)	28 (6%)	18	35
2	D	454/455 (100%)	427 (94%)	27 (6%)	19	37
All	All	1701/1740 (98%)	1589 (93%)	112 (7%)	16	32

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	512	MET
2	D	505	LEU
1	C	264	LEU
2	D	461	GLU
2	D	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	518	ASN
2	D	499	ASN
1	C	230	ASN
2	D	518	ASN
2	D	278	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	CLP	C	499	1,2	0,21,25	-	-	-		
4	CFM	C	497	1	0,24,24	-	-	-		
3	HCA	C	495	-	4,13,13	0.54	0	4,18,18	1.27	1 (25%)
3	HCA	A	494	-	4,13,13	0.38	0	4,18,18	1.22	1 (25%)
5	CLP	A	498	1,2	0,21,25	-	-	-		
4	CFM	A	496	1	0,24,24	-	-	-		

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	CLP	A	498	1,2	-	-	0/9/9/10
5	CLP	C	499	1,2	-	-	0/9/9/10
3	HCA	C	495	-	-	4/7/17/17	-
3	HCA	A	494	-	-	4/7/17/17	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	494	HCA	C4-C5-C6	2.13	114.62	111.39
3	C	495	HCA	C4-C5-C6	2.11	114.59	111.39

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C2-C3-C4-C5
3	A	494	HCA	C7-C3-C4-C5
3	A	494	HCA	O7-C3-C4-C5
3	A	494	HCA	C3-C4-C5-C6
3	C	495	HCA	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	499	CLP	2	0
4	C	497	CFM	6	0
5	A	498	CLP	3	0
4	A	496	CFM	5	0

5.7 Other polymers ⓘ

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.