



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:32 am BST

PDB ID : 3TTQ
Title : Crystal structure of Leuconostoc mesenteroides NRRL B-1299 N-terminally truncated dextransucrase DSR-E in orthorhombic apo-form at 1.9 angstrom resolution
Authors : Brison, Y.; Pijning, T.; Fabre, E.; Mourey, L.; Morel, S.; Potocki-Veronese, G.; Monsan, P.; Remaud-Simeon, M.; Dijkstra, B.W.; Tranier, S.
Deposited on : 2011-09-15
Resolution : 1.90 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 ⓘ](#)) 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

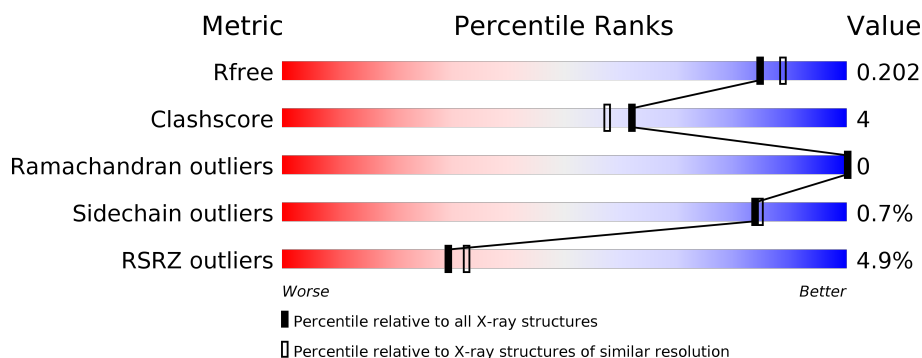
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	1108	<div> <div>5%</div> <div>85%</div> <div>8%</div> <div>6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	2866	-	-	-	X
4	GOL	A	2870	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	2885	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9331 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 Dextranucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1036	Total	C	N	O	S	0	5	0
			8128	5088	1387	1634	19			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1758	ALA	-	EXPRESSION TAG	UNP Q8G9Q2
A	2836	LYS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2837	GLY	-	EXPRESSION TAG	UNP Q8G9Q2
A	2838	GLU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2839	LEU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2840	LYS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2841	LEU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2842	GLU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2843	GLY	-	EXPRESSION TAG	UNP Q8G9Q2
A	2844	LYS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2845	PRO	-	EXPRESSION TAG	UNP Q8G9Q2
A	2846	ILE	-	EXPRESSION TAG	UNP Q8G9Q2
A	2847	PRO	-	EXPRESSION TAG	UNP Q8G9Q2
A	2848	ASN	-	EXPRESSION TAG	UNP Q8G9Q2
A	2849	PRO	-	EXPRESSION TAG	UNP Q8G9Q2
A	2850	LEU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2851	LEU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2852	GLY	-	EXPRESSION TAG	UNP Q8G9Q2
A	2853	LEU	-	EXPRESSION TAG	UNP Q8G9Q2
A	2854	ASP	-	EXPRESSION TAG	UNP Q8G9Q2
A	2855	SER	-	EXPRESSION TAG	UNP Q8G9Q2
A	2856	THR	-	EXPRESSION TAG	UNP Q8G9Q2
A	2857	ARG	-	EXPRESSION TAG	UNP Q8G9Q2
A	2858	THR	-	EXPRESSION TAG	UNP Q8G9Q2
A	2859	GLY	-	EXPRESSION TAG	UNP Q8G9Q2
A	2860	HIS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2861	HIS	-	EXPRESSION TAG	UNP Q8G9Q2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2862	HIS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2863	HIS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2864	HIS	-	EXPRESSION TAG	UNP Q8G9Q2
A	2865	HIS	-	EXPRESSION TAG	UNP Q8G9Q2

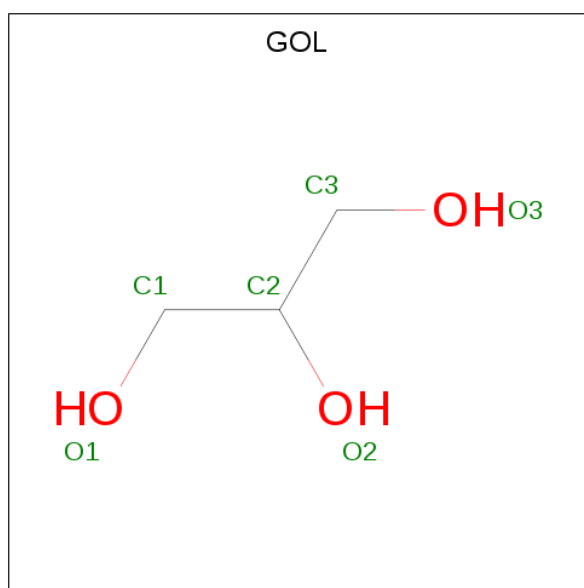
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



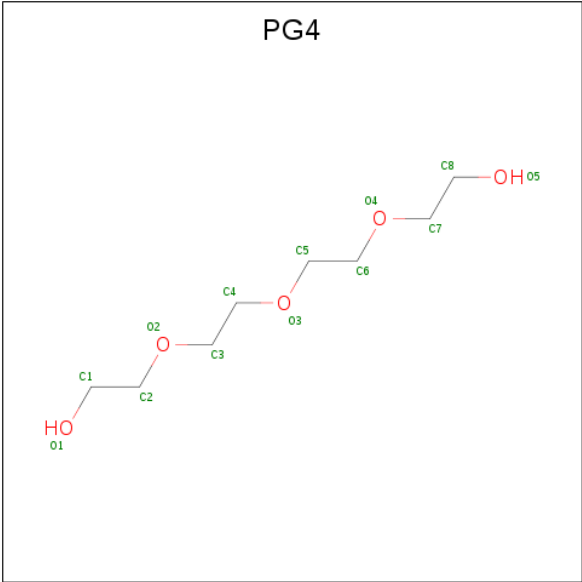
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

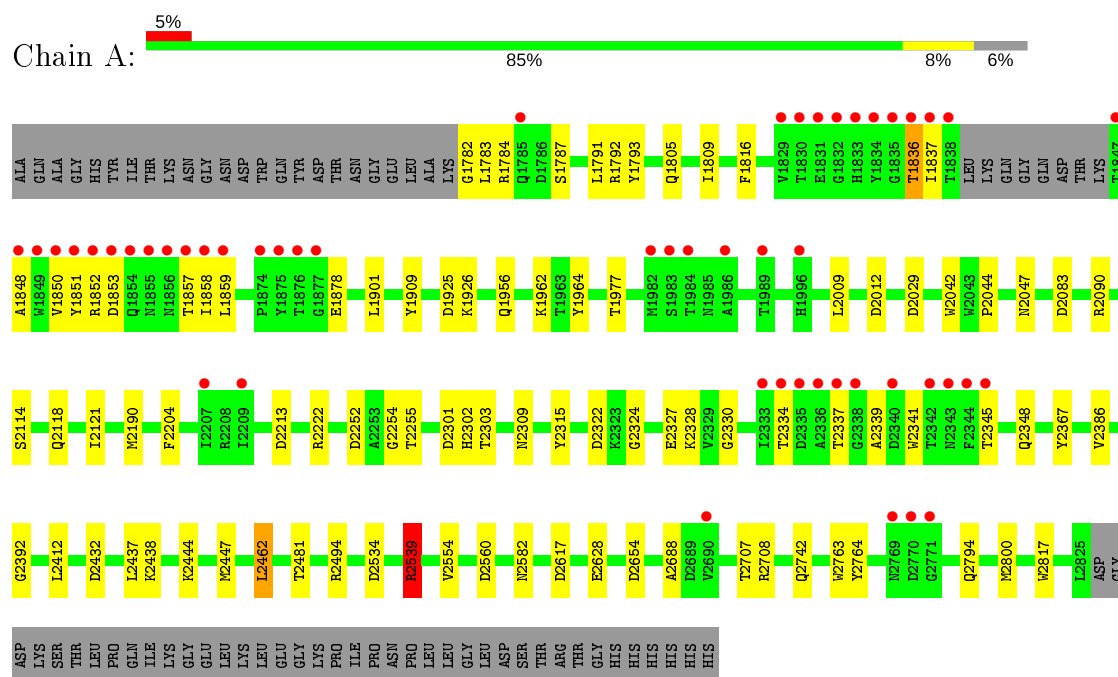
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1050	Total	O	0	0
			1050	1050		

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 ($\text{RSRZ} > 2$). 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: Dextranucrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.18Å 100.24Å 187.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 1.90 42.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (46.03-1.90) 97.2 (42.41-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.157 , 0.198 0.163 , 0.202	Depositor DCC
R_{free} test set	4950 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9331	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 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, CA, PG4, NA

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	1.03	7/8324 (0.1%)	0.96	24/11320 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2341	TRP	CD2-CE2	7.42	1.50	1.41
1	A	2042	TRP	CD2-CE2	5.38	1.47	1.41
1	A	1782	GLY	N-CA	5.36	1.54	1.46
1	A	2817	TRP	CD2-CE2	5.22	1.47	1.41
1	A	1787	SER	CB-OG	-5.12	1.35	1.42
1	A	2539	ARG	CZ-NH1	5.09	1.39	1.33
1	A	2628	GLU	CD-OE1	-5.01	1.20	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2190	MET	CG-SD-CE	-9.55	84.92	100.20
1	A	2222	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	2539	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	1925	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	2252[A]	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	2252[B]	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	2539	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	2322	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	2494	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	1792	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	2432	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	2090	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	1792	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	2029	ASP	CB-CG-OD1	5.84	123.56	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2301	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	2494	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	2412	LEU	CB-CG-CD2	5.66	120.62	111.00
1	A	2654	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	2534	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	1784	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	2012	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	2083	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	2090	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	2213	ASP	CB-CG-OD2	-5.10	113.71	118.30

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	8128	0	7618	66	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	138	0	184	19	0
5	A	13	0	18	0	0
6	A	1050	0	0	18	1
All	All	9331	0	7820	70	1

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 4.

All (70) 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:2255:THR:HG22	6:A:3445:HOH:O	1.20	1.35
1:A:2764:TYR:HE1	4:A:2879:GOL:HO2	0.94	0.93
1:A:2617[A]:ASP:OD1	6:A:3733:HOH:O	1.92	0.86
1:A:1977:THR:H	1:A:2047:ASN:HD21	1.24	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2334:THR:HG22	1:A:2339:ALA:O	1.79	0.83
1:A:2337:THR:HG23	6:A:3434:HOH:O	1.79	0.82
1:A:2345:THR:OG1	1:A:2348:GLN:HG3	1.82	0.79
1:A:2327:GLU:HB2	4:A:2888:GOL:H2	1.73	0.69
1:A:2044:PRO:HG3	1:A:2121:ILE:HD11	1.76	0.67
1:A:1850:VAL:CG1	1:A:1858:ILE:HG23	2.25	0.67
1:A:1909:TYR:HD1	4:A:2870:GOL:H32	1.60	0.66
1:A:1850:VAL:HG11	1:A:1858:ILE:HG23	1.78	0.66
1:A:2617[A]:ASP:OD1	6:A:3483:HOH:O	2.13	0.64
1:A:2337:THR:HG22	1:A:2339:ALA:H	1.63	0.64
1:A:2764:TYR:HE1	4:A:2879:GOL:O2	1.74	0.63
1:A:1837:ILE:HD11	1:A:1848:ALA:HB3	1.81	0.63
1:A:2302:HIS:HD2	6:A:2917:HOH:O	1.80	0.62
1:A:2303[B]:THR:HG21	6:A:3682:HOH:O	2.02	0.60
1:A:1783:LEU:HD22	1:A:1791:LEU:HD22	1.84	0.59
1:A:2328:LYS:HD3	1:A:2367:TYR:O	2.04	0.58
1:A:1850:VAL:HG12	1:A:1851:TYR:N	2.18	0.58
1:A:1837:ILE:CD1	1:A:1848:ALA:HB3	2.34	0.58
1:A:2334:THR:HG21	6:A:3367:HOH:O	2.05	0.56
1:A:2330:GLY:O	1:A:2334:THR:HG23	2.06	0.56
1:A:1926:LYS:HG3	4:A:2870:GOL:C3	2.36	0.56
4:A:2889:GOL:O1	6:A:3244:HOH:O	2.18	0.54
1:A:2392:GLY:O	4:A:2885:GOL:H12	2.07	0.54
1:A:2114:SER:O	1:A:2118:GLN:HG3	2.08	0.54
4:A:2871:GOL:H11	6:A:3686:HOH:O	2.08	0.53
1:A:1848:ALA:HB1	1:A:1878:GLU:HG3	1.90	0.53
1:A:1850:VAL:HG12	1:A:1851:TYR:H	1.73	0.53
1:A:1805:GLN:HB2	4:A:2875:GOL:H31	1.89	0.52
1:A:1850:VAL:HG11	1:A:1858:ILE:HD12	1.91	0.52
1:A:2324:GLY:N	4:A:2888:GOL:H32	2.25	0.52
1:A:2337:THR:HG21	1:A:2348:GLN:HB3	1.93	0.51
1:A:1926:LYS:HG3	4:A:2870:GOL:H31	1.90	0.51
1:A:1977:THR:H	1:A:2047:ASN:ND2	2.01	0.50
1:A:2437:LEU:HD23	1:A:2437:LEU:C	2.33	0.49
1:A:2481:THR:HG1	4:A:2884:GOL:HO2	1.56	0.49
1:A:2444:LYS:CE	6:A:3031:HOH:O	2.59	0.49
1:A:2481:THR:OG1	4:A:2884:GOL:O2	2.23	0.49
1:A:2044:PRO:CG	1:A:2121:ILE:HD11	2.42	0.48
1:A:2560:ASP:CB	6:A:3806:HOH:O	2.60	0.48
1:A:2047:ASN:H	1:A:2047:ASN:HD22	1.61	0.48
1:A:1926:LYS:HG3	4:A:2870:GOL:H2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1836:THR:O	1:A:1837:ILE:HG23	2.15	0.47
1:A:2324:GLY:H	4:A:2888:GOL:H32	1.80	0.47
1:A:2462:LEU:HB3	1:A:2554:VAL:HG12	1.96	0.46
1:A:2707:THR:HG22	1:A:2708:ARG:N	2.30	0.46
4:A:2889:GOL:O2	6:A:3773:HOH:O	2.17	0.46
1:A:1853:ASP:OD1	1:A:1857:THR:N	2.46	0.46
1:A:2254:GLY:HA3	1:A:2763:TRP:O	2.15	0.46
1:A:1783:LEU:HG	1:A:1809:ILE:HD13	1.97	0.46
1:A:1851:TYR:CD2	1:A:1859:LEU:HD12	2.51	0.45
1:A:2315:TYR:HA	1:A:2386:VAL:O	2.17	0.44
1:A:2539:ARG:HD3	1:A:2539:ARG:O	2.18	0.43
4:A:2887:GOL:H11	6:A:3176:HOH:O	2.18	0.43
1:A:2309:ASN:HD21	4:A:2886:GOL:H32	1.83	0.43
1:A:2444:LYS:HE2	6:A:3031:HOH:O	2.18	0.42
1:A:1901:LEU:HD23	1:A:1901:LEU:C	2.40	0.42
1:A:1793:TYR:HB2	1:A:1816:PHE:CZ	2.55	0.42
1:A:1962:LYS:HE2	6:A:3245:HOH:O	2.20	0.41
1:A:2794:GLN:NE2	6:A:3844:HOH:O	2.40	0.41
1:A:2447:MET:HA	1:A:2447:MET:HE2	2.01	0.41
1:A:2582:ASN:HD22	4:A:2886:GOL:H31	1.85	0.41
1:A:1852:ARG:CZ	1:A:1858:ILE:HD11	2.51	0.41
1:A:2742:GLN:NE2	6:A:3155:HOH:O	2.54	0.41
1:A:2204:PHE:CG	1:A:2688:ALA:HB2	2.56	0.40
1:A:1956:GLN:HA	1:A:1964:TYR:O	2.21	0.40
1:A:2303[A]:THR:HG23	6:A:3238:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:3703:HOH:O	6:A:3939:HOH:O[3_544]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1037/1108 (94%)	999 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	856/925 (92%)	850 (99%)	6 (1%)	84	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1836	THR
1	A	2009	LEU
1	A	2438	LYS
1	A	2462	LEU
1	A	2539	ARG
1	A	2800	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2047	ASN
1	A	2071	HIS
1	A	2232	GLN
1	A	2242	GLN
1	A	2302	HIS
1	A	2490	ASN
1	A	2528	GLN
1	A	2639	HIS
1	A	2661	ASN
1	A	2742	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2773	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	GOL	A	2883	-	5,5,5	0.45	0	5,5,5	0.16	0
4	GOL	A	2886	-	5,5,5	0.77	0	5,5,5	1.50	1 (20%)
4	GOL	A	2874	-	5,5,5	0.56	0	5,5,5	0.71	0
4	GOL	A	2870	-	5,5,5	0.91	0	5,5,5	1.69	2 (40%)
4	GOL	A	2884	-	5,5,5	0.44	0	5,5,5	0.28	0
4	GOL	A	2872	-	5,5,5	0.37	0	5,5,5	0.54	0
4	GOL	A	2888	-	5,5,5	0.46	0	5,5,5	0.74	0
4	GOL	A	2877	-	5,5,5	0.33	0	5,5,5	0.77	0
4	GOL	A	2869	-	5,5,5	0.83	0	5,5,5	1.13	1 (20%)
4	GOL	A	2875	-	5,5,5	0.31	0	5,5,5	0.96	0
4	GOL	A	2890	-	5,5,5	0.47	0	5,5,5	0.72	0
4	GOL	A	2879	-	5,5,5	0.57	0	5,5,5	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	2882	-	5,5,5	0.30	0	5,5,5	1.08	0
4	GOL	A	2868	-	5,5,5	0.94	0	5,5,5	0.82	0
4	GOL	A	2889	-	5,5,5	0.17	0	5,5,5	1.04	0
4	GOL	A	2887	-	5,5,5	0.27	0	5,5,5	0.66	0
4	GOL	A	2880	-	5,5,5	0.43	0	5,5,5	0.81	0
5	PG4	A	2891	-	12,12,12	0.97	0	11,11,11	0.74	0
4	GOL	A	2873	-	5,5,5	0.27	0	5,5,5	0.74	0
4	GOL	A	2885	-	5,5,5	1.19	1 (20%)	5,5,5	1.52	1 (20%)
4	GOL	A	2881	-	5,5,5	0.82	0	5,5,5	0.98	0
4	GOL	A	2878	-	5,5,5	0.68	0	5,5,5	0.98	0
4	GOL	A	2876	-	5,5,5	0.40	0	5,5,5	0.55	0
4	GOL	A	2871	-	5,5,5	0.63	0	5,5,5	1.38	1 (20%)

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	GOL	A	2883	-	-	2/4/4/4	-
4	GOL	A	2886	-	-	0/4/4/4	-
4	GOL	A	2874	-	-	0/4/4/4	-
4	GOL	A	2870	-	-	0/4/4/4	-
4	GOL	A	2884	-	-	2/4/4/4	-
4	GOL	A	2872	-	-	4/4/4/4	-
4	GOL	A	2888	-	-	3/4/4/4	-
4	GOL	A	2877	-	-	4/4/4/4	-
4	GOL	A	2869	-	-	4/4/4/4	-
4	GOL	A	2875	-	-	2/4/4/4	-
4	GOL	A	2890	-	-	2/4/4/4	-
4	GOL	A	2879	-	-	2/4/4/4	-
4	GOL	A	2882	-	-	2/4/4/4	-
4	GOL	A	2868	-	-	2/4/4/4	-
4	GOL	A	2889	-	-	2/4/4/4	-
4	GOL	A	2887	-	-	3/4/4/4	-
4	GOL	A	2880	-	-	1/4/4/4	-
5	PG4	A	2891	-	-	5/10/10/10	-
4	GOL	A	2873	-	-	4/4/4/4	-
4	GOL	A	2885	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	2881	-	-	1/4/4/4	-
4	GOL	A	2878	-	-	2/4/4/4	-
4	GOL	A	2876	-	-	2/4/4/4	-
4	GOL	A	2871	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2885	GOL	O2-C2	2.09	1.49	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2886	GOL	O3-C3-C2	2.57	122.52	110.20
4	A	2870	GOL	C3-C2-C1	2.51	121.47	111.70
4	A	2885	GOL	O3-C3-C2	2.51	122.22	110.20
4	A	2871	GOL	O3-C3-C2	2.35	121.46	110.20
4	A	2869	GOL	O3-C3-C2	2.20	120.77	110.20
4	A	2870	GOL	O1-C1-C2	-2.17	99.81	110.20

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2877	GOL	O1-C1-C2-C3
4	A	2877	GOL	C1-C2-C3-O3
4	A	2869	GOL	O1-C1-C2-C3
4	A	2890	GOL	O1-C1-C2-C3
4	A	2887	GOL	C1-C2-C3-O3
4	A	2885	GOL	C1-C2-C3-O3
4	A	2878	GOL	C1-C2-C3-O3
4	A	2871	GOL	C1-C2-C3-O3
4	A	2869	GOL	O2-C2-C3-O3
4	A	2885	GOL	O2-C2-C3-O3
4	A	2871	GOL	O2-C2-C3-O3
4	A	2884	GOL	C1-C2-C3-O3
4	A	2872	GOL	O1-C1-C2-C3
4	A	2872	GOL	C1-C2-C3-O3
4	A	2869	GOL	C1-C2-C3-O3
4	A	2875	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2879	GOL	O1-C1-C2-C3
4	A	2882	GOL	C1-C2-C3-O3
4	A	2889	GOL	C1-C2-C3-O3
4	A	2880	GOL	O1-C1-C2-C3
4	A	2873	GOL	C1-C2-C3-O3
4	A	2885	GOL	O1-C1-C2-C3
4	A	2881	GOL	C1-C2-C3-O3
4	A	2877	GOL	O1-C1-C2-O2
4	A	2877	GOL	O2-C2-C3-O3
4	A	2890	GOL	O1-C1-C2-O2
4	A	2879	GOL	O1-C1-C2-O2
4	A	2878	GOL	O2-C2-C3-O3
5	A	2891	PG4	O2-C3-C4-O3
4	A	2869	GOL	O1-C1-C2-O2
4	A	2882	GOL	O2-C2-C3-O3
4	A	2887	GOL	O2-C2-C3-O3
4	A	2873	GOL	O1-C1-C2-O2
4	A	2876	GOL	O1-C1-C2-O2
5	A	2891	PG4	O1-C1-C2-O2
5	A	2891	PG4	C5-C6-O4-C7
4	A	2883	GOL	O1-C1-C2-O2
4	A	2888	GOL	O1-C1-C2-O2
4	A	2868	GOL	O1-C1-C2-O2
4	A	2889	GOL	O2-C2-C3-O3
4	A	2873	GOL	O1-C1-C2-C3
4	A	2872	GOL	O1-C1-C2-O2
4	A	2875	GOL	O1-C1-C2-O2
5	A	2891	PG4	C1-C2-O2-C3
4	A	2872	GOL	O2-C2-C3-O3
4	A	2873	GOL	O2-C2-C3-O3
5	A	2891	PG4	O4-C7-C8-O5
4	A	2887	GOL	O1-C1-C2-O2
4	A	2883	GOL	C1-C2-C3-O3
4	A	2888	GOL	C1-C2-C3-O3
4	A	2876	GOL	C1-C2-C3-O3
4	A	2884	GOL	O2-C2-C3-O3
4	A	2885	GOL	O1-C1-C2-O2
4	A	2888	GOL	O1-C1-C2-C3
4	A	2868	GOL	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2886	GOL	2	0
4	A	2870	GOL	4	0
4	A	2884	GOL	2	0
4	A	2888	GOL	3	0
4	A	2875	GOL	1	0
4	A	2879	GOL	2	0
4	A	2889	GOL	2	0
4	A	2887	GOL	1	0
4	A	2885	GOL	1	0
4	A	2871	GOL	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, 95th 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	1036/1108 (93%)	-0.10	51 (4%)	29 33	13, 24, 48, 82	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1838	THR	6.9
1	A	1848	ALA	6.8
1	A	1875	TYR	5.9
1	A	1837	ILE	5.7
1	A	1847	THR	5.1
1	A	1836	THR	4.9
1	A	1849	TRP	4.9
1	A	2334	THR	4.8
1	A	1857	THR	4.7
1	A	1850	VAL	4.6
1	A	1858	ILE	4.6
1	A	1854	GLN	4.2
1	A	1835	GLY	4.1
1	A	2344	PHE	3.9
1	A	1876	THR	3.9
1	A	1856	ASN	3.9
1	A	1855	ASN	3.9
1	A	1984	THR	3.7
1	A	1852	ARG	3.7
1	A	2343	ASN	3.6
1	A	2337	THR	3.6
1	A	1834	TYR	3.6
1	A	2333	ILE	3.5
1	A	1859	LEU	3.4
1	A	1874	PRO	3.2
1	A	1833	HIS	3.2
1	A	2769	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1996[A]	HIS	3.1
1	A	1986	ALA	3.0
1	A	1853	ASP	2.9
1	A	2771	GLY	2.8
1	A	2209	ILE	2.8
1	A	2345	THR	2.7
1	A	1877	GLY	2.7
1	A	1831	GLU	2.7
1	A	2338	GLY	2.6
1	A	1851	TYR	2.6
1	A	2336	ALA	2.4
1	A	1983	SER	2.4
1	A	2207	ILE	2.4
1	A	1830	THR	2.3
1	A	1829	VAL	2.3
1	A	1982	MET	2.2
1	A	1785	GLN	2.2
1	A	1832	GLY	2.1
1	A	2335	ASP	2.1
1	A	2340	ASP	2.1
1	A	2690	VAL	2.1
1	A	1989	THR	2.0
1	A	2342	THR	2.0
1	A	2770	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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
2	NA	A	2866	1/1	-0.26	0.82	94,94,94,94	0
4	GOL	A	2886	6/6	0.68	0.28	52,67,72,74	0
4	GOL	A	2888	6/6	0.73	0.35	51,56,71,79	0
4	GOL	A	2890	6/6	0.80	0.28	65,69,71,76	0
4	GOL	A	2884	6/6	0.82	0.39	55,59,65,66	0
4	GOL	A	2875	6/6	0.85	0.24	51,56,58,58	0
5	PG4	A	2891	13/13	0.85	0.16	48,57,68,70	0
4	GOL	A	2872	6/6	0.86	0.33	39,47,52,52	0
4	GOL	A	2882	6/6	0.87	0.17	45,55,61,61	0
4	GOL	A	2870	6/6	0.87	0.26	39,42,49,55	0
4	GOL	A	2881	6/6	0.87	0.37	41,54,56,64	0
4	GOL	A	2876	6/6	0.87	0.17	51,57,62,69	0
4	GOL	A	2874	6/6	0.88	0.13	44,47,49,49	0
4	GOL	A	2878	6/6	0.88	0.28	34,44,46,59	0
4	GOL	A	2883	6/6	0.88	0.17	42,58,64,72	0
4	GOL	A	2889	6/6	0.89	0.18	58,64,67,71	0
4	GOL	A	2887	6/6	0.89	0.32	41,60,63,70	0
4	GOL	A	2869	6/6	0.89	0.16	24,40,48,50	0
4	GOL	A	2885	6/6	0.92	0.26	33,35,39,40	0
4	GOL	A	2877	6/6	0.92	0.11	47,47,49,53	0
4	GOL	A	2871	6/6	0.92	0.17	32,39,41,53	0
4	GOL	A	2879	6/6	0.93	0.14	29,44,54,58	0
4	GOL	A	2873	6/6	0.94	0.10	33,40,44,53	0
4	GOL	A	2880	6/6	0.94	0.11	43,55,62,69	0
4	GOL	A	2868	6/6	0.96	0.12	23,24,25,27	0
3	CA	A	2867	1/1	1.00	0.11	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.