WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 03:47 PM EDT

PDB ID	:	3NNK
Title	:	Biochemical and Structural Characterization of a Ureidoglycine Aminotransferase in the Klebsiella pneumoniae Uric Acid Catabolic Pathway
Authors	:	French, J.B.; Ealick, S.E.
Deposited on	:	2010-06-23
Resolution	:	2.58 Å(reported)

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	:	2.35
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)	:	2.35

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 2.58 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.
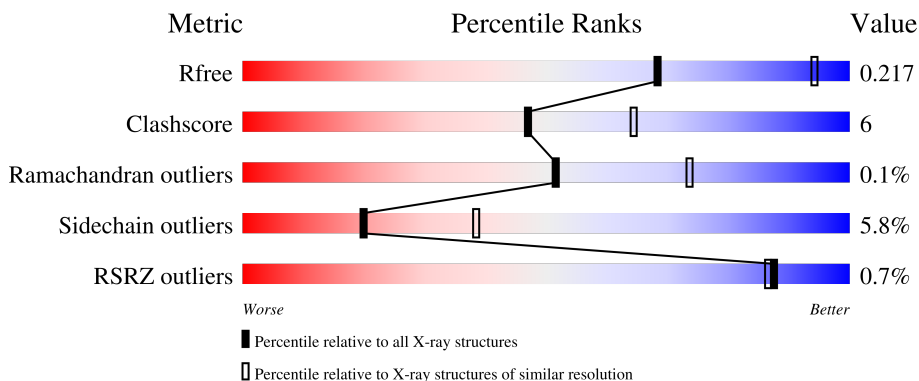
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	411	81% 18% •
1	B	411	.% 79% 20% •
1	C	411	.% 81% 17% •
1	D	411	79% 19% •
1	E	411	80% 18% •

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Mol	Chain	Length	Quality of chain
1	F	411	81% 18%
1	G	411	% 79% 19%
1	H	411	82% 16%
1	J	411	82% 17%
1	K	411	86% 13%
1	L	411	2% 82% 15%
1	M	411	80% 19%
1	O	411	84% 15%
1	P	411	81% 18%
1	R	411	2% 80% 18%
1	S	411	81% 17%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 51634 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 Ureidoglycine-glyoxylate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	P	S	0	0	0
			3158	1987	558	586	1	26			
1	B	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	C	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	D	410	Total	C	N	O	P	S	0	0	0
			3180	1999	567	588	1	25			
1	E	410	Total	C	N	O	P	S	0	0	0
			3147	1981	557	583	1	25			
1	F	410	Total	C	N	O	P	S	0	0	0
			3171	1994	566	585	1	25			
1	G	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	H	410	Total	C	N	O	P	S	0	0	0
			3183	2000	567	590	1	25			
1	J	410	Total	C	N	O	P	S	0	0	0
			3154	1984	558	586	1	25			
1	K	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	L	409	Total	C	N	O	P	S	0	0	0
			3156	1982	564	584	1	25			
1	M	410	Total	C	N	O	P	S	0	0	0
			3183	2000	567	590	1	25			
1	O	410	Total	C	N	O	P	S	0	0	0
			3154	1984	558	586	1	25			
1	P	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	R	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	S	410	Total	C	N	O	P	S	0	0	0
			3179	1999	567	587	1	25			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total 41	O 41	0	0
2	B	51	Total 51	O 51	0	0
2	C	39	Total 39	O 39	0	0
2	D	33	Total 33	O 33	0	0
2	E	49	Total 49	O 49	0	0
2	F	73	Total 73	O 73	0	0
2	G	66	Total 66	O 66	0	0
2	H	59	Total 59	O 59	0	0
2	J	73	Total 73	O 73	0	0
2	K	71	Total 71	O 71	0	0
2	L	64	Total 64	O 64	0	0
2	M	59	Total 59	O 59	0	0
2	O	69	Total 69	O 69	0	0
2	P	76	Total 76	O 76	0	0
2	R	69	Total 69	O 69	0	0
2	S	60	Total 60	O 60	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: Ureidoglycine-glyoxylate aminotransferase

Chain A:

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain B:

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain C:

V324 L325 V328 I329 P330 Q331 G351 M367 G368 M377 L383 K391 W404 R411

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain D:

79%　　　19%

MET D2 Q5 L9 N10 P11 D25 P26 R27 M32 I37 Y40 M52 R56 S73 E78 A79 I80 L81 V82 S83 A84 I85 R86 V91 L92 V93 R98 E105 I106 R109 A112 W121 G122 E123 V124 F125 T126 P127 D128 Q129 I137 R138
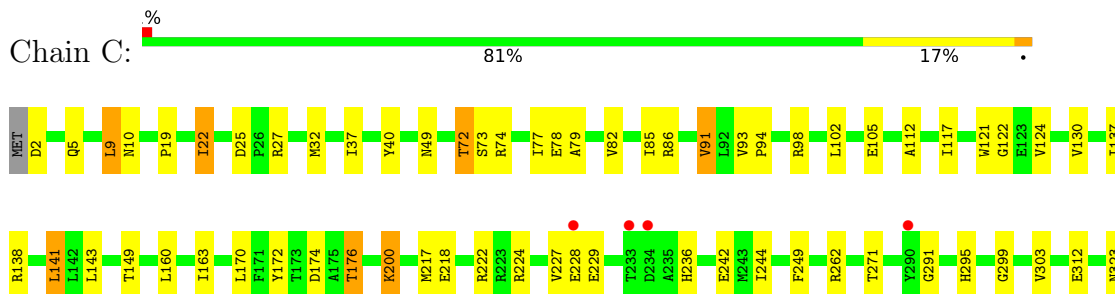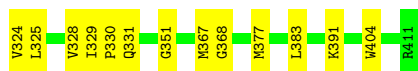
P139 R140 L141 L142 L143 Q146 T152 G161 E162 R165 L170 D174 A175 T176 A177 S178 W189 S195 Q199 K200 G203 G204 M217 E218 R224 E228 E229 G230 I231 R237 I244 M253 V254 W258 R262 L263 H266 T271 R277

G291 H295 G299 V303 M321 N322 N323 V324 L325 P330 Q331 F354 M367 G368 M377 L383 W404 R411

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain E:

80%　　　18%

MET D2 Q5 L9 N10 P11 P19 I22 D25 P26 R27 A31 M32 S33 I37 I77 E78 A79 V82 I85 R86 V91 L92 V93 F96 G97 R98 L102 E105 A112 W121 G122 E123 V124 F125 T126 Q129 K135 R136 I137 R138

L143 Q146 L154 Y167 Y172 T173 D174 A175 T176 A177 L184 K200 M217 E218 R224 E228 E229 G230 I231 R237 S246 F249 M253 T271 A272 L273 E278 R281 G291 H295 N323 V324 L325 I329 G335 R339 K340 L341

D345 I348 G351 T352 S353 F354 G359 W362 M367 G368 K373 D374 M377 T378 L383 L390 W404 R411

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain F:

81%　　　18%

MET D2 L9 N10 P11 D25 P26 R27 R30 A31 M32 S33 L36 I37 N49 M52 R56 S73 E78 A79 I80 L81 V82 S83 A84 I85 R86 V91 L92 V93 R98 E105 R109 A112 T116 W121 G122 E123 V124 F125 T126 Q129

K135 R136 I137 L141 T149 T152 M153 L154 L157 Y167 L170 D174 A175 T176 L179 E185 V188 D192 S195 A196 K200 C201 L202 G203 S214 A215 R216 R224 E229 R237 E241 I244 R262 T270 T271 H295 K296 L297

K304 M321 N322 N323 V324 L325 I348 M367 G368 M377 T378 L383 W404 D405 H406 E410 R411

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain G:

%　　79%　　　19%

- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain H:

- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain J:

- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain K:

- Molecule 1: Ureidoglycine-glyoxylate aminotransferase
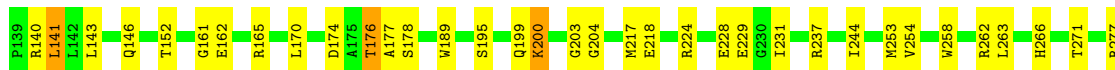
Chain L:

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain M:

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase
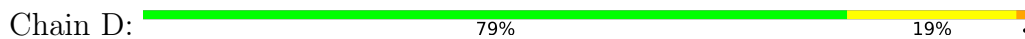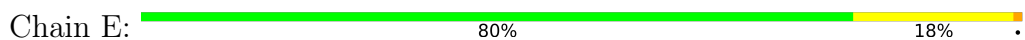
Chain O:

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase
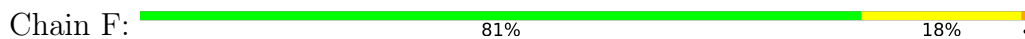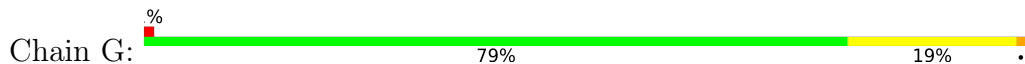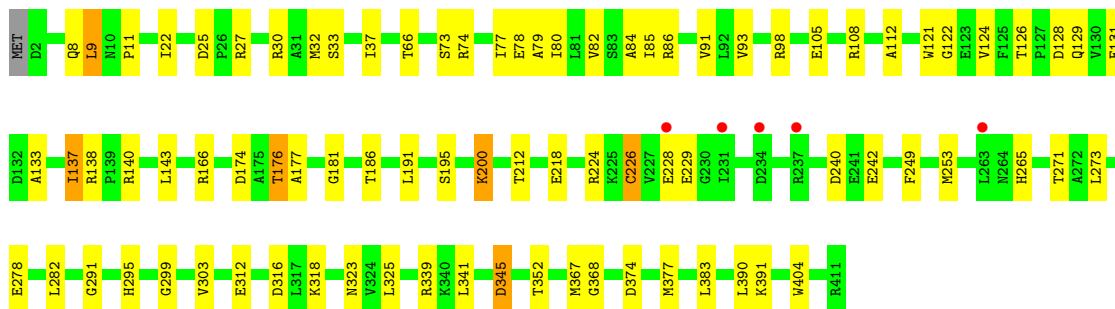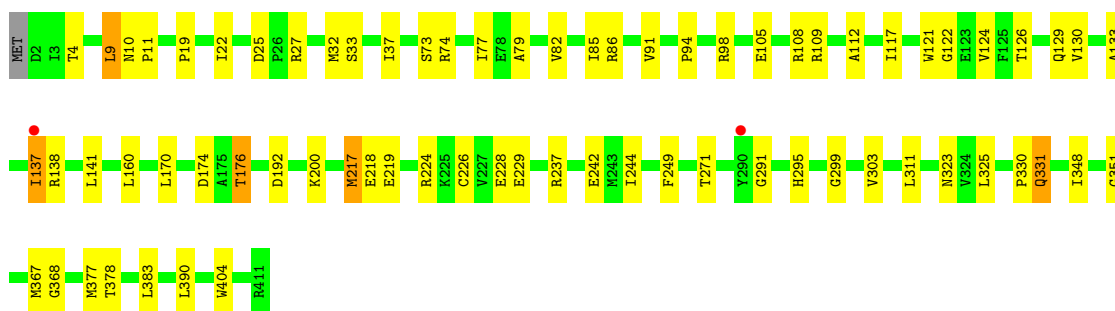
Chain P:
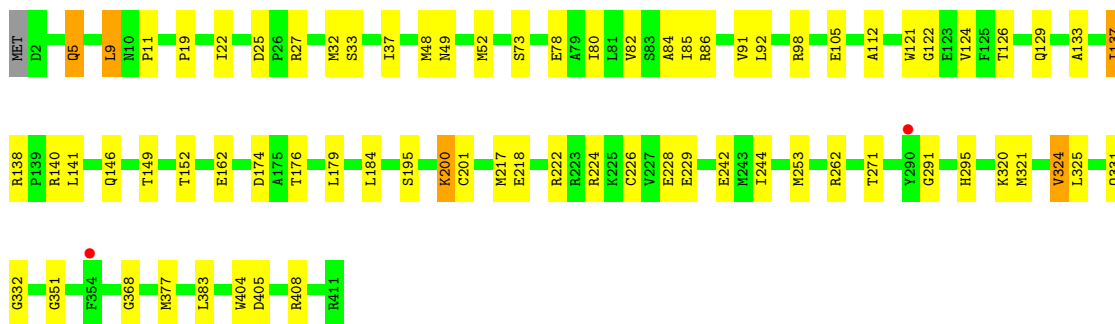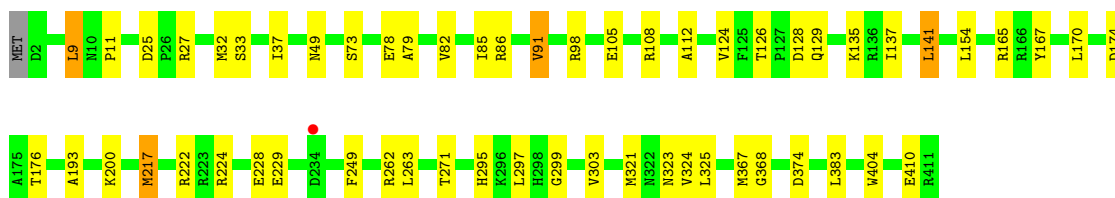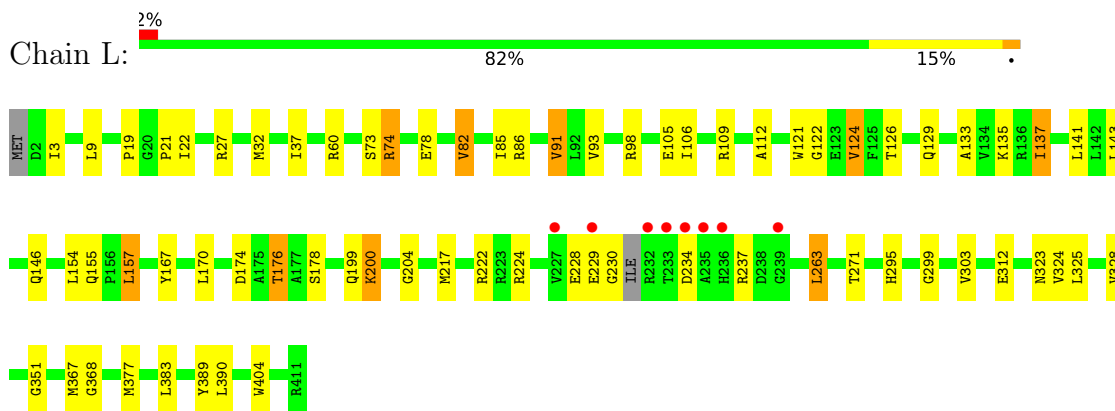
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain R:

• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain S:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	142.15Å 149.20Å 198.00Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.58 49.85 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.58) 93.9 (49.85-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.246 0.192 , 0.217	Depositor DCC
R_{free} test set	12155 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 9.1	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -k,-h,-l 0.048 for k,h,-l 0.420 for h,-k,-l	Xtriage
Reported twinning fraction	0.549 for H, K, L 0.451 for h,-k,-l	Depositor
Outliers	2 of 242432 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	51634	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 11.96% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: LLP

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	0.31	0/3198	0.52	0/4335
1	B	0.31	0/3215	0.51	0/4354
1	C	0.31	0/3204	0.52	1/4341 (0.0%)
1	D	0.32	0/3220	0.52	1/4360 (0.0%)
1	E	0.31	0/3187	0.51	0/4321
1	F	0.31	0/3211	0.52	0/4349
1	G	0.31	0/3204	0.51	0/4341
1	H	0.31	0/3223	0.51	0/4364
1	J	0.31	0/3194	0.52	0/4330
1	K	0.31	0/3215	0.52	2/4354 (0.0%)
1	L	0.31	0/3195	0.52	1/4327 (0.0%)
1	M	0.32	0/3223	0.51	0/4364
1	O	0.31	0/3194	0.52	1/4330 (0.0%)
1	P	0.31	0/3215	0.53	0/4354
1	R	0.31	0/3204	0.51	0/4341
1	S	0.32	0/3219	0.51	0/4358
All	All	0.31	0/51321	0.52	6/69523 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	141	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	141	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	141	LEU	CA-CB-CG	5.22	127.31	115.30
1	L	263	LEU	CA-CB-CG	5.14	127.13	115.30
1	O	141	LEU	CA-CB-CG	5.03	126.87	115.30

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	3158	0	3090	45	0
1	B	3175	0	3127	51	0
1	C	3164	0	3101	46	0
1	D	3180	0	3133	52	0
1	E	3147	0	3076	41	0
1	F	3171	0	3121	47	0
1	G	3164	0	3101	52	0
1	H	3183	0	3135	45	0
1	J	3154	0	3084	42	0
1	K	3175	0	3127	35	0
1	L	3156	0	3089	40	0
1	M	3183	0	3135	47	0
1	O	3154	0	3084	36	0
1	P	3175	0	3127	45	0
1	R	3164	0	3101	45	0
1	S	3179	0	3133	46	0
2	A	41	0	0	0	0
2	B	51	0	0	3	0
2	C	39	0	0	1	0
2	D	33	0	0	0	0
2	E	49	0	0	0	0
2	F	73	0	0	2	0
2	G	66	0	0	2	0
2	H	59	0	0	0	0
2	J	73	0	0	0	0
2	K	71	0	0	0	0
2	L	64	0	0	0	0
2	M	59	0	0	0	0
2	O	69	0	0	0	0
2	P	76	0	0	3	0
2	R	69	0	0	0	0
2	S	60	0	0	0	0
All	All	51634	0	49764	626	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 626 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:72:THR:HG23	1:C:200:LLP:OP2	1.58	1.03
1:H:126:THR:H	1:H:129:GLN:HE21	1.14	0.96
1:K:174:ASP:OD1	1:K:176:THR:HG23	1.69	0.92
1:O:295:HIS:HE1	1:O:368:GLY:H	1.14	0.91
1:K:9:LEU:HD13	1:K:11:PRO:HD3	1.53	0.90

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	408/411 (99%)	388 (95%)	20 (5%)	0	100	100
1	B	407/411 (99%)	390 (96%)	17 (4%)	0	100	100
1	C	407/411 (99%)	384 (94%)	22 (5%)	1 (0%)	47	69
1	D	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	47	69
1	E	407/411 (99%)	391 (96%)	15 (4%)	1 (0%)	47	69
1	F	407/411 (99%)	390 (96%)	17 (4%)	0	100	100
1	G	407/411 (99%)	391 (96%)	15 (4%)	1 (0%)	47	69
1	H	407/411 (99%)	395 (97%)	11 (3%)	1 (0%)	47	69
1	J	407/411 (99%)	392 (96%)	15 (4%)	0	100	100
1	K	407/411 (99%)	395 (97%)	12 (3%)	0	100	100
1	L	404/411 (98%)	391 (97%)	13 (3%)	0	100	100
1	M	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	47	69
1	O	407/411 (99%)	393 (97%)	14 (3%)	0	100	100
1	P	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	47	69
1	R	407/411 (99%)	395 (97%)	11 (3%)	1 (0%)	47	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	407/411 (99%)	394 (97%)	12 (3%)	1 (0%)	47	69
All	All	6510/6576 (99%)	6265 (96%)	236 (4%)	9 (0%)	51	73

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	331	GLN
1	R	391	LYS
1	D	331	GLN
1	G	226	CYS
1	S	246	SER

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	323/336 (96%)	304 (94%)	19 (6%)	19	37
1	B	327/336 (97%)	308 (94%)	19 (6%)	20	38
1	C	324/336 (96%)	305 (94%)	19 (6%)	19	37
1	D	328/336 (98%)	312 (95%)	16 (5%)	25	46
1	E	321/336 (96%)	300 (94%)	21 (6%)	17	33
1	F	326/336 (97%)	312 (96%)	14 (4%)	29	52
1	G	324/336 (96%)	303 (94%)	21 (6%)	17	33
1	H	329/336 (98%)	310 (94%)	19 (6%)	20	38
1	J	323/336 (96%)	305 (94%)	18 (6%)	21	40
1	K	327/336 (97%)	313 (96%)	14 (4%)	29	52
1	L	323/336 (96%)	297 (92%)	26 (8%)	12	22
1	M	329/336 (98%)	312 (95%)	17 (5%)	23	44
1	O	323/336 (96%)	305 (94%)	18 (6%)	21	40
1	P	327/336 (97%)	308 (94%)	19 (6%)	20	38
1	R	324/336 (96%)	305 (94%)	19 (6%)	19	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	328/336 (98%)	307 (94%)	21 (6%)	17	34
All	All	5206/5376 (97%)	4906 (94%)	300 (6%)	20	38

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	137	ILE
1	S	138	ARG
1	O	383	LEU
1	R	9	LEU
1	F	91	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	5	GLN
1	R	129	GLN
1	S	406	HIS
1	G	49	ASN
1	G	46	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	LLP	O	200	1	23,24,25	1.61	2 (8%)	25,32,34	1.67	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	LLP	B	200	1	23,24,25	1.61	2 (8%)	25,32,34	1.74	6 (24%)
1	LLP	C	200	1	23,24,25	1.64	2 (8%)	25,32,34	1.59	6 (24%)
1	LLP	E	200	1	23,24,25	1.61	2 (8%)	25,32,34	1.70	5 (20%)
1	LLP	F	200	1	23,24,25	1.62	2 (8%)	25,32,34	1.52	5 (20%)
1	LLP	J	200	1	23,24,25	1.64	2 (8%)	25,32,34	1.47	5 (20%)
1	LLP	A	200	1	23,24,25	1.64	2 (8%)	25,32,34	1.43	4 (16%)
1	LLP	K	200	1	23,24,25	1.63	2 (8%)	25,32,34	1.68	4 (16%)
1	LLP	S	200	1	23,24,25	1.64	2 (8%)	25,32,34	1.65	5 (20%)
1	LLP	G	200	1	23,24,25	1.63	2 (8%)	25,32,34	1.59	5 (20%)
1	LLP	L	200	1	23,24,25	1.63	2 (8%)	25,32,34	1.46	4 (16%)
1	LLP	P	200	1	23,24,25	1.62	2 (8%)	25,32,34	1.68	5 (20%)
1	LLP	H	200	1	23,24,25	1.62	2 (8%)	25,32,34	1.64	5 (20%)
1	LLP	R	200	1	23,24,25	1.63	2 (8%)	25,32,34	1.54	5 (20%)
1	LLP	D	200	1	23,24,25	1.64	2 (8%)	25,32,34	1.54	4 (16%)
1	LLP	M	200	1	23,24,25	1.63	2 (8%)	25,32,34	1.73	5 (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
1	LLP	O	200	1	-	4/16/17/19	0/1/1/1
1	LLP	B	200	1	-	8/16/17/19	0/1/1/1
1	LLP	C	200	1	-	10/16/17/19	0/1/1/1
1	LLP	E	200	1	-	5/16/17/19	0/1/1/1
1	LLP	F	200	1	-	7/16/17/19	0/1/1/1
1	LLP	J	200	1	-	6/16/17/19	0/1/1/1
1	LLP	A	200	1	-	7/16/17/19	0/1/1/1
1	LLP	K	200	1	-	4/16/17/19	0/1/1/1
1	LLP	S	200	1	-	7/16/17/19	0/1/1/1
1	LLP	G	200	1	-	7/16/17/19	0/1/1/1
1	LLP	L	200	1	-	5/16/17/19	0/1/1/1
1	LLP	P	200	1	-	3/16/17/19	0/1/1/1
1	LLP	H	200	1	-	5/16/17/19	0/1/1/1
1	LLP	R	200	1	-	7/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	200	1	-	5/16/17/19	0/1/1/1
1	LLP	M	200	1	-	6/16/17/19	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	200	LLP	C4'-NZ	6.46	1.49	1.27
1	F	200	LLP	C4'-NZ	6.45	1.48	1.27
1	S	200	LLP	C4'-NZ	6.45	1.48	1.27
1	J	200	LLP	C4'-NZ	6.45	1.48	1.27
1	K	200	LLP	C4'-NZ	6.44	1.48	1.27

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	LLP	OP4-C5'-C5	5.53	119.90	109.35
1	K	200	LLP	OP4-C5'-C5	5.39	119.62	109.35
1	E	200	LLP	OP4-C5'-C5	5.30	119.44	109.35
1	M	200	LLP	OP4-C5'-C5	5.10	119.07	109.35
1	P	200	LLP	OP4-C5'-C5	5.05	118.98	109.35

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	200	LLP	C4-C4'-NZ-CE
1	A	200	LLP	C5'-OP4-P-OP2
1	A	200	LLP	C-CA-CB-CG
1	B	200	LLP	C-CA-CB-CG
1	C	200	LLP	C4-C4'-NZ-CE

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	200	LLP	3	0
1	E	200	LLP	1	0
1	J	200	LLP	1	0
1	S	200	LLP	1	0
1	G	200	LLP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	200	LLP	2	0
1	P	200	LLP	1	0
1	R	200	LLP	1	0
1	D	200	LLP	2	0

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	410/411 (99%)	-0.08	1 (0%)	95	95	26, 36, 45, 53	0
1	B	409/411 (99%)	-0.11	4 (0%)	82	81	27, 33, 43, 57	0
1	C	409/411 (99%)	-0.08	4 (0%)	82	81	26, 34, 47, 57	0
1	D	409/411 (99%)	-0.17	2 (0%)	91	90	26, 33, 42, 46	0
1	E	409/411 (99%)	-0.09	2 (0%)	91	90	25, 35, 44, 48	0
1	F	409/411 (99%)	-0.14	0	100	100	26, 32, 43, 56	0
1	G	409/411 (99%)	-0.05	5 (1%)	79	77	26, 34, 45, 58	0
1	H	409/411 (99%)	-0.13	2 (0%)	91	90	25, 32, 41, 47	0
1	J	409/411 (99%)	-0.17	2 (0%)	91	90	25, 31, 41, 46	0
1	K	409/411 (99%)	-0.07	1 (0%)	95	95	25, 31, 44, 55	0
1	L	408/411 (99%)	-0.03	8 (1%)	65	62	25, 32, 43, 61	0
1	M	409/411 (99%)	-0.13	0	100	100	25, 33, 42, 46	0
1	O	409/411 (99%)	-0.12	1 (0%)	95	95	24, 31, 41, 46	0
1	P	409/411 (99%)	-0.13	1 (0%)	95	95	25, 32, 44, 55	0
1	R	409/411 (99%)	-0.03	10 (2%)	59	55	27, 32, 43, 61	0
1	S	409/411 (99%)	-0.13	1 (0%)	95	95	27, 33, 43, 46	0
All	All	6544/6576 (99%)	-0.10	44 (0%)	87	86	24, 33, 44, 61	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	234	ASP	5.2
1	R	236	HIS	5.1
1	L	235	ALA	5.0
1	L	234	ASP	4.7
1	R	233	THR	4.2

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

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
1	LLP	A	200	24/25	0.95	0.15	32,33,35,35	0
1	LLP	M	200	24/25	0.95	0.15	30,33,34,35	0
1	LLP	E	200	24/25	0.96	0.15	31,32,33,33	0
1	LLP	D	200	24/25	0.97	0.13	29,30,30,31	0
1	LLP	B	200	24/25	0.97	0.14	29,30,32,32	0
1	LLP	H	200	24/25	0.97	0.16	28,31,32,33	0
1	LLP	J	200	24/25	0.97	0.16	28,30,30,30	0
1	LLP	K	200	24/25	0.97	0.15	29,31,31,32	0
1	LLP	L	200	24/25	0.97	0.16	28,29,30,30	0
1	LLP	C	200	24/25	0.97	0.15	32,33,33,34	0
1	LLP	O	200	24/25	0.97	0.15	28,30,31,31	0
1	LLP	R	200	24/25	0.97	0.14	29,31,31,32	0
1	LLP	S	200	24/25	0.97	0.13	31,32,33,33	0
1	LLP	G	200	24/25	0.98	0.14	30,31,31,31	0
1	LLP	P	200	24/25	0.98	0.15	30,32,32,32	0
1	LLP	F	200	24/25	0.99	0.13	28,30,30,31	0

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.