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 ⓘ

Feb 15, 2017 – 03:45 am GMT

PDB ID	:	2ZCI
Title	:	Structure of a GTP-dependent bacterial PEP-carboxykinase from Corynebacterium glutamicum
Authors	:	Aich, S.; Prasad, L.; Delbaere, L.T.J.
Deposited on	:	2007-11-09
Resolution	:	2.30 Å(reported)

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

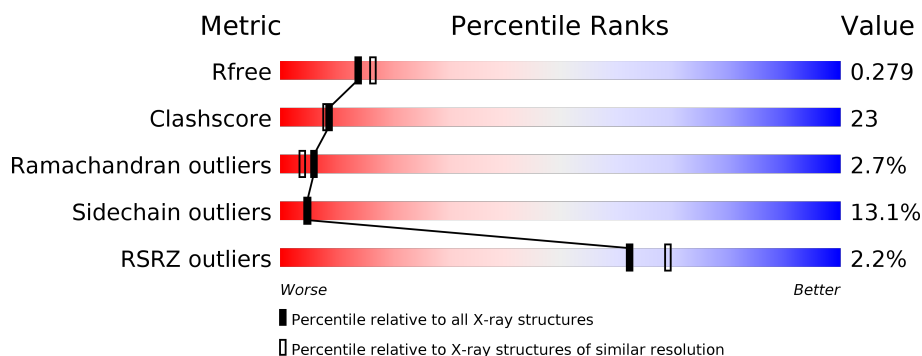|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.30 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		0.279
Clashscore		23
Ramachandran outliers		2.7%
Sidechain outliers		13.1%
RSRZ outliers		2.2%

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$_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	610	% — 61% · 26% · 7% · ·
1	B	610	2% — 52% · 34% · 8% · ·
1	C	610	2% — 56% · 31% · 8% · ·
1	D	610	3% — 50% · 33% · 10% · 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18407 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 Phosphoenolpyruvate carboxykinase [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4539	2871	764	874	30			
1	B	584	Total	C	N	O	S	0	0	0
			4518	2858	761	869	30			
1	C	586	Total	C	N	O	S	0	0	0
			4535	2869	763	873	30			
1	D	578	Total	C	N	O	S	0	0	0
			4489	2840	755	864	30			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	109	Total	O	0	0
			109	109		
2	B	69	Total	O	0	0
			69	69		
2	C	89	Total	O	0	0
			89	89		
2	D	59	Total	O	0	0
			59	59		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Phosphoenolpyruvate carboxykinase [GTP]

• Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]

K255 L256 I257 N258 P259 E260 A263 A268 P271 S272 A273 C274 G275 K276 T277 N278 L279 A280 T285 I286 P287 G288 W289 T290 A291 Q292 V293 D296 D297 I298 L301 K302 L303 R304 E305 D306 Y309 A310 V311 N315 G316 F317 F318 N325 Y326 A327 P330 T335

N340 T344 L348 T349 D350 D351 G352 D353 I354 D360 G361 D362 A363 P364 A365 H366 L367 I368 D369 W370 P377 E378 S379 D380 N382 A383 A384 S388 R389 Y390 C391 I394 S397 P398 A399 E403 F404 N405 D406 W407 E408 G409 V410 K411 I412 L416 R420 R421

P426 L427 V428 T429 Q430 T431 Y432 D433 W434 E435 H436 M439 L443 G447 GLN THR ALA ALA SER ALA GLU ALA LYS VAL G458 T459 L460 R461 H462 D463 P464 M465 L468 P469 F470 E477 N481 W482 G486 G490 D491 M493 F497 L498 V499 R503 R504 G505
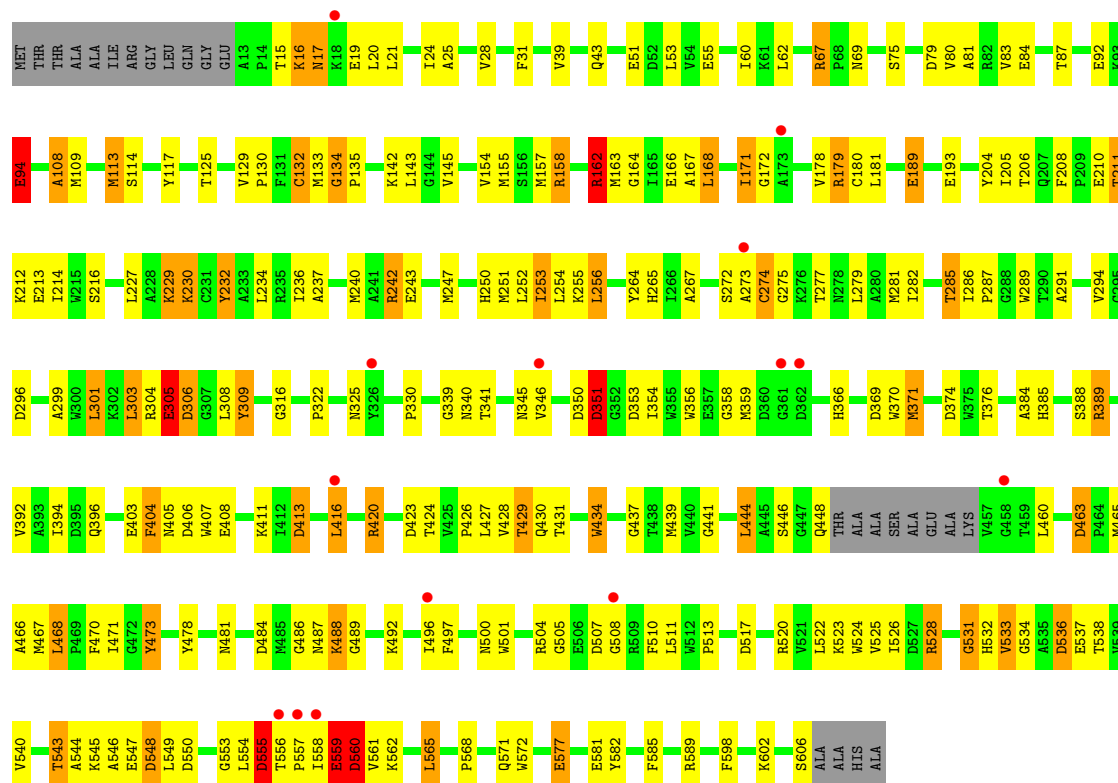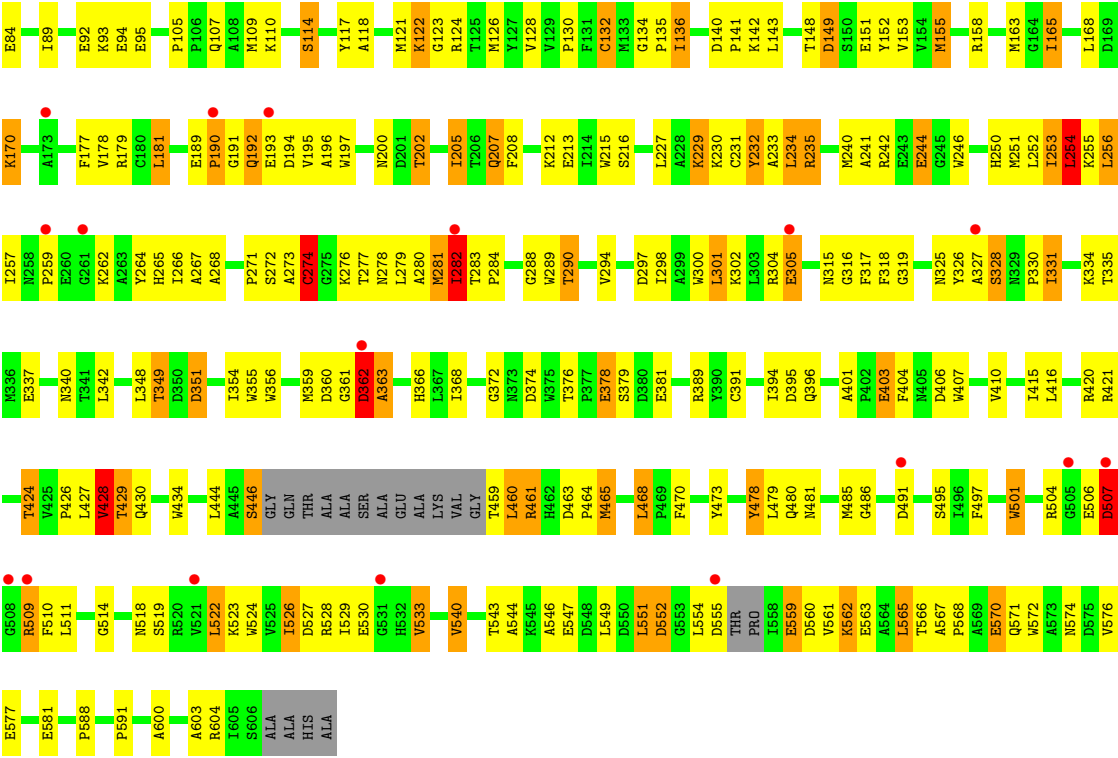
E506 D507 G508 R509 F510 L511 W512 P513 G514 D517 N518 V521 L522 K523 W524 V525 I526 D527 R528 I529 E530 G531 H532 V533 G534 A535 V540 G541 H542 T543 A544 K545 A546 E547 D548 L551 D552 G553 L554 D555 T556 P557 I558 E559 D560 V561 K562 L565 E570 Q571 W572 E577 D578

E581 Y582 F585 A600 R604 I605 S606 ALA ALA HIS ALA

● Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]

Chain C:

2%

56%   31%   8% ● ●

MET THR THR ALA ALA ILE ARG GLY LEU GLN GLN GLU A13 P14 T15 K16 N17 K18 E19 L20 L21 I24 A25 V28 F31 V39 Q43 E51 D52 L53 V54 E55 I60 K61 L62 R67 P68 N69 S75 D79 V80 A81 R82 V83 E84 T87 E92 K93

E94 A108 M109 M113 S114 Y117 T125 V129 P130 F131 C132 M133 G134 P135 K142 L143 G144 V145 V154 M155 S156 M157 R158 R162 M163 G164 I165 E166 A167 L168 I171 G172 A173 V178 R179 C180 L181 E189 E193 Y204 I205 T206 Q207 F208 P209 E210 T211

K212 E213 I214 W215 S216 L227 A228 K229 K230 C231 Y232 A233 L234 R235 I236 A237 M240 A241 R242 E243 M247 H250 M251 L252 I253 L254 K255 L256 Y264 H265 A267 S272 A273 C274 G275 K276 T277 N278 L279 A280 M281 I282 T285 I286 P287 G288 W289 T290 A291 V294 G295

D296 A299 W300 L301 K302 L303 R304 E305 D306 G307 L308 Y309 G316 P322 N325 Y326 P330 G339 N340 T341 N345 V346 D350 D351 G352 D353 I354 W355 S356 E357 G358 M359 D360 G361 D362 H366 D369 W370 M371 D374 W375 T376 A384 H385 S388 R389

V392 A393 I394 D395 Q396 E403 F404 N405 D406 W407 E408 K411 I412 D413 L416 R420 D423 T424 V425 P426 L427 V428 T429 Q430 T431 W434 G437 T438 M439 V440 G441 L444 A445 S446 G447 Q448 THR ALA ALA SER ALA GLU ALA LYS V457 G458 T459 L460 D463 P464 M465

A466 M467 L468 P469 F470 I471 G472 Y473 Y478 N481 D484 M485 G486 N487 K488 G489 K492 I496 F497 N500 W501 R504 G505 E506 D507 G508 R509 F510 L511 W512 P513 D517 R520 V521 L522 K523 W524 V525 I526 D527 R528 G531 H532 V533 G534 A535 D536 E537 T538 V539

V540 T543 A544 K545 A546 E547 D548 L549 D550 G553 L554 D555 T556 P557 I558 E559 D560 V561 K562 L565 P568 Q571 W572 E577 E581 Y582 F585 R589 F598 K602 S606 ALA ALA HIS ALA

● Molecule 1: Phosphoenolpyruvate carboxykinase [GTP]

Chain D:

3%

50%   33%   10% ● 5%

MET THR THR ALA ALA ILE ARG GLY LEU GLN GLN GLU ALA PRO T15 K16 N17 K18 E19 L20 W23 E29 L30 F31 E34 F38 Q43 W46 M49 A50 E51 D52 L53 V54 K61 L62 N63 E64 E65 K66 R67 P68 N69 S70 Y71 S75 S78 D79 V83

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.34Å 118.06Å 152.93Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	24.83 – 2.30 24.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.0 (24.83-2.30) 77.0 (24.83-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.63 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.188 , 0.279 0.189 , 0.279	Depositor DCC
R_{free} test set	4256 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.8	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	0.94	EDS
Total number of atoms	18407	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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 ⓘ

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	1.39	16/4658 (0.3%)	1.27	33/6342 (0.5%)
1	B	1.31	8/4637 (0.2%)	1.21	35/6313 (0.6%)
1	C	1.40	24/4654 (0.5%)	1.23	21/6337 (0.3%)
1	D	1.25	12/4605 (0.3%)	1.17	14/6266 (0.2%)
All	All	1.34	60/18554 (0.3%)	1.22	103/25258 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	3
1	D	0	2
All	All	0	9

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	CG-CD	9.11	1.65	1.51
1	C	577	GLU	CB-CG	7.57	1.66	1.52
1	C	274	CYS	CB-SG	7.41	1.94	1.82
1	C	305	GLU	CB-CG	7.28	1.66	1.52
1	C	108	ALA	CA-CB	7.20	1.67	1.52

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	B	30	LEU	CA-CB-CG	11.09	140.81	115.30
1	C	158	ARG	NE-CZ-NH2	-9.78	115.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	LEU	CB-CG-CD2	-9.46	94.92	111.00
1	D	30	LEU	CA-CB-CG	9.45	137.04	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	559	GLU	Peptide
1	A	81	ALA	Peptide
1	B	350	ASP	Peptide
1	C	81	ALA	Peptide

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	4539	0	4342	151	0
1	B	4518	0	4320	225	0
1	C	4535	0	4336	209	0
1	D	4489	0	4292	228	0
2	A	109	0	0	9	0
2	B	69	0	0	6	0
2	C	89	0	0	8	0
2	D	59	0	0	9	0
All	All	18407	0	17290	802	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 23.

The worst 5 of 802 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:D:355:TRP:HA	1:D:359:MET:CE	1.70	1.22
1:B:129:VAL:HG13	1:B:163:MET:CE	1.70	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:GLY:HA3	1:C:548:ASP:OD2	1.38	1.18
1:D:132:CYS:HB2	1:D:143:LEU:HD23	1.18	1.16
1:A:558:ILE:H	1:A:558:ILE:HD12	1.00	1.16

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	582/610 (95%)	528 (91%)	39 (7%)	15 (3%)	6	4
1	B	580/610 (95%)	523 (90%)	38 (7%)	19 (3%)	4	2
1	C	582/610 (95%)	527 (90%)	42 (7%)	13 (2%)	8	6
1	D	572/610 (94%)	519 (91%)	37 (6%)	16 (3%)	6	4
All	All	2316/2440 (95%)	2097 (90%)	156 (7%)	63 (3%)	6	4

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLU
1	A	273	ALA
1	A	362	ASP
1	A	551	LEU
1	A	556	THR

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	474/487 (97%)	420 (89%)	54 (11%)	7	7
1	B	471/487 (97%)	408 (87%)	63 (13%)	4	4
1	C	473/487 (97%)	423 (89%)	50 (11%)	8	9
1	D	469/487 (96%)	389 (83%)	80 (17%)	2	2
All	All	1887/1948 (97%)	1640 (87%)	247 (13%)	5	5

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	551	LEU
1	C	282	ILE
1	D	491	ASP
1	B	565	LEU
1	C	132	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	571	GLN
1	C	207	GLN
1	D	278	ASN
1	C	17	ASN
1	C	101	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 carbohydrates 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	586/610 (96%)	-0.30	7 (1%)	79	82	14, 25, 44, 62	0
1	B	584/610 (95%)	-0.06	14 (2%)	59	66	15, 32, 51, 62	0
1	C	586/610 (96%)	-0.14	14 (2%)	59	66	17, 28, 46, 72	0
1	D	578/610 (94%)	0.03	17 (2%)	52	59	23, 35, 54, 74	0
All	All	2334/2440 (95%)	-0.12	52 (2%)	62	69	14, 30, 50, 74	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	557	PRO	7.0
1	D	508	GLY	6.5
1	C	556	THR	6.2
1	D	327	ALA	4.5
1	D	507	ASP	4.1

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 carbohydrates 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.