



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:04 AM EDT

PDB ID : 1MIO / pdb_00001mio
Title : X-RAY CRYSTAL STRUCTURE OF THE NITROGENASE
MOLYBDENUM-IRON PROTEIN FROM CLOSTRIDIUM PASTEURIANUM AT 3.0 ANGSTROMS RESOLUTION
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Deposited on : 1993-03-24
Resolution : 3.00 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

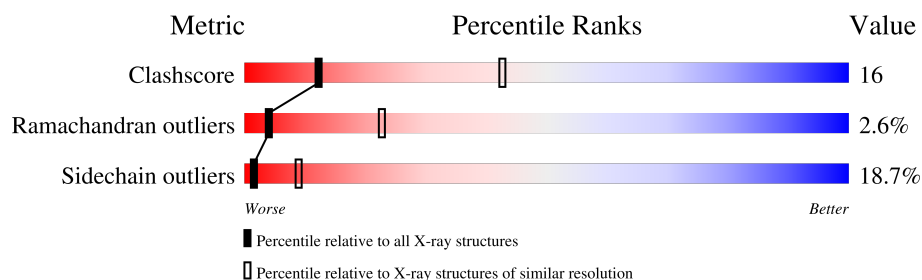
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	
1	C	533	
2	B	458	
2	D	458	

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
5	CFM	B	496	-	-	X	-
5	CFM	D	496	-	-	X	-
6	CLP	B	498	-	-	X	-
6	CLP	D	498	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15269 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	525	Total	C	N	O	S	0	0	0
			4074	2588	682	777	27			
1	C	525	Total	C	N	O	S	0	0	0
			4077	2589	683	778	27			

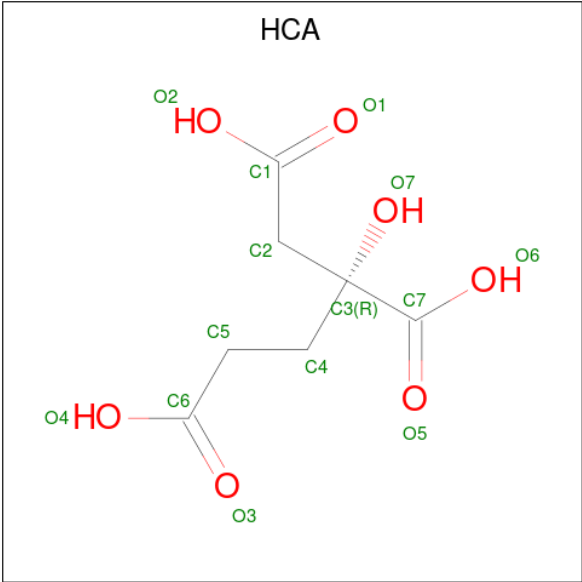
- Molecule 2 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			
2	D	457	Total	C	N	O	S	0	0	0
			3511	2231	579	681	20			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

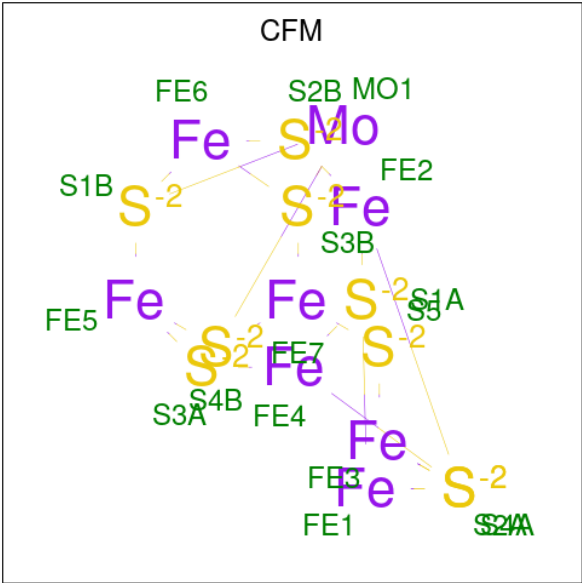
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇).



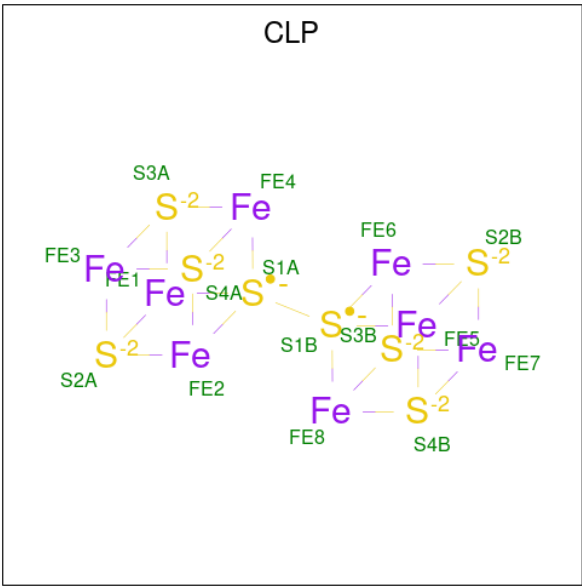
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			14	7	7		
4	D	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe₇MoS₉).

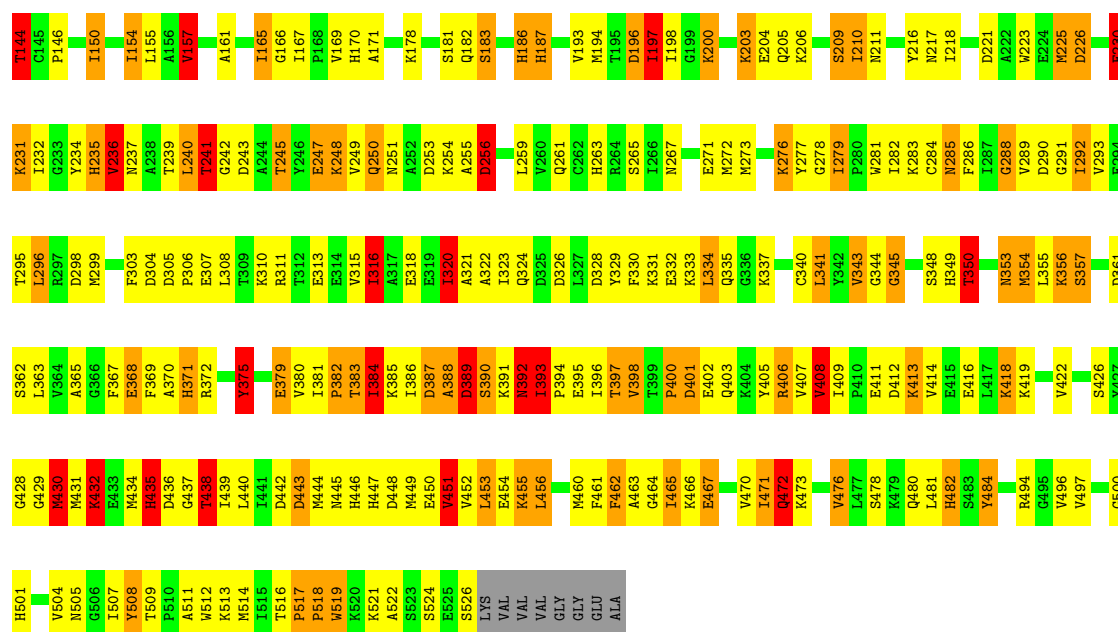


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	D	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE-S CLUSTER (CCD ID: CLP) (formula: Fe₈S₈).

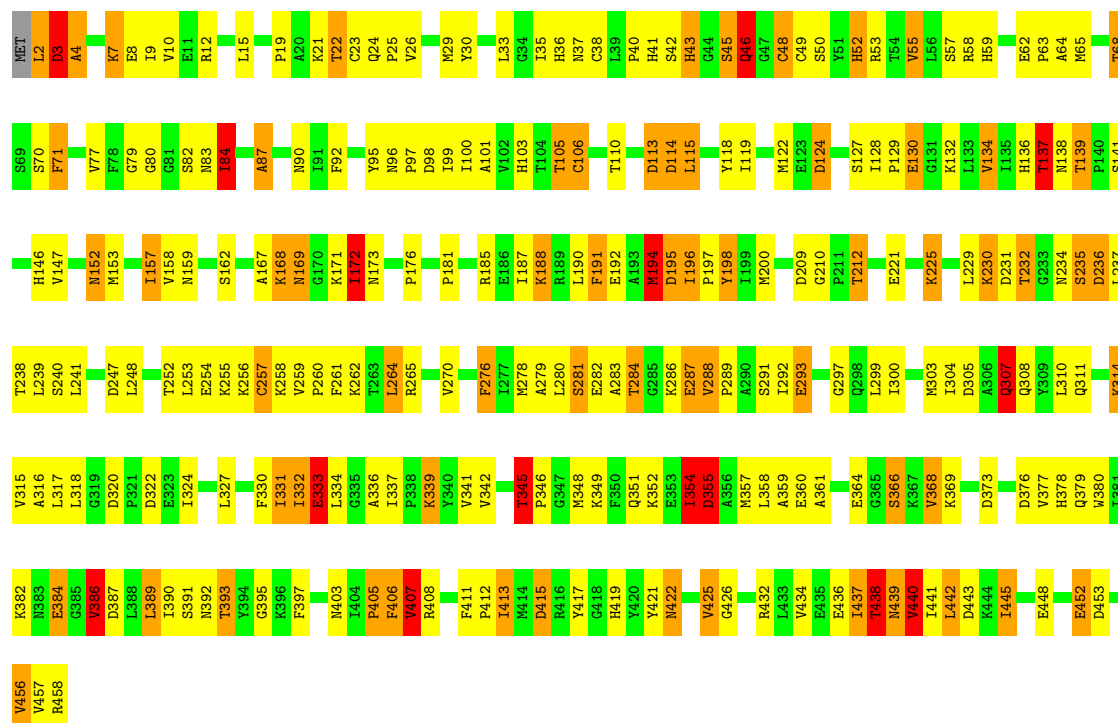


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			16	8	8		
6	D	1	Total	Fe	S	0	0
			16	8	8		



• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain B: 44% 38% 14%



• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN (BETA CHAIN)

Chain D: 44% 40% 13%

E455	V370	R296	K217	H146	F78	MET
V456	D373	L299	M218	V147	G81	L2
V457		I300	E221	F150	S82	D3
R458	D376	D301		A151	N83	A4
	V377	L302	T224	N152	I84	E8
	H378	M303	E227	M153	K85	I9
	Q379	I304	D228	V154	T86	V10
	W380	D305	L229		A87	E11
		A306	E227	I157	V88	R12
	V386	Q307	K230	V158	K89	
	D387	Q308	D231	N159	N90	L15
	L388		T232	Y160	I91	R16
	L389	Q311	G233	L161	F92	I17
	I390	V315	N234	S162	S93	N18
	S391	A316	S235	E163	L94	
	N392	L317	L239	N164	Y95	T22
	T393	L318	S240	T165	N96	
		G319	L241		P97	P25
	K396	D320		K168	D98	
	A399	P321	A245	M169	D99	P25
	R400	D322	S246		I99	A28
	E401	E323	D247	I172	I100	M29
	E402	I324	L248	N173	H103	Y30
N403		I325	G249	I175	T104	G34
I404		A326	A250	P176	T105	I35
F406		L327		G177	C106	H36
V407		S328	L253	F178	S108	N37
H408		V407	E254		C38	
F409		K329	K255	P181	L39	L39
G410			K256	A182	P40	
F411		E333	C257	D183	H41	
		L394	K258	M184	S42	
		I337	V259	R185	H43	
H419		P338	P260		S45	
Y420		K339	F261	K188	Q46	
Y421		Y340	K262	R189		
N422		V341	T263	L190	Q121	H52
		V342	L264	F191	M122	R53
Y427		T343	R265	E192	E123	T54
K428		G344	T266	A193	D124	
		T345	P267	M194	S127	L56
I431		P346	L268	D195	I128	S57
			G269		P129	R58
E436		K349	V270	Y198	E130	H59
I437		F350		I199	F60	
T438		Q351	E275	M200	L133	K61
N439			F276	F201	V134	A64
V440			I277	P202	I135	M65
				D203	H136	A66
				T204	T137	S67
D443		D355	E282		N138	T68
E448		A356	K286	L208	T139	S69
G449		M357	E287	D209	P140	S70
T450		L358		G210	S141	
E451				P211	Y142	F71
E452		G365	S291	T212	V143	T72
D453		S366	L292		G144	
F454		K367	E293	Y216	S145	V77

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	69.96Å 151.30Å 121.90Å 90.00° 110.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15269	wwPDB-VP
Average B, all atoms (Å ²)	8.0	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: CLP, CFM, HCA, CA

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	1.29	34/4163 (0.8%)	2.38	237/5629 (4.2%)
1	C	1.33	47/4166 (1.1%)	2.34	241/5631 (4.3%)
2	B	1.21	23/3582 (0.6%)	2.24	184/4845 (3.8%)
2	D	1.24	26/3582 (0.7%)	2.27	190/4845 (3.9%)
All	All	1.27	130/15493 (0.8%)	2.31	852/20950 (4.1%)

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	2
1	C	0	5
2	B	0	2
2	D	0	4
All	All	0	13

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	ILE	CA-CB	10.01	1.68	1.54
2	D	43	HIS	CD2-NE2	-9.05	1.27	1.37
1	C	236	VAL	CA-CB	8.71	1.63	1.53
1	C	186	HIS	CD2-NE2	-8.68	1.28	1.37
1	C	407	VAL	CA-CB	8.51	1.64	1.53

The worst 5 of 852 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	443	ASP	CA-CB-CG	20.04	132.64	112.60
2	D	124	ASP	CA-CB-CG	18.36	130.97	112.60
1	A	102	ASN	CA-CB-CG	15.65	128.25	112.60
1	A	390	SER	N-CA-C	15.30	143.38	110.80
1	A	240	LEU	O-C-N	14.92	140.83	122.63

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ILE	Peptide
1	A	240	LEU	Mainchain
2	B	198	TYR	Sidechain
2	B	337	ILE	Peptide
1	C	32	THR	Peptide

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4074	0	3992	144	0
1	C	4077	0	3999	159	0
2	B	3511	0	3495	104	0
2	D	3511	0	3495	94	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	14	0	6	0	0
4	D	14	0	6	2	0
5	B	17	0	0	4	0
5	D	17	0	0	4	0
6	B	16	0	0	4	0
6	D	16	0	0	5	0
All	All	15269	0	14993	469	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 16.

The worst 5 of 469 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)
6:B:498:CLP:S1A	6:B:498:CLP:S1B	2.30	1.28
6:D:498:CLP:S1A	6:D:498:CLP:S1B	2.33	1.26
1:C:345:GLY:HA3	5:D:496:CFM:S1A	2.01	0.99
1:C:197:ILE:HD11	1:C:249:VAL:HB	1.43	0.99
2:D:162:SER:HB3	2:D:257:CYS:SG	2.06	0.96

There are no symmetry-related clashes.

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	523/533 (98%)	447 (86%)	58 (11%)	18 (3%)	3	17
1	C	523/533 (98%)	452 (86%)	51 (10%)	20 (4%)	2	15
2	B	455/458 (99%)	414 (91%)	35 (8%)	6 (1%)	9	38
2	D	455/458 (99%)	411 (90%)	37 (8%)	7 (2%)	8	35
All	All	1956/1982 (99%)	1724 (88%)	181 (9%)	51 (3%)	4	23

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	143	ALA
1	A	241	THR
1	A	387	ASP
1	A	411	GLU

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	434/446 (97%)	344 (79%)	90 (21%)	1	7
1	C	435/446 (98%)	353 (81%)	82 (19%)	1	9
2	B	383/384 (100%)	309 (81%)	74 (19%)	1	8
2	D	383/384 (100%)	323 (84%)	60 (16%)	2	13
All	All	1635/1660 (98%)	1329 (81%)	306 (19%)	1	9

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	416	GLU
2	D	311	GLN
1	C	443	ASP
2	D	115	LEU
2	D	420	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	18	ASN
2	D	403	ASN
2	D	37	ASN
2	D	298	GLN
1	A	501	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 oligosaccharides 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	CFM	D	496	4,1	0,24,24	-	-	-		
5	CFM	B	496	4,1	0,24,24	-	-	-		
6	CLP	D	498	1,2	0,25,25	-	-	-		
6	CLP	B	498	1,2	0,25,25	-	-	-		
4	HCA	D	494	5	13,13,13	2.38	4 (30%)	15,18,18	2.34	6 (40%)
4	HCA	B	494	5	13,13,13	2.38	4 (30%)	15,18,18	1.87	3 (20%)

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
6	CLP	D	498	1,2	-	-	0/12/10/10
4	HCA	D	494	5	-	6/17/17/17	-
4	HCA	B	494	5	-	10/17/17/17	-
6	CLP	B	498	1,2	-	-	0/12/10/10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	494	HCA	O5-C7	7.05	1.44	1.22
4	D	494	HCA	O5-C7	6.72	1.43	1.22
4	B	494	HCA	O3-C6	2.84	1.31	1.22
4	D	494	HCA	O1-C1	2.67	1.30	1.22
4	D	494	HCA	O3-C6	2.62	1.30	1.22

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	494	HCA	O6-C7-C3	5.39	123.49	113.14
4	B	494	HCA	O6-C7-C3	4.53	121.84	113.14
4	D	494	HCA	O2-C1-O1	-3.24	115.00	123.33
4	D	494	HCA	O4-C6-C5	3.14	123.92	114.00
4	D	494	HCA	O3-C6-C5	-2.82	114.16	123.09

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	494	HCA	C1-C2-C3-C4
4	B	494	HCA	C1-C2-C3-C7
4	B	494	HCA	C1-C2-C3-O7
4	B	494	HCA	C2-C3-C4-C5
4	B	494	HCA	C7-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	496	CFM	4	0
5	B	496	CFM	4	0
6	D	498	CLP	5	0
6	B	498	CLP	4	0
4	D	494	HCA	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.