



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:03 PM BST

PDB ID : 3JBB
EMDB ID: : EMD-6430
Title : Characterization of red-shifted phycobiliprotein complexes isolated from the chlorophyll f-containing cyanobacterium Halomicronema hongdechloris
Authors : Li, Y.; Lin, Y.; Garvey, C.; Birch, D.; Corkery, R.W.; Loughlin, P.C.; Scheer, H.; Willows, R.D.; Chen, M.
Deposited on : 2015-08-26
Resolution : 26.00 Å(reported)
Based on PDB ID : 4PO5

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

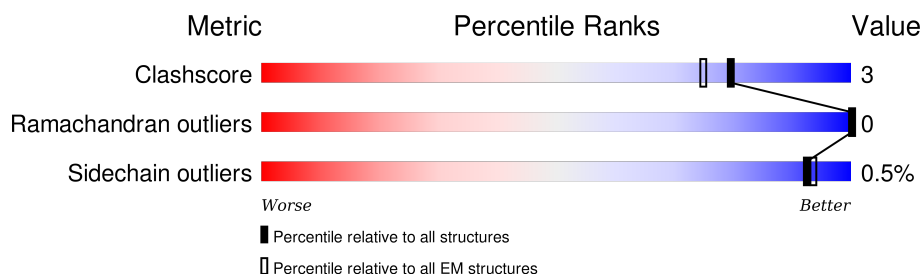
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 26.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	167	90% 7% .
1	C	167	92% 5% .
1	E	167	92% 5% .
1	G	167	90% 7% .
1	I	167	92% 5% .
1	K	167	92% 5% .
2	B	161	96% . .
2	D	161	97% .
2	F	161	98% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	161	<div><div></div><div>96%</div><div></div></div> <div><div></div><div></div></div>
2	J	161	<div><div></div><div>97%</div><div></div></div> <div><div></div><div></div></div>
2	L	161	<div><div></div><div>98%</div><div></div></div> <div><div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18492 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

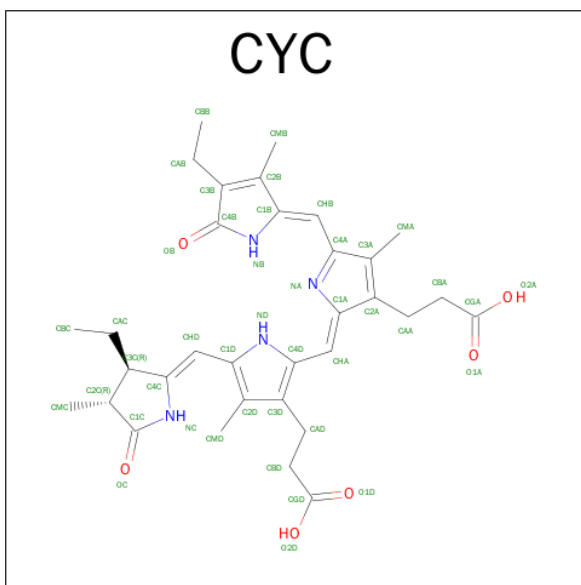
- Molecule 1 is a protein called allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		
1	C	162	Total	C	N	O	S	6	0
			1308	832	225	247	4		
1	E	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		
1	G	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		
1	I	162	Total	C	N	O	S	6	0
			1308	832	225	247	4		
1	K	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		

- Molecule 2 is a protein called allophycocyanin beta chain.

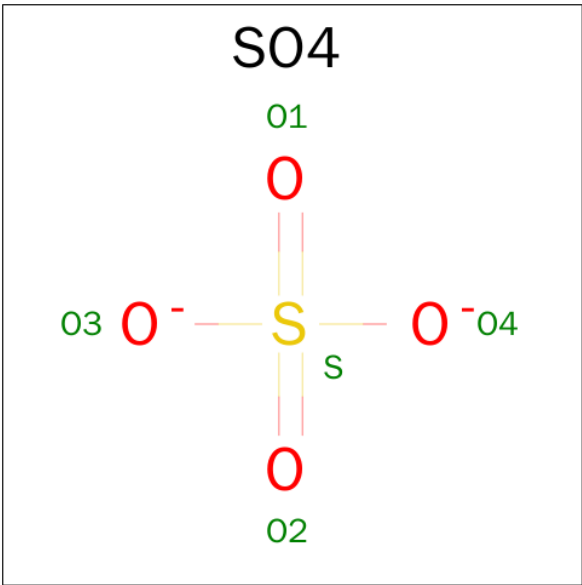
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	161	Total	C	N	O	S	9	0
			1257	789	212	249	7		
2	D	161	Total	C	N	O	S	9	0
			1259	789	213	250	7		
2	F	161	Total	C	N	O	S	7	0
			1248	782	210	249	7		
2	H	161	Total	C	N	O	S	9	0
			1257	789	212	249	7		
2	J	161	Total	C	N	O	S	9	0
			1259	789	213	250	7		
2	L	161	Total	C	N	O	S	7	0
			1248	782	210	249	7		

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	1
			46	34	4	8	
3	B	1	Total	C	N	O	0
			43	33	4	6	
3	C	1	Total	C	N	O	1
			46	34	4	8	
3	D	1	Total	C	N	O	0
			43	33	4	6	
3	E	1	Total	C	N	O	1
			46	34	4	8	
3	F	1	Total	C	N	O	0
			43	33	4	6	
3	G	1	Total	C	N	O	1
			46	34	4	8	
3	H	1	Total	C	N	O	0
			43	33	4	6	
3	I	1	Total	C	N	O	1
			46	34	4	8	
3	J	1	Total	C	N	O	0
			43	33	4	6	
3	K	1	Total	C	N	O	1
			46	34	4	8	
3	L	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	O	S	0
			10	8	2	
4	A	1	Total	O	S	0
			10	8	2	
4	B	1	Total	O	S	0
			25	20	5	
4	B	1	Total	O	S	0
			25	20	5	
4	B	1	Total	O	S	0
			25	20	5	
4	B	1	Total	O	S	0
			25	20	5	
4	C	1	Total	O	S	0
			10	8	2	
4	C	1	Total	O	S	0
			10	8	2	
4	D	1	Total	O	S	0
			25	20	5	
4	D	1	Total	O	S	0
			25	20	5	
4	D	1	Total	O	S	0
			25	20	5	
4	D	1	Total	O	S	0
			25	20	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	E	1	Total	O	S	0
			10	8	2	
4	E	1	Total	O	S	0
			10	8	2	
4	F	1	Total	O	S	0
			25	20	5	
4	F	1	Total	O	S	0
			25	20	5	
4	F	1	Total	O	S	0
			25	20	5	
4	F	1	Total	O	S	0
			25	20	5	
4	F	1	Total	O	S	0
			25	20	5	
4	G	1	Total	O	S	0
			10	8	2	
4	G	1	Total	O	S	0
			10	8	2	
4	H	1	Total	O	S	0
			25	20	5	
4	H	1	Total	O	S	0
			25	20	5	
4	H	1	Total	O	S	0
			25	20	5	
4	H	1	Total	O	S	0
			25	20	5	
4	H	1	Total	O	S	0
			25	20	5	
4	I	1	Total	O	S	0
			10	8	2	
4	I	1	Total	O	S	0
			10	8	2	
4	J	1	Total	O	S	0
			25	20	5	
4	J	1	Total	O	S	0
			25	20	5	
4	J	1	Total	O	S	0
			25	20	5	
4	J	1	Total	O	S	0
			25	20	5	
4	J	1	Total	O	S	0
			25	20	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	K	1	Total	O	S	0
			10	8	2	
4	K	1	Total	O	S	0
			10	8	2	
4	L	1	Total	O	S	0
			25	20	5	
4	L	1	Total	O	S	0
			25	20	5	
4	L	1	Total	O	S	0
			25	20	5	
4	L	1	Total	O	S	0
			25	20	5	
4	L	1	Total	O	S	0
			25	20	5	

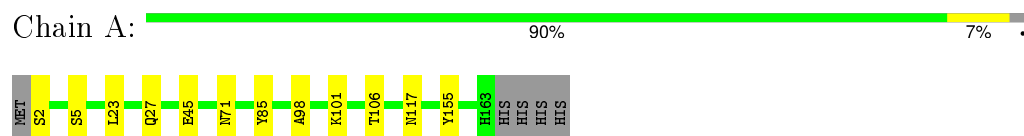
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	177	Total	O	0
			177	177	
5	B	218	Total	O	0
			218	218	
5	C	188	Total	O	0
			188	188	
5	D	212	Total	O	0
			212	212	
5	E	185	Total	O	0
			185	185	
5	F	218	Total	O	0
			218	218	
5	G	178	Total	O	0
			178	178	
5	H	217	Total	O	0
			217	217	
5	I	188	Total	O	0
			188	188	
5	J	212	Total	O	0
			212	212	
5	K	185	Total	O	0
			185	185	
5	L	218	Total	O	0
			218	218	

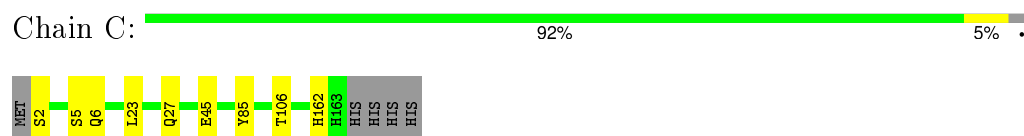
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

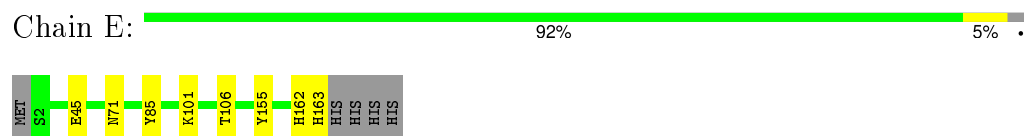
- Molecule 1: allophycocyanin subunit alpha-B



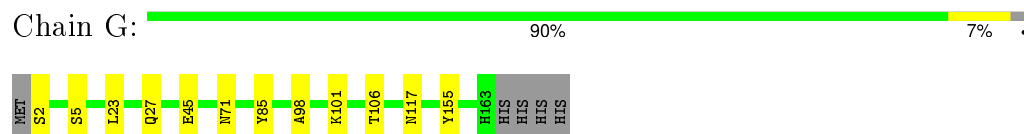
- Molecule 1: allophycocyanin subunit alpha-B



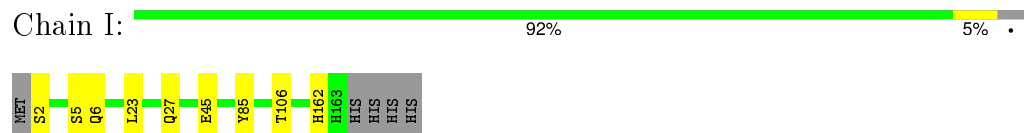
- Molecule 1: allophycocyanin subunit alpha-B



- Molecule 1: allophycocyanin subunit alpha-B



- Molecule 1: allophycocyanin subunit alpha-B



- Molecule 1: allophycocyanin subunit alpha-B





- Molecule 2: allophycocyanin beta chain

Chain B:  96%



- Molecule 2: allophycocyanin beta chain

Chain D:  97%



- Molecule 2: allophycocyanin beta chain

Chain F:  98%



- Molecule 2: allophycocyanin beta chain

Chain H:  96%



- Molecule 2: allophycocyanin beta chain

Chain J:  97%



- Molecule 2: allophycocyanin beta chain

Chain L:  98%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	420	Depositor
Resolution determination method	FSC 0.333	Depositor
CTF correction method	Each particle	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	180000	Depositor
Image detector	GENERIC IMAGE PLATES	Depositor

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: CYC, MEN, SO4

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.36	0/1342	0.47	0/1817
1	C	0.35	0/1348	0.48	0/1825
1	E	0.35	0/1342	0.48	0/1817
1	G	0.36	0/1342	0.47	0/1817
1	I	0.36	0/1348	0.48	0/1825
1	K	0.35	0/1342	0.48	0/1817
2	B	0.36	0/1279	0.54	1/1726 (0.1%)
2	D	0.35	0/1278	0.52	0/1725
2	F	0.36	0/1261	0.53	0/1703
2	H	0.36	0/1279	0.54	1/1726 (0.1%)
2	J	0.35	0/1278	0.52	0/1725
2	L	0.36	0/1261	0.53	0/1703
All	All	0.36	0/15700	0.50	2/21226 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	36	LEU	CA-CB-CG	5.71	128.42	115.30
2	B	36	LEU	CA-CB-CG	5.70	128.41	115.30

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	1302	0	1311	10	0
1	C	1308	0	1315	7	0
1	E	1302	0	1311	7	0
1	G	1302	0	1311	10	0
1	I	1308	0	1315	8	0
1	K	1302	0	1311	7	0
2	B	1257	0	1284	7	0
2	D	1259	0	1282	5	0
2	F	1248	0	1264	4	0
2	H	1257	0	1284	7	0
2	J	1259	0	1282	6	0
2	L	1248	0	1264	4	0
3	A	46	0	4	1	0
3	B	43	0	35	3	0
3	C	46	0	4	1	0
3	D	43	0	35	5	0
3	E	46	0	4	1	0
3	F	43	0	35	3	0
3	G	46	0	4	1	0
3	H	43	0	35	3	0
3	I	46	0	4	1	0
3	J	43	0	35	4	0
3	K	46	0	4	1	0
3	L	43	0	35	3	0
4	A	10	0	0	0	0
4	B	25	0	0	0	0
4	C	10	0	0	0	0
4	D	25	0	0	0	0
4	E	10	0	0	0	0
4	F	25	0	0	0	0
4	G	10	0	0	0	0
4	H	25	0	0	0	0
4	I	10	0	0	0	0
4	J	25	0	0	0	0
4	K	10	0	0	0	0
4	L	25	0	0	0	0
5	A	177	0	0	2	0
5	B	218	0	0	2	0
5	C	188	0	0	3	0
5	D	212	0	0	1	0
5	E	185	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	218	0	0	2	0
5	G	178	0	0	2	0
5	H	217	0	0	2	0
5	I	188	0	0	3	0
5	J	212	0	0	1	0
5	K	185	0	0	1	0
5	L	218	0	0	2	0
All	All	18492	0	15768	86	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 3.

The worst 5 of 86 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:62:TYR:OH	3:C:201[B]:CYC:O1D	2.12	0.67
2:H:62:TYR:OH	3:I:201[B]:CYC:O1D	2.12	0.67
2:D:62:TYR:OH	3:E:201[B]:CYC:O1D	2.12	0.66
2:J:62:TYR:OH	3:K:201[B]:CYC:O1D	2.12	0.66
3:G:201[B]:CYC:O1D	2:L:62:TYR:OH	2.14	0.62

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 PDB entries followed by that with respect to all EM entries.

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	165/167 (99%)	165 (100%)	0	0	100	100
1	C	166/167 (99%)	166 (100%)	0	0	100	100
1	E	165/167 (99%)	165 (100%)	0	0	100	100
1	G	165/167 (99%)	165 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	166/167 (99%)	166 (100%)	0	0	100	100
1	K	165/167 (99%)	165 (100%)	0	0	100	100
2	B	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	D	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	F	165/161 (102%)	163 (99%)	2 (1%)	0	100	100
2	H	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	J	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	L	165/161 (102%)	163 (99%)	2 (1%)	0	100	100
All	All	1990/1968 (101%)	1978 (99%)	12 (1%)	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 PDB entries followed by that with respect to all EM entries.

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	139/139 (100%)	138 (99%)	1 (1%)	88	94
1	C	140/139 (101%)	139 (99%)	1 (1%)	88	94
1	E	139/139 (100%)	138 (99%)	1 (1%)	88	94
1	G	139/139 (100%)	138 (99%)	1 (1%)	88	94
1	I	140/139 (101%)	139 (99%)	1 (1%)	88	94
1	K	139/139 (100%)	138 (99%)	1 (1%)	88	94
2	B	133/124 (107%)	132 (99%)	1 (1%)	86	94
2	D	133/124 (107%)	133 (100%)	0	100	100
2	F	131/124 (106%)	131 (100%)	0	100	100
2	H	133/124 (107%)	132 (99%)	1 (1%)	86	94
2	J	133/124 (107%)	133 (100%)	0	100	100
2	L	131/124 (106%)	131 (100%)	0	100	100
All	All	1630/1578 (103%)	1622 (100%)	8 (0%)	92	96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	85	TYR
1	K	85	TYR
2	H	36	LEU
1	C	85	TYR
1	G	85	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	163	HIS
1	K	163	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
2	MEN	B	71	2	6,8,9	0.66	0	6,9,11	1.16	0
2	MEN	D	71	2	6,8,9	0.74	0	6,9,11	1.17	0
2	MEN	F	71	2	6,8,9	0.74	0	6,9,11	1.10	0
2	MEN	H	71	2	6,8,9	0.65	0	6,9,11	1.18	0
2	MEN	J	71	2	6,8,9	0.75	0	6,9,11	1.19	0
2	MEN	L	71	2	6,8,9	0.76	0	6,9,11	1.10	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
2	MEN	B	71	2	-	0/6/8/10	0/0/0/0
2	MEN	D	71	2	-	0/6/8/10	0/0/0/0
2	MEN	F	71	2	-	0/6/8/10	0/0/0/0
2	MEN	H	71	2	-	0/6/8/10	0/0/0/0
2	MEN	J	71	2	-	0/6/8/10	0/0/0/0
2	MEN	L	71	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

60 ligands 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	$\# Z > 2$
3	CYC	A	201[A]	-	35,46,46	4.20	12 (34%)	44,67,67	2.16	19 (43%)
3	CYC	A	201[B]	-	35,46,46	4.20	12 (34%)	44,67,67	2.15	19 (43%)
4	SO4	A	202	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	A	203	-	4,4,4	0.24	0	6,6,6	0.07	0
3	CYC	B	201	2	35,46,46	4.46	13 (37%)	44,67,67	2.32	15 (34%)
4	SO4	B	202	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	B	203	-	4,4,4	0.21	0	6,6,6	0.16	0
4	SO4	B	204	-	4,4,4	0.21	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	205	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	B	206	-	4,4,4	0.21	0	6,6,6	0.08	0
3	CYC	C	201[A]	-	35,46,46	4.31	10 (28%)	44,67,67	2.22	20 (45%)
3	CYC	C	201[B]	-	35,46,46	4.31	10 (28%)	44,67,67	2.22	20 (45%)
4	SO4	C	202	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	C	203	-	4,4,4	0.23	0	6,6,6	0.06	0
3	CYC	D	201	2	35,46,46	4.48	12 (34%)	44,67,67	2.33	13 (29%)
4	SO4	D	202	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	D	203	-	4,4,4	0.20	0	6,6,6	0.17	0
4	SO4	D	204	-	4,4,4	0.21	0	6,6,6	0.08	0
4	SO4	D	205	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	D	206	-	4,4,4	0.22	0	6,6,6	0.08	0
3	CYC	E	201[A]	-	35,46,46	4.25	13 (37%)	44,67,67	2.15	18 (40%)
3	CYC	E	201[B]	-	35,46,46	4.25	13 (37%)	44,67,67	2.15	18 (40%)
4	SO4	E	202	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	E	203	-	4,4,4	0.27	0	6,6,6	0.06	0
3	CYC	F	201	2	35,46,46	4.42	12 (34%)	44,67,67	2.11	13 (29%)
4	SO4	F	202	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	F	203	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	F	204	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	F	205	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	F	206	-	4,4,4	0.23	0	6,6,6	0.09	0
3	CYC	G	201[A]	-	35,46,46	4.22	12 (34%)	44,67,67	2.15	19 (43%)
3	CYC	G	201[B]	-	35,46,46	4.22	12 (34%)	44,67,67	2.14	19 (43%)
4	SO4	G	202	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	G	203	-	4,4,4	0.23	0	6,6,6	0.07	0
3	CYC	H	201	2	35,46,46	4.48	13 (37%)	44,67,67	2.31	15 (34%)
4	SO4	H	202	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	H	203	-	4,4,4	0.22	0	6,6,6	0.16	0
4	SO4	H	204	-	4,4,4	0.22	0	6,6,6	0.07	0
4	SO4	H	205	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	H	206	-	4,4,4	0.22	0	6,6,6	0.09	0
3	CYC	I	201[A]	-	35,46,46	4.28	10 (28%)	44,67,67	2.21	20 (45%)
3	CYC	I	201[B]	-	35,46,46	4.28	10 (28%)	44,67,67	2.21	20 (45%)
4	SO4	I	202	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	I	203	-	4,4,4	0.24	0	6,6,6	0.06	0
3	CYC	J	201	2	35,46,46	4.48	12 (34%)	44,67,67	2.33	14 (31%)
4	SO4	J	202	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	J	203	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SO4	J	204	-	4,4,4	0.21	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	J	205	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	J	206	-	4,4,4	0.24	0	6,6,6	0.08	0
3	CYC	K	201[A]	-	35,46,46	4.27	13 (37%)	44,67,67	2.15	18 (40%)
3	CYC	K	201[B]	-	35,46,46	4.27	13 (37%)	44,67,67	2.15	18 (40%)
4	SO4	K	202	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	K	203	-	4,4,4	0.26	0	6,6,6	0.06	0
3	CYC	L	201	2	35,46,46	4.42	12 (34%)	44,67,67	2.12	14 (31%)
4	SO4	L	202	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	L	203	-	4,4,4	0.20	0	6,6,6	0.19	0
4	SO4	L	204	-	4,4,4	0.22	0	6,6,6	0.07	0
4	SO4	L	205	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	L	206	-	4,4,4	0.22	0	6,6,6	0.08	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
3	CYC	A	201[A]	-	-	2/21/74/74	0/4/4/4
3	CYC	A	201[B]	-	-	2/21/74/74	0/4/4/4
4	SO4	A	202	-	-	0/0/0/0	0/0/0/0
4	SO4	A	203	-	-	0/0/0/0	0/0/0/0
3	CYC	B	201	2	-	2/21/74/74	0/4/4/4
4	SO4	B	202	-	-	0/0/0/0	0/0/0/0
4	SO4	B	203	-	-	0/0/0/0	0/0/0/0
4	SO4	B	204	-	-	0/0/0/0	0/0/0/0
4	SO4	B	205	-	-	0/0/0/0	0/0/0/0
4	SO4	B	206	-	-	0/0/0/0	0/0/0/0
3	CYC	C	201[A]	-	-	2/21/74/74	0/4/4/4
3	CYC	C	201[B]	-	-	2/21/74/74	0/4/4/4
4	SO4	C	202	-	-	0/0/0/0	0/0/0/0
4	SO4	C	203	-	-	0/0/0/0	0/0/0/0
3	CYC	D	201	2	-	2/21/74/74	0/4/4/4
4	SO4	D	202	-	-	0/0/0/0	0/0/0/0
4	SO4	D	203	-	-	0/0/0/0	0/0/0/0
4	SO4	D	204	-	-	0/0/0/0	0/0/0/0
4	SO4	D	205	-	-	0/0/0/0	0/0/0/0
4	SO4	D	206	-	-	0/0/0/0	0/0/0/0
3	CYC	E	201[A]	-	-	2/21/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	E	201[B]	-	-	2/21/74/74	0/4/4/4
4	SO4	E	202	-	-	0/0/0/0	0/0/0/0
4	SO4	E	203	-	-	0/0/0/0	0/0/0/0
3	CYC	F	201	2	-	2/21/74/74	0/4/4/4
4	SO4	F	202	-	-	0/0/0/0	0/0/0/0
4	SO4	F	203	-	-	0/0/0/0	0/0/0/0
4	SO4	F	204	-	-	0/0/0/0	0/0/0/0
4	SO4	F	205	-	-	0/0/0/0	0/0/0/0
4	SO4	F	206	-	-	0/0/0/0	0/0/0/0
3	CYC	G	201[A]	-	-	2/21/74/74	0/4/4/4
3	CYC	G	201[B]	-	-	2/21/74/74	0/4/4/4
4	SO4	G	202	-	-	0/0/0/0	0/0/0/0
4	SO4	G	203	-	-	0/0/0/0	0/0/0/0
3	CYC	H	201	2	-	2/21/74/74	0/4/4/4
4	SO4	H	202	-	-	0/0/0/0	0/0/0/0
4	SO4	H	203	-	-	0/0/0/0	0/0/0/0
4	SO4	H	204	-	-	0/0/0/0	0/0/0/0
4	SO4	H	205	-	-	0/0/0/0	0/0/0/0
4	SO4	H	206	-	-	0/0/0/0	0/0/0/0
3	CYC	I	201[A]	-	-	2/21/74/74	0/4/4/4
3	CYC	I	201[B]	-	-	2/21/74/74	0/4/4/4
4	SO4	I	202	-	-	0/0/0/0	0/0/0/0
4	SO4	I	203	-	-	0/0/0/0	0/0/0/0
3	CYC	J	201	2	-	2/21/74/74	0/4/4/4
4	SO4	J	202	-	-	0/0/0/0	0/0/0/0
4	SO4	J	203	-	-	0/0/0/0	0/0/0/0
4	SO4	J	204	-	-	0/0/0/0	0/0/0/0
4	SO4	J	205	-	-	0/0/0/0	0/0/0/0
4	SO4	J	206	-	-	0/0/0/0	0/0/0/0
3	CYC	K	201[A]	-	-	2/21/74/74	0/4/4/4
3	CYC	K	201[B]	-	-	2/21/74/74	0/4/4/4
4	SO4	K	202	-	-	0/0/0/0	0/0/0/0
4	SO4	K	203	-	-	0/0/0/0	0/0/0/0
3	CYC	L	201	2	-	2/21/74/74	0/4/4/4
4	SO4	L	202	-	-	0/0/0/0	0/0/0/0
4	SO4	L	203	-	-	0/0/0/0	0/0/0/0
4	SO4	L	204	-	-	0/0/0/0	0/0/0/0
4	SO4	L	205	-	-	0/0/0/0	0/0/0/0
4	SO4	L	206	-	-	0/0/0/0	0/0/0/0

The worst 5 of 214 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	CYC	C2C-C1C	-19.52	1.33	1.52
3	J	201	CYC	C2C-C1C	-19.52	1.33	1.52
3	H	201	CYC	C2C-C1C	-19.40	1.33	1.52
3	B	201	CYC	C2C-C1C	-19.36	1.34	1.52
3	F	201	CYC	C2C-C1C	-19.12	1.34	1.52

The worst 5 of 312 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	201[B]	CYC	CHB-C4A-NA	-4.12	117.20	124.89
3	I	201[A]	CYC	CHB-C4A-NA	-4.12	117.20	124.89
3	C	201[A]	CYC	CHB-C4A-NA	-4.08	117.26	124.89
3	C	201[B]	CYC	CHB-C4A-NA	-4.08	117.26	124.89
3	E	201[B]	CYC	CHB-C4A-NA	-3.99	117.44	124.89

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	201	CYC	C1B-CHB-C4A-C3A
3	F	201	CYC	C1B-CHB-C4A-C3A
3	D	201	CYC	C1B-CHB-C4A-C3A
3	J	201	CYC	C1B-CHB-C4A-C3A
3	H	201	CYC	C1B-CHB-C4A-C3A

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201[B]	CYC	1	0
3	B	201	CYC	3	0
3	C	201[B]	CYC	1	0
3	D	201	CYC	5	0
3	E	201[B]	CYC	1	0
3	F	201	CYC	3	0
3	G	201[B]	CYC	1	0
3	H	201	CYC	3	0
3	I	201[B]	CYC	1	0
3	J	201	CYC	4	0
3	K	201[B]	CYC	1	0
3	L	201	CYC	3	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.