



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:09 PM GMT

PDB ID : 3W9T
Title : pore-forming CEL-III
Authors : Unno, H.; Goda, S.; Hatakeyama, T.
Deposited on : 2013-04-16
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

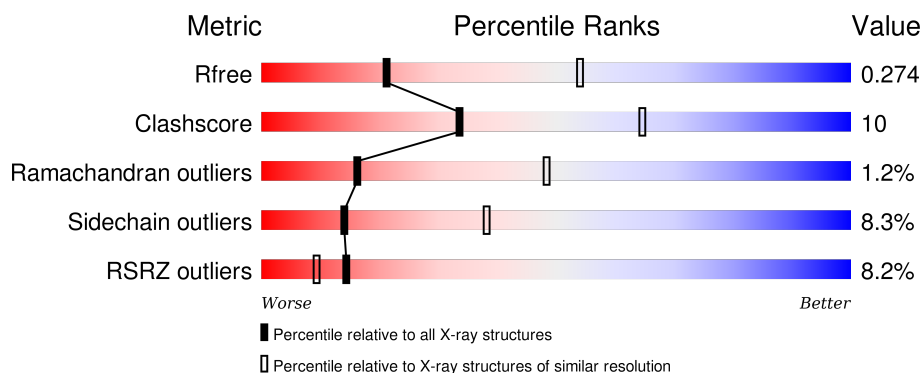
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	<div> <div>7%</div> <div>73% 23% . .</div> </div>
1	B	432	<div> <div>7%</div> <div>75% 20% .</div> </div>
1	C	432	<div> <div>6%</div> <div>76% 20% . .</div> </div>
1	D	432	<div> <div>7%</div> <div>78% 18% .</div> </div>
1	E	432	<div> <div>8%</div> <div>78% 18% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	432	
1	G	432	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	W9T	E	505	-	-	-	X
2	W9T	G	505	-	-	-	X
3	CA	C	1014	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24175 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemolytic lectin CEL-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	C	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	G	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	B	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	F	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	E	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	D	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	-	EXPRESSION TAG	UNP Q868M7
A	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
A	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
A	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
A	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
A	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
A	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
A	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
A	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
A	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
A	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
A	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
A	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
A	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
C	1	PCA	-	EXPRESSION TAG	UNP Q868M7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
C	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
C	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
C	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
C	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
C	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
C	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
C	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
C	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
C	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
C	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
C	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
C	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
G	1	PCA	-	EXPRESSION TAG	UNP Q868M7
G	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
G	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
G	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
G	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
G	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
G	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
G	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
G	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
G	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
G	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
G	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
G	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
G	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
B	1	PCA	-	EXPRESSION TAG	UNP Q868M7
B	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
B	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
B	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
B	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
B	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
B	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
B	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
B	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
B	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
B	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
B	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
B	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
B	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
F	1	PCA	-	EXPRESSION TAG	UNP Q868M7

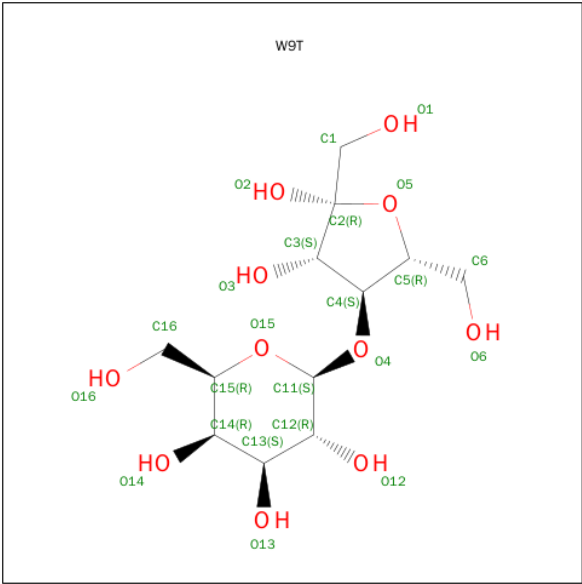
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Chain	Residue	Modelled	Actual	Comment	Reference
F	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
F	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
F	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
F	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
F	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
F	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
F	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
F	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
F	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
F	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
F	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
F	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
F	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
E	1	PCA	-	EXPRESSION TAG	UNP Q868M7
E	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
E	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
E	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
E	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
E	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
E	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
E	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
E	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
E	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
E	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
E	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
E	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
E	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
D	1	PCA	-	EXPRESSION TAG	UNP Q868M7
D	15	SER	ASN	ENGINEERED MUTATION	UNP Q868M7
D	16	PHE	TYR	ENGINEERED MUTATION	UNP Q868M7
D	36	TYR	HIS	ENGINEERED MUTATION	UNP Q868M7
D	48	ILE	MET	ENGINEERED MUTATION	UNP Q868M7
D	92	GLN	LEU	ENGINEERED MUTATION	UNP Q868M7
D	95	ARG	LYS	ENGINEERED MUTATION	UNP Q868M7
D	97	THR	ALA	ENGINEERED MUTATION	UNP Q868M7
D	122	ILE	VAL	ENGINEERED MUTATION	UNP Q868M7
D	146	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7
D	173	ASP	GLU	ENGINEERED MUTATION	UNP Q868M7
D	204	SER	GLN	ENGINEERED MUTATION	UNP Q868M7
D	340	THR	SER	ENGINEERED MUTATION	UNP Q868M7
D	404	VAL	ILE	ENGINEERED MUTATION	UNP Q868M7

- Molecule 2 is 4-O-BETA-D-GALACTOPYRANOSYL-BETA-D-FRUCTOFURANOSE

(three-letter code: W9T) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			23	12	11		
2	G	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	6	Total	Ca	0	0
			6	6		
3	D	6	Total	Ca	0	0
			6	6		
3	E	7	Total	Ca	0	0
			7	7		
3	B	6	Total	Ca	0	0
			6	6		
3	C	7	Total	Ca	0	0
			7	7		
3	A	6	Total	Ca	0	0
			6	6		
3	F	6	Total	Ca	0	0
			6	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

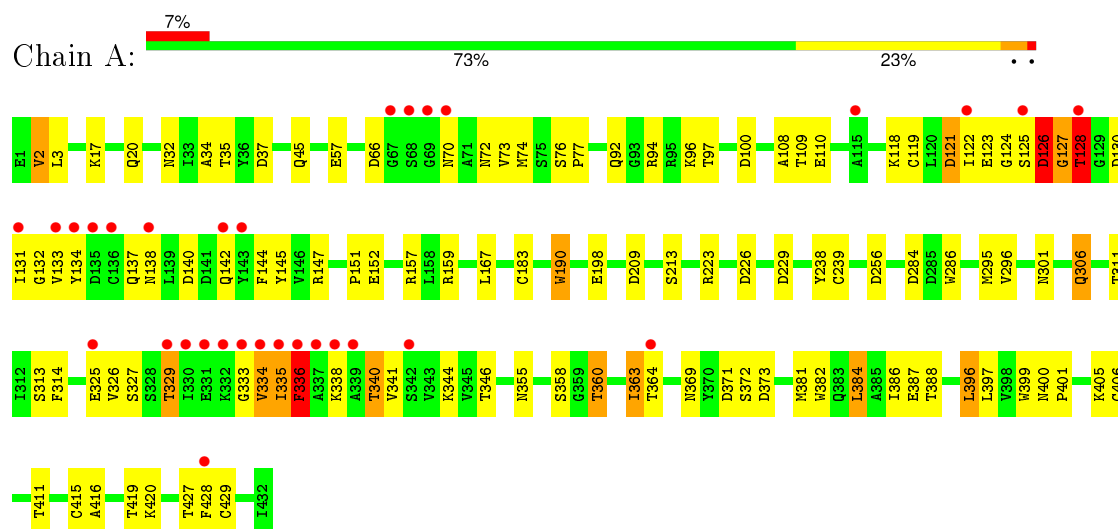
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	C	9	Total 9	O 9	0	0
5	G	5	Total 5	O 5	0	0
5	B	14	Total 14	O 14	0	0
5	F	13	Total 13	O 13	0	0
5	E	10	Total 10	O 10	0	0
5	D	14	Total 14	O 14	0	0

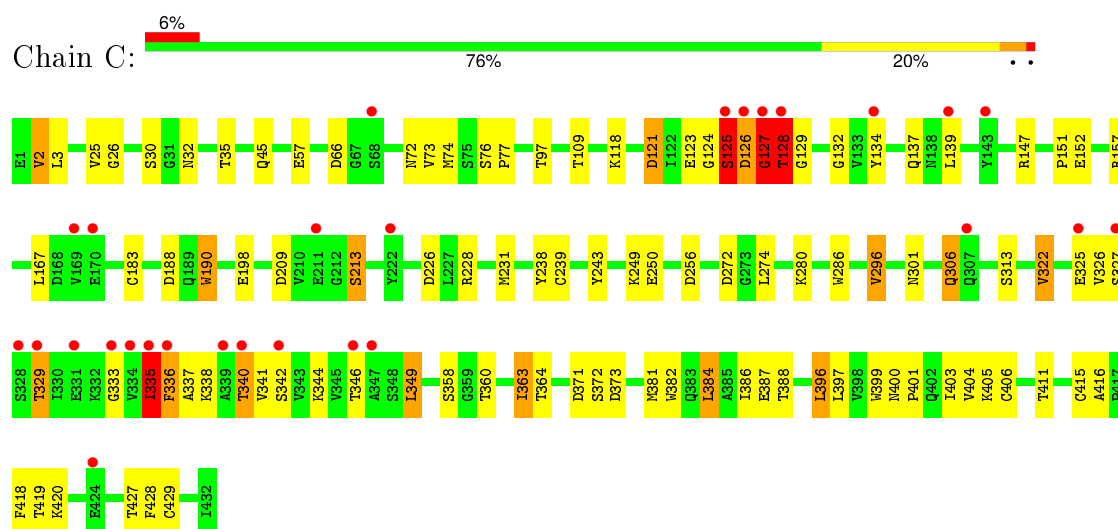
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 ($\text{RSRZ} > 2$). 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.

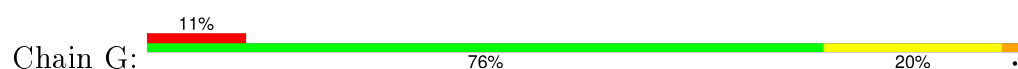
• Molecule 1: Hemolytic lectin CEL-III

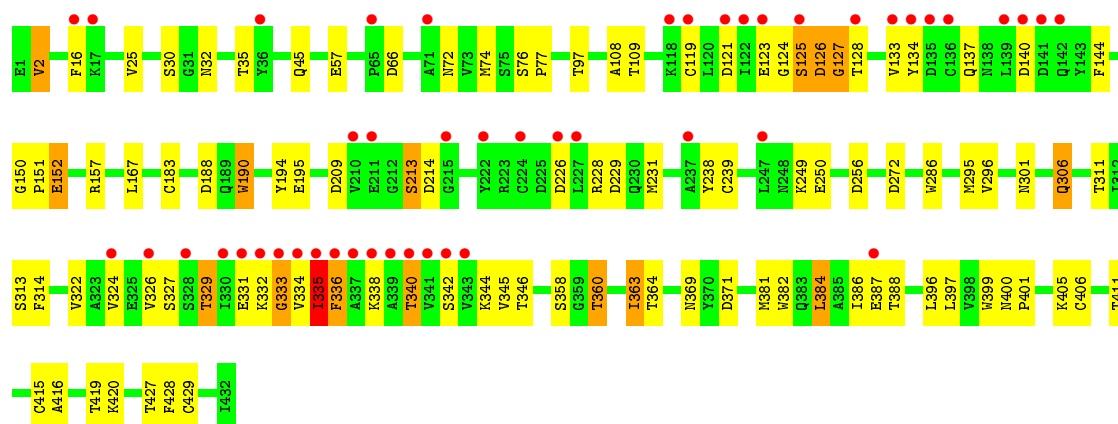


• Molecule 1: Hemolytic lectin CEL-III

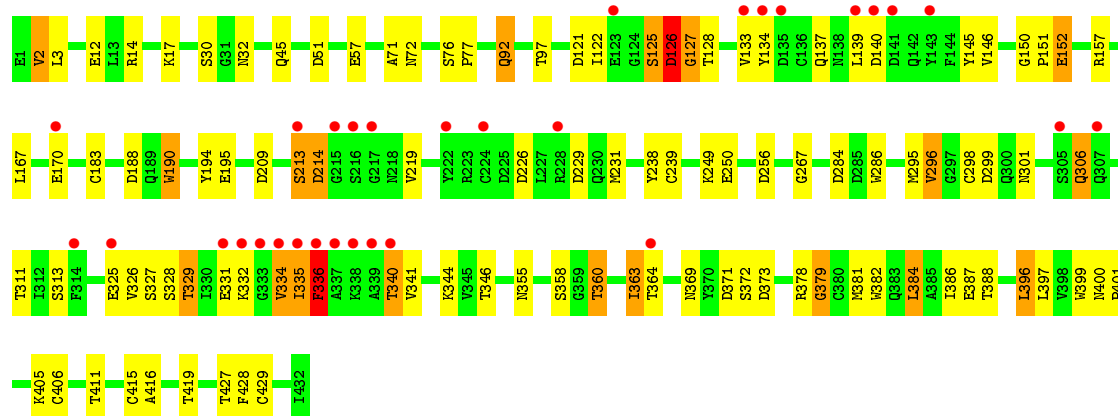
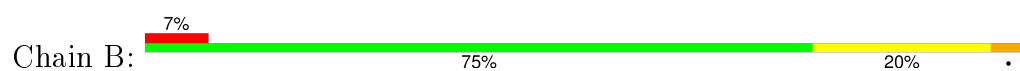


• Molecule 1: Hemolytic lectin CEL-III

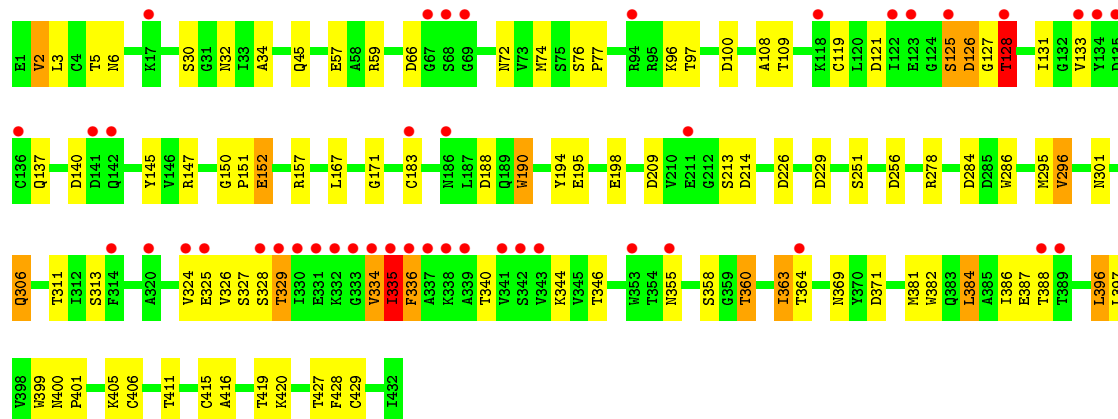
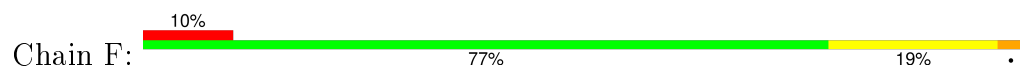




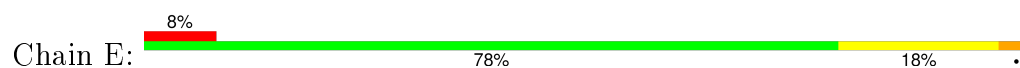
• Molecule 1: Hemolytic lectin CEL-III

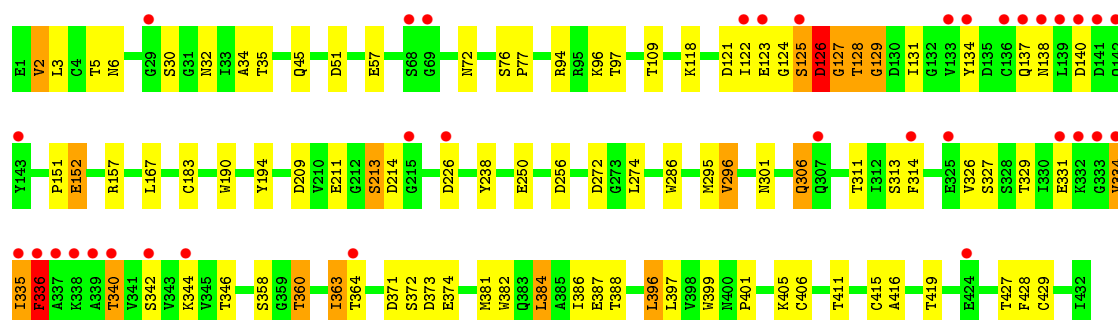


• Molecule 1: Hemolytic lectin CEL-III

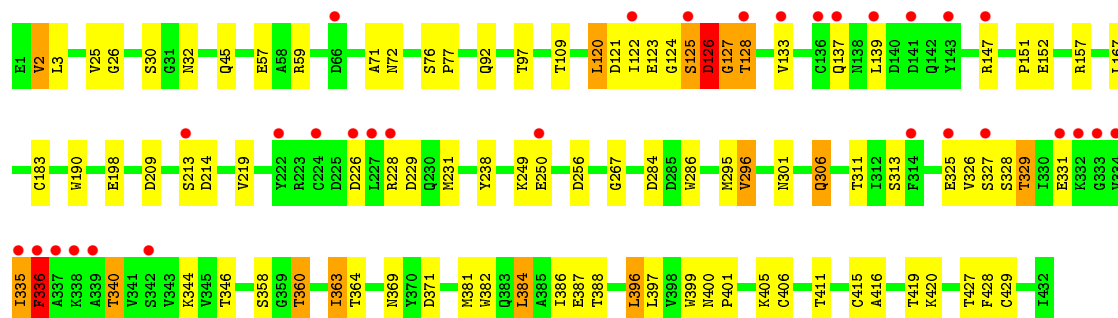
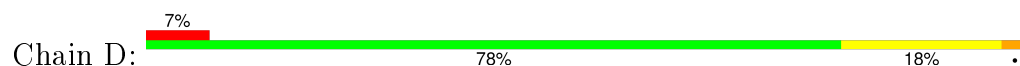


• Molecule 1: Hemolytic lectin CEL-III





• Molecule 1: Hemolytic lectin CEL-III



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.80Å 228.65Å 133.02Å 90.00° 127.13° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.90) 98.4 (48.20-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.273 0.239 , 0.274	Depositor DCC
R_{free} test set	5793 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
Estimated twinning fraction	0.000 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 113677 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24175	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, W9T, PCA, MG

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	0.47	1/3366 (0.0%)	0.70	3/4566 (0.1%)
1	B	0.47	1/3366 (0.0%)	0.72	4/4566 (0.1%)
1	C	0.46	0/3366	0.71	5/4566 (0.1%)
1	D	0.45	0/3366	0.68	2/4566 (0.0%)
1	E	0.47	0/3366	0.69	2/4566 (0.0%)
1	F	0.49	0/3366	0.70	2/4566 (0.0%)
1	G	0.45	0/3366	0.71	1/4566 (0.0%)
All	All	0.47	2/23562 (0.0%)	0.70	19/31962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
1	G	0	4
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	CG-OD2	-7.12	1.08	1.25
1	B	379	GLY	N-CA	-5.95	1.37	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CB-CG-OD1	13.30	130.27	118.30
1	C	128	THR	N-CA-C	-10.58	82.44	111.00
1	B	378	ARG	C-N-CA	9.70	142.68	122.30
1	A	126	ASP	OD1-CG-OD2	-8.37	107.39	123.30
1	B	378	ARG	CA-C-N	7.94	132.07	116.20

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PRO	Peptide
1	A	335	ILE	Peptide
1	C	125	SER	Peptide
1	C	127	GLY	Peptide
1	C	151	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3313	0	3083	92	2
1	B	3313	0	3082	90	1
1	C	3313	0	3083	90	0
1	D	3313	0	3082	69	1
1	E	3313	0	3083	71	1
1	F	3313	0	3083	77	0
1	G	3313	0	3083	79	0
2	A	115	0	107	3	0
2	B	138	0	128	6	0
2	C	115	0	106	8	0
2	D	115	0	106	4	0
2	E	138	0	129	11	0
2	F	115	0	108	8	0
2	G	115	0	105	5	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	7	0	0	0	2
3	D	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	7	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
5	A	10	0	0	1	0
5	B	14	0	0	0	0
5	C	9	0	0	1	0
5	D	14	0	0	0	0
5	E	10	0	0	0	0
5	F	13	0	0	0	0
5	G	5	0	0	0	0
All	All	24175	0	22368	472	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 472 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:THR:HG23	1:B:329:THR:HG23	1.12	1.07
1:B:125:SER:HB3	1:B:139:LEU:HD13	1.39	1.05
1:E:340:THR:HG23	1:D:329:THR:HG23	1.42	1.02
2:E:506:W9T:O15	2:E:506:W9T:H17	1.61	0.97
1:E:6:ASN:HB2	2:E:506:W9T:H3	1.50	0.92

All (4) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:C	3:C:1014:CA:CA[4_555]	1.19	1.01
1:A:127:GLY:CA	3:C:1014:CA:CA[4_555]	1.68	0.52
1:E:211:GLU:OE2	1:E:211:GLU:OE2[2_654]	1.69	0.51
1:B:127:GLY:O	1:D:123:GLU:OE2[4_555]	2.07	0.13

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	430/432 (100%)	407 (95%)	18 (4%)	5 (1%)	16	48
1	B	430/432 (100%)	410 (95%)	16 (4%)	4 (1%)	21	57
1	C	430/432 (100%)	410 (95%)	13 (3%)	7 (2%)	12	40
1	D	430/432 (100%)	411 (96%)	15 (4%)	4 (1%)	21	57
1	E	430/432 (100%)	408 (95%)	17 (4%)	5 (1%)	16	48
1	F	430/432 (100%)	410 (95%)	15 (4%)	5 (1%)	16	48
1	G	430/432 (100%)	411 (96%)	12 (3%)	7 (2%)	12	40
All	All	3010/3024 (100%)	2867 (95%)	106 (4%)	37 (1%)	16	48

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	ASP
1	C	128	THR
1	C	336	PHE
1	G	126	ASP
1	G	336	PHE

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	370/370 (100%)	340 (92%)	30 (8%)	15	39
1	B	370/370 (100%)	337 (91%)	33 (9%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	370/370 (100%)	340 (92%)	30 (8%)	15	39
1	D	370/370 (100%)	337 (91%)	33 (9%)	12	35
1	E	370/370 (100%)	339 (92%)	31 (8%)	14	37
1	F	370/370 (100%)	341 (92%)	29 (8%)	16	41
1	G	370/370 (100%)	340 (92%)	30 (8%)	15	39
All	All	2590/2590 (100%)	2374 (92%)	216 (8%)	14	38

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	137	GLN
1	B	397	LEU
1	D	256	ASP
1	B	190	TRP
1	B	334	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	301	ASN
1	F	138	ASN
1	D	270	GLN
1	B	306	GLN
1	F	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PCA	A	1	1	7,8,9	0.52	0	9,10,12	2.24	2 (22%)
1	PCA	B	1	1	7,8,9	0.46	0	9,10,12	2.11	2 (22%)
1	PCA	C	1	1	7,8,9	0.48	0	9,10,12	2.22	2 (22%)
1	PCA	D	1	1	7,8,9	0.58	0	9,10,12	2.21	2 (22%)
1	PCA	E	1	1	7,8,9	0.42	0	9,10,12	2.30	2 (22%)
1	PCA	F	1	1	7,8,9	0.46	0	9,10,12	2.16	2 (22%)
1	PCA	G	1	1	7,8,9	0.60	0	9,10,12	2.10	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	F	1	1	-	0/0/11/13	0/1/1/1
1	PCA	G	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	PCA	CA-N-CD	-4.48	98.79	113.81
1	A	1	PCA	CA-N-CD	-4.09	100.12	113.81
1	C	1	PCA	CA-N-CD	-3.88	100.80	113.81
1	E	1	PCA	CA-N-CD	-3.88	100.81	113.81
1	B	1	PCA	CA-N-CD	-3.81	101.05	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 95 ligands modelled in this entry, 58 are monoatomic - leaving 37 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$
2	W9T	A	1001	3	23,24,24	0.58	0	28,36,36	1.21	2 (7%)
2	W9T	A	1002	3	23,24,24	0.67	0	28,36,36	1.30	3 (10%)
2	W9T	A	1003	3	23,24,24	0.51	0	28,36,36	0.86	2 (7%)
2	W9T	A	1004	3	23,24,24	0.59	1 (4%)	28,36,36	0.95	0
2	W9T	A	1012	3	23,24,24	0.50	0	28,36,36	0.90	0
2	W9T	B	501	3	23,24,24	0.61	0	28,36,36	1.18	2 (7%)
2	W9T	B	502	3	23,24,24	0.73	0	28,36,36	1.46	4 (14%)
2	W9T	B	503	3	23,24,24	0.54	0	28,36,36	0.90	1 (3%)
2	W9T	B	504	3	23,24,24	0.60	0	28,36,36	1.73	6 (21%)
2	W9T	B	507	3	23,24,24	0.54	0	28,36,36	1.41	2 (7%)
2	W9T	B	513	-	23,24,24	0.83	1 (4%)	28,36,36	2.17	6 (21%)
2	W9T	C	1001	3	23,24,24	0.77	0	28,36,36	1.45	3 (10%)
2	W9T	C	1002	3	23,24,24	0.53	0	28,36,36	1.17	2 (7%)
2	W9T	C	1003	3	23,24,24	0.59	0	28,36,36	1.23	2 (7%)
2	W9T	C	1004	3	23,24,24	0.60	0	28,36,36	1.47	5 (17%)
2	W9T	C	1005	3	23,24,24	0.65	0	28,36,36	0.84	1 (3%)
2	W9T	D	501	3	23,24,24	0.60	1 (4%)	28,36,36	1.05	1 (3%)
2	W9T	D	502	3	23,24,24	0.60	0	28,36,36	1.15	2 (7%)
2	W9T	D	506	3	23,24,24	0.59	0	28,36,36	0.98	0
2	W9T	D	507	3	23,24,24	0.59	0	28,36,36	1.43	4 (14%)
2	W9T	D	512	3	23,24,24	0.45	0	28,36,36	1.24	3 (10%)
2	W9T	E	501	3	23,24,24	0.63	0	28,36,36	1.27	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	W9T	E	502	3	23,24,24	0.58	0	28,36,36	1.13	2 (7%)
2	W9T	E	503	3	23,24,24	0.61	1 (4%)	28,36,36	1.09	3 (10%)
2	W9T	E	504	3	23,24,24	0.63	0	28,36,36	1.04	1 (3%)
2	W9T	E	505	3	23,24,24	0.63	0	28,36,36	1.24	4 (14%)
2	W9T	E	506	-	23,24,24	0.61	0	28,36,36	1.64	6 (21%)
2	W9T	F	501	3	23,24,24	0.64	0	28,36,36	0.94	1 (3%)
2	W9T	F	502	3	23,24,24	0.60	0	28,36,36	0.78	1 (3%)
2	W9T	F	503	3	23,24,24	0.81	1 (4%)	28,36,36	1.61	5 (17%)
2	W9T	F	504	3	23,24,24	0.57	0	28,36,36	0.98	2 (7%)
2	W9T	F	512	-	23,24,24	0.80	0	28,36,36	1.82	9 (32%)
2	W9T	G	501	3	23,24,24	0.55	0	28,36,36	0.89	2 (7%)
2	W9T	G	502	3	23,24,24	0.59	0	28,36,36	0.94	1 (3%)
2	W9T	G	503	3	23,24,24	0.55	0	28,36,36	1.49	4 (14%)
2	W9T	G	504	3	23,24,24	0.53	0	28,36,36	0.93	1 (3%)
2	W9T	G	505	3	23,24,24	0.56	0	28,36,36	1.28	3 (10%)

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	W9T	A	1001	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1002	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1003	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1004	3	-	0/11/50/50	0/2/2/2
2	W9T	A	1012	3	-	0/11/50/50	0/2/2/2
2	W9T	B	501	3	-	0/11/50/50	0/2/2/2
2	W9T	B	502	3	-	0/11/50/50	0/2/2/2
2	W9T	B	503	3	-	0/11/50/50	0/2/2/2
2	W9T	B	504	3	-	0/11/50/50	0/2/2/2
2	W9T	B	507	3	-	0/11/50/50	0/2/2/2
2	W9T	B	513	-	-	0/11/50/50	0/2/2/2
2	W9T	C	1001	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1002	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1003	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1004	3	-	0/11/50/50	0/2/2/2
2	W9T	C	1005	3	-	0/11/50/50	0/2/2/2
2	W9T	D	501	3	-	0/11/50/50	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	W9T	D	502	3	-	0/11/50/50	0/2/2/2
2	W9T	D	506	3	-	0/11/50/50	0/2/2/2
2	W9T	D	507	3	-	0/11/50/50	0/2/2/2
2	W9T	D	512	3	-	0/11/50/50	0/2/2/2
2	W9T	E	501	3	-	0/11/50/50	0/2/2/2
2	W9T	E	502	3	-	0/11/50/50	0/2/2/2
2	W9T	E	503	3	-	0/11/50/50	0/2/2/2
2	W9T	E	504	3	-	0/11/50/50	0/2/2/2
2	W9T	E	505	3	-	0/11/50/50	0/2/2/2
2	W9T	E	506	-	-	0/11/50/50	0/2/2/2
2	W9T	F	501	3	-	0/11/50/50	0/2/2/2
2	W9T	F	502	3	-	0/11/50/50	0/2/2/2
2	W9T	F	503	3	-	0/11/50/50	0/2/2/2
2	W9T	F	504	3	-	0/11/50/50	0/2/2/2
2	W9T	F	512	-	-	0/11/50/50	0/2/2/2
2	W9T	G	501	3	-	0/11/50/50	0/2/2/2
2	W9T	G	502	3	-	0/11/50/50	0/2/2/2
2	W9T	G	503	3	-	0/11/50/50	0/2/2/2
2	W9T	G	504	3	-	0/11/50/50	0/2/2/2
2	W9T	G	505	3	-	0/11/50/50	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	W9T	O2-C2	2.00	1.44	1.41
2	B	513	W9T	O2-C2	2.02	1.44	1.41
2	A	1004	W9T	O2-C2	2.02	1.44	1.41
2	E	503	W9T	O2-C2	2.05	1.44	1.41
2	F	503	W9T	O2-C2	2.06	1.44	1.41

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	513	W9T	C11-O15-C15	-7.51	99.17	113.75
2	E	506	W9T	O13-C13-C12	-4.14	101.03	110.34
2	C	1003	W9T	C11-O4-C4	-3.94	107.71	118.01
2	F	503	W9T	O4-C11-O15	-3.78	101.11	110.68
2	B	507	W9T	C11-O4-C4	-3.64	108.50	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	W9T	3	0
2	B	502	W9T	2	0
2	B	504	W9T	2	0
2	B	513	W9T	2	0
2	C	1001	W9T	2	0
2	C	1004	W9T	6	0
2	D	502	W9T	2	0
2	D	506	W9T	2	0
2	E	505	W9T	3	0
2	E	506	W9T	8	0
2	F	503	W9T	3	0
2	F	512	W9T	5	0
2	G	504	W9T	1	0
2	G	505	W9T	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	431/432 (99%)	0.60	31 (7%) 18 12	42, 73, 121, 211	0
1	B	431/432 (99%)	0.52	31 (7%) 18 12	44, 73, 111, 196	0
1	C	431/432 (99%)	0.50	28 (6%) 22 16	47, 75, 114, 165	0
1	D	431/432 (99%)	0.48	31 (7%) 18 12	43, 77, 119, 218	0
1	E	431/432 (99%)	0.60	35 (8%) 15 9	45, 73, 123, 193	0
1	F	431/432 (99%)	0.68	43 (9%) 9 5	46, 74, 137, 209	0
1	G	431/432 (99%)	0.84	47 (10%) 7 4	43, 77, 138, 211	0
All	All	3017/3024 (99%)	0.60	246 (8%) 14 9	42, 75, 124, 218	0

The worst 5 of 246 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	334	VAL	12.9
1	G	337	ALA	12.0
1	E	335	ILE	11.6
1	G	334	VAL	11.3
1	G	333	GLY	10.6

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

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PCA	F	1	8/9	0.82	0.25	-	65,67,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	PCA	G	1	8/9	0.93	0.24	-	74,76,80,81	0
1	PCA	E	1	8/9	0.84	0.27	-	86,95,99,101	0
1	PCA	C	1	8/9	0.86	0.31	-	76,88,94,96	0
1	PCA	A	1	8/9	0.84	0.24	-	83,87,93,93	0
1	PCA	B	1	8/9	0.93	0.24	-	68,77,80,82	0
1	PCA	D	1	8/9	0.88	0.23	-	76,82,87,88	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	W9T	F	512	23/23	0.91	0.26	1.74	68,78,85,91	0
2	W9T	B	513	23/23	0.93	0.24	1.05	61,70,76,86	0
2	W9T	E	506	23/23	0.94	0.24	0.69	78,85,94,102	0
2	W9T	B	501	23/23	0.93	0.22	0.45	79,86,115,120	0
2	W9T	F	503	23/23	0.84	0.27	0.18	85,100,105,112	0
2	W9T	B	503	23/23	0.90	0.21	0.10	94,105,118,121	0
2	W9T	D	502	23/23	0.86	0.24	0.09	109,121,134,139	0
2	W9T	C	1004	23/23	0.86	0.30	0.06	100,120,137,138	0
3	CA	C	1008	1/1	0.93	0.19	0.03	69,69,69,69	0
2	W9T	G	505	23/23	0.81	0.42	0.02	140,157,166,168	0
2	W9T	E	505	23/23	0.78	0.40	0.00	132,151,158,161	0
3	CA	D	508	1/1	0.93	0.19	-0.05	80,80,80,80	0
3	CA	F	505	1/1	0.96	0.19	-0.21	61,61,61,61	0
2	W9T	D	501	23/23	0.92	0.19	-0.30	75,86,102,104	0
2	W9T	A	1012	23/23	0.92	0.18	-0.37	72,79,105,116	0
2	W9T	C	1002	23/23	0.90	0.25	-0.42	73,83,117,119	0
2	W9T	A	1004	23/23	0.94	0.20	-0.48	67,80,103,121	0
2	W9T	B	504	23/23	0.85	0.25	-0.48	92,116,139,148	0
2	W9T	E	503	23/23	0.91	0.19	-0.49	58,74,104,107	0
2	W9T	E	504	23/23	0.90	0.18	-0.53	79,86,120,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	W9T	B	502	23/23	0.92	0.23	-0.56	69,81,98,105	0
2	W9T	F	501	23/23	0.93	0.16	-0.58	69,78,101,102	0
3	CA	C	1006	1/1	0.97	0.18	-0.59	65,65,65,65	0
2	W9T	D	512	23/23	0.92	0.18	-0.60	75,89,106,108	0
3	CA	D	505	1/1	0.97	0.17	-0.63	68,68,68,68	0
4	MG	E	512	1/1	0.97	0.16	-0.68	54,54,54,54	0
3	CA	C	1014	1/1	0.97	0.21	-0.71	60,60,60,60	0
2	W9T	A	1002	23/23	0.80	0.23	-0.72	100,117,129,132	0
3	CA	B	508	1/1	0.98	0.17	-0.75	79,79,79,79	0
2	W9T	C	1003	23/23	0.94	0.18	-0.75	74,89,117,130	0
3	CA	A	1008	1/1	0.98	0.16	-0.78	66,66,66,66	0
3	CA	A	1005	1/1	0.98	0.16	-0.78	70,70,70,70	0
2	W9T	F	502	23/23	0.94	0.19	-0.79	74,82,99,101	0
3	CA	F	507	1/1	0.99	0.15	-0.82	76,76,76,76	0
2	W9T	E	501	23/23	0.96	0.16	-0.83	59,67,80,88	0
2	W9T	E	502	23/23	0.91	0.20	-0.84	65,82,101,103	0
3	CA	E	509	1/1	0.97	0.15	-0.87	65,65,65,65	0
2	W9T	C	1001	23/23	0.85	0.16	-0.91	85,103,132,143	0
2	W9T	F	504	23/23	0.87	0.20	-0.92	90,101,105,109	0
2	W9T	D	507	23/23	0.91	0.18	-1.05	69,90,112,121	0
2	W9T	C	1005	23/23	0.83	0.17	-1.08	96,114,124,125	0
3	CA	F	508	1/1	0.91	0.18	-1.09	70,70,70,70	0
2	W9T	G	502	23/23	0.93	0.16	-1.11	63,72,99,106	0
3	CA	A	1009	1/1	0.98	0.18	-1.11	68,68,68,68	0
2	W9T	G	503	23/23	0.90	0.21	-1.18	86,101,126,130	0
2	W9T	A	1003	23/23	0.92	0.18	-1.19	73,87,119,125	0
3	CA	C	1010	1/1	0.91	0.14	-1.19	91,91,91,91	0
3	CA	E	508	1/1	0.98	0.16	-1.21	55,55,55,55	0
3	CA	G	509	1/1	0.96	0.15	-1.21	66,66,66,66	0
2	W9T	B	507	23/23	0.93	0.16	-1.32	70,96,115,121	0
2	W9T	D	506	23/23	0.91	0.18	-1.34	98,111,133,137	0
2	W9T	A	1001	23/23	0.94	0.14	-1.50	79,83,98,100	0
2	W9T	G	504	23/23	0.91	0.14	-1.51	92,96,110,112	0
3	CA	B	505	1/1	0.95	0.13	-1.51	64,64,64,64	0
3	CA	E	510	1/1	0.97	0.11	-1.66	95,95,95,95	0
3	CA	G	508	1/1	0.88	0.12	-1.73	84,84,84,84	0
4	MG	D	510	1/1	0.86	0.10	-1.74	85,85,85,85	0
3	CA	C	1007	1/1	0.88	0.12	-1.81	64,64,64,64	0
3	CA	B	506	1/1	0.97	0.14	-1.84	75,75,75,75	0
4	MG	B	512	1/1	0.92	0.07	-1.91	70,70,70,70	0
3	CA	C	1009	1/1	0.96	0.11	-1.97	75,75,75,75	0
3	CA	A	1007	1/1	0.96	0.12	-1.98	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	G	511	1/1	0.99	0.09	-2.02	74,74,74,74	0
3	CA	B	510	1/1	0.94	0.11	-2.04	85,85,85,85	0
3	CA	A	1006	1/1	0.94	0.09	-2.09	92,92,92,92	0
4	MG	D	511	1/1	0.96	0.11	-2.11	83,83,83,83	0
3	CA	G	510	1/1	0.98	0.09	-2.13	83,83,83,83	0
4	MG	A	1011	1/1	0.88	0.08	-2.15	72,72,72,72	0
3	CA	B	509	1/1	0.96	0.08	-2.16	96,96,96,96	0
3	CA	D	504	1/1	0.98	0.05	-2.18	84,84,84,84	0
4	MG	A	1010	1/1	0.90	0.12	-2.20	59,59,59,59	0
3	CA	D	503	1/1	0.91	0.11	-2.21	73,73,73,73	0
2	W9T	G	501	23/23	0.95	0.14	-2.24	85,95,99,104	0
4	MG	E	513	1/1	0.69	0.12	-2.29	109,109,109,109	0
3	CA	G	506	1/1	0.94	0.06	-2.29	116,116,116,116	0
4	MG	C	1011	1/1	0.95	0.05	-2.34	86,86,86,86	0
3	CA	F	506	1/1	0.98	0.14	-2.39	92,92,92,92	0
4	MG	F	509	1/1	0.94	0.10	-2.42	53,53,53,53	0
3	CA	E	507	1/1	0.97	0.12	-2.53	60,60,60,60	0
3	CA	D	509	1/1	0.96	0.07	-2.83	97,97,97,97	0
3	CA	F	511	1/1	0.85	0.06	-2.86	127,127,127,127	0
3	CA	G	507	1/1	0.98	0.11	-2.97	72,72,72,72	0
4	MG	G	512	1/1	0.95	0.10	-3.05	108,108,108,108	0
4	MG	F	510	1/1	0.91	0.10	-3.21	68,68,68,68	0
3	CA	E	511	1/1	0.94	0.10	-3.26	123,123,123,123	0
4	MG	B	511	1/1	0.96	0.09	-3.60	84,84,84,84	0
4	MG	C	1012	1/1	0.96	0.07	-3.75	67,67,67,67	0
3	CA	C	1013	1/1	0.91	0.10	-	94,94,94,94	0
3	CA	B	514	1/1	0.92	0.06	-	88,88,88,88	0
3	CA	G	513	1/1	0.84	0.05	-	87,87,87,87	0
3	CA	E	514	1/1	0.84	0.10	-	88,88,88,88	0
3	CA	E	515	1/1	0.99	0.23	-	37,37,37,37	1
3	CA	A	1013	1/1	0.76	0.06	-	96,96,96,96	0
3	CA	D	513	1/1	0.91	0.04	-	93,93,93,93	0
3	CA	F	513	1/1	0.95	0.07	-	93,93,93,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.