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 ⓘ

Mar 23, 2024 – 07:52 PM EDT

|		
PDB ID	:	2AP9
Title	:	Crystal structure of acetylglutamate kinase from Mycobacterium tuberculosis CDC1551
Authors	:	Rajashankar, K.R.; Kniewel, R.; Lee, K.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2005-08-15
Resolution	:	2.80 Å(reported)

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 2.80 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.
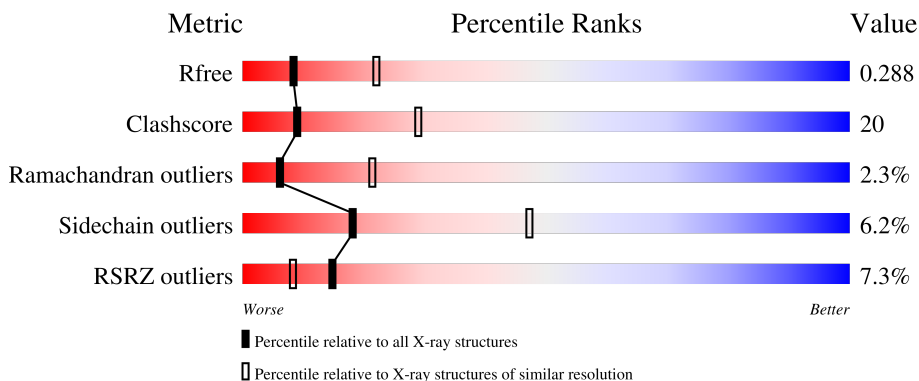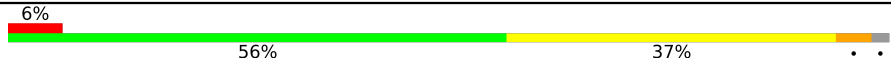
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	299	5% / 56% / 39% / ..
1	B	299	3% / 54% / 39% / ..
1	C	299	8% / 57% / 37% / ..
1	D	299	2% / 55% / 37% / 5% ..
1	E	299	17% / 54% / 39% / 6% .

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Mol	Chain	Length	Quality of chain
1	F	299	6% / 56% / 37%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13141 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 acetylglutamate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	Se	0	0	0
			2221	1400	399	412	3	7			
1	B	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			
1	C	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			
1	D	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			
1	E	295	Total	C	N	O	S	Se	0	0	0
			2180	1376	387	407	3	7			
1	F	292	Total	C	N	O	S	Se	0	0	0
			2156	1362	380	404	3	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MSE	MET	modified residue	UNP P0A4Y6
A	55	MSE	MET	modified residue	UNP P0A4Y6
A	78	MSE	MET	modified residue	UNP P0A4Y6
A	105	MSE	MET	modified residue	UNP P0A4Y6
A	167	MSE	MET	modified residue	UNP P0A4Y6
A	213	MSE	MET	modified residue	UNP P0A4Y6
A	248	LEU	SER	conflict	UNP P0A4Y6
A	250	MSE	MET	modified residue	UNP P0A4Y6
A	297	GLU	-	expression tag	UNP P0A4Y6
A	298	GLY	-	expression tag	UNP P0A4Y6
A	299	HIS	-	expression tag	UNP P0A4Y6
A	300	HIS	-	expression tag	UNP P0A4Y6
A	301	HIS	-	expression tag	UNP P0A4Y6
A	302	HIS	-	expression tag	UNP P0A4Y6
A	303	HIS	-	expression tag	UNP P0A4Y6
A	304	HIS	-	expression tag	UNP P0A4Y6
B	42	MSE	MET	modified residue	UNP P0A4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	MSE	MET	modified residue	UNP P0A4Y6
B	78	MSE	MET	modified residue	UNP P0A4Y6
B	105	MSE	MET	modified residue	UNP P0A4Y6
B	167	MSE	MET	modified residue	UNP P0A4Y6
B	213	MSE	MET	modified residue	UNP P0A4Y6
B	248	LEU	SER	conflict	UNP P0A4Y6
B	250	MSE	MET	modified residue	UNP P0A4Y6
B	297	GLU	-	expression tag	UNP P0A4Y6
B	298	GLY	-	expression tag	UNP P0A4Y6
B	299	HIS	-	expression tag	UNP P0A4Y6
B	300	HIS	-	expression tag	UNP P0A4Y6
B	301	HIS	-	expression tag	UNP P0A4Y6
B	302	HIS	-	expression tag	UNP P0A4Y6
B	303	HIS	-	expression tag	UNP P0A4Y6
B	304	HIS	-	expression tag	UNP P0A4Y6
C	42	MSE	MET	modified residue	UNP P0A4Y6
C	55	MSE	MET	modified residue	UNP P0A4Y6
C	78	MSE	MET	modified residue	UNP P0A4Y6
C	105	MSE	MET	modified residue	UNP P0A4Y6
C	167	MSE	MET	modified residue	UNP P0A4Y6
C	213	MSE	MET	modified residue	UNP P0A4Y6
C	248	LEU	SER	conflict	UNP P0A4Y6
C	250	MSE	MET	modified residue	UNP P0A4Y6
C	297	GLU	-	expression tag	UNP P0A4Y6
C	298	GLY	-	expression tag	UNP P0A4Y6
C	299	HIS	-	expression tag	UNP P0A4Y6
C	300	HIS	-	expression tag	UNP P0A4Y6
C	301	HIS	-	expression tag	UNP P0A4Y6
C	302	HIS	-	expression tag	UNP P0A4Y6
C	303	HIS	-	expression tag	UNP P0A4Y6
C	304	HIS	-	expression tag	UNP P0A4Y6
D	42	MSE	MET	modified residue	UNP P0A4Y6
D	55	MSE	MET	modified residue	UNP P0A4Y6
D	78	MSE	MET	modified residue	UNP P0A4Y6
D	105	MSE	MET	modified residue	UNP P0A4Y6
D	167	MSE	MET	modified residue	UNP P0A4Y6
D	213	MSE	MET	modified residue	UNP P0A4Y6
D	248	LEU	SER	conflict	UNP P0A4Y6
D	250	MSE	MET	modified residue	UNP P0A4Y6
D	297	GLU	-	expression tag	UNP P0A4Y6
D	298	GLY	-	expression tag	UNP P0A4Y6
D	299	HIS	-	expression tag	UNP P0A4Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	300	HIS	-	expression tag	UNP P0A4Y6
D	301	HIS	-	expression tag	UNP P0A4Y6
D	302	HIS	-	expression tag	UNP P0A4Y6
D	303	HIS	-	expression tag	UNP P0A4Y6
D	304	HIS	-	expression tag	UNP P0A4Y6
E	42	MSE	MET	modified residue	UNP P0A4Y6
E	55	MSE	MET	modified residue	UNP P0A4Y6
E	78	MSE	MET	modified residue	UNP P0A4Y6
E	105	MSE	MET	modified residue	UNP P0A4Y6
E	167	MSE	MET	modified residue	UNP P0A4Y6
E	213	MSE	MET	modified residue	UNP P0A4Y6
E	248	LEU	SER	conflict	UNP P0A4Y6
E	250	MSE	MET	modified residue	UNP P0A4Y6
E	297	GLU	-	expression tag	UNP P0A4Y6
E	298	GLY	-	expression tag	UNP P0A4Y6
E	299	HIS	-	expression tag	UNP P0A4Y6
E	300	HIS	-	expression tag	UNP P0A4Y6
E	301	HIS	-	expression tag	UNP P0A4Y6
E	302	HIS	-	expression tag	UNP P0A4Y6
E	303	HIS	-	expression tag	UNP P0A4Y6
E	304	HIS	-	expression tag	UNP P0A4Y6
F	42	MSE	MET	modified residue	UNP P0A4Y6
F	55	MSE	MET	modified residue	UNP P0A4Y6
F	78	MSE	MET	modified residue	UNP P0A4Y6
F	105	MSE	MET	modified residue	UNP P0A4Y6
F	167	MSE	MET	modified residue	UNP P0A4Y6
F	213	MSE	MET	modified residue	UNP P0A4Y6
F	248	LEU	SER	conflict	UNP P0A4Y6
F	250	MSE	MET	modified residue	UNP P0A4Y6
F	297	GLU	-	expression tag	UNP P0A4Y6
F	298	GLY	-	expression tag	UNP P0A4Y6
F	299	HIS	-	expression tag	UNP P0A4Y6
F	300	HIS	-	expression tag	UNP P0A4Y6
F	301	HIS	-	expression tag	UNP P0A4Y6
F	302	HIS	-	expression tag	UNP P0A4Y6
F	303	HIS	-	expression tag	UNP P0A4Y6
F	304	HIS	-	expression tag	UNP P0A4Y6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ni 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total 34	O 34	0	0
4	B	24	Total 24	O 24	0	0
4	C	13	Total 13	O 13	0	0
4	D	17	Total 17	O 17	0	0
4	E	15	Total 15	O 15	0	0
4	F	10	Total 10	O 10	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: acetylglutamate kinase

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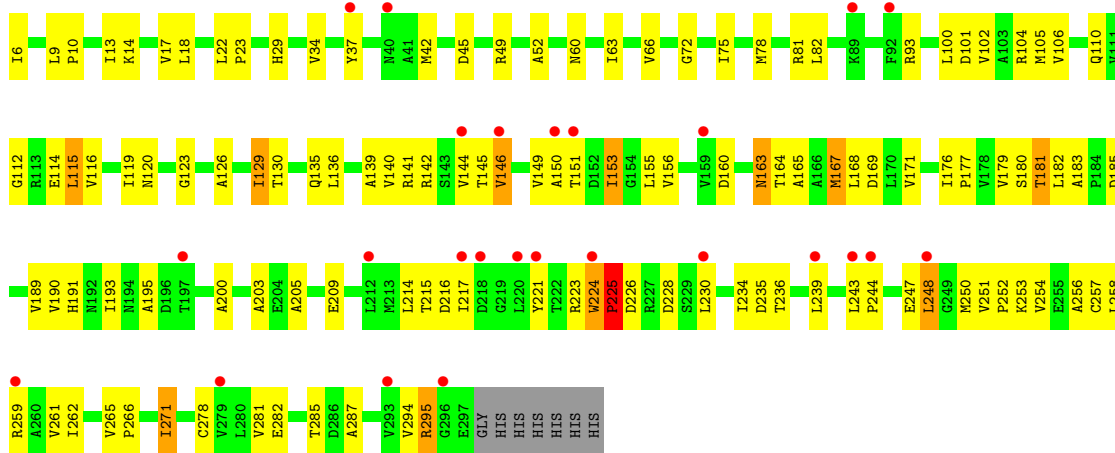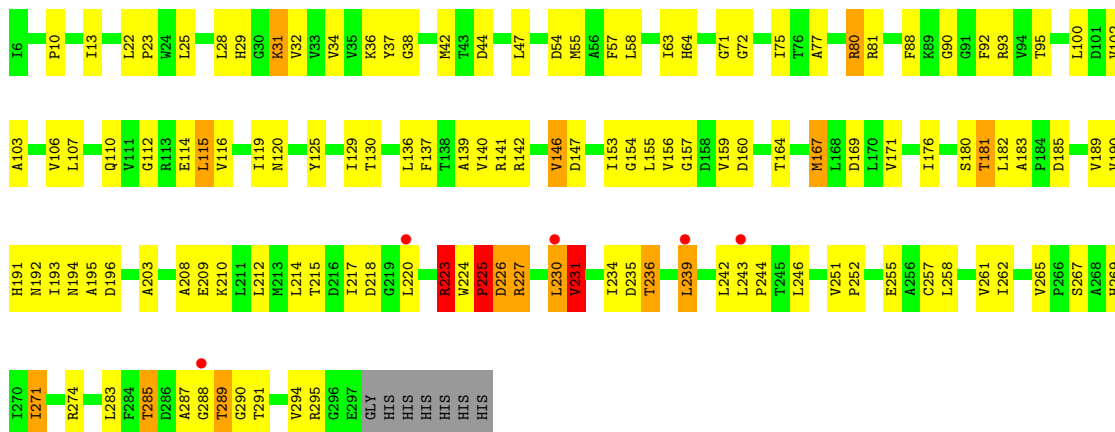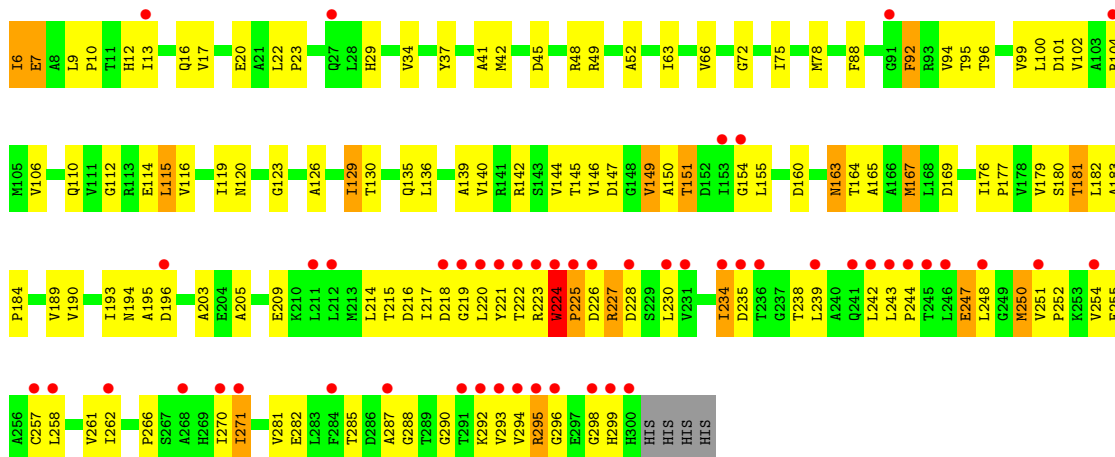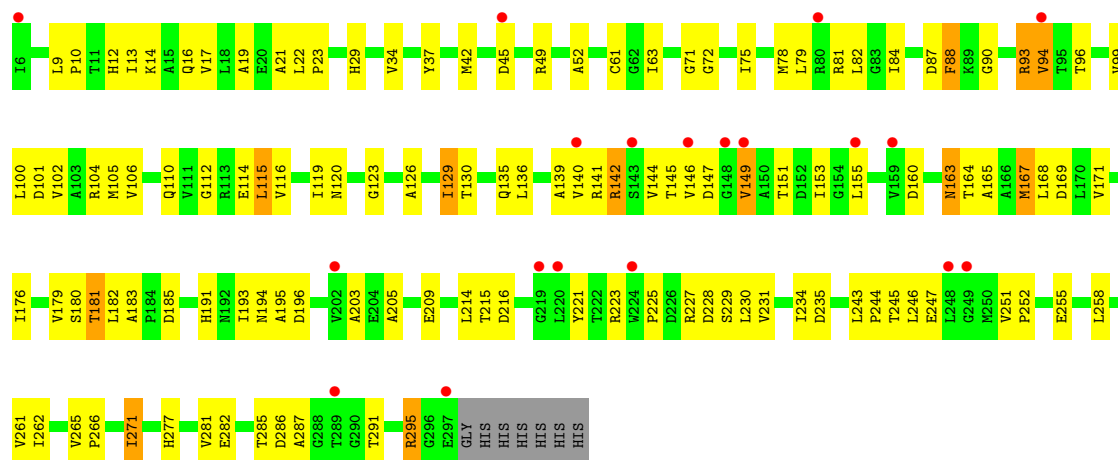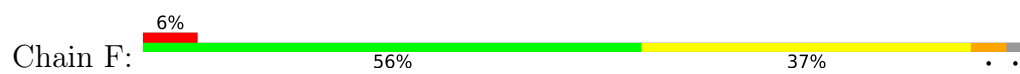I6 L9 P10 I13 K14 V17 L18 L22 P23 H29 V34 Y37 N40 A41 M42 D45 R49 A52 N60 I63 V66 G72 I75 M78 R81 L82 K89 F92 R93 L100 D101 V102 A103 R104 M105 V106 Q110 V111

G112 R113 E114 L115 V116 I119 N120 G123 A126 I129 T130 Q135 L136 A139 V140 R141 R142 S143 V144 T145 V146 V149 A150 T151 D152 I153 G154 L155 V156 V159 D160 N163 T164 A165 A166 M167 L168 D169 L170 V171 I176 P177 V178 V179 S180 T181 L182 A183 P184 D185

V189 V190 H191 N192 I193 N194 A195 D196 T197 A200 A203 E204 A205 E209 L212 M213 L214 T215 D216 I217 D218 G219 L220 Y221 T222 R223 W224 P225 D226 R227 D228 S229 L230 I234 D235 T236 L239 L243 P244 E247 L248 G249 M250 V251 P252 K253 V254 E255 A256 C257 L258

R259 A260 V261 I262 V265 P266 I271 C278 V279 L280 V281 E282 T285 D286 A287 V293 V294 R295 G296 E297 GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: acetylglutamate kinase

Chain D:

2%
55%   37%   5%

I6 P10 I13 L22 P23 W24 L25 L28 H29 G30 K31 V32 V33 V34 V35 K36 Y37 G38 M42 T43 D44 L47 D54 M55 A56 F57 L58 I63 H64 G71 G72 I75 I76 A77 R80 R81 F88 K89 G90 G91 F92 R93 V94 T95 L100 D101 V102

A103 V106 L107 Q110 V111 G112 R113 E114 L115 V116 I119 N120 Y125 I129 T130 L136 F137 T138 A139 V140 R141 R142 V146 D147 I153 G154 L155 V156 G157 D158 V159 D160 T164 M167 L168 D169 L170 V171 I176 S180 T181 L182 A183 P184 D185 V189 V190

H191 N192 I193 N194 A195 D196 A203 A208 E209 K210 L211 L212 M213 L214 T215 D216 I217 D218 G219 L220 R223 W224 P225 D226 R227 L230 V231 I234 D235 T236 L239 L242 L243 P244 T245 L246 V251 P252 E255 A256 C257 L258 V261 I262 V265 P266 S267 A268 H269

I270 I271 R274 L283 F284 T285 D286 A287 G288 T289 G290 T291 V294 R295 G296 E297 GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: acetylglutamate kinase

Chain E:

17%
54%   39%   6%

I6 E7 A8 L9 P10 T11 H12 I13 Q16 V17 E20 A21 L22 P23 Q27 L28 H29 V34 Y37 A41 M42 D45 R48 R49 A52 I63 V66 G72 I75 M78 F88 G91 F92 R93 V94 T95 T96 V99 L100 D101 V102 A103 R104

M105 V106 Q110 V111 G112 R113 E114 L115 V116 I119 N120 G123 A126 I129 T130 Q135 L136 A139 V140 R141 R142 S143 V144 T145 V146 D147 V149 A150 T151 D152 I153 G154 L155 D160 N163 T164 A165 A166 M167 L168 D169 I176 P177 V178 V179 S180 T181 L182 A183

P184 V189 V190 I193 N194 A195 D196 A203 E204 A205 E209 K210 L211 L212 M213 L214 T215 D216 I217 D218 G219 L220 Y221 T222 R223 W224 P225 D226 R227 D228 S229 L230 V231 I234 D235 G237 T238 L239 A240 Q241 L242 L243 P244 T245 L246 E247 L248 G249 M250 V251 P252 K253 V254 E255

A256 C257 L258 V261 I262 P266 S267 A268 H269 I270 I271 V281 E282 L283 F284 T285 D286 A287 G288 T289 G290 T291 K292 V293 V294 R295 G296 E297 G298 H299 H300 HIS HIS HIS HIS

• Molecule 1: acetylglutamate kinase

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.02Å 123.00Å 194.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.80 48.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.9 (48.80-2.80) 93.7 (48.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.284 0.267 , 0.288	Depositor DCC
R_{free} test set	4582 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	67.7	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.8	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	0.92	EDS
Total number of atoms	13141	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NI

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	0.29	0/2253	0.60	1/3058 (0.0%)
1	B	0.28	0/2182	0.60	2/2963 (0.1%)
1	C	0.28	0/2182	0.75	4/2963 (0.1%)
1	D	0.28	0/2182	0.71	7/2963 (0.2%)
1	E	0.28	0/2208	0.64	4/2998 (0.1%)
1	F	0.28	0/2182	0.63	1/2963 (0.0%)
All	All	0.28	0/13189	0.65	19/17908 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	224	TRP	C-N-CD	-19.46	77.79	120.60
1	C	224	TRP	C-N-CA	13.74	179.73	122.00
1	A	146	VAL	N-CA-C	-8.79	87.25	111.00
1	E	228	ASP	N-CA-C	8.08	132.81	111.00
1	E	226	ASP	N-CA-C	7.66	131.69	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.

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PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2221	0	2250	98	0
1	B	2156	0	2205	87	0
1	C	2156	0	2205	84	0
1	D	2156	0	2205	93	0
1	E	2180	0	2222	96	0
1	F	2156	0	2205	95	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
4	A	34	0	0	3	0
4	B	24	0	0	7	0
4	C	13	0	0	1	0
4	D	17	0	0	0	0
4	E	15	0	0	2	0
4	F	10	0	0	1	0
All	All	13141	0	13292	532	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 20.

The worst 5 of 532 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:HB3	4:A:1034:HOH:O	1.57	1.02
1:E:48:ARG:HD3	4:E:305:HOH:O	1.63	0.99
1:B:72:GLY:H	1:B:75:ILE:HD13	1.30	0.97
1:A:236:THR:HG21	1:A:262:ILE:HD11	1.45	0.96
1:E:72:GLY:H	1:E:75:ILE:HD13	1.30	0.96

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	297/299 (99%)	264 (89%)	27 (9%)	6 (2%)	7	24
1	B	290/299 (97%)	250 (86%)	31 (11%)	9 (3%)	4	14
1	C	290/299 (97%)	258 (89%)	27 (9%)	5 (2%)	9	29
1	D	290/299 (97%)	250 (86%)	32 (11%)	8 (3%)	5	17
1	E	293/299 (98%)	251 (86%)	34 (12%)	8 (3%)	5	17
1	F	290/299 (97%)	255 (88%)	30 (10%)	5 (2%)	9	29
All	All	1750/1794 (98%)	1528 (87%)	181 (10%)	41 (2%)	6	21

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	A	149	VAL
1	A	181	THR
1	B	181	THR
1	B	224	TRP

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	232/225 (103%)	217 (94%)	15 (6%)	17	44
1	B	226/225 (100%)	214 (95%)	12 (5%)	22	54
1	C	226/225 (100%)	213 (94%)	13 (6%)	20	50
1	D	226/225 (100%)	210 (93%)	16 (7%)	14	39
1	E	228/225 (101%)	213 (93%)	15 (7%)	16	44
1	F	226/225 (100%)	212 (94%)	14 (6%)	18	47
All	All	1364/1350 (101%)	1279 (94%)	85 (6%)	18	47

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	7	GLU

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type
1	F	87	ASP
1	E	101	ASP
1	E	169	ASP
1	F	129	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	191	HIS
1	F	163	ASN
1	D	40	ASN
1	F	16	GLN
1	C	163	ASN

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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	292/299 (97%)	0.33	15 (5%)	28	19	53, 74, 117, 135	0
1	B	285/299 (95%)	0.37	10 (3%)	44	34	51, 73, 111, 133	0
1	C	285/299 (95%)	0.55	25 (8%)	10	5	49, 76, 119, 135	0
1	D	285/299 (95%)	0.21	5 (1%)	68	61	49, 70, 121, 140	0
1	E	288/299 (96%)	0.92	51 (17%)	1	1	52, 81, 134, 146	0
1	F	285/299 (95%)	0.52	19 (6%)	17	10	53, 78, 129, 142	0
All	All	1720/1794 (95%)	0.48	125 (7%)	15	8	49, 75, 125, 146	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	299	HIS	6.8
1	A	149	VAL	6.0
1	E	220	LEU	5.9
1	E	239	LEU	5.9
1	E	254	VAL	5.8

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	1001	1/1	0.44	0.37	99,99,99,99	0
2	MG	A	1002	1/1	0.81	0.25	59,59,59,59	0
3	NI	A	1003	1/1	0.85	0.44	90,90,90,90	1

6.5 Other polymers (i)

There are no such residues in this entry.