



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 04:25 PM BST

PDB ID : 1LOB  
Title : THREE-DIMENSIONAL STRUCTURES OF COMPLEXES OF LATHYRUS OCHRUS ISOLECTIN I WITH GLUCOSE AND MANNOSE: FINE SPECIFICITY OF THE MONOSACCHARIDE-BINDING SITE  
Authors : Bourne, Y.; Cambillau, C.  
Deposited on : 1993-01-27  
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

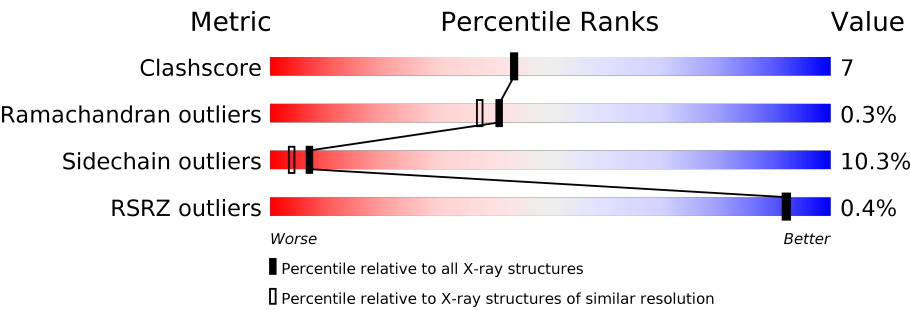
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	181	
1	C	181	
1	E	181	
1	G	181	
2	B	52	
2	D	52	
2	F	52	

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Mol	Chain	Length	Quality of chain
2	H	52	<div><div></div><div>73%</div><div>12%</div><div>6%</div><div>10%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7460 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 LEGUME ISOLECTIN I (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	C	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	E	180	Total	C	N	O	0	0	0
			1397	890	230	277			
1	G	180	Total	C	N	O	0	0	0
			1397	890	230	277			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	LYS	conflict	UNP P04122
C	153	ALA	LYS	conflict	UNP P04122
E	153	ALA	LYS	conflict	UNP P04122
G	153	ALA	LYS	conflict	UNP P04122

- Molecule 2 is a protein called LEGUME ISOLECTIN I (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	D	47	Total	C	N	O	0	0	0
			376	248	58	70			
2	F	47	Total	C	N	O	0	0	0
			381	251	58	72			
2	H	47	Total	C	N	O	0	0	0
			376	248	58	70			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	TYR	PHE	conflict	UNP P12306
D	41	TYR	PHE	conflict	UNP P12306
F	41	TYR	PHE	conflict	UNP P12306
H	41	TYR	PHE	conflict	UNP P12306

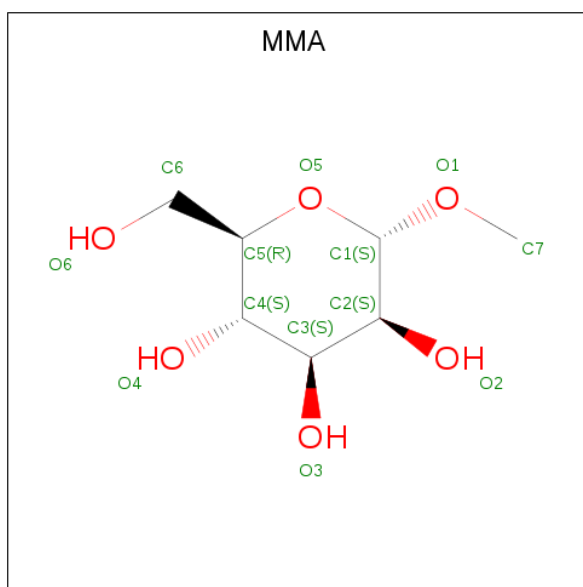
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mn 1 1	0	0
4	A	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	E	1	Total Mn 1 1	0	0

- Molecule 5 is methyl alpha-D-mannopyranoside (three-letter code: MMA) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	7	6		
5	C	1	Total	C	O	0	0
			13	7	6		
5	E	1	Total	C	O	0	0
			13	7	6		
5	G	1	Total	C	O	0	0
			13	7	6		

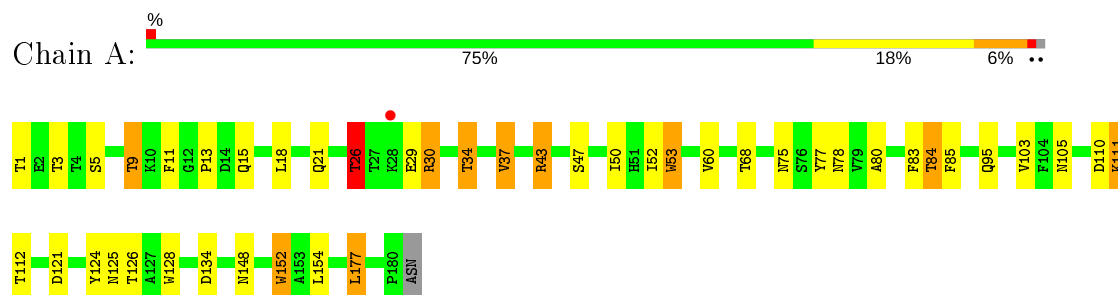
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	B	14	Total	O	0	0
			14	14		
6	C	58	Total	O	0	0
			58	58		
6	D	10	Total	O	0	0
			10	10		
6	E	51	Total	O	0	0
			51	51		
6	F	13	Total	O	0	0
			13	13		
6	G	64	Total	O	0	0
			64	64		
6	H	13	Total	O	0	0
			13	13		

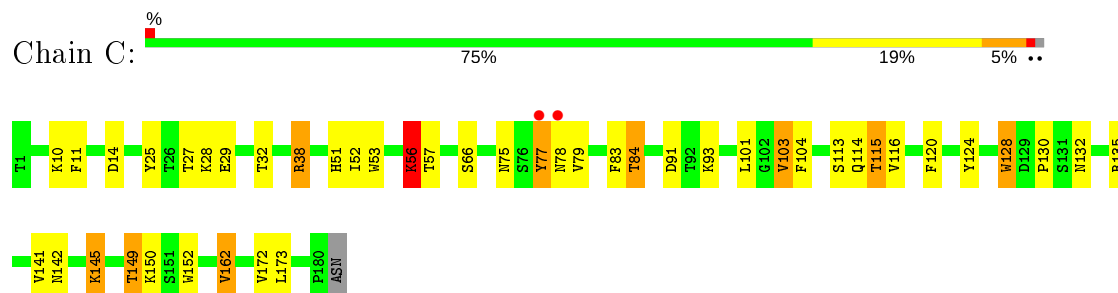
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

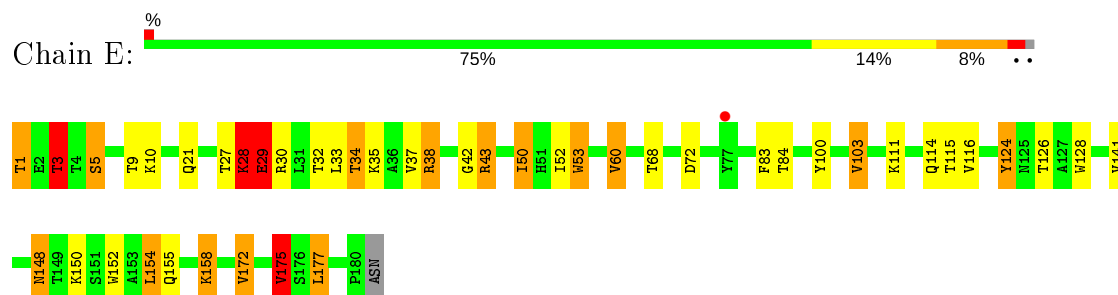
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



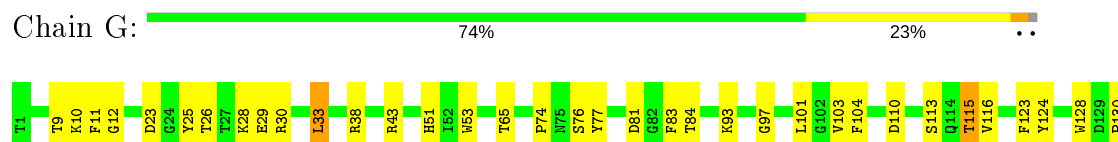
- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

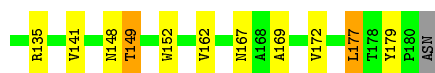


- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

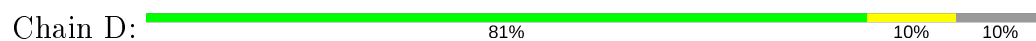




• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.30Å 139.80Å 62.70Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 7.99 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 77.5 (7.99-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 1.97Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.182 , (Not available) 0.173 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 98.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, MN, MMA

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	0.88	0/1431	1.63	23/1954 (1.2%)
1	C	0.85	0/1431	1.62	21/1954 (1.1%)
1	E	0.88	0/1431	1.61	23/1954 (1.2%)
1	G	0.87	1/1431 (0.1%)	1.57	24/1954 (1.2%)
2	B	1.01	0/394	1.62	8/539 (1.5%)
2	D	0.96	0/389	1.61	7/532 (1.3%)
2	F	0.93	0/394	1.53	8/539 (1.5%)
2	H	1.00	1/389 (0.3%)	1.62	8/532 (1.5%)
All	All	0.89	2/7290 (0.0%)	1.61	122/9958 (1.2%)

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
2	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	10	VAL	CA-CB	6.07	1.67	1.54
1	G	115	THR	CA-CB	5.31	1.67	1.53

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	38	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	C	172	VAL	CG1-CB-CG2	-9.89	95.07	110.90
1	G	177	LEU	CA-CB-CG	9.18	136.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	TRP	CD1-CG-CD2	9.12	113.59	106.30
1	C	152	TRP	CD1-CG-CD2	8.99	113.50	106.30
1	E	152	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	A	53	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	C	128	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	G	172	VAL	CG1-CB-CG2	-8.42	97.43	110.90
1	G	38	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	G	128	TRP	CE2-CD2-CG	-8.26	100.69	107.30
1	E	3	THR	N-CA-CB	-8.22	94.67	110.30
1	E	177	LEU	CA-CB-CG	8.22	134.20	115.30
2	B	19	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	G	128	TRP	CD1-CG-CD2	8.18	112.84	106.30
2	H	19	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	C	128	TRP	CE2-CD2-CG	-7.96	100.93	107.30
1	A	30	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	26	THR	N-CA-CB	-7.90	95.30	110.30
1	G	152	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	C	56	LYS	CA-CB-CG	7.52	129.94	113.40
1	E	53	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	G	53	TRP	CD1-CG-CD2	7.42	112.23	106.30
1	A	152	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	C	53	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	G	135	ARG	NE-CZ-NH2	-7.28	116.66	120.30
2	H	21	ARG	CA-CB-CG	-7.21	97.54	113.40
2	F	21	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	43	ARG	NE-CZ-NH1	7.17	123.88	120.30
2	F	19	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	E	103	VAL	CG1-CB-CG2	-7.01	99.68	110.90
1	A	128	TRP	CE2-CD2-CG	-7.00	101.70	107.30
2	D	40	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	G	53	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	E	152	TRP	CE2-CD2-CG	-6.96	101.74	107.30
1	E	128	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	E	53	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	E	30	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	53	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	G	152	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	E	124	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	C	152	TRP	CE2-CD2-CG	-6.75	101.90	107.30
2	H	40	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	C	152	TRP	CG-CD1-NE1	-6.74	103.36	110.10
2	B	19	TRP	CE2-CD2-CG	-6.73	101.91	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	TRP	CE2-CD2-CG	-6.72	101.93	107.30
2	D	19	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	C	53	TRP	CE2-CD2-CG	-6.62	102.00	107.30
2	D	19	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	G	135	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	128	TRP	NE1-CE2-CZ2	-6.56	123.18	130.40
1	G	43	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	177	LEU	CA-CB-CG	6.50	130.26	115.30
1	E	152	TRP	CG-CD1-NE1	-6.49	103.61	110.10
1	C	135	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	B	40	TRP	CE2-CD2-CG	-6.37	102.20	107.30
2	F	40	TRP	CD1-CG-CD2	6.34	111.37	106.30
1	A	37	VAL	N-CA-CB	-6.31	97.62	111.50
1	E	128	TRP	CD1-CG-CD2	6.25	111.30	106.30
2	D	40	TRP	CE2-CD2-CG	-6.24	102.31	107.30
2	H	21	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	D	21	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	77	TYR	CB-CG-CD2	-6.15	117.31	121.00
2	B	40	TRP	CD1-CG-CD2	6.14	111.21	106.30
1	A	128	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	G	9	THR	N-CA-CB	-6.05	98.80	110.30
1	C	135	ARG	NE-CZ-NH2	-5.99	117.30	120.30
2	B	16	VAL	N-CA-CB	-5.94	98.44	111.50
1	A	53	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	A	30	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	38	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	B	19	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	E	154	LEU	CA-CB-CG	5.83	128.71	115.30
2	F	16	VAL	N-CA-CB	-5.79	98.76	111.50
1	C	124	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	E	50	ILE	CB-CG1-CD1	-5.76	97.77	113.90
1	C	14	ASP	CB-CG-OD2	-5.76	113.12	118.30
2	F	40	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	E	175	VAL	CG1-CB-CG2	-5.75	101.69	110.90
2	H	40	TRP	CE2-CD2-CG	-5.75	102.70	107.30
1	G	33	LEU	CA-CB-CG	5.75	128.52	115.30
2	F	19	TRP	CE2-CD2-CG	-5.74	102.71	107.30
1	E	100	TYR	CB-CG-CD1	-5.70	117.58	121.00
2	F	21	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	128	TRP	CD1-CG-CD2	5.64	110.81	106.30
1	G	179	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	C	84	THR	N-CA-CB	-5.61	99.64	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	83	PHE	N-CA-CB	-5.59	100.53	110.60
1	A	9	THR	N-CA-CB	-5.55	99.76	110.30
1	E	83	PHE	N-CA-CB	-5.53	100.64	110.60
1	A	121	ASP	CB-CG-OD1	5.53	123.28	118.30
1	G	124	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	C	120	PHE	N-CA-C	-5.48	96.19	111.00
2	B	41	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	C	77	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	E	37	VAL	CA-CB-CG2	-5.45	102.73	110.90
2	D	21	ARG	CA-CB-CG	-5.44	101.42	113.40
1	A	152	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	F	19	TRP	CG-CD1-NE1	-5.42	104.68	110.10
2	H	31	GLU	CA-CB-CG	-5.38	101.55	113.40
2	H	19	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	125	ASN	N-CA-C	-5.37	96.51	111.00
2	D	4	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	103	VAL	N-CA-CB	-5.33	99.78	111.50
1	G	30	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	43	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	172	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	C	84	THR	CA-CB-CG2	5.28	119.79	112.40
2	B	21	ARG	CA-CB-CG	-5.21	101.93	113.40
1	G	53	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	C	91	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	128	TRP	NE1-CE2-CD2	5.16	112.45	107.30
1	E	38	ARG	N-CA-CB	-5.14	101.36	110.60
1	G	77	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	C	83	PHE	N-CA-CB	-5.11	101.40	110.60
1	E	29	GLU	CA-C-N	5.09	128.41	117.20
1	E	38	ARG	CA-CB-CG	5.07	124.56	113.40
1	A	85	PHE	N-CA-C	-5.07	97.32	111.00
1	G	43	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	G	25	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	A	43	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	G	123	PHE	CA-C-N	-5.01	106.18	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	41	TYR	Sidechain

## 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	1397	0	1346	22	0
1	C	1397	0	1346	18	0
1	E	1397	0	1346	22	0
1	G	1397	0	1346	10	0
2	B	381	0	357	10	0
2	D	376	0	351	2	0
2	F	381	0	357	8	0
2	H	376	0	351	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	B	13	0	14	0	0
5	C	13	0	14	0	0
5	E	13	0	14	0	0
5	G	13	0	14	0	0
6	A	75	0	0	3	0
6	B	14	0	0	2	0
6	C	58	0	0	1	0
6	D	10	0	0	0	0
6	E	51	0	0	0	0
6	F	13	0	0	0	0
6	G	64	0	0	1	0
6	H	13	0	0	0	0
All	All	7460	0	6856	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (76) 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:130:PRO:HG3	1:C:149:THR:HG21	1.52	0.92
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.30	0.79
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.35	0.75
1:E:21:GLN:HE21	1:E:43:ARG:HE	1.41	0.67
1:A:83:PHE:HB2	6:B:67:HOH:O	1.96	0.64
1:A:11:PHE:O	1:A:29:GLU:HA	1.98	0.64
1:C:11:PHE:O	1:C:29:GLU:HA	1.98	0.63
1:G:103:VAL:HG13	1:G:104:PHE:CD2	2.35	0.61
1:C:114:GLN:HA	1:C:142:ASN:HD21	1.67	0.59
1:E:124:TYR:CE2	1:E:126:THR:HG22	2.37	0.59
1:C:128:TRP:HB2	1:C:145:LYS:HG2	1.86	0.58
1:A:110:ASP:OD1	1:A:112:THR:HB	2.04	0.57
1:E:5:SER:OG	2:F:43:HIS:HD2	1.88	0.56
1:G:130:PRO:HG3	1:G:149:THR:HG21	1.87	0.54
1:E:1:THR:HA	2:F:46:LEU:O	2.07	0.54
1:A:5:SER:OG	2:B:43:HIS:HD2	1.91	0.54
1:E:21:GLN:NE2	1:E:43:ARG:HE	2.06	0.53
1:A:15:GLN:HG2	1:A:18:LEU:HD22	1.91	0.52
1:G:148:ASN:HD22	2:H:8:GLU:HG2	1.74	0.52
1:A:75:ASN:HD21	1:A:78:ASN:HD22	1.58	0.52
1:C:10:LYS:HZ2	1:C:29:GLU:HG2	1.75	0.51
1:G:12:GLY:O	1:G:26:THR:HG21	2.11	0.50
1:E:28:LYS:HG2	1:E:29:GLU:HG2	1.93	0.50
1:A:34:THR:CG2	2:B:35:HIS:HD2	2.25	0.49
1:E:21:GLN:NE2	1:E:43:ARG:HH21	2.06	0.49
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.59	0.49
1:C:25:TYR:CE2	1:C:27:THR:HB	2.47	0.49
1:A:52:ILE:HG23	1:A:53:TRP:HD1	1.78	0.49
1:G:167:ASN:HD21	1:G:169:ALA:HB3	1.78	0.49
1:E:53:TRP:HB3	1:E:60:VAL:HB	1.95	0.48
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.10	0.48
1:E:114:GLN:HB3	2:F:17:PRO:HD3	1.95	0.48
1:E:21:GLN:HE22	1:E:43:ARG:NH2	2.08	0.48
1:G:97:GLY:HA2	2:H:27:THR:HG21	1.96	0.47
1:E:34:THR:CG2	2:F:35:HIS:HD2	2.27	0.47
1:C:103:VAL:HG13	1:C:104:PHE:CD2	2.49	0.47
1:C:75:ASN:HD22	1:C:77:TYR:HD2	1.61	0.47
2:H:41:TYR:OH	2:H:43:HIS:HB2	2.15	0.47
1:A:34:THR:HG21	2:B:28:THR:HG23	1.97	0.47
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.50	0.46
1:C:128:TRP:CB	1:C:145:LYS:HG2	2.46	0.46
1:A:13:PRO:HA	1:A:26:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ARG:HG2	2:D:32:PHE:HD2	1.79	0.46
1:C:56:LYS:HD3	1:C:57:THR:HG23	1.98	0.46
1:G:65:THR:HA	2:H:41:TYR:O	2.15	0.46
1:A:34:THR:HG21	2:B:35:HIS:HD2	1.81	0.46
1:E:33:LEU:O	1:E:42:GLY:HA3	2.15	0.46
1:E:103:VAL:HG13	1:E:115:THR:HG21	1.98	0.46
1:C:38:ARG:HG2	2:D:32:PHE:CD2	2.51	0.45
1:A:111:LYS:HG3	6:A:242:HOH:O	2.18	0.44
1:G:11:PHE:O	1:G:29:GLU:HA	2.18	0.44
1:A:47:SER:O	2:B:21:ARG:NH1	2.51	0.44
1:C:113:SER:O	1:C:115:THR:HG22	2.17	0.44
1:C:130:PRO:HB2	1:C:132:ASN:HD21	1.82	0.44
1:A:95:GLN:HB3	1:A:105:ASN:OD1	2.18	0.44
1:E:148:ASN:CG	2:F:6:LEU:HD11	2.38	0.44
1:E:158:LYS:HB3	1:E:158:LYS:HE2	1.53	0.43
2:B:35:HIS:CG	6:B:67:HOH:O	2.71	0.43
1:G:23:ASP:HB3	6:G:965:HOH:O	2.19	0.43
1:E:3:THR:HA	2:F:44:SER:O	2.18	0.43
1:A:84:THR:HG21	1:A:103:VAL:HG11	2.01	0.43
1:A:15:GLN:CG	1:A:18:LEU:HD22	2.49	0.42
1:C:66:SER:HA	1:C:162:VAL:O	2.20	0.42
1:E:21:GLN:HB2	1:E:43:ARG:HB2	2.02	0.42
1:A:1:THR:HA	2:B:46:LEU:O	2.20	0.41
1:C:78:ASN:HB3	6:C:511:HOH:O	2.19	0.41
1:E:155:GLN:NE2	1:E:158:LYS:HD3	2.35	0.41
1:C:27:THR:HG22	1:C:32:THR:OG1	2.20	0.41
1:E:52:ILE:HG23	1:E:53:TRP:HD1	1.85	0.41
1:E:38:ARG:HD3	2:F:30:ALA:O	2.21	0.41
1:A:80:ALA:HB3	2:B:31:GLU:HB2	2.03	0.41
1:E:175:VAL:HG13	2:F:6:LEU:HB3	2.02	0.40
6:A:265:HOH:O	2:B:35:HIS:HE1	2.04	0.40
1:C:130:PRO:HB2	1:C:132:ASN:ND2	2.36	0.40
6:A:265:HOH:O	2:B:35:HIS:CE1	2.73	0.40
1:G:110:ASP:O	1:G:113:SER:HB3	2.21	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
1	C	178/181 (98%)	169 (95%)	8 (4%)	1 (1%)	25	19
1	E	178/181 (98%)	172 (97%)	4 (2%)	2 (1%)	14	8
1	G	178/181 (98%)	171 (96%)	7 (4%)	0	100	100
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	D	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	F	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	H	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
All	All	892/932 (96%)	858 (96%)	31 (4%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	29	GLU
1	E	28	LYS
1	C	28	LYS

### 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	154/155 (99%)	138 (90%)	16 (10%)	7	4
1	C	154/155 (99%)	139 (90%)	15 (10%)	8	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	154/155 (99%)	128 (83%)	26 (17%)	2	1
1	G	154/155 (99%)	138 (90%)	16 (10%)	7	4
2	B	40/44 (91%)	38 (95%)	2 (5%)	24	20
2	D	39/44 (89%)	39 (100%)	0	100	100
2	F	40/44 (91%)	37 (92%)	3 (8%)	13	9
2	H	39/44 (89%)	37 (95%)	2 (5%)	24	19
All	All	774/796 (97%)	694 (90%)	80 (10%)	7	4

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	9	THR
1	A	26	THR
1	A	30	ARG
1	A	34	THR
1	A	37	VAL
1	A	50	ILE
1	A	60	VAL
1	A	68	THR
1	A	84	THR
1	A	111	LYS
1	A	134	ASP
1	A	148	ASN
1	A	152	TRP
1	A	154	LEU
1	A	177	LEU
2	B	3	SER
2	B	16	VAL
1	C	51	HIS
1	C	52	ILE
1	C	56	LYS
1	C	79	VAL
1	C	84	THR
1	C	93	LYS
1	C	101	LEU
1	C	115	THR
1	C	116	VAL
1	C	141	VAL
1	C	145	LYS

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Mol	Chain	Res	Type
1	C	149	THR
1	C	150	LYS
1	C	162	VAL
1	C	173	LEU
1	E	1	THR
1	E	3	THR
1	E	5	SER
1	E	9	THR
1	E	10	LYS
1	E	27	THR
1	E	28	LYS
1	E	29	GLU
1	E	32	THR
1	E	34	THR
1	E	35	LYS
1	E	50	ILE
1	E	60	VAL
1	E	68	THR
1	E	72	ASP
1	E	84	THR
1	E	111	LYS
1	E	116	VAL
1	E	141	VAL
1	E	148	ASN
1	E	150	LYS
1	E	154	LEU
1	E	158	LYS
1	E	172	VAL
1	E	175	VAL
1	E	177	LEU
2	F	1	GLU
2	F	12	LEU
2	F	16	VAL
1	G	10	LYS
1	G	28	LYS
1	G	33	LEU
1	G	51	HIS
1	G	74	PRO
1	G	76	SER
1	G	81	ASP
1	G	84	THR
1	G	93	LYS

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Mol	Chain	Res	Type
1	G	101	LEU
1	G	115	THR
1	G	116	VAL
1	G	141	VAL
1	G	149	THR
1	G	162	VAL
1	G	177	LEU
2	H	10	VAL
2	H	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	78	ASN
2	B	7	ASN
2	B	35	HIS
2	B	43	HIS
1	C	51	HIS
1	C	142	ASN
1	C	167	ASN
1	C	171	ASN
1	E	21	GLN
1	E	148	ASN
1	E	155	GLN
2	F	35	HIS
2	F	43	HIS
1	G	51	HIS
1	G	142	ASN
1	G	161	ASN
1	G	167	ASN
1	G	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	MMA	E	182	-	13,13,13	0.76	0	18,18,18	1.05	0
5	MMA	G	182	-	13,13,13	0.89	0	18,18,18	1.23	2 (11%)
5	MMA	C	182	-	13,13,13	1.05	1 (7%)	18,18,18	1.77	4 (22%)
5	MMA	B	53	-	13,13,13	0.92	0	18,18,18	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MMA	E	182	-	-	2/4/24/24	0/1/1/1
5	MMA	G	182	-	-	1/4/24/24	0/1/1/1
5	MMA	C	182	-	-	0/4/24/24	0/1/1/1
5	MMA	B	53	-	-	0/4/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	182	MMA	O1-C1	2.55	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	182	MMA	O4-C4-C3	-3.98	101.15	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	182	MMA	O3-C3-C2	2.78	116.78	110.35
5	C	182	MMA	O2-C2-C1	-2.70	103.48	110.05
5	C	182	MMA	O5-C1-C2	-2.59	104.88	110.35
5	G	182	MMA	O1-C1-C2	2.30	110.85	108.15
5	G	182	MMA	O3-C3-C2	-2.20	105.27	110.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	182	MMA	C4-C5-C6-O6
5	E	182	MMA	O5-C5-C6-O6
5	G	182	MMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	180/181 (99%)	-0.79	1 (0%) 89 88	7, 14, 28, 44	0
1	C	180/181 (99%)	-0.50	2 (1%) 80 79	8, 23, 39, 46	0
1	E	180/181 (99%)	-0.54	1 (0%) 89 88	10, 19, 40, 49	0
1	G	180/181 (99%)	-0.73	0 100 100	7, 17, 32, 42	0
2	B	47/52 (90%)	-0.83	0 100 100	4, 14, 26, 35	0
2	D	47/52 (90%)	-0.63	0 100 100	10, 20, 34, 43	0
2	F	47/52 (90%)	-0.77	0 100 100	7, 19, 29, 37	0
2	H	47/52 (90%)	-0.81	0 100 100	7, 15, 31, 37	0
All	All	908/932 (97%)	-0.67	4 (0%) 92 92	4, 18, 35, 49	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LYS	3.0
1	E	77	TYR	2.9
1	C	78	ASN	2.7
1	C	77	TYR	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	E	688	1/1	0.64	0.18	36,36,36,36	0
3	CA	C	458	1/1	0.68	0.20	46,46,46,46	0
4	MN	C	459	1/1	0.91	0.06	30,30,30,30	0
5	MMA	C	182	13/13	0.92	0.10	27,29,31,31	0
5	MMA	E	182	13/13	0.94	0.10	20,24,29,30	0
3	CA	A	228	1/1	0.95	0.10	13,13,13,13	0
5	MMA	G	182	13/13	0.95	0.09	14,17,20,20	0
5	MMA	B	53	13/13	0.96	0.08	7,13,17,18	0
3	CA	G	918	1/1	0.97	0.12	11,11,11,11	0
4	MN	E	689	1/1	0.97	0.04	27,27,27,27	0
4	MN	G	919	1/1	0.98	0.05	19,19,19,19	0
4	MN	A	229	1/1	0.99	0.05	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.