Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:22 pm BST

PDB ID	:	5LFC
Title	:	Crystal structure of Leuconostoc citreum NRRL B-1299 N-terminally truncated dextransucrase DSR-M
Authors	:	Claverie, M.; Cioci, G.; Remaud-simeon, M.; Moulis, C.; Tranier, S.
Deposited on	:	2016-07-01
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

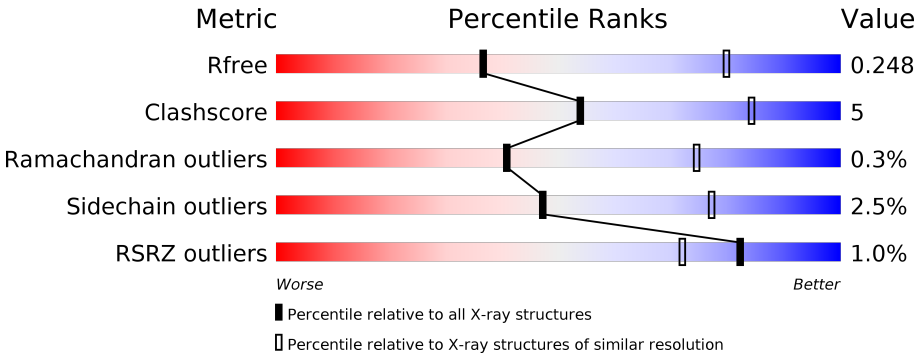
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1293	% 78% 10% • 11%
1	B	1293	% 76% 12% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18029 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.

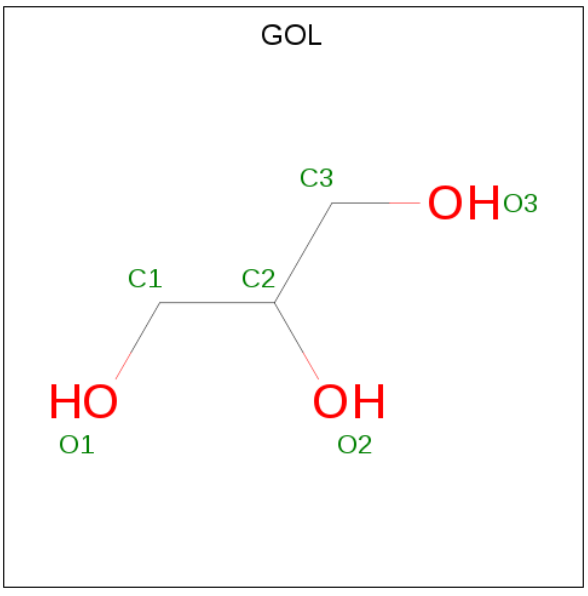
- Molecule 1 is a protein called DsrV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1148	Total	C	N	O	S	0	0	0
			9008	5643	1521	1825	19			
1	B	1148	Total	C	N	O	S	0	0	0
			8995	5634	1519	1823	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

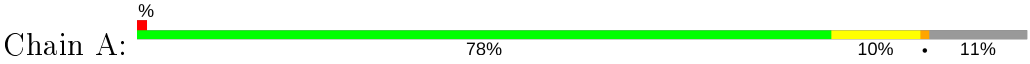
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0

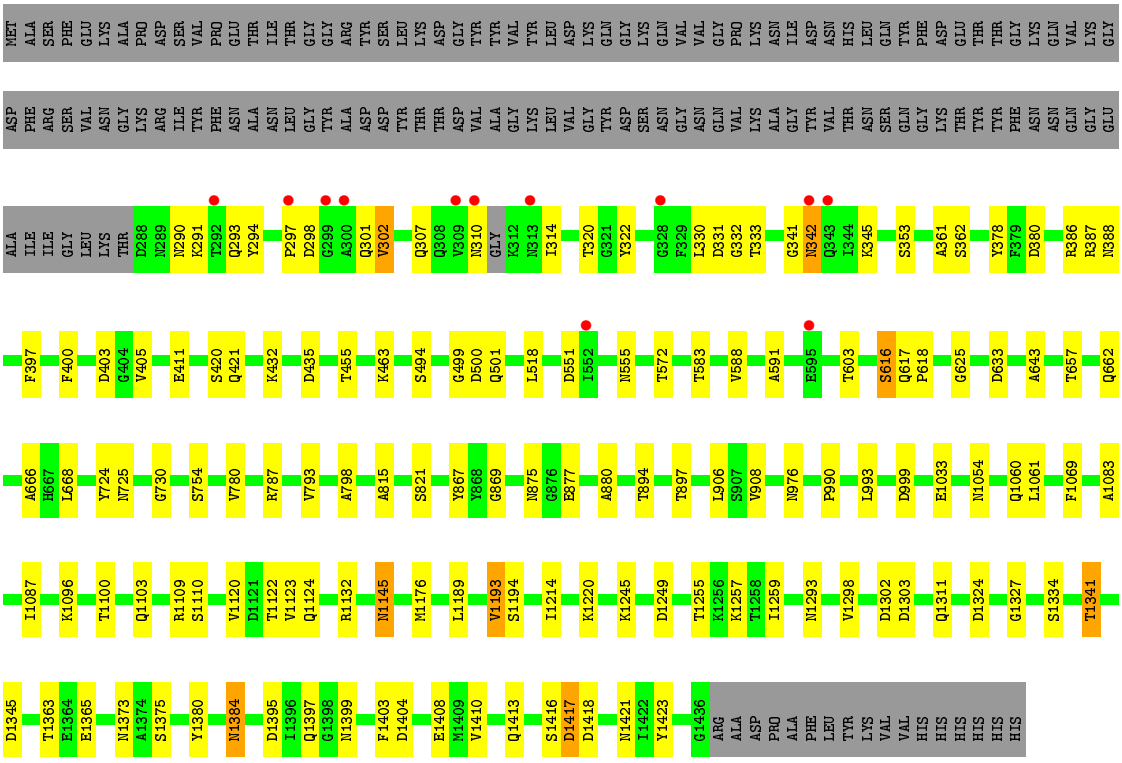
3 Residue-property plots (i)

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

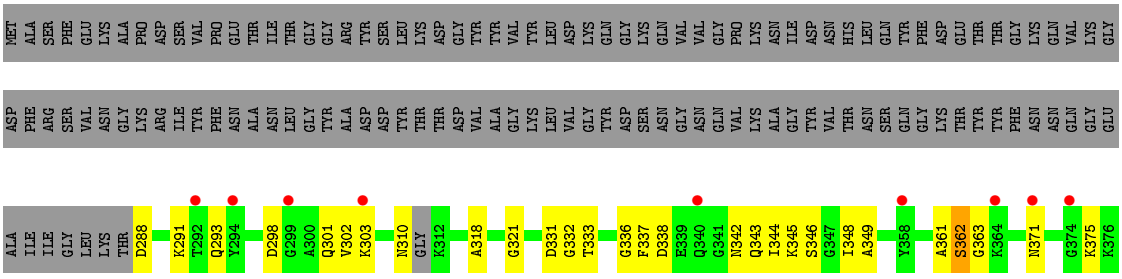
Chain A:

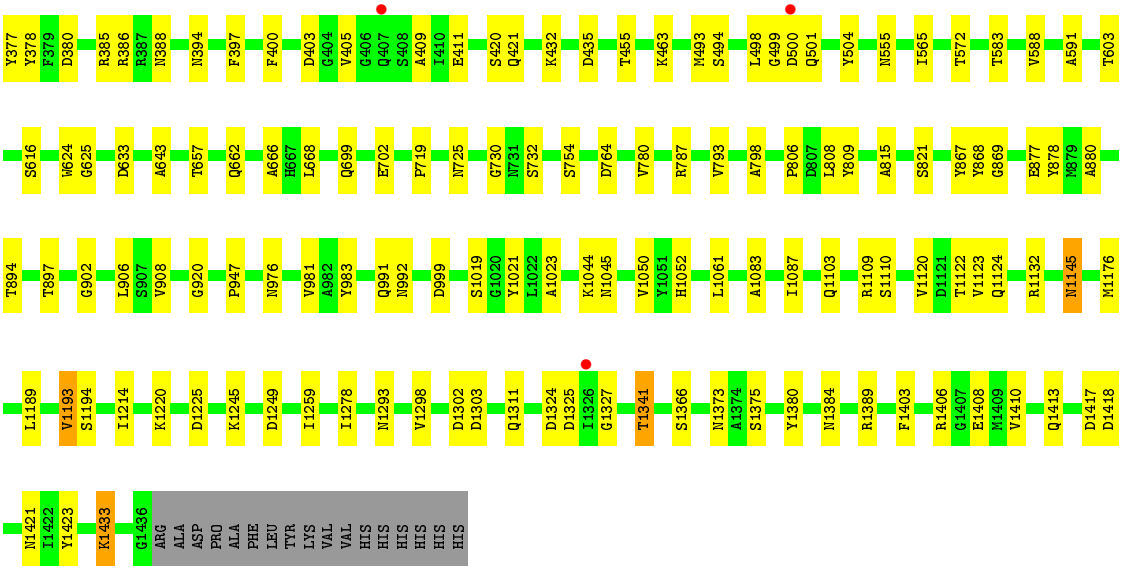




- Molecule 1: DsrV

Chain B:




Y377 Y378 F379 D380 R385 R386 R387 N388 N394 F397 F400 D403 G404 V405 G406 Q407 S408 A409 I410 E411 S420 Q421 K432 D435 T455 K463 M493 S494 L498 G499 D500 Q501 Y504 N555 I565 T572 T583 V588 A591 T603
S616 W624 G625 D633 A643 T657 Q662 A666 H667 L668 Q699 E702 P719 N725 G730 N731 S732 S754 D764 V780 R787 V793 A798 P806 D807 L808 Y809 A815 S821 Y867 Y868 G869 E877 Y878 M879 A880
T894 T897 G902 L906 S907 V908 G920 P947 N976 V981 A982 Y983 Q991 N992 D999 S1019 G1020 Y1021 L1022 A1023 K1044 N1045 V1050 Y1051 H1052 L1061 A1083 I1087 Q1103 R1109 S1110 V1120 D1121 T1122 V1123 Q1124 R1132 M1145 M1176
L1189 V1193 S1194 I1214 K1220 D1225 K1245 D1249 I1259 I1278 N1293 V1298 D1302 D1303 Q1311 D1324 D1325 I1326 G1327 T1341 S1366 N1373 A1374 S1375 Y1380 N1384 R1389 F1403 R1406 G1407 E1408 M1409 V1410 Q1413 D1417 D1418
N1421 I1422 Y1423 K1433 G1436 ARG ALA ASP PRO ALA PHE LEU TYR LYS VAL VAL HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.84Å 128.71Å 229.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.67 – 3.20 49.23 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (114.67-3.20) 98.4 (49.23-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.248 0.222 , 0.248	Depositor DCC
R_{free} test set	2531 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18029	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.333 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: GOL, CA

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	0.48	0/9204	0.64	2/12502 (0.0%)
1	B	0.44	0/9191	0.62	1/12488 (0.0%)
All	All	0.47	0/18395	0.63	3/24990 (0.0%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1417	ASP	N-CA-CB	-5.45	100.79	110.60
1	B	1225	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	1384	ASN	CB-CA-C	-5.11	100.19	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	616	SER	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	9008	0	8514	90	0
1	B	8995	0	8486	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	12	0	0	0	0
All	All	18029	0	17016	186	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 5.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:CB	1:A:322:TYR:CE1	2.46	0.98
1:B:344:ILE:HD13	1:B:349:ALA:HB2	1.43	0.96
1:B:565:ILE:HD11	1:B:1278:ILE:HD12	1.48	0.95
1:B:1044:LYS:HE2	1:B:1045:ASN:O	1.68	0.94
1:B:662:GLN:N	1:B:662:GLN:OE1	2.11	0.83
1:B:500:ASP:OD1	1:B:504:TYR:OH	1.97	0.81
1:B:336:GLY:C	1:B:344:ILE:HG22	2.03	0.79
1:B:303:LYS:O	1:B:318:ALA:HA	1.84	0.76
1:B:338:ASP:OD2	1:B:342:ASN:HB2	1.89	0.73
1:B:565:ILE:CD1	1:B:1278:ILE:HD12	2.20	0.72
1:B:565:ILE:HD11	1:B:1278:ILE:CD1	2.19	0.72
1:B:500:ASP:O	1:B:501:GLN:HB3	1.88	0.72
1:B:821:SER:HB3	1:B:1122:THR:HG21	1.71	0.71
1:A:302:VAL:O	1:A:302:VAL:HG12	1.91	0.70
1:A:293:GLN:HE22	1:A:301:GLN:CD	1.96	0.69
1:B:371:ASN:HA	1:B:375:LYS:O	1.93	0.68
1:B:947:PRO:HG3	1:B:1019:SER:HB2	1.74	0.68
1:B:293:GLN:HE21	1:B:321:GLY:HA3	1.58	0.67
1:A:361:ALA:O	1:A:362:SER:OG	2.10	0.67
1:B:1302:ASP:OD1	1:B:1303:ASP:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:GLN:HB2	1:A:618:PRO:HD3	1.75	0.67
1:B:345:LYS:HE2	1:B:362:SER:C	2.16	0.66
1:A:1302:ASP:OD1	1:A:1303:ASP:N	2.29	0.65
1:A:314:ILE:HD13	1:A:341:GLY:CA	2.27	0.64
1:A:403:ASP:HB3	1:A:405:VAL:HG23	1.80	0.64
1:B:411:GLU:O	1:B:1384:ASN:ND2	2.30	0.63
1:B:301:GLN:O	1:B:301:GLN:HG2	1.97	0.63
1:A:1120:VAL:HG22	1:A:1123:VAL:HG22	1.79	0.63
1:B:403:ASP:HB3	1:B:405:VAL:HG23	1.81	0.62
1:A:330:LEU:HD12	1:A:331:ASP:H	1.63	0.62
1:B:1120:VAL:HG22	1:B:1123:VAL:HG22	1.81	0.62
1:A:1380:TYR:HB2	1:A:1403:PHE:CZ	2.35	0.61
1:A:821:SER:HB3	1:A:1122:THR:HG21	1.81	0.61
1:A:1373:ASN:OD1	1:A:1375:SER:HB3	2.01	0.61
1:A:1120:VAL:CG2	1:A:1123:VAL:HG22	2.32	0.60
1:B:1373:ASN:OD1	1:B:1375:SER:HB3	2.01	0.59
1:B:1120:VAL:CG2	1:B:1123:VAL:HG22	2.32	0.59
1:A:990:PRO:HD2	1:A:993:LEU:HD12	1.83	0.58
1:A:494:SER:HA	1:A:499:GLY:HA3	1.85	0.58
1:A:1324:ASP:HB3	1:A:1327:GLY:O	2.03	0.58
1:A:494:SER:OG	1:A:500:ASP:O	2.16	0.58
1:A:293:GLN:NE2	1:A:301:GLN:CG	2.66	0.58
1:B:336:GLY:O	1:B:344:ILE:HG22	2.03	0.58
1:B:288:ASP:CB	1:B:291:LYS:O	2.52	0.58
1:A:1083:ALA:O	1:A:1087:ILE:HG12	2.04	0.58
1:B:1293:ASN:HB2	1:B:1341:THR:HG21	1.86	0.58
1:A:293:GLN:HE22	1:A:301:GLN:NE2	2.02	0.58
1:B:1045:ASN:ND2	1:B:1052:HIS:CE1	2.72	0.57
1:A:494:SER:HA	1:A:499:GLY:CA	2.35	0.57
1:B:1083:ALA:O	1:B:1087:ILE:HG12	2.03	0.57
1:B:1324:ASP:HB3	1:B:1327:GLY:O	2.05	0.56
1:B:798:ALA:HB1	1:B:815:ALA:HB3	1.87	0.56
1:A:1123:VAL:O	1:A:1123:VAL:HG23	2.06	0.56
1:A:1293:ASN:HB2	1:A:1341:THR:HG21	1.87	0.56
1:B:409:ALA:O	1:B:1384:ASN:ND2	2.39	0.55
1:A:341:GLY:O	1:A:342:ASN:CB	2.54	0.55
1:A:314:ILE:CD1	1:A:341:GLY:HA3	2.36	0.55
1:A:345:LYS:HD2	1:A:362:SER:H	1.71	0.55
1:A:1417:ASP:HB2	1:A:1423:TYR:HE1	1.72	0.55
1:B:377:TYR:CD1	1:B:385:ARG:HD2	2.42	0.55
1:A:798:ALA:HB1	1:A:815:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:TYR:HB2	1:B:1403:PHE:CZ	2.42	0.55
1:A:551:ASP:OD1	1:A:555:ASN:N	2.35	0.54
1:B:1123:VAL:O	1:B:1123:VAL:HG23	2.05	0.54
1:A:1417:ASP:OD2	1:A:1421:ASN:HB2	2.08	0.54
1:A:411:GLU:O	1:A:1384:ASN:ND2	2.40	0.53
1:B:380:ASP:HB3	1:B:386:ARG:HD2	1.90	0.53
1:B:732:SER:HA	1:B:1050:VAL:HG11	1.91	0.53
1:A:293:GLN:NE2	1:A:301:GLN:CD	2.63	0.53
1:A:297:PRO:O	1:A:298:ASP:OD1	2.26	0.53
1:A:361:ALA:O	1:A:362:SER:CB	2.55	0.53
1:B:1417:ASP:HB2	1:B:1423:TYR:HE1	1.73	0.53
1:B:493:MET:CE	1:B:498:LEU:HD12	2.39	0.53
1:B:493:MET:HE3	1:B:498:LEU:HD12	1.91	0.52
1:B:361:ALA:O	1:B:362:SER:OG	2.17	0.52
1:A:494:SER:CA	1:A:499:GLY:HA3	2.40	0.52
1:B:908:VAL:HG23	1:B:908:VAL:O	2.10	0.52
1:B:583:THR:O	1:B:1194:SER:HB3	2.10	0.51
1:B:1021:TYR:CE2	1:B:1023:ALA:HB2	2.46	0.51
1:A:1033:GLU:N	1:A:1033:GLU:OE1	2.39	0.51
1:B:1021:TYR:HE2	1:B:1023:ALA:HB2	1.76	0.51
1:A:1404:ASP:OD1	1:A:1408:GLU:O	2.29	0.51
1:A:1189:LEU:HB2	1:A:1220:LYS:HB3	1.92	0.50
1:B:1189:LEU:HB2	1:B:1220:LYS:HB3	1.93	0.50
1:A:908:VAL:HG23	1:A:908:VAL:O	2.11	0.50
1:B:293:GLN:NE2	1:B:301:GLN:OE1	2.45	0.50
1:A:583:THR:O	1:A:1194:SER:HB3	2.12	0.50
1:B:1103:GLN:HA	1:B:1176:MET:HB3	1.93	0.49
1:B:501:GLN:O	1:B:501:GLN:HG2	2.12	0.49
1:A:894:THR:HG22	1:A:1096:LYS:O	2.13	0.49
1:A:1103:GLN:HA	1:A:1176:MET:HB3	1.95	0.49
1:A:588:VAL:HG12	1:A:591:ALA:HB3	1.95	0.48
1:B:624:TRP:CZ2	1:B:719:PRO:HD3	2.47	0.48
1:A:1410:VAL:HG13	1:A:1413:GLN:OE1	2.14	0.48
1:B:432:LYS:HA	1:B:455:THR:HG22	1.96	0.48
1:B:494:SER:CB	1:B:499:GLY:HA3	2.43	0.48
1:A:331:ASP:CG	1:A:332:GLY:H	2.17	0.48
1:A:314:ILE:CD1	1:A:341:GLY:CA	2.92	0.48
1:A:494:SER:HA	1:A:499:GLY:N	2.29	0.47
1:B:725:ASN:O	1:B:730:GLY:O	2.32	0.47
1:A:1363:THR:OG1	1:A:1365:GLU:HG2	2.13	0.47
1:A:432:LYS:HA	1:A:455:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:O	1:A:302:VAL:CG1	2.60	0.47
1:B:657:THR:HA	1:B:666:ALA:HB1	1.96	0.47
1:A:657:THR:HA	1:A:666:ALA:HB1	1.96	0.47
1:B:643:ALA:HA	1:B:1259:ILE:HD11	1.97	0.46
1:B:337:PHE:CE1	1:B:343:GLN:NE2	2.83	0.46
1:A:867:TYR:CE2	1:A:869:GLY:HA3	2.50	0.46
1:B:1417:ASP:HB3	1:B:1421:ASN:HB2	1.96	0.46
1:B:361:ALA:O	1:B:362:SER:CB	2.63	0.46
1:B:588:VAL:HG12	1:B:591:ALA:HB3	1.96	0.46
1:A:725:ASN:O	1:A:730:GLY:O	2.33	0.46
1:A:314:ILE:HD11	1:A:341:GLY:HA3	1.97	0.46
1:A:291:LYS:CB	1:A:322:TYR:CD1	2.97	0.46
1:B:1410:VAL:HG13	1:B:1413:GLN:OE1	2.16	0.46
1:A:291:LYS:CB	1:A:322:TYR:HE1	2.19	0.45
1:A:894:THR:O	1:A:897:THR:HB	2.16	0.45
1:B:821:SER:CB	1:B:1122:THR:HG21	2.44	0.45
1:B:494:SER:HA	1:B:499:GLY:N	2.32	0.45
1:A:294:TYR:CE2	1:A:307:GLN:OE1	2.70	0.45
1:A:662:GLN:OE1	1:A:662:GLN:N	2.48	0.45
1:B:336:GLY:CA	1:B:344:ILE:HG22	2.46	0.45
1:A:293:GLN:HG2	1:A:294:TYR:N	2.32	0.45
1:B:787:ARG:NH2	1:B:793:VAL:HG22	2.31	0.45
1:B:867:TYR:CE2	1:B:869:GLY:HA3	2.51	0.45
1:B:894:THR:O	1:B:897:THR:HB	2.16	0.45
1:B:1109:ARG:NH2	1:B:1145:ASN:HD22	2.15	0.45
1:B:1245:LYS:HE3	1:B:1249:ASP:OD2	2.16	0.45
1:B:344:ILE:HD11	1:B:348:ILE:O	2.17	0.45
1:A:435:ASP:C	1:A:1298:VAL:HG12	2.37	0.45
1:B:421:GLN:HB3	1:B:1311:GLN:HG2	1.98	0.45
1:A:294:TYR:O	1:A:301:GLN:O	2.35	0.45
1:A:572:THR:HG22	1:A:572:THR:O	2.16	0.45
1:A:787:ARG:NH2	1:A:793:VAL:HG22	2.31	0.44
1:B:572:THR:O	1:B:572:THR:HG22	2.17	0.44
1:B:591:ALA:HB1	1:B:1193:VAL:HG12	1.99	0.44
1:A:421:GLN:HB3	1:A:1311:GLN:HG2	1.99	0.44
1:B:1389:ARG:CZ	1:B:1406:ARG:O	2.66	0.44
1:B:346:SER:OG	1:B:361:ALA:N	2.51	0.44
1:B:388:ASN:N	1:B:400:PHE:O	2.51	0.44
1:B:902:GLY:HA3	1:B:920:GLY:O	2.18	0.44
1:A:1245:LYS:HE3	1:A:1249:ASP:OD2	2.17	0.43
1:B:1109:ARG:NH2	1:B:1145:ASN:ND2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LYS:C	1:B:318:ALA:HA	2.39	0.43
1:A:591:ALA:HB1	1:A:1193:VAL:HG12	2.00	0.43
1:B:1433:LYS:H	1:B:1433:LYS:HG2	1.65	0.43
1:A:294:TYR:HE2	1:A:307:GLN:CD	2.22	0.43
1:A:1060:GLN:HE22	1:A:1100:THR:HB	1.83	0.42
1:A:378:TYR:HB2	1:A:400:PHE:CE2	2.53	0.42
1:A:616:SER:HB3	1:A:617:GLN:H	1.68	0.42
1:B:1324:ASP:OD1	1:B:1325:ASP:N	2.52	0.42
1:A:1109:ARG:NH2	1:A:1145:ASN:HD22	2.17	0.42
1:B:394:ASN:N	1:B:394:ASN:HD22	2.18	0.42
1:B:806:PRO:HA	1:B:809:TYR:O	2.18	0.42
1:B:588:VAL:HG21	1:B:1214:ILE:HD12	2.02	0.42
1:B:394:ASN:N	1:B:394:ASN:ND2	2.68	0.42
1:A:1110:SER:HB3	1:A:1124:GLN:HB3	2.01	0.42
1:A:1109:ARG:NH2	1:A:1145:ASN:ND2	2.68	0.42
1:A:724:TYR:CD1	1:A:724:TYR:C	2.93	0.42
1:B:345:LYS:HE2	1:B:363:GLY:N	2.35	0.42
1:A:643:ALA:HA	1:A:1259:ILE:HD11	2.01	0.42
1:B:603:THR:HG21	1:B:625:GLY:HA3	2.02	0.42
1:B:1110:SER:HB3	1:B:1124:GLN:HB3	2.01	0.41
1:A:1255:THR:C	1:A:1257:LYS:H	2.23	0.41
1:A:875:ASN:HA	1:A:1069:PHE:O	2.20	0.41
1:B:780:VAL:O	1:B:780:VAL:HG23	2.20	0.41
1:A:293:GLN:HE21	1:A:301:GLN:CG	2.32	0.41
1:A:1311:GLN:HE22	1:A:1334:SER:HA	1.86	0.41
1:A:1395:ASP:OD2	1:A:1399:ASN:HB2	2.21	0.41
1:B:699:GLN:HB3	1:B:702:GLU:CG	2.50	0.41
1:B:877:GLU:HB2	1:B:880:ALA:CB	2.51	0.41
1:A:588:VAL:HG21	1:A:1214:ILE:HD12	2.01	0.41
1:B:332:GLY:O	1:B:333:THR:HG23	2.19	0.41
1:A:1417:ASP:OD1	1:A:1418:ASP:N	2.54	0.41
1:A:780:VAL:HG23	1:A:780:VAL:O	2.21	0.41
1:A:877:GLU:HB2	1:A:880:ALA:CB	2.51	0.41
1:B:991:GLN:O	1:B:992:ASN:CB	2.69	0.41
1:B:868:TYR:CE1	1:B:878:TYR:CE1	3.09	0.41
1:B:378:TYR:HB2	1:B:400:PHE:CE2	2.57	0.40
1:A:294:TYR:HE2	1:A:307:GLN:OE1	2.03	0.40
1:A:603:THR:HG21	1:A:625:GLY:HA3	2.02	0.40
1:B:435:ASP:C	1:B:1298:VAL:HG12	2.41	0.40
1:B:332:GLY:C	1:B:333:THR:HG23	2.42	0.40
1:A:380:ASP:HB3	1:A:386:ARG:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ASN:N	1:A:400:PHE:O	2.54	0.40
1:B:981:VAL:HG11	1:B:983:TYR:CZ	2.57	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	1144/1293 (88%)	1085 (95%)	56 (5%)	3 (0%)	41	74
1	B	1144/1293 (88%)	1083 (95%)	57 (5%)	4 (0%)	41	74
All	All	2288/2586 (88%)	2168 (95%)	113 (5%)	7 (0%)	41	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	ASN
1	A	501	GLN
1	B	331	ASP
1	B	1418	ASP
1	A	302	VAL
1	B	362	SER
1	B	302	VAL

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	971/1097 (88%)	946 (97%)	25 (3%)	46 76
1	B	968/1097 (88%)	945 (98%)	23 (2%)	49 77
All	All	1939/2194 (88%)	1891 (98%)	48 (2%)	47 77

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
1	A	310	ASN
1	A	320	THR
1	A	333	THR
1	A	353	SER
1	A	387	ARG
1	A	397	PHE
1	A	420	SER
1	A	463	LYS
1	A	518	LEU
1	A	633	ASP
1	A	668	LEU
1	A	754	SER
1	A	906	LEU
1	A	976	ASN
1	A	999	ASP
1	A	1054	ASN
1	A	1061	LEU
1	A	1132	ARG
1	A	1145	ASN
1	A	1193	VAL
1	A	1341	THR
1	A	1345	ASP
1	A	1397	GLN
1	A	1416	SER
1	B	298	ASP
1	B	310	ASN
1	B	397	PHE
1	B	420	SER
1	B	463	LYS
1	B	555	ASN
1	B	616	SER
1	B	633	ASP
1	B	668	LEU
1	B	754	SER

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Mol	Chain	Res	Type
1	B	764	ASP
1	B	808	LEU
1	B	906	LEU
1	B	976	ASN
1	B	999	ASP
1	B	1061	LEU
1	B	1132	ARG
1	B	1145	ASN
1	B	1193	VAL
1	B	1341	THR
1	B	1366	SER
1	B	1408	GLU
1	B	1433	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
1	A	293	GLN
1	A	301	GLN
1	A	310	ASN
1	A	343	GLN
1	A	555	ASN
1	A	742	ASN
1	A	953	ASN
1	A	1048	ASN
1	A	1060	GLN
1	A	1145	ASN
1	A	1212	ASN
1	A	1277	ASN
1	A	1311	GLN
1	A	1394	GLN
1	B	293	GLN
1	B	310	ASN
1	B	343	GLN
1	B	394	ASN
1	B	555	ASN
1	B	742	ASN
1	B	953	ASN
1	B	1060	GLN
1	B	1145	ASN
1	B	1212	ASN

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Mol	Chain	Res	Type
1	B	1311	GLN
1	B	1394	GLN
1	B	1427	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	GOL	A	2002	-	5,5,5	0.26	0	5,5,5	0.68	0
3	GOL	B	2002	-	5,5,5	0.41	0	5,5,5	0.41	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	GOL	A	2002	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	2002	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2002	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	1148/1293 (88%)	-0.23	12 (1%)	82	72	30, 44, 73, 108	0
1	B	1148/1293 (88%)	-0.00	12 (1%)	82	72	46, 60, 86, 106	0
All	All	2296/2586 (88%)	-0.12	24 (1%)	82	72	30, 53, 81, 108	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	THR	3.4
1	B	294	TYR	3.1
1	A	310	ASN	3.0
1	A	300	ALA	2.8
1	B	340	GLN	2.8
1	B	500	ASP	2.8
1	A	342	ASN	2.7
1	B	299	GLY	2.7
1	A	297	PRO	2.7
1	B	374	GLY	2.6
1	B	358	TYR	2.6
1	A	299	GLY	2.6
1	A	309	VAL	2.6
1	B	292	THR	2.6
1	A	343	GLN	2.3
1	A	313	ASN	2.2
1	A	328	GLY	2.2
1	B	364	LYS	2.2
1	B	371	ASN	2.2
1	B	303	LYS	2.2
1	A	552	ILE	2.2
1	B	407	GLN	2.1
1	B	1326	ILE	2.1
1	A	595	GLU	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. 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	B-factors(Å^2)	Q<0.9
3	GOL	B	2002	6/6	0.86	0.28	52,53,53,55	0
3	GOL	A	2002	6/6	0.91	0.25	42,43,43,46	0
2	CA	B	2001	1/1	0.94	0.07	55,55,55,55	0
2	CA	A	2001	1/1	0.98	0.11	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.