



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:19 AM UTC

PDB ID : 2DGK / pdb_00002dgk
Title : Crystal structure of an N-terminal deletion mutant of Escherichia coli GadB in an autoinhibited state (aldamine)
Authors : Gruetter, M.G.; Capitani, G.; Gut, H.
Deposited on : 2006-03-14
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

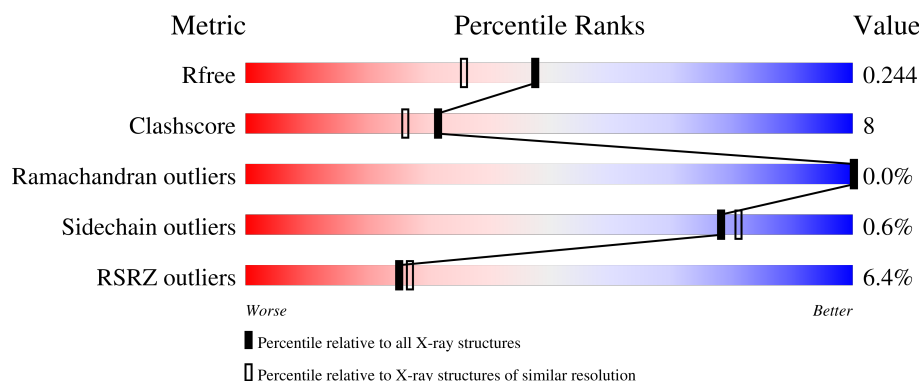
1 Overall quality at a glance

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	452	5% 79% 17% .
1	B	452	4% 76% 20% ..
1	C	452	4% 79% 18% .
1	D	452	5% 80% 17% .
1	E	452	12% 76% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	452	8% 79% 17% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22818 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 Glutamate decarboxylase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	2	0
			3497	2236	596	640	25			
1	B	438	Total	C	N	O	S	0	3	0
			3497	2234	596	642	25			
1	C	437	Total	C	N	O	S	0	1	0
			3485	2227	595	638	25			
1	D	438	Total	C	N	O	S	0	2	0
			3497	2236	596	640	25			
1	E	438	Total	C	N	O	S	0	3	0
			3499	2236	596	642	25			
1	F	438	Total	C	N	O	S	0	2	0
			3494	2231	597	641	25			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP P69910
A	?	-	ASP	deletion	UNP P69910
A	?	-	LYS	deletion	UNP P69910
A	?	-	LYS	deletion	UNP P69910
A	?	-	GLN	deletion	UNP P69910
A	?	-	VAL	deletion	UNP P69910
A	?	-	THR	deletion	UNP P69910
A	?	-	ASP	deletion	UNP P69910
A	?	-	LEU	deletion	UNP P69910
A	?	-	ARG	deletion	UNP P69910
A	?	-	SER	deletion	UNP P69910
A	?	-	GLU	deletion	UNP P69910
A	?	-	LEU	deletion	UNP P69910
A	?	-	LEU	deletion	UNP P69910
B	?	-	MET	deletion	UNP P69910
B	?	-	ASP	deletion	UNP P69910
B	?	-	LYS	deletion	UNP P69910

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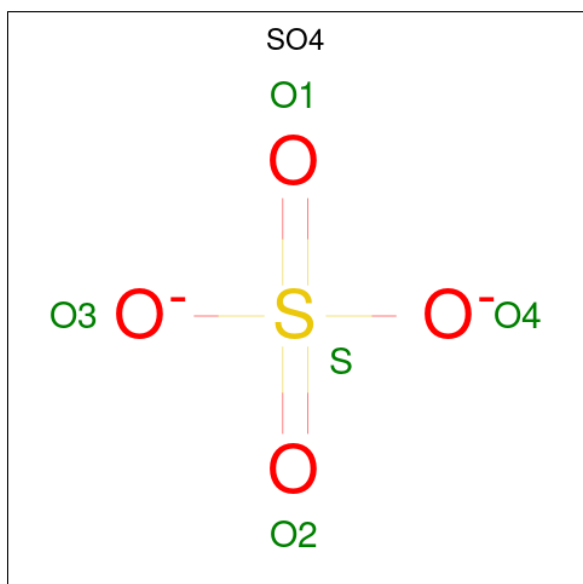
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP P69910
B	?	-	GLN	deletion	UNP P69910
B	?	-	VAL	deletion	UNP P69910
B	?	-	THR	deletion	UNP P69910
B	?	-	ASP	deletion	UNP P69910
B	?	-	LEU	deletion	UNP P69910
B	?	-	ARG	deletion	UNP P69910
B	?	-	SER	deletion	UNP P69910
B	?	-	GLU	deletion	UNP P69910
B	?	-	LEU	deletion	UNP P69910
B	?	-	LEU	deletion	UNP P69910
C	?	-	MET	deletion	UNP P69910
C	?	-	ASP	deletion	UNP P69910
C	?	-	LYS	deletion	UNP P69910
C	?	-	LYS	deletion	UNP P69910
C	?	-	GLN	deletion	UNP P69910
C	?	-	VAL	deletion	UNP P69910
C	?	-	THR	deletion	UNP P69910
C	?	-	ASP	deletion	UNP P69910
C	?	-	LEU	deletion	UNP P69910
C	?	-	ARG	deletion	UNP P69910
C	?	-	SER	deletion	UNP P69910
C	?	-	GLU	deletion	UNP P69910
C	?	-	LEU	deletion	UNP P69910
C	?	-	LEU	deletion	UNP P69910
D	?	-	MET	deletion	UNP P69910
D	?	-	ASP	deletion	UNP P69910
D	?	-	LYS	deletion	UNP P69910
D	?	-	LYS	deletion	UNP P69910
D	?	-	GLN	deletion	UNP P69910
D	?	-	VAL	deletion	UNP P69910
D	?	-	THR	deletion	UNP P69910
D	?	-	ASP	deletion	UNP P69910
D	?	-	LEU	deletion	UNP P69910
D	?	-	ARG	deletion	UNP P69910
D	?	-	SER	deletion	UNP P69910
D	?	-	GLU	deletion	UNP P69910
D	?	-	LEU	deletion	UNP P69910
D	?	-	LEU	deletion	UNP P69910
E	?	-	MET	deletion	UNP P69910
E	?	-	ASP	deletion	UNP P69910
E	?	-	LYS	deletion	UNP P69910

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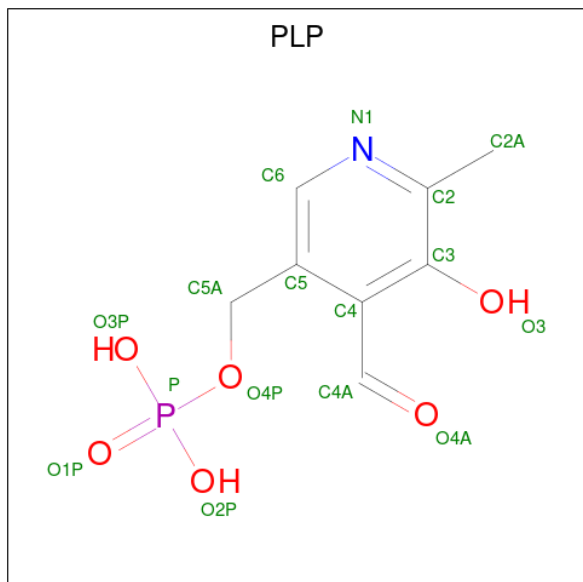
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LYS	deletion	UNP P69910
E	?	-	GLN	deletion	UNP P69910
E	?	-	VAL	deletion	UNP P69910
E	?	-	THR	deletion	UNP P69910
E	?	-	ASP	deletion	UNP P69910
E	?	-	LEU	deletion	UNP P69910
E	?	-	ARG	deletion	UNP P69910
E	?	-	SER	deletion	UNP P69910
E	?	-	GLU	deletion	UNP P69910
E	?	-	LEU	deletion	UNP P69910
E	?	-	LEU	deletion	UNP P69910
F	?	-	MET	deletion	UNP P69910
F	?	-	ASP	deletion	UNP P69910
F	?	-	LYS	deletion	UNP P69910
F	?	-	LYS	deletion	UNP P69910
F	?	-	GLN	deletion	UNP P69910
F	?	-	VAL	deletion	UNP P69910
F	?	-	THR	deletion	UNP P69910
F	?	-	ASP	deletion	UNP P69910
F	?	-	LEU	deletion	UNP P69910
F	?	-	ARG	deletion	UNP P69910
F	?	-	SER	deletion	UNP P69910
F	?	-	GLU	deletion	UNP P69910
F	?	-	LEU	deletion	UNP P69910
F	?	-	LEU	deletion	UNP P69910

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



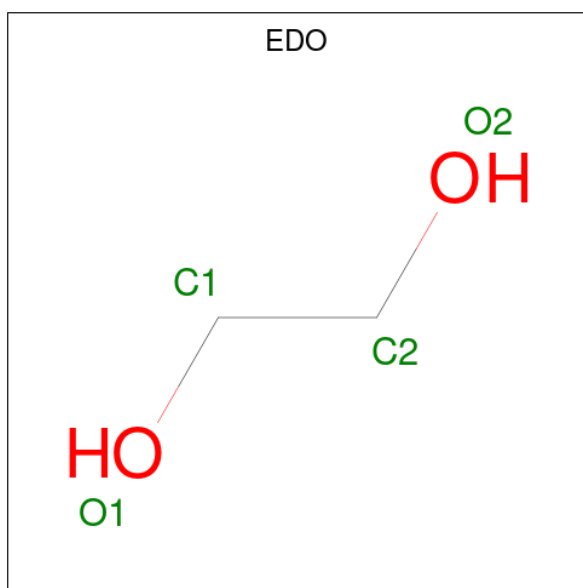
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 15 8 1 5 1	0	0
3	B	1	Total C N O P 15 8 1 5 1	0	0
3	C	1	Total C N O P 15 8 1 5 1	0	0
3	D	1	Total C N O P 15 8 1 5 1	0	0
3	E	1	Total C N O P 15 8 1 5 1	0	0
3	F	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	1
			5	2	3		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	1
			5	2	3		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	267	Total	O	0	0
			267	267		
5	B	301	Total	O	0	0
			301	301		
5	C	327	Total	O	0	0
			327	327		

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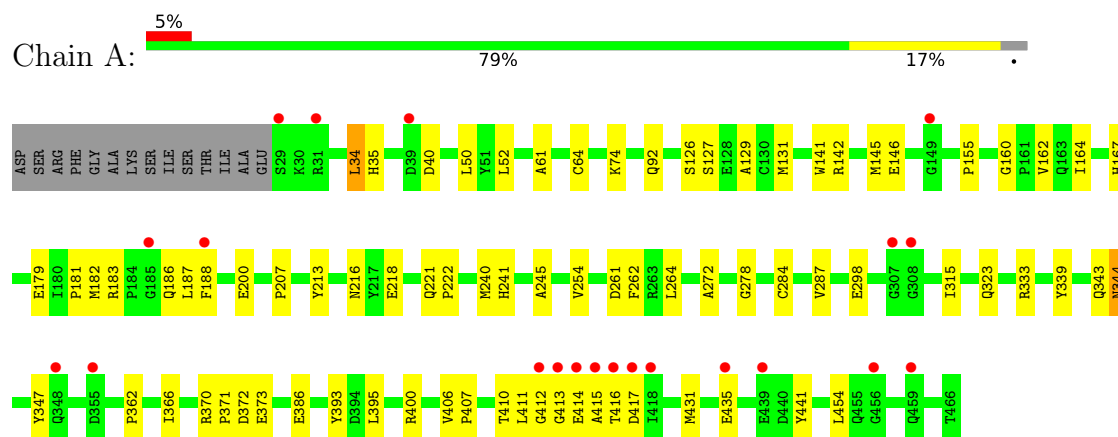
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	311	Total 311	O 311	0	0
5	E	231	Total 231	O 231	0	0
5	F	258	Total 258	O 258	0	0

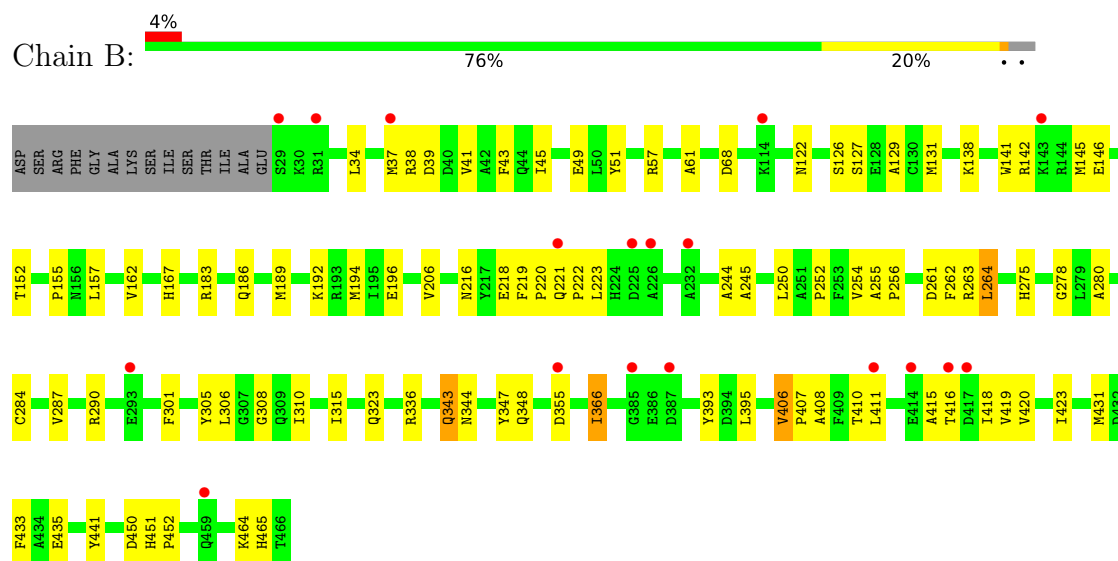
3 Residue-property plots [i](#)

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: Glutamate decarboxylase beta

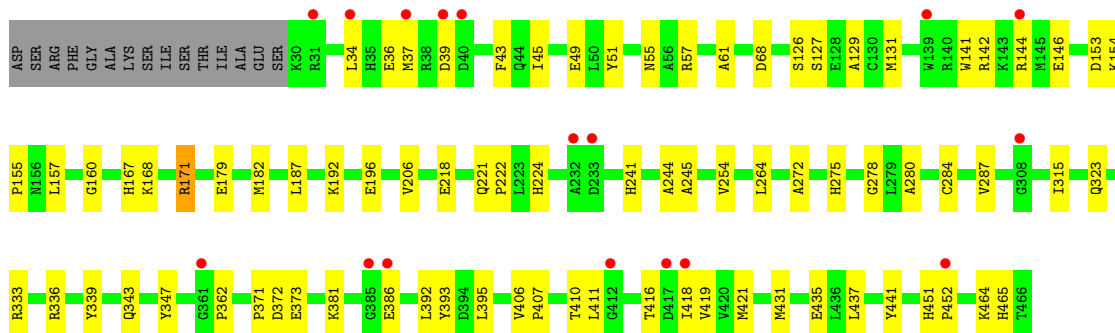


• Molecule 1: Glutamate decarboxylase beta

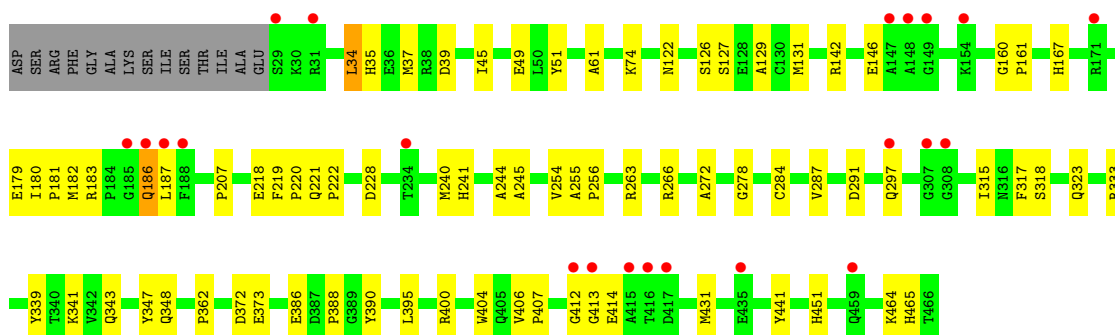
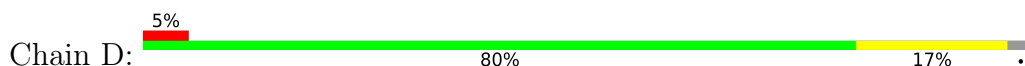


• Molecule 1: Glutamate decarboxylase beta

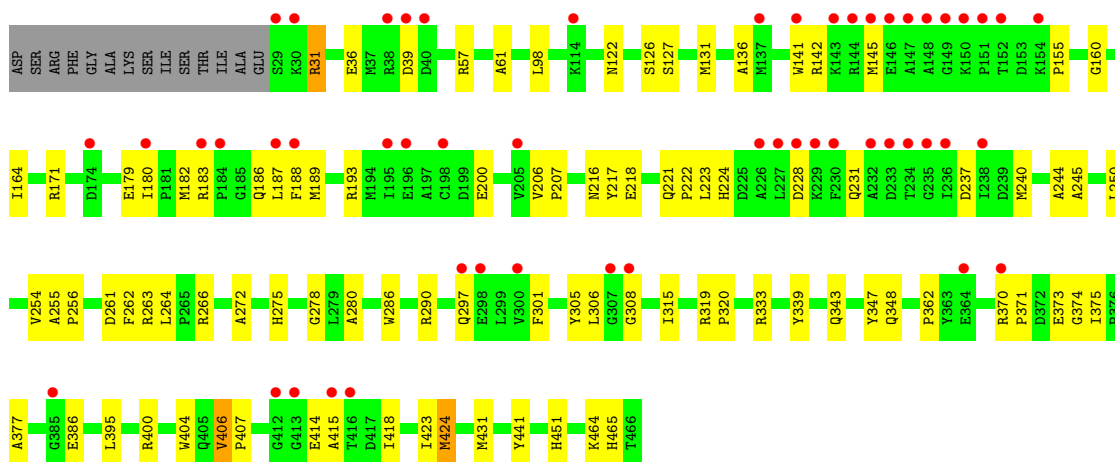
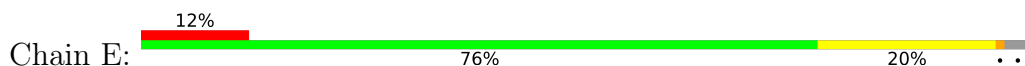




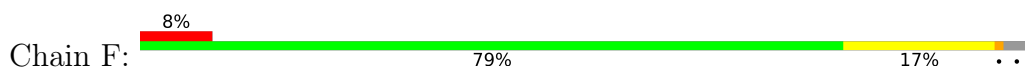
• Molecule 1: Glutamate decarboxylase beta

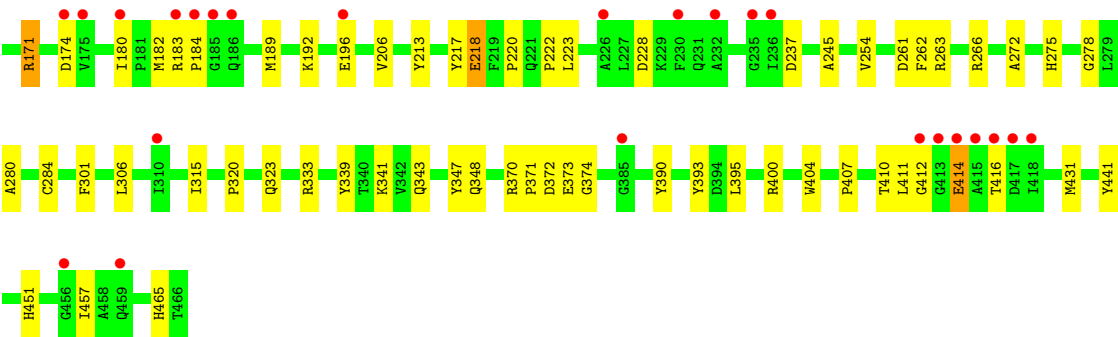


• Molecule 1: Glutamate decarboxylase beta



• Molecule 1: Glutamate decarboxylase beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.77Å 158.56Å 201.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.90) 98.9 (30.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 1.91Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.246 0.217 , 0.244	Depositor DCC
R_{free} test set	2308 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22818	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0904e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PLP, 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	0.37	0/3601	0.88	10/4881 (0.2%)
1	B	0.38	0/3605	0.89	11/4887 (0.2%)
1	C	0.38	0/3583	0.88	5/4857 (0.1%)
1	D	0.38	0/3601	0.87	9/4881 (0.2%)
1	E	0.36	0/3610	0.87	9/4893 (0.2%)
1	F	0.35	0/3598	0.88	9/4878 (0.2%)
All	All	0.37	0/21598	0.88	53/29277 (0.2%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	GLU	N-CA-C	-7.48	96.54	108.73
1	D	218	GLU	N-CA-C	-7.46	96.57	108.73
1	F	218	GLU	N-CA-C	-6.80	96.57	108.20
1	A	278	GLY	N-CA-C	-6.60	106.67	115.32
1	A	218	GLU	N-CA-C	-6.60	96.92	108.20
1	D	278	GLY	N-CA-C	-6.53	106.77	115.32
1	C	218	GLU	N-CA-C	-6.48	97.12	108.20
1	B	406	VAL	N-CA-C	-6.45	101.77	108.15
1	F	278	GLY	N-CA-C	-6.38	107.65	114.67
1	E	278	GLY	N-CA-C	-6.17	107.23	115.32
1	E	206	VAL	N-CA-C	6.11	114.20	108.15
1	A	213	TYR	N-CA-C	5.96	117.78	111.28
1	B	433	PHE	N-CA-C	-5.90	104.93	111.36
1	A	167	HIS	N-CA-C	-5.87	104.97	111.36
1	B	278	GLY	N-CA-C	-5.85	108.23	114.67
1	E	218	GLU	N-CA-C	-5.81	98.27	108.20
1	C	406	VAL	N-CA-C	-5.79	102.41	108.15
1	F	213	TYR	N-CA-C	5.79	117.59	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	406	VAL	N-CA-C	-5.77	102.44	108.15
1	E	406	VAL	N-CA-C	-5.67	102.54	108.15
1	F	451	HIS	CA-C-N	5.63	126.00	119.47
1	F	451	HIS	C-N-CA	5.63	126.00	119.47
1	D	167	HIS	N-CA-C	-5.63	105.23	111.36
1	C	167	HIS	N-CA-C	-5.49	105.38	111.36
1	E	263	ARG	N-CA-C	-5.47	105.86	112.54
1	B	264	LEU	CA-C-N	5.44	124.90	119.24
1	B	264	LEU	C-N-CA	5.44	124.90	119.24
1	E	406	VAL	CA-C-N	5.42	125.68	119.83
1	E	406	VAL	C-N-CA	5.42	125.68	119.83
1	F	457	ILE	N-CA-C	5.40	115.61	110.53
1	D	451	HIS	CA-C-N	5.39	125.72	119.47
1	D	451	HIS	C-N-CA	5.39	125.72	119.47
1	F	263	ARG	N-CA-C	-5.34	105.86	112.38
1	A	241	HIS	N-CA-C	-5.33	99.60	108.34
1	B	263	ARG	N-CA-C	-5.32	105.89	112.38
1	C	278	GLY	N-CA-C	-5.30	108.37	115.32
1	D	122	ASN	N-CA-C	-5.27	102.67	110.48
1	A	162	VAL	N-CA-C	5.23	116.12	110.21
1	B	366	ILE	N-CA-C	-5.22	107.67	111.90
1	A	64	CYS	N-CA-C	5.18	117.81	110.50
1	A	264	LEU	CA-C-N	5.16	124.61	119.24
1	A	264	LEU	C-N-CA	5.16	124.61	119.24
1	D	241	HIS	N-CA-C	-5.16	99.88	108.34
1	E	451	HIS	CA-C-N	5.16	125.45	119.47
1	E	451	HIS	C-N-CA	5.16	125.45	119.47
1	F	206	VAL	N-CA-C	5.13	113.23	108.15
1	C	241	HIS	N-CA-C	-5.12	99.95	108.34
1	B	162	VAL	N-CA-C	5.09	115.96	110.21
1	B	122	ASN	N-CA-C	-5.07	102.98	110.48
1	D	263	ARG	N-CA-C	-5.07	106.20	112.38
1	B	167	HIS	N-CA-C	-5.04	105.86	111.36
1	F	62	THR	N-CA-C	5.04	117.94	110.48
1	A	406	VAL	N-CA-C	-5.01	103.19	108.15

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	3497	0	3394	56	0
1	B	3497	0	3396	65	0
1	C	3485	0	3385	62	0
1	D	3497	0	3395	56	0
1	E	3499	0	3388	76	0
1	F	3494	0	3389	64	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	15	0	6	1	0
3	B	15	0	6	1	0
3	C	15	0	6	1	0
3	D	15	0	6	1	0
3	E	15	0	6	1	0
3	F	15	0	6	1	0
4	A	4	0	6	0	0
4	B	9	0	12	0	0
4	C	9	0	12	0	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	A	267	0	0	2	0
5	B	301	0	0	3	0
5	C	327	0	0	1	0
5	D	311	0	0	3	0
5	E	231	0	0	5	0
5	F	258	0	0	5	0
All	All	22818	0	20431	335	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 8.

All (335) 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:B:250:LEU:HD23	1:B:343:GLN:HG3	1.56	0.86
1:A:362:PRO:HB2	1:A:386:GLU:HG2	1.60	0.83
1:C:221:GLN:HB3	1:C:222:PRO:HD3	1.61	0.83
1:D:362:PRO:HB2	1:D:386:GLU:HG2	1.59	0.83
1:E:348:GLN:HE21	1:E:431:MET:HE3	1.42	0.83
1:E:183:ARG:HG2	1:E:414:GLU:HB2	1.61	0.82
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.59	0.82
1:A:333:ARG:HD3	1:B:39:ASP:HA	1.63	0.81
1:C:333:ARG:HD3	1:D:39:ASP:HA	1.63	0.81
1:E:145:MET:HE1	1:E:200:GLU:HG2	1.64	0.80
1:A:182:MET:HE2	1:A:187:LEU:HB3	1.65	0.79
1:A:221:GLN:HB3	1:A:222:PRO:HD3	1.64	0.79
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.63	0.79
1:E:362:PRO:HB2	1:E:386:GLU:HG2	1.63	0.79
1:E:127:SER:O	1:E:131[B]:MET:HG3	1.83	0.78
1:C:127:SER:O	1:C:131[B]:MET:HG2	1.83	0.77
1:E:127:SER:O	1:E:131[A]:MET:HG2	1.84	0.77
1:C:39:ASP:HA	1:D:333:ARG:HD3	1.67	0.76
1:E:375:ILE:HD11	1:E:424:MET:HE1	1.68	0.74
1:C:362:PRO:HB2	1:C:386:GLU:HG2	1.69	0.74
1:B:127:SER:O	1:B:131[B]:MET:HG2	1.86	0.74
1:F:127:SER:O	1:F:131[B]:MET:HG2	1.89	0.72
1:E:182:MET:HE2	1:E:187:LEU:HB3	1.72	0.71
1:E:228:ASP:HA	1:E:266:ARG:HH21	1.55	0.71
1:A:127:SER:O	1:A:131[B]:MET:HG2	1.92	0.70
1:F:182:MET:HE3	1:F:412:GLY:H	1.57	0.68
1:D:182:MET:H	1:D:413:GLY:HA3	1.61	0.66
1:A:181:PRO:HB2	1:A:414:GLU:HG3	1.76	0.66
1:C:410:THR:HG22	1:C:419:VAL:HG22	1.78	0.66
1:D:142:ARG:O	1:D:146:GLU:HG3	1.95	0.65
1:B:410:THR:HG22	1:B:419:VAL:HG22	1.78	0.65
1:A:362:PRO:CB	1:A:386:GLU:HG2	2.26	0.65
1:C:142:ARG:O	1:C:146:GLU:HG3	1.97	0.65
1:A:145:MET:HE1	1:A:200:GLU:HG2	1.77	0.65
1:C:182:MET:HE2	1:C:187:LEU:HB3	1.78	0.65
1:F:171:ARG:HH11	1:F:171:ARG:HB2	1.63	0.64
1:A:431:MET:O	1:A:435:GLU:HG2	1.98	0.64
1:E:375:ILE:CD1	1:E:424:MET:HE1	2.27	0.63
1:A:61:ALA:HB2	1:A:407:PRO:HD3	1.80	0.63
1:F:348:GLN:HG2	1:F:431:MET:HE1	1.80	0.63
1:C:315:ILE:HG23	1:D:131[A]:MET:SD	2.39	0.63
1:D:127:SER:O	1:D:131[B]:MET:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:348:GLN:HE21	1:E:431:MET:CE	2.11	0.62
1:F:182:MET:CE	1:F:412:GLY:H	2.13	0.61
1:F:370:ARG:HD3	1:F:373:GLU:OE2	2.00	0.61
1:C:154:LYS:N	1:C:155:PRO:HD3	2.16	0.61
1:F:348:GLN:HE21	1:F:431:MET:HE2	1.66	0.60
1:C:171:ARG:HH11	1:C:171:ARG:HB2	1.67	0.60
1:D:362:PRO:CB	1:D:386:GLU:HG2	2.32	0.60
1:A:142:ARG:O	1:A:146:GLU:HG3	2.02	0.59
1:C:381:LYS:HE3	1:C:418:ILE:HD12	1.84	0.59
1:E:31:ARG:HB3	1:E:31:ARG:NH1	2.18	0.59
1:C:61:ALA:HB2	1:C:407:PRO:HD3	1.85	0.59
1:F:61:ALA:HB2	1:F:407:PRO:HD3	1.84	0.59
1:C:411:LEU:O	1:C:416:THR:HA	2.03	0.59
1:A:141:TRP:CZ3	1:A:155:PRO:HB3	2.38	0.58
1:F:339:TYR:O	1:F:343:GLN:HG2	2.03	0.58
1:A:216:ASN:HD21	1:A:366:ILE:HG22	1.68	0.58
1:B:57:ARG:NH2	1:B:68:ASP:OD2	2.36	0.58
1:A:415:ALA:C	1:A:417:ASP:H	2.11	0.58
1:B:250:LEU:HD23	1:B:343:GLN:CG	2.31	0.58
1:E:333:ARG:NE	1:F:39:ASP:OD1	2.35	0.58
1:D:339:TYR:O	1:D:343:GLN:HG2	2.02	0.57
1:E:31:ARG:HB3	1:E:31:ARG:HH11	1.69	0.57
1:C:171:ARG:HB2	1:C:171:ARG:NH1	2.19	0.57
1:B:51:TYR:CB	1:C:57:ARG:HG3	2.34	0.57
1:C:144:ARG:HH11	1:C:144:ARG:HB3	1.69	0.57
1:D:207:PRO:HG2	1:D:240:MET:HE2	1.85	0.57
1:E:164:ILE:HD11	1:F:301:PHE:HB3	1.87	0.57
1:C:339:TYR:O	1:C:343:GLN:HG2	2.05	0.57
1:B:250:LEU:CD2	1:B:343:GLN:HG3	2.31	0.57
1:A:372:ASP:OD1	1:A:373:GLU:HG3	2.05	0.57
1:B:142:ARG:O	1:B:146:GLU:HG3	2.05	0.57
1:A:207:PRO:CG	1:A:240:MET:HE2	2.35	0.56
1:C:315:ILE:HG21	1:D:315:ILE:HD13	1.87	0.56
1:E:39:ASP:HA	1:F:333:ARG:HG3	1.86	0.56
1:D:181:PRO:HB3	1:D:414:GLU:HG3	1.88	0.56
1:A:34:LEU:HD12	1:A:35:HIS:CE1	2.41	0.56
1:C:395:LEU:HD21	1:C:441:TYR:CZ	2.40	0.56
1:E:142:ARG:HH22	1:F:174:ASP:CG	2.13	0.56
1:B:395:LEU:HD21	1:B:441:TYR:CZ	2.40	0.56
1:D:254:VAL:HG21	1:D:347:TYR:CE2	2.41	0.56
1:E:126:SER:HB2	3:E:1504:PLP:O4P	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:GLN:NE2	1:E:237:ASP:HB2	2.20	0.55
1:C:57:ARG:NH2	1:C:68:ASP:OD2	2.39	0.55
1:C:141:TRP:CZ3	1:C:155:PRO:HG3	2.40	0.55
1:E:315:ILE:HG21	1:F:315:ILE:HD13	1.88	0.55
1:B:305:TYR:HB2	1:B:308:GLY:O	2.06	0.55
1:D:207:PRO:CG	1:D:240:MET:HE2	2.37	0.55
1:B:57:ARG:HG3	1:C:51:TYR:CB	2.37	0.55
1:C:393:TYR:OH	1:C:410:THR:HG23	2.07	0.55
1:A:131[A]:MET:SD	1:B:315:ILE:HG23	2.47	0.55
1:C:431:MET:O	1:C:435:GLU:HG3	2.07	0.55
1:A:333:ARG:HE	1:B:39:ASP:HB3	1.73	0.54
1:D:388:PRO:HB2	1:D:390:TYR:CE2	2.42	0.54
1:B:157[B]:LEU:HD11	1:B:206:VAL:HG23	1.89	0.54
1:D:372:ASP:OD1	1:D:373:GLU:HG3	2.07	0.54
1:D:61:ALA:HB2	1:D:407:PRO:HD3	1.90	0.54
1:E:415:ALA:HB1	1:E:418:ILE:HD12	1.90	0.54
1:A:339:TYR:O	1:A:343:GLN:HG2	2.07	0.54
1:B:415:ALA:HB1	1:B:418:ILE:HD12	1.89	0.53
1:C:153:ASP:C	1:C:155:PRO:HD3	2.33	0.53
1:E:39:ASP:HB2	5:E:4987:HOH:O	2.08	0.53
1:C:34:LEU:HD23	1:C:34:LEU:C	2.34	0.53
1:F:126:SER:HB2	3:F:1505:PLP:O4P	2.08	0.53
1:E:224:HIS:CD2	1:E:264:LEU:HB3	2.44	0.53
1:E:370:ARG:HD3	1:E:373:GLU:OE2	2.08	0.53
1:A:315:ILE:HG23	1:B:131[A]:MET:SD	2.48	0.52
1:B:264:LEU:O	1:B:290:ARG:NH2	2.42	0.52
1:E:31:ARG:NH1	1:F:106:ASP:OD2	2.42	0.52
1:F:393:TYR:OH	1:F:410:THR:HG23	2.09	0.52
1:A:254:VAL:HG21	1:A:347:TYR:CE2	2.45	0.52
1:D:161:PRO:CB	1:D:182:MET:HE3	2.40	0.52
1:A:74:LYS:HE2	1:B:43:PHE:CZ	2.44	0.52
1:C:157:LEU:HD11	1:C:206:VAL:HG23	1.91	0.52
1:E:301:PHE:HB3	1:F:164:ILE:HD11	1.91	0.51
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.92	0.51
1:E:189:MET:HE3	1:E:223:LEU:HD13	1.91	0.51
1:A:245:ALA:HA	1:A:272:ALA:HA	1.92	0.51
1:E:255:ALA:N	1:E:256:PRO:HD3	2.24	0.51
1:B:275:HIS:HA	1:B:280:ALA:O	2.11	0.51
1:C:131[A]:MET:SD	1:D:315:ILE:HG23	2.51	0.51
1:C:333:ARG:HE	1:D:39:ASP:HB3	1.76	0.51
1:D:228:ASP:HA	1:D:266:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:GLY:O	1:E:179:GLU:HG3	2.11	0.51
1:A:411:LEU:O	1:A:416:THR:HA	2.11	0.51
1:E:362:PRO:CB	1:E:386:GLU:HG2	2.36	0.51
1:F:87:LYS:NZ	5:F:5006:HOH:O	2.43	0.51
1:B:61:ALA:HB2	1:B:407:PRO:HD3	1.93	0.50
1:C:144:ARG:HB3	1:C:144:ARG:NH1	2.25	0.50
1:C:336:ARG:HD2	1:D:34:LEU:HD22	1.92	0.50
1:E:306:LEU:HD21	1:F:400:ARG:NE	2.25	0.50
1:E:315:ILE:HD13	1:F:315:ILE:HG21	1.93	0.50
1:C:192:LYS:O	1:C:196:GLU:HG3	2.12	0.50
1:E:348:GLN:HG2	1:E:431:MET:HE1	1.93	0.50
1:A:182:MET:H	1:A:413:GLY:HA3	1.77	0.50
1:E:145:MET:CE	1:E:200:GLU:HG2	2.39	0.50
1:C:37:MET:O	1:D:333:ARG:HD2	2.12	0.49
1:E:395:LEU:HD21	1:E:441:TYR:CZ	2.46	0.49
1:F:141:TRP:CZ3	1:F:155:PRO:HB3	2.47	0.49
1:B:343:GLN:HA	1:B:343:GLN:OE1	2.12	0.49
1:E:207:PRO:CG	1:E:240:MET:HE2	2.43	0.49
1:E:61:ALA:HB2	1:E:407:PRO:HD3	1.93	0.49
1:E:171:ARG:HH11	1:E:171:ARG:HG2	1.77	0.49
1:E:371:PRO:HD2	5:E:4999:HOH:O	2.13	0.49
1:A:207:PRO:HG2	1:A:240:MET:HE2	1.93	0.49
1:C:372:ASP:OD1	1:C:373:GLU:HG3	2.12	0.49
1:B:344:ASN:O	1:B:348:GLN:HG3	2.12	0.49
1:E:136:ALA:HB3	5:E:4801:HOH:O	2.13	0.49
1:E:188[A]:PHE:CZ	1:E:216:ASN:HB2	2.48	0.49
1:B:38:ARG:HB2	1:B:41:VAL:HG23	1.95	0.49
1:F:411:LEU:O	1:F:416:THR:HA	2.12	0.49
1:F:228:ASP:HA	1:F:266:ARG:HH21	1.78	0.48
1:C:392:LEU:HD13	1:C:421:MET:HB2	1.95	0.48
1:A:315:ILE:O	1:B:131[A]:MET:HE1	2.14	0.48
1:F:254:VAL:HG21	1:F:347:TYR:CE2	2.47	0.48
1:B:192:LYS:O	1:B:196:GLU:HG3	2.14	0.48
1:D:51:TYR:CB	1:E:57:ARG:HG3	2.44	0.48
1:A:284:CYS:HB2	1:A:323:GLN:HB3	1.96	0.48
1:D:464:LYS:HE3	5:D:4990:HOH:O	2.13	0.48
1:C:254:VAL:HG21	1:C:347:TYR:CE2	2.48	0.48
1:A:187:LEU:O	1:A:188[A]:PHE:CD1	2.67	0.48
1:C:34:LEU:HD23	1:C:34:LEU:O	2.13	0.48
1:D:255:ALA:N	1:D:256:PRO:HD3	2.29	0.48
1:E:131[B]:MET:SD	1:F:315:ILE:HG23	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:MET:O	1:B:435:GLU:HG3	2.14	0.47
1:F:348:GLN:NE2	1:F:431:MET:HE2	2.28	0.47
1:A:395:LEU:HD21	1:A:441:TYR:CZ	2.49	0.47
1:E:264:LEU:O	1:E:290:ARG:NH2	2.48	0.47
1:A:216:ASN:ND2	1:A:366:ILE:HG22	2.29	0.47
1:B:411:LEU:O	1:B:416:THR:HA	2.14	0.47
1:A:181:PRO:CB	1:A:414:GLU:HG3	2.42	0.47
1:D:182:MET:HG2	1:D:187:LEU:CD2	2.45	0.47
1:E:339:TYR:O	1:E:343:GLN:HG2	2.15	0.47
1:A:40:ASP:HB2	5:A:4952:HOH:O	2.15	0.47
1:A:415:ALA:C	1:A:417:ASP:N	2.74	0.47
1:B:255:ALA:N	1:B:256:PRO:HD3	2.30	0.46
1:D:400:ARG:HA	1:D:404:TRP:O	2.16	0.46
1:A:371:PRO:HD2	5:A:4916:HOH:O	2.15	0.46
1:D:183:ARG:NH2	1:D:186:GLN:OE1	2.45	0.46
1:D:348:GLN:HG2	1:D:431:MET:HE1	1.96	0.46
1:D:297:GLN:HG2	5:D:4967:HOH:O	2.14	0.46
1:E:186:GLN:HE21	1:E:193:ARG:CZ	2.29	0.46
1:F:465:HIS:CG	1:F:465:HIS:O	2.68	0.46
1:B:138:LYS:HE2	1:B:142:ARG:HH21	1.80	0.46
1:A:126:SER:HB2	3:A:1500:PLP:O4P	2.16	0.46
1:B:465:HIS:O	1:B:465:HIS:CG	2.68	0.46
1:C:129:ALA:HB1	1:C:287:VAL:HB	1.97	0.46
1:C:275:HIS:HA	1:C:280:ALA:O	2.16	0.46
1:D:160:GLY:O	1:D:179:GLU:HG3	2.16	0.46
1:D:245:ALA:HA	1:D:272:ALA:HA	1.97	0.46
1:C:284:CYS:HB2	1:C:323:GLN:HB3	1.98	0.46
1:E:244:ALA:O	1:E:245:ALA:C	2.58	0.46
1:E:306:LEU:HD21	1:F:400:ARG:CZ	2.46	0.46
1:E:36:GLU:OE2	1:F:341:LYS:NZ	2.48	0.46
1:E:141:TRP:CZ3	1:E:155:PRO:HB3	2.50	0.46
1:E:180:ILE:HD12	1:E:180:ILE:N	2.30	0.46
1:E:400:ARG:HA	1:E:404:TRP:O	2.15	0.46
1:E:254:VAL:HG21	1:E:347:TYR:CE2	2.51	0.45
1:E:343:GLN:OE1	1:E:343:GLN:HA	2.16	0.45
1:F:142:ARG:O	1:F:146:GLU:HG3	2.16	0.45
1:D:129:ALA:HB1	1:D:287:VAL:HB	1.97	0.45
1:E:122:ASN:HB2	1:E:286:TRP:CZ3	2.52	0.45
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.51	0.45
1:A:344:ASN:HD22	1:A:344:ASN:HA	1.60	0.45
1:C:43:PHE:CZ	1:D:74:LYS:HE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:372:ASP:OD1	1:F:373:GLU:HG3	2.17	0.45
1:B:216:ASN:HD21	1:B:366:ILE:HG22	1.82	0.45
1:C:55:ASN:O	1:C:57:ARG:NH1	2.50	0.45
1:C:333:ARG:HD3	1:D:39:ASP:CA	2.42	0.45
1:B:284:CYS:HB2	1:B:323:GLN:HB3	1.98	0.45
1:D:395:LEU:HD21	1:D:441:TYR:CZ	2.51	0.45
1:F:171:ARG:HH11	1:F:171:ARG:CB	2.28	0.45
1:A:207:PRO:HG3	1:A:240:MET:HE2	1.98	0.45
1:E:39:ASP:OD1	1:F:333:ARG:NH2	2.50	0.45
1:F:192:LYS:HG2	1:F:196:GLU:OE2	2.17	0.45
1:C:371:PRO:HD2	5:C:4829:HOH:O	2.17	0.44
1:E:217:TYR:CD2	1:E:374:GLY:HA2	2.51	0.44
1:F:371:PRO:HD2	5:F:4931:HOH:O	2.16	0.44
1:C:245:ALA:HA	1:C:272:ALA:HA	2.00	0.44
1:A:92:GLN:HG2	1:B:49:GLU:O	2.18	0.44
1:E:377:ALA:HB2	1:E:424:MET:CE	2.48	0.44
1:F:57:ARG:CZ	1:F:66:THR:O	2.66	0.44
1:C:224:HIS:CD2	1:C:264:LEU:HB3	2.52	0.44
1:A:164:ILE:HD11	1:B:301:PHE:HB3	1.99	0.44
1:D:465:HIS:CG	1:D:465:HIS:O	2.71	0.44
1:A:298:GLU:H	1:A:298:GLU:CD	2.26	0.44
1:B:183:ARG:NH2	1:B:186:GLN:OE1	2.47	0.44
1:F:180:ILE:N	1:F:180:ILE:HD12	2.32	0.44
1:D:284:CYS:HB2	1:D:323:GLN:HB3	1.99	0.44
1:F:189:MET:HE3	1:F:223:LEU:HD13	1.99	0.44
1:B:57:ARG:HG3	1:C:51:TYR:CG	2.53	0.43
1:F:217:TYR:CD2	1:F:374:GLY:HA2	2.53	0.43
1:B:41:VAL:O	1:B:45:ILE:HG13	2.18	0.43
1:B:393:TYR:OH	1:B:410:THR:HG23	2.18	0.43
1:E:261:ASP:HB2	1:E:262:PHE:H	1.62	0.43
1:F:261:ASP:HB2	1:F:262:PHE:H	1.64	0.43
1:A:34:LEU:HD13	1:A:34:LEU:C	2.42	0.43
1:A:400:ARG:NE	1:B:306:LEU:HD21	2.33	0.43
1:C:464:LYS:O	1:C:465:HIS:HB3	2.17	0.43
1:F:142:ARG:HG3	1:F:152:THR:HG21	1.99	0.43
1:F:370:ARG:HD3	1:F:373:GLU:CD	2.43	0.43
1:A:34:LEU:HD13	1:A:34:LEU:O	2.18	0.43
1:B:450:ASP:C	1:B:452:PRO:HD3	2.42	0.43
1:C:333:ARG:HD2	1:D:37:MET:O	2.18	0.43
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.53	0.43
1:B:254:VAL:HG21	1:B:347:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HG3	1:B:186:GLN:O	2.18	0.43
1:B:408:ALA:HA	1:B:420:VAL:O	2.18	0.43
1:C:160:GLY:O	1:C:179:GLU:HG3	2.19	0.43
1:C:465:HIS:O	1:C:465:HIS:CG	2.72	0.43
1:D:291:ASP:HB2	2:D:4773:SO4:O3	2.19	0.43
1:E:400:ARG:NH1	1:F:306:LEU:HD11	2.33	0.43
1:F:183:ARG:NH2	1:F:414:GLU:OE2	2.46	0.43
1:B:126:SER:HB2	3:B:1501:PLP:O4P	2.18	0.43
1:B:310:ILE:HD11	5:B:5052:HOH:O	2.19	0.43
1:C:45:ILE:O	1:C:49:GLU:HG3	2.19	0.43
1:C:244:ALA:O	1:C:245:ALA:C	2.61	0.43
1:E:465:HIS:CG	1:E:465:HIS:O	2.72	0.43
1:C:36:GLU:OE2	1:D:341:LYS:HD3	2.19	0.42
1:D:182:MET:HG2	1:D:187:LEU:HD22	2.01	0.42
1:C:34:LEU:C	1:C:34:LEU:CD2	2.92	0.42
1:C:126:SER:HB2	3:C:1502:PLP:O4P	2.18	0.42
1:F:128:GLU:O	1:F:132:LEU:HG	2.19	0.42
1:B:189:MET:HE3	1:B:223:LEU:HD13	2.01	0.42
1:D:34:LEU:HD12	1:D:35:HIS:CE1	2.53	0.42
1:A:412:GLY:O	1:A:413:GLY:C	2.62	0.42
1:B:145:MET:HB2	1:B:152:THR:HG22	2.02	0.42
1:F:390:TYR:CD1	1:F:390:TYR:C	2.98	0.42
1:A:393:TYR:OH	1:A:410:THR:HG23	2.19	0.42
1:B:244:ALA:O	1:B:245:ALA:C	2.63	0.42
1:E:250:LEU:HD12	1:E:375:ILE:HG22	2.00	0.42
1:F:171:ARG:HH11	1:F:171:ARG:CG	2.33	0.42
1:A:160:GLY:O	1:A:179:GLU:HG3	2.19	0.42
1:A:333:ARG:HD2	1:B:37:MET:O	2.19	0.42
1:A:370:ARG:HA	1:A:371:PRO:HD3	1.92	0.42
1:D:126:SER:HB2	3:D:1503:PLP:O4P	2.20	0.42
1:F:400:ARG:HA	1:F:404:TRP:O	2.20	0.42
1:A:183:ARG:NH2	1:A:186:GLN:OE1	2.53	0.42
1:C:315:ILE:HG21	1:D:315:ILE:CD1	2.50	0.42
1:C:451:HIS:N	1:C:452:PRO:HD3	2.35	0.42
1:D:45:ILE:O	1:D:49:GLU:HG3	2.20	0.42
1:B:194:MET:HE1	1:B:223:LEU:O	2.20	0.42
1:E:250:LEU:CD1	1:E:375:ILE:HG22	2.50	0.42
1:E:464:LYS:O	1:E:465:HIS:HB3	2.20	0.42
1:A:261:ASP:HB2	1:A:262:PHE:H	1.64	0.41
1:D:348:GLN:HG2	1:D:431:MET:CE	2.50	0.41
1:E:406:VAL:HG13	1:E:423:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ARG:HG3	1:F:184:PRO:HD2	2.02	0.41
1:A:129:ALA:HB1	1:A:287:VAL:HB	2.01	0.41
1:E:31:ARG:HH11	1:F:106:ASP:CG	2.27	0.41
1:E:98:LEU:HG	5:E:4984:HOH:O	2.20	0.41
1:E:319:ARG:HB2	1:E:320:PRO:HD2	2.01	0.41
1:F:38:ARG:HG3	5:F:4914:HOH:O	2.19	0.41
1:F:284:CYS:HB2	1:F:323:GLN:HB3	2.02	0.41
1:F:275:HIS:HA	1:F:280:ALA:O	2.21	0.41
1:F:320:PRO:HB2	5:F:4978:HOH:O	2.19	0.41
1:B:406:VAL:HG13	1:B:423:ILE:HG12	2.02	0.41
1:D:362:PRO:HG3	1:D:388:PRO:HG3	2.02	0.41
1:C:168:LYS:HE2	5:D:4986:HOH:O	2.21	0.41
1:D:180:ILE:HA	1:D:181:PRO:HD3	1.92	0.41
1:E:221:GLN:HB3	1:E:222:PRO:CD	2.41	0.41
1:F:245:ALA:HA	1:F:272:ALA:HA	2.03	0.41
1:B:415:ALA:HA	5:B:4941:HOH:O	2.21	0.41
1:D:244:ALA:O	1:D:245:ALA:C	2.64	0.41
1:D:362:PRO:CG	1:D:388:PRO:HG3	2.51	0.41
1:D:412:GLY:O	1:D:413:GLY:C	2.64	0.41
1:B:219:PHE:HA	1:B:220:PRO:HD3	1.90	0.41
1:B:261:ASP:HB2	1:B:262:PHE:H	1.66	0.41
1:D:317:PHE:HB3	1:D:318:SER:H	1.77	0.41
1:F:182:MET:HE3	1:F:412:GLY:N	2.32	0.41
1:F:237:ASP:OD1	1:F:266:ARG:NH1	2.52	0.41
1:B:216:ASN:ND2	1:B:366:ILE:HG22	2.35	0.41
1:B:464:LYS:O	1:B:465:HIS:HB3	2.19	0.41
1:C:362:PRO:CB	1:C:386:GLU:HG2	2.45	0.41
1:E:221:GLN:CB	1:E:222:PRO:HD3	2.42	0.41
1:F:411:LEU:O	1:F:416:THR:HG22	2.21	0.41
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.96	0.40
1:D:219:PHE:HA	1:D:220:PRO:HD3	1.88	0.40
1:E:245:ALA:HA	1:E:272:ALA:HA	2.02	0.40
1:E:333:ARG:HG3	1:F:39:ASP:HA	2.02	0.40
1:B:129:ALA:HB1	1:B:287:VAL:HB	2.03	0.40
1:E:297:GLN:HG2	5:E:4898:HOH:O	2.21	0.40
1:F:218:GLU:O	1:F:220:PRO:HD3	2.22	0.40
1:B:451:HIS:N	1:B:452:PRO:HD3	2.36	0.40
1:F:112:ALA:HA	1:F:113:PRO:HD3	1.85	0.40
1:A:34:LEU:HD22	1:B:336:ARG:HD2	2.03	0.40
1:E:305:TYR:HB2	1:E:308:GLY:O	2.20	0.40
1:A:454:LEU:HD21	5:F:4819:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PRO:HA	5:B:4991:HOH:O	2.22	0.40
1:E:275:HIS:HA	1:E:280:ALA:O	2.21	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	438/452 (97%)	424 (97%)	14 (3%)	0	100	100
1	B	439/452 (97%)	428 (98%)	11 (2%)	0	100	100
1	C	436/452 (96%)	423 (97%)	13 (3%)	0	100	100
1	D	438/452 (97%)	422 (96%)	15 (3%)	1 (0%)	43	36
1	E	439/452 (97%)	420 (96%)	19 (4%)	0	100	100
1	F	438/452 (97%)	427 (98%)	11 (2%)	0	100	100
All	All	2628/2712 (97%)	2544 (97%)	83 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	GLN

5.3.2 Protein sidechains [i](#)

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	367/376 (98%)	364 (99%)	3 (1%)	73	75
1	B	368/376 (98%)	365 (99%)	3 (1%)	73	75
1	C	365/376 (97%)	363 (100%)	2 (0%)	81	84
1	D	367/376 (98%)	366 (100%)	1 (0%)	86	88
1	E	368/376 (98%)	366 (100%)	2 (0%)	81	84
1	F	367/376 (98%)	365 (100%)	2 (0%)	81	84
All	All	2202/2256 (98%)	2189 (99%)	13 (1%)	78	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	52	LEU
1	A	344	ASN
1	B	34	LEU
1	B	343	GLN
1	B	355	ASP
1	C	171	ARG
1	C	437	LEU
1	D	34	LEU
1	E	31	ARG
1	E	424	MET
1	F	171	ARG
1	F	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	65	GLN
1	A	71	ASN
1	A	109	HIS
1	A	216	ASN
1	A	297	GLN
1	A	302	ASN
1	A	309	GLN
1	A	344	ASN
1	A	459	GLN
1	B	47	ASN
1	B	109	HIS

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Mol	Chain	Res	Type
1	B	117	GLN
1	B	201	ASN
1	B	216	ASN
1	B	302	ASN
1	B	309	GLN
1	C	47	ASN
1	C	65	GLN
1	C	109	HIS
1	C	117	GLN
1	C	221	GLN
1	C	309	GLN
1	C	344	ASN
1	D	47	ASN
1	D	221	GLN
1	D	309	GLN
1	D	348	GLN
1	E	35	HIS
1	E	65	GLN
1	E	186	GLN
1	E	309	GLN
1	E	344	ASN
1	E	348	GLN
1	E	455	GLN
1	F	35	HIS
1	F	309	GLN
1	F	344	ASN
1	F	348	GLN
1	F	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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	SO4	C	4772	-	4,4,4	1.06	0	6,6,6	1.31	1 (16%)
3	PLP	D	1503	1	15,15,16	1.01	0	21,22,23	1.25	3 (14%)
2	SO4	E	4774	-	4,4,4	1.08	0	6,6,6	1.31	1 (16%)
3	PLP	E	1504	1	15,15,16	1.07	1 (6%)	21,22,23	1.26	4 (19%)
3	PLP	B	1501	1	15,15,16	0.89	1 (6%)	21,22,23	1.28	3 (14%)
4	EDO	B	2191[B]	-	3,3,3	0.44	0	2,2,2	0.35	0
2	SO4	D	4773	-	4,4,4	1.08	0	6,6,6	1.30	1 (16%)
3	PLP	C	1502	1	15,15,16	0.97	1 (6%)	21,22,23	1.27	4 (19%)
2	SO4	A	4770	-	4,4,4	1.05	0	6,6,6	1.31	1 (16%)
4	EDO	B	2191[A]	-	3,3,3	0.44	0	2,2,2	0.36	0
2	SO4	F	4775	-	4,4,4	1.11	0	6,6,6	1.31	1 (16%)
3	PLP	A	1500	1	15,15,16	1.06	1 (6%)	21,22,23	1.25	3 (14%)
4	EDO	E	2197	-	3,3,3	0.39	0	2,2,2	0.43	0
4	EDO	C	2192[B]	-	3,3,3	0.42	0	2,2,2	0.40	0
3	PLP	F	1505	1	15,15,16	1.21	2 (13%)	21,22,23	1.22	3 (14%)
4	EDO	C	2195	-	3,3,3	0.41	0	2,2,2	0.40	0
4	EDO	A	2193	-	3,3,3	0.40	0	2,2,2	0.40	0
4	EDO	C	2192[A]	-	3,3,3	0.42	0	2,2,2	0.42	0
2	SO4	B	4771	-	4,4,4	1.08	0	6,6,6	1.30	1 (16%)
4	EDO	D	2196	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	F	2198	-	3,3,3	0.38	0	2,2,2	0.43	0
4	EDO	B	2194	-	3,3,3	0.46	0	2,2,2	0.36	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	PLP	B	1501	1	-	0/6/6/8	0/1/1/1
4	EDO	A	2193	-	-	1/1/1/1	-
3	PLP	D	1503	1	-	0/6/6/8	0/1/1/1
3	PLP	A	1500	1	-	0/6/6/8	0/1/1/1
4	EDO	B	2191[A]	-	-	0/1/1/1	-
4	EDO	B	2191[B]	-	-	1/1/1/1	-
4	EDO	C	2192[A]	-	-	1/1/1/1	-
4	EDO	E	2197	-	-	0/1/1/1	-
3	PLP	C	1502	1	-	0/6/6/8	0/1/1/1
4	EDO	D	2196	-	-	0/1/1/1	-
4	EDO	C	2192[B]	-	-	1/1/1/1	-
3	PLP	E	1504	1	-	0/6/6/8	0/1/1/1
4	EDO	F	2198	-	-	1/1/1/1	-
3	PLP	F	1505	1	-	0/6/6/8	0/1/1/1
4	EDO	B	2194	-	-	0/1/1/1	-
4	EDO	C	2195	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1505	PLP	C5-C4	2.56	1.43	1.40
3	C	1502	PLP	C5-C4	2.20	1.43	1.40
3	A	1500	PLP	C5-C4	2.17	1.43	1.40
3	B	1501	PLP	C5-C4	2.04	1.42	1.40
3	F	1505	PLP	C4A-C4	2.02	1.55	1.51
3	E	1504	PLP	C5-C4	2.01	1.42	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4775	SO4	O4-S-O3	2.88	124.40	108.54
2	E	4774	SO4	O4-S-O3	2.87	124.37	108.54
2	C	4772	SO4	O4-S-O3	2.87	124.36	108.54
2	A	4770	SO4	O4-S-O3	2.87	124.36	108.54
2	D	4773	SO4	O4-S-O3	2.87	124.34	108.54
2	B	4771	SO4	O4-S-O3	2.85	124.26	108.54
3	B	1501	PLP	C3-C2-N1	-2.72	117.53	120.96
3	C	1502	PLP	C3-C2-N1	-2.69	117.56	120.96
3	B	1501	PLP	C6-N1-C2	2.68	124.06	119.20
3	A	1500	PLP	C3-C2-N1	-2.67	117.60	120.96
3	C	1502	PLP	C6-N1-C2	2.65	124.01	119.20
3	D	1503	PLP	C3-C2-N1	-2.64	117.63	120.96
3	E	1504	PLP	C3-C2-N1	-2.62	117.66	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1503	PLP	C6-N1-C2	2.59	123.90	119.20
3	E	1504	PLP	C6-N1-C2	2.59	123.89	119.20
3	A	1500	PLP	C6-N1-C2	2.56	123.84	119.20
3	F	1505	PLP	C6-N1-C2	2.56	123.84	119.20
3	F	1505	PLP	C3-C2-N1	-2.49	117.82	120.96
3	A	1500	PLP	C2A-C2-C3	2.48	123.69	120.80
3	E	1504	PLP	C2A-C2-C3	2.45	123.66	120.80
3	D	1503	PLP	C2A-C2-C3	2.40	123.61	120.80
3	C	1502	PLP	C2A-C2-C3	2.28	123.46	120.80
3	B	1501	PLP	C2A-C2-C3	2.26	123.44	120.80
3	F	1505	PLP	C2A-C2-C3	2.25	123.43	120.80
3	E	1504	PLP	O3P-P-O1P	2.03	118.75	110.83
3	C	1502	PLP	O3P-P-O1P	2.03	118.73	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2192[B]	EDO	O1-C1-C2-O2
4	B	2191[B]	EDO	O1-C1-C2-O2
4	C	2192[A]	EDO	O1-C1-C2-O2
4	A	2193	EDO	O1-C1-C2-O2
4	F	2198	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1503	PLP	1	0
3	E	1504	PLP	1	0
3	B	1501	PLP	1	0
2	D	4773	SO4	1	0
3	C	1502	PLP	1	0
3	A	1500	PLP	1	0
3	F	1505	PLP	1	0

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	438/452 (96%)	0.37	21 (4%)	35	38	15, 26, 37, 41	2 (0%)
1	B	438/452 (96%)	0.38	18 (4%)	41	44	14, 26, 37, 42	3 (0%)
1	C	437/452 (96%)	0.37	17 (3%)	43	46	14, 26, 37, 42	1 (0%)
1	D	438/452 (96%)	0.31	22 (5%)	34	36	15, 25, 36, 41	2 (0%)
1	E	438/452 (96%)	0.76	52 (11%)	9	9	17, 29, 47, 52	3 (0%)
1	F	438/452 (96%)	0.63	37 (8%)	17	18	16, 29, 43, 48	2 (0%)
All	All	2627/2712 (96%)	0.47	167 (6%)	25	27	14, 27, 40, 52	13 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	GLY	5.4
1	E	148	ALA	4.8
1	E	235	GLY	4.8
1	A	416	THR	4.5
1	E	416	THR	4.5
1	E	147	ALA	4.5
1	F	153	ASP	4.2
1	D	412	GLY	4.1
1	C	233	ASP	4.1
1	E	188[A]	PHE	4.0
1	F	412	GLY	4.0
1	E	236	ILE	4.0
1	F	29	SER	4.0
1	D	416	THR	3.9
1	F	385	GLY	3.9
1	A	415	ALA	3.8
1	E	149	GLY	3.7
1	F	417	ASP	3.7
1	F	144	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	417	ASP	3.6
1	E	412	GLY	3.6
1	E	230	PHE	3.5
1	D	147	ALA	3.5
1	D	415	ALA	3.4
1	E	145	MET	3.4
1	F	148	ALA	3.3
1	F	415	ALA	3.3
1	C	232	ALA	3.2
1	E	198	CYS	3.2
1	F	416	THR	3.1
1	F	413	GLY	3.1
1	A	417	ASP	3.1
1	A	188[A]	PHE	3.1
1	E	183	ARG	3.1
1	E	184	PRO	3.0
1	F	147	ALA	3.0
1	B	31	ARG	3.0
1	E	229	LYS	3.0
1	A	412	GLY	3.0
1	F	459	GLN	2.9
1	D	31	ARG	2.9
1	B	29	SER	2.9
1	F	310	ILE	2.9
1	E	234	THR	2.9
1	E	232	ALA	2.9
1	E	238	ILE	2.9
1	A	308	GLY	2.9
1	F	183	ARG	2.8
1	F	414	GLU	2.8
1	E	152	THR	2.8
1	A	149	GLY	2.7
1	C	361	GLY	2.7
1	E	39	ASP	2.7
1	E	114	LYS	2.7
1	F	230	PHE	2.7
1	E	151	PRO	2.7
1	B	416	THR	2.7
1	E	29	SER	2.7
1	A	418	ILE	2.7
1	F	232	ALA	2.6
1	F	235	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	221	GLN	2.6
1	C	34	LEU	2.6
1	A	413	GLY	2.6
1	B	143	LYS	2.6
1	A	355	ASP	2.5
1	C	417	ASP	2.5
1	C	385	GLY	2.5
1	A	29	SER	2.5
1	B	459	GLN	2.5
1	B	355	ASP	2.5
1	E	144	ARG	2.5
1	F	196	GLU	2.5
1	B	387	ASP	2.5
1	E	195	ILE	2.5
1	D	459	GLN	2.5
1	E	40	ASP	2.5
1	E	196	GLU	2.4
1	D	29	SER	2.4
1	E	226	ALA	2.4
1	B	385	GLY	2.4
1	F	149	GLY	2.4
1	E	297	GLN	2.4
1	D	308	GLY	2.4
1	A	39	ASP	2.4
1	D	148	ALA	2.4
1	C	308	GLY	2.4
1	E	233	ASP	2.3
1	A	31	ARG	2.3
1	D	188[A]	PHE	2.3
1	E	146	GLU	2.3
1	C	418	ILE	2.3
1	E	415	ALA	2.3
1	F	226	ALA	2.3
1	E	137	MET	2.3
1	E	413	GLY	2.3
1	B	417	ASP	2.3
1	F	40	ASP	2.3
1	E	141	TRP	2.3
1	B	293	GLU	2.3
1	E	187	LEU	2.3
1	F	456	GLY	2.3
1	C	139	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	141	TRP	2.3
1	B	225	ASP	2.3
1	C	40	ASP	2.3
1	A	348	GLN	2.3
1	C	37	MET	2.3
1	E	30	LYS	2.3
1	E	227	LEU	2.3
1	F	139	TRP	2.2
1	A	439	GLU	2.2
1	B	232	ALA	2.2
1	D	185	GLY	2.2
1	E	307	GLY	2.2
1	F	39	ASP	2.2
1	F	236	ILE	2.2
1	D	297	GLN	2.2
1	A	435	GLU	2.2
1	A	307	GLY	2.2
1	E	308	GLY	2.2
1	E	228	ASP	2.2
1	F	145	MET	2.2
1	C	144	ARG	2.2
1	A	414	GLU	2.2
1	D	435	GLU	2.2
1	B	37	MET	2.2
1	E	150	LYS	2.2
1	B	414	GLU	2.2
1	E	298	GLU	2.2
1	D	186	GLN	2.2
1	D	234	THR	2.2
1	D	413	GLY	2.2
1	F	184	PRO	2.2
1	D	154	LYS	2.2
1	E	364	GLU	2.1
1	E	180	ILE	2.1
1	F	186	GLN	2.1
1	E	174	ASP	2.1
1	B	411	LEU	2.1
1	B	114	LYS	2.1
1	F	180	ILE	2.1
1	F	418	ILE	2.1
1	F	174	ASP	2.1
1	E	143	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	386	GLU	2.1
1	C	452	PRO	2.1
1	C	39	ASP	2.1
1	C	31	ARG	2.1
1	F	114	LYS	2.1
1	A	185	GLY	2.1
1	A	456	GLY	2.1
1	E	300	VAL	2.1
1	F	175	VAL	2.1
1	D	187	LEU	2.1
1	B	226	ALA	2.1
1	D	171	ARG	2.1
1	E	370	ARG	2.1
1	E	154	LYS	2.0
1	C	412	GLY	2.0
1	E	385	GLY	2.0
1	F	185	GLY	2.0
1	E	38	ARG	2.0
1	F	146	GLU	2.0
1	A	459	GLN	2.0
1	D	307	GLY	2.0
1	E	205	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	EDO	B	2191[A]	4/4	0.71	0.17	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	2191[B]	4/4	0.71	0.17	47,47,47,47	1
4	EDO	C	2192[A]	4/4	0.73	0.18	47,47,47,47	1
4	EDO	C	2192[B]	4/4	0.73	0.18	47,47,47,47	1
2	SO4	F	4775	5/5	0.79	0.15	52,52,52,52	5
4	EDO	E	2197	4/4	0.83	0.13	38,38,38,39	0
2	SO4	A	4770	5/5	0.86	0.20	37,37,37,37	5
4	EDO	A	2193	4/4	0.88	0.10	32,33,33,33	0
4	EDO	F	2198	4/4	0.88	0.10	32,32,32,33	0
2	SO4	B	4771	5/5	0.89	0.14	50,50,50,50	0
2	SO4	C	4772	5/5	0.90	0.14	38,38,38,38	5
2	SO4	E	4774	5/5	0.91	0.12	53,53,53,53	5
4	EDO	C	2195	4/4	0.91	0.09	29,30,30,30	0
2	SO4	D	4773	5/5	0.93	0.17	31,31,31,31	5
4	EDO	D	2196	4/4	0.93	0.10	33,33,33,33	0
3	PLP	F	1505	15/16	0.95	0.10	22,23,24,24	0
3	PLP	B	1501	15/16	0.95	0.08	19,20,21,22	0
3	PLP	C	1502	15/16	0.96	0.07	18,20,21,21	0
3	PLP	E	1504	15/16	0.96	0.08	22,22,22,22	0
4	EDO	B	2194	4/4	0.96	0.05	27,27,27,27	0
3	PLP	A	1500	15/16	0.97	0.06	19,20,21,21	0
3	PLP	D	1503	15/16	0.97	0.06	17,18,19,19	0

6.5 Other polymers

There are no such residues in this entry.