



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:34 AM GMT

PDB ID : 3OFL
Title : Crystal structure of Humanpapillomavirus18(HPV18) capsid L1 pentamers
bound to heparin oligosaccharides
Authors : Chen, X.S.; Dasgupta, J.
Deposited on : 2010-08-15
Resolution : 3.40 Å(reported)

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

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

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

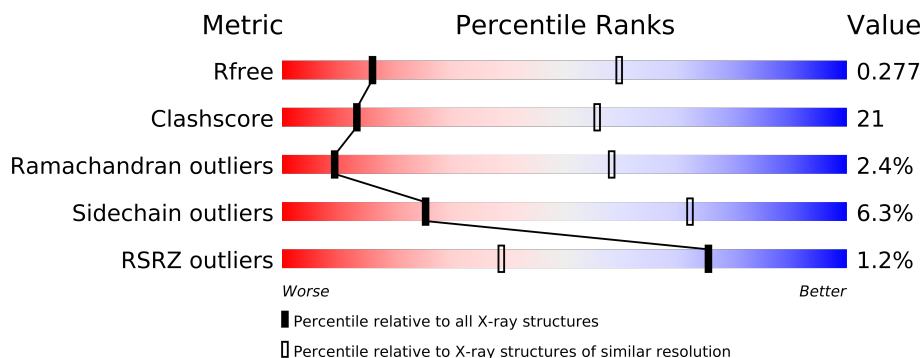
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	427	
1	B	427	
1	C	427	
1	D	427	
1	E	427	
1	F	427	
1	G	427	
1	H	427	
1	I	427	
1	J	427	
1	K	427	
1	L	427	
1	M	427	
1	N	427	

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Mol	Chain	Length	Quality of chain
1	O	427	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	JHM	E	501	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 51547 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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	B	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	C	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	D	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	E	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	F	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	G	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	H	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	I	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	J	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	K	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	L	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	M	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	N	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	O	421	Total	C	N	O	S	0	0	0
			3307	2088	559	640	20			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	EXPRESSION TAG	UNP Q80B70
A	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
A	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
A	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
A	433	GLY	-	LINKER	UNP Q80B70
A	434	GLY	-	LINKER	UNP Q80B70
A	435	SER	-	LINKER	UNP Q80B70
A	436	GLY	-	LINKER	UNP Q80B70
A	437	GLY	-	LINKER	UNP Q80B70
B	20	ALA	-	EXPRESSION TAG	UNP Q80B70
B	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
B	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
B	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
B	433	GLY	-	LINKER	UNP Q80B70
B	434	GLY	-	LINKER	UNP Q80B70
B	435	SER	-	LINKER	UNP Q80B70
B	436	GLY	-	LINKER	UNP Q80B70
B	437	GLY	-	LINKER	UNP Q80B70
C	20	ALA	-	EXPRESSION TAG	UNP Q80B70
C	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
C	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
C	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
C	433	GLY	-	LINKER	UNP Q80B70
C	434	GLY	-	LINKER	UNP Q80B70
C	435	SER	-	LINKER	UNP Q80B70
C	436	GLY	-	LINKER	UNP Q80B70
C	437	GLY	-	LINKER	UNP Q80B70
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
E	20	ALA	-	EXPRESSION TAG	UNP Q80B70
E	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
E	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
E	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
E	433	GLY	-	LINKER	UNP Q80B70
E	434	GLY	-	LINKER	UNP Q80B70
E	435	SER	-	LINKER	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLY	-	LINKER	UNP Q80B70
E	437	GLY	-	LINKER	UNP Q80B70
F	20	ALA	-	EXPRESSION TAG	UNP Q80B70
F	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
F	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
F	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
F	433	GLY	-	LINKER	UNP Q80B70
F	434	GLY	-	LINKER	UNP Q80B70
F	435	SER	-	LINKER	UNP Q80B70
F	436	GLY	-	LINKER	UNP Q80B70
F	437	GLY	-	LINKER	UNP Q80B70
G	20	ALA	-	EXPRESSION TAG	UNP Q80B70
G	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
G	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
G	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
G	433	GLY	-	LINKER	UNP Q80B70
G	434	GLY	-	LINKER	UNP Q80B70
G	435	SER	-	LINKER	UNP Q80B70
G	436	GLY	-	LINKER	UNP Q80B70
G	437	GLY	-	LINKER	UNP Q80B70
H	20	ALA	-	EXPRESSION TAG	UNP Q80B70
H	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
H	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
H	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
H	433	GLY	-	LINKER	UNP Q80B70
H	434	GLY	-	LINKER	UNP Q80B70
H	435	SER	-	LINKER	UNP Q80B70
H	436	GLY	-	LINKER	UNP Q80B70
H	437	GLY	-	LINKER	UNP Q80B70
I	20	ALA	-	EXPRESSION TAG	UNP Q80B70
I	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
I	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
I	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
I	433	GLY	-	LINKER	UNP Q80B70
I	434	GLY	-	LINKER	UNP Q80B70
I	435	SER	-	LINKER	UNP Q80B70
I	436	GLY	-	LINKER	UNP Q80B70
I	437	GLY	-	LINKER	UNP Q80B70
J	20	ALA	-	EXPRESSION TAG	UNP Q80B70
J	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
J	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
J	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70

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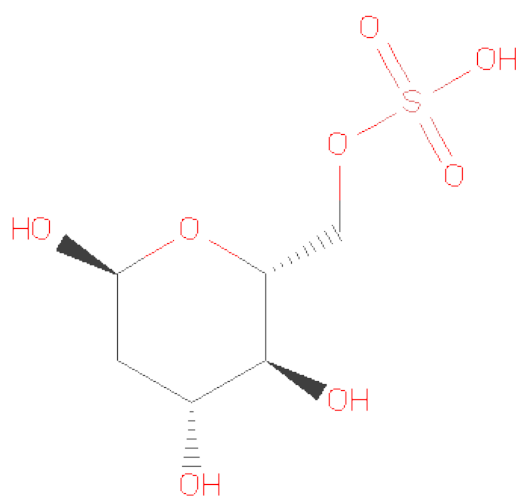
Chain	Residue	Modelled	Actual	Comment	Reference
J	433	GLY	-	LINKER	UNP Q80B70
J	434	GLY	-	LINKER	UNP Q80B70
J	435	SER	-	LINKER	UNP Q80B70
J	436	GLY	-	LINKER	UNP Q80B70
J	437	GLY	-	LINKER	UNP Q80B70
K	20	ALA	-	EXPRESSION TAG	UNP Q80B70
K	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
K	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
K	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
K	433	GLY	-	LINKER	UNP Q80B70
K	434	GLY	-	LINKER	UNP Q80B70
K	435	SER	-	LINKER	UNP Q80B70
K	436	GLY	-	LINKER	UNP Q80B70
K	437	GLY	-	LINKER	UNP Q80B70
L	20	ALA	-	EXPRESSION TAG	UNP Q80B70
L	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
L	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
L	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
L	433	GLY	-	LINKER	UNP Q80B70
L	434	GLY	-	LINKER	UNP Q80B70
L	435	SER	-	LINKER	UNP Q80B70
L	436	GLY	-	LINKER	UNP Q80B70
L	437	GLY	-	LINKER	UNP Q80B70
M	20	ALA	-	EXPRESSION TAG	UNP Q80B70
M	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
M	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
M	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
M	433	GLY	-	LINKER	UNP Q80B70
M	434	GLY	-	LINKER	UNP Q80B70
M	435	SER	-	LINKER	UNP Q80B70
M	436	GLY	-	LINKER	UNP Q80B70
M	437	GLY	-	EXPRESSION TAG	UNP Q80B70
N	20	ALA	-	LINKER	UNP Q80B70
N	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
N	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
N	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
N	433	GLY	-	LINKER	UNP Q80B70
N	434	GLY	-	LINKER	UNP Q80B70
N	435	SER	-	LINKER	UNP Q80B70
N	436	GLY	-	LINKER	UNP Q80B70
N	437	GLY	-	LINKER	UNP Q80B70
O	20	ALA	-	EXPRESSION TAG	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
O	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
O	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
O	433	GLY	-	LINKER	UNP Q80B70
O	434	GLY	-	LINKER	UNP Q80B70
O	435	SER	-	LINKER	UNP Q80B70
O	436	GLY	-	LINKER	UNP Q80B70
O	437	GLY	-	EXPRESSION TAG	UNP Q80B70

- Molecule 2 is 2-DEOXY-6-O-SULFO-ALPHA-D-ARABINO-HEXOPYRANOSE (three-letter code: JHM) (formula: C₆H₁₂O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	O	S	0	0
			15	6	8	1		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	3	Total	C	O	S	0	0
			45	18	24	3		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	20	ALA	-	EXPRESSION TAG	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
E	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
E	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
E	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
E	433	GLY	-	LINKER	UNP Q80B70
E	434	GLY	-	LINKER	UNP Q80B70
E	435	SER	-	LINKER	UNP Q80B70
E	436	GLY	-	LINKER	UNP Q80B70
E	437	GLY	-	LINKER	UNP Q80B70

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	E	2	Total	C	O	S	0	0
			30	12	16	2		
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	C	2	Total	C	O	S	0	0
			30	12	16	2		
4	N	2	Total	C	O	S	0	0
			30	12	16	2		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
E	20	ALA	-	EXPRESSION TAG	UNP Q80B70
E	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
E	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
E	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
E	433	GLY	-	LINKER	UNP Q80B70
E	434	GLY	-	LINKER	UNP Q80B70
E	435	SER	-	LINKER	UNP Q80B70
E	436	GLY	-	LINKER	UNP Q80B70
E	437	GLY	-	LINKER	UNP Q80B70
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
C	20	ALA	-	EXPRESSION TAG	UNP Q80B70
C	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
C	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
C	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
C	433	GLY	-	LINKER	UNP Q80B70
C	434	GLY	-	LINKER	UNP Q80B70
C	435	SER	-	LINKER	UNP Q80B70
C	436	GLY	-	LINKER	UNP Q80B70
C	437	GLY	-	LINKER	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
N	20	ALA	-	LINKER	UNP Q80B70
N	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
N	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
N	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
N	433	GLY	-	LINKER	UNP Q80B70
N	434	GLY	-	LINKER	UNP Q80B70
N	435	SER	-	LINKER	UNP Q80B70
N	436	GLY	-	LINKER	UNP Q80B70
N	437	GLY	-	LINKER	UNP Q80B70

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	4	Total	C	O	S	0	0
			60	24	32	4		
5	A	4	Total	C	O	S	0	0
			60	24	32	4		
5	D	4	Total	C	O	S	0	0
			60	24	32	4		
5	B	4	Total	C	O	S	0	0
			60	24	32	4		
5	A	4	Total	C	O	S	0	0
			60	24	32	4		
5	C	4	Total	C	O	S	0	0
			60	24	32	4		
5	F	4	Total	C	O	S	0	0
			60	24	32	4		
5	O	4	Total	C	O	S	0	0
			60	24	32	4		
5	N	4	Total	C	O	S	0	0
			60	24	32	4		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	20	ALA	-	EXPRESSION TAG	UNP Q80B70
E	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
E	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
E	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
E	433	GLY	-	LINKER	UNP Q80B70
E	434	GLY	-	LINKER	UNP Q80B70
E	435	SER	-	LINKER	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLY	-	LINKER	UNP Q80B70
E	437	GLY	-	LINKER	UNP Q80B70
A	20	ALA	-	EXPRESSION TAG	UNP Q80B70
A	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
A	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
A	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
A	433	GLY	-	LINKER	UNP Q80B70
A	434	GLY	-	LINKER	UNP Q80B70
A	435	SER	-	LINKER	UNP Q80B70
A	436	GLY	-	LINKER	UNP Q80B70
A	437	GLY	-	LINKER	UNP Q80B70
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
B	20	ALA	-	EXPRESSION TAG	UNP Q80B70
B	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
B	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
B	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
B	433	GLY	-	LINKER	UNP Q80B70
B	434	GLY	-	LINKER	UNP Q80B70
B	435	SER	-	LINKER	UNP Q80B70
B	436	GLY	-	LINKER	UNP Q80B70
B	437	GLY	-	LINKER	UNP Q80B70
A	20	ALA	-	EXPRESSION TAG	UNP Q80B70
A	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
A	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
A	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
A	433	GLY	-	LINKER	UNP Q80B70
A	434	GLY	-	LINKER	UNP Q80B70
A	435	SER	-	LINKER	UNP Q80B70
A	436	GLY	-	LINKER	UNP Q80B70
A	437	GLY	-	LINKER	UNP Q80B70
C	20	ALA	-	EXPRESSION TAG	UNP Q80B70
C	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
C	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
C	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
C	433	GLY	-	LINKER	UNP Q80B70
C	434	GLY	-	LINKER	UNP Q80B70
C	435	SER	-	LINKER	UNP Q80B70
C	436	GLY	-	LINKER	UNP Q80B70
C	437	GLY	-	LINKER	UNP Q80B70
F	20	ALA	-	EXPRESSION TAG	UNP Q80B70
F	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
F	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
F	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
F	433	GLY	-	LINKER	UNP Q80B70
F	434	GLY	-	LINKER	UNP Q80B70
F	435	SER	-	LINKER	UNP Q80B70
F	436	GLY	-	LINKER	UNP Q80B70
F	437	GLY	-	LINKER	UNP Q80B70
O	20	ALA	-	EXPRESSION TAG	UNP Q80B70
O	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
O	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
O	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
O	433	GLY	-	LINKER	UNP Q80B70
O	434	GLY	-	LINKER	UNP Q80B70
O	435	SER	-	LINKER	UNP Q80B70
O	436	GLY	-	LINKER	UNP Q80B70
O	437	GLY	-	EXPRESSION TAG	UNP Q80B70
N	20	ALA	-	LINKER	UNP Q80B70
N	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
N	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
N	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
N	433	GLY	-	LINKER	UNP Q80B70
N	434	GLY	-	LINKER	UNP Q80B70
N	435	SER	-	LINKER	UNP Q80B70
N	436	GLY	-	LINKER	UNP Q80B70
N	437	GLY	-	LINKER	UNP Q80B70

- Molecule 6 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	10	Total	C	O	S	0	0
			150	60	80	10		
6	F	10	Total	C	O	S	0	0
			150	60	80	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ALA	-	EXPRESSION TAG	UNP Q80B70
B	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
B	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
B	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
B	433	GLY	-	LINKER	UNP Q80B70
B	434	GLY	-	LINKER	UNP Q80B70
B	435	SER	-	LINKER	UNP Q80B70
B	436	GLY	-	LINKER	UNP Q80B70
B	437	GLY	-	LINKER	UNP Q80B70
F	20	ALA	-	EXPRESSION TAG	UNP Q80B70
F	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
F	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
F	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
F	433	GLY	-	LINKER	UNP Q80B70
F	434	GLY	-	LINKER	UNP Q80B70
F	435	SER	-	LINKER	UNP Q80B70
F	436	GLY	-	LINKER	UNP Q80B70
F	437	GLY	-	LINKER	UNP Q80B70

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	6	Total	C	O	S	0	0
			90	36	48	6		
7	J	6	Total	C	O	S	0	0
			90	36	48	6		
7	J	6	Total	C	O	S	0	0
			90	36	48	6		
7	F	6	Total	C	O	S	0	0
			90	36	48	6		
7	H	6	Total	C	O	S	0	0
			90	36	48	6		
7	J	6	Total	C	O	S	0	0
			90	36	48	6		
7	L	6	Total	C	O	S	0	0
			90	36	48	6		
7	L	6	Total	C	O	S	0	0
			90	36	48	6		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	20	ALA	-	EXPRESSION TAG	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
E	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
E	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
E	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
E	433	GLY	-	LINKER	UNP Q80B70
E	434	GLY	-	LINKER	UNP Q80B70
E	435	SER	-	LINKER	UNP Q80B70
E	436	GLY	-	LINKER	UNP Q80B70
E	437	GLY	-	LINKER	UNP Q80B70
J	20	ALA	-	EXPRESSION TAG	UNP Q80B70
J	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
J	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
J	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
J	433	GLY	-	LINKER	UNP Q80B70
J	434	GLY	-	LINKER	UNP Q80B70
J	435	SER	-	LINKER	UNP Q80B70
J	436	GLY	-	LINKER	UNP Q80B70
J	437	GLY	-	LINKER	UNP Q80B70
J	20	ALA	-	EXPRESSION TAG	UNP Q80B70
J	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
J	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
J	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
J	433	GLY	-	LINKER	UNP Q80B70
J	434	GLY	-	LINKER	UNP Q80B70
J	435	SER	-	LINKER	UNP Q80B70
J	436	GLY	-	LINKER	UNP Q80B70
J	437	GLY	-	LINKER	UNP Q80B70
F	20	ALA	-	EXPRESSION TAG	UNP Q80B70
F	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
F	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
F	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
F	433	GLY	-	LINKER	UNP Q80B70
F	434	GLY	-	LINKER	UNP Q80B70
F	435	SER	-	LINKER	UNP Q80B70
F	436	GLY	-	LINKER	UNP Q80B70
F	437	GLY	-	LINKER	UNP Q80B70
H	20	ALA	-	EXPRESSION TAG	UNP Q80B70
H	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
H	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
H	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
H	433	GLY	-	LINKER	UNP Q80B70
H	434	GLY	-	LINKER	UNP Q80B70
H	435	SER	-	LINKER	UNP Q80B70

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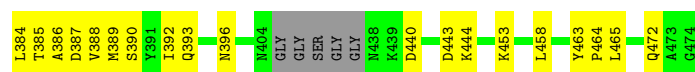
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Chain	Residue	Modelled	Actual	Comment	Reference
H	436	GLY	-	LINKER	UNP Q80B70
H	437	GLY	-	LINKER	UNP Q80B70
J	20	ALA	-	EXPRESSION TAG	UNP Q80B70
J	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
J	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
J	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
J	433	GLY	-	LINKER	UNP Q80B70
J	434	GLY	-	LINKER	UNP Q80B70
J	435	SER	-	LINKER	UNP Q80B70
J	436	GLY	-	LINKER	UNP Q80B70
J	437	GLY	-	LINKER	UNP Q80B70
L	20	ALA	-	EXPRESSION TAG	UNP Q80B70
L	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
L	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
L	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
L	433	GLY	-	LINKER	UNP Q80B70
L	434	GLY	-	LINKER	UNP Q80B70
L	435	SER	-	LINKER	UNP Q80B70
L	436	GLY	-	LINKER	UNP Q80B70
L	437	GLY	-	LINKER	UNP Q80B70
L	20	ALA	-	EXPRESSION TAG	UNP Q80B70
L	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
L	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
L	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
L	433	GLY	-	LINKER	UNP Q80B70
L	434	GLY	-	LINKER	UNP Q80B70
L	435	SER	-	LINKER	UNP Q80B70
L	436	GLY	-	LINKER	UNP Q80B70
L	437	GLY	-	LINKER	UNP Q80B70



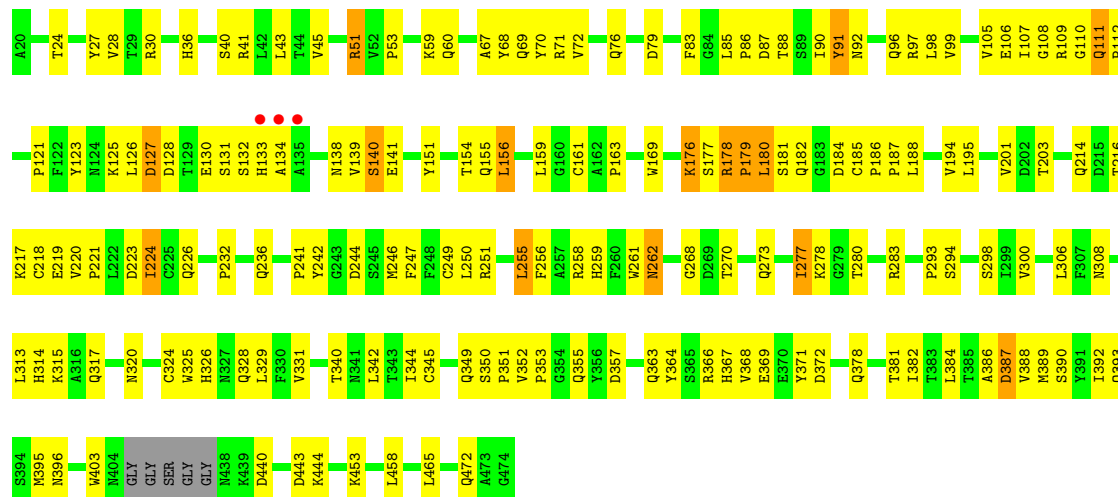
Age Group	Percentage
18-24	35%
25-34	30%
35-44	20%
45-54	10%
55-64	5%
65-74	3%
75-84	2%
85+	1%





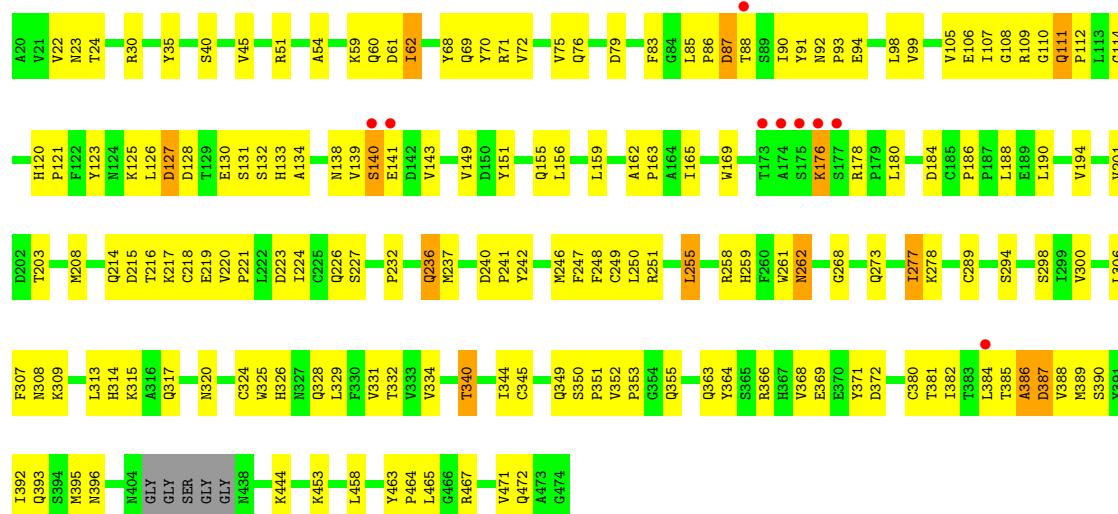
• Molecule 1: L1

Chain F:



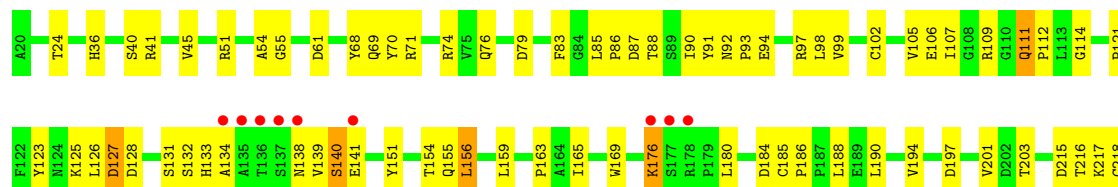
• Molecule 1: L1

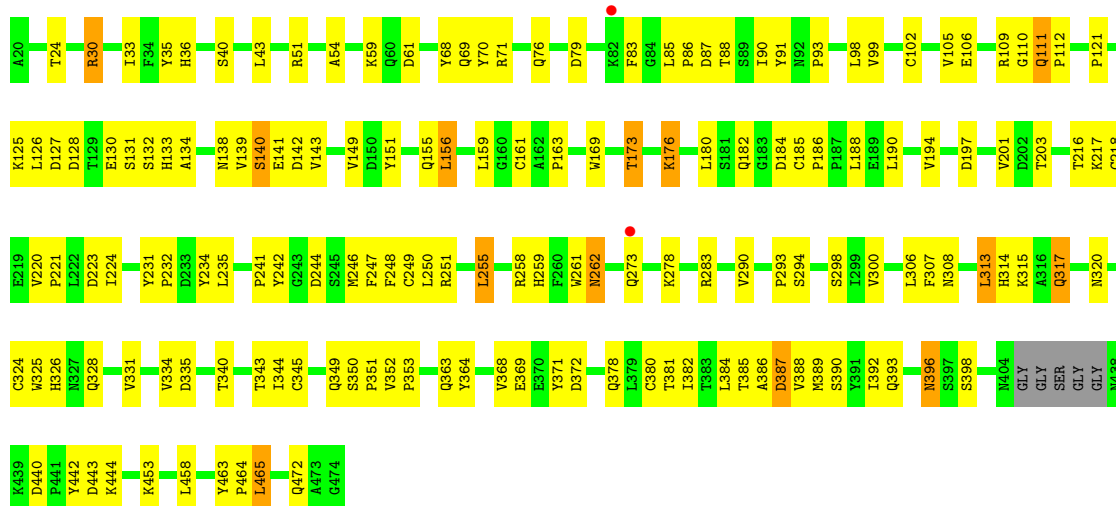
Chain G:



• Molecule 1: L1

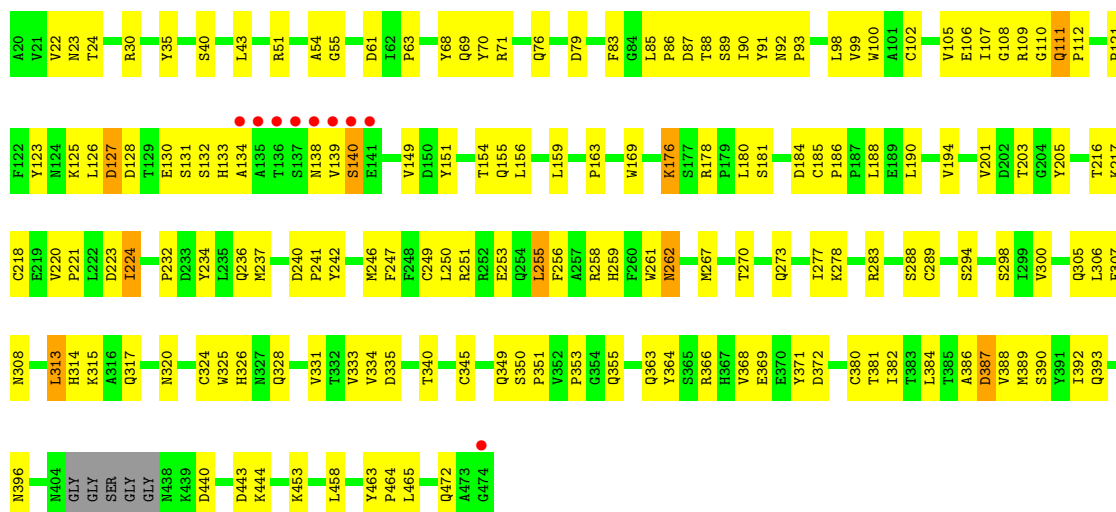
Chain H:





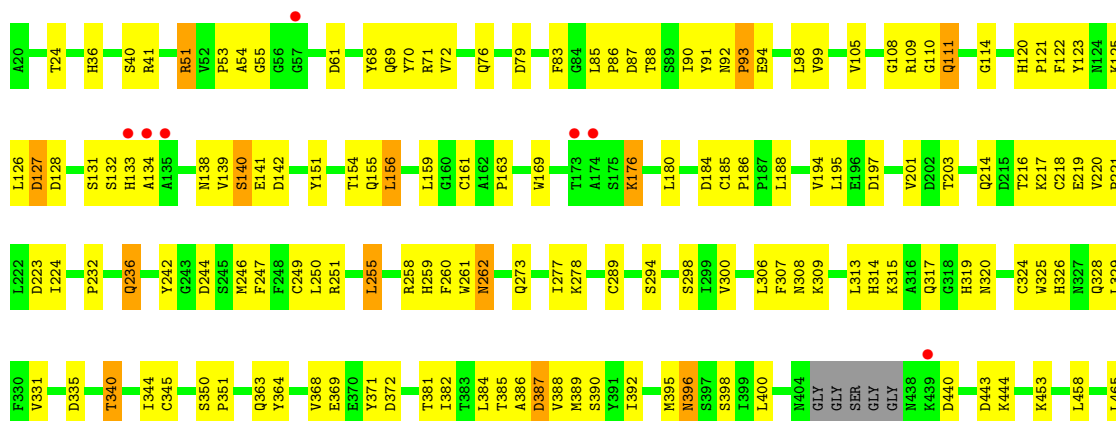
• Molecule 1: L1

Chain L:



• Molecule 1: L1

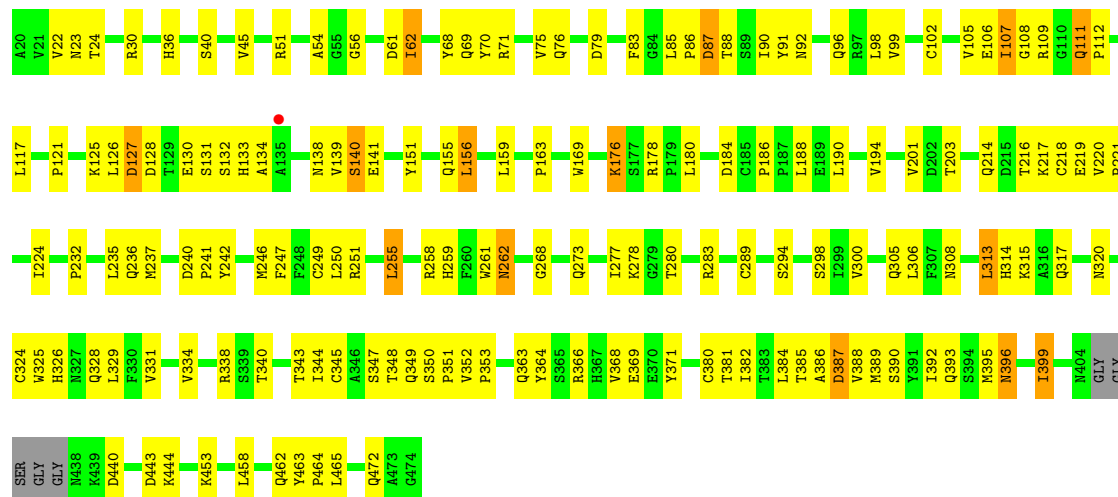
Chain M:





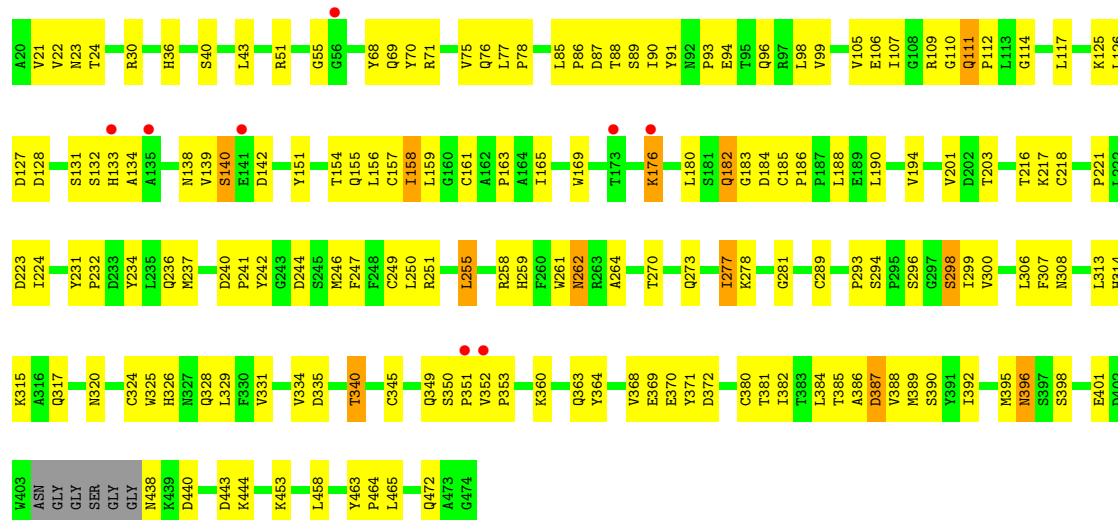
• Molecule 1: L1

Chain N:



• Molecule 1: L1

Chain O:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.99Å 106.49Å 237.66Å 88.46° 85.75° 69.02°	Depositor
Resolution (Å)	42.80 – 3.40 42.79 – 3.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.80-3.40) 84.3 (42.79-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 3.40Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.281 0.253 , 0.277	Depositor DCC
R_{free} test set	4354 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , -3.5	EDS
Estimated twinning fraction	0.017 for -h,-h+k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 92923 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	51547	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: JHM, IDS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.76	10/3400 (0.3%)	0.77	2/4622 (0.0%)
1	B	0.63	2/3400 (0.1%)	0.67	0/4622
1	C	0.66	1/3400 (0.0%)	0.70	1/4622 (0.0%)
1	D	0.66	2/3400 (0.1%)	0.75	3/4622 (0.1%)
1	E	0.71	3/3400 (0.1%)	0.72	1/4622 (0.0%)
1	F	0.60	0/3400	0.70	0/4622
1	G	0.59	0/3400	0.70	0/4622
1	H	0.64	2/3400 (0.1%)	0.69	2/4622 (0.0%)
1	I	0.62	0/3400	0.68	0/4622
1	J	0.60	0/3400	0.69	3/4622 (0.1%)
1	K	0.61	1/3400 (0.0%)	0.69	1/4622 (0.0%)
1	L	0.58	0/3400	0.68	0/4622
1	M	0.59	0/3400	0.67	0/4622
1	N	0.60	0/3400	0.69	0/4622
1	O	0.61	0/3392	0.68	0/4611
All	All	0.63	21/50992 (0.0%)	0.70	13/69319 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	1	0
5	C	1	0
5	N	1	0
6	B	2	0
7	E	2	0
7	H	1	0
7	J	5	0
7	L	4	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	17	0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	56	GLY	C-O	12.55	1.43	1.23
1	A	172	GLY	C-O	11.64	1.42	1.23
1	A	176	LYS	CE-NZ	-11.37	1.20	1.49
1	C	278	LYS	CE-NZ	-9.26	1.25	1.49
1	D	280	THR	CB-CG2	-8.92	1.23	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LYS	CD-CE-NZ	-19.64	66.52	111.70
1	D	176	LYS	CA-CB-CG	12.45	140.78	113.40
1	D	278	LYS	CD-CE-NZ	-10.97	86.48	111.70
1	E	444	LYS	CD-CE-NZ	-6.82	96.02	111.70
1	D	176	LYS	CB-CA-C	-5.90	98.59	110.40

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	518	IDS	C4
6	B	534	IDS	C4
6	B	538	IDS	C4
5	C	572	IDS	C4
7	E	548	IDS	C4

There are no planarity outliers.

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	A	3315	0	3178	143	0
1	B	3315	0	3181	153	0
1	C	3315	0	3181	153	0
1	D	3315	0	3181	125	0
1	E	3315	0	3181	131	0
1	F	3315	0	3181	172	0
1	G	3315	0	3181	157	1
1	H	3315	0	3181	125	0
1	I	3315	0	3181	134	0
1	J	3315	0	3181	186	2
1	K	3315	0	3181	127	1
1	L	3315	0	3181	140	1
1	M	3315	0	3181	120	4
1	N	3315	0	3181	154	1
1	O	3307	0	3175	144	6
2	E	15	0	10	8	0
3	E	45	0	17	6	0
4	C	30	0	14	0	0
4	D	120	0	55	12	0
4	E	30	0	14	3	0
4	N	30	0	14	1	0
5	A	120	0	54	1	3
5	B	60	0	26	17	0
5	C	60	0	27	5	0
5	D	60	0	26	4	2
5	E	60	0	26	5	1
5	F	60	0	27	1	1
5	N	60	0	27	18	1
5	O	60	0	26	1	0
6	B	150	0	66	9	0
6	F	150	0	66	6	4
7	E	90	0	40	5	0
7	F	90	0	40	13	0
7	H	90	0	40	10	0
7	J	270	0	120	49	0
7	L	180	0	80	17	4
All	All	51547	0	48521	2052	16

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 21.

The worst 5 of 2052 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:J:561:JHM:H2A	7:J:564:IDS:C3	1.42	1.38
5:B:530:IDS:O61	1:C:274:SER:CB	1.76	1.31
1:C:95:THR:HB	5:C:572:IDS:O61	1.30	1.28
5:B:530:IDS:O61	1:C:274:SER:HB2	1.12	1.28
7:L:611:JHM:H1	7:L:614:IDS:O62	1.18	1.24

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:53:PRO:CB	6:F:583:JHM:O7[1_655]	1.52	0.68
1:M:61:ASP:OD1	6:F:584:IDS:O2S[1_655]	1.81	0.39
1:O:86:PRO:O	5:A:519:JHM:O7[1_666]	1.83	0.37
1:L:89:SER:CB	7:L:613:JHM:O9[1_655]	1.89	0.31
1:K:173:THR:CG2	5:E:514:IDS:O1S[1_566]	1.95	0.25

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/427 (98%)	366 (88%)	40 (10%)	12 (3%)	7	54
1	B	418/427 (98%)	368 (88%)	41 (10%)	9 (2%)	10	60
1	C	418/427 (98%)	364 (87%)	44 (10%)	10 (2%)	9	58
1	D	418/427 (98%)	366 (88%)	43 (10%)	9 (2%)	10	60
1	E	418/427 (98%)	368 (88%)	41 (10%)	9 (2%)	10	60
1	F	418/427 (98%)	364 (87%)	44 (10%)	10 (2%)	9	58
1	G	418/427 (98%)	366 (88%)	42 (10%)	10 (2%)	9	58
1	H	418/427 (98%)	367 (88%)	39 (9%)	12 (3%)	7	54
1	I	418/427 (98%)	367 (88%)	40 (10%)	11 (3%)	8	56
1	J	418/427 (98%)	363 (87%)	44 (10%)	11 (3%)	8	56
1	K	418/427 (98%)	366 (88%)	43 (10%)	9 (2%)	10	60
1	L	418/427 (98%)	370 (88%)	39 (9%)	9 (2%)	10	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	418/427 (98%)	365 (87%)	43 (10%)	10 (2%)	9	58
1	N	418/427 (98%)	365 (87%)	45 (11%)	8 (2%)	12	64
1	O	417/427 (98%)	362 (87%)	44 (11%)	11 (3%)	8	56
All	All	6269/6405 (98%)	5487 (88%)	632 (10%)	150 (2%)	9	58

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	B	131	SER
1	B	140	SER
1	B	298	SER
1	C	131	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/370 (100%)	343 (93%)	26 (7%)	21	68
1	B	369/370 (100%)	347 (94%)	22 (6%)	27	73
1	C	369/370 (100%)	343 (93%)	26 (7%)	21	68
1	D	369/370 (100%)	348 (94%)	21 (6%)	29	75
1	E	369/370 (100%)	342 (93%)	27 (7%)	20	65
1	F	369/370 (100%)	341 (92%)	28 (8%)	19	64
1	G	369/370 (100%)	345 (94%)	24 (6%)	24	71
1	H	369/370 (100%)	346 (94%)	23 (6%)	26	72
1	I	369/370 (100%)	345 (94%)	24 (6%)	24	71
1	J	369/370 (100%)	348 (94%)	21 (6%)	29	75
1	K	369/370 (100%)	350 (95%)	19 (5%)	33	78
1	L	369/370 (100%)	348 (94%)	21 (6%)	29	75
1	M	369/370 (100%)	348 (94%)	21 (6%)	29	75
1	N	369/370 (100%)	345 (94%)	24 (6%)	24	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	368/370 (100%)	345 (94%)	23 (6%)	25	72
All	All	5534/5550 (100%)	5184 (94%)	350 (6%)	25	72

5 of 350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	215	ASP
1	H	465	LEU
1	N	396	ASN
1	G	251	ARG
1	H	133	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 237 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	396	ASN
1	I	308	ASN
1	N	363	GLN
1	H	138	ASN
1	H	341	ASN

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 ⓘ

121 carbohydrates 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
5	JHM	A	517	5	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	A	518	5	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
5	JHM	A	519	5	15,15,15	1.15	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	A	520	5	14,15,17	1.91	2 (14%)	14,22,26	2.03	5 (35%)
5	JHM	A	543	5	15,15,15	1.12	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	A	544	5	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	A	545	5	15,15,15	1.15	2 (13%)	22,22,22	1.89	4 (18%)
5	IDS	A	546	5	14,15,17	1.89	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	B	527	5	15,15,15	1.14	2 (13%)	22,22,22	1.87	4 (18%)
5	IDS	B	528	5	14,15,17	1.89	2 (14%)	14,22,26	2.05	5 (35%)
5	JHM	B	529	5	15,15,15	1.13	2 (13%)	22,22,22	1.89	4 (18%)
5	IDS	B	530	5	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
6	JHM	B	533	6	15,15,15	1.16	2 (13%)	22,22,22	1.88	4 (18%)
6	IDS	B	534	6	14,15,17	1.91	2 (14%)	14,22,26	2.03	5 (35%)
6	JHM	B	535	6	15,15,15	1.14	2 (13%)	22,22,22	1.89	4 (18%)
6	IDS	B	536	6	14,15,17	1.91	2 (14%)	14,22,26	2.05	5 (35%)
6	JHM	B	537	6	15,15,15	1.15	2 (13%)	22,22,22	1.87	4 (18%)
6	IDS	B	538	6	14,15,17	1.89	2 (14%)	14,22,26	2.05	5 (35%)
6	JHM	B	539	6	15,15,15	1.14	2 (13%)	22,22,22	1.89	4 (18%)
6	IDS	B	540	6	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
6	JHM	B	541	6	15,15,15	1.14	2 (13%)	22,22,22	1.87	4 (18%)
6	IDS	B	542	6	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
4	JHM	C	531	4	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
4	IDS	C	532	4	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
5	JHM	C	571	5	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
5	IDS	C	572	5	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	C	573	5	15,15,15	1.12	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	C	574	5	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
4	JHM	D	503	4	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
4	IDS	D	504	4	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
4	JHM	D	507	4	15,15,15	1.16	2 (13%)	22,22,22	1.89	4 (18%)
4	IDS	D	508	4	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
4	JHM	D	509	4	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
4	IDS	D	510	4	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
4	JHM	D	521	4	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IDS	D	522	5,4	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
5	JHM	D	523	5,4	15,15,15	1.13	2 (13%)	22,22,22	1.89	4 (18%)
5	IDS	D	524	5	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	D	525	5	15,15,15	1.16	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	D	526	5	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
3	IDS	E	502	3,2	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
3	JHM	E	505	3	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
3	IDS	E	506	3	14,15,17	1.89	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	E	511	5	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	E	512	5	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	E	513	5	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
5	IDS	E	514	5	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
4	JHM	E	515	4	15,15,15	1.12	2 (13%)	22,22,22	1.87	4 (18%)
4	IDS	E	516	4	14,15,17	1.89	2 (14%)	14,22,26	2.03	5 (35%)
7	JHM	E	547	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	E	548	7	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	E	549	7	15,15,15	1.13	2 (13%)	22,22,22	1.89	4 (18%)
7	IDS	E	550	7	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	E	551	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	E	552	7	14,15,17	1.89	2 (14%)	14,22,26	2.02	5 (35%)
7	JHM	F	565	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	F	566	7	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	F	567	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	F	568	7	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
7	JHM	F	569	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	F	570	7	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
6	JHM	F	581	6	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
6	IDS	F	582	6	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
6	JHM	F	583	6	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
6	IDS	F	584	6	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
6	JHM	F	585	6	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
6	IDS	F	586	6	14,15,17	1.89	2 (14%)	14,22,26	2.04	5 (35%)
6	JHM	F	587	6	15,15,15	1.14	2 (13%)	22,22,22	1.87	4 (18%)
6	IDS	F	588	6	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
6	JHM	F	589	6	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	IDS	F	590	6	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
5	JHM	F	591	5	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
5	IDS	F	592	5	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
5	JHM	F	593	5	15,15,15	1.12	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	F	594	5	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	H	575	7	15,15,15	1.15	2 (13%)	22,22,22	1.89	4 (18%)
7	IDS	H	576	7	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
7	JHM	H	577	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	H	578	7	14,15,17	1.89	2 (14%)	14,22,26	2.03	5 (35%)
7	JHM	H	579	7	15,15,15	1.15	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	H	580	7	14,15,17	1.89	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	J	553	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	J	554	7	14,15,17	1.91	2 (14%)	14,22,26	2.05	5 (35%)
7	JHM	J	555	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	J	556	7	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
7	JHM	J	557	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	J	558	7	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	J	559	7	15,15,15	1.12	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	J	560	7	14,15,17	1.89	2 (14%)	14,22,26	2.05	5 (35%)
7	JHM	J	561	7	15,15,15	1.13	2 (13%)	22,22,22	1.89	4 (18%)
7	IDS	J	562	7	14,15,17	1.90	2 (14%)	14,22,26	2.03	5 (35%)
7	JHM	J	563	7	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	J	564	7	14,15,17	1.89	2 (14%)	14,22,26	2.03	5 (35%)
7	JHM	J	595	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	J	596	7	14,15,17	1.91	2 (14%)	14,22,26	2.05	5 (35%)
7	JHM	J	597	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	J	598	7	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	J	599	7	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	J	600	7	14,15,17	1.89	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	L	611	7	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	L	612	7	14,15,17	1.90	2 (14%)	14,22,26	2.06	5 (35%)
7	JHM	L	613	7	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
7	IDS	L	614	7	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
7	JHM	L	615	7	15,15,15	1.14	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	L	616	7	14,15,17	1.91	2 (14%)	14,22,26	2.06	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	JHM	L	617	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	L	618	7	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
7	JHM	L	619	7	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	L	620	7	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
7	JHM	L	621	7	15,15,15	1.14	2 (13%)	22,22,22	1.87	4 (18%)
7	IDS	L	622	7	14,15,17	1.88	2 (14%)	14,22,26	2.05	5 (35%)
4	JHM	N	601	4	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
4	IDS	N	602	4	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	N	607	5	15,15,15	1.13	2 (13%)	22,22,22	1.88	4 (18%)
5	IDS	N	608	5	14,15,17	1.90	2 (14%)	14,22,26	2.05	5 (35%)
5	JHM	N	609	5	15,15,15	1.13	2 (13%)	22,22,22	1.87	4 (18%)
5	IDS	N	610	5	14,15,17	1.89	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	O	603	5	15,15,15	1.12	2 (13%)	22,22,22	1.86	4 (18%)
5	IDS	O	604	5	14,15,17	1.91	2 (14%)	14,22,26	2.04	5 (35%)
5	JHM	O	605	5	15,15,15	1.12	2 (13%)	22,22,22	1.87	4 (18%)
5	IDS	O	606	5	14,15,17	1.90	2 (14%)	14,22,26	2.04	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JHM	A	517	5	-	0/6/22/22	0/1/1/1
5	IDS	A	518	5	1/1/5/7	0/9/22/29	0/1/1/1
5	JHM	A	519	5	-	0/6/22/22	0/1/1/1
5	IDS	A	520	5	-	0/9/22/29	0/1/1/1
5	JHM	A	543	5	-	0/6/22/22	0/1/1/1
5	IDS	A	544	5	-	0/9/22/29	0/1/1/1
5	JHM	A	545	5	-	0/6/22/22	0/1/1/1
5	IDS	A	546	5	-	0/9/22/29	0/1/1/1
5	JHM	B	527	5	-	0/6/22/22	0/1/1/1
5	IDS	B	528	5	-	0/9/22/29	0/1/1/1
5	JHM	B	529	5	-	0/6/22/22	0/1/1/1
5	IDS	B	530	5	-	0/9/22/29	0/1/1/1
6	JHM	B	533	6	-	0/6/22/22	0/1/1/1
6	IDS	B	534	6	1/1/5/7	0/9/22/29	0/1/1/1
6	JHM	B	535	6	-	0/6/22/22	0/1/1/1
6	IDS	B	536	6	-	0/9/22/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	JHM	B	537	6	-	0/6/22/22	0/1/1/1
6	IDS	B	538	6	1/1/5/7	0/9/22/29	0/1/1/1
6	JHM	B	539	6	-	0/6/22/22	0/1/1/1
6	IDS	B	540	6	-	0/9/22/29	0/1/1/1
6	JHM	B	541	6	-	0/6/22/22	0/1/1/1
6	IDS	B	542	6	-	0/9/22/29	0/1/1/1
4	JHM	C	531	4	-	0/6/22/22	0/1/1/1
4	IDS	C	532	4	-	0/9/22/29	0/1/1/1
5	JHM	C	571	5	-	0/6/22/22	0/1/1/1
5	IDS	C	572	5	1/1/5/7	0/9/22/29	0/1/1/1
5	JHM	C	573	5	-	0/6/22/22	0/1/1/1
5	IDS	C	574	5	-	0/9/22/29	0/1/1/1
4	JHM	D	503	4	-	0/6/22/22	0/1/1/1
4	IDS	D	504	4	-	0/9/22/29	0/1/1/1
4	JHM	D	507	4	-	0/6/22/22	0/1/1/1
4	IDS	D	508	4	-	0/9/22/29	0/1/1/1
4	JHM	D	509	4	-	0/6/22/22	0/1/1/1
4	IDS	D	510	4	-	0/9/22/29	0/1/1/1
4	JHM	D	521	4	-	0/6/22/22	0/1/1/1
4	IDS	D	522	5,4	-	0/9/22/29	0/1/1/1
5	JHM	D	523	5,4	-	0/6/22/22	0/1/1/1
5	IDS	D	524	5	-	0/9/22/29	0/1/1/1
5	JHM	D	525	5	-	0/6/22/22	0/1/1/1
5	IDS	D	526	5	-	0/9/22/29	0/1/1/1
3	IDS	E	502	3,2	-	0/9/22/29	0/1/1/1
3	JHM	E	505	3	-	0/6/22/22	0/1/1/1
3	IDS	E	506	3	-	0/9/22/29	0/1/1/1
5	JHM	E	511	5	-	0/6/22/22	0/1/1/1
5	IDS	E	512	5	-	0/9/22/29	0/1/1/1
5	JHM	E	513	5	-	0/6/22/22	0/1/1/1
5	IDS	E	514	5	-	0/9/22/29	0/1/1/1
4	JHM	E	515	4	-	0/6/22/22	0/1/1/1
4	IDS	E	516	4	-	0/9/22/29	0/1/1/1
7	JHM	E	547	7	-	0/6/22/22	0/1/1/1
7	IDS	E	548	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	E	549	7	-	0/6/22/22	0/1/1/1
7	IDS	E	550	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	E	551	7	-	0/6/22/22	0/1/1/1
7	IDS	E	552	7	-	0/9/22/29	0/1/1/1
7	JHM	F	565	7	-	0/6/22/22	0/1/1/1
7	IDS	F	566	7	-	0/9/22/29	0/1/1/1
7	JHM	F	567	7	-	0/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IDS	F	568	7	-	0/9/22/29	0/1/1/1
7	JHM	F	569	7	-	0/6/22/22	0/1/1/1
7	IDS	F	570	7	-	0/9/22/29	0/1/1/1
6	JHM	F	581	6	-	0/6/22/22	0/1/1/1
6	IDS	F	582	6	-	0/9/22/29	0/1/1/1
6	JHM	F	583	6	-	0/6/22/22	0/1/1/1
6	IDS	F	584	6	-	0/9/22/29	0/1/1/1
6	JHM	F	585	6	-	0/6/22/22	0/1/1/1
6	IDS	F	586	6	-	0/9/22/29	0/1/1/1
6	JHM	F	587	6	-	0/6/22/22	0/1/1/1
6	IDS	F	588	6	-	0/9/22/29	0/1/1/1
6	JHM	F	589	6	-	0/6/22/22	0/1/1/1
6	IDS	F	590	6	-	0/9/22/29	0/1/1/1
5	JHM	F	591	5	-	0/6/22/22	0/1/1/1
5	IDS	F	592	5	-	0/9/22/29	0/1/1/1
5	JHM	F	593	5	-	0/6/22/22	0/1/1/1
5	IDS	F	594	5	-	0/9/22/29	0/1/1/1
7	JHM	H	575	7	-	0/6/22/22	0/1/1/1
7	IDS	H	576	7	-	0/9/22/29	0/1/1/1
7	JHM	H	577	7	-	0/6/22/22	0/1/1/1
7	IDS	H	578	7	-	0/9/22/29	0/1/1/1
7	JHM	H	579	7	-	0/6/22/22	0/1/1/1
7	IDS	H	580	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	J	553	7	-	0/6/22/22	0/1/1/1
7	IDS	J	554	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	J	555	7	-	0/6/22/22	0/1/1/1
7	IDS	J	556	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	J	557	7	-	0/6/22/22	0/1/1/1
7	IDS	J	558	7	-	0/9/22/29	0/1/1/1
7	JHM	J	559	7	-	0/6/22/22	0/1/1/1
7	IDS	J	560	7	-	0/9/22/29	0/1/1/1
7	JHM	J	561	7	-	0/6/22/22	0/1/1/1
7	IDS	J	562	7	-	0/9/22/29	0/1/1/1
7	JHM	J	563	7	-	0/6/22/22	0/1/1/1
7	IDS	J	564	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	J	595	7	-	0/6/22/22	0/1/1/1
7	IDS	J	596	7	-	0/9/22/29	0/1/1/1
7	JHM	J	597	7	-	0/6/22/22	0/1/1/1
7	IDS	J	598	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	J	599	7	-	0/6/22/22	0/1/1/1
7	IDS	J	600	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	L	611	7	-	0/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IDS	L	612	7	-	0/9/22/29	0/1/1/1
7	JHM	L	613	7	-	0/6/22/22	0/1/1/1
7	IDS	L	614	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	L	615	7	-	0/6/22/22	0/1/1/1
7	IDS	L	616	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	L	617	7	-	0/6/22/22	0/1/1/1
7	IDS	L	618	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	L	619	7	-	0/6/22/22	0/1/1/1
7	IDS	L	620	7	1/1/5/7	0/9/22/29	0/1/1/1
7	JHM	L	621	7	-	0/6/22/22	0/1/1/1
7	IDS	L	622	7	-	0/9/22/29	0/1/1/1
4	JHM	N	601	4	-	0/6/22/22	0/1/1/1
4	IDS	N	602	4	-	0/9/22/29	0/1/1/1
5	JHM	N	607	5	-	0/6/22/22	0/1/1/1
5	IDS	N	608	5	1/1/5/7	0/9/22/29	0/1/1/1
5	JHM	N	609	5	-	0/6/22/22	0/1/1/1
5	IDS	N	610	5	-	0/9/22/29	0/1/1/1
5	JHM	O	603	5	-	0/6/22/22	0/1/1/1
5	IDS	O	604	5	-	0/9/22/29	0/1/1/1
5	JHM	O	605	5	-	0/6/22/22	0/1/1/1
5	IDS	O	606	5	-	0/9/22/29	0/1/1/1

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	594	IDS	O2-C2	-4.91	1.37	1.46
7	J	596	IDS	O2-C2	-4.90	1.37	1.46
5	A	544	IDS	O2-C2	-4.89	1.37	1.46
7	J	598	IDS	O2-C2	-4.88	1.37	1.46
5	D	526	IDS	O2-C2	-4.88	1.37	1.46

The worst 5 of 545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	549	JHM	C6-O6-S	6.92	125.67	116.76
6	B	539	JHM	C6-O6-S	6.91	125.65	116.76
7	J	561	JHM	C6-O6-S	6.91	125.65	116.76
5	D	523	JHM	C6-O6-S	6.90	125.63	116.76
7	F	567	JHM	C6-O6-S	6.90	125.63	116.76

5 of 17 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	J	556	IDS	C4
7	L	614	IDS	C4
7	L	616	IDS	C4
7	J	554	IDS	C4
7	L	620	IDS	C4

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry i

1 ligand is 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	JHM	E	501	3	15,15,15	1.14	2 (13%)	22,22,22	1.88	4 (18%)

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	JHM	E	501	3	-	0/6/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	JHM	O1-C1	2.65	1.45	1.39
2	E	501	JHM	C3-C4	2.26	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	JHM	C6-O6-S	6.87	125.60	116.76
2	E	501	JHM	C3-C4-C5	-3.10	106.75	109.92
2	E	501	JHM	C2-C3-C4	-2.56	107.16	110.61
2	E	501	JHM	C1-C2-C3	-2.38	107.03	111.16

There are no chirality outliers.

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, 95th 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 ²)	Q<0.9
1	A	422/427 (98%)	-0.06	4 (0%)	81 47	13, 51, 103, 135	0
1	B	422/427 (98%)	-0.05	5 (1%)	75 39	12, 49, 101, 134	0
1	C	422/427 (98%)	-0.09	8 (1%)	64 29	11, 44, 102, 137	0
1	D	422/427 (98%)	-0.11	4 (0%)	81 47	11, 43, 96, 137	0
1	E	422/427 (98%)	-0.12	1 (0%)	93 77	11, 44, 101, 137	0
1	F	422/427 (98%)	-0.09	3 (0%)	84 52	13, 51, 103, 143	0
1	G	422/427 (98%)	0.01	9 (2%)	60 27	15, 52, 102, 124	0
1	H	422/427 (98%)	-0.08	9 (2%)	60 27	11, 42, 99, 141	0
1	I	422/427 (98%)	-0.12	3 (0%)	84 52	12, 43, 97, 135	0
1	J	422/427 (98%)	-0.01	3 (0%)	84 52	11, 48, 102, 131	0
1	K	422/427 (98%)	-0.06	2 (0%)	88 61	14, 52, 99, 140	0
1	L	422/427 (98%)	0.05	9 (2%)	60 27	14, 50, 104, 131	0
1	M	422/427 (98%)	-0.04	7 (1%)	67 31	12, 50, 101, 130	0
1	N	422/427 (98%)	-0.10	1 (0%)	93 77	16, 55, 99, 135	0
1	O	421/427 (98%)	-0.01	8 (1%)	64 29	12, 51, 102, 136	0
All	All	6329/6405 (98%)	-0.06	76 (1%)	75 39	11, 48, 102, 143	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	138	ASN	8.3
1	G	174	ALA	5.5
1	L	136	THR	5.2
1	D	134	ALA	5.1
1	H	135	ALA	4.8

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 ⓘ

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, 95th 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(Å ²)	Q<0.9
5	IDS	O	604	15/17	0.87	439.67	26,28,35,39	0
6	JHM	F	589	15/15	0.73	187.82	42,62,84,85	0
5	JHM	C	573	15/15	0.68	87.55	42,62,84,85	0
5	JHM	O	603	15/15	0.79	29.48	42,62,84,85	0
6	IDS	F	590	15/17	0.62	29.44	26,28,35,39	0
7	JHM	E	549	15/15	0.74	25.57	42,62,84,85	0
7	JHM	J	599	15/15	0.54	23.70	42,62,84,85	0
7	IDS	J	556	15/17	0.74	21.18	26,28,35,39	0
7	IDS	L	618	15/17	0.53	19.39	26,28,35,39	0
6	JHM	F	587	15/15	0.59	19.03	42,62,84,85	0
4	IDS	D	510	15/17	0.78	19.01	26,28,35,39	0
5	IDS	B	530	15/17	0.54	18.02	26,28,35,39	0
7	JHM	H	579	15/15	0.52	17.01	42,62,84,85	0
7	JHM	E	547	15/15	0.84	16.13	42,62,84,85	0
5	JHM	A	519	15/15	0.55	14.47	42,62,84,85	0
7	IDS	J	598	15/17	0.69	14.34	26,28,35,39	0
4	IDS	N	602	15/17	0.62	13.85	26,28,35,39	0
7	IDS	E	548	15/17	0.68	13.41	26,28,35,39	0
7	IDS	J	564	15/17	0.52	13.01	26,28,35,39	0
6	IDS	F	588	15/17	0.50	12.09	26,28,35,39	0
7	IDS	F	568	15/17	0.64	11.49	26,28,35,39	0
5	JHM	D	525	15/15	0.43	11.46	42,62,84,85	0
7	IDS	J	600	15/17	0.55	11.22	26,28,35,39	0
7	JHM	J	561	15/15	0.49	10.78	42,62,84,85	0
3	JHM	E	505	15/15	0.57	10.16	42,62,84,85	0
7	JHM	J	553	15/15	0.51	10.15	42,62,84,85	0
5	IDS	C	572	15/17	0.64	10.04	26,28,35,39	0
4	JHM	D	509	15/15	0.55	9.66	42,62,84,85	0
6	JHM	F	581	15/15	0.75	9.58	42,62,84,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	JHM	N	607	15/15	0.59	9.16	42,62,84,85	0
5	IDS	D	524	15/17	0.51	8.62	26,28,35,39	0
7	JHM	H	575	15/15	0.89	8.50	42,62,84,85	0
5	IDS	A	518	15/17	0.56	8.46	26,28,35,39	0
7	JHM	J	597	15/15	0.50	8.43	42,62,84,85	0
4	JHM	D	503	15/15	0.74	8.35	42,62,84,85	0
4	IDS	D	504	15/17	0.53	8.00	26,28,35,39	0
6	JHM	B	537	15/15	0.51	7.97	42,62,84,85	0
4	JHM	E	515	15/15	0.53	7.80	42,62,84,85	0
6	JHM	F	583	15/15	0.69	7.71	42,62,84,85	0
7	JHM	J	595	15/15	0.54	7.60	42,62,84,85	0
7	JHM	J	555	15/15	0.68	7.59	42,62,84,85	0
7	IDS	H	578	15/17	0.83	7.54	26,28,35,39	0
6	JHM	F	585	15/15	0.71	7.43	42,62,84,85	0
7	JHM	F	565	15/15	0.60	7.18	42,62,84,85	0
3	IDS	E	502	15/17	0.49	7.11	26,28,35,39	0
7	JHM	L	619	15/15	0.52	7.00	42,62,84,85	0
7	JHM	H	577	15/15	0.74	6.96	42,62,84,85	0
5	IDS	N	610	15/17	0.69	6.87	26,28,35,39	0
5	IDS	D	526	15/17	0.50	6.84	26,28,35,39	0
5	JHM	D	523	15/15	0.56	6.73	42,62,84,85	0
7	IDS	J	554	15/17	0.49	6.64	26,28,35,39	0
4	JHM	D	521	15/15	0.59	6.23	42,62,84,85	0
5	IDS	A	520	15/17	0.46	6.06	26,28,35,39	0
6	IDS	F	584	15/17	0.82	5.90	26,28,35,39	0
7	IDS	H	576	15/17	0.65	5.87	26,28,35,39	0
7	IDS	F	570	15/17	0.62	5.74	26,28,35,39	0
4	IDS	D	508	15/17	0.54	5.44	26,28,35,39	0
7	JHM	J	563	15/15	0.58	5.35	42,62,84,85	0
4	JHM	D	507	15/15	0.72	5.24	42,62,84,85	0
7	JHM	L	615	15/15	0.69	5.15	42,62,84,85	0
7	IDS	E	550	15/17	0.66	5.04	26,28,35,39	0
4	JHM	N	601	15/15	0.63	4.97	42,62,84,85	0
3	IDS	E	506	15/17	0.74	4.92	26,28,35,39	0
7	JHM	F	567	15/15	0.47	4.80	42,62,84,85	0
7	IDS	H	580	15/17	0.71	4.67	26,28,35,39	0
5	IDS	N	608	15/17	0.63	4.66	26,28,35,39	0
6	IDS	F	586	15/17	0.58	4.55	26,28,35,39	0
5	JHM	E	511	15/15	0.51	4.29	42,62,84,85	0
4	IDS	D	522	15/17	0.54	4.23	26,28,35,39	0
4	IDS	C	532	15/17	0.73	4.09	26,28,35,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	JHM	L	613	15/15	0.41	4.04	42,62,84,85	0
6	IDS	B	542	15/17	0.71	3.87	26,28,35,39	0
5	JHM	O	605	15/15	0.79	3.74	42,62,84,85	0
6	IDS	B	534	15/17	0.50	3.74	26,28,35,39	0
5	JHM	B	529	15/15	0.68	3.70	42,62,84,85	0
5	JHM	C	571	15/15	0.57	3.56	42,62,84,85	0
7	JHM	F	569	15/15	0.51	3.13	42,62,84,85	0
5	IDS	C	574	15/17	0.58	3.11	26,28,35,39	0
5	JHM	A	517	15/15	0.42	2.79	42,62,84,85	0
7	IDS	J	596	15/17	0.52	2.74	26,28,35,39	0
5	JHM	B	527	15/15	0.47	2.72	42,62,84,85	0
5	IDS	B	528	15/17	0.47	2.49	26,28,35,39	0
6	JHM	B	541	15/15	0.51	2.45	42,62,84,85	0
7	IDS	L	616	15/17	0.46	2.40	26,28,35,39	0
5	IDS	O	606	15/17	0.62	2.15	26,28,35,39	0
5	IDS	A	546	15/17	0.52	2.14	26,28,35,39	0
4	JHM	C	531	15/15	0.56	2.12	42,62,84,85	0
7	JHM	L	611	15/15	0.55	2.01	42,62,84,85	0
7	IDS	L	614	15/17	0.44	2.00	26,28,35,39	0
5	IDS	A	544	15/17	0.49	1.88	26,28,35,39	0
7	JHM	L	617	15/15	0.46	1.88	42,62,84,85	0
5	JHM	N	609	15/15	0.62	1.80	42,62,84,85	0
7	IDS	J	562	15/17	0.59	1.66	26,28,35,39	0
5	IDS	E	514	15/17	0.55	1.65	26,28,35,39	0
5	IDS	F	592	15/17	0.53	1.59	26,28,35,39	0
5	JHM	F	593	15/15	0.61	1.53	42,62,84,85	0
5	IDS	F	594	15/17	0.55	1.38	26,28,35,39	0
5	JHM	A	543	15/15	0.45	1.13	42,62,84,85	0
5	JHM	F	591	15/15	0.50	0.71	42,62,84,85	0
7	IDS	L	612	15/17	0.44	0.53	26,28,35,39	0
6	JHM	B	539	15/15	0.61	-	42,62,84,85	0
6	IDS	B	538	15/17	0.60	-	26,28,35,39	0
7	IDS	F	566	15/17	0.65	-	26,28,35,39	0
7	JHM	E	551	15/15	0.66	-	42,62,84,85	0
7	JHM	J	557	15/15	0.68	-	42,62,84,85	0
7	IDS	L	622	15/17	0.64	-	26,28,35,39	0
7	JHM	L	621	15/15	0.50	-	42,62,84,85	0
5	JHM	A	545	15/15	0.56	-	42,62,84,85	0
6	JHM	B	533	15/15	0.82	-	42,62,84,85	0
7	IDS	L	620	15/17	0.59	-	26,28,35,39	0
6	IDS	F	582	15/17	0.65	-	26,28,35,39	0
7	IDS	J	560	15/17	0.60	-	26,28,35,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	IDS	B	540	15/17	0.53	-	26,28,35,39	0
7	IDS	J	558	15/17	0.83	-	26,28,35,39	0
7	IDS	E	552	15/17	0.50	-	26,28,35,39	0
6	JHM	B	535	15/15	0.58	-	42,62,84,85	0
5	IDS	E	512	15/17	0.69	-	26,28,35,39	0
7	JHM	J	559	15/15	0.69	-	42,62,84,85	0
6	IDS	B	536	15/17	0.61	-	26,28,35,39	0
4	IDS	E	516	15/17	0.55	-	26,28,35,39	0
5	JHM	E	513	15/15	0.56	-	42,62,84,85	0

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, 95th 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(\AA^2)	Q<0.9
2	JHM	E	501	15/15	0.45	33.56	42,62,84,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.