Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 05:08 PM EDT

PDB ID	:	2DGK
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:

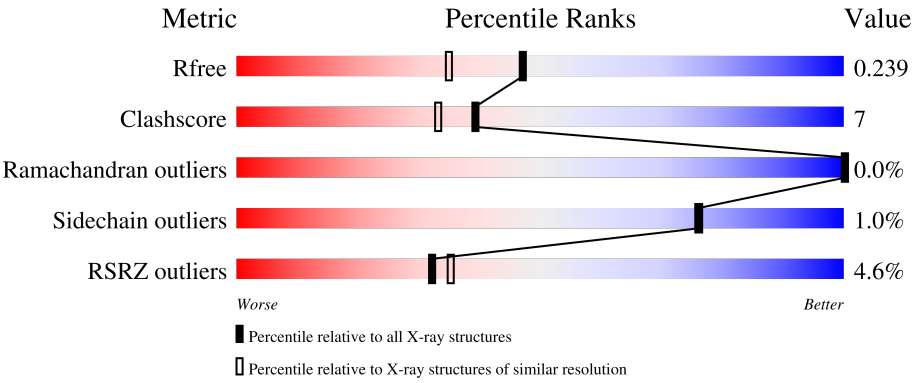
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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% 82% 14% ·
1	B	452	3% 78% 18% ·
1	C	452	4% 80% 17% ·
1	D	452	4% 82% 14% ·
1	E	452	6% 78% 18% · ·

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Mol	Chain	Length	Quality of chain
1	F	452	

2 Entry composition (i)

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 3497	C 2236	N 596	O 640	S 25	0	2	0
1	B	438	Total 3497	C 2234	N 596	O 642	S 25	0	3	0
1	C	437	Total 3485	C 2227	N 595	O 638	S 25	0	1	0
1	D	438	Total 3497	C 2236	N 596	O 640	S 25	0	2	0
1	E	438	Total 3499	C 2236	N 596	O 642	S 25	0	3	0
1	F	438	Total 3494	C 2231	N 597	O 641	S 25	0	2	0

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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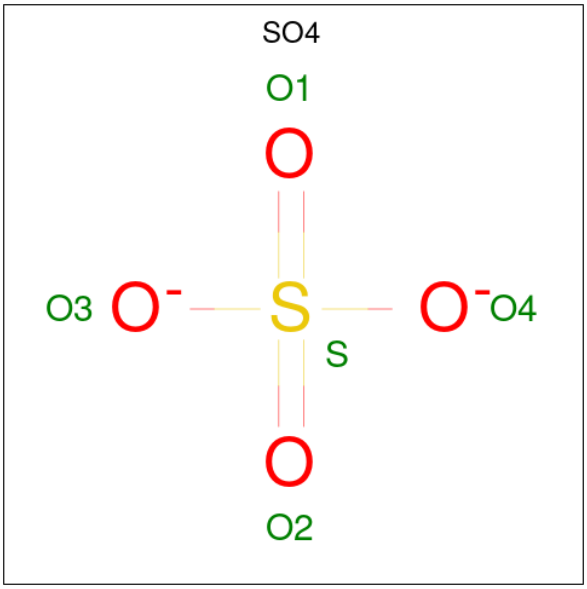
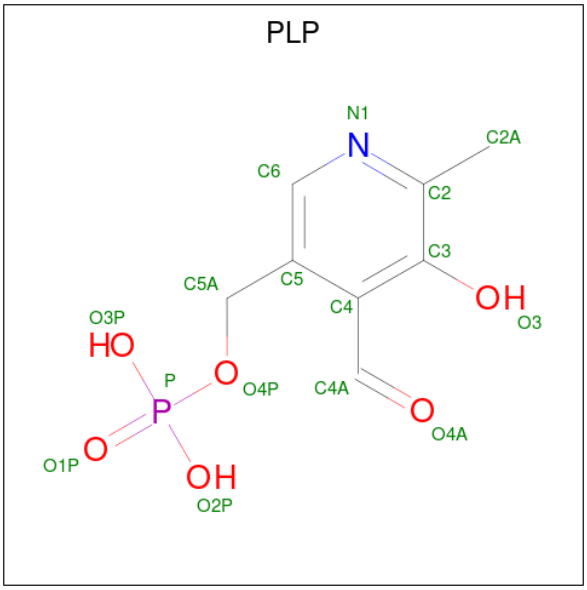
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LYS	deletion	UNP P69910
E	?	-	GLN	deletion	UNP P69910
E	?	-	VAL	deletion	UNP P69910
E	?	-	THR	deletion	UNP P69910
E	?	-	ASP	deletion	UNP P69910
E	?	-	LEU	deletion	UNP P69910
E	?	-	ARG	deletion	UNP P69910
E	?	-	SER	deletion	UNP P69910
E	?	-	GLU	deletion	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 (three-letter code: SO4) (formula: O_4S).



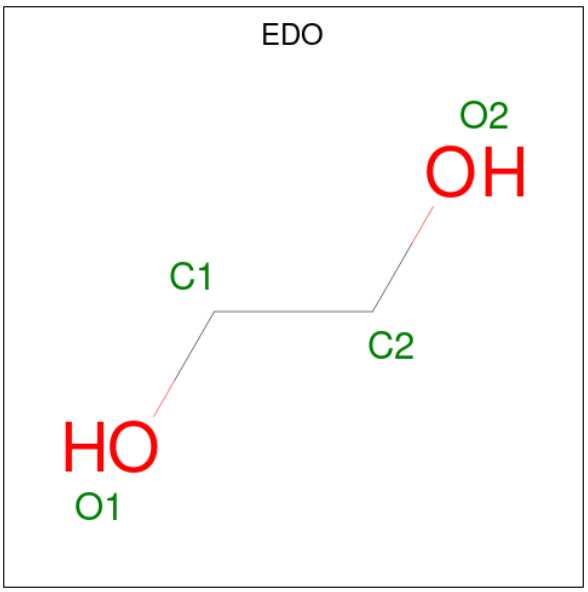
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

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

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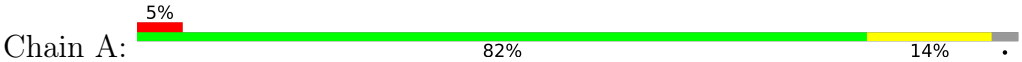
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	311	Total O 311 311	0	0
5	E	231	Total O 231 231	0	0
5	F	258	Total O 258 258	0	0

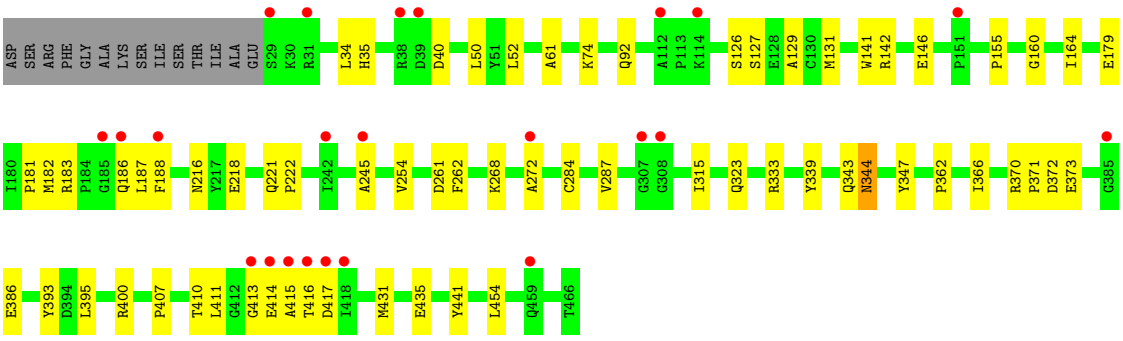
3 Residue-property plots (i)

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

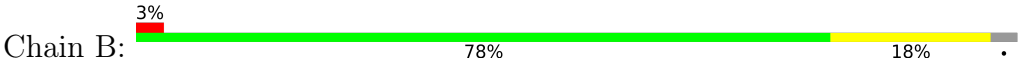
Chain A:

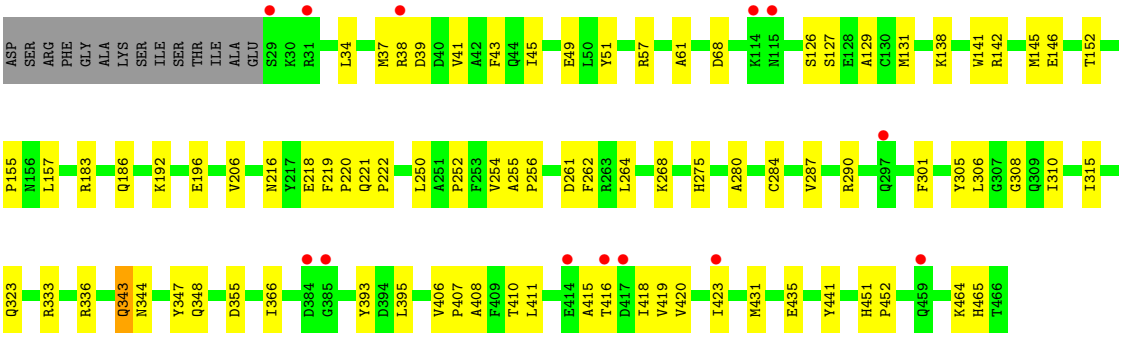




• Molecule 1: Glutamate decarboxylase beta

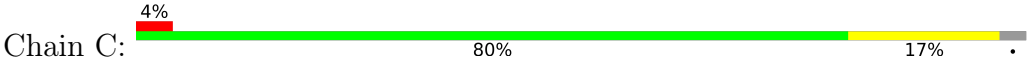
Chain B:

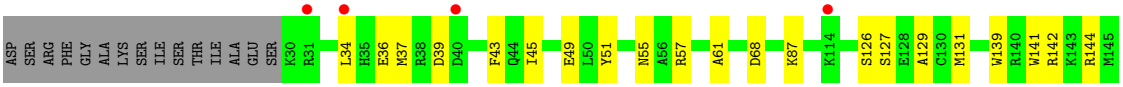


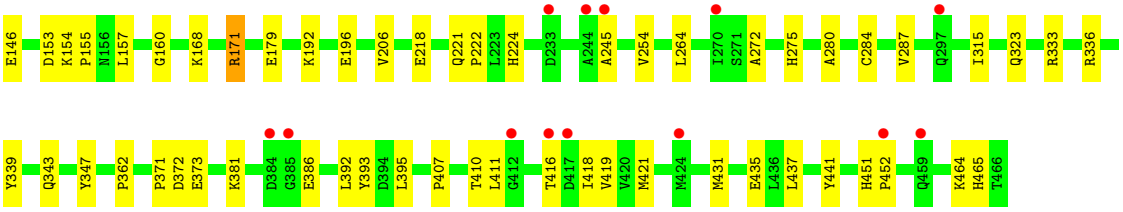


• Molecule 1: Glutamate decarboxylase beta

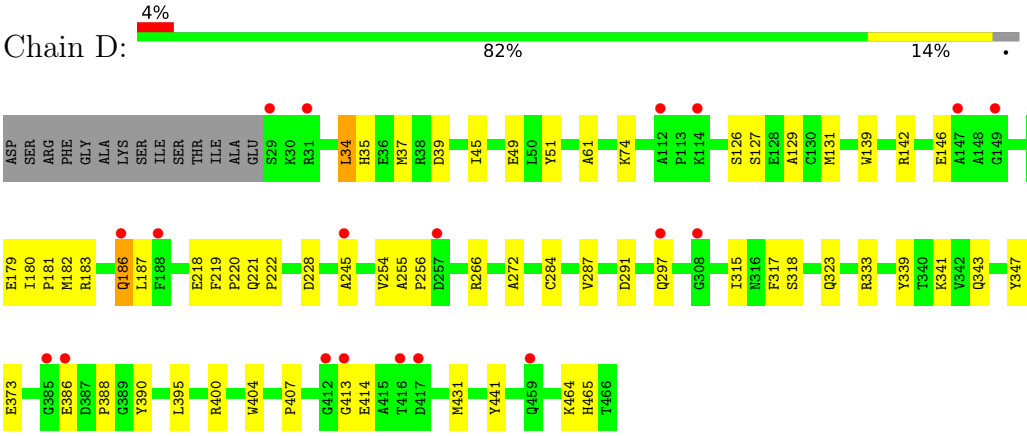
Chain C:



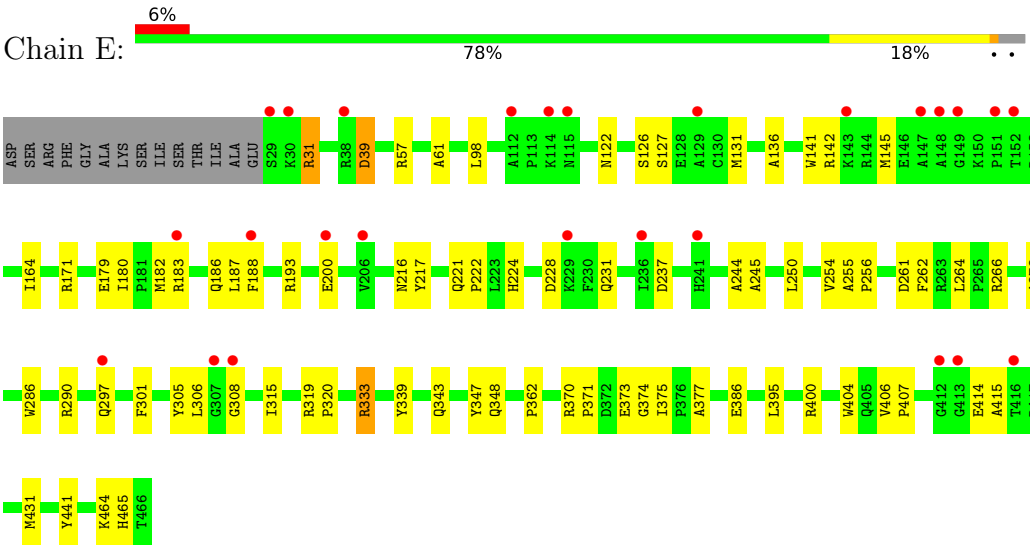




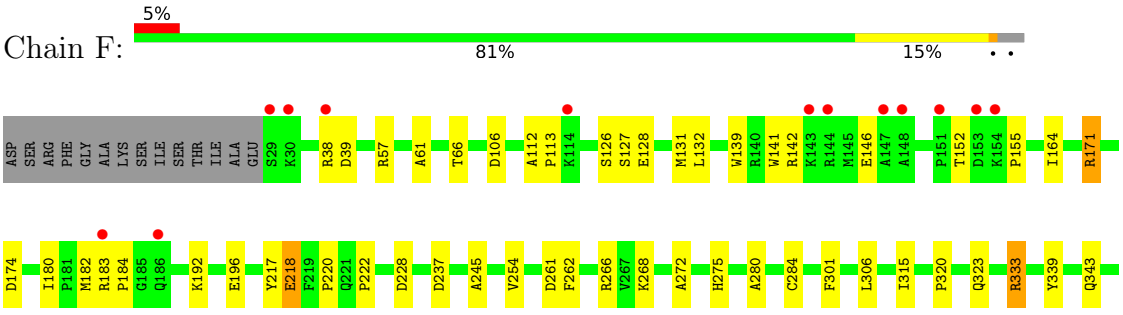
• Molecule 1: Glutamate decarboxylase beta

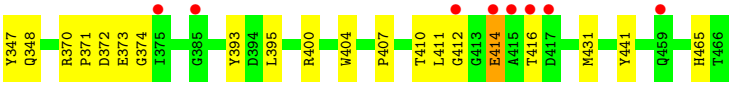


• Molecule 1: Glutamate decarboxylase beta



• Molecule 1: Glutamate decarboxylase beta




Y347
Q348
R370
P371
D372
E373
G374
I375
G385
Y393
D394
L395
R400
W404
P407
T410
L411
G412
G413
E414
A415
T416
D417
M431
Y441
Q459
H465
T466

4 Data and refinement statistics (i)

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 29.33 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.90) 99.0 (29.33-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.93 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.246 0.211 , 0.239	Depositor DCC
R_{free} test set	2308 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PLP, EDO, SO4

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	0.33	0/3601	0.58	1/4881 (0.0%)
1	B	0.33	0/3605	0.59	1/4887 (0.0%)
1	C	0.34	0/3583	0.58	1/4857 (0.0%)
1	D	0.33	0/3601	0.58	1/4881 (0.0%)
1	E	0.31	0/3610	0.57	0/4893
1	F	0.31	0/3598	0.57	1/4878 (0.0%)
All	All	0.33	0/21598	0.58	5/29277 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	218	GLU	N-CA-C	-5.36	96.54	111.00
1	D	218	GLU	N-CA-C	-5.35	96.57	111.00
1	F	218	GLU	N-CA-C	-5.34	96.57	111.00
1	A	218	GLU	N-CA-C	-5.22	96.92	111.00
1	C	218	GLU	N-CA-C	-5.14	97.12	111.00

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	47	0
1	B	3497	0	3396	60	0
1	C	3485	0	3385	59	0
1	D	3497	0	3395	52	0
1	E	3499	0	3388	73	0
1	F	3494	0	3389	56	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	4	0
All	All	22818	0	20431	306	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 7.

All (306) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:348:GLN:HG2	1:F:431:MET:HE1	1.69	0.74
1:F:127:SER:O	1:F:131[B]:MET:HG2	1.89	0.72
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: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:348:GLN:HE21	1:E:431:MET:CE	2.11	0.63
1:A:61:ALA:HB2	1:A:407:PRO:HD3	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
1:E:348:GLN:HE21	1:E:431:MET:HE3	1.64	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:TYR:O	1:A:343:GLN:HG2	2.07	0.54
1:A:415:ALA:C	1:A:417:ASP:H	2.11	0.53
1:B:415:ALA:HB1	1:B:418:ILE:HD12	1.89	0.53
1:E:39:ASP:HB2	5:E:4987:HOH:O	2.08	0.53
1:E:145:MET:CE	1:E:200:GLU:HG2	2.39	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:E:377:ALA:HB2	1:E:424:MET:HE1	1.91	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: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: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:E:142:ARG:HH22	1:F:174:ASP:CG	2.13	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
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: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:A:182:MET:H	1:A:413:GLY:HA3	1.77	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:375:ILE:HD11	1:E:424:MET:HE1	1.93	0.49
1:E:61:ALA:HB2	1:E:407:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:153:ASP:C	1:C:155:PRO:HD3	2.33	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: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:34:LEU:HD23	1:C:34:LEU:C	2.34	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
1:B:431:MET:O	1:B:435:GLU:HG3	2.14	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:B:465:HIS:CG	1:B:465:HIS:O	2.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:306:LEU:HD21	1:F:400:ARG:CZ	2.46	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
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:E:182:MET:HE2	1:E:187:LEU:O	2.16	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:E:145:MET:HE1	1:E:200:GLU:HG2	1.99	0.45
1:F:171:ARG:HH11	1:F:171:ARG:CB	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:34:LEU:HD13	1:A:34:LEU:O	2.18	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
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: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: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:D:34:LEU:HD12	1:D:35:HIS:CE1	2.53	0.42
1:D:348:GLN:HG2	1:D:431:MET:HE1	2.00	0.42
1:B:145:MET:HB2	1:B:152:THR:HG22	2.02	0.42
1:A:393:TYR:OH	1:A:410:THR:HG23	2.19	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:E:244:ALA:O	1:E:245:ALA:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ALA:C	1:A:417:ASP:N	2.74	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: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
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: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:E:348:GLN:HG2	1:E:431:MET:HE3	2.02	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:362:PRO:CG	1:D:388:PRO:HG3	2.51	0.41
1:E:375:ILE:CD1	1:E:424:MET:HE1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:161:PRO:HG3	1:D:182:MET:HE3	2.04	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
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%)	47	38
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%)	81	82
1	B	368/376 (98%)	363 (99%)	5 (1%)	67	65
1	C	365/376 (97%)	361 (99%)	4 (1%)	73	73
1	D	367/376 (98%)	365 (100%)	2 (0%)	88	89
1	E	368/376 (98%)	365 (99%)	3 (1%)	81	82
1	F	367/376 (98%)	362 (99%)	5 (1%)	67	65
All	All	2202/2256 (98%)	2180 (99%)	22 (1%)	76	76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	268	LYS
1	A	344	ASN
1	B	34	LEU
1	B	268	LYS
1	B	333	ARG
1	B	343	GLN
1	B	355	ASP
1	C	87	LYS
1	C	139	TRP
1	C	171	ARG
1	C	437	LEU
1	D	34	LEU
1	D	139	TRP
1	E	31	ARG
1	E	39	ASP
1	E	333	ARG
1	F	139	TRP
1	F	171	ARG
1	F	268	LYS
1	F	333	ARG
1	F	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	109	HIS
1	A	216	ASN
1	A	309	GLN
1	A	344	ASN
1	A	451	HIS
1	A	459	GLN
1	B	109	HIS
1	B	216	ASN
1	C	109	HIS
1	C	309	GLN
1	C	344	ASN
1	D	309	GLN
1	D	348	GLN
1	E	109	HIS
1	E	186	GLN
1	E	309	GLN
1	E	344	ASN
1	E	348	GLN
1	E	455	GLN
1	F	201	ASN
1	F	309	GLN
1	F	344	ASN
1	F	348	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	PLP	A	1500	1	15,15,16	1.07	1 (6%)	20,22,23	1.23	3 (15%)
3	PLP	C	1502	1	15,15,16	0.97	1 (6%)	20,22,23	1.25	4 (20%)
4	EDO	A	2193	-	3,3,3	0.43	0	2,2,2	0.36	0
2	SO4	E	4774	-	4,4,4	1.02	0	6,6,6	1.56	1 (16%)
3	PLP	F	1505	1	15,15,16	1.21	2 (13%)	20,22,23	1.19	3 (15%)
2	SO4	B	4771	-	4,4,4	1.02	0	6,6,6	1.55	1 (16%)
4	EDO	C	2195	-	3,3,3	0.44	0	2,2,2	0.36	0
3	PLP	B	1501	1	15,15,16	0.89	1 (6%)	20,22,23	1.25	3 (15%)
4	EDO	B	2191[A]	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	C	2192[A]	-	3,3,3	0.45	0	2,2,2	0.37	0
3	PLP	D	1503	1	15,15,16	1.00	1 (6%)	20,22,23	1.23	3 (15%)
4	EDO	E	2197	-	3,3,3	0.42	0	2,2,2	0.38	0
2	SO4	D	4773	-	4,4,4	1.02	0	6,6,6	1.56	1 (16%)
4	EDO	B	2191[B]	-	3,3,3	0.48	0	2,2,2	0.31	0
2	SO4	F	4775	-	4,4,4	1.05	0	6,6,6	1.57	1 (16%)
4	EDO	B	2194	-	3,3,3	0.50	0	2,2,2	0.31	0
4	EDO	C	2192[B]	-	3,3,3	0.45	0	2,2,2	0.36	0
2	SO4	A	4770	-	4,4,4	0.99	0	6,6,6	1.56	1 (16%)
4	EDO	F	2198	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	D	2196	-	3,3,3	0.47	0	2,2,2	0.35	0
2	SO4	C	4772	-	4,4,4	1.00	0	6,6,6	1.56	1 (16%)
3	PLP	E	1504	1	15,15,16	1.07	1 (6%)	20,22,23	1.23	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	2191[A]	-	-	0/1/1/1	-
3	PLP	C	1502	1	-	0/6/6/8	0/1/1/1
4	EDO	A	2193	-	-	1/1/1/1	-
4	EDO	B	2191[B]	-	-	1/1/1/1	-
3	PLP	E	1504	1	-	0/6/6/8	0/1/1/1
3	PLP	F	1505	1	-	0/6/6/8	0/1/1/1
4	EDO	B	2194	-	-	0/1/1/1	-
4	EDO	C	2192[A]	-	-	1/1/1/1	-
4	EDO	C	2192[B]	-	-	1/1/1/1	-
3	PLP	D	1503	1	-	0/6/6/8	0/1/1/1
4	EDO	E	2197	-	-	0/1/1/1	-
4	EDO	C	2195	-	-	0/1/1/1	-
4	EDO	D	2196	-	-	0/1/1/1	-
4	EDO	F	2198	-	-	1/1/1/1	-
3	PLP	B	1501	1	-	0/6/6/8	0/1/1/1
3	PLP	A	1500	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1505	PLP	C5-C4	2.65	1.43	1.40
3	C	1502	PLP	C5-C4	2.28	1.43	1.40
3	A	1500	PLP	C5-C4	2.24	1.43	1.40
3	F	1505	PLP	C3-C2	2.14	1.43	1.40
3	B	1501	PLP	C5-C4	2.11	1.42	1.40
3	E	1504	PLP	C5-C4	2.08	1.42	1.40
3	D	1503	PLP	C5-C4	2.02	1.42	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4775	SO4	O4-S-O3	3.59	124.40	109.06
2	E	4774	SO4	O4-S-O3	3.59	124.37	109.06
2	C	4772	SO4	O4-S-O3	3.58	124.36	109.06
2	A	4770	SO4	O4-S-O3	3.58	124.36	109.06
2	D	4773	SO4	O4-S-O3	3.58	124.34	109.06
2	B	4771	SO4	O4-S-O3	3.56	124.26	109.06
3	B	1501	PLP	C6-N1-C2	2.64	124.06	119.17
3	C	1502	PLP	C6-N1-C2	2.61	124.01	119.17
3	D	1503	PLP	C6-N1-C2	2.56	123.90	119.17
3	E	1504	PLP	C6-N1-C2	2.55	123.89	119.17
3	A	1500	PLP	C6-N1-C2	2.53	123.84	119.17
3	F	1505	PLP	C6-N1-C2	2.53	123.84	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1501	PLP	C3-C2-N1	-2.51	117.53	120.77
3	C	1502	PLP	C3-C2-N1	-2.48	117.56	120.77
3	A	1500	PLP	C3-C2-N1	-2.45	117.60	120.77
3	D	1503	PLP	C3-C2-N1	-2.43	117.63	120.77
3	E	1504	PLP	C3-C2-N1	-2.41	117.66	120.77
3	F	1505	PLP	C3-C2-N1	-2.28	117.82	120.77
3	A	1500	PLP	C2A-C2-C3	2.27	123.69	120.89
3	E	1504	PLP	C2A-C2-C3	2.25	123.66	120.89
3	D	1503	PLP	C2A-C2-C3	2.20	123.61	120.89
3	C	1502	PLP	C2A-C2-C3	2.08	123.46	120.89
3	B	1501	PLP	C2A-C2-C3	2.07	123.44	120.89
3	E	1504	PLP	O3P-P-O1P	2.06	118.75	110.68
3	F	1505	PLP	C2A-C2-C3	2.06	123.43	120.89
3	C	1502	PLP	O3P-P-O1P	2.06	118.73	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2191[B]	EDO	O1-C1-C2-O2
4	C	2192[A]	EDO	O1-C1-C2-O2
4	C	2192[B]	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	A	1500	PLP	1	0
3	C	1502	PLP	1	0
3	F	1505	PLP	1	0
3	B	1501	PLP	1	0
3	D	1503	PLP	1	0
2	D	4773	SO4	1	0
3	E	1504	PLP	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, 95^{th} 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%)	0.33	23 (5%)	26	29	17, 26, 37, 41	0
1	B	438/452 (96%)	0.27	13 (2%)	50	53	15, 26, 37, 42	0
1	C	437/452 (96%)	0.30	17 (3%)	39	42	15, 26, 37, 42	0
1	D	438/452 (96%)	0.28	20 (4%)	32	35	16, 25, 36, 41	0
1	E	438/452 (96%)	0.52	27 (6%)	20	23	17, 29, 47, 52	0
1	F	438/452 (96%)	0.45	21 (4%)	30	33	16, 29, 43, 48	0
All	All	2627/2712 (96%)	0.36	121 (4%)	32	35	15, 27, 40, 52	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	114	LYS	5.2
1	E	236	ILE	5.1
1	E	148	ALA	4.9
1	B	114	LYS	4.2
1	A	416	THR	4.1
1	D	416	THR	4.1
1	F	114	LYS	4.1
1	C	385	GLY	4.0
1	E	151	PRO	4.0
1	A	114	LYS	3.9
1	E	416	THR	3.8
1	F	417	ASP	3.7
1	D	149	GLY	3.7
1	F	414	GLU	3.6
1	F	459	GLN	3.6
1	C	114	LYS	3.6
1	F	385	GLY	3.6
1	F	153	ASP	3.5
1	B	31	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	114	LYS	3.5
1	E	188[A]	PHE	3.5
1	F	416	THR	3.4
1	A	188[A]	PHE	3.3
1	F	412	GLY	3.3
1	E	29	SER	3.2
1	A	31	ARG	3.1
1	D	31	ARG	3.1
1	E	308	GLY	3.1
1	E	115	ASN	3.1
1	A	39	ASP	3.0
1	D	147	ALA	3.0
1	F	144	ARG	3.0
1	E	183	ARG	3.0
1	F	183	ARG	2.9
1	F	29	SER	2.9
1	D	413	GLY	2.9
1	D	112	ALA	2.8
1	D	29	SER	2.8
1	E	30	LYS	2.7
1	C	417	ASP	2.7
1	E	149	GLY	2.7
1	F	143	LYS	2.7
1	B	414	GLU	2.7
1	F	148	ALA	2.7
1	E	297	GLN	2.7
1	B	29	SER	2.7
1	D	188[A]	PHE	2.6
1	E	152	THR	2.6
1	A	112	ALA	2.6
1	D	417	ASP	2.6
1	A	186	GLN	2.6
1	E	112	ALA	2.6
1	B	385	GLY	2.6
1	C	459	GLN	2.6
1	F	30	LYS	2.5
1	A	29	SER	2.5
1	B	115	ASN	2.5
1	F	415	ALA	2.5
1	E	206	VAL	2.5
1	D	459	GLN	2.5
1	A	245	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	245	ALA	2.5
1	E	147	ALA	2.5
1	A	459	GLN	2.5
1	D	297	GLN	2.5
1	A	417	ASP	2.5
1	C	416	THR	2.5
1	B	423	ILE	2.4
1	D	308	GLY	2.4
1	E	412	GLY	2.4
1	A	308	GLY	2.4
1	C	40	ASP	2.4
1	C	384	ASP	2.4
1	C	31	ARG	2.4
1	B	416	THR	2.4
1	A	185	GLY	2.4
1	A	272	ALA	2.4
1	C	233	ASP	2.4
1	D	385	GLY	2.3
1	B	384	ASP	2.3
1	C	244	ALA	2.3
1	C	245	ALA	2.3
1	C	412	GLY	2.3
1	A	38	ARG	2.3
1	A	385	GLY	2.3
1	D	386	GLU	2.3
1	F	154	LYS	2.3
1	A	414	GLU	2.2
1	C	270	ILE	2.2
1	B	417	ASP	2.2
1	E	413	GLY	2.2
1	B	297	GLN	2.2
1	B	459	GLN	2.2
1	E	241	HIS	2.2
1	A	307	GLY	2.2
1	F	186	GLN	2.2
1	F	38	ARG	2.2
1	B	38	ARG	2.2
1	C	424	MET	2.2
1	D	412	GLY	2.2
1	F	147	ALA	2.2
1	A	151	PRO	2.1
1	E	307	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	154	LYS	2.1
1	E	129	ALA	2.1
1	E	38	ARG	2.1
1	A	418	ILE	2.1
1	F	151	PRO	2.1
1	E	229	LYS	2.1
1	A	413	GLY	2.1
1	A	242	ILE	2.1
1	C	34	LEU	2.1
1	E	143	LYS	2.1
1	C	297	GLN	2.1
1	D	186	GLN	2.1
1	C	452	PRO	2.0
1	A	415	ALA	2.0
1	E	200	GLU	2.0
1	D	257	ASP	2.0
1	F	375	ILE	2.0
1	E	154	LYS	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 monosaccharides 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, 95^{th} 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	0.56	0.27	47,47,47,47	1
4	EDO	B	2191[B]	4/4	0.56	0.27	47,47,47,47	1
4	EDO	C	2192[A]	4/4	0.62	0.27	47,47,47,47	1
4	EDO	C	2192[B]	4/4	0.62	0.27	47,47,47,47	1
4	EDO	E	2197	4/4	0.83	0.19	38,38,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	F	2198	4/4	0.83	0.15	32,32,32,33	0
4	EDO	A	2193	4/4	0.87	0.15	32,33,33,33	0
2	SO4	A	4770	5/5	0.90	0.19	37,37,37,37	5
4	EDO	C	2195	4/4	0.90	0.12	29,30,30,30	0
2	SO4	F	4775	5/5	0.91	0.16	52,52,52,52	5
4	EDO	D	2196	4/4	0.92	0.15	33,33,33,33	0
2	SO4	C	4772	5/5	0.93	0.14	38,38,38,38	5
2	SO4	B	4771	5/5	0.94	0.20	50,50,50,50	0
3	PLP	F	1505	15/16	0.95	0.15	22,23,24,24	0
2	SO4	D	4773	5/5	0.95	0.16	31,31,31,31	5
3	PLP	B	1501	15/16	0.96	0.12	19,20,21,22	0
3	PLP	E	1504	15/16	0.96	0.14	22,22,22,22	0
2	SO4	E	4774	5/5	0.96	0.14	53,53,53,53	5
3	PLP	C	1502	15/16	0.97	0.13	18,20,21,21	0
3	PLP	A	1500	15/16	0.97	0.13	19,20,21,21	0
4	EDO	B	2194	4/4	0.97	0.07	27,27,27,27	0
3	PLP	D	1503	15/16	0.98	0.14	17,18,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.