



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:06 AM UTC

PDB ID : 4LHD / pdb_00004lhd
Title : Crystal structure of Synechocystis sp. PCC 6803 glycine decarboxylase (P-protein), holo form with pyridoxal-5'-phosphate and glycine, closed flexible loop
Authors : Hasse, D.; Andersson, E.; Carlsson, G.; Masloboy, A.; Hagemann, M.; Bauwe, H.; Andersson, I.
Deposited on : 2013-07-01
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

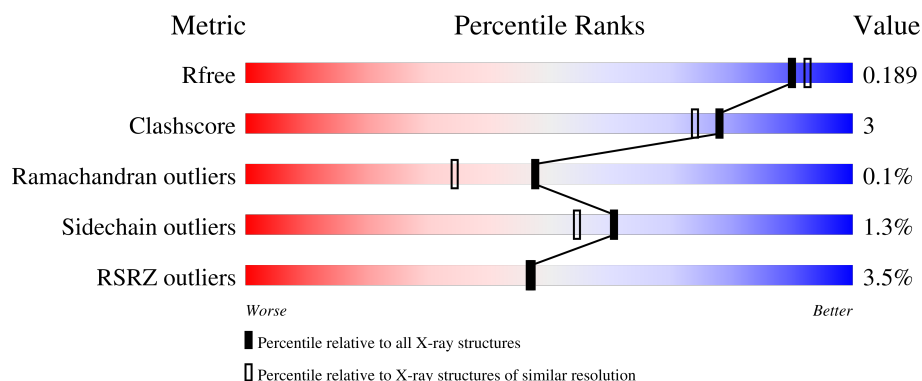
1 Overall quality at a glance

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	983	3% 90% 7% ••
1	B	983	4% 89% 6% •

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	GLY	A	1002	-	X	-	-
2	GLY	A	1004	-	X	-	-
2	GLY	B	1001	-	X	-	-

2 Entry composition [i](#)

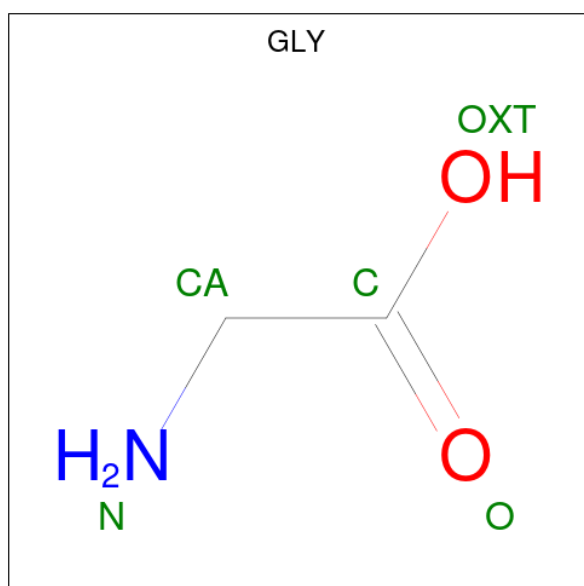
There are 6 unique types of molecules in this entry. The entry contains 16216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycine dehydrogenase [decarboxylating].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	952	Total	C	N	O	P	S	0	22	0
			7424	4724	1253	1401	1	45			
1	B	940	Total	C	N	O	P	S	0	17	0
			7298	4645	1227	1380	1	45			

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



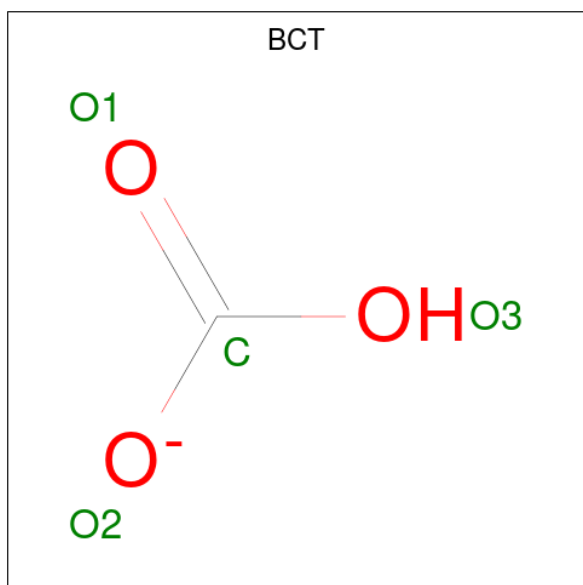
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

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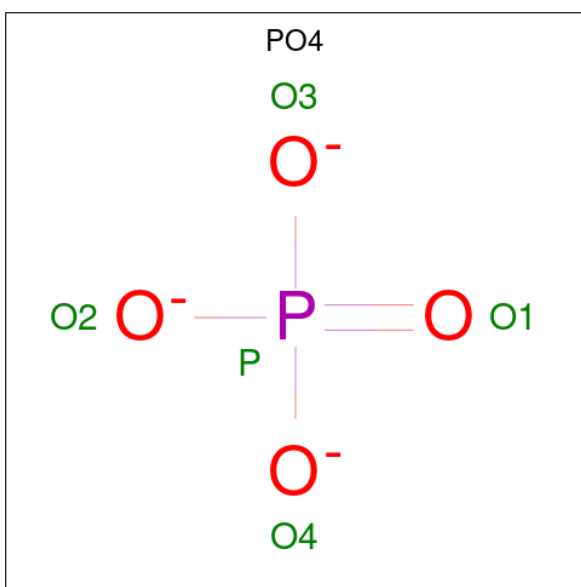
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			5	2	1	2		
2	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



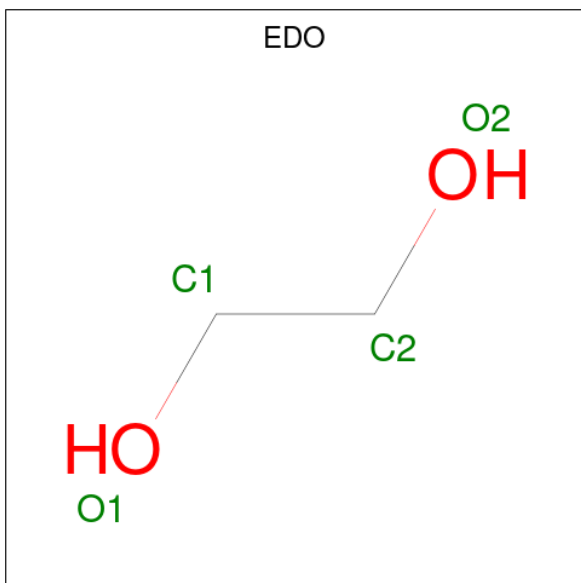
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: 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	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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

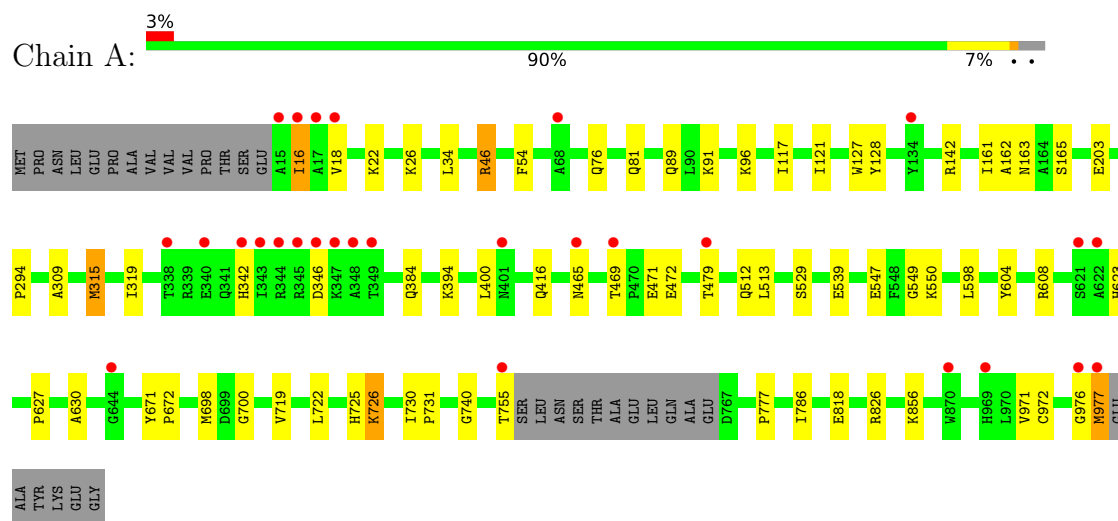
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	697	Total O 698 698	0	1
6	B	675	Total O 678 678	0	3

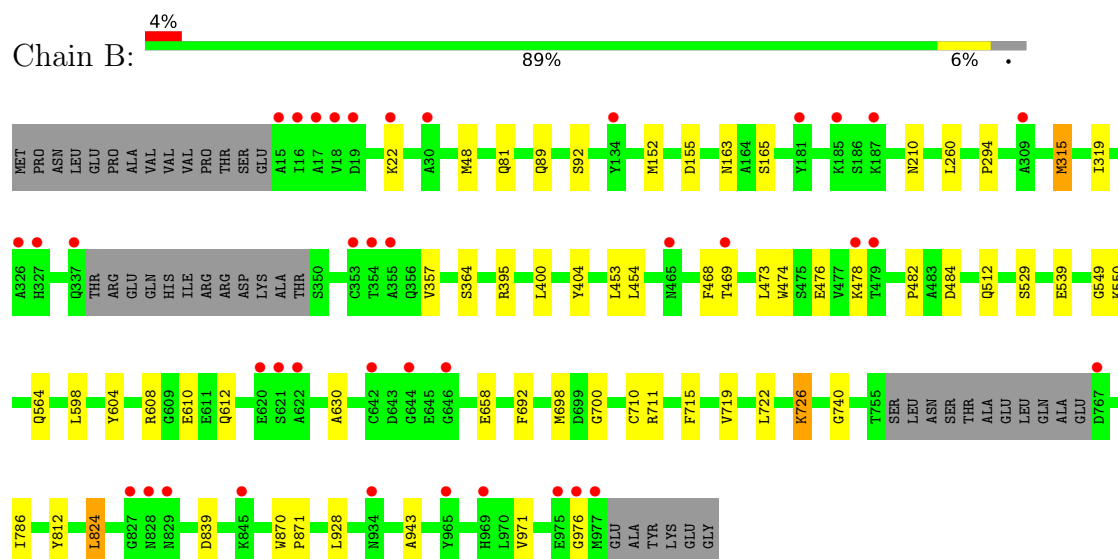
3 Residue-property plots [i](#)

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: Glycine dehydrogenase [decarboxylating]



- Molecule 1: Glycine dehydrogenase [decarboxylating]



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.99Å 159.99Å 159.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.76 – 1.80 49.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.76-1.80) 99.3 (49.76-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.163 , 0.191 0.161 , 0.189	Depositor DCC
R_{free} test set	10959 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16216	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: BCT, EDO, PO4, LLP

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	0.41	0/7653	0.73	0/10407
1	B	0.41	0/7509	0.73	1/10212 (0.0%)
All	All	0.41	0/15162	0.73	1/20619 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	VAL	N-CA-C	5.10	115.72	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7424	0	7316	46	0
1	B	7298	0	7170	39	0
2	A	20	0	8	3	0
2	B	10	0	4	1	0
3	A	12	0	0	0	0
3	B	4	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	32	0	48	7	0
5	B	20	0	30	5	0
6	A	698	0	0	8	0
6	B	678	0	0	4	0
All	All	16216	0	14576	83	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 3.

All (83) 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:346:ASP:HB3	1:A:627:PRO:HB2	1.52	0.89
1:A:416:GLN:HB3	2:A:1003:GLY:HA2	1.63	0.81
1:A:16:ILE:HD11	1:B:454:LEU:HD21	1.67	0.77
1:B:48:MET:HG2	1:B:812:TYR:CD1	2.22	0.74
1:A:161[A]:ILE:HD13	1:A:309:ALA:HA	1.71	0.72
1:A:550:LYS:HG2	5:A:1011:EDO:H11	1.72	0.71
1:B:210[B]:ASN:ND2	6:B:1709:HOH:O	2.25	0.69
1:A:549:GLY:HA3	5:A:1011:EDO:H21	1.76	0.68
1:B:152:MET:HE1	1:B:364:SER:HA	1.77	0.67
1:B:604:TYR:OH	1:B:608:ARG:NH1	2.30	0.65
1:A:623:HIS:NE2	2:A:1001:GLY:HA2	2.13	0.63
1:B:48:MET:HG2	1:B:812:TYR:CG	2.34	0.63
1:A:604:TYR:CZ	1:A:608:ARG:HD2	2.34	0.62
1:B:294:PRO:HB3	5:B:1006:EDO:H21	1.82	0.60
1:A:818:GLU:OE2	1:A:826:ARG:NH2	2.35	0.59
1:A:96:LYS:NZ	6:A:1670:HOH:O	2.37	0.57
1:A:384:GLN:HG2	1:A:479:THR:HG21	1.85	0.57
1:A:294:PRO:HB3	5:A:1011:EDO:H22	1.87	0.56
1:B:92:SER:HA	5:B:1010:EDO:H21	1.86	0.56
1:A:117:ILE:HG23	1:A:121:ILE:HD12	1.86	0.56
1:B:604:TYR:CZ	1:B:608:ARG:HD2	2.41	0.56
1:B:824:LEU:HD22	1:B:839:ASP:HB2	1.88	0.55
1:B:971:VAL:HG11	1:B:976:GLY:HA3	1.87	0.55
1:B:395:ARG:NH2	1:B:476:GLU:OE2	2.26	0.55
1:B:726:LLP:O3	1:B:726:LLP:NZ	2.40	0.55
1:B:658:GLU:HG3	1:B:692:PHE:CZ	2.42	0.54
1:B:698[A]:MET:HE1	1:B:715:PHE:CZ	2.42	0.54
1:B:163:ASN:HB3	1:B:315:MET:HE1	1.89	0.53
1:A:471:GLU:HG3	1:B:22:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:VAL:HG11	1:A:976:GLY:HA3	1.90	0.52
1:A:698[B]:MET:HE3	1:A:700:GLY:HA2	1.92	0.52
1:A:54:PHE:HA	5:A:1014:EDO:H22	1.92	0.51
1:A:512[B]:GLN:HG3	1:A:513:LEU:N	2.26	0.51
1:A:726:LLP:NZ	1:A:726:LLP:O3	2.40	0.50
1:B:482:PRO:HB2	1:B:484:ASP:OD1	2.12	0.49
1:B:698[B]:MET:HE3	1:B:700:GLY:HA2	1.94	0.49
1:B:81:GLN:NE2	1:B:89:GLN:OE1	2.40	0.49
1:B:564[B]:GLN:HG2	6:B:1498:HOH:O	2.13	0.48
1:B:610:GLU:OE1	1:B:612:GLN:NE2	2.46	0.48
1:A:394:LYS:NZ	6:A:1598:HOH:O	2.47	0.48
1:B:564[B]:GLN:NE2	6:B:1395:HOH:O	2.28	0.48
1:A:777:PRO:HG2	6:A:1441:HOH:O	2.14	0.47
1:A:319[B]:ILE:HD11	1:A:972[B]:CYS:SG	2.54	0.47
1:B:598:LEU:HD13	1:B:630:ALA:HA	1.97	0.47
1:A:81:GLN:NE2	1:A:89:GLN:OE1	2.40	0.46
1:A:394:LYS:HG3	1:A:400:LEU:HD22	1.97	0.46
1:B:870:TRP:CD1	1:B:871:PRO:HA	2.51	0.46
1:A:127:TRP:HA	5:A:1012:EDO:H11	1.97	0.46
1:B:928:LEU:HD11	1:B:943:ALA:HB2	1.96	0.46
1:A:203:GLU:HG3	6:A:1336:HOH:O	2.16	0.46
1:B:870:TRP:CG	1:B:871:PRO:HA	2.51	0.46
1:A:18:VAL:O	1:A:22:LYS:HG2	2.15	0.45
1:B:315:MET:HB3	1:B:315:MET:HE3	1.70	0.45
1:A:162:ALA:O	1:A:319[B]:ILE:HD12	2.17	0.45
1:A:725:HIS:HA	1:A:730:ILE:HB	1.99	0.45
1:A:91:LYS:NZ	1:A:547:GLU:OE1	2.44	0.44
1:A:512[A]:GLN:HG3	6:A:1504:HOH:O	2.16	0.44
1:A:469:THR:O	1:A:472:GLU:HB3	2.17	0.44
1:B:549:GLY:HA3	5:B:1006:EDO:H11	1.99	0.44
1:A:598:LEU:HD13	1:A:630:ALA:HA	2.00	0.44
1:B:710:CYS:HA	5:B:1009:EDO:H22	2.00	0.43
1:B:928:LEU:CD1	1:B:943:ALA:HB2	2.48	0.43
1:A:26:LYS:HB3	1:B:474:TRP:CE2	2.54	0.43
1:A:34:LEU:HD22	5:A:1013:EDO:H11	2.01	0.42
1:A:342:HIS:HD2	6:A:1711:HOH:O	2.03	0.42
1:B:468:PHE:CE1	1:B:473:LEU:HD11	2.55	0.42
1:B:711:ARG:H	5:B:1009:EDO:C2	2.32	0.42
1:A:722:LEU:O	1:A:740:GLY:HA2	2.19	0.42
1:A:46:ARG:NH2	6:A:1622:HOH:O	2.53	0.41
2:A:1002:GLY:N	6:A:1551:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ASP:OD1	2:B:1002:GLY:N	2.52	0.41
1:A:977:MET:HE2	1:A:977:MET:HB3	1.73	0.41
1:B:512:GLN:HG3	6:B:1420:HOH:O	2.20	0.41
1:B:722:LEU:O	1:B:740:GLY:HA2	2.21	0.41
1:B:404:TYR:CE1	1:B:482:PRO:HD3	2.55	0.41
1:B:539:GLU:HB3	1:B:786:ILE:HG23	2.03	0.41
1:A:142:ARG:HH11	5:A:1012:EDO:H21	1.85	0.40
1:A:539:GLU:HB3	1:A:786:ILE:HG23	2.01	0.40
1:A:671:TYR:HA	1:A:672:PRO:C	2.46	0.40
1:A:128:TYR:O	1:A:731:PRO:HB2	2.21	0.40
1:A:161[A]:ILE:HG13	1:A:315:MET:HE1	2.03	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	969/983 (99%)	942 (97%)	26 (3%)	1 (0%)	48	34
1	B	950/983 (97%)	925 (97%)	24 (2%)	1 (0%)	48	34
All	All	1919/1966 (98%)	1867 (97%)	50 (3%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

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

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	794/798 (100%)	785 (99%)	9 (1%)	65	60
1	B	778/798 (98%)	766 (98%)	12 (2%)	57	49
All	All	1572/1596 (98%)	1551 (99%)	21 (1%)	61	54

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	46	ARG
1	A	76	GLN
1	A	315	MET
1	A	465	ASN
1	A	529	SER
1	A	719	VAL
1	A	755	THR
1	A	977	MET
1	B	260	LEU
1	B	315	MET
1	B	319[A]	ILE
1	B	319[B]	ILE
1	B	400	LEU
1	B	453	LEU
1	B	469	THR
1	B	478	LYS
1	B	529	SER
1	B	550	LYS
1	B	719	VAL
1	B	824	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	626	ASN
1	A	797	GLN
1	A	934	ASN
1	B	47	GLN
1	B	50	GLN
1	B	120	ASN
1	B	431	ASN
1	B	559	GLN
1	B	768	GLN
1	B	829	ASN

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	B	726	1	23,24,25	1.72	5 (21%)	25,32,34	2.26	3 (12%)
1	LLP	A	726	1	23,24,25	1.72	5 (21%)	25,32,34	2.06	3 (12%)

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	B	726	1	-	4/16/17/19	0/1/1/1
1	LLP	A	726	1	-	2/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	LLP	O3-C3	-5.65	1.24	1.36
1	A	726	LLP	O3-C3	-5.44	1.24	1.36
1	B	726	LLP	C2-N1	2.62	1.38	1.33
1	A	726	LLP	C2-N1	2.56	1.38	1.33
1	A	726	LLP	CE-NZ	2.39	1.52	1.46
1	B	726	LLP	C4'-NZ	2.17	1.34	1.27
1	A	726	LLP	C4'-NZ	2.17	1.34	1.27
1	A	726	LLP	C4-C4'	2.07	1.51	1.46
1	B	726	LLP	CE-NZ	2.04	1.51	1.46
1	B	726	LLP	C4-C4'	2.00	1.50	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	726	LLP	OP4-C5'-C5	9.54	127.25	109.36
1	A	726	LLP	OP4-C5'-C5	8.30	124.91	109.36
1	B	726	LLP	C4-C4'-NZ	-3.34	108.61	124.04
1	A	726	LLP	C4-C4'-NZ	-3.28	108.90	124.04
1	B	726	LLP	CE-NZ-C4'	-2.11	111.97	118.72
1	A	726	LLP	CE-NZ-C4'	-2.03	112.23	118.72

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	726	LLP	C4-C4'-NZ-CE
1	B	726	LLP	C4-C5-C5'-OP4
1	B	726	LLP	C6-C5-C5'-OP4
1	B	726	LLP	C4-C4'-NZ-CE
1	A	726	LLP	C3-C4-C4'-NZ
1	B	726	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	726	LLP	1	0
1	A	726	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 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	B	1002	-	4,4,4	1.14	1 (25%)	3,4,4	1.49	0
5	EDO	B	1009	-	3,3,3	0.41	0	2,2,2	0.49	0
3	BCT	A	1007	-	3,3,3	0.53	0	2,3,3	0.29	0
4	PO4	A	1008	-	4,4,4	1.06	0	6,6,6	0.52	0
2	GLY	A	1004	-	4,4,4	1.12	1 (25%)	3,4,4	1.82	2 (66%)
5	EDO	B	1010	-	3,3,3	0.48	0	2,2,2	0.17	0
4	PO4	B	1005	-	4,4,4	0.87	0	6,6,6	0.49	0
2	GLY	A	1002	-	4,4,4	1.15	1 (25%)	3,4,4	1.59	1 (33%)
5	EDO	A	1012	-	3,3,3	0.44	0	2,2,2	0.49	0
5	EDO	A	1011	-	3,3,3	0.43	0	2,2,2	0.24	0
5	EDO	A	1014	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	A	1013	-	3,3,3	0.49	0	2,2,2	0.16	0
2	GLY	A	1001	-	4,4,4	1.14	1 (25%)	3,4,4	1.55	0
5	EDO	A	1017	-	3,3,3	0.42	0	2,2,2	0.49	0
5	EDO	B	1008	-	3,3,3	0.45	0	2,2,2	0.40	0
4	PO4	A	1009	-	4,4,4	0.91	0	6,6,6	0.49	0
5	EDO	B	1006	-	3,3,3	0.46	0	2,2,2	0.20	0
5	EDO	A	1015	-	3,3,3	0.45	0	2,2,2	0.40	0
3	BCT	B	1003	-	3,3,3	0.46	0	2,3,3	0.53	0
5	EDO	B	1007	-	3,3,3	0.48	0	2,2,2	0.42	0
3	BCT	A	1005	-	3,3,3	0.49	0	2,3,3	0.22	0
5	EDO	A	1010	-	3,3,3	0.47	0	2,2,2	0.49	0
2	GLY	A	1003	-	4,4,4	1.20	1 (25%)	3,4,4	1.55	0
3	BCT	A	1006	-	3,3,3	0.53	0	2,3,3	0.13	0
4	PO4	B	1004	-	4,4,4	0.92	0	6,6,6	0.44	0
2	GLY	B	1001	-	4,4,4	1.14	1 (25%)	3,4,4	1.68	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1016	-	3,3,3	0.37	0	2,2,2	0.57	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	B	1002	-	-	2/2/2/2	-
5	EDO	B	1009	-	-	1/1/1/1	-
2	GLY	A	1004	-	-	2/2/2/2	-
5	EDO	B	1010	-	-	0/1/1/1	-
2	GLY	A	1002	-	-	2/2/2/2	-
5	EDO	A	1012	-	-	0/1/1/1	-
5	EDO	A	1011	-	-	0/1/1/1	-
5	EDO	A	1014	-	-	0/1/1/1	-
5	EDO	A	1013	-	-	1/1/1/1	-
2	GLY	A	1001	-	-	2/2/2/2	-
5	EDO	A	1017	-	-	1/1/1/1	-
5	EDO	B	1008	-	-	0/1/1/1	-
5	EDO	B	1006	-	-	0/1/1/1	-
5	EDO	A	1015	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	0/1/1/1	-
5	EDO	A	1010	-	-	0/1/1/1	-
2	GLY	A	1003	-	-	1/2/2/2	-
2	GLY	B	1001	-	-	2/2/2/2	-
5	EDO	A	1016	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	GLY	OXT-C	-2.24	1.23	1.30
2	B	1001	GLY	OXT-C	-2.18	1.23	1.30
2	A	1004	GLY	OXT-C	-2.16	1.23	1.30
2	A	1002	GLY	OXT-C	-2.16	1.23	1.30
2	A	1001	GLY	OXT-C	-2.13	1.23	1.30
2	B	1002	GLY	OXT-C	-2.12	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	GLY	OXT-C-O	-2.24	117.57	123.33
2	B	1001	GLY	OXT-C-O	-2.18	117.72	123.33
2	A	1004	GLY	OXT-C-CA	2.16	121.98	113.38
2	A	1002	GLY	OXT-C-O	-2.12	117.89	123.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	GLY	O-C-CA-N
2	A	1001	GLY	OXT-C-CA-N
2	A	1002	GLY	O-C-CA-N
2	A	1002	GLY	OXT-C-CA-N
2	A	1004	GLY	OXT-C-CA-N
2	B	1001	GLY	O-C-CA-N
2	B	1001	GLY	OXT-C-CA-N
2	B	1002	GLY	O-C-CA-N
2	B	1002	GLY	OXT-C-CA-N
2	A	1004	GLY	O-C-CA-N
5	A	1013	EDO	O1-C1-C2-O2
5	A	1017	EDO	O1-C1-C2-O2
5	B	1009	EDO	O1-C1-C2-O2
2	A	1003	GLY	OXT-C-CA-N

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	GLY	1	0
5	B	1009	EDO	2	0
5	B	1010	EDO	1	0
2	A	1002	GLY	1	0
5	A	1012	EDO	2	0
5	A	1011	EDO	3	0
5	A	1014	EDO	1	0
5	A	1013	EDO	1	0
2	A	1001	GLY	1	0
5	B	1006	EDO	2	0
2	A	1003	GLY	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	951/983 (96%)	-0.24	28 (2%)	53 53	7, 15, 37, 66	22 (2%)
1	B	939/983 (95%)	-0.13	39 (4%)	40 40	8, 16, 40, 68	17 (1%)
All	All	1890/1966 (96%)	-0.19	67 (3%)	47 47	7, 15, 39, 68	39 (2%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	ALA	7.1
1	B	15	ALA	6.5
1	B	16	ILE	5.8
1	B	18	VAL	5.1
1	A	343	ILE	4.9
1	A	622	ALA	4.7
1	A	16	ILE	4.6
1	B	644	GLY	4.4
1	A	755	THR	4.4
1	A	342	HIS	4.3
1	B	977	MET	4.3
1	B	828	ASN	4.1
1	B	767	ASP	4.1
1	A	621	SER	4.1
1	B	478	LYS	4.0
1	B	622	ALA	3.9
1	A	977	MET	3.7
1	B	185	LYS	3.7
1	A	18	VAL	3.6
1	B	355	ALA	3.6
1	B	642	CYS	3.5
1	A	17	ALA	3.5
1	A	349	THR	3.5
1	B	969	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	344	ARG	3.0
1	A	348	ALA	2.9
1	A	340	GLU	2.9
1	B	354	THR	2.8
1	B	646	GLY	2.8
1	B	976	GLY	2.8
1	A	969	HIS	2.8
1	B	309	ALA	2.8
1	A	68	ALA	2.7
1	B	134	TYR	2.7
1	B	479	THR	2.7
1	B	187	LYS	2.7
1	B	17	ALA	2.7
1	A	346	ASP	2.6
1	A	347	LYS	2.6
1	B	845	LYS	2.6
1	B	326	ALA	2.6
1	B	975	GLU	2.6
1	A	469	THR	2.5
1	A	345	ARG	2.5
1	B	337	GLN	2.5
1	B	465	ASN	2.4
1	B	353	CYS	2.4
1	B	327	HIS	2.4
1	A	644	GLY	2.4
1	B	469	THR	2.4
1	B	965	TYR	2.4
1	A	976	GLY	2.3
1	B	827	GLY	2.3
1	B	829	ASN	2.3
1	A	338	THR	2.3
1	B	22	LYS	2.3
1	A	479	THR	2.3
1	B	19	ASP	2.3
1	B	621	SER	2.2
1	A	465	ASN	2.2
1	B	620	GLU	2.2
1	B	30	ALA	2.1
1	B	934	ASN	2.1
1	A	870	TRP	2.1
1	A	401	ASN	2.0
1	A	134	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	181	TYR	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	726	24/25	0.93	0.12	11,27,36,40	11
1	LLP	A	726	24/25	0.96	0.10	8,20,32,36	0

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
2	GLY	A	1003	5/5	0.70	0.22	35,35,41,42	5
2	GLY	A	1002	5/5	0.75	0.23	35,36,39,43	5
2	GLY	B	1001	5/5	0.75	0.22	55,59,64,65	0
2	GLY	B	1002	5/5	0.77	0.20	34,43,45,49	0
2	GLY	A	1001	5/5	0.79	0.22	33,35,49,53	0
2	GLY	A	1004	5/5	0.79	0.20	39,39,41,47	0
5	EDO	A	1016	4/4	0.79	0.17	22,25,28,30	4
5	EDO	B	1008	4/4	0.81	0.17	42,43,47,49	0
5	EDO	A	1017	4/4	0.82	0.18	20,29,32,32	4
5	EDO	A	1013	4/4	0.82	0.23	39,43,44,44	0
3	BCT	A	1007	4/4	0.84	0.14	20,26,26,34	4
5	EDO	B	1010	4/4	0.84	0.18	34,35,39,42	4
5	EDO	A	1012	4/4	0.85	0.20	12,12,17,27	4
3	BCT	B	1003	4/4	0.86	0.17	18,33,35,38	4
5	EDO	B	1009	4/4	0.87	0.14	9,13,15,15	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BCT	A	1006	4/4	0.87	0.16	37,37,41,45	4
4	PO4	B	1004	5/5	0.88	0.11	28,50,52,56	0
5	EDO	B	1007	4/4	0.89	0.14	29,30,30,33	0
5	EDO	A	1014	4/4	0.89	0.15	33,42,46,46	0
4	PO4	A	1009	5/5	0.90	0.11	20,24,26,32	5
3	BCT	A	1005	4/4	0.90	0.13	15,27,30,31	4
5	EDO	A	1011	4/4	0.90	0.14	16,17,21,26	4
4	PO4	A	1008	5/5	0.91	0.14	12,36,38,42	5
5	EDO	A	1010	4/4	0.91	0.12	27,28,30,33	0
5	EDO	A	1015	4/4	0.93	0.10	19,23,34,36	4
4	PO4	B	1005	5/5	0.94	0.08	21,27,30,31	5
5	EDO	B	1006	4/4	0.94	0.16	21,23,30,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.