



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:14 AM UTC

PDB ID : 4RIT / pdb_00004rit
Title : The yellow crystal structure of pyridoxal-dependent decarboxylase from
sphaerobacter thermophilus dsm 20745
Authors : Wu, R.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics
(MCSG)
Deposited on : 2014-10-07
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

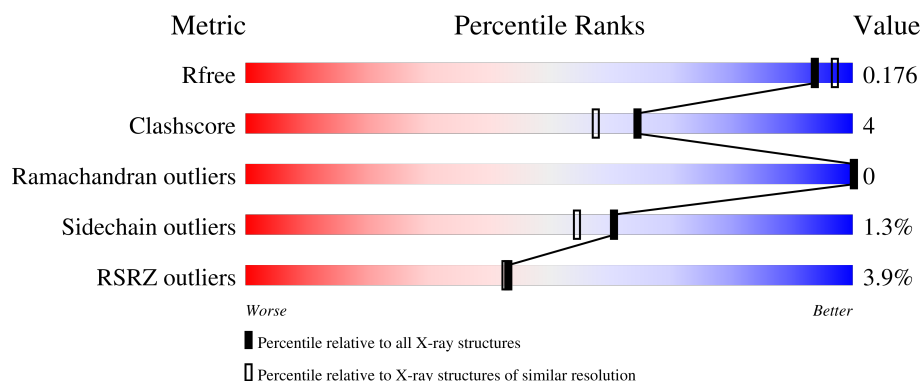
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of 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	486	
1	B	486	

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
3	GOL	B	506	-	-	X	-
4	TRS	B	508	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7997 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 Pyridoxal-dependent decarboxylase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	B	469	Total	C	N	O	P	S	Se	0	13	0
			3695	2335	665	674	1	4	16			
1	A	461	Total	C	N	O	P	S	Se	0	14	0
			3651	2309	655	668	1	3	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP D1C7D8
B	-1	ASN	-	expression tag	UNP D1C7D8
B	0	ALA	-	expression tag	UNP D1C7D8
A	-2	SER	-	expression tag	UNP D1C7D8
A	-1	ASN	-	expression tag	UNP D1C7D8
A	0	ALA	-	expression tag	UNP D1C7D8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

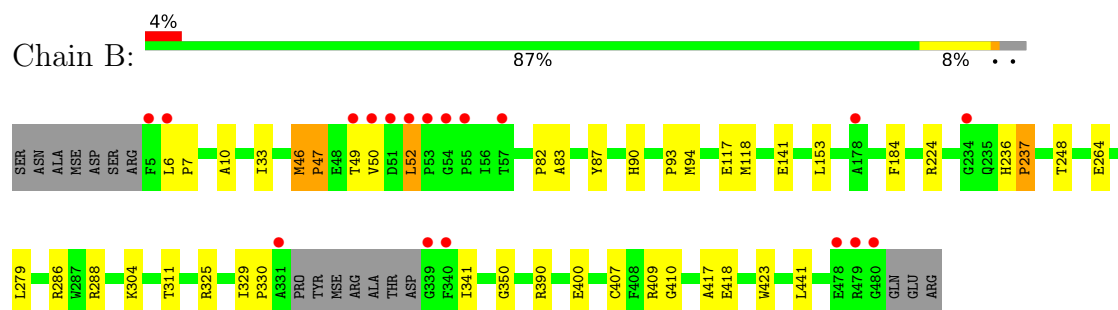
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	291	Total	O	0	0
			291	291		
5	A	267	Total	O	0	0
			267	267		

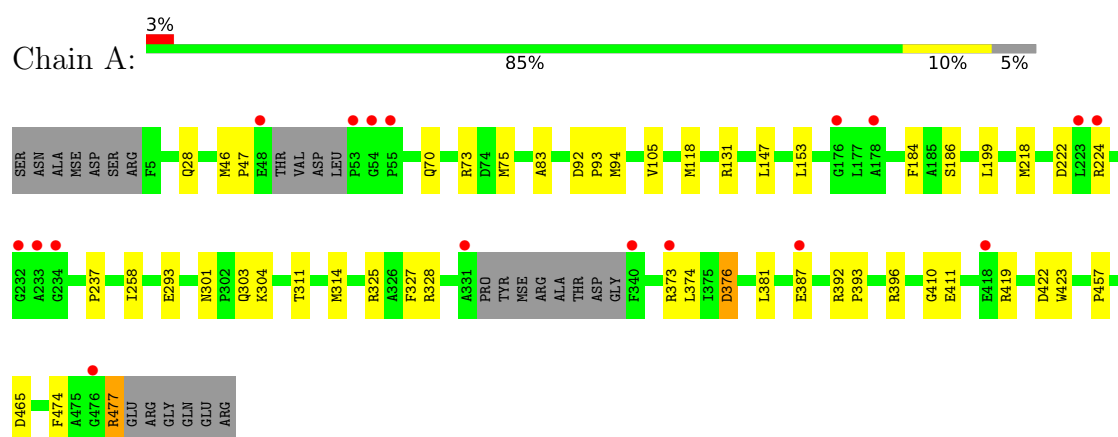
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Pyridoxal-dependent decarboxylase



- Molecule 1: Pyridoxal-dependent decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.48Å 118.57Å 126.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 1.80 39.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.59-1.80) 99.3 (39.59-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.150 , 0.173 0.158 , 0.176	Depositor DCC
R_{free} test set	5354 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7997	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, LLP, GOL, TRS

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	0.90	8/3685 (0.2%)	0.93	5/4984 (0.1%)
1	B	0.90	7/3730 (0.2%)	0.95	9/5045 (0.2%)
All	All	0.90	15/7415 (0.2%)	0.94	14/10029 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328[A]	ARG	C-N	-8.80	1.23	1.33
1	A	328[B]	ARG	C-N	-8.80	1.23	1.33
1	A	327	PHE	C-N	-7.73	1.23	1.33
1	A	222	ASP	C-N	-7.06	1.25	1.33
1	B	46	MSE	C-N	5.91	1.40	1.33
1	B	330	PRO	N-CD	5.61	1.55	1.47
1	B	93	PRO	N-CD	5.53	1.55	1.47
1	B	47	PRO	N-CD	5.47	1.55	1.47
1	A	93	PRO	N-CD	5.42	1.55	1.47
1	B	236	HIS	C-N	5.38	1.40	1.33
1	B	237	PRO	N-CD	5.35	1.55	1.47
1	A	392	ARG	C-N	5.34	1.40	1.33
1	B	329	ILE	C-N	5.27	1.40	1.33
1	A	393	PRO	N-CD	5.13	1.54	1.47
1	A	75	MSE	SE-CE	-5.09	1.80	1.95

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	VAL	N-CA-C	9.08	119.88	110.62
1	B	350	GLY	N-CA-C	-6.81	104.01	110.21
1	B	46	MSE	CA-C-N	-6.63	113.47	120.03
1	B	46	MSE	C-N-CA	-6.63	113.47	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ARG	N-CA-C	-6.14	104.58	111.28
1	A	325	ARG	N-CA-C	6.03	117.93	111.36
1	B	236	HIS	CA-C-N	-6.00	113.58	119.76
1	B	236	HIS	C-N-CA	-6.00	113.58	119.76
1	B	329	ILE	CA-C-N	-5.99	113.61	119.78
1	B	329	ILE	C-N-CA	-5.99	113.61	119.78
1	B	325	ARG	N-CA-C	5.98	117.88	111.36
1	A	224	ARG	CA-C-N	5.81	128.34	120.44
1	A	224	ARG	C-N-CA	5.81	128.34	120.44
1	A	199	LEU	N-CA-C	-5.15	105.75	111.36

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	3651	0	3642	32	0
1	B	3695	0	3680	31	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	36	0	48	6	0
3	B	30	0	40	4	0
4	A	8	0	12	1	0
4	B	16	0	24	1	0
5	A	267	0	0	4	0
5	B	291	0	0	3	0
All	All	7997	0	7446	58	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 4.

All (58) 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:457:PRO:HA	3:A:504:GOL:H31	1.57	0.84
1:B:409:ARG:HH22	3:B:506:GOL:H2	1.43	0.80
1:B:46:MSE:HE3	1:B:47:PRO:HD2	1.64	0.78
1:B:288[A]:ARG:NH1	5:B:829:HOH:O	2.21	0.73
1:A:131:ARG:HH22	3:A:503:GOL:H32	1.52	0.73
1:B:409:ARG:HH22	3:B:506:GOL:C2	2.01	0.72
1:A:396:ARG:HE	1:A:411:GLU:CD	1.97	0.72
1:A:46:MSE:HE3	1:A:47:PRO:HD2	1.76	0.68
1:A:387:GLU:HG3	5:A:728:HOH:O	1.95	0.66
1:A:28:GLN:NE2	5:A:843:HOH:O	2.31	0.64
1:B:83:ALA:HA	1:B:94:MSE:HE2	1.81	0.63
1:B:409:ARG:NH2	3:B:506:GOL:H2	2.14	0.62
1:A:83:ALA:HA	1:A:94:MSE:HE2	1.85	0.59
1:B:52:LEU:HD12	1:B:52:LEU:O	2.01	0.59
1:B:83:ALA:HA	1:B:94:MSE:CE	2.33	0.58
1:B:83:ALA:CB	1:B:94:MSE:HE2	2.33	0.58
1:B:286:ARG:HD2	4:B:508:TRS:H12	1.84	0.58
1:A:184:PHE:HE2	1:A:237:PRO:HB3	1.69	0.57
1:B:184:PHE:HE2	1:B:237:PRO:HB3	1.69	0.57
1:B:90:HIS:CG	1:A:118[A]:MSE:HE1	2.41	0.56
1:A:293:GLU:OE1	4:A:508:TRS:O1	2.22	0.56
1:A:474:PHE:O	1:A:477:ARG:HG2	2.07	0.55
1:B:441:LEU:H	3:A:506:GOL:C1	2.21	0.53
1:B:83:ALA:CA	1:B:94:MSE:HE2	2.39	0.53
1:A:419:ARG:NH1	1:A:422:ASP:OD2	2.43	0.52
1:A:396:ARG:NH2	1:A:411:GLU:OE1	2.44	0.51
1:B:141:GLU:O	1:B:141:GLU:HG3	2.10	0.51
1:B:390:ARG:NH2	1:B:400[B]:GLU:OE2	2.45	0.50
1:A:465:ASP:OD1	3:A:505:GOL:H11	2.14	0.48
1:B:248:THR:O	1:B:407[A]:CYS:SG	2.71	0.48
1:B:118[B]:MSE:SE	5:B:876:HOH:O	2.81	0.48
1:B:417:ALA:HB1	3:B:506:GOL:H31	1.95	0.48
1:A:131:ARG:NH2	3:A:503:GOL:H32	2.25	0.47
1:A:376[A]:ASP:OD2	5:A:768:HOH:O	2.20	0.47
1:A:410:GLY:HA3	1:A:423:TRP:CZ3	2.50	0.47
1:B:410:GLY:HA3	1:B:423:TRP:CZ3	2.49	0.47
1:A:474:PHE:O	1:A:477:ARG:CG	2.64	0.46
1:A:83:ALA:HA	1:A:94:MSE:CE	2.46	0.46
1:B:418:GLU:H	1:B:418:GLU:CD	2.23	0.45
1:B:33:ILE:HD11	1:A:105:VAL:HG22	2.00	0.44
1:A:153:LEU:HG	5:A:848:HOH:O	2.17	0.43
1:A:465:ASP:OD1	3:A:505:GOL:C1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118[B]:MSE:CE	1:A:92:ASP:OD1	2.67	0.43
1:A:396:ARG:NE	1:A:411:GLU:OE1	2.51	0.43
1:B:6:LEU:HD11	1:A:374:LEU:HD21	2.01	0.43
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.80	0.42
1:B:82:PRO:HA	1:B:87:TYR:CG	2.55	0.42
1:A:186:SER:HB2	1:A:218[B]:MSE:HB2	2.02	0.41
1:A:218[A]:MSE:HB3	1:A:258[A]:ILE:HD11	2.01	0.41
1:B:418:GLU:CD	1:B:418:GLU:N	2.79	0.41
1:B:118[B]:MSE:HE1	1:A:92:ASP:OD1	2.20	0.41
1:A:301:ASN:HB3	1:A:303:GLN:HG2	2.02	0.41
1:B:224:ARG:HH12	1:B:264[A]:GLU:CD	2.24	0.41
1:B:153:LEU:HG	5:B:832:HOH:O	2.21	0.40
1:A:147:LEU:HD23	1:A:314:MSE:HB3	2.04	0.40
1:A:70:GLN:O	1:A:73[B]:ARG:HB3	2.21	0.40
1:B:279:LEU:O	1:B:286:ARG:HB3	2.21	0.40
1:B:7:PRO:HG2	1:B:10:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

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	468/486 (96%)	455 (97%)	13 (3%)	0	100	100
1	B	477/486 (98%)	463 (97%)	14 (3%)	0	100	100
All	All	945/972 (97%)	918 (97%)	27 (3%)	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	369/362 (102%)	364 (99%)	5 (1%)	59	52
1	B	371/362 (102%)	366 (99%)	5 (1%)	61	54
All	All	740/724 (102%)	730 (99%)	10 (1%)	61	52

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

Mol	Chain	Res	Type
1	B	49	THR
1	B	52	LEU
1	B	117	GLU
1	B	311	THR
1	B	341	ILE
1	A	311	THR
1	A	373	ARG
1	A	376[A]	ASP
1	A	376[B]	ASP
1	A	477	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
1	A	27	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
1	LLP	A	304	1	23,24,25	1.97	6 (26%)	25,32,34	1.71	6 (24%)
1	LLP	B	304	1	23,24,25	2.06	5 (21%)	25,32,34	1.71	5 (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
1	LLP	A	304	1	-	4/16/17/19	0/1/1/1
1	LLP	B	304	1	-	4/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	LLP	C4'-NZ	6.44	1.48	1.27
1	A	304	LLP	C4'-NZ	6.42	1.48	1.27
1	B	304	LLP	C4-C4'	3.57	1.54	1.46
1	A	304	LLP	C2'-C2	2.99	1.55	1.50
1	A	304	LLP	C4-C4'	2.96	1.52	1.46
1	B	304	LLP	C2'-C2	2.85	1.54	1.50
1	B	304	LLP	C3-C2	-2.77	1.38	1.41
1	B	304	LLP	CB-CA	-2.44	1.49	1.53
1	A	304	LLP	OP4-C5'	-2.36	1.36	1.44
1	A	304	LLP	C3-C2	-2.27	1.38	1.41
1	A	304	LLP	O3-C3	2.08	1.41	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	LLP	OP4-C5'-C5	4.09	117.02	109.36
1	B	304	LLP	OP4-C5'-C5	3.99	116.83	109.36
1	B	304	LLP	C5-C6-N1	-3.70	117.82	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	LLP	C5-C6-N1	-3.20	118.62	123.83
1	A	304	LLP	C4-C4'-NZ	-2.91	110.64	124.04
1	B	304	LLP	C6-N1-C2	2.88	124.43	119.20
1	B	304	LLP	CD-CE-NZ	2.77	118.17	110.83
1	B	304	LLP	C4-C4'-NZ	-2.37	113.09	124.04
1	A	304	LLP	C2'-C2-C3	-2.08	118.36	120.80
1	A	304	LLP	C6-N1-C2	2.02	122.86	119.20
1	A	304	LLP	C2'-C2-N1	2.00	121.42	117.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	304	LLP	C4-C4'-NZ-CE
1	A	304	LLP	C4-C4'-NZ-CE
1	A	304	LLP	CG-CD-CE-NZ
1	B	304	LLP	CG-CD-CE-NZ
1	B	304	LLP	C3-C4-C4'-NZ
1	A	304	LLP	C3-C4-C4'-NZ
1	B	304	LLP	CD-CE-NZ-C4'
1	A	304	LLP	CD-CE-NZ-C4'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	B	504	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	B	503	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	A	505	-	5,5,5	0.32	0	5,5,5	0.54	0
4	TRS	B	508	-	7,7,7	0.98	1 (14%)	9,9,9	2.92	4 (44%)
4	TRS	B	509	-	7,7,7	0.42	0	9,9,9	1.09	0
3	GOL	A	507	-	5,5,5	0.26	0	5,5,5	0.31	0
4	TRS	A	508	-	7,7,7	0.55	0	9,9,9	1.55	1 (11%)
3	GOL	A	502	-	5,5,5	0.15	0	5,5,5	1.00	0
3	GOL	A	503	-	5,5,5	0.35	0	5,5,5	0.34	0
3	GOL	A	506	-	5,5,5	0.30	0	5,5,5	0.46	0
3	GOL	B	505	-	5,5,5	0.47	0	5,5,5	0.89	0
3	GOL	B	507	-	5,5,5	0.17	0	5,5,5	0.72	0
3	GOL	A	504	-	5,5,5	0.79	0	5,5,5	0.63	0
3	GOL	B	506	-	5,5,5	0.26	0	5,5,5	0.32	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	B	504	-	-	1/4/4/4	-
3	GOL	B	503	-	-	4/4/4/4	-
3	GOL	A	505	-	-	3/4/4/4	-
4	TRS	B	508	-	-	5/9/9/9	-
4	TRS	B	509	-	-	6/9/9/9	-
3	GOL	A	507	-	-	2/4/4/4	-
4	TRS	A	508	-	-	3/9/9/9	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	A	506	-	-	3/4/4/4	-
3	GOL	B	505	-	-	2/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
3	GOL	A	504	-	-	4/4/4/4	-
3	GOL	B	506	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	508	TRS	C2-C	-2.14	1.47	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	508	TRS	O2-C2-C	-6.92	91.60	110.88
4	B	508	TRS	C2-C-N	-3.45	99.37	108.17
4	A	508	TRS	O3-C3-C	-3.02	102.45	110.88
4	B	508	TRS	O1-C1-C	2.88	118.90	110.88
4	B	508	TRS	C1-C-N	2.32	114.09	108.17

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-C3
3	B	503	GOL	C1-C2-C3-O3
3	B	507	GOL	O1-C1-C2-O2
3	B	507	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	A	504	GOL	O1-C1-C2-C3
3	A	506	GOL	O1-C1-C2-C3
4	B	509	TRS	C1-C-C3-O3
4	B	509	TRS	C2-C-C3-O3
4	B	509	TRS	N-C-C3-O3
3	B	506	GOL	O1-C1-C2-C3
3	B	506	GOL	C1-C2-C3-O3
3	A	504	GOL	C1-C2-C3-O3
3	A	505	GOL	C1-C2-C3-O3
3	A	506	GOL	C1-C2-C3-O3
3	A	507	GOL	C1-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
3	B	506	GOL	O2-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
3	A	504	GOL	O1-C1-C2-O2
3	A	506	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	B	505	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	504	GOL	O2-C2-C3-O3
4	B	508	TRS	C3-C-C2-O2
4	B	508	TRS	N-C-C3-O3
4	B	509	TRS	N-C-C1-O1
4	A	508	TRS	C2-C-C1-O1
4	A	508	TRS	N-C-C1-O1
3	B	505	GOL	O1-C1-C2-O2
4	B	508	TRS	C1-C-C2-O2
4	B	509	TRS	C2-C-C1-O1
4	B	509	TRS	C3-C-C1-O1
4	A	508	TRS	C3-C-C1-O1
3	A	507	GOL	O2-C2-C3-O3
4	B	508	TRS	N-C-C2-O2
3	B	504	GOL	O1-C1-C2-C3
3	B	506	GOL	O1-C1-C2-O2
3	A	505	GOL	O1-C1-C2-C3
4	B	508	TRS	C1-C-C3-O3
3	A	502	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	GOL	2	0
4	B	508	TRS	1	0
4	A	508	TRS	1	0
3	A	503	GOL	2	0
3	A	506	GOL	1	0
3	A	504	GOL	1	0
3	B	506	GOL	4	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	448/486 (92%)	-0.15	17 (3%) 44 44	10, 26, 50, 71	11 (2%)
1	B	456/486 (93%)	-0.23	18 (3%) 43 43	10, 23, 49, 76	9 (1%)
All	All	904/972 (93%)	-0.19	35 (3%) 43 43	10, 24, 49, 76	20 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	6.9
1	B	51	ASP	6.0
1	B	50	VAL	4.9
1	B	339	GLY	4.3
1	A	55	PRO	4.2
1	B	5	PHE	4.2
1	B	53	PRO	4.1
1	B	340	PHE	4.0
1	A	223	LEU	4.0
1	A	54	GLY	4.0
1	B	49	THR	3.9
1	B	55	PRO	3.8
1	A	331	ALA	3.6
1	A	476	GLY	3.6
1	A	53	PRO	3.4
1	B	331	ALA	3.3
1	B	479	ARG	3.3
1	A	233	ALA	3.1
1	B	54	GLY	3.1
1	A	340	PHE	2.9
1	B	178	ALA	2.9
1	A	418	GLU	2.9
1	A	232	GLY	2.8
1	A	176	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	57	THR	2.6
1	A	48	GLU	2.5
1	B	6	LEU	2.5
1	A	178	ALA	2.3
1	A	373	ARG	2.3
1	A	387	GLU	2.2
1	A	234	GLY	2.2
1	B	478	GLU	2.1
1	B	480	GLY	2.1
1	A	224	ARG	2.1
1	B	234	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
1	LLP	B	304	24/25	0.96	0.08	14,21,36,39	2
1	LLP	A	304	24/25	0.96	0.08	16,22,33,36	3

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
3	GOL	A	507	6/6	0.56	0.25	46,47,74,81	0
3	GOL	B	506	6/6	0.72	0.20	64,72,77,78	0
3	GOL	B	507	6/6	0.77	0.20	42,55,70,72	0
3	GOL	A	503	6/6	0.78	0.15	60,66,73,74	0
4	TRS	B	509	8/8	0.78	0.17	58,62,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TRS	A	508	8/8	0.80	0.20	49,58,64,65	0
3	GOL	A	504	6/6	0.81	0.20	54,58,60,66	0
3	GOL	B	505	6/6	0.82	0.17	60,67,72,74	0
4	TRS	B	508	8/8	0.83	0.16	51,57,61,65	0
3	GOL	A	506	6/6	0.84	0.19	34,69,74,81	0
3	GOL	B	503	6/6	0.85	0.15	56,61,63,65	0
3	GOL	B	504	6/6	0.86	0.12	33,35,38,53	0
3	GOL	A	505	6/6	0.87	0.17	63,69,71,73	0
3	GOL	A	502	6/6	0.88	0.13	43,48,49,49	0
2	CL	A	501	1/1	0.94	0.14	45,45,45,45	0
2	CL	B	501	1/1	0.97	0.09	31,31,31,31	0
2	CL	B	502	1/1	0.99	0.10	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.