



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:36 PM UTC

PDB ID : 4LHC / pdb_00004lhc
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 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

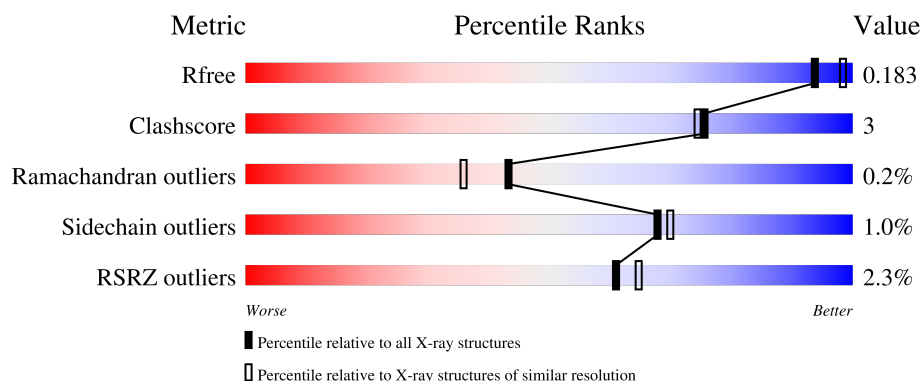
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	% 90% 5% .
1	B	983	3% 88% 7% .

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	1003	-	X	-	-
2	GLY	A	1004	-	X	-	-
2	GLY	B	1001	-	X	-	-
6	BCN	A	1017	-	-	X	-

2 Entry composition [i](#)

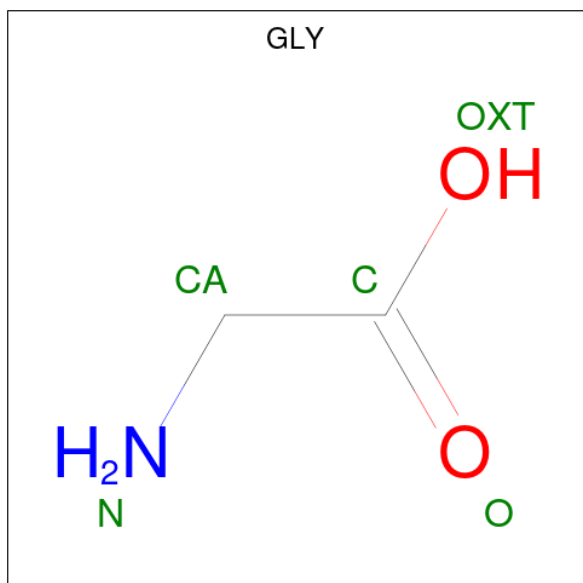
There are 7 unique types of molecules in this entry. The entry contains 16238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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 (CCD ID: GLY) (formula: $C_2H_5NO_2$).



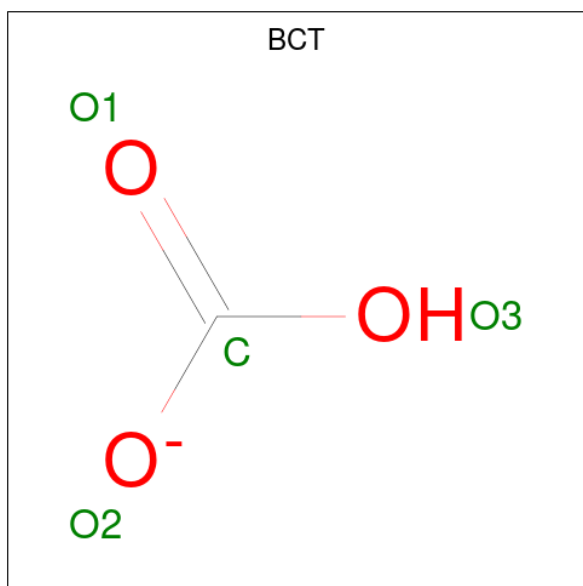
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

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

- 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	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	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 (CCD ID: EDO) (formula: C₂H₆O₂).



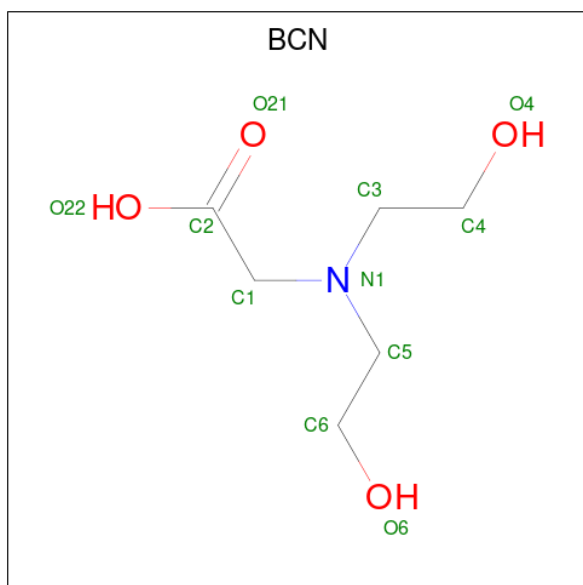
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

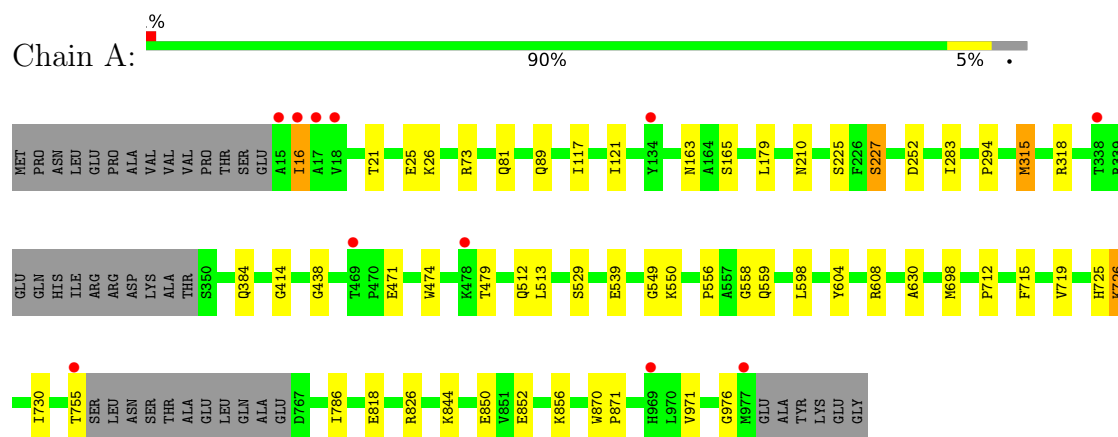
- Molecule 7 is water.

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

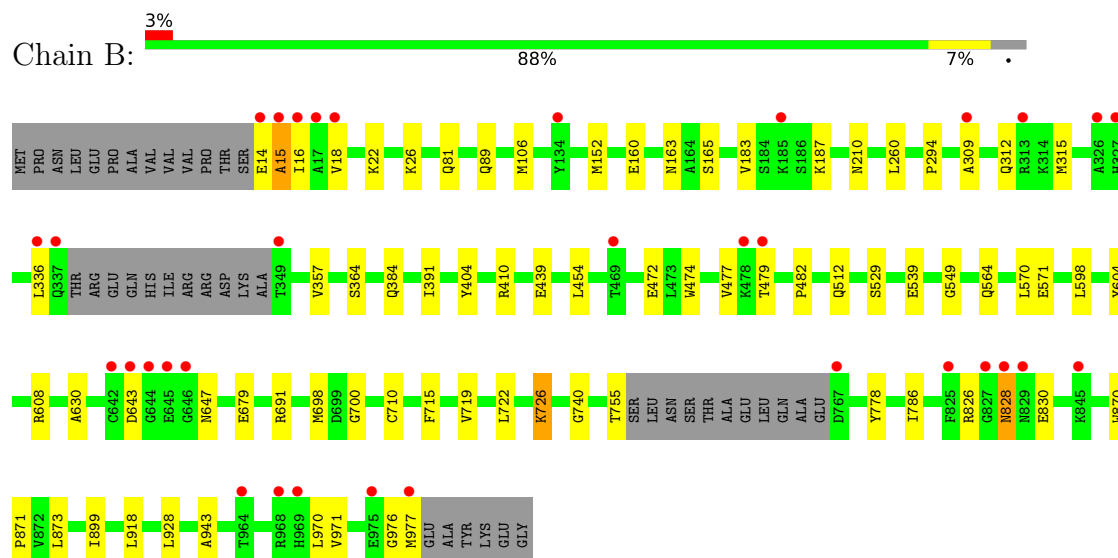
3 Residue-property plots [i](#)

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	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	9313 reflections (5.02%)	wwPDB-VP
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 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	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.

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, LLP, PO4, BCN, 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	0.42	0/7533	0.73	0/10245
1	B	0.42	0/7526	0.72	1/10236 (0.0%)
All	All	0.42	0/15059	0.72	1/20481 (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	5.66	116.31	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	7355	0	7220	41	0
1	B	7347	0	7211	47	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	42	5	0
5	B	36	0	54	7	0
6	A	11	0	12	7	0
7	A	705	0	0	5	0
7	B	689	0	0	6	0
All	All	16238	0	14549	89	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 (89) 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:559:GLN:HE21	6:A:1017:BCN:H41	1.42	0.83
1:A:210[B]:ASN:ND2	7:A:1637:HOH:O	2.24	0.71
1:A:384:GLN:HG2	1:A:479:THR:HG21	1.77	0.66
1:B:210[B]:ASN:ND2	7:B:1634:HOH:O	2.31	0.63
1:A:16:ILE:HD11	1:B:454:LEU:HD21	1.81	0.63
1:A:818:GLU:OE2	1:A:826:ARG:NH2	2.32	0.62
1:A:549:GLY:HA3	5:A:1011:EDO:H21	1.82	0.61
1:A:604:TYR:CZ	1:A:608[A]:ARG:HD2	2.34	0.61
1:B:971:VAL:HG11	1:B:976:GLY:HA3	1.83	0.61
2:A:1004:GLY:N	7:A:1576:HOH:O	2.34	0.59
1:A:73:ARG:HH22	5:A:1013:EDO:H11	1.66	0.59
1:B:755:THR:H	5:B:1011:EDO:H21	1.68	0.59
1:B:14:GLU:HA	1:B:16:ILE:N	2.19	0.57
1:B:698[B]:MET:HE1	1:B:715:PHE:CZ	2.39	0.57
1:A:252:ASP:OD1	5:A:1014:EDO:H11	2.05	0.57
1:B:152:MET:HE1	1:B:364:SER:HA	1.86	0.56
1:A:471:GLU:HG3	1:B:22:LYS:HB2	1.88	0.56
1:A:550:LYS:HG2	5:A:1011:EDO:H11	1.87	0.56
1:A:870:TRP:CD1	1:A:871:PRO:HA	2.43	0.53
1:A:698[B]:MET:HE1	1:A:715:PHE:CZ	2.43	0.53
1:B:726:LLP:O3	1:B:726:LLP:NZ	2.41	0.53
1:B:698[A]:MET:HE3	1:B:700:GLY:HA2	1.91	0.53
1:A:558:GLY:HA3	6:A:1017:BCN:H51	1.91	0.53
1:A:726:LLP:NZ	1:A:726:LLP:O3	2.41	0.53
1:B:81:GLN:NE2	1:B:89:GLN:OE1	2.29	0.51
1:B:294:PRO:HB3	5:B:1006:EDO:H21	1.92	0.51
1:A:294:PRO:HB3	5:A:1011:EDO:H22	1.92	0.51
1:B:512[A]:GLN:HG3	7:B:1367:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:TYR:CZ	1:B:608:ARG:HD2	2.46	0.51
1:B:474:TRP:O	1:B:477:VAL:HG22	2.11	0.50
2:B:1001:GLY:N	7:B:1513:HOH:O	2.45	0.50
1:A:179:LEU:HD22	1:A:283:ILE:HD11	1.94	0.49
1:B:870:TRP:CG	1:B:871:PRO:HA	2.48	0.49
1:B:870:TRP:CD1	1:B:871:PRO:HA	2.48	0.49
1:A:26:LYS:HB3	1:B:474:TRP:CE2	2.48	0.49
1:A:852[B]:GLU:O	1:A:856:LYS:HG2	2.13	0.48
1:A:556:PRO:HB3	6:A:1017:BCN:H62	1.96	0.48
1:A:844:LYS:NZ	1:A:850:GLU:OE2	2.45	0.47
1:A:512[A]:GLN:HG3	7:A:1494:HOH:O	2.14	0.47
1:B:549:GLY:HA3	5:B:1006:EDO:H11	1.96	0.47
1:A:598:LEU:HD13	1:A:630:ALA:HA	1.97	0.47
1:B:571:GLU:OE2	5:B:1013:EDO:H21	2.15	0.47
5:B:1011:EDO:H22	7:B:1678:HOH:O	2.16	0.46
1:A:512[B]:GLN:HG3	1:A:513:LEU:N	2.30	0.46
1:A:539:GLU:HB3	1:A:786:ILE:HG23	1.97	0.46
1:A:726:LLP:H4'1	7:A:1698:HOH:O	2.15	0.45
1:B:14:GLU:N	1:B:15:ALA:HB3	2.31	0.45
1:A:21:THR:O	1:A:25:GLU:HG3	2.15	0.45
1:B:404:TYR:CE1	1:B:482:PRO:HD3	2.52	0.45
1:B:691:ARG:NH1	7:B:1557:HOH:O	2.49	0.45
1:B:722:LEU:O	1:B:740:GLY:HA2	2.16	0.45
1:A:971:VAL:HG11	1:A:976:GLY:HA3	1.99	0.44
1:B:598:LEU:HD13	1:B:630:ALA:HA	1.99	0.44
1:B:826:ARG:HD2	1:B:830:GLU:HG3	1.99	0.44
1:A:870:TRP:CG	1:A:871:PRO:HA	2.53	0.44
1:A:315:MET:HB3	1:A:315:MET:HE2	1.66	0.44
1:B:384:GLN:HG2	1:B:479:THR:HG21	1.99	0.44
1:A:163:ASN:HB2	1:A:318:ARG:O	2.17	0.44
1:A:414:GLY:C	1:A:438:GLY:HA2	2.43	0.44
1:A:559:GLN:NE2	6:A:1017:BCN:H41	2.20	0.44
1:B:643:ASP:OD2	1:B:647:ASN:N	2.51	0.44
1:B:183:VAL:HG21	1:B:260:LEU:HD11	1.99	0.43
6:A:1017:BCN:H42	6:A:1017:BCN:H12	1.67	0.43
1:B:160:GLU:OE1	1:B:309:ALA:N	2.28	0.43
1:A:81:GLN:NE2	1:A:89:GLN:OE1	2.36	0.43
1:B:152:MET:HE3	1:B:152:MET:HB2	1.70	0.43
1:A:725:HIS:HA	1:A:730:ILE:HB	2.02	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564[B]:GLN:HG2	7:B:1448:HOH:O	2.18	0.42
1:B:828:ASN:OD1	1:B:828:ASN:N	2.52	0.42
1:A:559:GLN:HE21	6:A:1017:BCN:C4	2.22	0.42
1:B:106:MET:HE2	1:B:106:MET:HB3	1.79	0.42
1:B:336:LEU:HD11	1:B:970:LEU:HD22	2.01	0.42
1:B:539:GLU:HB3	1:B:786:ILE:HG23	2.01	0.42
1:B:710:CYS:HA	5:B:1012:EDO:H22	2.02	0.41
1:A:117:ILE:HG23	1:A:121:ILE:HD12	2.01	0.41
1:A:225:SER:OG	1:A:227:SER:HB3	2.19	0.41
1:A:474:TRP:CE2	1:B:26:LYS:HB3	2.56	0.41
1:B:187:LYS:HE2	1:B:187:LYS:HB2	1.95	0.41
1:B:899:ILE:HG23	1:B:918:LEU:HD21	2.02	0.41
1:B:391:ILE:HD12	1:B:477:VAL:HG12	2.02	0.41
1:B:928:LEU:HD11	1:B:943:ALA:HB2	2.03	0.40
1:A:698[A]:MET:HE1	1:A:712:PRO:HG3	2.03	0.40
1:B:163:ASN:HB3	1:B:315:MET:CE	2.51	0.40
1:B:315:MET:HE3	1:B:315:MET:HB3	1.90	0.40
1:B:778:TYR:OH	5:B:1013:EDO:H11	2.20	0.40
1:A:384:GLN:CG	1:A:479:THR:HG21	2.49	0.40
1:B:928:LEU:CD1	1:B:943:ALA:HB2	2.51	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	953/983 (97%)	929 (98%)	23 (2%)	1 (0%)	48	40
1	B	952/983 (97%)	926 (97%)	24 (2%)	2 (0%)	43	36
All	All	1905/1966 (97%)	1855 (97%)	47 (2%)	3 (0%)	43	36

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	781/798 (98%)	775 (99%)	6 (1%)	73	75
1	B	780/798 (98%)	770 (99%)	10 (1%)	61	61
All	All	1561/1596 (98%)	1545 (99%)	16 (1%)	68	70

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

Mol	Chain	Res	Type
1	A	16	ILE
1	A	227	SER
1	A	315	MET
1	A	529	SER
1	A	719	VAL
1	A	755	THR
1	B	18	VAL
1	B	312	GLN
1	B	472	GLU
1	B	529	SER
1	B	570	LEU
1	B	679	GLU
1	B	719	VAL
1	B	828	ASN
1	B	873	LEU
1	B	977	MET

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	47	GLN
1	A	50	GLN
1	A	401	ASN
1	A	431	ASN
1	A	559	GLN
1	B	47	GLN
1	B	50	GLN
1	B	120	ASN
1	B	329	ASN
1	B	511	HIS
1	B	626	ASN
1	B	768	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	B	726	1	23,24,25	1.80	5 (21%)	25,32,34	2.15	2 (8%)
1	LLP	A	726	1	23,24,25	1.74	5 (21%)	25,32,34	2.14	2 (8%)

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	-	2/16/17/19	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	A	726	LLP	O3-C3	-5.57	1.24	1.36
1	B	726	LLP	O3-C3	-5.50	1.24	1.36
1	B	726	LLP	CE-NZ	2.72	1.52	1.46
1	B	726	LLP	C2-N1	2.59	1.38	1.33
1	A	726	LLP	C2-N1	2.43	1.38	1.33
1	A	726	LLP	C4'-NZ	2.34	1.35	1.27
1	B	726	LLP	C4'-NZ	2.29	1.34	1.27
1	A	726	LLP	CE-NZ	2.25	1.51	1.46
1	A	726	LLP	C6-N1	2.13	1.38	1.34
1	B	726	LLP	C4-C4'	2.05	1.51	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	726	LLP	OP4-C5'-C5	9.12	126.45	109.36
1	A	726	LLP	OP4-C5'-C5	8.82	125.88	109.36
1	A	726	LLP	C4-C4'-NZ	-3.57	107.58	124.04
1	B	726	LLP	C4-C4'-NZ	-3.34	108.65	124.04

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	726	LLP	C4-C4'-NZ-CE
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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	726	LLP	1	0
1	A	726	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1002	-	4,4,4	1.14	1 (25%)	3,4,4	1.75	1 (33%)
5	EDO	A	1010	-	3,3,3	0.46	0	2,2,2	0.43	0
3	BCT	A	1006	-	3,3,3	0.55	0	2,3,3	0.25	0
4	PO4	A	1007	-	4,4,4	0.99	0	6,6,6	0.59	0
5	EDO	B	1006	-	3,3,3	0.41	0	2,2,2	0.24	0
5	EDO	B	1014	-	3,3,3	0.42	0	2,2,2	0.30	0
4	PO4	A	1009	-	4,4,4	0.96	0	6,6,6	0.43	0
5	EDO	B	1011	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	A	1016	-	3,3,3	0.41	0	2,2,2	0.31	0
2	GLY	A	1001	-	4,4,4	1.17	1 (25%)	3,4,4	1.55	0
5	EDO	A	1014	-	3,3,3	0.47	0	2,2,2	0.15	0
5	EDO	B	1008	-	3,3,3	0.44	0	2,2,2	0.47	0
5	EDO	B	1010	-	3,3,3	0.42	0	2,2,2	0.46	0
2	GLY	A	1004	-	4,4,4	1.13	1 (25%)	3,4,4	1.72	2 (66%)
5	EDO	B	1013	-	3,3,3	0.45	0	2,2,2	0.23	0
4	PO4	A	1008	-	4,4,4	0.92	0	6,6,6	0.51	0
5	EDO	A	1012	-	3,3,3	0.37	0	2,2,2	0.25	0
5	EDO	A	1013	-	3,3,3	0.46	0	2,2,2	0.27	0
3	BCT	A	1005	-	3,3,3	0.51	0	2,3,3	0.24	0
4	PO4	B	1005	-	4,4,4	0.94	0	6,6,6	0.69	0
3	BCT	B	1002	-	3,3,3	0.51	0	2,3,3	0.42	0
5	EDO	B	1009	-	3,3,3	0.45	0	2,2,2	0.48	0
2	GLY	B	1001	-	4,4,4	1.14	1 (25%)	3,4,4	1.68	1 (33%)
5	EDO	B	1012	-	3,3,3	0.41	0	2,2,2	0.45	0
5	EDO	A	1015	-	3,3,3	0.42	0	2,2,2	0.39	0
5	EDO	A	1011	-	3,3,3	0.41	0	2,2,2	0.33	0
6	BCN	A	1017	-	10,10,10	0.75	0	11,11,11	1.09	0
4	PO4	B	1003	-	4,4,4	0.93	0	6,6,6	0.46	0
4	PO4	B	1004	-	4,4,4	0.91	0	6,6,6	0.55	0
5	EDO	B	1007	-	3,3,3	0.32	0	2,2,2	0.76	0
2	GLY	A	1003	-	4,4,4	1.11	1 (25%)	3,4,4	1.68	2 (66%)

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	1002	-	-	2/2/2/2	-
5	EDO	A	1010	-	-	0/1/1/1	-
5	EDO	B	1006	-	-	0/1/1/1	-
5	EDO	B	1014	-	-	1/1/1/1	-
5	EDO	B	1011	-	-	1/1/1/1	-
5	EDO	A	1016	-	-	0/1/1/1	-
2	GLY	A	1001	-	-	2/2/2/2	-
5	EDO	A	1014	-	-	0/1/1/1	-
5	EDO	B	1008	-	-	0/1/1/1	-
5	EDO	B	1010	-	-	0/1/1/1	-
2	GLY	A	1004	-	-	2/2/2/2	-
5	EDO	B	1013	-	-	1/1/1/1	-
5	EDO	A	1012	-	-	0/1/1/1	-
5	EDO	A	1013	-	-	0/1/1/1	-
5	EDO	B	1009	-	-	0/1/1/1	-
2	GLY	B	1001	-	-	2/2/2/2	-
5	EDO	B	1012	-	-	1/1/1/1	-
5	EDO	A	1015	-	-	1/1/1/1	-
5	EDO	A	1011	-	-	0/1/1/1	-
6	BCN	A	1017	-	-	1/10/10/10	-
5	EDO	B	1007	-	-	0/1/1/1	-
2	GLY	A	1003	-	-	2/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GLY	OXT-C	-2.21	1.23	1.30
2	A	1002	GLY	OXT-C	-2.19	1.23	1.30
2	B	1001	GLY	OXT-C	-2.19	1.23	1.30
2	A	1004	GLY	OXT-C	-2.16	1.23	1.30
2	A	1003	GLY	OXT-C	-2.09	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	GLY	OXT-C-O	-2.33	117.34	123.33
2	B	1001	GLY	OXT-C-O	-2.20	117.69	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	GLY	OXT-C-CA	2.10	121.72	113.38
2	A	1003	GLY	OXT-C-CA	2.05	121.55	113.38
2	A	1004	GLY	OXT-C-O	-2.04	118.08	123.33
2	A	1003	GLY	OXT-C-O	-2.01	118.17	123.33

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	GLY	O-C-CA-N
2	A	1003	GLY	OXT-C-CA-N
2	A	1004	GLY	O-C-CA-N
2	A	1004	GLY	OXT-C-CA-N
6	A	1017	BCN	N1-C5-C6-O6
2	A	1001	GLY	OXT-C-CA-N
2	B	1001	GLY	OXT-C-CA-N
2	A	1001	GLY	O-C-CA-N
2	B	1001	GLY	O-C-CA-N
2	A	1002	GLY	OXT-C-CA-N
5	B	1012	EDO	O1-C1-C2-O2
5	A	1015	EDO	O1-C1-C2-O2
2	A	1002	GLY	O-C-CA-N
5	B	1013	EDO	O1-C1-C2-O2
5	B	1011	EDO	O1-C1-C2-O2
5	B	1014	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1006	EDO	2	0
5	B	1011	EDO	2	0
5	A	1014	EDO	1	0
2	A	1004	GLY	1	0
5	B	1013	EDO	2	0
5	A	1013	EDO	1	0
2	B	1001	GLY	1	0
5	B	1012	EDO	1	0
5	A	1011	EDO	3	0
6	A	1017	BCN	7	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	941/983 (95%)	-0.41	11 (1%) 76 79	6, 16, 38, 62	20 (2%)
1	B	941/983 (95%)	-0.29	33 (3%) 47 50	7, 17, 43, 86	17 (1%)
All	All	1882/1966 (95%)	-0.35	44 (2%) 61 65	6, 17, 41, 86	37 (1%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	ALA	7.4
1	B	15	ALA	6.2
1	B	828	ASN	5.5
1	B	646	GLY	5.2
1	B	644	GLY	4.9
1	B	349	THR	4.5
1	B	18	VAL	4.0
1	B	16	ILE	3.8
1	A	16	ILE	3.7
1	B	767	ASP	3.7
1	B	185	LYS	3.6
1	A	969	HIS	3.6
1	B	478	LYS	3.6
1	A	977	MET	3.5
1	A	338	THR	3.4
1	A	755	THR	3.4
1	A	18	VAL	3.3
1	B	14	GLU	3.1
1	B	977	MET	3.1
1	A	17	ALA	3.1
1	B	134	TYR	3.0
1	B	829	ASN	2.8
1	B	969	HIS	2.7
1	B	968	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	643	ASP	2.6
1	B	337	GLN	2.6
1	B	642	CYS	2.4
1	A	134	TYR	2.3
1	B	645	GLU	2.3
1	B	309	ALA	2.3
1	B	327	HIS	2.3
1	A	478	LYS	2.3
1	B	17	ALA	2.3
1	B	313	ARG	2.2
1	B	326	ALA	2.2
1	B	827	GLY	2.2
1	B	469	THR	2.2
1	B	964	THR	2.2
1	B	336	LEU	2.2
1	B	845	LYS	2.1
1	B	975	GLU	2.0
1	B	825	PHE	2.0
1	A	469	THR	2.0
1	B	479	THR	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	0.96	0.07	10,19,24,25	9
1	LLP	A	726	24/25	0.97	0.07	7,17,24,27	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($\text{\AA}^2$)	Q<0.9
5	EDO	B	1011	4/4	0.70	0.20	20,23,27,27	4
5	EDO	B	1008	4/4	0.71	0.23	19,22,26,34	4
6	BCN	A	1017	11/11	0.73	0.26	32,45,64,67	11
5	EDO	A	1013	4/4	0.76	0.22	49,50,54,60	0
5	EDO	B	1013	4/4	0.77	0.22	40,45,51,52	0
2	GLY	A	1002	5/5	0.78	0.17	44,47,48,51	0
2	GLY	A	1003	5/5	0.80	0.20	35,36,41,43	5
5	EDO	B	1010	4/4	0.82	0.17	42,43,47,51	0
5	EDO	B	1014	4/4	0.83	0.17	40,42,43,47	0
2	GLY	B	1001	5/5	0.83	0.18	44,51,60,61	0
4	PO4	B	1005	5/5	0.84	0.14	23,29,38,43	5
5	EDO	A	1014	4/4	0.84	0.17	34,40,43,43	0
2	GLY	A	1004	5/5	0.85	0.16	53,56,58,61	0
5	EDO	A	1012	4/4	0.86	0.18	34,37,42,42	0
2	GLY	A	1001	5/5	0.87	0.17	31,35,51,52	0
5	EDO	A	1015	4/4	0.87	0.13	25,32,32,34	4
3	BCT	A	1006	4/4	0.89	0.13	40,41,44,50	4
5	EDO	A	1011	4/4	0.89	0.15	19,21,29,33	4
5	EDO	B	1006	4/4	0.90	0.18	29,34,41,56	0
4	PO4	A	1009	5/5	0.90	0.12	16,19,31,37	5
5	EDO	B	1012	4/4	0.90	0.17	10,11,21,25	4
3	BCT	B	1002	4/4	0.91	0.12	18,35,37,40	4
5	EDO	A	1016	4/4	0.91	0.10	21,23,37,40	2
5	EDO	B	1009	4/4	0.91	0.13	25,27,32,32	0
4	PO4	A	1008	5/5	0.92	0.10	24,27,32,35	5
3	BCT	A	1005	4/4	0.92	0.10	16,30,32,32	4
4	PO4	B	1003	5/5	0.92	0.11	25,45,47,51	0
4	PO4	B	1004	5/5	0.92	0.09	22,23,29,29	5
4	PO4	A	1007	5/5	0.92	0.12	14,32,39,41	5
5	EDO	A	1010	4/4	0.93	0.12	26,26,27,35	0
5	EDO	B	1007	4/4	0.94	0.13	16,36,38,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.