



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 12:09 PM EDT

PDB ID : 2Z2P  
Title : Crystal Structure of catalytically inactive H270A virginiamycin B lyase from *Staphylococcus aureus* with Quinupristin  
Authors : Korczynska, M.; Berghuis, A.M.  
Deposited on : unknown  
Resolution : 2.80 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

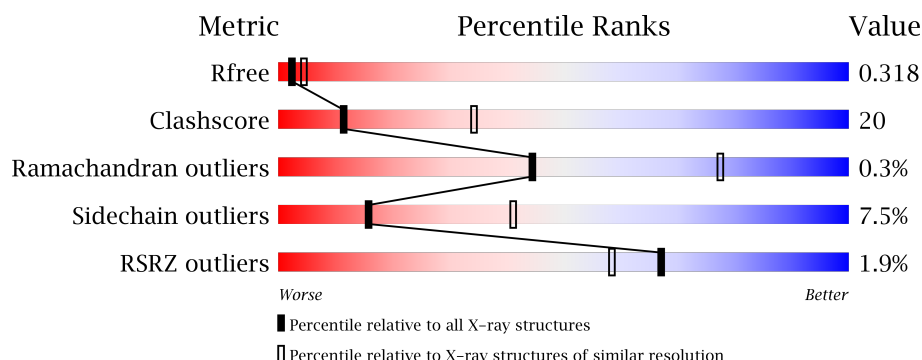
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	299	<div> <div>2%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>
1	B	299	<div> <div>2%</div> <div>69%</div> <div>27%</div> <div>• • •</div> </div>
2	C	7	<div> <div>86%</div> <div>14%</div> </div>
2	D	7	<div> <div>57%</div> <div>43%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DOL	A	2002	X	-	X	-
4	DOL	B	2003	X	-	X	-
5	MHT	C	8	X	-	-	X
5	MHT	D	8	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4794 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 VIRGINIAMYCIN B LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	1	0
			2274	1444	377	444	9			
1	B	293	Total	C	N	O	S	0	1	0
			2274	1444	377	444	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLU	PRO	SEE REMARK 999	UNP Q53744
A	54	ASN	THR	SEE REMARK 999	UNP Q53744
A	55	LYS	PRO	SEE REMARK 999	UNP Q53744
A	56	GLY	ASP	SEE REMARK 999	UNP Q53744
A	211	THR	PRO	SEE REMARK 999	UNP Q53744
A	212	SER	LEU	SEE REMARK 999	UNP Q53744
A	270	ALA	HIS	ENGINEERED MUTATION	UNP Q53744
B	51	GLU	PRO	SEE REMARK 999	UNP Q53744
B	54	ASN	THR	SEE REMARK 999	UNP Q53744
B	55	LYS	PRO	SEE REMARK 999	UNP Q53744
B	56	GLY	ASP	SEE REMARK 999	UNP Q53744
B	211	THR	PRO	SEE REMARK 999	UNP Q53744
B	212	SER	LEU	SEE REMARK 999	UNP Q53744
B	270	ALA	HIS	ENGINEERED MUTATION	UNP Q53744

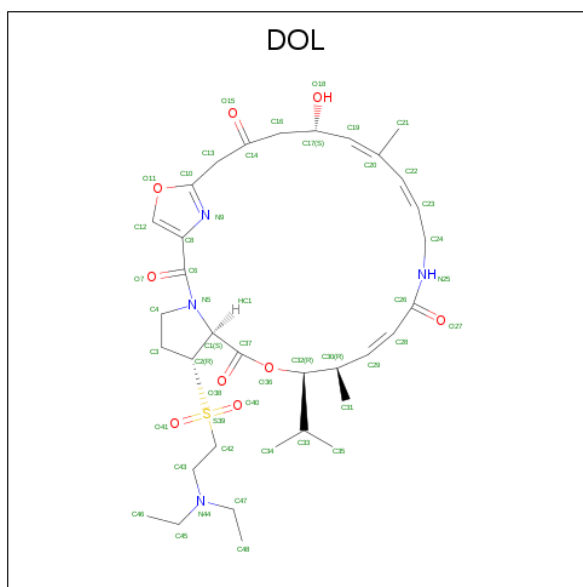
- Molecule 2 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			63	45	8	10			
2	D	7	Total	C	N	O	0	0	0
			63	45	8	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

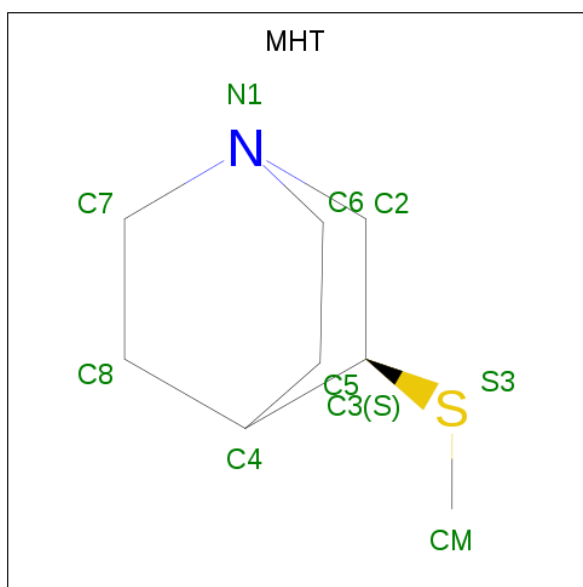
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0

- Molecule 4 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula:  $C_{34}H_{50}N_4O_9S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 48 34 4 9 1	0	0
4	B	1	Total C N O S 48 34 4 9 1	0	0

- Molecule 5 is (3S)-3-(methylsulfonyl)-1-azabicyclo[2.2.2]octane (three-letter code: MHT) (formula:  $C_8H_{15}NS$ ).

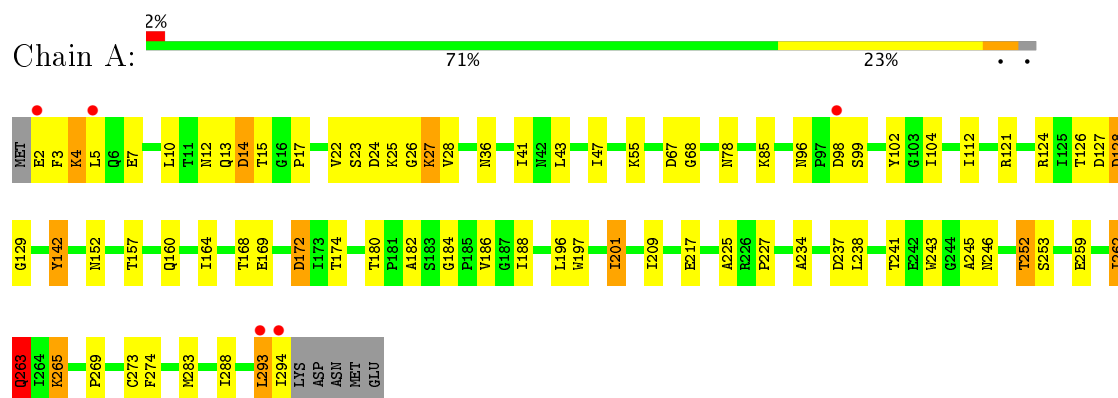


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	S	0	0
			10	8	1	1		
5	D	1	Total	C	N	S	0	0
			10	8	1	1		

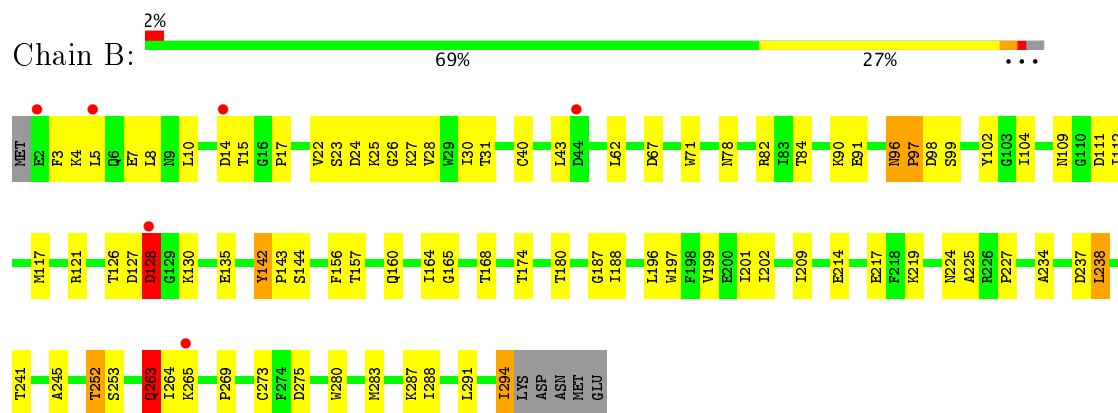
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

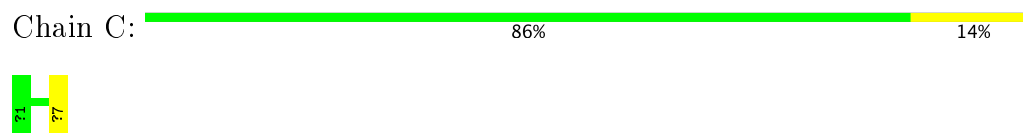
#### • Molecule 1: VIRGINIAMYCIN B LYASE



#### • Molecule 1: VIRGINIAMYCIN B LYASE



#### • Molecule 2: QUINUPRISTIN



#### • Molecule 2: QUINUPRISTIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.00Å 93.70Å 95.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.18 – 2.80 36.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (36.18-2.80) 91.2 (36.18-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.262 , 0.318 0.272 , 0.318	Depositor DCC
$R_{free}$ test set	1587 reflections (12.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.45 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.1572e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MG, DOL, DBB, 004, MHV, MHW, MHT, MHU

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	0.37	0/2325	0.57	1/3158 (0.0%)
1	B	0.38	0/2325	0.62	3/3158 (0.1%)
2	C	0.83	0/13	0.93	0/15
2	D	0.85	0/13	0.89	0/15
All	All	0.38	0/4676	0.60	4/6346 (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	5
1	B	0	5
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	PRO	O-C-N	6.35	132.85	122.70
1	A	14	ASP	O-C-N	-5.24	114.32	122.70
1	B	96	ASN	C-N-CD	5.05	139.02	128.40
1	B	98	ASP	CA-C-N	-5.02	106.16	117.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Peptide
1	A	14	ASP	Peptide
1	A	24	ASP	Peptide
1	A	262	ILE	Peptide
1	A	263	GLN	Peptide
1	B	128	ASP	Peptide
1	B	14	ASP	Peptide
1	B	24	ASP	Peptide
1	B	263	GLN	Peptide
1	B	97	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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	2274	0	2231	66	0
1	B	2274	0	2232	58	0
2	C	63	0	49	2	0
2	D	63	0	49	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	48	0	50	34	0
4	B	48	0	48	33	0
5	C	10	0	14	1	0
5	D	10	0	14	0	0
All	All	4794	0	4687	187	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 20.

All (187) 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)
4:B:2003:DOL:H351	4:B:2003:DOL:C42	1.65	1.23
1:A:23:SER:OG	1:A:27:LYS:HD2	1.36	1.22
4:B:2003:DOL:H353	4:B:2003:DOL:C37	1.76	1.16
4:B:2003:DOL:HC42	4:B:2003:DOL:HC12	1.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2002:DOL:H312	4:A:2002:DOL:C35	1.69	1.12
4:A:2002:DOL:H353	4:A:2002:DOL:HC28	1.32	1.12
4:B:2003:DOL:C4	4:B:2003:DOL:HC12	1.80	1.12
4:B:2003:DOL:C35	4:B:2003:DOL:C42	2.30	1.10
4:A:2002:DOL:H463	4:A:2002:DOL:C48	1.82	1.08
4:B:2003:DOL:H353	4:B:2003:DOL:O38	1.54	1.06
4:B:2003:DOL:H421	4:B:2003:DOL:H351	1.32	1.06
4:B:2003:DOL:H483	4:B:2003:DOL:C46	1.85	1.04
4:A:2002:DOL:H212	4:A:2002:DOL:H162	1.38	1.03
4:A:2002:DOL:C31	4:A:2002:DOL:H353	1.87	1.02
4:A:2002:DOL:C21	4:A:2002:DOL:C14	2.40	1.00
4:B:2003:DOL:C4	4:B:2003:DOL:C12	2.36	1.00
4:B:2003:DOL:H483	4:B:2003:DOL:H463	1.02	0.98
4:A:2002:DOL:H212	4:A:2002:DOL:C16	1.91	0.98
4:A:2002:DOL:H483	4:A:2002:DOL:H463	1.43	0.97
4:A:2002:DOL:C21	4:A:2002:DOL:C16	2.42	0.97
1:A:263:GLN:O	1:A:263:GLN:HG2	1.67	0.93
1:A:25:LYS:HE3	1:A:27:LYS:HG3	1.51	0.92
4:A:2002:DOL:H312	4:A:2002:DOL:H353	0.93	0.92
4:B:2003:DOL:H463	4:B:2003:DOL:C48	1.91	0.92
4:B:2003:DOL:C35	4:B:2003:DOL:H422	2.01	0.91
4:B:2003:DOL:HC42	4:B:2003:DOL:C12	1.97	0.91
4:A:2002:DOL:C14	4:A:2002:DOL:H213	2.01	0.90
4:A:2002:DOL:C4	4:A:2002:DOL:HC12	2.02	0.90
1:A:12:ASN:HB3	1:A:15:THR:HG21	1.54	0.90
4:B:2003:DOL:C35	4:B:2003:DOL:C37	2.47	0.89
4:A:2002:DOL:H212	4:A:2002:DOL:C14	1.99	0.89
4:A:2002:DOL:HC42	4:A:2002:DOL:HC12	1.54	0.89
4:B:2003:DOL:C35	4:B:2003:DOL:C2	2.52	0.88
4:B:2003:DOL:HC41	4:B:2003:DOL:C12	2.07	0.85
4:B:2003:DOL:O36	4:B:2003:DOL:HC28	1.76	0.85
4:A:2002:DOL:C35	4:A:2002:DOL:HC28	2.07	0.84
1:A:25:LYS:HG2	1:A:26:GLY:N	1.93	0.84
4:B:2003:DOL:C35	4:B:2003:DOL:S39	2.67	0.83
1:A:25:LYS:HG2	1:A:26:GLY:H	1.43	0.82
4:A:2002:DOL:H463	4:A:2002:DOL:H482	1.62	0.82
4:A:2002:DOL:C4	4:A:2002:DOL:C12	2.57	0.80
4:B:2003:DOL:S39	4:B:2003:DOL:H351	2.21	0.80
4:B:2003:DOL:C2	4:B:2003:DOL:C33	2.60	0.80
1:B:263:GLN:OE1	1:B:263:GLN:HA	1.80	0.79
1:A:17:PRO:HG2	1:A:283:MET:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HD2	1:A:43:LEU:HB2	1.66	0.77
1:B:3:PHE:HB3	1:B:291:LEU:HD11	1.66	0.77
1:A:23:SER:HG	1:A:27:LYS:HD2	1.46	0.77
4:A:2002:DOL:C46	4:A:2002:DOL:C48	2.48	0.77
4:A:2002:DOL:C10	4:A:2002:DOL:H213	2.15	0.75
4:A:2002:DOL:C28	4:A:2002:DOL:H353	2.15	0.73
1:B:30:ILE:HD13	1:B:288:ILE:HD11	1.70	0.73
4:A:2002:DOL:H483	4:A:2002:DOL:C46	2.18	0.72
1:B:264:ILE:HG13	1:B:287:LYS:NZ	2.04	0.71
4:A:2002:DOL:HC42	4:A:2002:DOL:C12	2.21	0.70
4:B:2003:DOL:H353	4:B:2003:DOL:C2	2.18	0.70
4:A:2002:DOL:C35	4:A:2002:DOL:C28	2.68	0.70
1:B:7:GLU:HG2	1:B:283:MET:HE3	1.73	0.69
1:B:263:GLN:OE1	1:B:263:GLN:CA	2.40	0.69
1:B:25:LYS:HG2	1:B:26:GLY:H	1.57	0.69
1:B:263:GLN:O	1:B:263:GLN:CD	2.31	0.68
1:A:263:GLN:CG	1:A:263:GLN:O	2.41	0.68
1:A:12:ASN:HB3	1:A:15:THR:CG2	2.22	0.68
1:B:25:LYS:HG2	1:B:26:GLY:N	2.10	0.66
4:B:2003:DOL:H353	4:B:2003:DOL:S39	2.35	0.66
1:B:7:GLU:HG2	1:B:283:MET:CE	2.25	0.66
4:A:2002:DOL:C13	4:A:2002:DOL:H213	2.26	0.65
1:A:25:LYS:HE3	1:A:27:LYS:CG	2.26	0.65
4:A:2002:DOL:N9	4:A:2002:DOL:H213	2.13	0.64
4:A:2002:DOL:HC12	4:A:2002:DOL:HC41	1.78	0.64
1:A:22:VAL:HG22	1:A:28:VAL:HG12	1.79	0.64
4:A:2002:DOL:HC41	4:A:2002:DOL:C12	2.29	0.62
1:B:3:PHE:HB3	1:B:291:LEU:CD1	2.28	0.62
1:A:3:PHE:CE1	1:A:293:LEU:HB3	2.33	0.62
1:A:262:ILE:O	1:A:262:ILE:HG22	1.98	0.62
1:A:152:ASN:HB2	4:B:2003:DOL:C3	2.30	0.62
1:B:4:LYS:HG2	1:B:294:ILE:HG12	1.82	0.61
4:B:2003:DOL:HC12	4:B:2003:DOL:HC41	1.67	0.61
1:B:25:LYS:HD2	1:B:43:LEU:HB2	1.83	0.61
1:A:5:LEU:CD2	1:A:262:ILE:HA	2.31	0.60
4:A:2002:DOL:C46	4:A:2002:DOL:H482	2.25	0.60
1:A:265:LYS:CD	1:A:265:LYS:H	2.14	0.60
1:B:27:LYS:HG2	1:B:40:CYS:SG	2.42	0.60
1:B:252:THR:HG22	1:B:253:SER:H	1.67	0.59
4:B:2003:DOL:H353	4:B:2003:DOL:C42	2.26	0.59
1:B:96:ASN:HB2	1:B:121:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:ND2	1:A:99:SER:H	2.00	0.59
4:A:2002:DOL:H212	4:A:2002:DOL:O15	2.01	0.59
1:A:152:ASN:HB2	4:B:2003:DOL:HC3A	1.83	0.59
4:A:2002:DOL:C37	4:A:2002:DOL:O41	2.51	0.58
1:A:23:SER:OG	1:A:27:LYS:CD	2.30	0.58
1:A:68:GLY:HA3	1:A:85:LYS:HE2	1.86	0.57
4:B:2003:DOL:C48	4:B:2003:DOL:C46	2.55	0.57
1:B:78:ASN:OD1	1:B:99:SER:HB2	2.05	0.57
1:A:142:TYR:HB2	1:A:160:GLN:HG2	1.86	0.56
1:A:201:ILE:HA	1:A:227:PRO:HD2	1.85	0.56
1:B:275:ASP:OD1	1:B:280:TRP:NE1	2.38	0.56
4:B:2003:DOL:H353	4:B:2003:DOL:H422	1.82	0.56
1:B:22:VAL:HG22	1:B:28:VAL:HG12	1.86	0.56
4:A:2002:DOL:C35	4:A:2002:DOL:C31	2.52	0.56
1:A:180:THR:OG1	1:A:217:GLU:OE2	2.20	0.56
1:B:201:ILE:HA	1:B:227:PRO:HD2	1.88	0.56
1:A:241:THR:HB	1:A:269:PRO:HB2	1.88	0.56
1:A:22:VAL:HG12	1:A:23:SER:H	1.72	0.55
1:B:142:TYR:HB2	1:B:160:GLN:HG2	1.89	0.55
1:A:243:TRP:HA	1:A:269:PRO:HD2	1.88	0.55
1:B:164:ILE:HG21	1:B:209:ILE:HG21	1.88	0.55
1:A:5:LEU:HD21	1:A:262:ILE:HA	1.88	0.55
1:A:168:THR:OG1	1:A:172:ASP:OD2	2.25	0.54
1:A:184:GLY:O	1:A:201:ILE:HG22	2.06	0.54
1:B:102:TYR:CZ	2:D:7:004:HD1	2.43	0.54
1:A:168:THR:HB	4:B:2003:DOL:H343	1.90	0.53
1:B:10:LEU:HD21	1:B:288:ILE:HD12	1.90	0.53
1:B:264:ILE:HG13	1:B:287:LYS:HZ1	1.74	0.52
4:B:2003:DOL:O36	4:B:2003:DOL:C28	2.43	0.52
1:A:41:ILE:HG12	1:A:47:ILE:HG13	1.92	0.51
1:A:196:LEU:HB2	1:A:209:ILE:HG23	1.92	0.51
1:B:117:MET:HE3	2:D:7:004:HE	1.93	0.51
1:A:265:LYS:CD	1:A:265:LYS:N	2.74	0.51
1:B:17:PRO:HG2	1:B:283:MET:O	2.11	0.51
1:A:142:TYR:HB2	1:A:160:GLN:CG	2.41	0.51
1:A:36:ASN:ND2	1:A:55:LYS:HA	2.25	0.51
1:A:25:LYS:CG	1:A:26:GLY:H	2.18	0.50
1:A:293:LEU:O	1:A:294:ILE:HB	2.10	0.50
1:A:102:TYR:CZ	2:C:7:004:HD1	2.46	0.50
1:B:156:PHE:CE1	1:B:165:GLY:HA3	2.45	0.50
1:B:275:ASP:OD1	1:B:280:TRP:CD1	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:TRP:CZ2	1:B:82:ARG:HD2	2.46	0.50
1:A:225:ALA:HA	1:A:245:ALA:HB2	1.94	0.49
1:A:142:TYR:CB	1:A:160:GLN:HG2	2.42	0.49
1:A:265:LYS:HD3	1:A:265:LYS:N	2.27	0.49
1:B:142:TYR:HB2	1:B:160:GLN:CG	2.42	0.49
1:A:164:ILE:HG21	1:A:209:ILE:HG21	1.93	0.49
1:A:4:LYS:HE2	1:A:5:LEU:H	1.78	0.49
1:A:104:ILE:HD11	1:A:112:ILE:HG21	1.95	0.48
1:B:264:ILE:HG13	1:B:287:LYS:HZ3	1.76	0.48
1:B:22:VAL:HG11	1:B:275:ASP:HB3	1.94	0.48
1:A:124:ARG:HH22	1:A:169:GLU:CD	2.16	0.48
1:A:96:ASN:HB2	1:A:121:ARG:HH21	1.79	0.48
1:B:225:ALA:HA	1:B:245:ALA:HB2	1.95	0.48
1:B:117:MET:CE	2:D:7:004:HE	2.44	0.47
1:A:197:TRP:CD2	1:A:238:LEU:HD13	2.50	0.47
1:A:262:ILE:O	1:A:262:ILE:CG2	2.62	0.47
1:A:182:ALA:HB1	5:C:8:MHT:H5A	1.96	0.47
1:B:117:MET:HG2	1:B:143:PRO:O	2.15	0.47
1:B:142:TYR:CB	1:B:160:GLN:HG2	2.45	0.46
1:A:157:THR:HG23	1:A:188:ILE:HB	1.97	0.46
1:A:152:ASN:HB2	4:B:2003:DOL:HC31	1.97	0.45
1:B:197:TRP:CD2	1:B:238:LEU:HD13	2.51	0.45
1:A:4:LYS:HG3	1:A:5:LEU:N	2.31	0.45
1:A:25:LYS:CG	1:A:26:GLY:N	2.69	0.45
1:A:4:LYS:CE	1:A:5:LEU:H	2.30	0.45
1:B:31:THR:HG23	1:B:62:LEU:HD13	1.98	0.45
1:B:22:VAL:HG12	1:B:23:SER:H	1.81	0.45
1:B:187:GLY:H	1:B:199:VAL:HG22	1.81	0.45
1:A:172:ASP:N	1:A:172:ASP:OD2	2.39	0.45
1:B:109:ASN:HD21	1:B:111:ASP:CG	2.20	0.45
1:B:96:ASN:HB2	1:B:121:ARG:NH2	2.32	0.44
4:A:2002:DOL:H471	4:A:2002:DOL:O41	2.18	0.44
1:B:234:ALA:O	1:B:237:ASP:HB2	2.18	0.43
1:B:126:THR:OG1	1:B:128:ASP:O	2.31	0.43
4:A:2002:DOL:HC23	4:A:2002:DOL:H211	1.54	0.43
1:A:3:PHE:CZ	1:A:293:LEU:HB3	2.52	0.43
1:B:22:VAL:HG23	1:B:273[A]:CYS:SG	2.58	0.43
4:B:2003:DOL:O18	4:B:2003:DOL:C21	2.67	0.43
1:A:265:LYS:H	1:A:265:LYS:HE2	1.84	0.42
2:D:4:PRO:HA	2:D:5:MHU:HM1	1.85	0.42
4:B:2003:DOL:HC23	4:B:2003:DOL:H211	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:O	1:A:129:GLY:HA2	2.19	0.42
1:A:234:ALA:O	1:A:237:ASP:HB2	2.19	0.42
1:B:104:ILE:HD11	1:B:112:ILE:HG21	2.01	0.42
1:B:263:GLN:O	1:B:263:GLN:OE1	2.37	0.42
1:B:27:LYS:HE2	1:B:40:CYS:SG	2.59	0.42
1:B:90:LYS:HD3	1:B:91:GLU:N	2.34	0.42
1:B:157:THR:HG23	1:B:188:ILE:HB	2.03	0.41
1:A:102:TYR:OH	2:C:7:004:HD1	2.21	0.41
1:B:117:MET:HE2	1:B:144:SER:HA	2.02	0.41
1:A:252:THR:HG22	1:A:253:SER:H	1.86	0.41
1:A:273[B]:CYS:SG	1:A:274:PHE:N	2.94	0.41
1:B:7:GLU:HG2	1:B:283:MET:HE1	2.01	0.41
1:A:2:GLU:HB3	1:A:3:PHE:H	1.60	0.41
1:B:196:LEU:HB2	1:B:209:ILE:HG23	2.03	0.40
1:B:180:THR:OG1	1:B:217:GLU:OE2	2.36	0.40
1:B:241:THR:HB	1:B:269:PRO:HB2	2.03	0.40
1:A:67:ASP:HB3	1:B:202:ILE:HG23	2.03	0.40
4:A:2002:DOL:H312	4:A:2002:DOL:HC28	1.39	0.40
1:B:82:ARG:HE	1:B:84:THR:HG22	1.86	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	292/299 (98%)	269 (92%)	21 (7%)	2 (1%)	25	59
1	B	292/299 (98%)	267 (91%)	25 (9%)	0	100	100
2	C	2/7 (29%)	2 (100%)	0	0	100	100
2	D	2/7 (29%)	1 (50%)	1 (50%)	0	100	100
All	All	588/612 (96%)	539 (92%)	47 (8%)	2 (0%)	44	77



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	186	VAL

### 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	245/251 (98%)	227 (93%)	18 (7%)	16	42
1	B	245/251 (98%)	226 (92%)	19 (8%)	15	39
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	494/506 (98%)	457 (92%)	37 (8%)	16	41

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	GLU
1	A	10	LEU
1	A	13	GLN
1	A	27	LYS
1	A	98	ASP
1	A	127	ASP
1	A	128	ASP
1	A	142	TYR
1	A	172	ASP
1	A	174	THR
1	A	201	ILE
1	A	246	ASN
1	A	252	THR
1	A	259	GLU
1	A	265	LYS
1	A	288	ILE
1	A	293	LEU

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Mol	Chain	Res	Type
1	B	5	LEU
1	B	8	LEU
1	B	15	THR
1	B	67	ASP
1	B	127	ASP
1	B	128	ASP
1	B	130	LYS
1	B	135	GLU
1	B	142	TYR
1	B	168	THR
1	B	174	THR
1	B	214	GLU
1	B	219	LYS
1	B	224	ASN
1	B	238	LEU
1	B	252	THR
1	B	263	GLN
1	B	265	LYS
1	B	294	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	32	GLN
1	A	78	ASN
1	A	118	ASN
1	A	228	HIS
1	A	246	ASN
1	B	9	ASN
1	B	13	GLN
1	B	162	ASN
1	B	204	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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
2	MHW	C	1	3,2	9,9,10	0.99	0	9,11,13	1.82	1 (11%)
2	DBB	C	3	2	5,5,6	1.20	1 (20%)	3,5,7	1.52	1 (33%)
2	MHU	C	5	2	15,15,16	1.21	2 (13%)	18,19,21	1.24	1 (5%)
2	MHV	C	6	2,5	9,9,10	1.11	1 (11%)	9,11,13	1.34	2 (22%)
2	004	C	7	2	8,10,11	1.97	4 (50%)	11,12,14	1.82	3 (27%)
2	MHW	D	1	3,2	9,9,10	0.88	0	9,11,13	2.16	1 (11%)
2	DBB	D	3	2	5,5,6	1.23	1 (20%)	3,5,7	1.45	1 (33%)
2	MHU	D	5	2	15,15,16	1.24	3 (20%)	18,19,21	1.20	1 (5%)
2	MHV	D	6	2,5	9,9,10	1.07	1 (11%)	9,11,13	2.11	4 (44%)
2	004	D	7	2	8,10,11	1.96	3 (37%)	11,12,14	1.97	3 (27%)

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	MHW	C	1	3,2	-	0/2/2/4	0/1/1/1
2	DBB	C	3	2	-	0/2/4/6	0/0/0/0
2	MHU	C	5	2	-	0/8/12/14	0/1/1/1
2	MHV	C	6	2,5	-	0/1/12/14	0/1/1/1
2	004	C	7	2	-	0/4/6/8	0/1/1/1
2	MHW	D	1	3,2	-	0/2/2/4	0/1/1/1
2	DBB	D	3	2	-	0/2/4/6	0/0/0/0
2	MHU	D	5	2	-	0/8/12/14	0/1/1/1
2	MHV	D	6	2,5	-	0/1/12/14	0/1/1/1
2	004	D	7	2	-	0/4/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	004	CG1-CB	-3.66	1.33	1.39
2	C	7	004	CG1-CB	-3.40	1.33	1.39
2	D	7	004	CD1-CE	-2.45	1.32	1.38
2	D	5	MHU	CZ1-NZ	-2.41	1.39	1.45
2	D	7	004	CG2-CB	-2.32	1.35	1.39
2	C	7	004	CD1-CE	-2.32	1.32	1.38
2	C	5	MHU	CZ1-NZ	-2.30	1.40	1.45
2	C	7	004	CG2-CB	-2.23	1.35	1.39
2	D	5	MHU	CA-C	2.04	1.52	1.50
2	C	5	MHU	CZ-NZ	2.12	1.42	1.37
2	D	5	MHU	CZ-NZ	2.21	1.42	1.37
2	C	3	DBB	CA-C	2.42	1.53	1.50
2	C	7	004	CB-CA	2.44	1.55	1.52
2	D	3	DBB	CA-C	2.47	1.53	1.50
2	D	6	MHV	CA-C	2.77	1.53	1.50
2	C	6	MHV	CA-C	2.82	1.53	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	MHW	O-C-CA	-5.94	119.17	124.32
2	C	1	MHW	O-C-CA	-5.02	119.98	124.32
2	C	5	MHU	O-C-CA	-3.62	116.72	125.15
2	D	5	MHU	O-C-CA	-3.47	117.06	125.15
2	D	6	MHV	CB-CA-N	-2.90	106.36	112.48
2	C	3	DBB	O-C-CA	-2.63	117.75	125.02
2	D	3	DBB	O-C-CA	-2.49	118.13	125.02
2	C	6	MHV	CB-CA-N	-2.40	107.41	112.48
2	D	7	004	O-C-CA	-2.35	120.96	124.40
2	C	7	004	O-C-CA	-2.28	121.07	124.40
2	D	6	MHV	OD1-CG-CB	-2.26	119.05	121.98
2	C	6	MHV	CE-CD2-CG	2.13	115.47	111.89
2	D	7	004	CG1-CB-CA	2.53	124.89	120.66
2	C	7	004	CG1-CB-CA	2.58	124.98	120.66
2	D	6	MHV	CD2-CG-CB	2.84	119.67	115.84
2	D	6	MHV	CE-CD2-CG	3.54	117.84	111.89
2	C	7	004	C-CA-N	3.72	117.11	109.15
2	D	7	004	C-CA-N	4.57	118.94	109.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	004	2	0
2	D	5	MHU	1	0
2	D	7	004	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z  > 2$
4	DOL	A	2002	-	43,50,50	4.42	17 (39%)	54,70,70	3.28	24 (44%)
4	DOL	B	2003	-	43,50,50	4.88	19 (44%)	54,70,70	3.74	29 (53%)
5	MHT	C	8	2	9,11,11	1.32	1 (11%)	11,15,15	2.09	4 (36%)
5	MHT	D	8	2	9,11,11	1.28	1 (11%)	11,15,15	2.39	6 (54%)

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
4	DOL	A	2002	-	1/1/14/20	0/58/77/77	0/1/3/3
4	DOL	B	2003	-	3/3/14/20	2/58/77/77	0/1/3/3
5	MHT	C	8	2	1/1/3/3	0/0/20/20	0/0/2/2
5	MHT	D	8	2	1/1/3/3	0/0/20/20	0/0/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2003	DOL	C16-C14	-17.41	1.27	1.51
4	A	2002	DOL	C28-C26	-14.22	1.21	1.48
4	B	2003	DOL	C28-C26	-13.82	1.22	1.48
4	A	2002	DOL	C16-C14	-13.36	1.32	1.51
4	B	2003	DOL	C42-S39	-10.26	1.61	1.78
4	B	2003	DOL	C43-N44	-10.05	1.24	1.47
4	A	2002	DOL	C42-S39	-9.61	1.62	1.78
4	A	2002	DOL	C43-N44	-9.42	1.25	1.47
4	A	2002	DOL	C13-C14	-9.39	1.34	1.52
4	B	2003	DOL	C13-C14	-9.06	1.35	1.52
4	B	2003	DOL	C16-C17	-7.31	1.42	1.54
4	B	2003	DOL	C47-N44	-4.80	1.23	1.47
4	A	2002	DOL	C47-N44	-4.68	1.23	1.47
4	B	2003	DOL	C45-N44	-4.67	1.23	1.47
4	A	2002	DOL	C45-N44	-4.57	1.24	1.47
4	B	2003	DOL	O36-C32	-4.40	1.38	1.44
4	A	2002	DOL	O36-C32	-4.10	1.38	1.44
4	A	2002	DOL	C28-C29	-4.07	1.22	1.32
4	A	2002	DOL	O41-S39	-4.02	1.36	1.44
4	B	2003	DOL	C28-C29	-3.91	1.22	1.32
4	A	2002	DOL	O40-S39	-3.78	1.37	1.44
4	B	2003	DOL	O40-S39	-3.71	1.37	1.44
4	B	2003	DOL	C26-N25	-3.45	1.29	1.34
4	A	2002	DOL	C1-C2	-3.13	1.51	1.55
4	B	2003	DOL	O41-S39	-2.92	1.38	1.44
4	B	2003	DOL	C17-C19	-2.92	1.46	1.50
4	A	2002	DOL	O15-C14	-2.90	1.16	1.21
4	A	2002	DOL	C30-C32	-2.87	1.46	1.54
4	B	2003	DOL	C1-C2	-2.65	1.51	1.55
4	B	2003	DOL	O18-C17	-2.64	1.38	1.43
4	B	2003	DOL	C30-C32	-2.24	1.48	1.54
4	A	2002	DOL	C26-N25	-2.22	1.30	1.34
4	B	2003	DOL	C30-C29	-2.12	1.45	1.51
4	A	2002	DOL	C1-N5	2.32	1.49	1.46
5	D	8	MHT	C6-N1	2.44	1.53	1.47
5	C	8	MHT	C6-N1	2.58	1.54	1.47
4	A	2002	DOL	O36-C37	3.79	1.43	1.34
4	B	2003	DOL	O36-C37	4.14	1.43	1.34

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	DOL	O40-S39-O41	-14.07	105.01	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2003	DOL	O40-S39-O41	-13.36	105.66	117.94
4	B	2003	DOL	C43-C42-S39	-8.37	96.58	112.39
4	A	2002	DOL	C23-C22-C20	-7.72	114.23	125.89
4	B	2003	DOL	C16-C17-C19	-6.91	98.60	111.20
4	B	2003	DOL	O15-C14-C16	-6.80	111.50	121.50
4	A	2002	DOL	O15-C14-C16	-6.00	112.67	121.50
4	B	2003	DOL	C29-C28-C26	-5.67	108.10	122.90
4	B	2003	DOL	C23-C22-C20	-5.33	117.84	125.89
4	A	2002	DOL	C4-N5-C1	-5.07	106.73	112.33
4	A	2002	DOL	C30-C29-C28	-4.92	111.47	126.39
4	A	2002	DOL	O36-C37-O38	-4.48	115.13	123.90
4	B	2003	DOL	C4-N5-C1	-4.47	107.40	112.33
4	B	2003	DOL	C8-C6-N5	-4.30	114.75	119.77
4	B	2003	DOL	O38-C37-C1	-4.04	117.15	124.60
4	A	2002	DOL	C24-C23-C22	-3.78	115.22	125.36
4	A	2002	DOL	C43-C42-S39	-3.61	105.58	112.39
4	B	2003	DOL	C32-C30-C29	-3.44	97.64	109.40
4	B	2003	DOL	O36-C37-O38	-3.40	117.23	123.90
4	B	2003	DOL	C24-C23-C22	-3.27	116.58	125.36
4	B	2003	DOL	O27-C26-N25	-2.97	118.71	122.41
4	B	2003	DOL	C4-N5-C6	-2.94	114.36	125.27
5	D	8	MHT	C8-C4-C5	-2.67	104.89	109.43
5	D	8	MHT	C6-N1-C2	-2.40	105.97	109.74
5	D	8	MHT	C2-C3-S3	-2.39	105.50	110.35
4	A	2002	DOL	C4-N5-C6	-2.32	116.68	125.27
5	C	8	MHT	C7-N1-C6	-2.30	103.66	108.87
4	A	2002	DOL	C29-C28-C26	-2.28	116.94	122.90
5	C	8	MHT	C8-C4-C5	-2.24	105.61	109.43
5	D	8	MHT	C7-N1-C6	-2.21	103.88	108.87
4	A	2002	DOL	C31-C30-C32	-2.18	106.95	111.06
4	A	2002	DOL	O38-C37-C1	-2.17	120.60	124.60
4	B	2003	DOL	C30-C29-C28	-2.17	119.83	126.39
4	A	2002	DOL	O27-C26-C28	-2.14	118.89	122.88
4	A	2002	DOL	C1-N5-C6	2.04	128.49	120.93
4	A	2002	DOL	C43-N44-C45	2.17	120.32	111.47
4	A	2002	DOL	O18-C17-C16	2.24	115.71	109.77
4	B	2003	DOL	C1-N5-C6	2.25	129.27	120.93
4	B	2003	DOL	O36-C32-C33	2.36	111.45	107.33
4	B	2003	DOL	C3-C2-C1	2.37	108.84	104.31
5	C	8	MHT	C8-C4-C3	2.41	114.33	108.30
4	B	2003	DOL	C31-C30-C32	2.44	115.66	111.06
4	A	2002	DOL	C16-C17-C19	2.49	115.75	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	DOL	C3-C2-S39	2.58	120.67	113.19
4	A	2002	DOL	O27-C26-N25	2.60	125.65	122.41
4	B	2003	DOL	C34-C33-C32	2.68	120.47	111.81
5	D	8	MHT	C8-C4-C3	2.86	115.46	108.30
4	B	2003	DOL	C43-N44-C47	2.94	123.43	111.47
4	B	2003	DOL	O18-C17-C19	2.95	115.11	109.02
4	B	2003	DOL	C21-C20-C22	3.05	122.96	118.10
4	A	2002	DOL	C43-N44-C47	3.14	124.26	111.47
4	A	2002	DOL	C10-C13-C14	3.72	128.07	114.36
4	B	2003	DOL	C34-C33-C35	3.77	121.41	110.64
4	A	2002	DOL	O36-C32-C30	3.86	113.67	107.08
4	B	2003	DOL	C37-C1-N5	3.98	119.76	112.32
4	A	2002	DOL	C3-C4-N5	4.15	107.81	103.38
4	B	2003	DOL	C10-C13-C14	4.54	131.09	114.36
5	C	8	MHT	C7-N1-C2	4.81	117.32	109.74
5	D	8	MHT	C7-N1-C2	5.12	117.80	109.74
4	B	2003	DOL	O7-C6-N5	5.19	129.41	121.54
4	A	2002	DOL	C37-C1-N5	5.93	123.42	112.32
4	B	2003	DOL	C3-C4-N5	6.24	110.05	103.38
4	B	2003	DOL	O36-C37-C1	6.56	125.27	111.61

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2003	DOL	C30
4	B	2003	DOL	C32
4	B	2003	DOL	C17
4	A	2002	DOL	C32
5	D	8	MHT	C3
5	C	8	MHT	C3

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2003	DOL	C37-O36-C32-C33
4	B	2003	DOL	C32-O36-C37-C1

There are no ring outliers.

3 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	DOL	34	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2003	DOL	33	0
5	C	8	MHT	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	293/299 (97%)	0.08	5 (1%) 70 63	9, 18, 31, 50	3 (1%)
1	B	293/299 (97%)	0.10	6 (2%) 65 56	9, 18, 31, 50	5 (1%)
2	C	2/7 (28%)	0.08	0 100 100	22, 22, 22, 25	0
2	D	2/7 (28%)	-0.03	0 100 100	18, 18, 18, 21	0
All	All	590/612 (96%)	0.09	11 (1%) 67 58	9, 18, 31, 50	8 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	ILE	3.7
1	B	5	LEU	2.7
1	A	2	GLU	2.6
1	A	98	ASP	2.6
1	B	2	GLU	2.6
1	A	293	LEU	2.5
1	B	14	ASP	2.5
1	A	5	LEU	2.3
1	B	128	ASP	2.1
1	B	44	ASP	2.0
1	B	265	LYS	2.0

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

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
2	MHW	D	1	9/10	0.89	0.20	-	17,17,17,17	0
2	MHV	C	6	9/10	0.94	0.18	-	25,27,29,30	0
2	004	D	7	10/11	0.97	0.14	-	17,17,18,19	0
2	004	C	7	10/11	0.94	0.18	-	21,22,23,24	0
2	DBB	D	3	6/7	0.89	0.21	-	18,19,19,20	0
2	MHU	D	5	15/16	0.92	0.19	-	21,25,25,25	0
2	MHV	D	6	9/10	0.92	0.18	-	21,23,26,26	0
2	MHW	C	1	9/10	0.91	0.21	-	19,20,20,20	0
2	DBB	C	3	6/7	0.88	0.21	-	22,23,24,24	0
2	MHU	C	5	15/16	0.88	0.23	-	25,28,29,29	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
5	MHT	C	8	10/10	0.82	0.28	2.10	31,35,36,36	0
5	MHT	D	8	10/10	0.86	0.26	1.71	27,31,31,31	0
4	DOL	A	2002	48/48	0.80	0.27	0.90	28,32,34,35	0
4	DOL	B	2003	48/48	0.82	0.23	0.61	21,25,34,35	0
3	MG	A	1003	1/1	0.92	0.12	-1.63	18,18,18,18	0
3	MG	A	1001	1/1	0.94	0.23	-	2,2,2,2	0
3	MG	B	1004	1/1	0.89	0.10	-	15,15,15,15	0
3	MG	B	1002	1/1	0.96	0.26	-	2,2,2,2	0

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

There are no such residues in this entry.