



# wwPDB X-ray Structure Validation Summary Report

Jun 17, 2014 – 07:02 AM BST

PDB ID : 4V9G  
Title : RC-LH1-PufX dimer complex from Rhodobacter sphaeroides  
Authors : Qian, P.; Papiz, M.Z.; Jackson, P.J.; Brindley, A.A.; Ng, I.W.; Olsen, J.D.;  
Dickman, M.J.; Bullough, P.A.; Hunter, C.N.  
Deposited on : 2013-02-21  
Resolution : 7.78 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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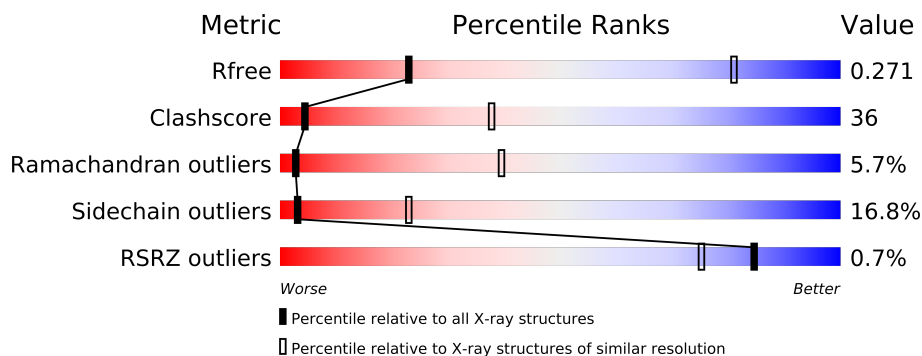
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23397
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 7.78 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))
$R_{free}$	66092	1106 (11.50-3.50)
Clashscore	79885	1006 (11.50-3.54)
Ramachandran outliers	78287	1301 (11.50-3.50)
Sidechain outliers	78261	1275 (11.50-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A1	58	
1	A2	58	
1	A3	58	
1	A5	58	
1	A7	58	
1	AD	58	
1	AF	58	
1	AJ	58	
1	AN	58	
1	AP	58	
1	AT	58	
1	AV	58	
1	AX	58	
1	AZ	58	

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Mol	Chain	Length	Quality of chain
1	B1	58	
1	B2	58	
1	B3	58	
1	B5	58	
1	B7	58	
1	BD	58	
1	BF	58	
1	BJ	58	
1	BN	58	
1	BP	58	
1	BT	58	
1	BV	58	
1	BX	58	
1	BZ	58	
2	AB	82	
2	BB	82	
3	A4	49	
3	A6	49	
3	A8	49	
3	A9	49	
3	AE	49	
3	AG	49	
3	AI	49	
3	AK	49	
3	AO	49	
3	AQ	49	
3	AS	49	
3	AU	49	
3	AW	49	
3	AY	49	
3	B4	49	
3	B6	49	
3	B8	49	
3	B9	49	
3	BE	49	
3	BG	49	
3	BI	49	
3	BK	49	
3	BO	49	
3	BQ	49	
3	BS	49	
3	BU	49	

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Mol	Chain	Length	Quality of chain
3	BW	49	
3	BY	49	
4	AH	260	
4	BH	260	
5	AL	282	
5	BL	282	
6	AM	308	
6	BM	308	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	BCL	B5	101	-	X
7	BCL	BL	303	-	X
7	BCL	BO	101	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 38108 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A5	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AT	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AV	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AX	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A3	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A7	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AD	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AF	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A1	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AJ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A2	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AN	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AP	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AZ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B5	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BT	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BV	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BX	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B3	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B7	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BD	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BF	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B1	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BJ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B2	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BN	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BP	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BZ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			

- Molecule 2 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	57	Total	C	N	O	S	0	0	0
			452	299	79	71	3			
2	BB	57	Total	C	N	O	S	0	0	0
			452	299	79	71	3			

- Molecule 3 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A9	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AO	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AQ	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	A6	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	AU	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	AW	48	Total 387	C 256	N 60	O 70	S 1	0	0	0
3	AY	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	A4	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	A8	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	AE	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	AG	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	AI	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	AK	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	BS	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	B9	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	BO	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	BQ	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	B6	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	BU	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	BW	48	Total 387	C 256	N 60	O 70	S 1	0	0	0
3	BY	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	B4	48	Total 388	C 256	N 61	O 70	S 1	0	0	0
3	B8	48	Total 388	C 256	N 61	O 70	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	BE	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BG	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BI	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BK	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AH	250	Total	C	N	O	S	0	0	0
			1901	1216	324	351	10			
4	BH	250	Total	C	N	O	S	0	0	0
			1901	1216	324	351	10			

- Molecule 5 is a protein called Reaction center protein L chain.

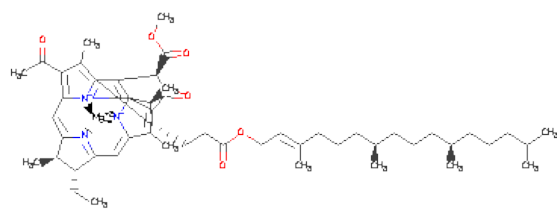
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AL	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
5	BL	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AM	304	Total	C	N	O	S	0	1	0
			2427	1619	398	399	11			
6	BM	304	Total	C	N	O	S	0	1	0
			2427	1619	398	399	11			

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AT	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AT	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AV	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A3	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A7	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AD	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AD	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AF	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A1	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AJ	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AN	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AP	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AP	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AZ	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AS	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A9	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AO	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A6	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A6	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AW	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AY	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AY	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A4	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A8	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AG	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AI	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AK	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	B5	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BT	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BV	1	Total 46	C 35	Mg 1	N 4	O 6	0	0

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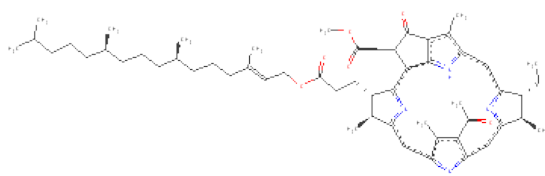
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7	B3	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B7	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BD	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BD	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BF	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BF	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B1	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B2	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BP	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BP	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BZ	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BZ	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B9	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BO	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BO	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B6	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BU	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BY	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BY	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B4	1	Total 46	C 35	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B8	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BI	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



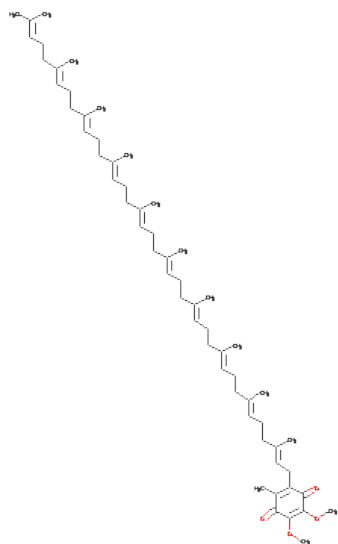
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	AL	1	Total	C	N	O		0	0
			65	55	4	6			
8	AM	1	Total	C	N	O		0	0
			65	55	4	6			
8	BL	1	Total	C	N	O		0	0
			65	55	4	6			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	BM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	AL	1	Total	C	O		0	0
			48	44	4			
9	AM	1	Total	C	O		0	0
			48	44	4			
9	BL	1	Total	C	O		0	0
			48	44	4			

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

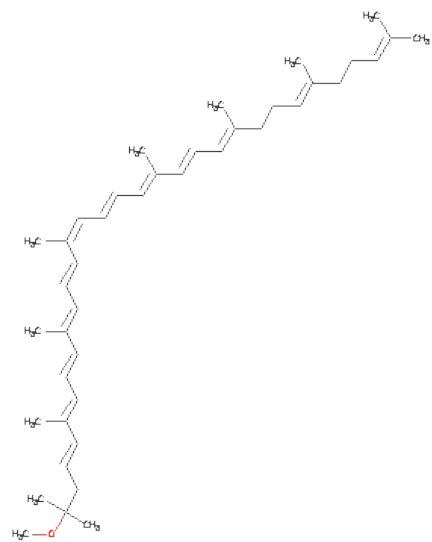


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AL	1	Total	O	P	0	0
			5	4	1		
10	BL	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	BL	1	Total	Fe	0	0
			1	1		
11	AM	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	AM	1	Total	C	O	0	0
			42	41	1		

### 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 errors 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.

- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A5: 



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AT: 



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AV: 



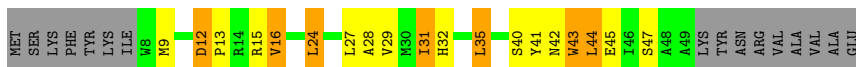
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AX: 



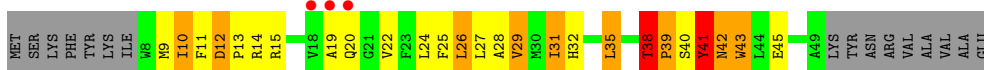
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A3: 



- Molecule 1: Light-harvesting protein B-875 alpha chain

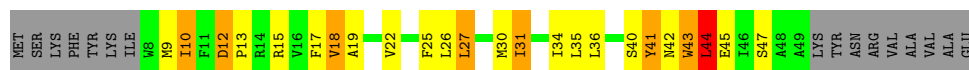
Chain A7: 



- Molecule 1: Light-harvesting protein B-875 alpha chain

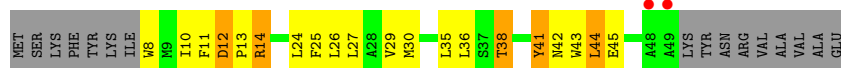


Chain AD:



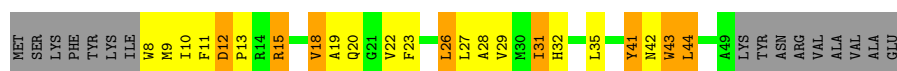
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AF:



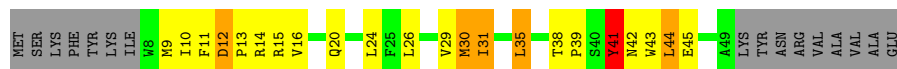
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A1:



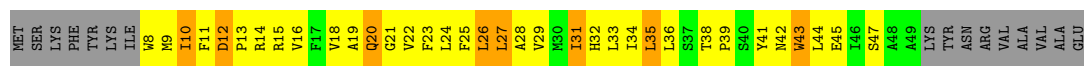
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AJ:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A2:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AN:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AP:



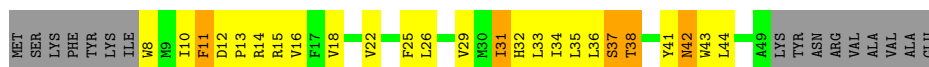
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AZ:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B5:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BT:



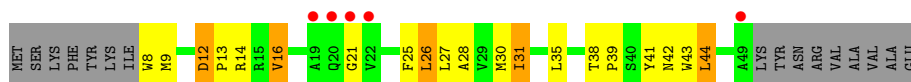
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BV:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BX:



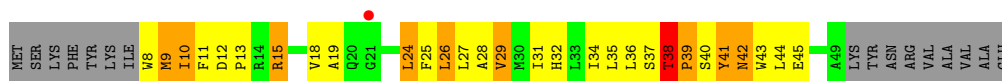
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B3:



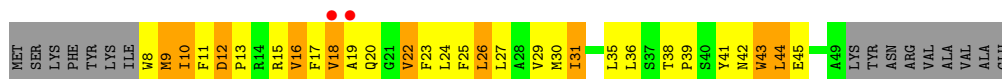
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B7:



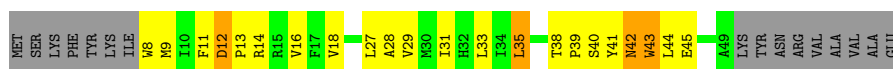
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BD:



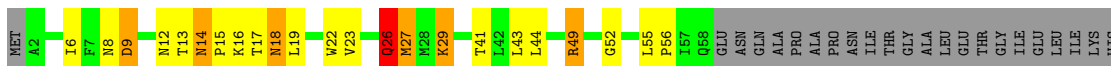
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain BF:



- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain B1:



LEU  
VAL

- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AS:



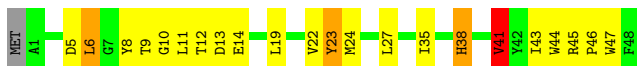
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A9:



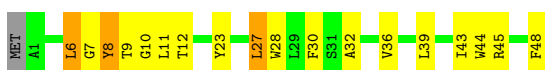
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AO:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AQ:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A6:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AU:



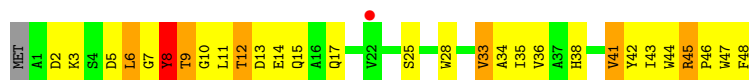
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AW:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AY:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A4:



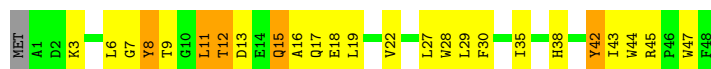
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A8:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AE:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AG:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AI:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AK:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BS:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain B9:



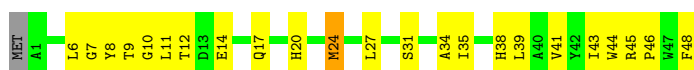
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BO:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BQ:



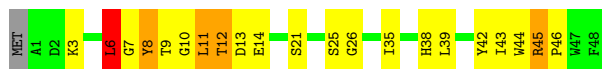
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain B6:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BU:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BW:



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BY:



- Molecule 3: Light-harvesting protein B-875 beta chain

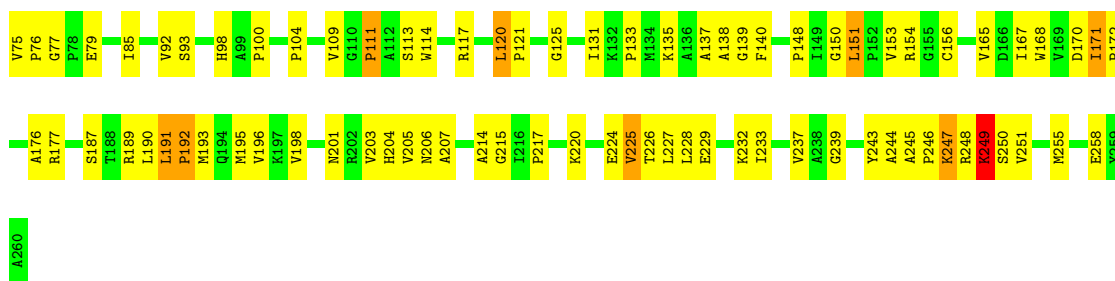
Chain B4:



- Molecule 3: Light-harvesting protein B-875 beta chain

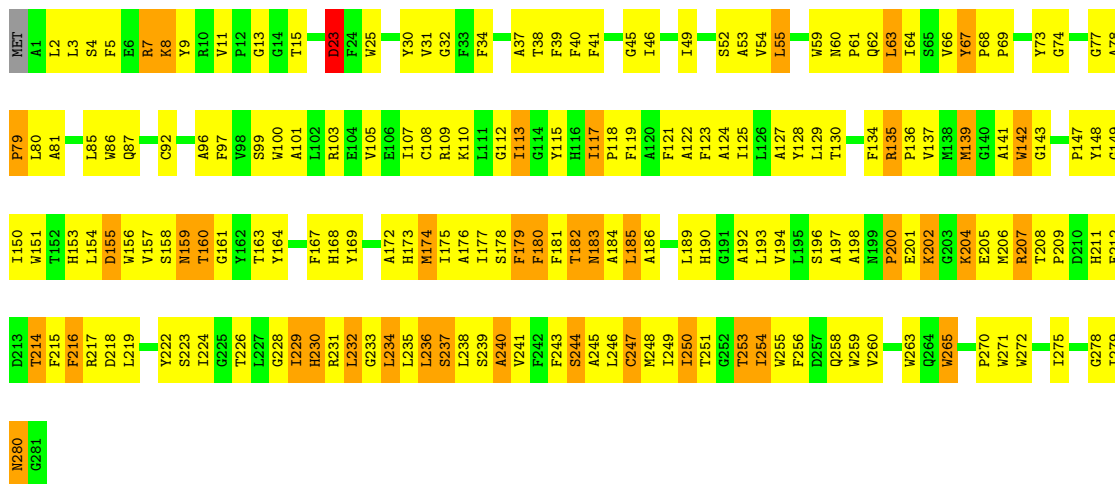
Chain B8:





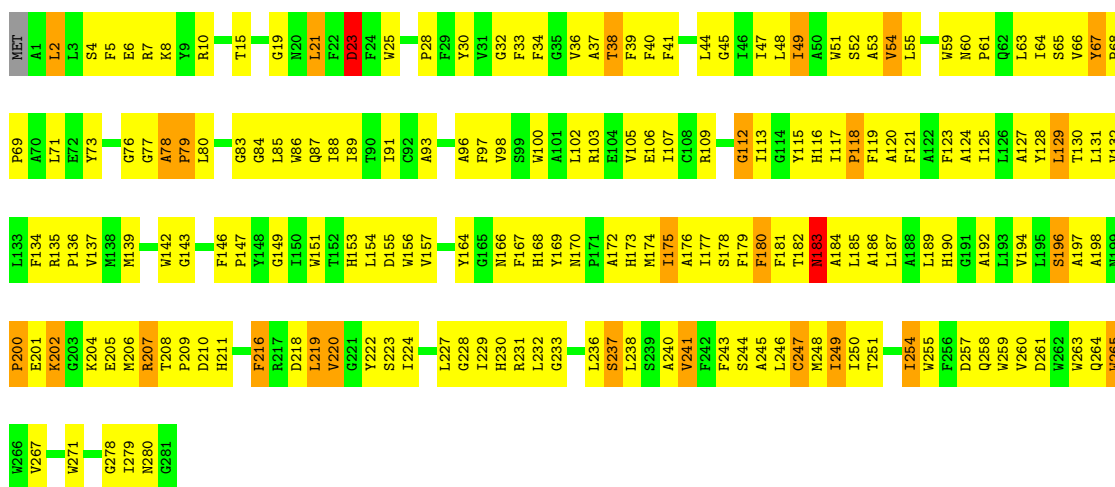
• Molecule 5: Reaction center protein L chain

Chain AL:



• Molecule 5: Reaction center protein L chain

Chain BL:

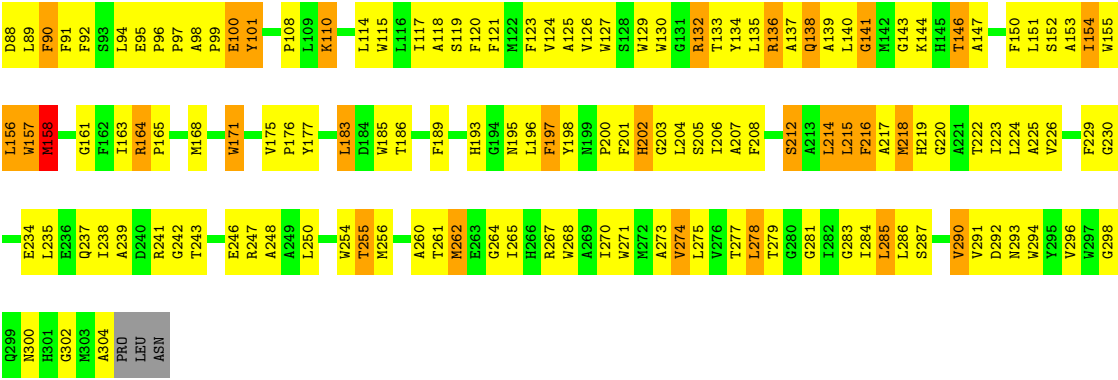


• Molecule 6: Reaction center protein M chain

Chain AM:

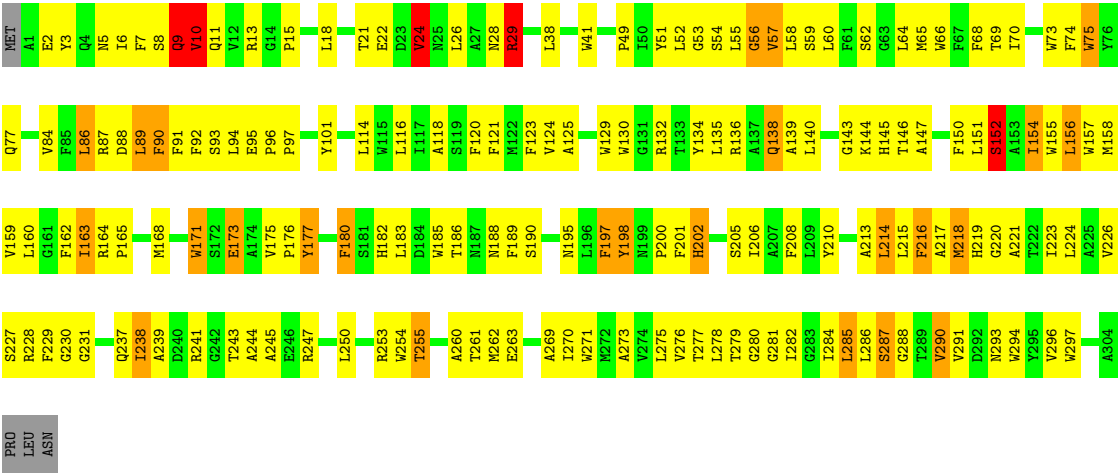






• Molecule 6: Reaction center protein M chain

Chain BM:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.08Å 415.07Å 129.82Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	20.39 – 7.78 20.07 – 8.00	Depositor EDS
% Data completeness (in resolution range)	73.7 (20.39-7.78) 73.6 (20.07-8.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 7.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.228 , 0.258 0.243 , 0.271	Depositor DCC
$R_{free}$ test set	319 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	430.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.09 , 308.6	EDS
Estimated twinning fraction	0.883 for H, K, L 0.117 for -H, -K, H+L 0.178 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.883 for H, K, L 0.117 for -H, -K, H+L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 6309 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	38108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	258.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, PO4, FE2, SPO, U10

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	A1	0.23	0/356	0.31	0/486
1	A2	0.24	0/356	0.31	0/486
1	A3	0.26	0/356	0.31	0/486
1	A5	0.25	0/356	0.31	0/486
1	A7	0.25	0/356	0.31	0/486
1	AD	0.25	0/356	0.31	0/486
1	AF	0.24	0/356	0.31	0/486
1	AJ	0.24	0/356	0.31	0/486
1	AN	0.25	0/356	0.31	0/486
1	AP	0.24	0/356	0.31	0/486
1	AT	0.26	0/356	0.31	0/486
1	AV	0.24	0/356	0.31	0/486
1	AX	0.25	0/356	0.31	0/486
1	AZ	0.26	0/356	0.31	0/486
1	B1	0.24	0/356	0.31	0/486
1	B2	0.25	0/356	0.31	0/486
1	B3	0.24	0/356	0.31	0/486
1	B5	0.24	0/356	0.31	0/486
1	B7	0.25	0/356	0.31	0/486
1	BD	0.26	0/356	0.31	0/486
1	BF	0.25	0/356	0.31	0/486
1	BJ	0.25	0/356	0.31	0/486
1	BN	0.24	0/356	0.31	0/486
1	BP	0.25	0/356	0.31	0/486
1	BT	0.24	0/356	0.31	0/486
1	BV	0.24	0/356	0.31	0/486
1	BX	0.26	0/356	0.31	0/486
1	BZ	0.25	0/356	0.31	0/486
2	AB	0.24	0/464	0.32	0/626
2	BB	0.24	0/464	0.32	0/626
3	A4	0.22	0/401	0.29	0/547
3	A6	0.22	0/401	0.29	0/547

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	A8	0.22	0/401	0.29	0/547
3	A9	0.22	0/401	0.29	0/547
3	AE	0.23	0/401	0.29	0/547
3	AG	0.22	0/401	0.29	0/547
3	AI	0.22	0/401	0.29	0/547
3	AK	0.22	0/401	0.29	0/547
3	AO	0.22	0/401	0.29	0/547
3	AQ	0.23	0/401	0.29	0/547
3	AS	0.24	0/401	0.29	0/547
3	AU	0.22	0/401	0.29	0/547
3	AW	0.21	0/400	0.29	0/545
3	AY	0.22	0/401	0.29	0/547
3	B4	0.23	0/401	0.29	0/547
3	B6	0.22	0/401	0.29	0/547
3	B8	0.21	0/401	0.29	0/547
3	B9	0.22	0/401	0.29	0/547
3	BE	0.23	0/401	0.29	0/547
3	BG	0.22	0/401	0.29	0/547
3	BI	0.22	0/401	0.29	0/547
3	BK	0.23	0/401	0.29	0/547
3	BO	0.22	0/401	0.29	0/547
3	BQ	0.24	0/401	0.29	0/547
3	BS	0.24	0/401	0.29	0/547
3	BU	0.22	0/401	0.29	0/547
3	BW	0.20	0/400	0.29	0/545
3	BY	0.22	0/401	0.29	0/547
4	AH	0.21	0/1950	0.34	0/2652
4	BH	0.21	0/1950	0.34	0/2652
5	AL	0.59	8/2320 (0.3%)	0.36	0/3175
5	BL	0.71	10/2320 (0.4%)	0.37	0/3175
6	AM	0.48	5/2524 (0.2%)	0.32	0/3445
6	BM	0.53	1/2524 (0.0%)	0.31	0/3445
All	All	0.36	24/35710 (0.1%)	0.32	0/48716

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	A7	0	1
1	AZ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B1	0	1
1	B7	0	1
3	AQ	0	1
3	AS	0	2
3	BS	0	2
4	BH	0	1
5	AL	0	3
6	AM	0	3
6	BM	0	1
All	All	0	17

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BM	152	SER	CB-OG	22.34	1.71	1.42
5	BL	196	SER	CB-OG	17.38	1.64	1.42
6	AM	212	SER	CB-OG	12.58	1.58	1.42
5	AL	212	GLU	CD-OE1	11.48	1.38	1.25
5	BL	247	CYS	CB-SG	11.36	2.01	1.82

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A7	38	THR	Peptide
3	AQ	27	LEU	Peptide
3	AS	11	LEU	Peptide
3	AS	12	THR	Peptide
1	AZ	38	THR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	345	0	355	25	0
1	A2	345	0	355	38	0
1	A3	345	0	355	22	0
1	A5	345	0	355	26	0
1	A7	345	0	355	33	0
1	AD	345	0	355	30	0
1	AF	345	0	355	19	0
1	AJ	345	0	355	21	0
1	AN	345	0	355	25	0
1	AP	345	0	355	25	0
1	AT	345	0	355	21	0
1	AV	345	0	355	15	0
1	AX	345	0	355	15	0
1	AZ	345	0	355	26	0
1	B1	345	0	355	27	0
1	B2	345	0	355	23	0
1	B3	345	0	355	15	0
1	B5	345	0	355	21	0
1	B7	345	0	355	39	0
1	BD	345	0	355	34	0
1	BF	345	0	355	25	0
1	BJ	345	0	355	23	0
1	BN	345	0	355	23	0
1	BP	345	0	355	27	0
1	BT	345	0	355	16	0
1	BV	345	0	355	14	0
1	BX	345	0	355	15	0
1	BZ	345	0	355	35	0
2	AB	452	0	462	19	0
2	BB	452	0	462	20	0
3	A4	388	0	370	31	0
3	A6	388	0	370	23	0
3	A8	388	0	370	18	0
3	A9	388	0	370	24	0
3	AE	388	0	370	32	0
3	AG	388	0	370	22	0
3	AI	388	0	370	29	0
3	AK	388	0	370	22	0
3	AO	388	0	370	22	0
3	AQ	388	0	370	18	0
3	AS	388	0	370	31	0
3	AU	388	0	370	24	0
3	AW	387	0	363	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AY	388	0	370	22	0
3	B4	388	0	370	16	0
3	B6	388	0	370	27	0
3	B8	388	0	370	18	0
3	B9	388	0	370	19	0
3	BE	388	0	370	38	0
3	BG	388	0	370	12	0
3	BI	388	0	370	26	0
3	BK	388	0	370	21	0
3	BO	388	0	370	23	0
3	BQ	388	0	370	27	0
3	BS	388	0	370	35	0
3	BU	388	0	370	19	0
3	BW	387	0	363	23	0
3	BY	388	0	370	13	0
4	AH	1901	0	1909	120	0
4	BH	1901	0	1909	109	0
5	AL	2232	0	2187	258	0
5	BL	2232	0	2187	284	0
6	AM	2427	0	2338	241	0
6	BM	2427	0	2338	220	0
7	A1	46	0	35	2	0
7	A2	46	0	35	3	0
7	A3	46	0	35	6	0
7	A4	46	0	35	6	0
7	A6	92	0	70	14	0
7	A7	46	0	35	9	0
7	A8	46	0	35	9	0
7	A9	46	0	35	11	0
7	AD	92	0	70	21	0
7	AF	46	0	35	12	0
7	AG	46	0	35	2	0
7	AI	46	0	35	11	0
7	AJ	46	0	35	8	0
7	AK	46	0	35	6	0
7	AL	132	0	148	55	0
7	AM	132	0	148	50	0
7	AN	46	0	35	4	0
7	AO	46	0	35	16	0
7	AP	92	0	70	21	0
7	AS	46	0	35	15	0
7	AT	92	0	70	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AV	46	0	35	6	0
7	AW	46	0	35	1	0
7	AY	92	0	70	7	0
7	AZ	46	0	35	12	0
7	B1	46	0	35	2	0
7	B2	46	0	35	9	0
7	B3	46	0	35	7	0
7	B4	46	0	35	3	0
7	B5	46	0	35	1	0
7	B6	46	0	35	5	0
7	B7	46	0	35	3	0
7	B8	46	0	35	11	0
7	B9	46	0	35	7	0
7	BD	92	0	70	14	0
7	BF	92	0	70	13	0
7	BI	46	0	35	12	0
7	BK	92	0	70	18	0
7	BL	198	0	222	87	0
7	BM	66	0	74	27	0
7	BO	92	0	70	25	0
7	BP	92	0	70	28	0
7	BT	46	0	35	7	0
7	BU	46	0	35	6	0
7	BV	92	0	70	12	0
7	BY	92	0	70	8	0
7	BZ	92	0	70	29	0
8	AL	65	0	76	27	0
8	AM	65	0	76	18	0
8	BL	65	0	76	45	0
8	BM	65	0	76	26	0
9	AL	48	0	63	21	0
9	AM	48	0	63	12	0
9	BL	48	0	63	20	0
10	AL	5	0	0	0	0
10	BL	5	0	0	0	0
11	AM	1	0	0	0	0
11	BL	1	0	0	0	0
12	AM	42	0	60	9	0
All	All	38108	0	37183	2683	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.



The worst 5 of 2683 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:BS:12:THR:CB	3:BS:13:ASP:HB2	1.15	1.62
5:BL:219:LEU:CG	5:BL:219:LEU:CD2	1.78	1.62
5:BL:219:LEU:CG	5:BL:219:LEU:CD1	1.75	1.58
6:AM:262:MET:CG	6:AM:262:MET:CB	1.75	1.57
5:BL:125:ILE:CG1	5:BL:125:ILE:CD1	1.75	1.57

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	A1	40/58 (69%)	29 (72%)	8 (20%)	3 (8%)	2	30
1	A2	40/58 (69%)	27 (68%)	7 (18%)	6 (15%)	0	9
1	A3	40/58 (69%)	24 (60%)	13 (32%)	3 (8%)	2	30
1	A5	40/58 (69%)	23 (58%)	12 (30%)	5 (12%)	1	14
1	A7	40/58 (69%)	23 (58%)	11 (28%)	6 (15%)	0	9
1	AD	40/58 (69%)	22 (55%)	13 (32%)	5 (12%)	1	14
1	AF	40/58 (69%)	26 (65%)	12 (30%)	2 (5%)	3	43
1	AJ	40/58 (69%)	29 (72%)	7 (18%)	4 (10%)	1	20
1	AN	40/58 (69%)	29 (72%)	6 (15%)	5 (12%)	1	14
1	AP	40/58 (69%)	28 (70%)	10 (25%)	2 (5%)	3	43
1	AT	40/58 (69%)	26 (65%)	9 (22%)	5 (12%)	1	14
1	AV	40/58 (69%)	28 (70%)	11 (28%)	1 (2%)	9	61
1	AX	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1	20
1	AZ	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1	20
1	B1	40/58 (69%)	28 (70%)	8 (20%)	4 (10%)	1	20
1	B2	40/58 (69%)	30 (75%)	7 (18%)	3 (8%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B3	40/58 (69%)	27 (68%)	12 (30%)	1 (2%)	9	61
1	B5	40/58 (69%)	24 (60%)	12 (30%)	4 (10%)	1	20
1	B7	40/58 (69%)	23 (58%)	12 (30%)	5 (12%)	1	14
1	BD	40/58 (69%)	26 (65%)	11 (28%)	3 (8%)	2	30
1	BF	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1	20
1	BJ	40/58 (69%)	27 (68%)	10 (25%)	3 (8%)	2	30
1	BN	40/58 (69%)	31 (78%)	8 (20%)	1 (2%)	9	61
1	BP	40/58 (69%)	26 (65%)	11 (28%)	3 (8%)	2	30
1	BT	40/58 (69%)	25 (62%)	13 (32%)	2 (5%)	3	43
1	BV	40/58 (69%)	29 (72%)	9 (22%)	2 (5%)	3	43
1	BX	40/58 (69%)	28 (70%)	11 (28%)	1 (2%)	9	61
1	BZ	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	1	20
2	AB	55/82 (67%)	24 (44%)	24 (44%)	7 (13%)	0	14
2	BB	55/82 (67%)	28 (51%)	22 (40%)	5 (9%)	1	25
3	A4	46/49 (94%)	30 (65%)	13 (28%)	3 (6%)	2	35
3	A6	46/49 (94%)	36 (78%)	9 (20%)	1 (2%)	10	64
3	A8	46/49 (94%)	30 (65%)	14 (30%)	2 (4%)	4	47
3	A9	46/49 (94%)	35 (76%)	8 (17%)	3 (6%)	2	35
3	AE	46/49 (94%)	34 (74%)	10 (22%)	2 (4%)	4	47
3	AG	46/49 (94%)	29 (63%)	16 (35%)	1 (2%)	10	64
3	AI	46/49 (94%)	34 (74%)	11 (24%)	1 (2%)	10	64
3	AK	46/49 (94%)	33 (72%)	10 (22%)	3 (6%)	2	35
3	AO	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	10	64
3	AQ	46/49 (94%)	40 (87%)	5 (11%)	1 (2%)	10	64
3	AS	46/49 (94%)	32 (70%)	12 (26%)	2 (4%)	4	47
3	AU	46/49 (94%)	31 (67%)	10 (22%)	5 (11%)	1	17
3	AW	46/49 (94%)	33 (72%)	11 (24%)	2 (4%)	4	47
3	AY	46/49 (94%)	31 (67%)	13 (28%)	2 (4%)	4	47
3	B4	46/49 (94%)	27 (59%)	14 (30%)	5 (11%)	1	17
3	B6	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	10	64
3	B8	46/49 (94%)	30 (65%)	14 (30%)	2 (4%)	4	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B9	46/49 (94%)	35 (76%)	8 (17%)	3 (6%)	2	35
3	BE	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	10	64
3	BG	46/49 (94%)	31 (67%)	15 (33%)	0	100	100
3	BI	46/49 (94%)	35 (76%)	11 (24%)	0	100	100
3	BK	46/49 (94%)	29 (63%)	15 (33%)	2 (4%)	4	47
3	BO	46/49 (94%)	33 (72%)	10 (22%)	3 (6%)	2	35
3	BQ	46/49 (94%)	38 (83%)	8 (17%)	0	100	100
3	BS	46/49 (94%)	31 (67%)	12 (26%)	3 (6%)	2	35
3	BU	46/49 (94%)	29 (63%)	13 (28%)	4 (9%)	1	25
3	BW	46/49 (94%)	32 (70%)	12 (26%)	2 (4%)	4	47
3	BY	46/49 (94%)	33 (72%)	11 (24%)	2 (4%)	4	47
4	AH	248/260 (95%)	178 (72%)	59 (24%)	11 (4%)	4	47
4	BH	248/260 (95%)	198 (80%)	43 (17%)	7 (3%)	8	59
5	AL	279/282 (99%)	203 (73%)	61 (22%)	15 (5%)	3	41
5	BL	279/282 (99%)	208 (75%)	61 (22%)	10 (4%)	5	53
6	AM	303/308 (98%)	223 (74%)	63 (21%)	17 (6%)	3	40
6	BM	303/308 (98%)	232 (77%)	56 (18%)	15 (5%)	3	43
All	All	4178/4860 (86%)	2942 (70%)	997 (24%)	239 (6%)	3	39

5 of 239 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A5	38	THR
1	A7	39	PRO
1	A7	41	TYR
1	AD	10	ILE
1	A1	12	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	A1	37/51 (72%)	31 (84%)	6 (16%)	3	25
1	A2	37/51 (72%)	31 (84%)	6 (16%)	3	25
1	A3	37/51 (72%)	29 (78%)	8 (22%)	1	11
1	A5	37/51 (72%)	33 (89%)	4 (11%)	9	46
1	A7	37/51 (72%)	27 (73%)	10 (27%)	1	6
1	AD	37/51 (72%)	32 (86%)	5 (14%)	6	34
1	AF	37/51 (72%)	32 (86%)	5 (14%)	6	34
1	AJ	37/51 (72%)	28 (76%)	9 (24%)	1	8
1	AN	37/51 (72%)	33 (89%)	4 (11%)	9	46
1	AP	37/51 (72%)	30 (81%)	7 (19%)	2	16
1	AT	37/51 (72%)	33 (89%)	4 (11%)	9	46
1	AV	37/51 (72%)	29 (78%)	8 (22%)	1	11
1	AX	37/51 (72%)	26 (70%)	11 (30%)	0	5
1	AZ	37/51 (72%)	27 (73%)	10 (27%)	1	6
1	B1	37/51 (72%)	29 (78%)	8 (22%)	1	11
1	B2	37/51 (72%)	33 (89%)	4 (11%)	9	46
1	B3	37/51 (72%)	27 (73%)	10 (27%)	1	6
1	B5	37/51 (72%)	31 (84%)	6 (16%)	3	25
1	B7	37/51 (72%)	28 (76%)	9 (24%)	1	8
1	BD	37/51 (72%)	26 (70%)	11 (30%)	0	5
1	BF	37/51 (72%)	33 (89%)	4 (11%)	9	46
1	BJ	37/51 (72%)	29 (78%)	8 (22%)	1	11
1	BN	37/51 (72%)	31 (84%)	6 (16%)	3	25
1	BP	37/51 (72%)	27 (73%)	10 (27%)	1	6
1	BT	37/51 (72%)	30 (81%)	7 (19%)	2	16
1	BV	37/51 (72%)	30 (81%)	7 (19%)	2	16
1	BX	37/51 (72%)	29 (78%)	8 (22%)	1	11
1	BZ	37/51 (72%)	28 (76%)	9 (24%)	1	8
2	AB	46/66 (70%)	34 (74%)	12 (26%)	1	7
2	BB	46/66 (70%)	35 (76%)	11 (24%)	1	8
3	A4	39/40 (98%)	29 (74%)	10 (26%)	1	7
3	A6	39/40 (98%)	34 (87%)	5 (13%)	6	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A8	39/40 (98%)	33 (85%)	6 (15%)	4	28
3	A9	39/40 (98%)	33 (85%)	6 (15%)	4	28
3	AE	39/40 (98%)	32 (82%)	7 (18%)	2	19
3	AG	39/40 (98%)	31 (80%)	8 (20%)	2	13
3	AI	39/40 (98%)	34 (87%)	5 (13%)	6	37
3	AK	39/40 (98%)	35 (90%)	4 (10%)	10	48
3	AO	39/40 (98%)	31 (80%)	8 (20%)	2	13
3	AQ	39/40 (98%)	36 (92%)	3 (8%)	18	64
3	AS	39/40 (98%)	34 (87%)	5 (13%)	6	37
3	AU	39/40 (98%)	34 (87%)	5 (13%)	6	37
3	AW	39/40 (98%)	35 (90%)	4 (10%)	10	48
3	AY	39/40 (98%)	26 (67%)	13 (33%)	0	3
3	B4	39/40 (98%)	35 (90%)	4 (10%)	10	48
3	B6	39/40 (98%)	32 (82%)	7 (18%)	2	19
3	B8	39/40 (98%)	35 (90%)	4 (10%)	10	48
3	B9	39/40 (98%)	36 (92%)	3 (8%)	18	64
3	BE	39/40 (98%)	32 (82%)	7 (18%)	2	19
3	BG	39/40 (98%)	32 (82%)	7 (18%)	2	19
3	BI	39/40 (98%)	37 (95%)	2 (5%)	33	78
3	BK	39/40 (98%)	33 (85%)	6 (15%)	4	28
3	BO	39/40 (98%)	33 (85%)	6 (15%)	4	28
3	BQ	39/40 (98%)	36 (92%)	3 (8%)	18	64
3	BS	39/40 (98%)	31 (80%)	8 (20%)	2	13
3	BU	39/40 (98%)	36 (92%)	3 (8%)	18	64
3	BW	39/40 (98%)	36 (92%)	3 (8%)	18	64
3	BY	39/40 (98%)	32 (82%)	7 (18%)	2	19
4	AH	201/208 (97%)	166 (83%)	35 (17%)	3	20
4	BH	201/208 (97%)	176 (88%)	25 (12%)	7	39
5	AL	220/221 (100%)	183 (83%)	37 (17%)	3	23
5	BL	220/221 (100%)	183 (83%)	37 (17%)	3	23
6	AM	238/241 (99%)	203 (85%)	35 (15%)	4	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BM	238/241 (99%)	199 (84%)	39 (16%)	3	24
All	All	3538/4020 (88%)	2944 (83%)	594 (17%)	3	23

5 of 594 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	AL	271	TRP
1	BX	44	LEU
5	BL	249	ILE
6	AM	75	TRP
6	AM	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
5	AL	173	HIS
1	B5	32	HIS
6	BM	9	GLN
5	AL	183	ASN
6	AM	4	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 76 ligands modelled in this entry, 2 are monoatomic - leaving 74 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
7	BCL	A1	101	-	52,54,74	2.34	16 (30%)	71,91,115	2.25	20 (28%)
7	BCL	A2	101	-	52,54,74	2.19	12 (23%)	71,91,115	2.27	19 (26%)
7	BCL	A3	101	-	52,54,74	2.32	16 (30%)	71,91,115	2.24	19 (26%)
7	BCL	A4	101	-	52,54,74	2.33	14 (26%)	71,91,115	2.26	20 (28%)
7	BCL	A6	101	-	52,54,74	2.18	12 (23%)	71,91,115	2.27	18 (25%)
7	BCL	A6	102	-	52,54,74	2.32	18 (34%)	71,91,115	2.29	20 (28%)
7	BCL	A7	101	-	52,54,74	2.16	11 (21%)	71,91,115	2.26	18 (25%)
7	BCL	A8	101	-	52,54,74	2.15	11 (21%)	71,91,115	2.26	18 (25%)
7	BCL	A9	101	-	52,54,74	2.31	14 (26%)	71,91,115	2.26	20 (28%)
7	BCL	AD	101	-	52,54,74	2.23	13 (25%)	71,91,115	2.17	21 (29%)
7	BCL	AD	102	-	52,54,74	2.27	12 (23%)	71,91,115	2.27	20 (28%)
7	BCL	AF	101	-	52,54,74	2.14	11 (21%)	71,91,115	2.28	19 (26%)
7	BCL	AG	101	-	52,54,74	2.32	15 (28%)	71,91,115	2.28	20 (28%)
7	BCL	AI	101	-	52,54,74	2.29	16 (30%)	71,91,115	2.28	20 (28%)
7	BCL	AJ	101	-	52,54,74	2.31	15 (28%)	71,91,115	2.27	20 (28%)
7	BCL	AK	101	-	52,54,74	2.22	13 (25%)	71,91,115	2.16	20 (28%)
7	BCL	AL	301	-	74,74,74	1.87	13 (17%)	98,115,115	2.00	23 (23%)
7	BCL	AL	302	-	74,74,74	2.00	15 (20%)	98,115,115	2.12	23 (23%)
8	BPH	AL	303	-	70,70,70	2.25	14 (20%)	94,101,101	1.84	15 (15%)
9	U10	AL	304	-	48,48,63	1.18	3 (6%)	59,61,79	1.77	14 (23%)
10	PO4	AL	305	-	4,4,4	0.32	0	6,6,6	0.29	0
7	BCL	AM	401	-	74,74,74	1.84	11 (14%)	98,115,115	2.03	22 (22%)
7	BCL	AM	402	-	74,74,74	2.01	15 (20%)	98,115,115	2.05	21 (21%)
8	BPH	AM	403	-	70,70,70	2.26	12 (17%)	94,101,101	1.83	14 (14%)
9	U10	AM	405	-	48,48,63	1.73	4 (8%)	59,61,79	1.92	15 (25%)
12	SPO	AM	406	-	41,41,41	1.30	2 (4%)	50,50,50	2.24	13 (26%)
7	BCL	AN	101	-	52,54,74	2.33	15 (28%)	71,91,115	2.23	18 (25%)
7	BCL	AO	101	-	52,54,74	2.26	13 (25%)	71,91,115	2.25	20 (28%)
7	BCL	AP	101	-	52,54,74	2.13	11 (21%)	71,91,115	2.28	19 (26%)
7	BCL	AP	102	-	52,54,74	2.31	17 (32%)	71,91,115	2.30	20 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCL	AS	101	-	52,54,74	2.28	14 (26%)	71,91,115	2.21	20 (28%)
7	BCL	AT	101	-	52,54,74	2.17	12 (23%)	71,91,115	2.28	18 (25%)
7	BCL	AT	102	-	52,54,74	2.33	18 (34%)	71,91,115	2.29	20 (28%)
7	BCL	AV	101	-	52,54,74	2.22	13 (25%)	71,91,115	2.17	20 (28%)
7	BCL	AW	101	-	52,54,74	2.19	12 (23%)	71,91,115	2.27	18 (25%)
7	BCL	AY	101	-	52,54,74	2.32	15 (28%)	71,91,115	2.24	20 (28%)
7	BCL	AY	102	-	52,54,74	2.32	17 (32%)	71,91,115	2.28	20 (28%)
7	BCL	AZ	101	-	52,54,74	2.30	14 (26%)	71,91,115	2.26	20 (28%)
7	BCL	B1	101	-	52,54,74	2.32	16 (30%)	71,91,115	2.24	20 (28%)
7	BCL	B2	101	-	52,54,74	2.19	13 (25%)	71,91,115	2.25	19 (26%)
7	BCL	B3	101	-	52,54,74	2.32	16 (30%)	71,91,115	2.24	19 (26%)
7	BCL	B4	101	-	52,54,74	2.33	14 (26%)	71,91,115	2.25	19 (26%)
7	BCL	B5	101	-	52,54,74	2.17	13 (25%)	71,91,115	2.29	18 (25%)
7	BCL	B6	101	-	52,54,74	2.31	18 (34%)	71,91,115	2.28	20 (28%)
7	BCL	B7	101	-	52,54,74	2.17	13 (25%)	71,91,115	2.30	18 (25%)
7	BCL	B8	101	-	52,54,74	2.15	11 (21%)	71,91,115	2.28	18 (25%)
7	BCL	B9	101	-	52,54,74	2.30	14 (26%)	71,91,115	2.25	20 (28%)
7	BCL	BD	101	-	52,54,74	2.25	13 (25%)	71,91,115	2.18	21 (29%)
7	BCL	BD	102	-	52,54,74	2.28	14 (26%)	71,91,115	2.28	20 (28%)
7	BCL	BF	101	-	52,54,74	2.15	12 (23%)	71,91,115	2.27	19 (26%)
7	BCL	BF	102	-	52,54,74	2.32	16 (30%)	71,91,115	2.28	20 (28%)
7	BCL	BI	101	-	52,54,74	2.31	16 (30%)	71,91,115	2.28	20 (28%)
7	BCL	BK	101	-	52,54,74	2.19	14 (26%)	71,91,115	2.18	19 (26%)
7	BCL	BK	102	-	52,54,74	2.32	14 (26%)	71,91,115	2.26	19 (26%)
7	BCL	BL	301	-	74,74,74	1.88	11 (14%)	98,115,115	2.02	22 (22%)
7	BCL	BL	302	-	74,74,74	1.95	13 (17%)	98,115,115	1.98	23 (23%)
7	BCL	BL	303	-	74,74,74	1.98	16 (21%)	98,115,115	2.07	23 (23%)
8	BPH	BL	304	-	70,70,70	2.26	14 (20%)	94,101,101	1.84	15 (15%)
9	U10	BL	306	-	48,48,63	1.24	4 (8%)	59,61,79	1.77	14 (23%)
10	PO4	BL	307	-	4,4,4	0.31	0	6,6,6	0.29	0
7	BCL	BM	401	-	74,74,74	2.29	18 (24%)	98,115,115	2.17	24 (24%)
8	BPH	BM	402	-	70,70,70	2.26	12 (17%)	94,101,101	1.83	14 (14%)
7	BCL	BO	101	-	52,54,74	2.32	15 (28%)	71,91,115	2.23	21 (29%)
7	BCL	BO	102	-	52,54,74	2.27	13 (25%)	71,91,115	2.25	20 (28%)
7	BCL	BP	101	-	52,54,74	2.14	11 (21%)	71,91,115	2.26	19 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCL	BP	102	-	52,54,74	2.30	16 (30%)	71,91,115	2.29	20 (28%)
7	BCL	BT	101	-	52,54,74	2.16	11 (21%)	71,91,115	2.26	18 (25%)
7	BCL	BU	101	-	52,54,74	2.33	18 (34%)	71,91,115	2.29	20 (28%)
7	BCL	BV	101	-	52,54,74	2.18	12 (23%)	71,91,115	2.21	19 (26%)
7	BCL	BV	102	-	52,54,74	2.15	11 (21%)	71,91,115	2.26	18 (25%)
7	BCL	BY	101	-	52,54,74	2.34	16 (30%)	71,91,115	2.25	19 (26%)
7	BCL	BY	102	-	52,54,74	2.30	16 (30%)	71,91,115	2.29	20 (28%)
7	BCL	BZ	101	-	52,54,74	2.31	14 (26%)	71,91,115	2.25	20 (28%)
7	BCL	BZ	102	-	52,54,74	2.30	14 (26%)	71,91,115	2.27	20 (28%)

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
7	BCL	A1	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A2	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A3	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A4	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A6	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A6	102	-	-	0/15/113/137	0/0/9/9
7	BCL	A7	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A8	101	-	-	0/15/113/137	0/0/9/9
7	BCL	A9	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AD	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AD	102	-	-	0/15/113/137	0/0/9/9
7	BCL	AF	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AG	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AI	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AJ	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AK	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AL	301	-	-	0/41/137/137	0/0/9/9
7	BCL	AL	302	-	-	0/41/137/137	0/0/9/9
8	BPH	AL	303	-	2/2/18/22	0/51/105/105	0/1/6/6
9	U10	AL	304	-	-	0/45/69/87	0/1/1/1
10	PO4	AL	305	-	-	0/0/0/0	0/0/0/0
7	BCL	AM	401	-	-	0/41/137/137	0/0/9/9
7	BCL	AM	402	-	-	0/41/137/137	0/0/9/9
8	BPH	AM	403	-	2/2/18/22	0/51/105/105	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	U10	AM	405	-	-	0/45/69/87	0/1/1/1
12	SPO	AM	406	-	-	0/47/47/47	0/0/0/0
7	BCL	AN	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AO	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AP	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AP	102	-	-	0/15/113/137	0/0/9/9
7	BCL	AS	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AT	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AT	102	-	-	0/15/113/137	0/0/9/9
7	BCL	AV	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AW	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AY	101	-	-	0/15/113/137	0/0/9/9
7	BCL	AY	102	-	-	0/15/113/137	0/0/9/9
7	BCL	AZ	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B1	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B2	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B3	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B4	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B5	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B6	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B7	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B8	101	-	-	0/15/113/137	0/0/9/9
7	BCL	B9	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BD	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BD	102	-	-	0/15/113/137	0/0/9/9
7	BCL	BF	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BF	102	-	-	0/15/113/137	0/0/9/9
7	BCL	BI	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BK	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BK	102	-	-	0/15/113/137	0/0/9/9
7	BCL	BL	301	-	-	0/41/137/137	0/0/9/9
7	BCL	BL	302	-	-	0/41/137/137	0/0/9/9
7	BCL	BL	303	-	-	0/41/137/137	0/0/9/9
8	BPH	BL	304	-	2/2/18/22	0/51/105/105	0/1/6/6
9	U10	BL	306	-	-	0/45/69/87	0/1/1/1
10	PO4	BL	307	-	-	0/0/0/0	0/0/0/0
7	BCL	BM	401	-	-	0/41/137/137	0/0/9/9
8	BPH	BM	402	-	2/2/18/22	0/51/105/105	0/1/6/6
7	BCL	BO	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BO	102	-	-	0/15/113/137	0/0/9/9
7	BCL	BP	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BP	102	-	-	0/15/113/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	BT	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BU	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BV	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BV	102	-	-	0/15/113/137	0/0/9/9
7	BCL	BY	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BY	102	-	-	0/15/113/137	0/0/9/9
7	BCL	BZ	101	-	-	0/15/113/137	0/0/9/9
7	BCL	BZ	102	-	-	0/15/113/137	0/0/9/9

The worst 5 of 961 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BM	402	BPH	C1D-CHD	11.17	1.47	1.35
8	AM	403	BPH	C1D-CHD	11.17	1.47	1.35
8	BL	304	BPH	C1D-CHD	9.69	1.46	1.35
8	AL	303	BPH	C1D-CHD	9.67	1.46	1.35
7	BF	102	BCL	C4D-C3D	-8.49	1.23	1.42

The worst 5 of 1383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B4	101	BCL	C1D-C2D-C3D	-7.83	99.29	106.97
7	B2	101	BCL	C1D-C2D-C3D	-7.83	99.30	106.97
7	AY	101	BCL	C1D-C2D-C3D	-7.83	99.30	106.97
7	A1	101	BCL	C1D-C2D-C3D	-7.82	99.30	106.97
7	BO	101	BCL	C1D-C2D-C3D	-7.80	99.32	106.97

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	BM	402	BPH	C8
8	BM	402	BPH	C13
8	AM	403	BPH	C8
8	AM	403	BPH	C13
8	BL	304	BPH	C8

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A1	42/58 (72%)	-0.35	0 100 100	135, 231, 388, 456	0
1	A2	42/58 (72%)	-0.27	0 100 100	182, 298, 500, 500	0
1	A3	42/58 (72%)	-0.11	0 100 100	162, 348, 498, 500	0
1	A5	42/58 (72%)	-0.35	0 100 100	87, 166, 318, 335	0
1	A7	42/58 (72%)	0.19	3 (7%) 16 23	217, 396, 500, 500	0
1	AD	42/58 (72%)	-0.27	0 100 100	120, 190, 361, 392	0
1	AF	42/58 (72%)	-0.02	2 (4%) 29 31	235, 399, 499, 500	0
1	AJ	42/58 (72%)	-0.31	0 100 100	42, 331, 460, 498	0
1	AN	42/58 (72%)	-0.24	0 100 100	149, 330, 490, 500	0
1	AP	42/58 (72%)	-0.23	0 100 100	163, 285, 365, 402	0
1	AT	42/58 (72%)	-0.17	0 100 100	171, 353, 500, 500	0
1	AV	42/58 (72%)	-0.09	0 100 100	310, 453, 500, 500	0
1	AX	42/58 (72%)	0.12	1 (2%) 56 48	270, 446, 500, 500	0
1	AZ	42/58 (72%)	-0.15	0 100 100	123, 321, 500, 500	0
1	B1	42/58 (72%)	-0.00	1 (2%) 56 48	230, 429, 500, 500	0
1	B2	42/58 (72%)	0.07	0 100 100	177, 354, 500, 500	0
1	B3	42/58 (72%)	-0.02	0 100 100	307, 434, 500, 500	0
1	B5	42/58 (72%)	-0.19	0 100 100	146, 321, 429, 492	0
1	B7	42/58 (72%)	-0.17	1 (2%) 56 48	162, 245, 500, 500	0
1	BD	42/58 (72%)	-0.13	2 (4%) 29 31	137, 211, 374, 482	0
1	BF	42/58 (72%)	0.08	0 100 100	206, 417, 500, 500	0
1	BJ	42/58 (72%)	-0.06	0 100 100	204, 333, 500, 500	0
1	BN	42/58 (72%)	-0.29	0 100 100	113, 245, 500, 500	0
1	BP	42/58 (72%)	0.33	1 (2%) 56 48	182, 415, 500, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	BT	42/58 (72%)	-0.05	0 100 100	214, 397, 484, 500	0
1	BV	42/58 (72%)	0.19	0 100 100	295, 443, 500, 500	0
1	BX	42/58 (72%)	0.75	5 (11%) 5 13	285, 448, 500, 500	0
1	BZ	42/58 (72%)	0.01	1 (2%) 56 48	243, 355, 499, 500	0
2	AB	57/82 (69%)	-0.47	0 100 100	145, 257, 378, 461	0
2	BB	57/82 (69%)	0.07	0 100 100	306, 464, 500, 500	0
3	A4	48/49 (97%)	-0.27	0 100 100	220, 382, 500, 500	0
3	A6	48/49 (97%)	-0.64	0 100 100	89, 180, 383, 405	0
3	A8	48/49 (97%)	-0.24	0 100 100	258, 408, 497, 500	0
3	A9	48/49 (97%)	-0.41	0 100 100	250, 475, 500, 500	0
3	AE	48/49 (97%)	-0.27	0 100 100	237, 329, 457, 500	0
3	AG	48/49 (97%)	0.29	0 100 100	149, 384, 500, 500	0
3	AI	48/49 (97%)	-0.15	0 100 100	233, 385, 491, 500	0
3	AK	48/49 (97%)	-0.36	0 100 100	235, 383, 499, 500	0
3	AO	48/49 (97%)	-0.37	0 100 100	117, 342, 494, 500	0
3	AQ	48/49 (97%)	-0.19	0 100 100	94, 446, 500, 500	0
3	AS	48/49 (97%)	-0.35	0 100 100	170, 319, 496, 500	0
3	AU	48/49 (97%)	-0.25	0 100 100	331, 417, 500, 500	0
3	AW	48/49 (97%)	0.05	3 (6%) 19 26	232, 405, 500, 500	0
3	AY	48/49 (97%)	-0.15	1 (2%) 60 51	262, 396, 500, 500	0
3	B4	48/49 (97%)	-0.12	1 (2%) 60 51	202, 353, 489, 500	0
3	B6	48/49 (97%)	-0.48	0 100 100	116, 241, 375, 438	0
3	B8	48/49 (97%)	0.22	2 (4%) 35 34	225, 472, 500, 500	0
3	B9	48/49 (97%)	-0.26	0 100 100	187, 374, 462, 494	0
3	BE	48/49 (97%)	-0.03	0 100 100	177, 387, 500, 500	0
3	BG	48/49 (97%)	0.20	1 (2%) 60 51	274, 482, 500, 500	0
3	BI	48/49 (97%)	-0.03	0 100 100	242, 480, 500, 500	0
3	BK	48/49 (97%)	0.16	0 100 100	356, 448, 500, 500	0
3	BO	48/49 (97%)	-0.21	0 100 100	206, 396, 500, 500	0
3	BQ	48/49 (97%)	-0.25	0 100 100	159, 401, 500, 500	0
3	BS	48/49 (97%)	-0.09	2 (4%) 35 34	235, 426, 500, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	BU	48/49 (97%)	-0.01	0 100 100	225, 487, 500, 500	0
3	BW	48/49 (97%)	-0.22	0 100 100	210, 382, 500, 500	0
3	BY	48/49 (97%)	-0.09	1 (2%) 60 51	279, 460, 500, 500	0
4	AH	250/260 (96%)	-0.34	0 100 100	2, 101, 447, 500	0
4	BH	250/260 (96%)	-0.18	0 100 100	16, 193, 470, 500	0
5	AL	281/282 (99%)	-0.51	0 100 100	2, 2, 194, 460	0
5	BL	281/282 (99%)	-0.51	0 100 100	2, 9, 249, 370	0
6	AM	304/308 (98%)	-0.41	0 100 100	2, 2, 215, 459	0
6	BM	304/308 (98%)	-0.31	0 100 100	2, 9, 269, 492	0
All	All	4304/4860 (88%)	-0.22	28 (0%) 84 75	2, 273, 500, 500	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A7	18	VAL	3.8
1	BX	21	GLY	3.8
1	BX	19	ALA	3.7
1	B1	12	ASP	3.3
1	BP	15	ARG	3.2

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BCL	B5	101	46/66	0.37	3.65	460,484,500,500	0
7	BCL	BO	101	46/66	0.36	3.21	500,500,500,500	0
7	BCL	BL	303	66/66	0.31	2.81	2,2,2,2	0
7	BCL	AO	101	46/66	0.28	1.75	247,260,266,272	0
7	BCL	B9	101	46/66	0.37	1.74	500,500,500,500	0
7	BCL	A6	101	46/66	0.27	1.61	391,461,488,498	0
7	BCL	BL	302	66/66	0.25	1.59	2,2,2,2	0
12	SPO	AM	406	42/42	0.26	1.52	2,2,2,2	0
7	BCL	AY	101	46/66	0.25	1.51	438,471,494,500	0
8	BPH	BL	304	65/65	0.23	1.50	2,2,2,2	0
7	BCL	B6	101	46/66	0.28	1.47	268,314,325,333	0
7	BCL	AM	401	66/66	0.20	1.46	2,2,2,2	0
9	U10	AM	405	48/63	0.25	1.40	2,2,2,2	0
9	U10	BL	306	48/63	0.22	1.40	2,2,2,2	0
7	BCL	BL	301	66/66	0.25	1.39	2,2,2,2	0
7	BCL	AM	402	66/66	0.21	1.36	2,2,2,2	0
7	BCL	AY	102	46/66	0.21	1.34	360,384,441,448	0
7	BCL	AK	101	46/66	0.26	1.31	422,500,500,500	0
8	BPH	AM	403	65/65	0.24	1.30	2,2,2,2	0
7	BCL	B4	101	46/66	0.27	1.23	467,500,500,500	0
8	BPH	AL	303	65/65	0.24	1.22	2,2,2,2	0
7	BCL	BK	101	46/66	0.25	1.16	471,500,500,500	0
7	BCL	AT	102	46/66	0.27	1.08	368,404,465,495	0
7	BCL	AL	302	66/66	0.23	1.02	2,2,2,2	0
7	BCL	BZ	101	46/66	0.31	0.88	411,455,500,500	0
7	BCL	AV	101	46/66	0.26	0.84	313,363,409,416	0
7	BCL	BM	401	66/66	0.20	0.80	2,2,2,2	0
7	BCL	A6	102	46/66	0.21	0.77	205,301,379,402	0
7	BCL	A1	101	46/66	0.18	0.75	317,355,399,417	0
7	BCL	BU	101	46/66	0.27	0.74	292,480,500,500	0
7	BCL	BF	102	46/66	0.29	0.71	418,498,500,500	0
7	BCL	AZ	101	46/66	0.25	0.67	500,500,500,500	0
7	BCL	AG	101	46/66	0.20	0.64	329,398,418,422	0
7	BCL	AD	102	46/66	0.17	0.64	145,169,200,210	0
7	BCL	BI	101	46/66	0.21	0.57	449,481,500,500	0
7	BCL	A4	101	46/66	0.18	0.50	289,335,362,369	0
7	BCL	B1	101	46/66	0.19	0.49	221,405,460,480	0
7	BCL	AD	101	46/66	0.16	0.49	133,145,160,169	0
7	BCL	AN	101	46/66	0.22	0.46	263,334,370,376	0
7	BCL	AP	101	46/66	0.25	0.35	196,268,280,290	0
7	BCL	BD	102	46/66	0.27	0.34	313,347,446,472	0
7	BCL	BV	101	46/66	0.28	0.34	326,464,500,500	0
7	BCL	B3	101	46/66	0.17	0.34	442,492,500,500	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BCL	BZ	102	46/66	0.26	0.33	340,425,460,469	0
8	BPH	BM	402	65/65	0.20	0.30	2,2,2,2	0
7	BCL	AI	101	46/66	0.16	0.27	277,287,302,304	0
7	BCL	AP	102	46/66	0.21	0.21	212,236,270,272	0
7	BCL	AJ	101	46/66	0.23	0.20	241,343,392,401	0
7	BCL	B7	101	46/66	0.26	0.15	159,184,195,199	0
7	BCL	A2	101	46/66	0.16	0.14	451,500,500,500	0
7	BCL	B2	101	46/66	0.24	0.12	171,220,230,232	0
7	BCL	BF	101	46/66	0.18	0.02	374,453,480,499	0
7	BCL	AW	101	46/66	0.23	0.01	388,435,462,478	0
7	BCL	A9	101	46/66	0.13	-0.00	318,386,396,414	0
7	BCL	AT	101	46/66	0.18	-0.00	241,267,280,281	0
7	BCL	A8	101	46/66	0.18	-0.01	301,369,400,413	0
10	PO4	BL	307	5/5	0.15	-0.09	2,2,2,2	0
7	BCL	A7	101	46/66	0.17	-0.12	180,198,207,213	0
10	PO4	AL	305	5/5	0.12	-0.13	2,2,2,2	0
7	BCL	BO	102	46/66	0.19	-0.14	152,179,187,204	0
7	BCL	AS	101	46/66	0.16	-0.15	275,321,356,360	0
7	BCL	AF	101	46/66	0.14	-0.22	204,214,229,239	0
7	BCL	BK	102	46/66	0.22	-0.22	321,390,455,471	0
7	BCL	BT	101	46/66	0.18	-0.26	274,316,329,331	0
7	BCL	BV	102	46/66	0.18	-0.28	332,395,420,424	0
7	BCL	BD	101	46/66	0.19	-0.32	233,299,305,307	0
7	BCL	B8	101	46/66	0.18	-0.41	233,268,304,309	0
7	BCL	BY	102	46/66	0.18	-0.57	192,221,234,245	0
7	BCL	BP	101	46/66	0.14	-0.63	142,147,153,161	0
7	BCL	BP	102	46/66	0.13	-0.66	172,203,216,217	0
7	BCL	A3	101	46/66	0.13	-0.68	245,269,314,322	0
7	BCL	BY	101	46/66	0.17	-0.68	283,306,315,316	0
11	FE2	BL	305	1/1	0.10	-1.74	2,2,2,2	0
9	U10	AL	304	48/63	0.20	-	2,2,2,2	0
7	BCL	AL	301	66/66	0.21	-	2,2,2,2	0
11	FE2	AM	404	1/1	0.04	-	2,2,2,2	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.