Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 08:56 PM GMT

PDB ID	:	1MRL
Title	:	Crystal structure of streptogramin A acetyltransferase with dalfopristin
Authors	:	Kehoe, L.E.; Snidwongse, J.; Courvalin, P.; Rafferty, J.B.; Murray, I.A.
Deposited on	:	2002-09-18
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

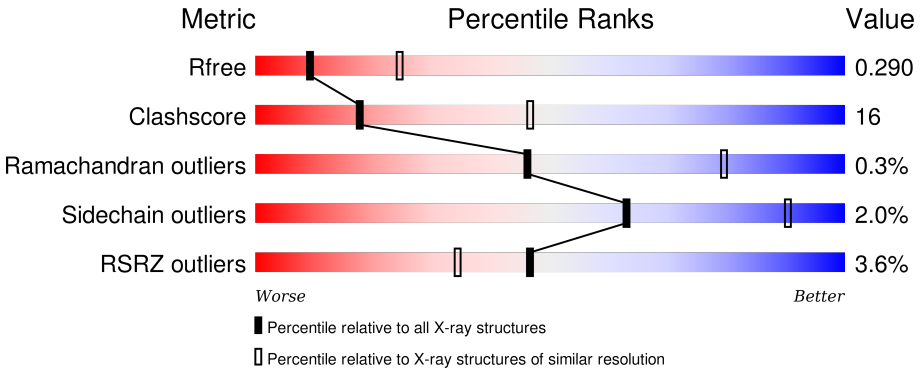
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 >=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 <=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	209	4% 73% 23%
1	B	209	2% 72% 24%
1	C	209	5% 76% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DOL	A	300	-	-	X	X
2	DOL	B	301	-	-	X	X
2	DOL	C	302	-	-	X	X

2 Entry composition

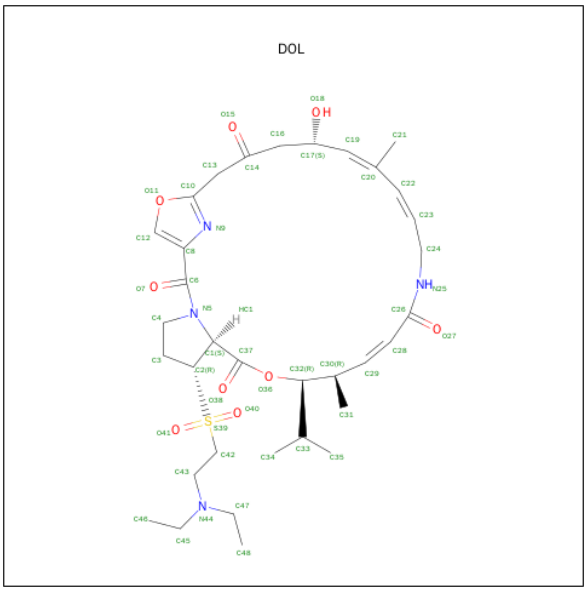
There are 2 unique types of molecules in this entry. The entry contains 4916 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Streptogramin A acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	2	0
			1586	1021	256	300	9			
1	B	204	Total	C	N	O	S	0	1	0
			1592	1027	260	297	8			
1	C	204	Total	C	N	O	S	0	1	0
			1594	1026	261	299	8			

- Molecule 2 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
2	A	1	Total	C	N	O	S	0	0
			48	34	4	9	1		
2	B	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

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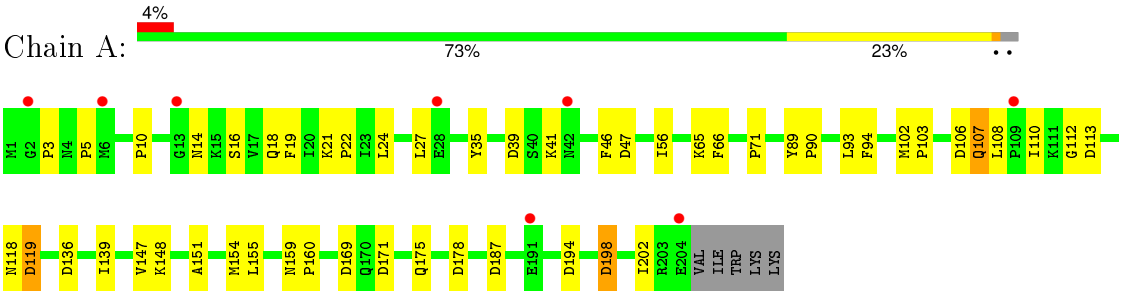
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			48	34	4	9	1		

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 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.

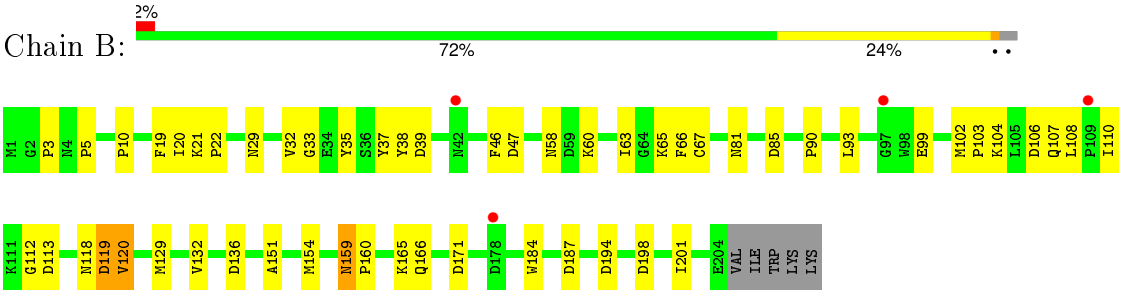
- Molecule 1: Streptogramin A acetyltransferase

Chain A:



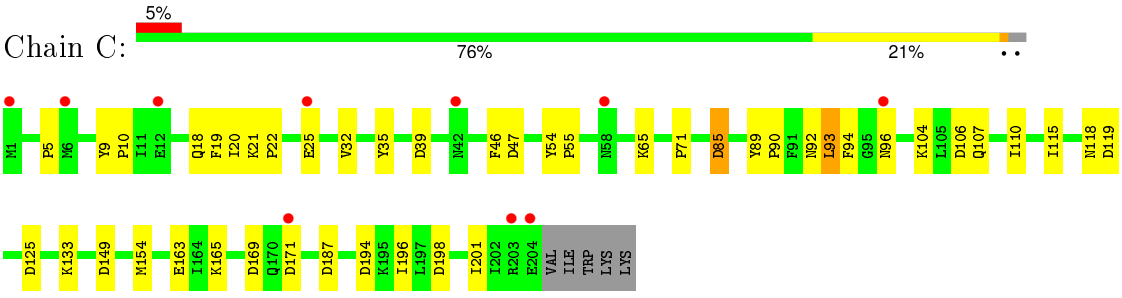
- Molecule 1: Streptogramin A acetyltransferase

Chain B:



- Molecule 1: Streptogramin A acetyltransferase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.91Å 90.91Å 104.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.80) 99.8 (14.99-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.271 , 0.304 0.257 , 0.290	Depositor DCC
R_{free} test set	1009 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 19862 reflections (0.010%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4916	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOL

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	0.22	0/1627	0.68	11/2220 (0.5%)
1	B	0.25	0/1632	0.68	11/2221 (0.5%)
1	C	0.22	0/1634	0.69	11/2225 (0.5%)
All	All	0.23	0/4893	0.68	33/6666 (0.5%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	198	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	119	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	119	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	47	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	47	ASP	CB-CG-OD2	5.41	123.16	118.30
1	A	113	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	149	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	178	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	187	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	106	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	187	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	39	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	106	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	194	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	119	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	171	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	125	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	198	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	85	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	113	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	47	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	106	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	169	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	194	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	187	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	136	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	198	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	194	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	171	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	169	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	171	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1586	0	1517	42	0
1	B	1592	0	1555	44	0
1	C	1594	0	1548	26	0
2	A	48	0	49	25	0
2	B	48	0	49	26	0
2	C	48	0	49	21	0
All	All	4916	0	4767	154	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 16.

All (154) 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)
2:C:302:DOL:C12	2:C:302:DOL:HC42	1.45	1.31
2:B:301:DOL:HC42	2:B:301:DOL:C12	1.46	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:DOL:C31	2:C:302:DOL:H343	1.60	1.26
2:B:301:DOL:C31	2:B:301:DOL:H343	1.63	1.25
2:A:300:DOL:C31	2:A:300:DOL:H343	1.58	1.25
1:B:102:MET:SD	2:B:301:DOL:H352	1.76	1.24
2:A:300:DOL:HC42	2:A:300:DOL:C12	1.45	1.22
2:C:302:DOL:C12	2:C:302:DOL:C4	2.20	1.19
2:A:300:DOL:C12	2:A:300:DOL:C4	2.20	1.19
1:B:93:LEU:HD22	2:B:301:DOL:HC41	1.23	1.18
2:B:301:DOL:C4	2:B:301:DOL:C12	2.20	1.17
2:B:301:DOL:C3	2:B:301:DOL:HC12	1.76	1.15
2:A:300:DOL:HC12	2:A:300:DOL:C3	1.77	1.13
2:C:302:DOL:HC12	2:C:302:DOL:C3	1.78	1.13
1:C:93:LEU:HD11	2:C:302:DOL:HC41	1.23	1.12
2:B:301:DOL:HC3A	2:B:301:DOL:HC12	1.31	1.12
2:A:300:DOL:HC3A	2:A:300:DOL:HC12	1.33	1.10
2:B:301:DOL:H312	2:B:301:DOL:H343	1.08	1.06
2:C:302:DOL:H312	2:C:302:DOL:C34	1.86	1.06
2:A:300:DOL:H312	2:A:300:DOL:C34	1.85	1.06
2:C:302:DOL:HC3A	2:C:302:DOL:HC12	1.33	1.05
2:A:300:DOL:H343	2:A:300:DOL:H312	1.04	1.02
2:B:301:DOL:C34	2:B:301:DOL:H312	1.89	1.02
2:C:302:DOL:H312	2:C:302:DOL:H343	1.05	1.01
2:C:302:DOL:C4	2:C:302:DOL:HC12	1.91	0.98
2:A:300:DOL:HC12	2:A:300:DOL:C4	1.91	0.97
1:B:65:LYS:H	1:B:118:ASN:HD22	1.09	0.97
2:B:301:DOL:C34	2:B:301:DOL:C31	2.42	0.94
1:B:102:MET:SD	2:B:301:DOL:H311	2.06	0.94
2:C:302:DOL:C31	2:C:302:DOL:C34	2.39	0.94
2:B:301:DOL:C4	2:B:301:DOL:HC12	1.92	0.93
1:B:65:LYS:H	1:B:118:ASN:ND2	1.67	0.92
2:A:300:DOL:C31	2:A:300:DOL:C34	2.37	0.92
1:C:93:LEU:HD11	2:C:302:DOL:C4	2.00	0.91
2:B:301:DOL:HC3A	2:B:301:DOL:C12	1.99	0.91
2:B:301:DOL:C3	2:B:301:DOL:C12	2.47	0.90
2:A:300:DOL:HC3A	2:A:300:DOL:C12	2.00	0.90
1:A:93:LEU:CD1	2:A:300:DOL:HC19	2.00	0.90
2:A:300:DOL:HC42	2:A:300:DOL:HC12	1.52	0.90
2:C:302:DOL:C12	2:C:302:DOL:HC3A	2.01	0.89
2:A:300:DOL:C12	2:A:300:DOL:C3	2.47	0.88
1:A:108:LEU:HD11	2:A:300:DOL:O27	1.74	0.86
1:B:93:LEU:CD2	2:B:301:DOL:HC41	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:H	1:B:107:GLN:HE21	1.28	0.81
2:A:300:DOL:H311	2:A:300:DOL:H343	1.61	0.81
1:A:56:ILE:HD13	2:A:300:DOL:H341	1.62	0.80
2:C:302:DOL:C12	2:C:302:DOL:C3	2.48	0.80
2:C:302:DOL:H311	2:C:302:DOL:H343	1.62	0.78
1:B:93:LEU:HD22	2:B:301:DOL:C4	2.12	0.77
1:B:108:LEU:HD11	2:B:301:DOL:O27	1.85	0.77
1:C:104:LYS:H	1:C:107:GLN:HE21	1.34	0.75
1:A:102:MET:HG3	1:A:103[A]:PRO:HD2	1.66	0.75
1:A:65:LYS:H	1:A:118:ASN:ND2	1.86	0.74
1:C:93:LEU:CD1	2:C:302:DOL:HC41	2.13	0.73
2:B:301:DOL:H311	2:B:301:DOL:H343	1.65	0.73
1:B:20:ILE:HD11	1:B:38:TYR:HB2	1.71	0.72
2:B:301:DOL:N9	2:B:301:DOL:O15	2.22	0.72
1:C:21:LYS:HB3	1:C:22:PRO:HD3	1.72	0.71
2:C:302:DOL:N9	2:C:302:DOL:O15	2.22	0.71
1:A:94:PHE:HB3	1:B:3:PRO:HG3	1.72	0.71
1:B:21:LYS:HB3	1:B:22:PRO:HD3	1.73	0.71
1:A:3:PRO:HG3	1:C:94:PHE:HB3	1.73	0.70
2:A:300:DOL:O15	2:A:300:DOL:N9	2.23	0.70
1:C:21:LYS:O	1:C:25:GLU:HG2	1.91	0.69
1:A:21:LYS:HB3	1:A:22:PRO:HD3	1.74	0.69
1:A:94:PHE:HB3	1:B:3:PRO:CG	2.24	0.67
1:A:65:LYS:H	1:A:118:ASN:HD22	1.43	0.67
1:B:21:LYS:HA	1:B:32:VAL:HG23	1.77	0.66
1:A:175:GLN:NE2	1:A:202:ILE:HB	2.12	0.65
1:A:93:LEU:HD11	2:A:300:DOL:HC22	1.80	0.64
1:B:10:PRO:HG3	1:B:19:PHE:CD1	2.34	0.63
1:B:165:LYS:HG3	1:B:166:GLN:N	2.13	0.61
1:B:32:VAL:HG12	1:B:63:ILE:HB	1.81	0.61
1:B:102:MET:CG	2:B:301:DOL:H311	2.31	0.60
1:C:5:PRO:HG3	1:C:35:TYR:CZ	2.37	0.59
1:B:21:LYS:HA	1:B:32:VAL:CG2	2.33	0.59
1:A:93:LEU:HD13	2:A:300:DOL:HC19	1.84	0.58
1:A:147:VAL:HG23	1:A:148:LYS:HG3	1.86	0.58
1:A:93:LEU:HD11	2:A:300:DOL:HC19	1.83	0.57
1:B:102:MET:CG	2:B:301:DOL:C31	2.83	0.57
1:A:5:PRO:HG3	1:A:35:TYR:CZ	2.39	0.57
1:A:139:ILE:HB	1:A:155:LEU:HD23	1.86	0.57
1:A:175:GLN:HE21	1:A:202:ILE:HB	1.70	0.55
1:B:33:GLY:HA3	1:B:65:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:TRP:CZ3	1:B:201:ILE:HD11	2.42	0.55
1:B:90[A]:PRO:HB2	1:B:93:LEU:HG	1.88	0.55
1:B:81:ASN:O	2:B:301:DOL:H241	2.08	0.54
1:A:10:PRO:HG3	1:A:19:PHE:CD1	2.41	0.54
1:A:110:ILE:HG22	1:A:112:GLY:H	1.73	0.54
1:A:39:ASP:HB3	1:A:71:PRO:HD3	1.90	0.54
1:A:14:ASN:OD1	1:A:16:SER:OG	2.24	0.53
1:B:104:LYS:H	1:B:107:GLN:NE2	2.02	0.53
1:C:93:LEU:HD23	2:C:302:DOL:HC19	1.91	0.52
1:B:67:CYS:SG	1:B:120:VAL:HG13	2.51	0.50
1:A:3:PRO:CG	1:C:94:PHE:HB3	2.39	0.50
1:B:65:LYS:N	1:B:118:ASN:HD22	1.93	0.50
1:B:110:ILE:HG22	1:B:112:GLY:H	1.77	0.50
1:B:102:MET:HG3	1:B:103:PRO:HD2	1.94	0.49
1:A:66:PHE:O	1:A:119:ASP:HA	2.12	0.49
1:A:18:GLN:HE22	1:A:46:PHE:H	1.61	0.48
1:C:154:MET:HE2	1:C:163:GLU:HB3	1.96	0.48
1:B:184:TRP:HZ3	1:B:201:ILE:HD11	1.76	0.48
1:A:5:PRO:HG3	1:A:35:TYR:OH	2.14	0.48
1:C:93:LEU:CD2	2:C:302:DOL:HC19	2.44	0.47
1:C:5:PRO:HG3	1:C:35:TYR:OH	2.15	0.47
1:C:65:LYS:H	1:C:118:ASN:HD22	1.63	0.47
1:C:65:LYS:H	1:C:118:ASN:ND2	2.12	0.47
1:A:89:TYR:HA	1:A:90[B]:PRO:HD3	1.78	0.46
1:A:18:GLN:NE2	1:A:46:PHE:H	2.14	0.46
1:C:39:ASP:HB3	1:C:71:PRO:HD3	1.97	0.46
1:C:20:ILE:HG22	1:C:32:VAL:HG11	1.98	0.46
1:C:196:ILE:HG12	1:C:201:ILE:HD13	1.97	0.46
2:C:302:DOL:HC31	2:C:302:DOL:H431	1.97	0.45
1:A:24:LEU:HD22	1:A:27:LEU:HD12	1.98	0.45
2:B:301:DOL:H431	2:B:301:DOL:HC31	1.98	0.44
2:B:301:DOL:HC33	2:B:301:DOL:O40	2.18	0.44
1:C:54:TYR:HA	1:C:55:PRO:HD3	1.90	0.44
2:A:300:DOL:HC31	2:A:300:DOL:H431	1.99	0.44
1:B:151:ALA:HB3	1:B:154:MET:HG3	2.00	0.44
1:A:102:MET:HG3	1:A:103[B]:PRO:HD2	1.99	0.44
1:A:151:ALA:HB3	1:A:154:MET:HG3	1.98	0.44
1:A:103[A]:PRO:HA	1:A:107:GLN:HE21	1.83	0.43
1:A:198:ASP:HA	1:C:85:ASP:OD2	2.19	0.43
1:A:103[B]:PRO:HA	1:A:107:GLN:HE21	1.84	0.43
1:C:115:ILE:HB	1:C:133:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:LEU:HD11	2:B:301:DOL:HC19	2.02	0.42
2:A:300:DOL:O18	1:B:37:TYR:OH	2.35	0.42
2:C:302:DOL:HC23	2:C:302:DOL:H211	1.89	0.42
1:B:93:LEU:CD1	2:B:301:DOL:HC19	2.48	0.42
2:A:300:DOL:H311	2:A:300:DOL:H352	2.02	0.42
1:B:104:LYS:HG3	1:B:107:GLN:NE2	2.34	0.42
1:C:89:TYR:HA	1:C:90[A]:PRO:HD3	1.74	0.42
1:C:19:PHE:O	1:C:22:PRO:HD2	2.20	0.42
1:C:89:TYR:HA	1:C:90[B]:PRO:HD3	1.78	0.42
2:C:302:DOL:H311	2:C:302:DOL:H352	2.02	0.41
1:B:159:ASN:C	1:B:159:ASN:ND2	2.73	0.41
1:B:20:ILE:HD12	1:B:46:PHE:CD2	2.56	0.41
1:A:159:ASN:HA	1:A:160:PRO:HA	1.94	0.41
1:B:29:ASN:HB3	1:B:60:LYS:HD3	2.01	0.41
1:C:9:TYR:HA	1:C:10:PRO:HD2	1.89	0.41
1:B:159:ASN:C	1:B:159:ASN:HD22	2.24	0.41
1:B:66:PHE:O	1:B:119:ASP:HA	2.21	0.41
2:A:300:DOL:O40	2:A:300:DOL:HC33	2.21	0.41
1:B:5:PRO:HG3	1:B:35:TYR:OH	2.21	0.41
1:A:94:PHE:HB3	1:B:3:PRO:HG2	2.00	0.41
1:C:110:ILE:HG23	1:C:110:ILE:O	2.21	0.41
1:A:93:LEU:HD22	2:A:300:DOL:HC41	2.03	0.40
1:B:159:ASN:HA	1:B:160:PRO:HA	1.93	0.40
1:A:89:TYR:HA	1:A:90[A]:PRO:HD3	1.88	0.40
1:B:129:MET:O	1:B:132:VAL:HG13	2.21	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	204/209 (98%)	192 (94%)	12 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	203/209 (97%)	195 (96%)	8 (4%)	0	100 100
1	C	203/209 (97%)	192 (95%)	9 (4%)	2 (1%)	19 52
All	All	610/627 (97%)	579 (95%)	29 (5%)	2 (0%)	46 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	ASN
1	C	46	PHE

5.3.2 Protein sidechains (i)

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	169/183 (92%)	167 (99%)	2 (1%)	78 95
1	B	171/183 (93%)	167 (98%)	4 (2%)	58 88
1	C	171/183 (93%)	167 (98%)	4 (2%)	58 88
All	All	511/549 (93%)	501 (98%)	10 (2%)	63 90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	107	GLN
1	B	58	ASN
1	B	99	GLU
1	B	120	VAL
1	B	159	ASN
1	C	18	GLN
1	C	93	LEU
1	C	96	ASN
1	C	165	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	58	ASN
1	A	107	GLN
1	A	118	ASN
1	A	162	ASN
1	A	175	GLN
1	B	58	ASN
1	B	107	GLN
1	B	118	ASN
1	B	159	ASN
1	B	162	ASN
1	C	96	ASN
1	C	107	GLN
1	C	118	ASN
1	C	166	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

3 ligands 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	DOL	A	300	-	43,50,50	5.36	14 (32%)	50,70,70	3.62	20 (40%)
2	DOL	B	301	-	43,50,50	5.71	15 (34%)	50,70,70	3.91	19 (38%)
2	DOL	C	302	-	43,50,50	5.38	14 (32%)	50,70,70	3.68	19 (38%)

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	DOL	A	300	-	-	1/58/77/77	0/1/3/3
2	DOL	B	301	-	-	1/58/77/77	0/1/3/3
2	DOL	C	302	-	-	1/58/77/77	0/1/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	DOL	C8-C6	-4.16	1.42	1.50
2	C	302	DOL	C1-C2	-2.52	1.51	1.55
2	B	301	DOL	C1-C2	-2.49	1.51	1.55
2	A	300	DOL	C1-C2	-2.46	1.51	1.55
2	B	301	DOL	C22-C20	2.95	1.52	1.45
2	A	300	DOL	C22-C20	2.97	1.52	1.45
2	C	302	DOL	C22-C20	3.05	1.52	1.45
2	B	301	DOL	O36-C37	4.41	1.44	1.34
2	A	300	DOL	O36-C37	4.49	1.44	1.34
2	C	302	DOL	O36-C37	4.49	1.44	1.34
2	C	302	DOL	C19-C20	5.31	1.52	1.34
2	B	301	DOL	C19-C20	5.35	1.53	1.34
2	A	300	DOL	C19-C20	5.37	1.53	1.34
2	B	301	DOL	C26-N25	7.08	1.44	1.34
2	A	300	DOL	C6-N5	7.09	1.47	1.35
2	C	302	DOL	C26-N25	7.11	1.44	1.34
2	A	300	DOL	C26-N25	7.15	1.44	1.34
2	B	301	DOL	C22-C23	7.33	1.52	1.31
2	A	300	DOL	C22-C23	7.36	1.52	1.31
2	C	302	DOL	C6-N5	7.39	1.47	1.35
2	C	302	DOL	C22-C23	7.41	1.52	1.31
2	B	301	DOL	C28-C29	7.47	1.52	1.32
2	A	300	DOL	C28-C29	7.52	1.52	1.32
2	C	302	DOL	C28-C29	7.52	1.52	1.32
2	A	300	DOL	O7-C6	8.33	1.39	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	DOL	O7-C6	8.38	1.39	1.22
2	B	301	DOL	O38-C37	8.85	1.43	1.21
2	A	300	DOL	O38-C37	8.90	1.43	1.21
2	C	302	DOL	O38-C37	8.95	1.43	1.21
2	A	300	DOL	O27-C26	9.33	1.43	1.24
2	C	302	DOL	O27-C26	9.35	1.43	1.24
2	B	301	DOL	O27-C26	9.43	1.43	1.24
2	B	301	DOL	O7-C6	10.22	1.43	1.22
2	C	302	DOL	O15-C14	11.81	1.43	1.21
2	A	300	DOL	O15-C14	11.85	1.43	1.21
2	B	301	DOL	O15-C14	11.90	1.43	1.21
2	B	301	DOL	C6-N5	12.72	1.56	1.35
2	C	302	DOL	O40-S39	16.82	1.76	1.44
2	B	301	DOL	O40-S39	16.83	1.76	1.44
2	A	300	DOL	O40-S39	16.84	1.76	1.44
2	A	300	DOL	O41-S39	16.89	1.76	1.44
2	C	302	DOL	O41-S39	16.93	1.76	1.44
2	B	301	DOL	O41-S39	16.96	1.76	1.44

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	302	DOL	C4-N5-C1	-13.68	97.46	112.39
2	B	301	DOL	C4-N5-C1	-13.54	97.61	112.39
2	A	300	DOL	C4-N5-C1	-13.38	97.79	112.39
2	C	302	DOL	C8-C6-N5	-8.44	112.56	119.89
2	B	301	DOL	C8-C6-N5	-8.36	112.62	119.89
2	A	300	DOL	C8-C6-N5	-7.98	112.96	119.89
2	B	301	DOL	C4-N5-C6	-7.71	99.52	125.73
2	B	301	DOL	C23-C22-C20	-7.66	114.07	125.75
2	C	302	DOL	C23-C22-C20	-7.46	114.37	125.75
2	A	300	DOL	C23-C22-C20	-7.44	114.40	125.75
2	B	301	DOL	O40-S39-O41	-7.42	110.84	117.98
2	C	302	DOL	O40-S39-O41	-7.36	110.90	117.98
2	A	300	DOL	O40-S39-O41	-7.32	110.94	117.98
2	A	300	DOL	C4-N5-C6	-6.99	101.97	125.73
2	C	302	DOL	C4-N5-C6	-6.95	102.10	125.73
2	A	300	DOL	C24-C23-C22	-6.81	105.39	125.31
2	B	301	DOL	C24-C23-C22	-6.78	105.49	125.31
2	C	302	DOL	C24-C23-C22	-6.70	105.72	125.31
2	B	301	DOL	O7-C6-N5	-6.02	113.21	121.52
2	B	301	DOL	C10-C13-C14	-5.30	96.24	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	302	DOL	C10-C13-C14	-5.29	96.25	113.47
2	A	300	DOL	C10-C13-C14	-5.27	96.35	113.47
2	B	301	DOL	O27-C26-N25	-3.82	117.61	122.53
2	A	300	DOL	O27-C26-N25	-3.63	117.85	122.53
2	C	302	DOL	O27-C26-N25	-3.59	117.91	122.53
2	B	301	DOL	O36-C37-O38	-3.13	117.45	123.89
2	A	300	DOL	O36-C37-O38	-3.05	117.62	123.89
2	C	302	DOL	O36-C37-O38	-3.03	117.66	123.89
2	A	300	DOL	O27-C26-C28	-2.75	117.72	123.01
2	C	302	DOL	O27-C26-C28	-2.64	117.93	123.01
2	B	301	DOL	O27-C26-C28	-2.64	117.94	123.01
2	A	300	DOL	O38-C37-C1	-2.57	119.96	124.61
2	C	302	DOL	C3-C2-S39	-2.54	108.52	112.77
2	B	301	DOL	C3-C2-S39	-2.48	108.62	112.77
2	C	302	DOL	O38-C37-C1	-2.45	120.17	124.61
2	B	301	DOL	O38-C37-C1	-2.41	120.25	124.61
2	A	300	DOL	C3-C2-S39	-2.34	108.85	112.77
2	A	300	DOL	O15-C14-C16	-2.24	117.95	121.47
2	C	302	DOL	O15-C14-C16	-2.14	118.11	121.47
2	A	300	DOL	O41-S39-C42	2.00	110.63	107.95
2	A	300	DOL	C1-N5-C6	2.26	130.67	121.30
2	A	300	DOL	C32-O36-C37	2.35	122.10	118.01
2	B	301	DOL	C32-O36-C37	2.53	122.43	118.01
2	C	302	DOL	C1-N5-C6	2.70	132.51	121.30
2	C	302	DOL	C32-O36-C37	2.76	122.81	118.01
2	B	301	DOL	C1-N5-C6	3.10	134.19	121.30
2	A	300	DOL	O7-C6-C8	3.60	126.76	118.75
2	A	300	DOL	C37-C1-N5	3.61	119.20	112.36
2	C	302	DOL	C37-C1-N5	3.65	119.27	112.36
2	B	301	DOL	C37-C1-N5	3.70	119.36	112.36
2	C	302	DOL	O7-C6-C8	3.97	127.58	118.75
2	C	302	DOL	O36-C37-C1	5.02	122.17	111.56
2	B	301	DOL	O36-C37-C1	5.07	122.29	111.56
2	A	300	DOL	O36-C37-C1	5.13	122.41	111.56
2	A	300	DOL	O36-C32-C30	5.36	116.22	107.08
2	C	302	DOL	O36-C32-C30	5.44	116.37	107.08
2	B	301	DOL	O36-C32-C30	5.55	116.54	107.08
2	B	301	DOL	O7-C6-C8	6.92	134.14	118.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	DOL	C32-O36-C37-C1
2	C	302	DOL	C32-O36-C37-C1
2	A	300	DOL	C32-O36-C37-C1

There are no ring outliers.

3 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	DOL	25	0
2	B	301	DOL	26	0
2	C	302	DOL	21	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	204/209 (97%)	0.05	8 (3%) 43 31	28, 28, 28, 28	0
1	B	204/209 (97%)	-0.19	4 (1%) 68 58	28, 28, 28, 28	0
1	C	204/209 (97%)	-0.09	10 (4%) 33 22	28, 28, 28, 28	0
All	All	612/627 (97%)	-0.08	22 (3%) 46 34	28, 28, 28, 28	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	GLU	3.9
1	C	25	GLU	3.2
1	A	2	GLY	3.0
1	B	109	PRO	2.9
1	A	6	MET	2.9
1	A	13	GLY	2.8
1	A	42	ASN	2.8
1	C	1	MET	2.4
1	B	178	ASP	2.4
1	C	42	ASN	2.4
1	C	58	ASN	2.4
1	C	96	ASN	2.4
1	A	204	GLU	2.2
1	C	12	GLU	2.2
1	A	109	PRO	2.2
1	B	42	ASN	2.1
1	C	6	MET	2.1
1	A	28	GLU	2.1
1	C	203	ARG	2.1
1	A	191	GLU	2.1
1	B	97	GLY	2.0
1	C	171	ASP	2.0

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 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DOL	B	301	48/48	0.53	0.51	6.90	53,53,53,53	0
2	DOL	C	302	48/48	0.53	0.42	5.95	53,53,53,53	0
2	DOL	A	300	48/48	0.57	0.43	5.50	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.