



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:06 AM GMT

PDB ID : 4LHC
Title : Crystal structure of Synechocystis sp. PCC 6803 glycine decarboxylase (P-protein), holo form with pyridoxal-5'-phosphate and glycine
Authors : Hasse, D.; Andersson, E.; Carlsson, G.; Masloboy, A.; Hagemann, M.; Bauwe, H.; Andersson, I.
Deposited on : 2013-07-01
Resolution : 1.90 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

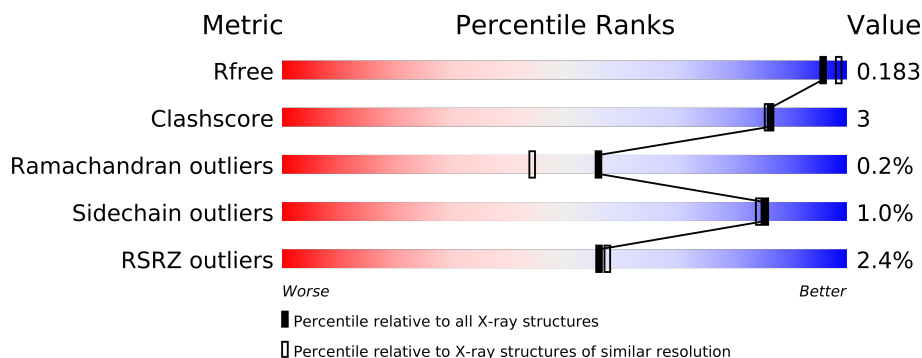
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	983	
1	B	983	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GLY	A	1001	-	X
2	GLY	A	1002	-	X
2	GLY	A	1004	-	X
2	GLY	B	1001	-	X
3	BCT	A	1005	-	X
3	BCT	A	1006	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	BCT	B	1002	-	X
4	PO4	A	1007	-	X
4	PO4	A	1009	-	X
4	PO4	B	1003	-	X
5	EDO	A	1010	-	X
5	EDO	A	1011	-	X
5	EDO	A	1012	-	X
5	EDO	A	1013	-	X
5	EDO	A	1014	-	X
5	EDO	A	1015	-	X
5	EDO	A	1016	-	X
5	EDO	B	1007	-	X
5	EDO	B	1008	-	X
5	EDO	B	1009	-	X
5	EDO	B	1010	-	X
5	EDO	B	1011	-	X
5	EDO	B	1012	-	X
5	EDO	B	1013	-	X
6	BCN	A	1017	-	X

2 Entry composition i

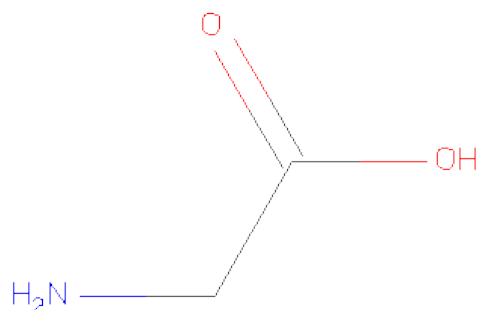
There are 7 unique types of molecules in this entry. The entry contains 16238 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glycine dehydrogenase [decarboxylating].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	942	Total	C	N	O	P	S	0	18	0
			7355	4676	1243	1390	1	45			
1	B	942	Total	C	N	O	P	S	0	17	0
			7347	4672	1238	1392	1	44			

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



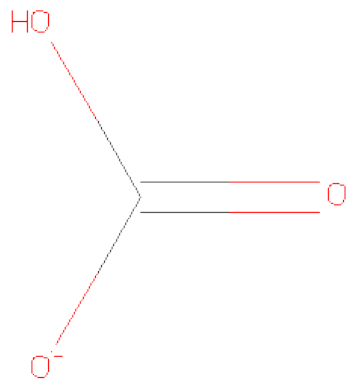
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

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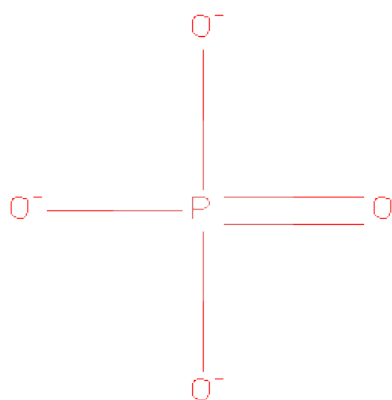
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



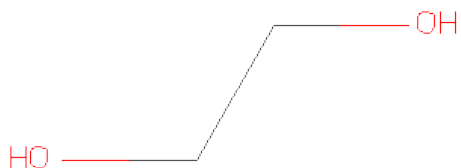
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



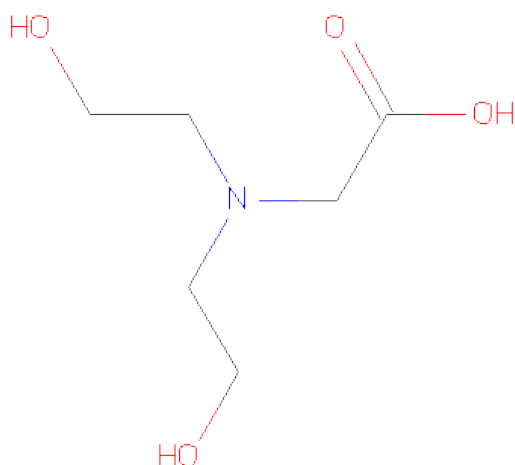
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 7 is water.

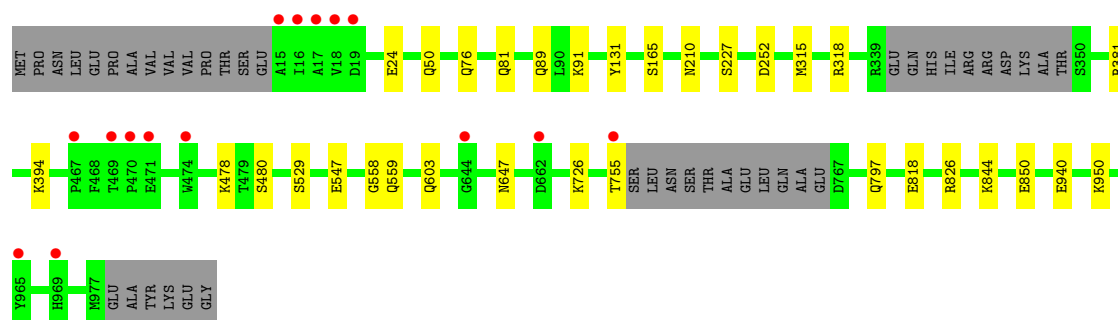
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	705	Total	O	0	0
			705	705		
7	B	689	Total	O	0	0
			689	689		

3 Residue-property plots

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.

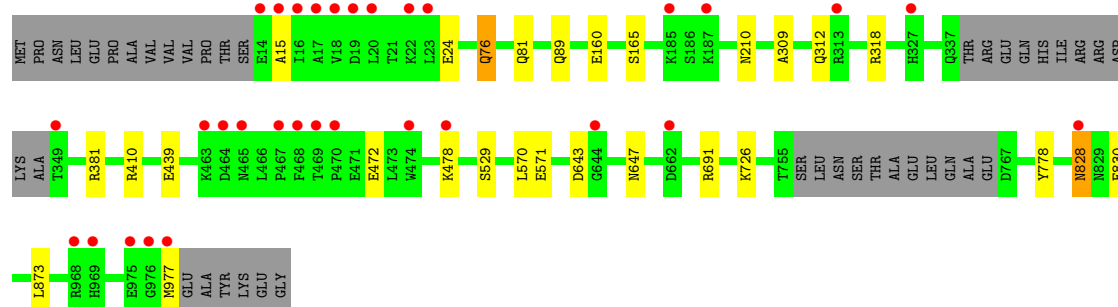
- Molecule 1: Glycine dehydrogenase [decarboxylating]

Chain A: 



- Molecule 1: Glycine dehydrogenase [decarboxylating]

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.05Å 160.05Å 159.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.78 – 1.90 49.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.78-1.90) 99.9 (49.78-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.155 , 0.186 0.153 , 0.183	Depositor DCC
R_{free} test set	9307 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.7	EDS
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 185417 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16238	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, BCN, LLP, PO4, EDO

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	0.34	0/7533	0.51	0/10245
1	B	0.35	0/7526	0.51	0/10236
All	All	0.35	0/15059	0.51	0/20481

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7355	0	0	19	0
1	B	7347	0	0	17	0
2	A	20	0	8	1	0
2	B	5	0	2	1	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	1	0
5	A	28	0	42	1	0
5	B	36	0	54	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	11	0	12	4	0
7	A	705	0	0	9	0
7	B	689	0	0	7	0
All	All	16238	0	118	39	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210[B]:ASN:ND2	7:A:1637:HOH:O	2.24	0.71
1:B:160:GLU:OE1	1:B:309:ALA:N	2.28	0.67
1:B:81:GLN:NE2	1:B:89:GLN:OE1	2.29	0.66
1:A:394:LYS:NZ	7:A:1537:HOH:O	2.29	0.66
1:A:558:GLY:N	6:A:1017:BCN:HO6	1.94	0.65
1:B:210[B]:ASN:ND2	7:B:1634:HOH:O	2.31	0.63
1:A:818:GLU:OE2	1:A:826:ARG:NH2	2.32	0.62
1:B:318:ARG:NH1	7:B:1588:HOH:O	2.33	0.62
1:A:318:ARG:NH1	7:A:1455:HOH:O	2.33	0.60
1:B:89:GLN:NE2	7:B:1621:HOH:O	2.33	0.60
2:A:1004:GLY:N	7:A:1576:HOH:O	2.34	0.59
1:A:89:GLN:NE2	7:A:1426:HOH:O	2.37	0.58
1:A:81:GLN:NE2	1:A:89:GLN:OE1	2.36	0.58
1:A:252:ASP:OD1	5:A:1014:EDO:H11	2.05	0.57
1:A:559:GLN:NE2	6:A:1017:BCN:H41	2.20	0.55
1:B:726:LLP:O3	1:B:726:LLP:NZ	2.41	0.53
1:A:726:LLP:NZ	1:A:726:LLP:O3	2.41	0.53
1:A:24:GLU:OE2	1:B:381:ARG:NH2	2.42	0.52
2:B:1001:GLY:N	7:B:1513:HOH:O	2.45	0.50
1:A:844:LYS:NZ	1:A:850:GLU:OE2	2.45	0.49
1:A:381:ARG:NH2	1:B:24:GLU:OE2	2.46	0.49
1:A:91:LYS:NZ	1:A:547:GLU:OE1	2.47	0.48
1:A:603:GLN:NE2	7:A:1421:HOH:O	2.46	0.47
1:A:478:LYS:NZ	1:A:480:SER:OG	2.48	0.47
1:B:571:GLU:OE2	5:B:1013:EDO:H21	2.15	0.47
1:A:797:GLN:NE2	7:A:1555:HOH:O	2.48	0.47
1:B:643:ASP:N	1:B:647:ASN:O	2.49	0.46
5:B:1011:EDO:H22	7:B:1678:HOH:O	2.16	0.46
1:B:691:ARG:NH1	7:B:1557:HOH:O	2.49	0.45
1:B:76:GLN:NE2	4:B:1004:PO4:O4	2.51	0.44
1:B:643:ASP:OD2	1:B:647:ASN:N	2.51	0.44
6:A:1017:BCN:H12	6:A:1017:BCN:H42	1.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:1017:BCN:O4	7:A:1729:HOH:O	2.22	0.42
1:B:410:ARG:NH2	1:B:439:GLU:OE1	2.53	0.42
1:B:828:ASN:OD1	1:B:828:ASN:N	2.52	0.42
1:B:478:LYS:N	7:B:1466:HOH:O	2.53	0.41
1:A:647:ASN:ND2	7:A:1619:HOH:O	2.53	0.40
1:A:940:GLU:OE2	1:A:950:LYS:NZ	2.54	0.40
1:B:778:TYR:OH	5:B:1013:EDO:H11	2.20	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	953/983 (97%)	929 (98%)	23 (2%)	1 (0%)	59 48
1	B	952/983 (97%)	926 (97%)	24 (2%)	2 (0%)	56 44
All	All	1905/1966 (97%)	1855 (97%)	47 (2%)	3 (0%)	56 44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	B	165	SER
1	B	15	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	781/798 (98%)	774 (99%)	7 (1%)	87	86
1	B	780/798 (98%)	771 (99%)	9 (1%)	82	80
All	All	1561/1596 (98%)	1545 (99%)	16 (1%)	85	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	76	GLN
1	A	131	TYR
1	A	227	SER
1	A	315	MET
1	A	529	SER
1	A	755	THR
1	B	76	GLN
1	B	312	GLN
1	B	472	GLU
1	B	529	SER
1	B	570	LEU
1	B	828	ASN
1	B	830	GLU
1	B	873	LEU
1	B	977	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	726	1	24,24,25	4.06	6 (25%)	30,32,34	2.05	4 (13%)
1	LLP	B	726	1	24,24,25	4.07	5 (20%)	30,32,34	2.07	2 (6%)

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	726	1	-	0/15/17/19	0/1/1/1
1	LLP	B	726	1	-	0/15/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	LLP	O-C	18.11	1.23	1.11
1	A	726	LLP	O-C	18.07	1.23	1.11
1	A	726	LLP	O3-C3	-5.33	1.24	1.37
1	B	726	LLP	O3-C3	-5.26	1.24	1.37
1	A	726	LLP	CA-C	2.68	1.53	1.48
1	B	726	LLP	CA-C	2.63	1.53	1.48
1	B	726	LLP	C2-N1	2.48	1.38	1.33
1	A	726	LLP	CB-CA	2.45	1.55	1.53
1	A	726	LLP	C2-N1	2.33	1.38	1.33
1	B	726	LLP	C4'-NZ	-2.12	1.34	1.45
1	A	726	LLP	C4'-NZ	-2.09	1.35	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	726	LLP	OP4-C5'-C5	8.45	126.45	109.26
1	A	726	LLP	OP4-C5'-C5	8.18	125.88	109.26
1	B	726	LLP	C-CA-N	-6.00	107.83	113.83
1	A	726	LLP	C-CA-N	-5.44	108.40	113.83
1	A	726	LLP	C4'-C4-C5	2.12	121.64	119.70
1	A	726	LLP	C4-C4'-NZ	-2.12	107.58	111.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

31 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	GLY	A	1001	-	4,4,4	1.06	0	4,4,4	1.19	0
2	GLY	A	1002	-	4,4,4	1.03	0	4,4,4	1.42	1 (25%)
2	GLY	A	1003	-	4,4,4	1.00	0	4,4,4	1.30	1 (25%)
2	GLY	A	1004	-	4,4,4	1.02	0	4,4,4	1.30	1 (25%)
3	BCT	A	1005	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	A	1006	-	0,3,3	0.00	-	0,3,3	0.00	-
4	PO4	A	1007	-	4,4,4	0.34	0	6,6,6	0.32	0
4	PO4	A	1008	-	4,4,4	0.26	0	6,6,6	0.31	0
4	PO4	A	1009	-	4,4,4	0.30	0	6,6,6	0.31	0
5	EDO	A	1010	-	3,3,3	0.57	0	2,2,2	0.43	0
5	EDO	A	1011	-	3,3,3	0.51	0	2,2,2	0.33	0
5	EDO	A	1012	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	A	1013	-	3,3,3	0.57	0	2,2,2	0.26	0
5	EDO	A	1014	-	3,3,3	0.58	0	2,2,2	0.14	0
5	EDO	A	1015	-	3,3,3	0.53	0	2,2,2	0.39	0
5	EDO	A	1016	-	3,3,3	0.53	0	2,2,2	0.31	0
6	BCN	A	1017	-	10,10,10	0.66	0	11,11,11	1.11	0
2	GLY	B	1001	-	4,4,4	1.03	0	4,4,4	1.35	1 (25%)
3	BCT	B	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	PO4	B	1003	-	4,4,4	0.27	0	6,6,6	0.31	0
4	PO4	B	1004	-	4,4,4	0.26	0	6,6,6	0.31	0
4	PO4	B	1005	-	4,4,4	0.28	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	1006	-	3,3,3	0.51	0	2,2,2	0.24	0
5	EDO	B	1007	-	3,3,3	0.43	0	2,2,2	0.79	0
5	EDO	B	1008	-	3,3,3	0.55	0	2,2,2	0.47	0
5	EDO	B	1009	-	3,3,3	0.57	0	2,2,2	0.49	0
5	EDO	B	1010	-	3,3,3	0.53	0	2,2,2	0.46	0
5	EDO	B	1011	-	3,3,3	0.56	0	2,2,2	0.34	0
5	EDO	B	1012	-	3,3,3	0.51	0	2,2,2	0.46	0
5	EDO	B	1013	-	3,3,3	0.55	0	2,2,2	0.22	0
5	EDO	B	1014	-	3,3,3	0.53	0	2,2,2	0.29	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
2	GLY	A	1001	-	-	0/2/2/2	0/0/0/0
2	GLY	A	1002	-	-	0/2/2/2	0/0/0/0
2	GLY	A	1003	-	-	0/2/2/2	0/0/0/0
2	GLY	A	1004	-	-	0/2/2/2	0/0/0/0
3	BCT	A	1005	-	-	0/0/0/0	0/0/0/0
3	BCT	A	1006	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1007	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1008	-	-	0/0/0/0	0/0/0/0
4	PO4	A	1009	-	-	0/0/0/0	0/0/0/0
5	EDO	A	1010	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1011	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1012	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1013	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1014	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1015	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1016	-	-	0/1/1/1	0/0/0/0
6	BCN	A	1017	-	-	0/10/10/10	0/0/0/0
2	GLY	B	1001	-	-	0/2/2/2	0/0/0/0
3	BCT	B	1002	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1003	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1004	-	-	0/0/0/0	0/0/0/0
4	PO4	B	1005	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1006	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1007	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1008	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1009	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1010	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1011	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1012	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1013	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1014	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	GLY	OXT-C-O	-2.34	117.34	123.30
2	B	1001	GLY	OXT-C-O	-2.21	117.69	123.30
2	A	1004	GLY	OXT-C-O	-2.05	118.08	123.30
2	A	1003	GLY	OXT-C-O	-2.02	118.17	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	942/983 (95%)	-0.33	15 (1%) 68 70	9, 16, 39, 62	2 (0%)
1	B	942/983 (95%)	-0.21	31 (3%) 44 45	9, 17, 43, 86	1 (0%)
All	All	1884/1966 (95%)	-0.27	46 (2%) 56 57	9, 17, 41, 86	3 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ILE	6.7
1	B	644	GLY	5.4
1	A	16	ILE	5.1
1	B	14	GLU	5.0
1	B	15	ALA	4.3
1	B	185	LYS	4.0
1	B	828	ASN	4.0
1	A	969	HIS	3.9
1	A	469	THR	3.8
1	B	469	THR	3.7
1	B	18	VAL	3.5
1	B	968	ARG	3.5
1	B	969	HIS	3.3
1	B	465	ASN	3.3
1	A	17	ALA	3.2
1	A	470	PRO	3.2
1	B	187	LYS	3.1
1	A	15	ALA	3.0
1	A	474	TRP	2.9
1	B	313	ARG	2.8
1	B	470	PRO	2.8
1	A	662	ASP	2.8
1	A	18	VAL	2.6
1	B	474	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	19	ASP	2.6
1	B	463	LYS	2.6
1	B	20	LEU	2.5
1	B	17	ALA	2.5
1	B	349	THR	2.4
1	B	22	LYS	2.4
1	B	478	LYS	2.4
1	A	19	ASP	2.3
1	A	467	PRO	2.3
1	B	327	HIS	2.2
1	B	975	GLU	2.2
1	A	965	TYR	2.2
1	A	644	GLY	2.2
1	B	464	ASP	2.1
1	B	977	MET	2.1
1	A	755	THR	2.1
1	B	662	ASP	2.1
1	B	468	PHE	2.1
1	B	467	PRO	2.0
1	A	471	GLU	2.0
1	B	23	LEU	2.0
1	B	976	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	B	726	24/25	0.14	2.62	10,19,24,25	9
1	LLP	A	726	24/25	0.08	-0.36	7,17,24,27	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	1009	4/4	0.18	26.34	25,27,32,32	0
6	BCN	A	1017	11/11	0.33	19.48	32,45,64,67	11
2	GLY	A	1002	5/5	0.20	16.65	44,47,48,51	0
5	EDO	B	1012	4/4	0.25	13.18	10,11,21,25	4
5	EDO	A	1010	4/4	0.17	12.13	26,26,27,35	0
3	BCT	A	1006	4/4	0.14	11.23	40,41,44,50	4
5	EDO	A	1013	4/4	0.19	10.91	49,50,54,60	0
5	EDO	A	1011	4/4	0.25	8.11	19,21,29,33	4
3	BCT	B	1002	4/4	0.13	7.37	18,35,37,40	4
5	EDO	B	1011	4/4	0.25	6.83	20,23,27,27	4
2	GLY	A	1001	5/5	0.21	6.62	31,35,51,52	0
5	EDO	A	1015	4/4	0.14	6.30	25,32,32,34	4
5	EDO	B	1008	4/4	0.34	5.96	19,22,26,34	4
2	GLY	B	1001	5/5	0.21	5.61	44,51,60,61	0
5	EDO	B	1013	4/4	0.20	5.10	40,45,51,52	0
5	EDO	B	1010	4/4	0.30	4.99	42,43,47,51	0
5	EDO	A	1012	4/4	0.13	4.53	34,37,42,42	0
5	EDO	A	1016	4/4	0.13	4.05	21,23,37,40	2
5	EDO	B	1007	4/4	0.20	3.90	16,36,38,41	0
3	BCT	A	1005	4/4	0.10	3.48	16,30,32,32	4
5	EDO	A	1014	4/4	0.17	3.43	34,40,43,43	0
4	PO4	A	1007	5/5	0.11	3.41	14,32,39,41	5
4	PO4	B	1003	5/5	0.12	2.66	25,45,47,51	0
2	GLY	A	1004	5/5	0.20	2.38	53,56,58,61	0
4	PO4	A	1009	5/5	0.21	2.22	16,19,31,37	5
2	GLY	A	1003	5/5	0.19	1.67	35,36,41,43	5
4	PO4	A	1008	5/5	0.12	1.58	24,27,32,35	5
5	EDO	B	1014	4/4	0.17	1.49	40,42,43,47	0
5	EDO	B	1006	4/4	0.15	1.43	29,34,41,56	0
4	PO4	B	1005	5/5	0.19	0.99	23,29,38,43	5
4	PO4	B	1004	5/5	0.09	0.75	22,23,29,29	5

6.5 Other polymers ⓘ

There are no such residues in this entry.