W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2024 – 11:28 AM EST

PDB ID	:	4FCC
Title	:	Glutamate dehydrogenase from E. coli
Authors	:	Bilokapic, S.; Schwartz, T.U.
Deposited on	:	2012-05-24
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

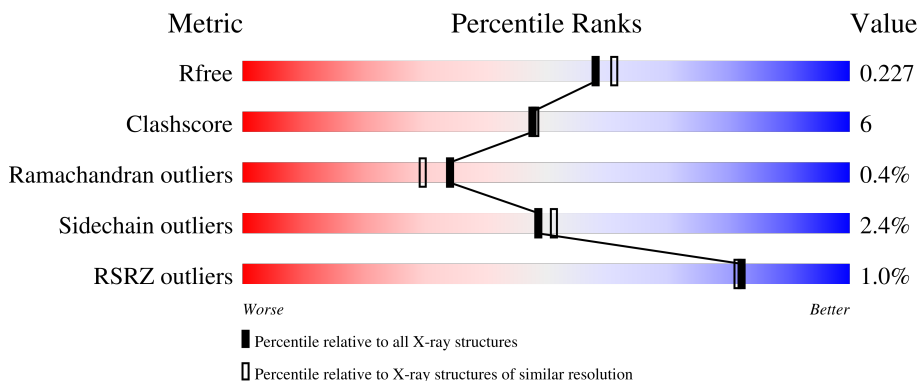|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		2.4%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	450	88% ⋯ 10% ··
1	B	450	.% 84% ⋯ 14% ··
1	C	450	4% 80% ⋯ 16% ··
1	D	450	2% 85% ⋯ 13% ·
1	E	450	87% ⋯ 10% ··

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Mol	Chain	Length	Quality of chain
1	F	450	87% 11% ··
1	G	450	88% 10% ··
1	H	450	2% 79% 18% ·
1	I	450	2% 82% 14% ··
1	J	450	86% 12% ·
1	K	450	84% 13% ··
1	L	450	89% 9% ··

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 44159 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 dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	B	442	Total 3370	C 2122	N 594	O 633	S 21	0	1	0
1	C	435	Total 3318	C 2094	N 582	O 621	S 21	0	1	0
1	D	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	E	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	F	442	Total 3373	C 2124	N 596	O 632	S 21	0	1	0
1	G	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	H	438	Total 3337	C 2104	N 587	O 625	S 21	0	0	0
1	I	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	J	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	K	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0
1	L	442	Total 3366	C 2119	N 594	O 632	S 21	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP Q8XDW9
A	-1	GLY	-	expression tag	UNP Q8XDW9
A	0	SER	-	expression tag	UNP Q8XDW9
B	-2	PRO	-	expression tag	UNP Q8XDW9
B	-1	GLY	-	expression tag	UNP Q8XDW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q8XDW9
C	-2	PRO	-	expression tag	UNP Q8XDW9
C	-1	GLY	-	expression tag	UNP Q8XDW9
C	0	SER	-	expression tag	UNP Q8XDW9
D	-2	PRO	-	expression tag	UNP Q8XDW9
D	-1	GLY	-	expression tag	UNP Q8XDW9
D	0	SER	-	expression tag	UNP Q8XDW9
E	-2	PRO	-	expression tag	UNP Q8XDW9
E	-1	GLY	-	expression tag	UNP Q8XDW9
E	0	SER	-	expression tag	UNP Q8XDW9
F	-2	PRO	-	expression tag	UNP Q8XDW9
F	-1	GLY	-	expression tag	UNP Q8XDW9
F	0	SER	-	expression tag	UNP Q8XDW9
G	-2	PRO	-	expression tag	UNP Q8XDW9
G	-1	GLY	-	expression tag	UNP Q8XDW9
G	0	SER	-	expression tag	UNP Q8XDW9
H	-2	PRO	-	expression tag	UNP Q8XDW9
H	-1	GLY	-	expression tag	UNP Q8XDW9
H	0	SER	-	expression tag	UNP Q8XDW9
I	-2	PRO	-	expression tag	UNP Q8XDW9
I	-1	GLY	-	expression tag	UNP Q8XDW9
I	0	SER	-	expression tag	UNP Q8XDW9
J	-2	PRO	-	expression tag	UNP Q8XDW9
J	-1	GLY	-	expression tag	UNP Q8XDW9
J	0	SER	-	expression tag	UNP Q8XDW9
K	-2	PRO	-	expression tag	UNP Q8XDW9
K	-1	GLY	-	expression tag	UNP Q8XDW9
K	0	SER	-	expression tag	UNP Q8XDW9
L	-2	PRO	-	expression tag	UNP Q8XDW9
L	-1	GLY	-	expression tag	UNP Q8XDW9
L	0	SER	-	expression tag	UNP Q8XDW9

- Molecule 2 is water.

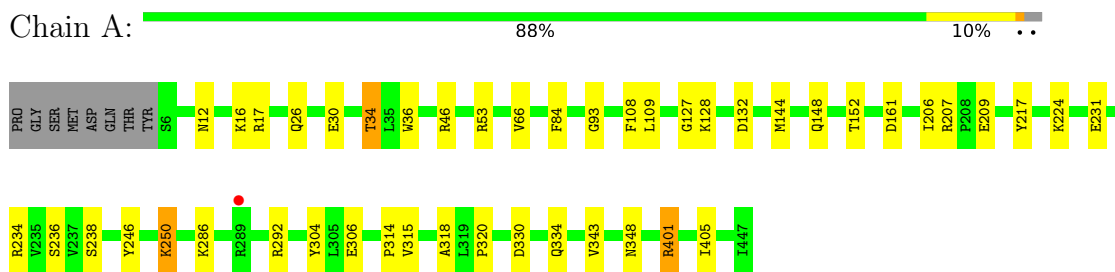| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	409	Total 409	O 409	0	0
2	B	277	Total 277	O 277	0	0
2	C	300	Total 300	O 300	0	0
2	D	254	Total 254	O 254	0	0

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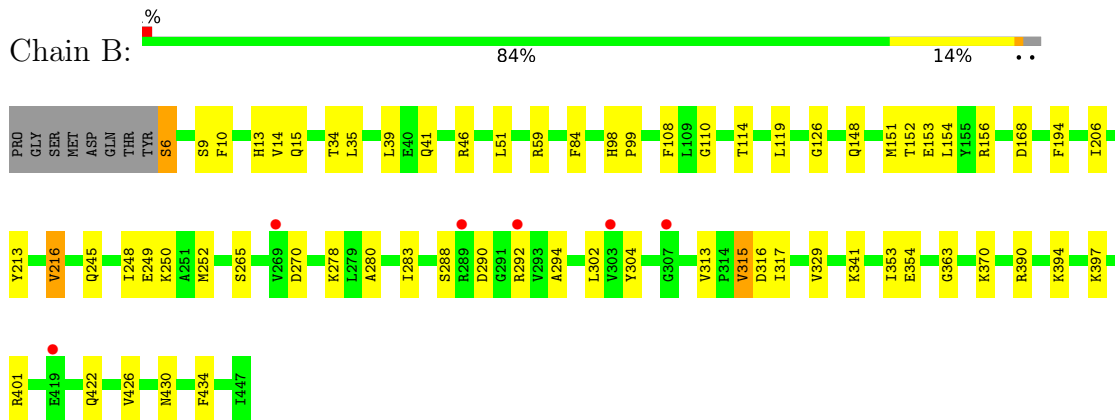| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	351	Total 351	O 351	0	0
2	F	323	Total 323	O 323	0	0
2	G	370	Total 370	O 370	0	0
2	H	288	Total 288	O 288	0	0
2	I	276	Total 276	O 276	0	0
2	J	325	Total 325	O 325	0	0
2	K	335	Total 335	O 335	0	0
2	L	325	Total 325	O 325	0	0

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.
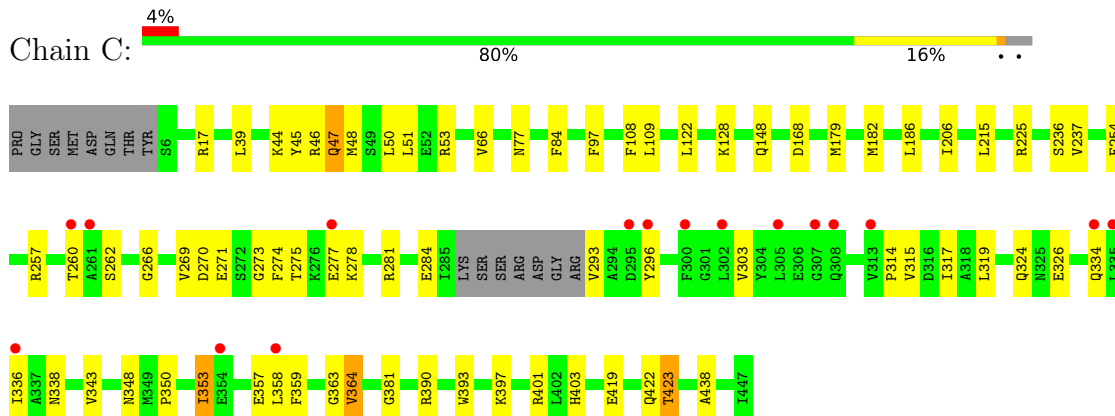
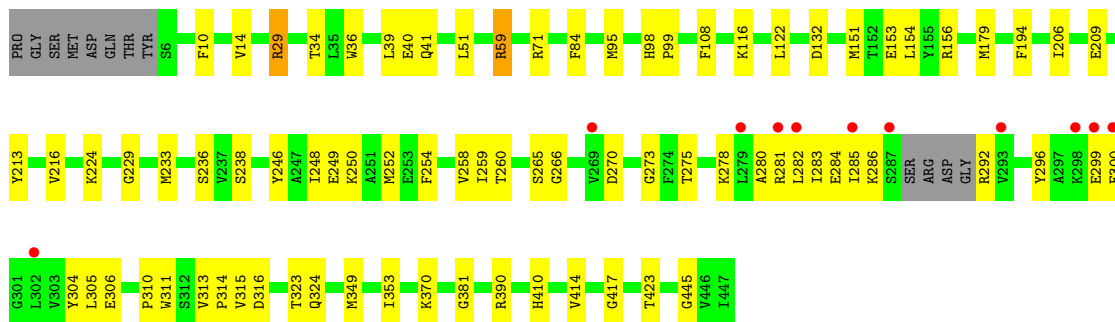• Molecule 1: Glutamate dehydrogenase

Chain A:

• Molecule 1: Glutamate dehydrogenase

Chain B:

• Molecule 1: Glutamate dehydrogenase

Chain C:

• Molecule 1: Glutamate dehydrogenase

Chain D:

• Molecule 1: Glutamate dehydrogenase

Chain E:

• Molecule 1: Glutamate dehydrogenase

Chain F:

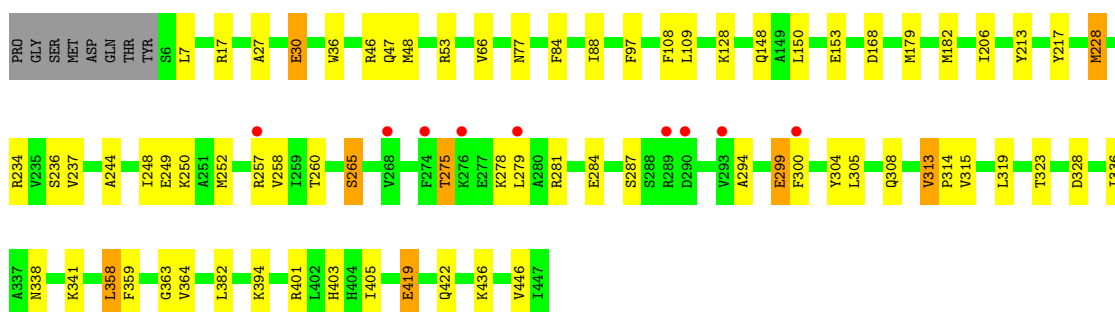• Molecule 1: Glutamate dehydrogenase
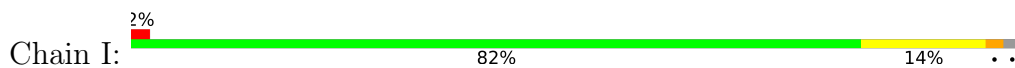
Chain G:

• Molecule 1: Glutamate dehydrogenase
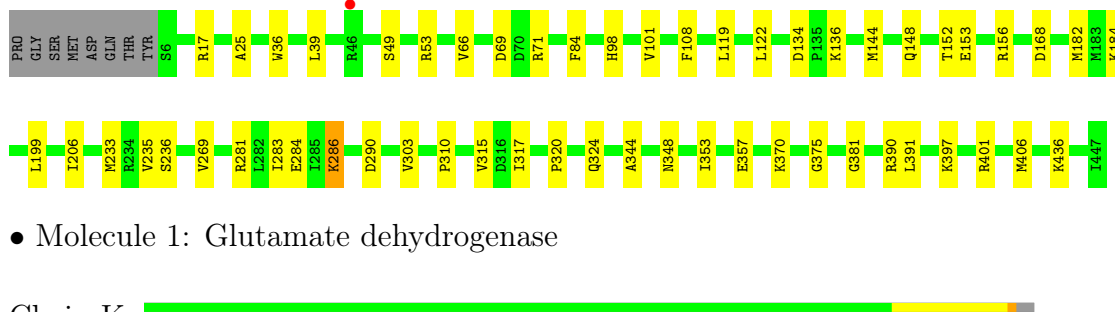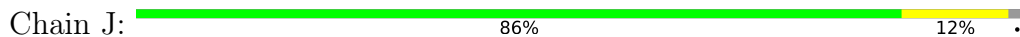
Chain H:

- Molecule 1: Glutamate dehydrogenase

- Molecule 1: Glutamate dehydrogenase

- Molecule 1: Glutamate dehydrogenase

- Molecule 1: Glutamate dehydrogenase

Chain L:
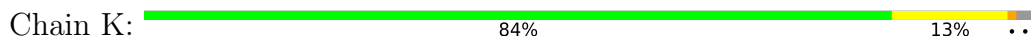
89%

9%

PRO GLY SER MET ASP GLN THR TYR S6 N12 T22 Q26 L35 W36 Q47 M48 V66 F108 L122 D132 Q148 T152 L205 I206 R207 V216 F230 S236 E271 S288 R289 D290 G291 R292 V315 N325 V329 H333

E345 G346 A347 N348 M349 P350 T351 T352 I353 L358 F359 Q360 Q361 F366 G381 R401 V426 N430 V446 I447

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.22Å 176.26Å 150.25Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	49.65 – 2.00 49.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.65-2.00) 98.9 (49.67-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.181 , 0.229 0.178 , 0.227	Depositor DCC
R_{free} test set	3646 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.4	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.346 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	44159	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1   Standard geometry (i)

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	0.40	0/3431	0.53	0/4630
1	B	0.35	0/3438	0.52	0/4640
1	C	0.38	0/3386	0.53	0/4571
1	D	0.35	0/3431	0.51	0/4630
1	E	0.39	0/3431	0.52	0/4630
1	F	0.38	0/3442	0.51	0/4645
1	G	0.41	0/3431	0.54	0/4630
1	H	0.36	0/3401	0.52	1/4589 (0.0%)
1	I	0.36	0/3431	0.50	0/4630
1	J	0.38	0/3431	0.52	0/4630
1	K	0.38	0/3431	0.54	0/4630
1	L	0.38	0/3431	0.51	0/4630
All	All	0.38	0/41115	0.52	1/55485 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	59	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3366	0	3324	37	0
1	B	3370	0	3331	49	0
1	C	3318	0	3274	55	0
1	D	3366	0	3324	43	0
1	E	3366	0	3324	30	0
1	F	3373	0	3331	37	0
1	G	3366	0	3324	32	0
1	H	3337	0	3298	59	0
1	I	3366	0	3324	48	0
1	J	3366	0	3324	46	0
1	K	3366	0	3324	41	0
1	L	3366	0	3324	32	0
2	A	409	0	0	16	0
2	B	277	0	0	14	0
2	C	300	0	0	12	0
2	D	254	0	0	18	0
2	E	351	0	0	8	0
2	F	323	0	0	12	0
2	G	370	0	0	10	0
2	H	288	0	0	16	0
2	I	276	0	0	4	0
2	J	325	0	0	14	0
2	K	335	0	0	11	0
2	L	325	0	0	12	0
All	All	44159	0	39826	485	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 6.

The worst 5 of 485 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:H:151:MET:SD	2:H:508:HOH:O	2.07	1.10
1:C:179:MET:SD	2:C:639:HOH:O	2.17	1.01
1:H:153:GLU:O	1:H:156:ARG:NH1	1.93	1.00
1:J:153:GLU:O	1:J:156:ARG:NH1	1.98	0.96
1:J:406:MET:SD	2:J:542:HOH:O	2.23	0.95

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	440/450 (98%)	433 (98%)	6 (1%)	1 (0%)	47	44
1	B	441/450 (98%)	427 (97%)	12 (3%)	2 (0%)	29	23
1	C	432/450 (96%)	420 (97%)	11 (2%)	1 (0%)	47	44
1	D	440/450 (98%)	421 (96%)	15 (3%)	4 (1%)	17	11
1	E	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	47	44
1	F	441/450 (98%)	429 (97%)	10 (2%)	2 (0%)	29	23
1	G	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	29	23
1	H	434/450 (96%)	418 (96%)	15 (4%)	1 (0%)	47	44
1	I	440/450 (98%)	429 (98%)	9 (2%)	2 (0%)	29	23
1	J	440/450 (98%)	428 (97%)	10 (2%)	2 (0%)	29	23
1	K	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	29	23
1	L	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	47	44
All	All	5268/5400 (98%)	5127 (97%)	120 (2%)	21 (0%)	34	30

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	E	206	ILE

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	347/354 (98%)	340 (98%)	7 (2%)	55	58
1	B	348/354 (98%)	340 (98%)	8 (2%)	50	53
1	C	342/354 (97%)	331 (97%)	11 (3%)	39	38
1	D	347/354 (98%)	340 (98%)	7 (2%)	55	58
1	E	347/354 (98%)	338 (97%)	9 (3%)	46	48
1	F	348/354 (98%)	342 (98%)	6 (2%)	60	65
1	G	347/354 (98%)	339 (98%)	8 (2%)	50	53
1	H	344/354 (97%)	336 (98%)	8 (2%)	50	53
1	I	347/354 (98%)	334 (96%)	13 (4%)	34	32
1	J	347/354 (98%)	342 (99%)	5 (1%)	67	72
1	K	347/354 (98%)	336 (97%)	11 (3%)	39	38
1	L	347/354 (98%)	340 (98%)	7 (2%)	55	58
All	All	4158/4248 (98%)	4058 (98%)	100 (2%)	49	51

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	71	ARG
1	I	299	GLU
1	L	401	ARG
1	H	108	PHE
1	I	84	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	422	GLN
1	F	422	GLN
1	L	26	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 ⓘ

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	442/450 (98%)	-0.57	1 (0%)	95	94	15, 26, 45, 79	0
1	B	442/450 (98%)	-0.38	6 (1%)	75	74	17, 32, 68, 129	0
1	C	435/450 (96%)	-0.14	16 (3%)	41	41	14, 31, 78, 104	0
1	D	442/450 (98%)	-0.36	7 (1%)	72	70	17, 33, 59, 108	0
1	E	442/450 (98%)	-0.56	1 (0%)	95	94	15, 28, 49, 80	0
1	F	442/450 (98%)	-0.58	0	100	100	15, 28, 47, 69	0
1	G	442/450 (98%)	-0.44	1 (0%)	95	94	14, 26, 48, 69	0
1	H	438/450 (97%)	-0.25	11 (2%)	57	56	17, 32, 75, 111	0
1	I	442/450 (98%)	-0.16	9 (2%)	65	63	14, 33, 81, 132	0
1	J	442/450 (98%)	-0.47	1 (0%)	95	94	15, 26, 48, 86	0
1	K	442/450 (98%)	-0.51	1 (0%)	95	94	15, 28, 50, 68	0
1	L	442/450 (98%)	-0.48	0	100	100	14, 29, 54, 77	0
All	All	5293/5400 (98%)	-0.41	54 (1%)	82	81	14, 29, 62, 132	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	ARG	7.0
1	H	302	LEU	5.2
1	H	281	ARG	4.7
1	D	288	SER	4.1
1	D	287	SER	3.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.