



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:43 PM GMT

PDB ID : 1LOC  
Title : INTERACTION OF A LEGUME LECTIN WITH TWO COMPONENTS OF  
THE BACTERIAL CELL WALL  
Authors : Bourne, Y.; Cambillau, C.  
Deposited on : 1993-01-27  
Resolution : 2.05 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

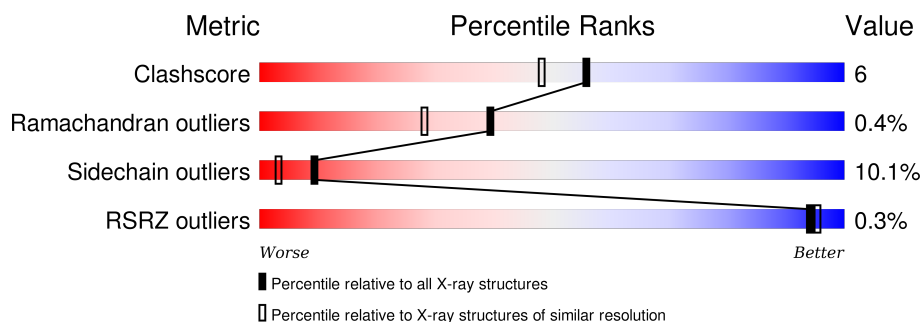
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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.




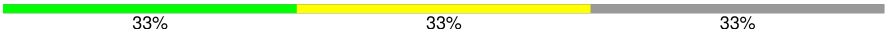


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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. 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	 74% 20% 6% .
1	C	181	 74% 20% 5% ..
1	E	181	 70% 22% 8% .
1	G	181	 77% 19% . ..
2	B	52	 69% 19% . 10%
2	D	52	 81% 6% . 10%
2	F	52	 62% 25% . . 10%

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Mol	Chain	Length	Quality of chain
2	H	52	
3	1	3	
3	2	3	
3	3	3	
3	4	3	

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
4	CA	A	228	-	-	-	X
4	CA	E	688	-	-	-	X
4	CA	G	918	-	-	-	X
5	MN	A	229	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7558 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 a protein called MURAMYL-DIPEPTIDE D-ALA-D-IGLN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	1	3	Total	C	N	O	0	0	0
			35	19	4	12			
3	2	2	Total	C	N	O	0	0	0
			25	14	2	9			
3	3	3	Total	C	N	O	0	0	0
			35	19	4	12			
3	4	3	Total	C	N	O	0	0	0
			35	19	4	12			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

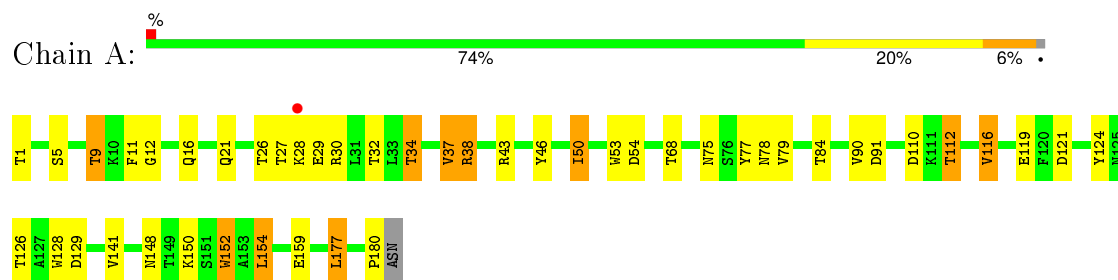
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total 78	O 78	0	0
6	B	13	Total 13	O 13	0	0
6	1	8	Total 8	O 8	0	0
6	C	54	Total 54	O 54	0	0
6	D	10	Total 10	O 10	0	0
6	E	55	Total 55	O 55	0	0
6	F	12	Total 12	O 12	0	0
6	3	6	Total 6	O 6	0	0
6	G	66	Total 66	O 66	0	0
6	H	8	Total 8	O 8	0	0
6	4	8	Total 8	O 8	0	0

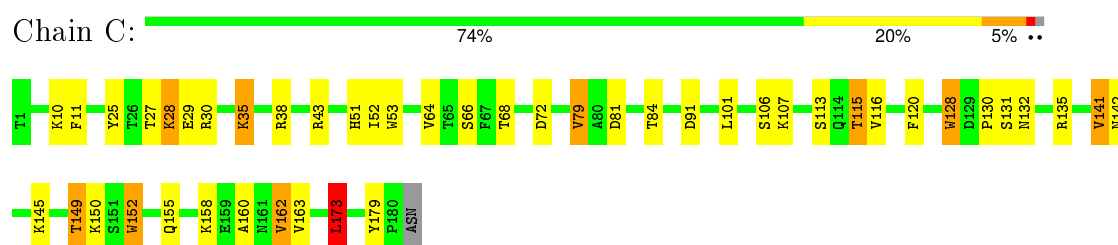
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

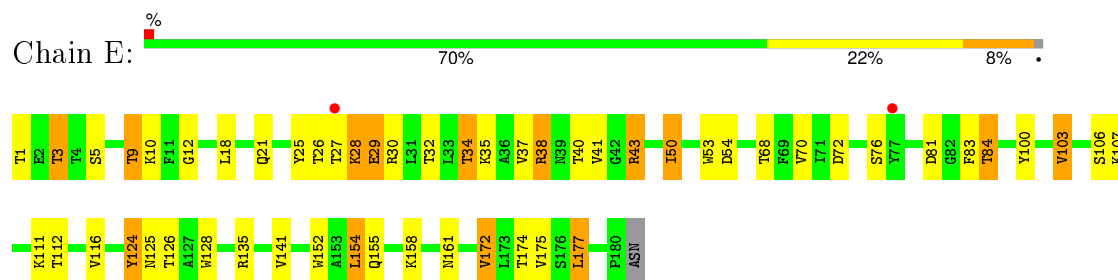
#### • Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



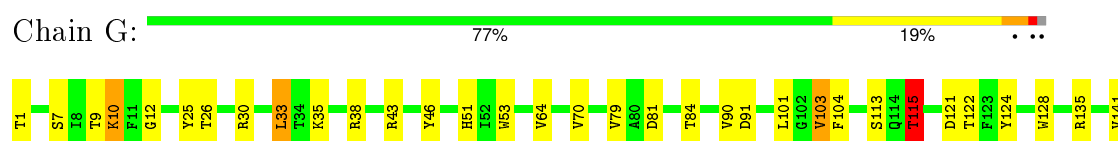
#### • Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

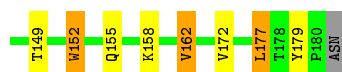


#### • Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)



#### • Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

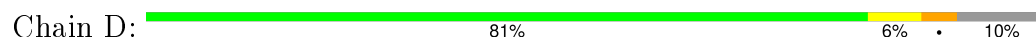




- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



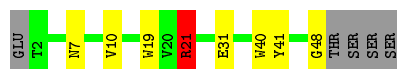
- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



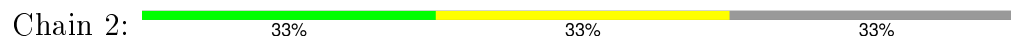
- Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)



- Molecule 3: MURAMYL-DIPEPTIDE D-ALA-D-IGLN



- Molecule 3: MURAMYL-DIPEPTIDE D-ALA-D-IGLN



- Molecule 3: MURAMYL-DIPEPTIDE D-ALA-D-IGLN





- Molecule 3: MURAMYL-DIPEPTIDE D-ALA-D-IGLN

Chain 4:  67% 33%

7950  
4951  
7952

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.58Å 139.80Å 63.40Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	6.00 – 2.05 6.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.05) 96.8 (6.00-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.37 (at 2.05Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.189 , (Not available) 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.52 , 123.8	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 57175 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, CA, MN, ZGL, MDP

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	0.95	3/1431 (0.2%)	1.68	27/1954 (1.4%)
1	C	0.83	2/1431 (0.1%)	1.54	19/1954 (1.0%)
1	E	0.90	0/1431	1.62	25/1954 (1.3%)
1	G	0.90	2/1431 (0.1%)	1.71	33/1954 (1.7%)
2	B	1.05	0/394	1.71	12/539 (2.2%)
2	D	1.00	0/389	1.67	7/532 (1.3%)
2	F	0.95	0/394	1.85	11/539 (2.0%)
2	H	1.02	0/389	1.94	10/532 (1.9%)
All	All	0.92	7/7290 (0.1%)	1.67	144/9958 (1.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	115	THR	CA-CB	5.96	1.68	1.53
1	A	116	VAL	CA-CB	5.57	1.66	1.54
1	C	141	VAL	CA-CB	5.56	1.66	1.54
1	A	141	VAL	CA-CB	5.55	1.66	1.54
1	C	115	THR	CA-CB	5.41	1.67	1.53
1	A	119	GLU	CD-OE2	-5.12	1.20	1.25
1	G	162	VAL	CA-CB	5.04	1.65	1.54

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	21	ARG	NE-CZ-NH1	21.85	131.22	120.30
2	F	21	ARG	NE-CZ-NH1	17.95	129.27	120.30
2	F	21	ARG	NE-CZ-NH2	-16.27	112.17	120.30
2	H	21	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	G	30	ARG	NE-CZ-NH2	-11.11	114.75	120.30
2	D	21	ARG	NE-CZ-NH1	10.88	125.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	30	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	E	103	VAL	CG1-CB-CG2	-10.23	94.53	110.90
1	G	38	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	A	38	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	B	19	TRP	CD1-CG-CD2	9.59	113.97	106.30
2	D	21	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	177	LEU	CA-CB-CG	9.21	136.50	115.30
1	E	177	LEU	CA-CB-CG	9.06	136.13	115.30
1	E	50	ILE	CB-CG1-CD1	-8.96	88.80	113.90
1	G	43	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	G	135	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	A	38	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	129	ASP	CB-CG-OD2	8.55	125.99	118.30
1	E	124	TYR	CB-CG-CD2	-8.51	115.90	121.00
1	G	135	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	152	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	G	53	TRP	CD1-CG-CD2	8.13	112.81	106.30
2	H	19	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	G	177	LEU	CA-CB-CG	7.99	133.68	115.30
1	C	152	TRP	CD1-CG-CD2	7.92	112.63	106.30
1	E	152	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	G	179	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	G	128	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	G	53	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	C	53	TRP	CD1-CG-CD2	7.79	112.54	106.30
2	D	19	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	G	64	VAL	CG1-CB-CG2	-7.63	98.69	110.90
2	D	40	TRP	CD1-CG-CD2	7.52	112.31	106.30
2	B	19	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	G	128	TRP	CE2-CD2-CG	-7.47	101.33	107.30
2	B	21	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	B	19	TRP	CG-CD1-NE1	-7.41	102.69	110.10
2	B	16	VAL	CG1-CB-CG2	7.37	122.70	110.90
1	A	53	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	G	152	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	G	124	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	C	128	TRP	CD1-CG-CD2	7.03	111.92	106.30
1	A	53	TRP	CD1-CG-CD2	6.98	111.88	106.30
1	E	128	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	C	152	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	E	128	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	G	128	TRP	CG-CD2-CE3	6.72	139.95	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	16	VAL	N-CA-CB	-6.71	96.73	111.50
1	A	128	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	C	128	TRP	CE2-CD2-CG	-6.61	102.01	107.30
2	D	40	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	C	53	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	E	152	TRP	CE2-CD2-CG	-6.54	102.06	107.30
1	A	152	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	30	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	G	152	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	G	38	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	91	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	100	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	E	154	LEU	CA-CB-CG	6.34	129.88	115.30
1	E	43	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	E	172	VAL	CB-CA-C	-6.31	99.41	111.40
2	F	19	TRP	CD1-CG-CD2	6.27	111.31	106.30
1	E	53	TRP	CD1-CG-CD2	6.26	111.31	106.30
2	D	19	TRP	CE2-CD2-CG	-6.26	102.30	107.30
1	E	3	THR	N-CA-CB	-6.26	98.41	110.30
2	B	21	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	128	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	A	79	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	A	37	VAL	N-CA-CB	-6.15	97.98	111.50
1	C	152	TRP	CG-CD1-NE1	-6.14	103.96	110.10
2	H	40	TRP	CD1-CG-CD2	6.12	111.20	106.30
1	A	50	ILE	CB-CG1-CD1	-6.08	96.87	113.90
2	B	40	TRP	CD1-CG-CD2	6.03	111.12	106.30
1	A	154	LEU	CA-CB-CG	6.00	129.09	115.30
1	E	125	ASN	N-CA-C	-5.97	94.89	111.00
1	E	41	VAL	CB-CA-C	-5.90	100.20	111.40
2	B	19	TRP	CG-CD2-CE3	5.89	139.20	133.90
2	B	16	VAL	N-CA-CB	-5.87	98.58	111.50
1	G	43	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	E	152	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	G	91	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	G	53	TRP	CA-CB-CG	5.82	124.76	113.70
1	G	53	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	C	30	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	152	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	A	53	TRP	CG-CD2-CE3	5.70	139.03	133.90
2	H	19	TRP	CE2-CD2-CG	-5.69	102.75	107.30
1	A	9	THR	N-CA-CB	-5.68	99.51	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASP	CB-CG-OD1	5.68	123.41	118.30
2	F	19	TRP	CG-CD1-NE1	-5.66	104.44	110.10
2	H	40	TRP	CE2-CD2-CG	-5.64	102.78	107.30
2	H	48	GLY	N-CA-C	-5.64	99.00	113.10
1	G	46	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	G	9	THR	N-CA-CB	-5.61	99.64	110.30
2	F	40	TRP	CD1-CG-CD2	5.60	110.78	106.30
1	E	30	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	53	TRP	CB-CG-CD1	-5.58	119.75	127.00
1	C	163	VAL	CG1-CB-CG2	-5.55	102.03	110.90
2	B	41	TYR	CB-CG-CD2	-5.54	117.67	121.00
2	B	40	TRP	CE2-CD2-CG	-5.54	102.87	107.30
1	C	38	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	H	19	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	C	152	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	E	53	TRP	CE2-CD2-CG	-5.48	102.92	107.30
1	G	121	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	128	TRP	CB-CG-CD1	-5.48	119.88	127.00
2	H	10	VAL	CG1-CB-CG2	-5.45	102.19	110.90
1	C	155	GLN	CA-CB-CG	-5.37	101.59	113.40
1	C	91	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	91	ASP	CB-CG-OD1	5.32	123.09	118.30
2	B	19	TRP	CB-CG-CD1	-5.31	120.09	127.00
1	A	54	ASP	CB-CG-OD1	5.31	123.08	118.30
2	D	40	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	C	120	PHE	N-CA-C	-5.29	96.72	111.00
2	F	19	TRP	CE2-CD2-CG	-5.29	103.07	107.30
1	C	173	LEU	CA-CB-CG	5.29	127.46	115.30
1	G	103	VAL	CB-CA-C	5.28	121.43	111.40
1	E	43	ARG	NE-CZ-NH2	-5.27	117.66	120.30
2	F	41	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	C	53	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	152	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	E	83	PHE	N-CA-CB	-5.25	101.16	110.60
1	G	33	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	46	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	G	152	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	A	77	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	E	38	ARG	CA-C-N	-5.22	105.72	117.20
2	F	16	VAL	CB-CA-C	5.21	121.31	111.40
1	E	70	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	G	81	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	21	ARG	CG-CD-NE	-5.14	101.00	111.80
1	G	70	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	E	53	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	C	25	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	E	54	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	H	31	GLU	CA-CB-CG	-5.08	102.23	113.40
1	C	43	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	179	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	90	VAL	CG1-CB-CG2	-5.05	102.82	110.90
2	F	21	ARG	CD-NE-CZ	5.05	130.67	123.60
1	G	152	TRP	CA-CB-CG	5.05	123.29	113.70
1	A	112	THR	N-CA-CB	-5.02	100.76	110.30

There are no chirality outliers.

There are no planarity outliers.

## 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	21	0
1	C	1397	0	1346	13	0
1	E	1397	0	1346	26	0
1	G	1397	0	1346	13	0
2	B	381	0	357	8	0
2	D	376	0	351	3	0
2	F	381	0	357	8	0
2	H	376	0	351	2	0
3	1	35	0	28	3	0
3	2	25	0	21	4	0
3	3	35	0	28	2	0
3	4	35	0	28	4	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	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	1	8	0	0	2	0
6	3	6	0	0	0	0
6	4	8	0	0	0	0
6	A	78	0	0	2	0
6	B	13	0	0	0	0
6	C	54	0	0	0	0
6	D	10	0	0	0	0
6	E	55	0	0	1	0
6	F	12	0	0	0	0
6	G	66	0	0	1	0
6	H	8	0	0	0	0
All	All	7558	0	6905	87	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 6.

All (87) 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)
3:4:950:MDP:H7	3:4:950:MDP:H113	1.38	1.05
3:3:950:MDP:H7	3:3:950:MDP:H113	1.54	0.89
3:2:950:MDP:H113	3:2:950:MDP:C8	2.03	0.89
3:4:950:MDP:C7	3:4:950:MDP:H113	2.07	0.84
3:1:950:MDP:H113	3:1:950:MDP:H7	1.62	0.82
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.32	0.75
3:4:950:MDP:C8	3:4:950:MDP:H113	2.18	0.72
1:G:12:GLY:O	1:G:26:THR:HG21	1.89	0.72
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.37	0.71
1:E:38:ARG:HB2	2:F:29:GLY:O	1.92	0.70
5:A:229:MN:MN	6:A:272:HOH:O	0.10	0.69
1:A:34:THR:HG21	2:B:35:HIS:HD2	1.58	0.69
1:C:11:PHE:O	1:C:29:GLU:HA	1.98	0.63
1:A:75:ASN:HD21	1:A:78:ASN:HD22	1.47	0.62
1:A:5:SER:OG	2:B:43:HIS:HD2	1.83	0.62
3:4:950:MDP:H7	3:4:950:MDP:C11	2.25	0.61
3:2:950:MDP:H113	3:2:950:MDP:H7	1.83	0.60
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.35	0.60
1:E:25:TYR:CE2	1:E:27:THR:HB	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:VAL:HG23	1:G:122:THR:HB	1.85	0.59
1:A:34:THR:CG2	2:B:35:HIS:HD2	2.14	0.59
3:1:950:MDP:C11	6:1:314:HOH:O	2.49	0.59
3:3:950:MDP:H113	3:3:950:MDP:C7	2.32	0.58
1:G:7:SER:HB3	2:H:41:TYR:HD1	1.67	0.58
1:E:5:SER:OG	2:F:43:HIS:HD2	1.86	0.58
1:C:35:LYS:HA	1:C:35:LYS:HE3	1.87	0.57
1:E:25:TYR:HE2	1:E:27:THR:HB	1.70	0.56
1:E:9:THR:HG22	1:G:1:THR:H3	1.70	0.56
1:C:10:LYS:HG2	1:C:29:GLU:HB3	1.87	0.56
1:C:79:VAL:HG13	1:C:135:ARG:NH2	2.21	0.55
1:E:155:GLN:NE2	1:E:158:LYS:HD2	2.20	0.55
1:E:10:LYS:HG3	1:E:29:GLU:HA	1.88	0.55
1:E:34:THR:CG2	2:F:35:HIS:HD2	2.19	0.55
1:C:128:TRP:HB2	1:C:145:LYS:HG2	1.88	0.55
1:E:21:GLN:HE21	1:E:43:ARG:HE	1.54	0.54
1:E:37:VAL:HG13	1:E:40:THR:HG21	1.88	0.54
1:G:155:GLN:OE1	1:G:158:LYS:HD3	2.07	0.54
1:A:124:TYR:CZ	1:A:126:THR:HG22	2.42	0.54
1:A:12:GLY:O	1:A:26:THR:HG21	2.07	0.54
1:E:21:GLN:NE2	1:E:43:ARG:HE	2.05	0.54
1:E:84:THR:HG21	1:E:103:VAL:HG21	1.89	0.54
1:A:21:GLN:HE21	1:A:43:ARG:HE	1.55	0.53
3:2:950:MDP:H7	3:2:950:MDP:C11	2.39	0.53
1:E:12:GLY:O	1:E:26:THR:HG21	2.08	0.52
1:G:115:THR:HG21	6:G:924:HOH:O	2.09	0.52
1:C:107:LYS:HB2	1:C:145:LYS:HG3	1.91	0.52
1:G:103:VAL:HG13	1:G:104:PHE:CD2	2.44	0.52
1:E:124:TYR:CE2	1:E:126:THR:HG22	2.46	0.51
1:A:159:GLU:HG2	6:A:287:HOH:O	2.10	0.50
1:A:150:LYS:HZ2	2:B:5:THR:H	1.60	0.50
1:C:27:THR:OG1	1:C:28:LYS:HD2	2.12	0.50
1:E:68:THR:HG22	1:E:161:ASN:HD22	1.76	0.49
1:A:21:GLN:NE2	1:A:43:ARG:HE	2.09	0.49
1:C:113:SER:HB3	1:C:142:ASN:HD22	1.76	0.49
3:2:950:MDP:C7	3:2:950:MDP:H113	2.43	0.49
1:E:38:ARG:HH21	2:F:32:PHE:HE2	1.61	0.49
1:E:27:THR:HG23	1:E:27:THR:O	2.13	0.48
1:C:68:THR:HA	1:C:160:ALA:O	2.13	0.48
1:E:35:LYS:HE2	1:E:35:LYS:HA	1.95	0.48
1:G:113:SER:O	1:G:115:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:PRO:HG2	1:C:149:THR:HG21	1.96	0.47
1:A:5:SER:OG	2:B:43:HIS:CD2	2.66	0.47
1:A:38:ARG:HD3	2:B:30:ALA:O	2.15	0.46
1:E:1:THR:N	1:G:10:LYS:HE3	2.30	0.46
1:C:66:SER:HA	1:C:162:VAL:O	2.16	0.45
1:E:174:THR:HG23	2:F:7:ASN:ND2	2.32	0.45
1:A:34:THR:HG21	2:B:35:HIS:CD2	2.44	0.45
1:A:11:PHE:O	1:A:29:GLU:HA	2.16	0.45
1:C:173:LEU:HB2	2:D:10:VAL:HG12	1.99	0.44
1:E:34:THR:HG22	2:F:35:HIS:HD2	1.82	0.44
1:E:1:THR:HA	2:F:46:LEU:O	2.18	0.44
1:G:79:VAL:CG2	1:G:122:THR:HB	2.48	0.43
1:A:150:LYS:HZ2	2:B:4:TYR:HA	1.83	0.43
1:E:34:THR:HG23	1:E:35:LYS:O	2.18	0.43
1:G:113:SER:OG	1:G:115:THR:HG23	2.19	0.43
2:D:10:VAL:HG13	2:D:10:VAL:O	2.19	0.43
2:F:16:VAL:HA	2:F:17:PRO:HD3	1.86	0.43
1:A:27:THR:HG22	1:A:32:THR:CG2	2.49	0.42
1:G:158:LYS:HE2	1:G:158:LYS:HB3	1.66	0.42
1:E:135:ARG:HD2	6:E:702:HOH:O	2.20	0.42
1:A:110:ASP:OD1	1:A:112:THR:HB	2.20	0.41
3:I:950:MDP:H112	6:I:314:HOH:O	2.15	0.41
1:A:27:THR:HG22	1:A:32:THR:HG21	2.02	0.41
1:E:111:LYS:HG3	1:E:112:THR:N	2.35	0.41
1:A:16:GLN:HB2	2:D:19:TRP:CD2	2.56	0.40
1:G:90:VAL:HA	2:H:21:ARG:HG3	2.03	0.40
1:C:145:LYS:HE2	1:C:145:LYS:HB3	1.82	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	175 (98%)	3 (2%)	0	100	100
1	E	178/181 (98%)	169 (95%)	8 (4%)	1 (1%)	30	18
1	G	178/181 (98%)	174 (98%)	4 (2%)	0	100	100
2	B	45/52 (86%)	43 (96%)	1 (2%)	1 (2%)	8	1
2	D	45/52 (86%)	43 (96%)	1 (2%)	1 (2%)	8	1
2	F	45/52 (86%)	42 (93%)	2 (4%)	1 (2%)	8	1
2	H	45/52 (86%)	44 (98%)	1 (2%)	0	100	100
All	All	892/932 (96%)	864 (97%)	24 (3%)	4 (0%)	39	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	28	LYS
2	B	11	PRO
2	F	11	PRO
2	D	11	PRO

### 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%)	140 (91%)	14 (9%)	12	5
1	C	154/155 (99%)	132 (86%)	22 (14%)	4	1
1	E	154/155 (99%)	134 (87%)	20 (13%)	5	1
1	G	154/155 (99%)	140 (91%)	14 (9%)	12	5
2	B	40/44 (91%)	39 (98%)	1 (2%)	55	48
2	D	39/44 (89%)	38 (97%)	1 (3%)	54	47
2	F	40/44 (91%)	36 (90%)	4 (10%)	9	3
2	H	39/44 (89%)	37 (95%)	2 (5%)	29	19
All	All	774/796 (97%)	696 (90%)	78 (10%)	9	3

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	9	THR
1	A	28	LYS
1	A	34	THR
1	A	37	VAL
1	A	50	ILE
1	A	68	THR
1	A	84	THR
1	A	116	VAL
1	A	148	ASN
1	A	152	TRP
1	A	154	LEU
1	A	177	LEU
1	A	180	PRO
2	B	16	VAL
1	C	28	LYS
1	C	35	LYS
1	C	51	HIS
1	C	52	ILE
1	C	64	VAL
1	C	72	ASP
1	C	79	VAL
1	C	81	ASP
1	C	84	THR
1	C	101	LEU
1	C	106	SER
1	C	115	THR
1	C	116	VAL
1	C	131	SER
1	C	132	ASN
1	C	141	VAL
1	C	149	THR
1	C	150	LYS
1	C	152	TRP
1	C	158	LYS
1	C	162	VAL
1	C	173	LEU
2	D	21	ARG
1	E	3	THR
1	E	9	THR
1	E	18	LEU
1	E	28	LYS

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Mol	Chain	Res	Type
1	E	29	GLU
1	E	32	THR
1	E	34	THR
1	E	50	ILE
1	E	72	ASP
1	E	76	SER
1	E	81	ASP
1	E	84	THR
1	E	106	SER
1	E	107	LYS
1	E	116	VAL
1	E	141	VAL
1	E	154	LEU
1	E	172	VAL
1	E	175	VAL
1	E	177	LEU
2	F	1	GLU
2	F	14	GLU
2	F	16	VAL
2	F	21	ARG
1	G	10	LYS
1	G	25	TYR
1	G	33	LEU
1	G	35	LYS
1	G	51	HIS
1	G	84	THR
1	G	101	LEU
1	G	115	THR
1	G	141	VAL
1	G	149	THR
1	G	152	TRP
1	G	162	VAL
1	G	172	VAL
1	G	177	LEU
2	H	7	ASN
2	H	21	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	GLN

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

11 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	$\# Z  > 2$
3	MDP	1	950	3	16,20,21	1.16	2 (12%)	16,28,30	2.49	5 (31%)
3	DAL	1	951	3	3,4,5	0.59	0	0,4,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ZGL	1	952	3	6,9,9	0.81	0	6,11,11	1.50	1 (16%)
3	MDP	2	950	3	16,20,21	1.93	2 (12%)	16,28,30	2.95	8 (50%)
3	DAL	2	951	3	3,4,5	1.75	2 (66%)	0,4,6	0.00	-
3	MDP	3	950	3	16,20,21	1.47	3 (18%)	16,28,30	1.77	2 (12%)
3	DAL	3	951	3	3,4,5	0.62	0	0,4,6	0.00	-
3	ZGL	3	952	3	6,9,9	0.42	0	6,11,11	1.48	2 (33%)
3	MDP	4	950	3	16,20,21	1.13	1 (6%)	16,28,30	1.78	4 (25%)
3	DAL	4	951	3	3,4,5	1.00	0	0,4,6	0.00	-
3	ZGL	4	952	3	6,9,9	1.05	1 (16%)	6,11,11	1.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MDP	1	950	3	-	0/10/36/38	0/1/1/1
3	DAL	1	951	3	-	0/0/2/4	0/0/0/0
3	ZGL	1	952	3	-	0/6/9/9	0/0/0/0
3	MDP	2	950	3	-	0/10/36/38	0/1/1/1
3	DAL	2	951	3	-	0/0/2/4	0/0/0/0
3	MDP	3	950	3	-	0/10/36/38	0/1/1/1
3	DAL	3	951	3	-	0/0/2/4	0/0/0/0
3	ZGL	3	952	3	-	0/6/9/9	0/0/0/0
3	MDP	4	950	3	-	0/10/36/38	0/1/1/1
3	DAL	4	951	3	-	0/0/2/4	0/0/0/0
3	ZGL	4	952	3	-	0/6/9/9	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	950	MDP	O5-C1	-2.83	1.37	1.43
3	3	950	MDP	O3-C7	-2.58	1.40	1.44
3	4	952	ZGL	CB-CA	-2.15	1.47	1.54
3	3	950	MDP	C7-C8	2.00	1.53	1.50
3	2	951	DAL	O-C	2.00	1.29	1.19
3	1	950	MDP	C7-C8	2.07	1.54	1.50
3	2	951	DAL	CB-CA	2.23	1.60	1.52
3	4	950	MDP	C7-C8	2.42	1.54	1.50
3	3	950	MDP	C1-C2	3.59	1.57	1.53
3	2	950	MDP	C4-C5	4.02	1.61	1.53

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	950	MDP	C7-C8	5.26	1.59	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	950	MDP	C1-O5-C5	-6.35	101.73	113.47
3	1	950	MDP	C11-N2-C10	-5.68	105.32	120.34
3	1	950	MDP	C1-O5-C5	-5.32	103.64	113.47
3	2	950	MDP	O6-C6-C5	-4.87	95.24	111.33
3	4	950	MDP	C11-N2-C10	-4.81	107.62	120.34
3	3	950	MDP	C11-N2-C10	-4.62	108.11	120.34
3	2	950	MDP	C11-N2-C10	-3.63	110.75	120.34
3	1	952	ZGL	O-C-N1	-3.53	117.85	123.08
3	2	950	MDP	O5-C5-C4	-2.77	104.48	109.68
3	1	950	MDP	O5-C1-C2	-2.64	106.50	109.66
3	2	950	MDP	O4-C4-C3	-2.54	103.86	109.87
3	3	952	ZGL	CA-C-N1	-2.42	112.74	116.62
3	4	950	MDP	O4-C4-C3	-2.24	104.57	109.87
3	3	952	ZGL	O-C-CA	2.26	123.42	120.33
3	2	950	MDP	C3-C4-C5	2.35	114.93	109.61
3	4	950	MDP	O3-C7-C9	2.64	113.84	107.26
3	1	950	MDP	O1-C1-C2	2.92	115.87	109.05
3	1	950	MDP	C6-C5-C4	2.98	120.37	113.02
3	4	950	MDP	O5-C1-C2	2.99	113.23	109.66
3	3	950	MDP	O5-C1-C2	3.29	113.59	109.66
3	2	950	MDP	C6-C5-C4	3.78	122.33	113.02
3	2	950	MDP	O5-C1-C2	4.52	115.06	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	950	MDP	3	0
3	2	950	MDP	4	0
3	3	950	MDP	2	0
3	4	950	MDP	4	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 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%)	-0.76	1 (0%) 90 92	11, 16, 29, 48	0
1	C	180/181 (99%)	-0.47	0 100 100	13, 24, 44, 61	0
1	E	180/181 (99%)	-0.47	2 (1%) 82 86	12, 21, 40, 61	0
1	G	180/181 (99%)	-0.65	0 100 100	12, 19, 36, 48	0
2	B	47/52 (90%)	-0.82	0 100 100	11, 17, 27, 34	0
2	D	47/52 (90%)	-0.56	0 100 100	13, 22, 39, 49	0
2	F	47/52 (90%)	-0.61	0 100 100	11, 22, 33, 42	0
2	H	47/52 (90%)	-0.74	0 100 100	11, 18, 30, 33	0
3	1	0/3	-	-	-	-
3	2	0/3	-	-	-	-
3	3	0/3	-	-	-	-
3	4	0/3	-	-	-	-
All	All	908/944 (96%)	-0.61	3 (0%) 94 95	11, 20, 37, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	77	TYR	2.2
1	A	28	LYS	2.1
1	E	27	THR	2.1

### 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZGL	1	952	10/10	0.86	0.17	-	22,28,44,46	0
3	MDP	3	950	20/21	0.92	0.14	-	27,30,36,36	0
3	ZGL	4	952	10/10	0.87	0.17	-	31,37,45,48	0
3	MDP	4	950	20/21	0.94	0.11	-	22,25,32,32	0
3	MDP	1	950	20/21	0.95	0.10	-	14,18,24,27	0
3	MDP	2	950	20/21	0.79	0.24	-	15,23,33,35	0
3	ZGL	3	952	10/10	0.86	0.19	-	38,41,54,55	0
3	DAL	1	951	5/6	0.96	0.08	-	15,16,18,20	0
3	DAL	4	951	5/6	0.96	0.10	-	24,25,26,29	0
3	DAL	3	951	5/6	0.92	0.11	-	29,31,35,37	0
3	DAL	2	951	5/6	0.78	0.19	-	15,20,25,33	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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	228	1/1	0.82	0.23	7.08	29,29,29,29	0
5	MN	A	229	1/1	0.98	0.21	6.59	18,18,18,18	0
4	CA	E	688	1/1	0.50	0.19	4.86	42,42,42,42	0
4	CA	G	918	1/1	0.87	0.16	3.52	41,41,41,41	0
4	CA	C	458	1/1	0.74	0.14	0.86	47,47,47,47	0
5	MN	E	689	1/1	0.96	0.06	-1.24	33,33,33,33	0
5	MN	C	459	1/1	0.98	0.05	-2.23	32,32,32,32	0
5	MN	G	919	1/1	0.97	0.06	-2.49	25,25,25,25	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.