



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:17 PM UTC

PDB ID : 2DGM / pdb_00002dgm
Title : Crystal structure of Escherichia coli GadB in complex with iodide
Authors : Gruetter, M.G.; Capitani, G.; Gut, H.
Deposited on : 2006-03-14
Resolution : 1.95 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

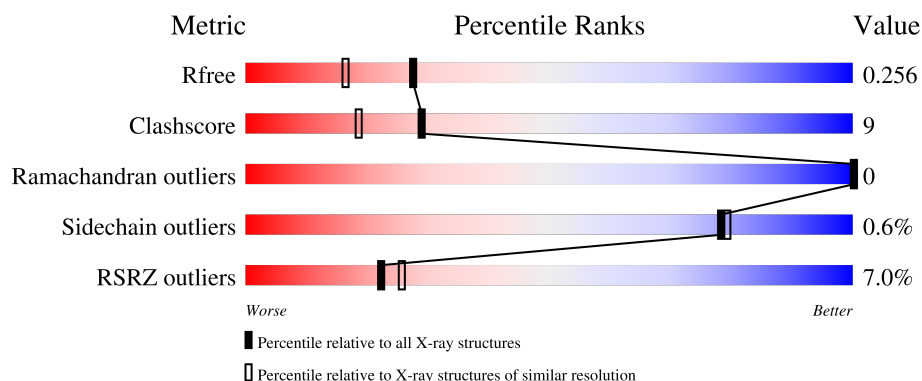
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	466	7% 77% 19% ..
1	B	466	6% 76% 20% .
1	C	466	8% 77% 20% ..
1	D	466	8% 81% 16% .
1	E	466	7% 78% 18% .

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Mol	Chain	Length	Quality of chain
1	F	466	

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	IOD	A	2331	-	-	X	-
2	IOD	A	2355	-	-	X	-
2	IOD	B	2333	-	-	X	-
2	IOD	B	2338	-	-	X	-
2	IOD	C	2351	-	-	X	-
2	IOD	D	2352	-	-	X	-
2	IOD	E	2335	-	-	X	-
2	IOD	E	2353	-	-	X	-
2	IOD	F	2336	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23729 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.

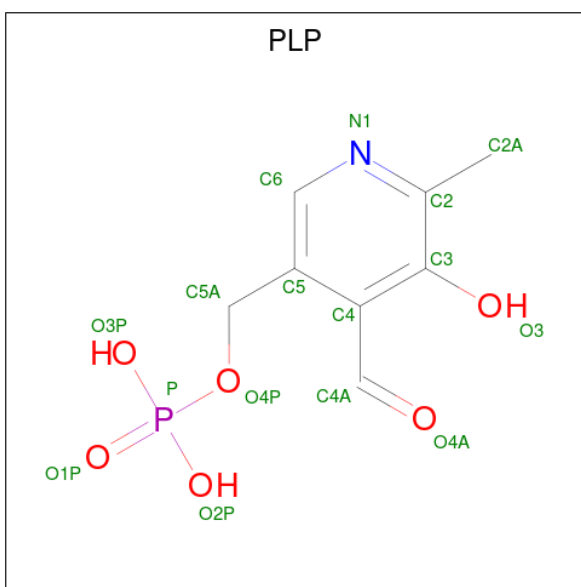
- Molecule 1 is a protein called Glutamate decarboxylase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	3	0
			3604	2300	616	663	25			
1	B	451	Total	C	N	O	S	0	2	0
			3591	2292	612	662	25			
1	C	454	Total	C	N	O	S	0	3	0
			3614	2306	616	666	26			
1	D	454	Total	C	N	O	S	0	4	0
			3621	2313	617	666	25			
1	E	450	Total	C	N	O	S	0	3	0
			3585	2288	610	661	26			
1	F	454	Total	C	N	O	S	0	2	0
			3619	2312	617	665	25			

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

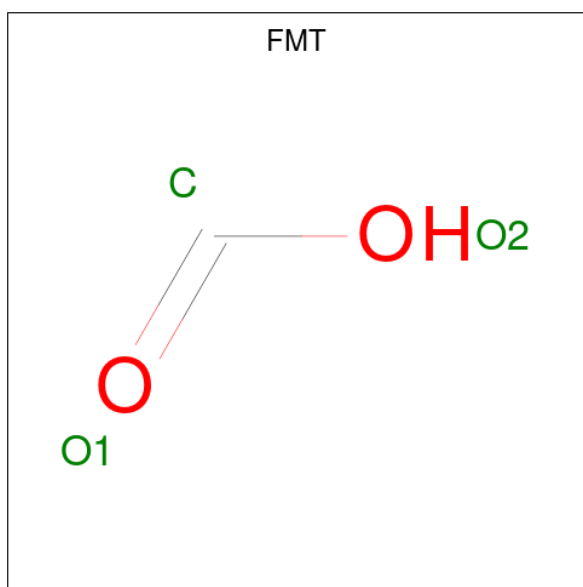
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	I	0	0
			6	6		
2	B	6	Total	I	0	0
			6	6		
2	C	4	Total	I	0	0
			4	4		
2	D	6	Total	I	0	0
			6	6		
2	E	5	Total	I	0	0
			5	5		
2	F	5	Total	I	0	0
			5	5		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



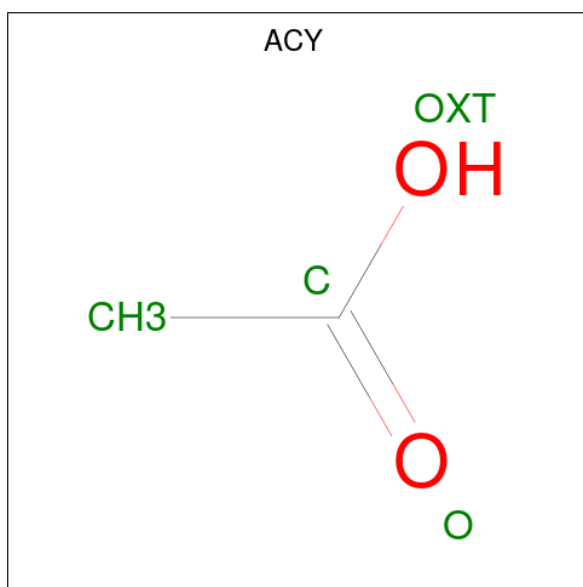
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



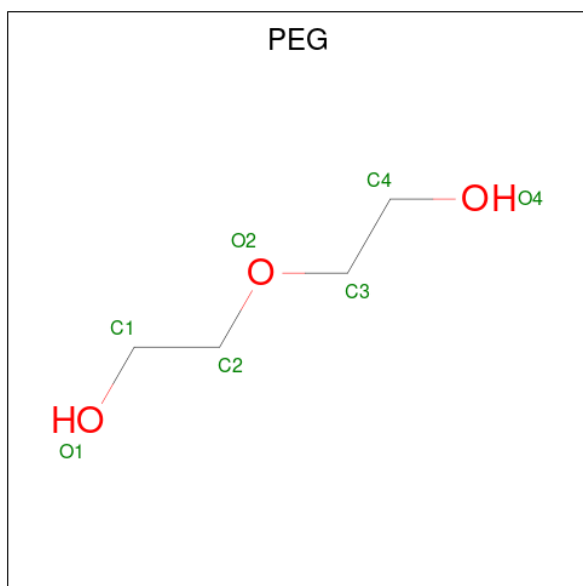
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total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

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		

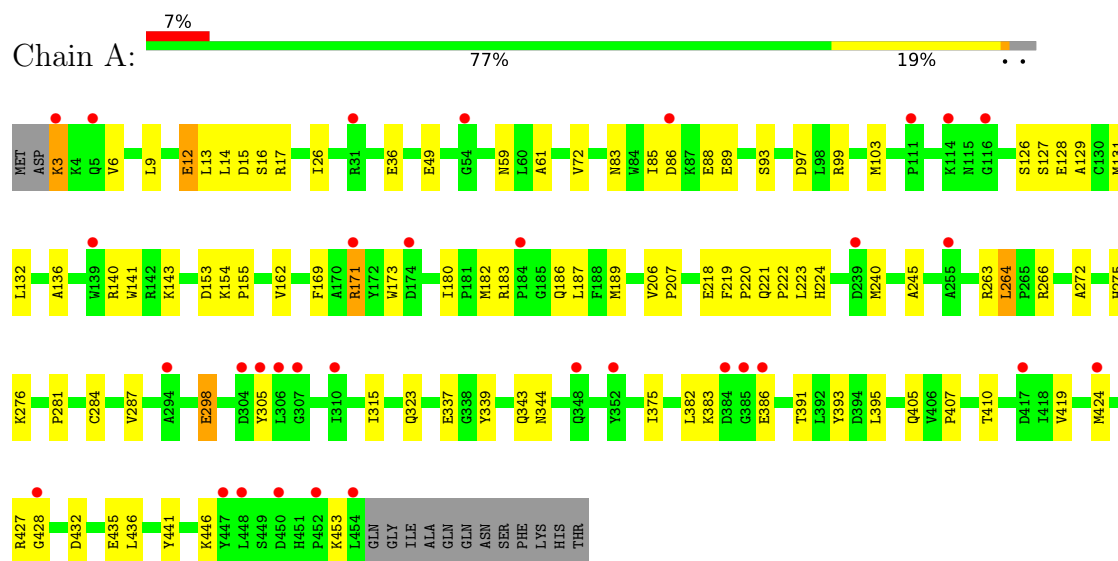
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	318	Total 318	O 318	0	0
7	B	339	Total 339	O 339	0	0
7	C	295	Total 295	O 295	0	0
7	D	346	Total 346	O 346	0	0
7	E	299	Total 299	O 299	0	0
7	F	326	Total 326	O 326	0	0

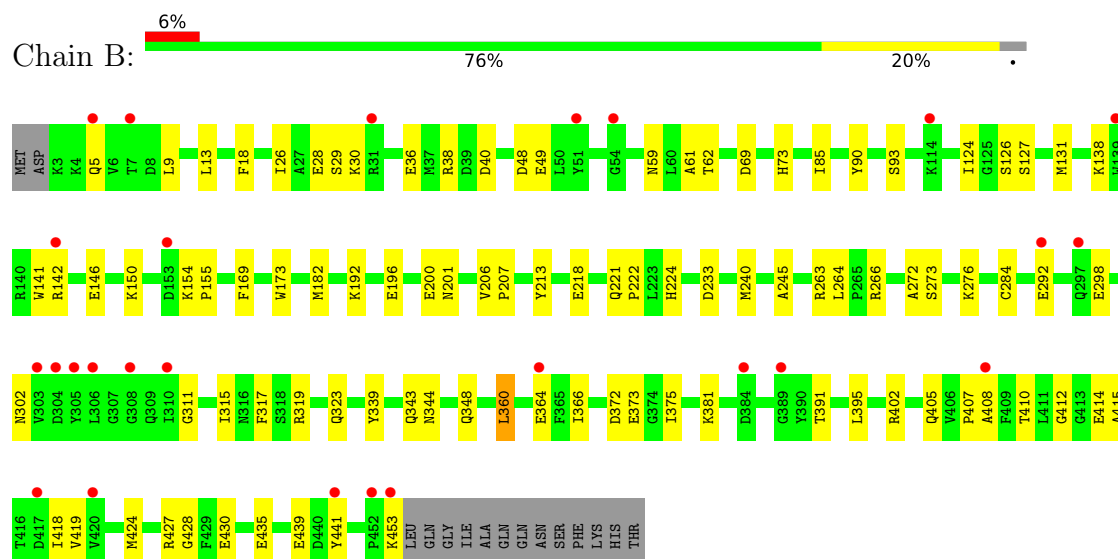
3 Residue-property plots

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.

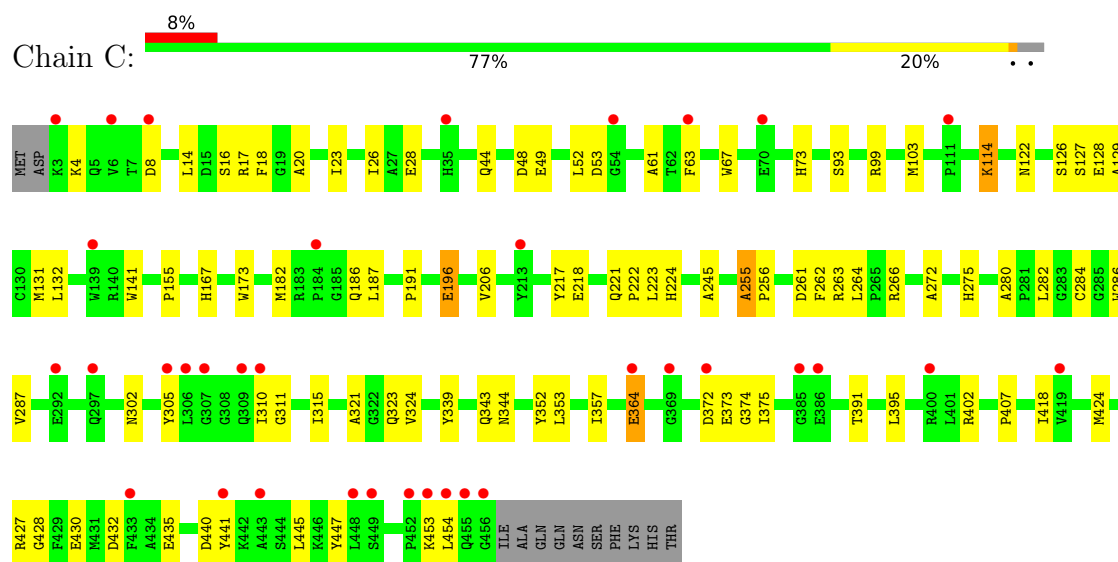
- Molecule 1: Glutamate decarboxylase beta



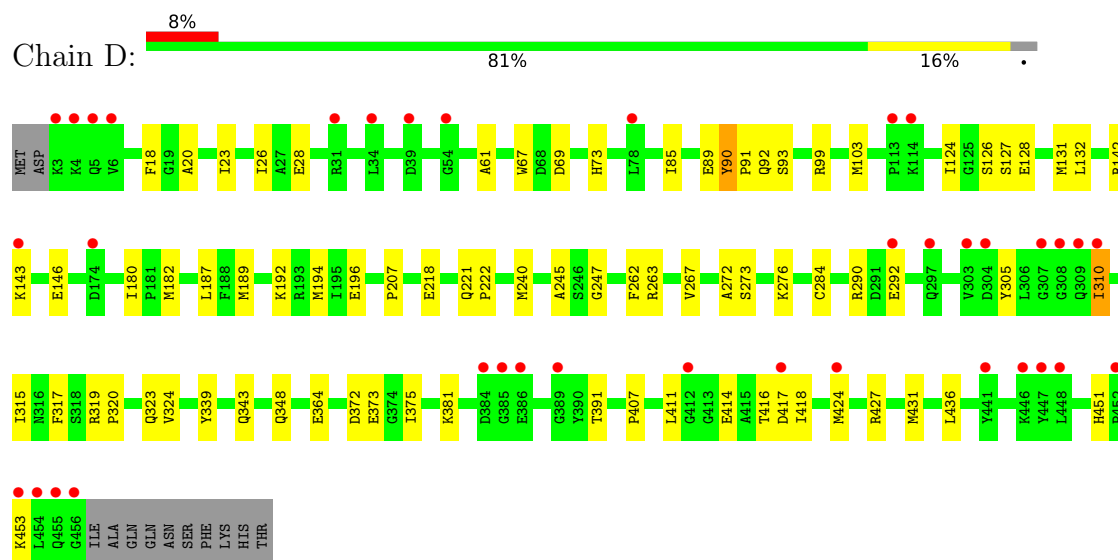
- Molecule 1: Glutamate decarboxylase beta



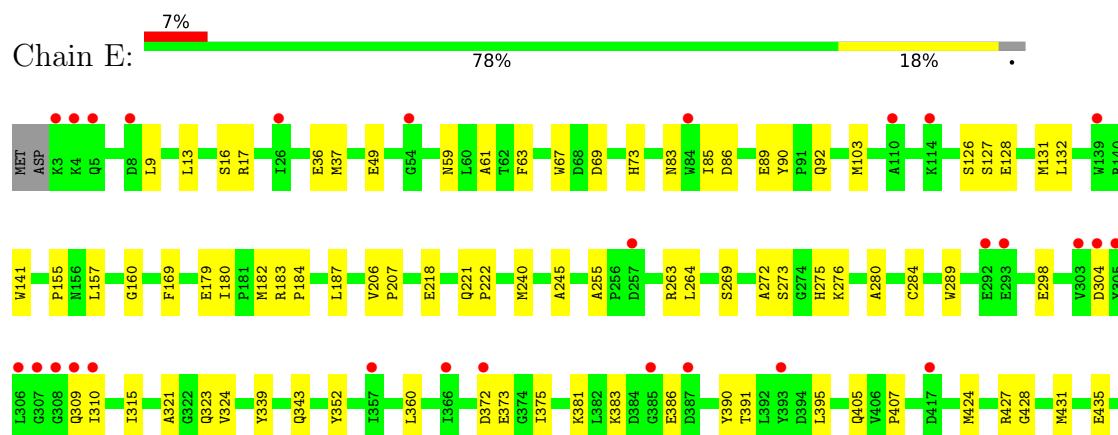
- Molecule 1: Glutamate decarboxylase beta

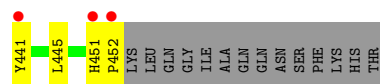


• Molecule 1: Glutamate decarboxylase beta

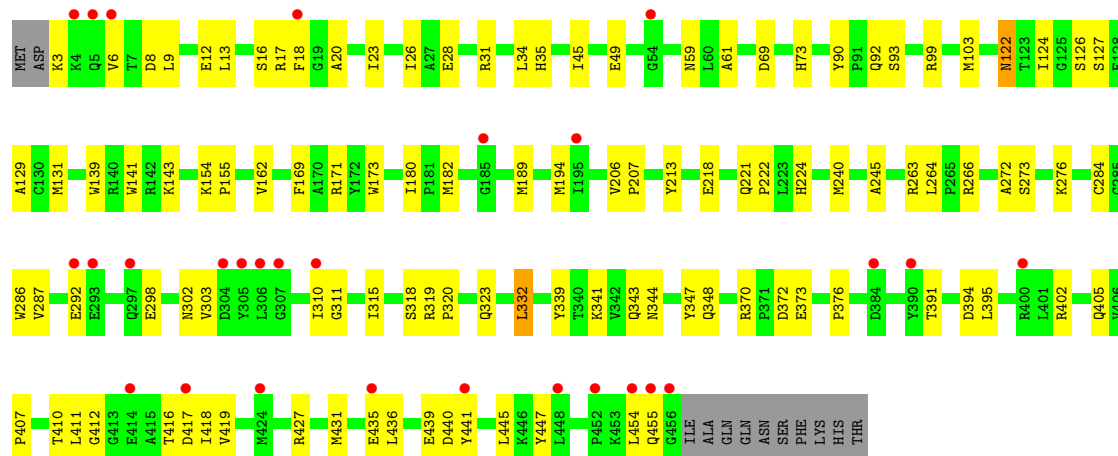
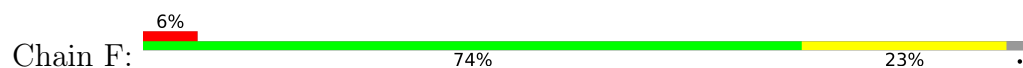


• Molecule 1: Glutamate decarboxylase beta





● Molecule 1: Glutamate decarboxylase beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.34Å 91.80Å 93.91Å 76.65° 76.94° 78.04°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-1.95) 92.1 (40.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.267 0.217 , 0.256	Depositor DCC
R_{free} test set	5338 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.156 for k,l,h 0.156 for l,h,k 0.013 for -k,-h,-l 0.002 for -l,-k,-h 0.008 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23729	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, PEG, PLP, FMT, IOD

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	0.39	0/3711	0.91	10/5028 (0.2%)
1	B	0.40	0/3692	0.89	12/5003 (0.2%)
1	C	0.38	0/3721	0.91	10/5041 (0.2%)
1	D	0.40	0/3737	0.90	8/5065 (0.2%)
1	E	0.39	0/3691	0.90	11/5002 (0.2%)
1	F	0.40	0/3723	0.89	11/5046 (0.2%)
All	All	0.39	0/22275	0.90	62/30185 (0.2%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	218	GLU	N-CA-C	-7.97	95.75	108.73
1	A	218	GLU	N-CA-C	-7.64	96.28	108.73
1	D	90	TYR	CA-C-N	7.60	127.98	119.32
1	D	90	TYR	C-N-CA	7.60	127.98	119.32
1	C	218	GLU	N-CA-C	-7.34	96.77	108.73
1	C	264	LEU	CA-C-N	6.70	126.95	119.32
1	C	264	LEU	C-N-CA	6.70	126.95	119.32
1	D	218	GLU	N-CA-C	-6.66	96.81	108.20
1	C	53	ASP	N-CA-C	-6.61	101.81	110.53
1	B	218	GLU	N-CA-C	-6.59	96.94	108.20
1	F	218	GLU	N-CA-C	-6.57	96.97	108.20
1	F	213	TYR	N-CA-C	6.43	118.29	111.28
1	B	93	SER	N-CA-C	-6.22	104.50	111.28
1	E	264	LEU	CA-C-N	6.14	126.32	119.32
1	E	264	LEU	C-N-CA	6.14	126.32	119.32
1	F	93	SER	N-CA-C	-5.88	104.95	111.36
1	E	90	TYR	CA-C-N	5.87	125.57	119.05
1	E	90	TYR	C-N-CA	5.87	125.57	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	263	ARG	N-CA-C	-5.74	105.54	112.54
1	B	366	ILE	N-CA-C	-5.73	106.88	111.81
1	B	90	TYR	CA-C-N	5.73	125.58	119.28
1	B	90	TYR	C-N-CA	5.73	125.58	119.28
1	B	263	ARG	N-CA-C	-5.73	105.56	112.54
1	B	206	VAL	N-CA-C	5.67	113.76	108.15
1	C	263	ARG	N-CA-C	-5.55	105.76	112.54
1	F	90	TYR	CA-C-N	5.50	125.33	119.28
1	F	90	TYR	C-N-CA	5.50	125.33	119.28
1	D	93	SER	N-CA-C	-5.47	105.32	111.28
1	A	263	ARG	N-CA-C	-5.46	105.87	112.54
1	C	255	ALA	CA-C-N	5.46	125.29	119.28
1	C	255	ALA	C-N-CA	5.46	125.29	119.28
1	E	206	VAL	N-CA-C	5.46	113.56	108.15
1	B	213	TYR	N-CA-C	5.42	117.19	111.28
1	C	206	VAL	N-CA-C	5.41	113.51	108.15
1	B	264	LEU	CA-C-N	5.39	126.57	119.84
1	B	264	LEU	C-N-CA	5.39	126.57	119.84
1	F	263	ARG	N-CA-C	-5.35	106.01	112.54
1	D	263	ARG	N-CA-C	-5.33	106.03	112.54
1	F	122	ASN	N-CA-C	-5.32	103.37	110.55
1	E	255	ALA	CA-C-N	5.32	124.98	119.56
1	E	255	ALA	C-N-CA	5.32	124.98	119.56
1	A	93	SER	N-CA-C	-5.29	105.52	111.28
1	A	264	LEU	CA-C-N	5.27	125.33	119.32
1	A	264	LEU	C-N-CA	5.27	125.33	119.32
1	A	36	GLU	N-CA-C	-5.25	102.70	110.48
1	A	206	VAL	N-CA-C	5.21	113.30	108.15
1	F	264	LEU	CA-C-N	5.17	125.22	119.32
1	F	264	LEU	C-N-CA	5.17	125.22	119.32
1	B	233	ASP	N-CA-C	5.17	116.99	111.36
1	A	162	VAL	N-CA-C	5.15	116.03	110.21
1	E	360	LEU	N-CA-C	5.13	119.81	113.50
1	C	167	HIS	N-CA-C	-5.12	105.88	111.82
1	D	247	GLY	N-CA-C	5.09	119.91	113.24
1	A	14	LEU	N-CA-C	5.09	119.76	113.50
1	D	451	HIS	CA-C-N	5.08	125.12	119.32
1	D	451	HIS	C-N-CA	5.08	125.12	119.32
1	B	408	ALA	N-CA-C	-5.07	100.64	108.90
1	F	162	VAL	N-CA-C	5.05	115.92	110.21
1	A	276	LYS	N-CA-C	-5.05	100.04	110.80
1	E	36	GLU	N-CA-C	-5.02	103.77	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	SER	N-CA-C	-5.02	105.81	111.28
1	F	206	VAL	N-CA-C	5.01	113.11	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	3604	0	3518	74	0
1	B	3591	0	3502	71	0
1	C	3614	0	3529	68	0
1	D	3621	0	3529	56	0
1	E	3585	0	3494	61	0
1	F	3619	0	3529	92	0
2	A	6	0	0	5	0
2	B	6	0	0	7	0
2	C	4	0	0	4	0
2	D	6	0	0	5	0
2	E	5	0	0	6	0
2	F	5	0	0	5	0
3	A	15	0	6	2	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	9	0	3	1	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	9	0	3	0	0
4	E	3	0	1	0	0
4	F	12	0	4	0	0
5	E	4	0	3	1	0
6	E	7	0	10	0	0
7	A	318	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	339	0	0	2	0
7	C	295	0	0	0	0
7	D	346	0	0	3	0
7	E	299	0	0	0	0
7	F	326	0	0	3	0
All	All	23729	0	21163	375	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 9.

All (375) 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:C:114:LYS:H	1:C:114:LYS:HD3	1.19	1.02
1:A:453:LYS:HB2	2:A:2343:IOD:I	2.36	0.95
1:E:431:MET:HE3	1:E:431:MET:HA	1.57	0.86
1:A:171:ARG:HH11	1:A:171:ARG:HB2	1.43	0.83
1:D:348:GLN:HE21	1:D:431:MET:HE2	1.45	0.80
1:D:26:ILE:HD13	1:E:435:GLU:HG3	1.64	0.77
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.66	0.76
1:E:339:TYR:O	1:E:343:GLN:HG2	1.85	0.75
1:F:348:GLN:HE21	1:F:431:MET:CE	2.00	0.75
1:A:131[B]:MET:SD	1:B:315:ILE:HG23	2.27	0.74
1:A:131[A]:MET:HE1	1:A:169:PHE:HB2	1.69	0.73
1:B:127:SER:O	1:B:131[B]:MET:HG2	1.89	0.73
1:B:131[B]:MET:HE3	1:B:173:TRP:HZ3	1.54	0.72
1:A:182:MET:HE2	1:A:187:LEU:HB3	1.71	0.72
1:F:339:TYR:O	1:F:343:GLN:HG2	1.90	0.72
1:B:142:ARG:O	1:B:146:GLU:HG3	1.89	0.71
1:B:182:MET:CE	1:B:412:GLY:H	2.03	0.71
1:C:339:TYR:O	1:C:343:GLN:HG2	1.91	0.71
1:B:207:PRO:HG2	1:B:240:MET:HE2	1.71	0.70
2:B:2332:IOD:I	1:C:427:ARG:HD2	2.62	0.70
1:D:436:LEU:HD11	1:E:49:GLU:HG2	1.74	0.70
1:A:153:ASP:O	1:A:154:LYS:HD3	1.91	0.69
1:E:61:ALA:HB2	1:E:407:PRO:HD3	1.73	0.69
1:E:131[B]:MET:SD	1:F:315:ILE:HG23	2.33	0.68
1:F:180:ILE:HD12	1:F:189:MET:HG3	1.75	0.68
1:F:182:MET:HE3	1:F:412:GLY:H	1.58	0.67
1:C:302:ASN:HD22	1:C:311:GLY:HA2	1.58	0.67
1:C:126:SER:HB2	3:C:501:PLP:O4P	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:348:GLN:HE21	1:F:431:MET:HE2	1.61	0.66
1:A:339:TYR:O	1:A:343:GLN:HG2	1.95	0.66
2:A:2331:IOD:I	1:F:427:ARG:HD2	2.66	0.66
1:C:131[B]:MET:SD	1:D:315:ILE:HG23	2.36	0.65
1:D:143:LYS:HD2	7:D:2772:HOH:O	1.96	0.65
1:B:339:TYR:O	1:B:343:GLN:HG2	1.97	0.65
1:F:302:ASN:HD22	1:F:311:GLY:HA2	1.60	0.65
1:F:143:LYS:HA	1:F:143:LYS:HE2	1.78	0.65
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.78	0.64
1:E:391:THR:HB	2:E:2359:IOD:I	2.67	0.64
1:C:127:SER:O	1:C:131[A]:MET:HG2	1.97	0.64
1:A:12:GLU:OE1	1:C:14:LEU:HD21	1.98	0.64
1:B:182:MET:HE3	1:B:412:GLY:H	1.62	0.64
1:C:375:ILE:HD12	1:C:424[A]:MET:HE1	1.79	0.64
1:B:292:GLU:HG3	7:B:2772:HOH:O	1.97	0.64
1:E:182:MET:HE2	1:E:187:LEU:HB3	1.79	0.63
1:A:298:GLU:H	1:A:298:GLU:CD	2.07	0.63
1:C:221:GLN:HB3	1:C:222:PRO:HD3	1.81	0.62
1:E:127:SER:O	1:E:131[A]:MET:HG2	1.99	0.62
1:F:127:SER:O	1:F:131[B]:MET:HG2	2.00	0.61
1:E:375:ILE:HD12	1:E:424[A]:MET:HE1	1.80	0.61
1:D:305:TYR:HB2	1:D:310[A]:ILE:HD12	1.82	0.61
1:D:339:TYR:O	1:D:343:GLN:HG2	2.01	0.61
1:E:103:MET:HE2	1:F:28:GLU:HG3	1.81	0.61
1:C:372:ASP:OD1	1:C:373:GLU:HG3	2.01	0.61
1:D:245:ALA:HA	1:D:272:ALA:HA	1.82	0.61
1:F:410:THR:HG22	1:F:419:VAL:HG22	1.82	0.61
1:B:298:GLU:CD	1:B:298:GLU:H	2.09	0.61
1:E:383:LYS:HB2	1:E:386:GLU:HG3	1.82	0.61
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.35	0.61
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.83	0.61
1:E:126:SER:HB2	3:E:502:PLP:O4P	2.01	0.60
1:F:245:ALA:HA	1:F:272:ALA:HA	1.82	0.60
1:F:182:MET:CE	1:F:412:GLY:H	2.14	0.60
1:B:391:THR:HB	2:B:2356:IOD:I	2.72	0.60
1:D:182:MET:HE2	1:D:187:LEU:HB3	1.84	0.60
1:B:427:ARG:HD2	2:B:2333:IOD:I	2.71	0.59
1:C:4:LYS:HD2	1:C:4:LYS:C	2.27	0.59
1:D:142:ARG:O	1:D:146:GLU:HG3	2.02	0.59
1:C:395:LEU:HD21	1:C:441:TYR:CZ	2.37	0.59
1:B:26:ILE:HD13	1:C:435:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASN:HA	1:A:405:GLN:HB2	1.84	0.59
1:C:61:ALA:HB2	1:C:407:PRO:HD3	1.85	0.58
1:B:418:ILE:HD13	2:B:2338:IOD:I	2.73	0.58
1:E:395:LEU:HD21	1:E:441:TYR:CZ	2.38	0.58
1:A:126:SER:HB2	3:A:500:PLP:O4P	2.03	0.58
1:D:180:ILE:HD12	1:D:189:MET:HG3	1.84	0.58
1:F:435:GLU:O	1:F:439:GLU:HG3	2.03	0.58
1:A:103:MET:HE2	1:B:28:GLU:HG3	1.85	0.57
1:D:89:GLU:C	1:D:91:PRO:HD3	2.29	0.57
1:C:441:TYR:HE1	1:C:445:LEU:HD11	1.69	0.57
1:A:315:ILE:HG21	1:B:315:ILE:HG21	1.86	0.57
1:A:3:LYS:O	1:A:6:VAL:HG12	2.04	0.57
1:B:372:ASP:OD1	1:B:373:GLU:HG3	2.05	0.57
1:D:305:TYR:CB	1:D:310[A]:ILE:HD12	2.33	0.57
1:F:180:ILE:HD11	1:F:194:MET:HA	1.87	0.57
1:B:138:LYS:O	1:B:142:ARG:HG3	2.04	0.57
1:F:154:LYS:HD2	7:F:2887:HOH:O	2.04	0.57
1:F:131[B]:MET:SD	1:F:169:PHE:HB2	2.44	0.56
1:F:298:GLU:H	1:F:298:GLU:CD	2.12	0.56
1:B:207:PRO:CG	1:B:240:MET:HE2	2.35	0.56
1:C:114:LYS:HD3	1:C:114:LYS:N	2.03	0.56
1:A:410:THR:HG22	1:A:419:VAL:HG22	1.87	0.56
1:E:375:ILE:CD1	1:E:424[A]:MET:HE1	2.36	0.56
1:A:207:PRO:HG2	1:A:240:MET:HE2	1.87	0.56
1:D:427:ARG:HD2	2:E:2335:IOD:I	2.75	0.56
1:A:131[B]:MET:HE2	1:A:173:TRP:HZ3	1.70	0.56
1:B:435:GLU:HG3	1:C:26:ILE:HD13	1.89	0.55
1:A:395:LEU:HD21	1:A:441:TYR:CZ	2.41	0.55
1:C:315:ILE:HG23	1:D:131[A]:MET:SD	2.47	0.55
1:D:126:SER:HB2	3:D:501:PLP:O4P	2.06	0.55
1:D:127:SER:O	1:D:131[B]:MET:HG2	2.07	0.55
1:D:391:THR:HB	2:D:2358:IOD:I	2.77	0.55
1:D:292:GLU:HG3	7:D:2836:HOH:O	2.07	0.54
1:F:348:GLN:HE21	1:F:431:MET:HE3	1.72	0.54
1:F:292:GLU:HG3	7:F:2810:HOH:O	2.08	0.54
1:A:16:SER:HB2	2:A:2331:IOD:I	2.78	0.54
1:A:221:GLN:HB3	1:A:222:PRO:HD3	1.90	0.54
1:B:126:SER:HB2	3:B:500:PLP:O4P	2.08	0.54
1:F:126:SER:HB2	3:F:502:PLP:O4P	2.08	0.54
1:F:411:LEU:O	1:F:416:THR:HA	2.08	0.54
1:D:418:ILE:HD12	1:D:418:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:PRO:HG2	1:E:240:MET:HE2	1.90	0.53
1:F:402:ARG:HD3	1:F:440:ASP:CG	2.33	0.53
1:D:411:LEU:O	1:D:416:THR:HA	2.09	0.53
1:A:127:SER:O	1:A:131[A]:MET:HG2	2.09	0.53
1:F:3:LYS:O	1:F:6:VAL:HG22	2.09	0.53
1:A:424:MET:HG2	7:A:2713:HOH:O	2.08	0.53
1:B:124:ILE:HD11	1:B:319:ARG:HD2	1.91	0.53
1:B:302:ASN:HD22	1:B:311:GLY:HA2	1.73	0.53
1:C:103:MET:HE2	1:D:28:GLU:HG3	1.90	0.53
1:E:372:ASP:OD1	1:E:373:GLU:HG3	2.09	0.53
1:E:451:HIS:N	1:E:452:PRO:HD3	2.24	0.53
1:F:61:ALA:HB2	1:F:407:PRO:HD3	1.90	0.52
1:A:49:GLU:HG2	1:F:436:LEU:HD11	1.90	0.52
1:A:375:ILE:HD12	1:A:424:MET:HE1	1.91	0.52
1:A:128:GLU:O	1:A:132:LEU:HG	2.09	0.52
1:D:372:ASP:OD1	1:D:373:GLU:HG3	2.09	0.52
1:F:34:LEU:HD22	1:F:35:HIS:CD2	2.44	0.52
1:A:428:GLY:HA2	1:F:18:PHE:CE1	2.44	0.52
1:F:221:GLN:HB3	1:F:222:PRO:HD3	1.91	0.52
1:E:245:ALA:HA	1:E:272:ALA:HA	1.90	0.52
1:E:49:GLU:O	1:F:92:GLN:HG2	2.10	0.51
1:E:131[A]:MET:HE1	1:E:169:PHE:HB2	1.92	0.51
1:C:99:ARG:O	1:C:103:MET:HG3	2.11	0.51
1:D:348:GLN:HE21	1:D:431:MET:CE	2.17	0.51
1:C:49:GLU:O	1:D:92:GLN:HG2	2.09	0.51
1:A:245:ALA:HA	1:A:272:ALA:HA	1.92	0.51
1:F:34:LEU:HD22	1:F:35:HIS:NE2	2.25	0.51
1:E:160:GLY:O	1:E:179:GLU:HG3	2.10	0.51
1:A:337:GLU:CD	1:B:36:GLU:HG2	2.36	0.51
1:D:73:HIS:NE2	2:D:2352:IOD:I	3.07	0.51
1:F:207:PRO:HG2	1:F:240:MET:HE2	1.93	0.51
1:F:171:ARG:HG2	1:F:171:ARG:HH11	1.76	0.51
1:F:370:ARG:HE	1:F:373:GLU:CD	2.18	0.51
1:A:131[A]:MET:CE	1:A:169:PHE:HB2	2.41	0.51
1:C:402:ARG:HE	1:C:440:ASP:CG	2.19	0.51
1:B:224:HIS:CD2	1:B:266:ARG:HB2	2.46	0.50
1:A:61:ALA:HB2	1:A:407:PRO:HD3	1.92	0.50
1:E:86:ASP:HB3	1:E:89:GLU:HB2	1.94	0.50
1:A:315:ILE:HG23	1:B:131[A]:MET:SD	2.52	0.50
1:E:92:GLN:HG2	1:F:49:GLU:O	2.11	0.50
1:F:447:TYR:HE2	1:F:454:LEU:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLU:HG3	1:D:103:MET:HE2	1.94	0.50
1:C:67:TRP:HA	2:C:2351:IOD:I	2.81	0.50
1:B:453:LYS:HE3	1:C:453:LYS:HE3	1.94	0.50
1:F:303:VAL:HG23	1:F:310:ILE:HG23	1.94	0.50
1:B:245:ALA:HA	1:B:272:ALA:HA	1.94	0.49
1:C:20:ALA:O	1:C:23:ILE:HG22	2.12	0.49
1:B:395:LEU:HD21	1:B:441:TYR:CZ	2.47	0.49
1:C:196:GLU:OE1	1:C:196:GLU:HA	2.12	0.49
1:A:88:GLU:OE1	1:A:305:TYR:HA	2.13	0.49
1:C:114:LYS:H	1:C:114:LYS:CD	2.00	0.49
1:A:141:TRP:CZ3	1:A:155:PRO:HB3	2.47	0.49
1:C:255:ALA:N	1:C:256:PRO:HD3	2.28	0.49
1:F:16:SER:HB2	2:F:2336:IOD:I	2.83	0.49
1:B:29:SER:C	1:B:30:LYS:HD2	2.38	0.49
1:D:180:ILE:HD11	1:D:194:MET:HA	1.94	0.49
1:C:63:PHE:CD2	1:C:424[A]:MET:HE2	2.48	0.48
1:A:435:GLU:HG3	1:F:26:ILE:HD13	1.95	0.48
1:C:315:ILE:HD13	1:D:315:ILE:HG21	1.95	0.48
1:A:284:CYS:HB2	1:A:323:GLN:HB3	1.96	0.48
1:F:391:THR:HB	2:F:2360:IOD:I	2.83	0.48
1:B:61:ALA:HB2	1:B:407:PRO:HD3	1.95	0.48
1:B:73:HIS:NE2	2:B:2350:IOD:I	3.16	0.48
1:B:375:ILE:HD12	1:B:424:MET:HE1	1.94	0.48
1:F:303:VAL:CG2	1:F:310:ILE:HG23	2.44	0.48
1:E:298:GLU:CD	1:E:298:GLU:H	2.21	0.48
1:F:348:GLN:NE2	1:F:431:MET:HE2	2.28	0.48
1:E:315:ILE:HG23	1:F:131[A]:MET:SD	2.54	0.48
1:C:352:TYR:OH	1:C:435:GLU:OE1	2.26	0.47
1:E:16:SER:HB2	2:E:2335:IOD:I	2.84	0.47
1:A:171:ARG:HH11	1:A:171:ARG:CB	2.21	0.47
1:C:441:TYR:CE1	1:C:445:LEU:HD11	2.47	0.47
1:F:319:ARG:HB2	1:F:320:PRO:HD2	1.97	0.47
1:F:124:ILE:HD11	1:F:319:ARG:HD2	1.95	0.47
1:A:129:ALA:HB1	1:A:287:VAL:HB	1.96	0.47
1:A:382:LEU:HD12	2:A:2355:IOD:I	2.85	0.47
1:D:364:GLU:OE1	1:D:381:LYS:NZ	2.44	0.47
1:A:9:LEU:HG	1:E:9:LEU:HD21	1.96	0.47
1:B:360:LEU:HD23	1:B:441:TYR:CD1	2.50	0.47
1:A:180:ILE:N	1:A:180:ILE:HD12	2.30	0.47
1:E:67:TRP:HA	2:E:2353:IOD:I	2.84	0.47
1:C:122:ASN:HB2	1:C:286:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131[B]:MET:HG2	1:C:173:TRP:CZ3	2.50	0.47
1:E:207:PRO:CG	1:E:240:MET:HE2	2.45	0.47
1:B:18:PHE:CE1	1:C:428:GLY:HA2	2.50	0.47
1:A:143:LYS:HD2	7:A:2718:HOH:O	2.14	0.47
1:A:186:GLN:O	1:A:186:GLN:HG3	2.15	0.47
1:E:103:MET:HE2	1:F:28:GLU:CG	2.44	0.47
1:C:141:TRP:CZ3	1:C:155:PRO:HB3	2.50	0.46
1:A:427:ARG:HD2	2:F:2336:IOD:I	2.84	0.46
1:C:128:GLU:O	1:C:132:LEU:HG	2.15	0.46
1:F:139[A]:TRP:CZ2	1:F:298:GLU:HG2	2.51	0.46
1:B:13:LEU:HD13	1:F:13:LEU:HD13	1.97	0.46
1:E:352:TYR:CD2	1:E:431:MET:HE1	2.50	0.46
1:A:383:LYS:HB2	1:A:386:GLU:CG	2.45	0.46
1:B:344:ASN:O	1:B:348:GLN:HG3	2.16	0.46
1:D:192:LYS:O	1:D:196:GLU:HG3	2.14	0.46
1:A:183:ARG:NH2	1:A:186:GLN:OE1	2.47	0.46
1:C:129:ALA:HB1	1:C:287:VAL:HB	1.97	0.46
1:A:207:PRO:CG	1:A:240:MET:HE2	2.46	0.46
1:E:273:SER:HB2	1:E:276:LYS:HG3	1.97	0.46
1:E:441:TYR:HE1	1:E:445:LEU:HD11	1.80	0.46
1:B:435:GLU:O	1:B:439:GLU:HG3	2.15	0.46
1:C:321:ALA:O	1:C:324:VAL:HG12	2.16	0.46
1:F:441:TYR:HE1	1:F:445:LEU:HD11	1.80	0.46
1:A:83:ASN:OD1	1:A:85:ILE:HG22	2.16	0.46
1:A:99:ARG:HG2	1:B:29:SER:HB2	1.97	0.46
1:E:284:CYS:HB2	1:E:323:GLN:HB3	1.98	0.46
1:C:305:TYR:HB2	1:C:310:ILE:HG22	1.97	0.45
1:A:183:ARG:NE	1:A:186:GLN:OE1	2.46	0.45
1:C:364:GLU:OE1	1:C:364:GLU:C	2.60	0.45
1:D:324:VAL:HG12	7:D:2804:HOH:O	2.16	0.45
1:E:315:ILE:HG21	1:F:315:ILE:HG21	1.98	0.45
1:D:61:ALA:HB2	1:D:407:PRO:HD3	1.99	0.45
1:F:131[B]:MET:HE3	1:F:173:TRP:HZ3	1.80	0.45
1:C:245:ALA:HA	1:C:272:ALA:HA	1.98	0.45
1:D:67:TRP:HA	2:D:2352:IOD:I	2.86	0.45
1:E:17:ARG:HE	1:E:17:ARG:HB2	1.66	0.45
1:B:5:GLN:OE1	1:F:6:VAL:HG21	2.17	0.45
1:B:182:MET:HE1	1:B:412:GLY:H	1.77	0.45
1:B:284:CYS:HB2	1:B:323:GLN:HB3	1.99	0.45
1:F:284:CYS:HB2	1:F:323:GLN:HB3	1.98	0.45
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:THR:HG22	1:B:419:VAL:HG22	1.97	0.45
1:A:395:LEU:HD21	1:A:441:TYR:CE2	2.52	0.45
1:E:269:SER:HB3	1:E:289:TRP:CD1	2.52	0.44
1:A:432:ASP:O	1:A:436:LEU:HD23	2.17	0.44
1:B:59:ASN:HA	1:B:405:GLN:HB2	1.99	0.44
1:C:284:CYS:HB2	1:C:323:GLN:HB3	1.98	0.44
1:A:428:GLY:HA2	1:F:18:PHE:CZ	2.53	0.44
1:D:128:GLU:O	1:D:132:LEU:HG	2.18	0.44
1:E:275:HIS:HA	1:E:280:ALA:O	2.18	0.44
1:E:381:LYS:HE2	2:E:2341:IOD:I	2.87	0.44
1:B:364:GLU:OE1	1:B:381:LYS:NZ	2.50	0.44
1:C:186:GLN:O	1:C:186:GLN:HG3	2.16	0.44
1:D:262:PHE:CD1	1:D:290:ARG:HB3	2.52	0.44
1:F:394:ASP:OD2	1:F:455:GLN:HA	2.18	0.44
1:A:13:LEU:HD13	1:E:13:LEU:HD13	1.99	0.44
1:B:124:ILE:CD1	1:B:319:ARG:HD2	2.47	0.44
1:E:273:SER:CB	1:E:276:LYS:HG3	2.47	0.44
1:C:191:PRO:HG3	1:C:223:LEU:HD23	1.98	0.44
1:E:321:ALA:O	1:E:324:VAL:HG12	2.18	0.44
1:B:48:ASP:OD2	1:C:430:GLU:OE2	2.36	0.44
1:D:273:SER:CB	1:D:276:LYS:HG3	2.47	0.44
1:B:192:LYS:O	1:B:196:GLU:HG3	2.16	0.44
1:B:414:GLU:N	1:B:414:GLU:OE1	2.51	0.44
1:B:424:MET:HG2	7:B:2701:HOH:O	2.16	0.44
1:D:20:ALA:O	1:D:23:ILE:HG22	2.18	0.44
1:D:207:PRO:HG2	1:D:240:MET:HE2	2.00	0.44
1:E:157:LEU:HD13	1:E:157:LEU:C	2.42	0.44
1:F:273:SER:CB	1:F:276:LYS:HG3	2.48	0.44
1:A:446:LYS:O	1:A:446:LYS:HD3	2.18	0.43
1:C:261:ASP:HB2	1:C:262:PHE:H	1.61	0.43
1:E:37:MET:HE3	1:F:332:LEU:O	2.17	0.43
1:D:417:ASP:CG	1:D:418:ILE:HD12	2.43	0.43
1:F:141:TRP:CZ3	1:F:155:PRO:HB3	2.53	0.43
1:C:447:TYR:HE1	1:C:454:LEU:HD11	1.82	0.43
1:A:26:ILE:HD13	1:F:435:GLU:HG3	2.00	0.43
1:A:153:ASP:OD2	1:A:154:LYS:HE2	2.18	0.43
1:B:273:SER:CB	1:B:276:LYS:HG3	2.49	0.43
1:C:73:HIS:NE2	2:C:2351:IOD:I	3.11	0.43
1:D:18:PHE:CE1	1:E:428:GLY:HA2	2.53	0.43
1:E:141:TRP:CZ3	1:E:155:PRO:HB3	2.53	0.43
1:E:180:ILE:HD12	1:E:180:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HE	1:A:17:ARG:HB2	1.60	0.43
1:B:154:LYS:O	1:B:201:ASN:HB3	2.18	0.43
1:D:375:ILE:HD12	1:D:424:MET:HE1	1.99	0.43
1:A:103:MET:HE2	1:B:28:GLU:CG	2.49	0.43
1:C:275:HIS:HA	1:C:280:ALA:O	2.18	0.43
1:B:49:GLU:OE2	1:C:432:ASP:OD2	2.37	0.43
1:D:284:CYS:HB2	1:D:323:GLN:HB3	2.00	0.43
1:F:28:GLU:HG2	1:F:31:ARG:O	2.19	0.43
1:F:122:ASN:HB2	1:F:286:TRP:CZ3	2.54	0.43
1:C:17:ARG:NH1	1:C:44:GLN:OE1	2.51	0.43
1:F:34:LEU:HD23	1:F:34:LEU:O	2.18	0.43
1:F:303:VAL:HG23	1:F:310:ILE:CG2	2.49	0.43
1:C:391:THR:HB	2:C:2357:IOD:I	2.88	0.43
1:F:182:MET:HE3	1:F:412:GLY:N	2.31	0.43
1:C:217:TYR:CD2	1:C:374:GLY:HA2	2.54	0.43
1:D:207:PRO:CG	1:D:240:MET:HE2	2.48	0.43
1:F:8:ASP:O	1:F:12:GLU:HG3	2.19	0.43
1:B:9:LEU:HD21	1:F:9:LEU:HG	2.01	0.42
1:D:85:ILE:HG12	1:D:317:PHE:CD1	2.54	0.42
1:F:45:ILE:O	1:F:49:GLU:HG3	2.20	0.42
1:A:275:HIS:NE2	3:A:500:PLP:O1P	2.47	0.42
1:C:4:LYS:HD3	1:C:8:ASP:OD2	2.18	0.42
1:F:69:ASP:C	1:F:69:ASP:OD1	2.62	0.42
1:A:143:LYS:NZ	1:A:298:GLU:OE2	2.43	0.42
1:D:273:SER:HB2	1:D:276:LYS:HG3	2.01	0.42
1:D:99:ARG:O	1:D:103:MET:HG3	2.19	0.42
1:F:129:ALA:HB1	1:F:287:VAL:HB	2.02	0.42
1:A:224:HIS:CD2	1:A:264:LEU:HB3	2.55	0.42
1:B:182:MET:HE3	1:B:412:GLY:N	2.30	0.42
1:D:124:ILE:HD11	1:D:319:ARG:HD2	2.00	0.42
1:E:69:ASP:OD1	1:E:69:ASP:C	2.63	0.42
2:D:2334:IOD:I	1:E:427:ARG:HD2	2.90	0.42
1:A:103:MET:CE	1:B:28:GLU:HG3	2.48	0.42
1:E:304:ASP:HA	1:E:309:GLN:HG2	2.01	0.42
1:F:124:ILE:HD13	1:F:124:ILE:HA	1.97	0.42
1:C:224:HIS:CD2	1:C:266:ARG:HB2	2.55	0.42
1:C:418:ILE:HD13	2:C:2339:IOD:I	2.89	0.42
1:F:347:TYR:CE2	1:F:376:PRO:HG3	2.55	0.42
1:A:343:GLN:OE1	1:A:343:GLN:HA	2.19	0.42
1:B:428:GLY:HA2	1:C:18:PHE:CE1	2.55	0.42
2:B:2333:IOD:I	1:C:16:SER:HB2	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:HIS:NE2	2:F:2354:IOD:I	3.17	0.42
1:F:224:HIS:CD2	1:F:266:ARG:HB2	2.54	0.42
1:F:441:TYR:CE1	1:F:445:LEU:HD11	2.55	0.42
1:A:219:PHE:HA	1:A:220:PRO:HD3	1.89	0.41
1:A:393:TYR:OH	1:A:410:THR:HG23	2.20	0.41
1:E:63:PHE:CD2	1:E:424[A]:MET:HE2	2.55	0.41
1:A:72:VAL:HG11	1:A:281:PRO:HG3	2.02	0.41
1:A:344:ASN:HD22	1:A:344:ASN:HA	1.67	0.41
1:A:391:THR:HB	2:A:2355:IOD:I	2.91	0.41
1:B:395:LEU:HD21	1:B:441:TYR:CE2	2.54	0.41
1:E:343:GLN:OE1	1:E:343:GLN:HA	2.21	0.41
1:F:124:ILE:CD1	1:F:319:ARG:HD2	2.50	0.41
1:E:390:TYR:CD1	1:E:390:TYR:C	2.98	0.41
1:F:20:ALA:O	1:F:23:ILE:HG22	2.20	0.41
1:F:99:ARG:O	1:F:103:MET:HG3	2.19	0.41
1:A:224:HIS:CD2	1:A:266:ARG:HB2	2.56	0.41
1:E:73:HIS:NE2	2:E:2353:IOD:I	3.10	0.41
1:F:34:LEU:HD23	1:F:34:LEU:C	2.46	0.41
1:B:402:ARG:NH2	1:C:52:LEU:HD12	2.35	0.41
1:D:69:ASP:OD1	1:D:69:ASP:C	2.64	0.41
1:F:59:ASN:HA	1:F:405:GLN:HB2	2.03	0.41
1:A:15:ASP:OD1	1:F:341:LYS:NZ	2.54	0.41
1:D:90:TYR:N	1:D:91:PRO:HD3	2.33	0.41
1:E:383:LYS:HB2	1:E:386:GLU:CG	2.49	0.41
1:F:395:LEU:HD21	1:F:441:TYR:CE2	2.56	0.41
1:A:86:ASP:HB3	1:A:89:GLU:HB2	2.02	0.41
1:A:298:GLU:CD	1:A:298:GLU:N	2.78	0.41
1:B:430:GLU:OE2	1:C:48:ASP:OD2	2.38	0.41
1:F:344:ASN:ND2	7:F:2982:HOH:O	2.53	0.41
1:F:418:ILE:HD13	2:F:2342:IOD:I	2.91	0.41
1:B:69:ASP:OD1	1:B:69:ASP:C	2.63	0.41
1:F:17:ARG:HE	1:F:17:ARG:HB2	1.59	0.41
1:F:34:LEU:HD22	1:F:35:HIS:CE1	2.56	0.41
1:F:344:ASN:HD22	1:F:344:ASN:HA	1.67	0.41
1:D:267:VAL:O	1:D:290:ARG:HD2	2.20	0.40
1:E:59:ASN:HA	1:E:405:GLN:HB2	2.01	0.40
1:F:370:ARG:NH2	1:F:372:ASP:OD2	2.54	0.40
1:B:38:ARG:HB3	1:B:40:ASP:OD1	2.21	0.40
1:B:150:LYS:NZ	1:B:200:GLU:OE1	2.45	0.40
1:C:344:ASN:HD22	1:C:344:ASN:HA	1.69	0.40
5:E:2519:ACY:H2	1:F:318:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:372:ASP:OD1	1:F:373:GLU:HG3	2.21	0.40
4:A:2550:FMT:H	1:B:62:THR:HA	2.02	0.40
1:B:85:ILE:HG12	1:B:317:PHE:CD1	2.56	0.40
1:B:381:LYS:HE2	2:B:2338:IOD:I	2.92	0.40
1:C:282:LEU:O	1:D:320:PRO:HG3	2.22	0.40
1:D:453:LYS:HD2	2:D:2346:IOD:I	2.92	0.40
1:E:83:ASN:OD1	1:E:85:ILE:HG22	2.21	0.40
1:E:183:ARG:O	1:E:184:PRO:C	2.65	0.40
1:B:415:ALA:HB1	1:B:418:ILE:HD12	2.02	0.40
1:C:395:LEU:HD21	1:C:441:TYR:CE2	2.56	0.40
1:E:128:GLU:O	1:E:132:LEU:HG	2.22	0.40
1:A:136:ALA:O	1:A:140:ARG:HG3	2.22	0.40
1:A:189:MET:HE3	1:A:223:LEU:HD13	2.04	0.40
1:B:131[B]:MET:SD	1:B:169:PHE:HB2	2.62	0.40
1:C:182:MET:HE2	1:C:187:LEU:HB3	2.03	0.40
1:C:353:LEU:O	1:C:357:ILE:HG13	2.21	0.40
1:F:402:ARG:HD3	1:F:440:ASP:OD1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/466 (97%)	444 (98%)	9 (2%)	0	100	100
1	B	451/466 (97%)	437 (97%)	14 (3%)	0	100	100
1	C	455/466 (98%)	441 (97%)	14 (3%)	0	100	100
1	D	456/466 (98%)	443 (97%)	13 (3%)	0	100	100
1	E	451/466 (97%)	437 (97%)	14 (3%)	0	100	100
1	F	454/466 (97%)	441 (97%)	13 (3%)	0	100	100
All	All	2720/2796 (97%)	2643 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	381/390 (98%)	376 (99%)	5 (1%)	61	58
1	B	379/390 (97%)	378 (100%)	1 (0%)	86	87
1	C	382/390 (98%)	379 (99%)	3 (1%)	73	74
1	D	383/390 (98%)	380 (99%)	3 (1%)	73	74
1	E	379/390 (97%)	378 (100%)	1 (0%)	86	87
1	F	381/390 (98%)	379 (100%)	2 (0%)	81	82
All	All	2285/2340 (98%)	2270 (99%)	15 (1%)	78	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	12	GLU
1	A	97	ASP
1	A	171	ARG
1	A	298	GLU
1	B	360	LEU
1	C	114	LYS
1	C	196	GLU
1	C	364	GLU
1	D	310[A]	ILE
1	D	310[B]	ILE
1	D	414	GLU
1	E	310	ILE
1	F	332	LEU
1	F	417	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	47	ASN
1	A	302	ASN
1	A	344	ASN
1	B	35	HIS
1	B	216	ASN
1	B	297	GLN
1	B	302	ASN
1	B	344	ASN
1	B	348	GLN
1	C	5	GLN
1	C	109	HIS
1	C	297	GLN
1	C	302	ASN
1	C	344	ASN
1	D	35	HIS
1	D	201	ASN
1	D	221	GLN
1	D	348	GLN
1	E	297	GLN
1	E	309	GLN
1	F	5	GLN
1	F	109	HIS
1	F	297	GLN
1	F	302	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 32 are monoatomic - leaving 21 for Mogul analysis.

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
4	FMT	F	2590	-	2,2,2	0.62	0	1,1,1	0.04	0
4	FMT	F	2670	-	2,2,2	0.63	0	1,1,1	0.04	0
4	FMT	F	2660	-	2,2,2	0.63	0	1,1,1	0.05	0
6	PEG	E	2833	-	6,6,6	0.53	0	5,5,5	0.47	0
5	ACY	E	2519	-	3,3,3	1.28	0	3,3,3	1.64	1 (33%)
3	PLP	A	500	1	15,15,16	0.92	0	21,22,23	1.48	6 (28%)
4	FMT	E	2620	-	2,2,2	0.63	0	1,1,1	0.08	0
3	PLP	B	500	1	15,15,16	0.85	0	21,22,23	1.45	5 (23%)
4	FMT	D	2630	-	2,2,2	0.63	0	1,1,1	0.07	0
4	FMT	B	2650	-	2,2,2	0.63	0	1,1,1	0.07	0
3	PLP	C	501	1	15,15,16	0.90	1 (6%)	21,22,23	1.51	6 (28%)
3	PLP	E	502	1	15,15,16	0.94	0	21,22,23	1.49	6 (28%)
3	PLP	F	502	1	15,15,16	0.84	0	21,22,23	1.47	5 (23%)
4	FMT	C	2610	-	2,2,2	0.62	0	1,1,1	0.06	0
4	FMT	F	2640	-	2,2,2	0.62	0	1,1,1	0.06	0
3	PLP	D	501	1	15,15,16	0.92	0	21,22,23	1.49	6 (28%)
4	FMT	D	2580	-	2,2,2	0.62	0	1,1,1	0.04	0
4	FMT	D	2570	-	2,2,2	0.63	0	1,1,1	0.05	0
4	FMT	A	2550	-	2,2,2	0.63	0	1,1,1	0.04	0
4	FMT	A	2560	-	2,2,2	0.62	0	1,1,1	0.04	0
4	FMT	A	2600	-	2,2,2	0.63	0	1,1,1	0.06	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	C	501	1	-	0/6/6/8	0/1/1/1
3	PLP	E	502	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	500	1	-	0/6/6/8	0/1/1/1
3	PLP	F	502	1	-	0/6/6/8	0/1/1/1
3	PLP	B	500	1	-	0/6/6/8	0/1/1/1
6	PEG	E	2833	-	-	0/4/4/4	-
3	PLP	D	501	1	-	0/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	PLP	C5-C4	2.12	1.42	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	C4A-C4-C5	3.18	124.21	120.94
3	E	502	PLP	C4A-C4-C5	3.03	124.07	120.94
3	A	500	PLP	C4A-C4-C5	2.98	124.02	120.94
3	D	501	PLP	C4A-C4-C5	2.89	123.92	120.94
3	F	502	PLP	C4A-C4-C5	2.84	123.86	120.94
3	B	500	PLP	C4A-C4-C5	2.70	123.72	120.94
3	A	500	PLP	C3-C2-N1	-2.69	117.56	120.96
3	D	501	PLP	C3-C2-N1	-2.68	117.58	120.96
3	E	502	PLP	C3-C2-N1	-2.67	117.59	120.96
3	B	500	PLP	C3-C2-N1	-2.66	117.61	120.96
3	F	502	PLP	C6-N1-C2	2.62	123.95	119.20
3	F	502	PLP	C3-C2-N1	-2.60	117.68	120.96
3	C	501	PLP	C6-N1-C2	2.60	123.92	119.20
3	C	501	PLP	C3-C2-N1	-2.59	117.69	120.96
3	B	500	PLP	C6-N1-C2	2.57	123.87	119.20
3	D	501	PLP	C6-N1-C2	2.56	123.84	119.20
3	A	500	PLP	C6-N1-C2	2.52	123.77	119.20
3	E	502	PLP	C6-N1-C2	2.52	123.76	119.20
3	D	501	PLP	C2A-C2-C3	2.36	123.56	120.80
3	C	501	PLP	C2A-C2-C3	2.35	123.55	120.80
3	E	502	PLP	C2A-C2-C3	2.31	123.50	120.80
3	A	500	PLP	C2A-C2-C3	2.30	123.49	120.80
3	B	500	PLP	C2A-C2-C3	2.30	123.49	120.80
3	F	502	PLP	C2A-C2-C3	2.30	123.49	120.80
5	E	2519	ACY	O-C-CH3	-2.22	113.44	122.53
3	C	501	PLP	C4A-C4-C3	-2.19	116.87	120.52
3	E	502	PLP	C4A-C4-C3	-2.11	117.00	120.52
3	C	501	PLP	O3P-P-O1P	2.11	119.07	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	PLP	C4A-C4-C3	-2.11	117.00	120.52
3	D	501	PLP	O3P-P-O1P	2.10	119.02	110.83
3	A	500	PLP	C4A-C4-C3	-2.10	117.03	120.52
3	B	500	PLP	C4A-C4-C3	-2.05	117.11	120.52
3	A	500	PLP	O3P-P-O1P	2.03	118.74	110.83
3	E	502	PLP	O3P-P-O1P	2.02	118.71	110.83
3	F	502	PLP	O3P-P-O1P	2.00	118.65	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2519	ACY	1	0
3	A	500	PLP	2	0
3	B	500	PLP	1	0
3	C	501	PLP	1	0
3	E	502	PLP	1	0
3	F	502	PLP	1	0
3	D	501	PLP	1	0
4	A	2550	FMT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	452/466 (96%)	0.79	33 (7%)	21	24	9, 18, 29, 43	3 (0%)
1	B	451/466 (96%)	0.74	26 (5%)	29	33	9, 18, 30, 42	2 (0%)
1	C	454/466 (97%)	0.86	35 (7%)	19	22	11, 19, 31, 48	3 (0%)
1	D	454/466 (97%)	0.82	37 (8%)	18	21	9, 18, 30, 46	4 (0%)
1	E	450/466 (96%)	0.79	31 (6%)	23	26	9, 18, 29, 40	3 (0%)
1	F	454/466 (97%)	0.81	28 (6%)	26	31	9, 18, 30, 45	2 (0%)
All	All	2715/2796 (97%)	0.80	190 (6%)	22	26	9, 18, 30, 48	17 (0%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	LEU	5.2
1	A	454	LEU	5.1
1	C	54	GLY	4.6
1	D	441	TYR	4.4
1	D	114	LYS	4.4
1	C	456	GLY	4.3
1	E	3	LYS	4.3
1	C	455	GLN	4.3
1	E	54	GLY	4.1
1	D	454	LEU	4.1
1	D	456	GLY	4.1
1	D	307	GLY	4.0
1	F	456	GLY	3.9
1	A	5	GLN	3.9
1	D	453	LYS	3.7
1	E	307	GLY	3.6
1	B	441	TYR	3.6
1	C	441	TYR	3.6
1	C	310	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	306	LEU	3.5
1	D	384	ASP	3.5
1	F	417	ASP	3.5
1	E	303	VAL	3.3
1	B	452	PRO	3.3
1	D	455	GLN	3.3
1	D	385	GLY	3.3
1	A	452	PRO	3.2
1	E	4	LYS	3.2
1	B	114	LYS	3.2
1	C	307	GLY	3.2
1	D	3	LYS	3.2
1	F	384	ASP	3.2
1	D	412	GLY	3.1
1	F	307	GLY	3.1
1	D	417	ASP	3.0
1	A	306	LEU	3.0
1	B	139	TRP	3.0
1	F	4	LYS	3.0
1	F	454	LEU	3.0
1	B	7	THR	3.0
1	B	417	ASP	3.0
1	D	304	ASP	2.9
1	E	257	ASP	2.9
1	E	310	ILE	2.9
1	E	8	ASP	2.9
1	C	453	LYS	2.9
1	D	292	GLU	2.9
1	A	424	MET	2.9
1	D	308	GLY	2.9
1	F	292	GLU	2.8
1	A	348	GLN	2.8
1	E	306	LEU	2.8
1	C	364	GLU	2.7
1	E	5	GLN	2.7
1	C	385	GLY	2.7
1	A	31	ARG	2.7
1	A	385	GLY	2.7
1	A	447	TYR	2.7
1	F	305	TYR	2.7
1	A	417	ASP	2.7
1	F	304	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	2.7
1	F	424	MET	2.6
1	E	304	ASP	2.6
1	C	433	PHE	2.6
1	D	386	GLU	2.6
1	F	293	GLU	2.6
1	C	386	GLU	2.6
1	D	448	LEU	2.6
1	E	309	GLN	2.6
1	D	6	VAL	2.6
1	D	4	LYS	2.6
1	D	143	LYS	2.6
1	C	305	TYR	2.6
1	E	452	PRO	2.6
1	A	304	ASP	2.5
1	B	308	GLY	2.5
1	C	443	ALA	2.5
1	E	292	GLU	2.5
1	A	305	TYR	2.5
1	F	390	TYR	2.5
1	F	297	GLN	2.5
1	F	414	GLU	2.5
1	A	255	ALA	2.5
1	A	174	ASP	2.5
1	A	54	GLY	2.4
1	B	384	ASP	2.4
1	A	111	PRO	2.4
1	C	184	PRO	2.4
1	E	305	TYR	2.4
1	C	372	ASP	2.4
1	D	452	PRO	2.4
1	C	297	GLN	2.4
1	D	389	GLY	2.4
1	A	384	ASP	2.4
1	B	31	ARG	2.4
1	C	292	GLU	2.4
1	B	5	GLN	2.4
1	C	369	GLY	2.4
1	F	6	VAL	2.4
1	B	304	ASP	2.3
1	A	352	TYR	2.3
1	E	110	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	385	GLY	2.3
1	A	114	LYS	2.3
1	E	139	TRP	2.3
1	F	435	GLU	2.3
1	B	306	LEU	2.3
1	F	5	GLN	2.3
1	A	310	ILE	2.3
1	F	310	ILE	2.3
1	D	31	ARG	2.3
1	C	70	GLU	2.3
1	C	35	HIS	2.3
1	C	3	LYS	2.3
1	B	142	ARG	2.3
1	C	449	SER	2.3
1	C	448	LEU	2.3
1	D	34	LEU	2.3
1	D	446	LYS	2.3
1	A	86	ASP	2.2
1	A	239	ASP	2.2
1	C	309	GLN	2.2
1	C	6	VAL	2.2
1	A	3	LYS	2.2
1	A	386	GLU	2.2
1	B	292	GLU	2.2
1	B	305	TYR	2.2
1	D	309	GLN	2.2
1	E	372	ASP	2.2
1	C	452	PRO	2.2
1	B	51	TYR	2.2
1	A	139	TRP	2.2
1	A	171	ARG	2.2
1	F	400	ARG	2.2
1	B	364	GLU	2.2
1	F	455	GLN	2.2
1	A	450	ASP	2.2
1	B	54	GLY	2.2
1	F	185	GLY	2.2
1	F	306	LEU	2.2
1	B	408	ALA	2.2
1	B	453	LYS	2.2
1	E	393	TYR	2.1
1	E	387	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	116	GLY	2.1
1	B	389	GLY	2.1
1	C	400	ARG	2.1
1	F	448	LEU	2.1
1	E	114	LYS	2.1
1	B	310	ILE	2.1
1	E	26	ILE	2.1
1	D	39	ASP	2.1
1	E	293	GLU	2.1
1	A	448	LEU	2.1
1	D	113	PRO	2.1
1	F	452	PRO	2.1
1	B	153	ASP	2.1
1	D	174	ASP	2.1
1	D	447	TYR	2.1
1	E	441	TYR	2.1
1	F	195	ILE	2.1
1	F	441	TYR	2.1
1	B	420	VAL	2.1
1	E	84	TRP	2.1
1	B	297	GLN	2.1
1	D	297	GLN	2.1
1	D	78	LEU	2.1
1	A	294	ALA	2.1
1	C	8	ASP	2.1
1	E	417	ASP	2.1
1	C	63	PHE	2.0
1	D	310[A]	ILE	2.0
1	E	357	ILE	2.0
1	C	213	TYR	2.0
1	D	424	MET	2.0
1	A	307	GLY	2.0
1	D	54	GLY	2.0
1	E	451	HIS	2.0
1	F	54	GLY	2.0
1	D	5	GLN	2.0
1	A	184	PRO	2.0
1	C	111	PRO	2.0
1	C	419	VAL	2.0
1	C	139	TRP	2.0
1	E	366	ILE	2.0
1	F	18	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	428	GLY	2.0
1	E	308	GLY	2.0
1	D	303	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($\text{\AA}^2$)	Q<0.9
6	PEG	E	2833	7/7	0.72	0.21	44,45,45,45	0
4	FMT	A	2560	3/3	0.76	0.22	31,31,31,31	0
4	FMT	D	2580	3/3	0.80	0.13	29,29,29,29	0
4	FMT	F	2670	3/3	0.82	0.12	27,27,28,28	0
4	FMT	B	2650	3/3	0.84	0.14	30,30,30,31	0
4	FMT	F	2660	3/3	0.84	0.14	30,30,30,30	0
5	ACY	E	2519	4/4	0.85	0.15	33,33,33,33	0
4	FMT	A	2600	3/3	0.87	0.11	28,28,28,28	0
2	IOD	A	2349	1/1	0.88	0.19	97,97,97,97	1
2	IOD	E	2353	1/1	0.88	0.18	50,50,50,50	1
4	FMT	D	2630	3/3	0.88	0.13	29,29,30,30	0
4	FMT	F	2590	3/3	0.88	0.12	33,33,33,33	0
4	FMT	E	2620	3/3	0.89	0.10	23,23,24,24	0
2	IOD	C	2351	1/1	0.90	0.17	53,53,53,53	1
4	FMT	D	2570	3/3	0.91	0.10	28,28,28,28	0
4	FMT	F	2640	3/3	0.91	0.09	29,29,29,30	0
3	PLP	D	501	15/16	0.92	0.09	15,15,16,16	0
2	IOD	B	2350	1/1	0.93	0.23	78,78,78,78	1
3	PLP	A	500	15/16	0.93	0.10	17,18,18,18	0
2	IOD	B	2356	1/1	0.94	0.12	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	C	2610	3/3	0.94	0.07	23,23,23,23	0
2	IOD	E	2359	1/1	0.94	0.10	49,49,49,49	1
2	IOD	F	2354	1/1	0.94	0.16	90,90,90,90	1
2	IOD	F	2360	1/1	0.94	0.14	43,43,43,43	1
2	IOD	C	2339	1/1	0.94	0.07	38,38,38,38	1
3	PLP	B	500	15/16	0.94	0.08	16,16,16,16	0
2	IOD	A	2361	1/1	0.94	0.09	39,39,39,39	1
3	PLP	F	502	15/16	0.94	0.08	16,16,17,17	0
4	FMT	A	2550	3/3	0.94	0.07	26,26,26,27	0
2	IOD	D	2352	1/1	0.94	0.20	76,76,76,76	1
2	IOD	D	2362	1/1	0.94	0.08	49,49,49,49	1
2	IOD	A	2337	1/1	0.95	0.06	36,36,36,36	1
2	IOD	E	2347	1/1	0.95	0.07	50,50,50,50	1
3	PLP	C	501	15/16	0.95	0.09	16,17,17,18	0
2	IOD	D	2358	1/1	0.95	0.10	45,45,45,45	1
2	IOD	C	2345	1/1	0.96	0.06	45,45,45,45	1
2	IOD	B	2338	1/1	0.96	0.06	35,35,35,35	1
2	IOD	C	2357	1/1	0.96	0.10	54,54,54,54	1
3	PLP	E	502	15/16	0.96	0.07	16,16,17,17	0
2	IOD	A	2355	1/1	0.96	0.12	48,48,48,48	1
2	IOD	F	2342	1/1	0.97	0.05	34,34,34,34	1
2	IOD	F	2348	1/1	0.97	0.05	42,42,42,42	1
2	IOD	D	2346	1/1	0.97	0.04	41,41,41,41	1
2	IOD	D	2340	1/1	0.97	0.05	30,30,30,30	1
2	IOD	E	2341	1/1	0.97	0.05	37,37,37,37	1
2	IOD	B	2344	1/1	0.98	0.06	39,39,39,39	1
2	IOD	B	2332	1/1	0.99	0.02	24,24,24,24	0
2	IOD	B	2333	1/1	0.99	0.02	22,22,22,22	0
2	IOD	A	2343	1/1	0.99	0.05	47,47,47,47	1
2	IOD	E	2335	1/1	0.99	0.02	20,20,20,20	1
2	IOD	F	2336	1/1	0.99	0.02	25,25,25,25	0
2	IOD	A	2331	1/1	1.00	0.01	20,20,20,20	0
2	IOD	D	2334	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.