wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 10:23 AM UTC

PDB ID	:	1EIY / pdb_00001eiy
Title	:	THE CRYSTAL STRUCTURE OF PHENYLALANYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS COMPLEXED WITH COGNATE TRNAPHE
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Deposited on	:	2000-02-29
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

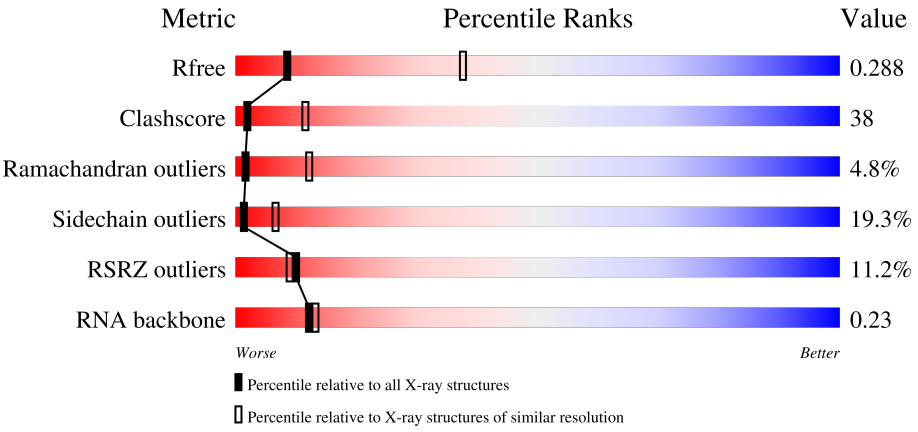
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	C	76	88% 7% 42% 36% 16%
2	A	350	14% 32% 47% 18%
3	B	785	2% 36% 44% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10485 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 RNA chain called TRNA(PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	76	1623	723	291	533	76	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	C	G	conflict	UNP Q5SGX1
C	65	G	C	conflict	UNP Q5SGX1

- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	345	2735	1768	477	482	8	0	0	0

- Molecule 3 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

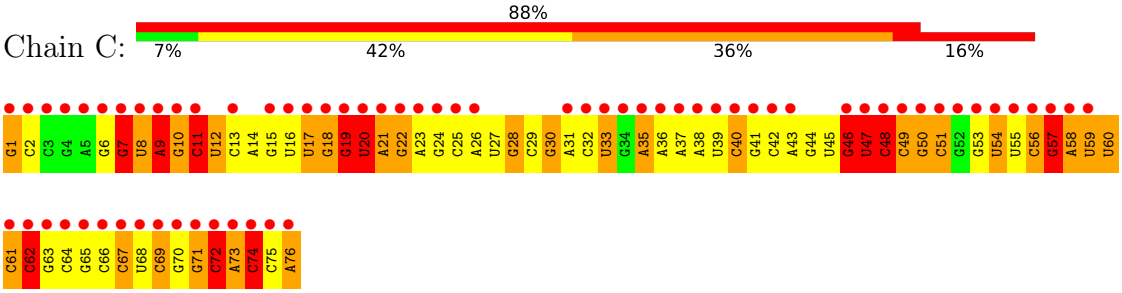
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	785	6127	3925	1091	1101	10	0	0	0

3 Residue-property plots (i)

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: TRNA(PHE)

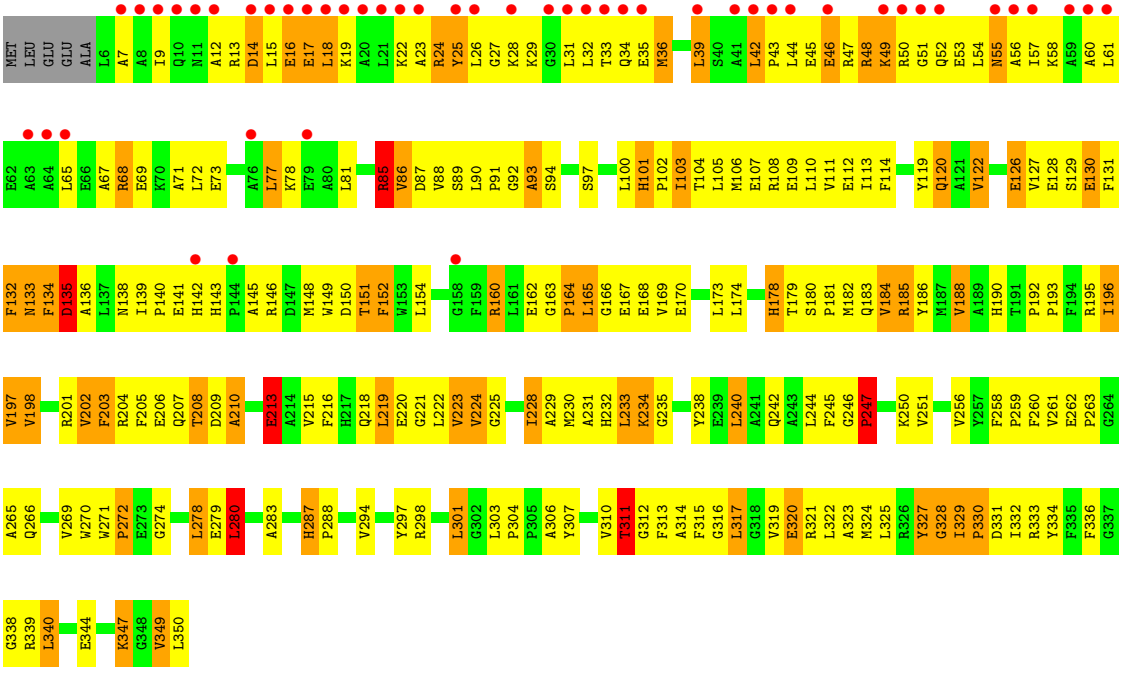
Chain C:



• Molecule 2: PHENYLALANYL-TRNA SYNTHETASE

Chain A:

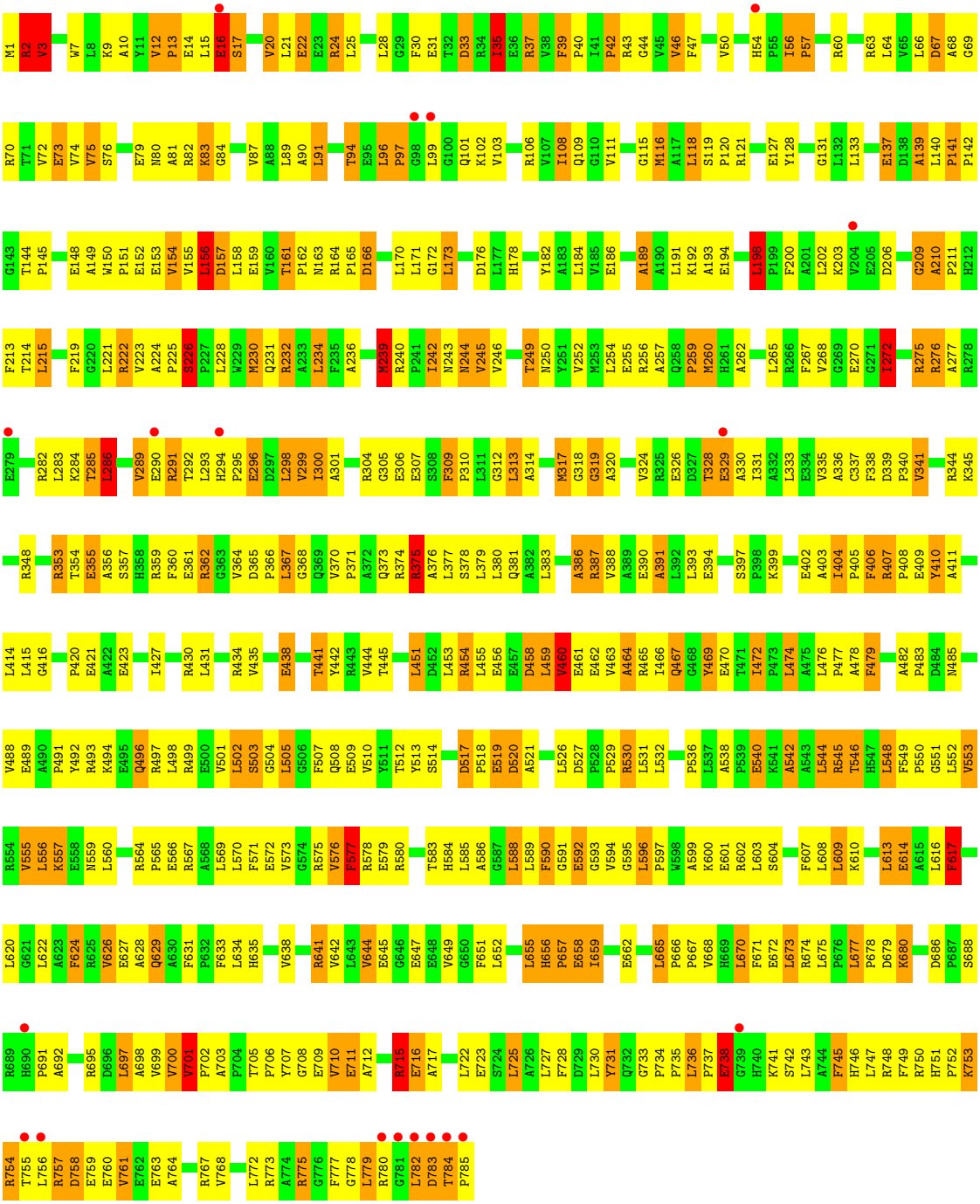




• Molecule 3: PHENYLALANYL-TRNA SYNTHETASE

Chain B:




M1 R2 V3 W7 L8 K9 A10 Y11 V12 P13 E14 L15 E16 S17 V20 L21 E22 E23 R24 L25 L28 G29 F30 E31 T32 D33 R34 I35 E36 R37 V38 F39 P40 I41 P42 R43 G44 V45 V46 F47 V50 H54 P55 I56 P57 R60 R63 L64 V65 L66 D67 A68 G69
R70 T71 V72 E73 V74 V75 S76 E79 N80 A81 R82 K83 G84 V87 A88 L89 A90 L91 T94 E95 L96 P97 G98 L99 G100 Q101 K102 V103 R106 V107 I108 Q109 G110 V111 G115 M116 A117 L118 S119 P120 R121 E127 Y128 G131 L132 L133 E137 D138 A139 L140 P141 P142
G143 T144 P145 E148 A149 W150 P151 E152 E153 V154 V155 L156 D157 L158 E159 V160 T161 P162 N163 R164 P165 D166 L170 L171 G172 L173 D176 L177 H178 Y182 A183 L184 V185 E186 A189 A190 L191 K192 A193 E194 L198 P199 F200 A201 L202 K203 V204 E205 D206 G209 A210 P211 H212
F213 T214 L215 F219 G220 L221 R222 V223 A224 P225 S226 P227 L228 W229 M230 Q231 R232 A233 L234 F235 A236 N239 R240 P241 I242 N243 N244 V245 V246 T249 N250 Y251 V252 M253 L254 E255 R256 A257 Q258 P259 M260 H261 A262 L265 R266 F267 V268 G269 E270 G271 I272 R275 R276 A277 R278
E279 R282 L283 K284 T285 L286 V289 E290 R291 T292 L293 H294 P295 E296 D297 L298 V299 I300 A301 R304 G305 E306 E307 S308 F309 P310 L311 G312 L313 A314 M317 G318 G319 A320 V324 R325 E326 D327 T328 E329 A330 I331 A332 L333 E334 V335 A336 C337 F338 D339 P340 V341 R344 K345
R348 R353 T354 E355 A356 S357 H358 R359 F360 E361 R362 G363 V364 D365 P366 L367 G368 Q369 V370 P371 A372 Q373 R374 R375 A376 L377 S378 L379 L380 Q381 A382 L383 A386 R387 V388 A389 E390 A391 L392 L393 E394 S397 P398 K399 E402 A403 T404 P405 F406 R407 P408 E409 Y410 A411
L414 L415 G416 P420 E421 A422 E423 I427 R430 L431 R434 V435 E438 T441 Y442 R443 V444 T445 L451 D452 L453 R454 L455 E456 E457 D458 L459 V460 E461 E462 V463 A464 R465 I466 Q467 G468 Y469 E470 T471 I472 P473 L474 A475 L476 P477 A478 F479 A482 P483 D484 N485
V488 E489 A490 P491 Y492 R493 K494 E495 Q496 R497 L498 R499 E500 V501 L502 S503 G504 L505 G506 F507 Q508 E509 V510 Y511 T512 Y513 S514 D517 P518 E519 D520 A521 L526 D527 F528 P529 R530 L531 L532 P536 L537 A538 F539 E540 K541 A542 A543 L544 R545 T546 H547 L548 F549 P550 G551 L552 V553
R554 V555 L556 K557 E558 N559 L560 R564 P565 E566 R567 A568 L569 L570 F571 E572 V573 G574 R575 V576 F577 R578 E579 R580 T583 H584 L585 A586 G587 L588 L589 F590 G591 E592 G593 V594 G595 L596 P597 W598 A599 K600 E601 R602 L603 S604 F607 L608 L609 K610 L613 E614 A615 L616 F617
L620 G621 L622 A623 F624 R625 V626 E627 A628 Q629 A630 F631 P632 F633 L634 H635 V638 R641 V642 L643 V644 E645 G646 E647 E648 V649 G650 F651 L652 L655 H656 P657 E658 I659 E662 L665 P666 P667 V668 H669 L670 F671 E672 L673 R674 L675 F676 L677 P678 D679 K680 D686 P687 S688
R689 H690 P691 A692 R695 D696 L697 A698 V699 V700 V701 P702 A703 P704 T705 P706 Y707 G708 E709 V710 E711 A712 R715 E716 A717 L722 E723 S724 L725 A726 L727 F728 D729 L730 Y731 Q732 G733 P734 P735 L736 P737 E738 G739 H740 K741 S742 L743 A744 F745 H746 L747 R748 F749 R750 H751 P752 K753
R754 T755 L756 R757 D758 E759 E760 V761 E762 E763 A764 R767 V768 L772 R773 A774 R775 G776 F777 G778 L779 R780 G781 L782 D783 T784 P785

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.00Å 175.00Å 140.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.00 – 3.30 28.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (28.00-3.30) 87.8 (28.00-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.30 (at 3.31Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.287 0.236 , 0.288	Depositor DCC
R_{free} test set	1657 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 75.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.080 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	C	0.68	1/1813 (0.1%)	1.11	16/2823 (0.6%)
2	A	1.12	2/2805 (0.1%)	1.52	47/3789 (1.2%)
3	B	1.03	9/6280 (0.1%)	1.52	120/8536 (1.4%)
All	All	1.00	12/10898 (0.1%)	1.45	183/15148 (1.2%)

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	C	0	6
3	B	0	1
All	All	0	7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	239	MET	SD-CE	12.98	2.12	1.79
3	B	249	THR	CA-CB	7.45	1.65	1.53
2	A	197	VAL	CA-CB	7.00	1.63	1.54
3	B	460	VAL	CA-CB	7.00	1.62	1.54
1	C	1	G	OP3-P	6.74	1.61	1.48

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	163	GLY	CA-C-N	11.49	134.20	119.84
2	A	163	GLY	C-N-CA	11.49	134.20	119.84
3	B	224	ALA	CA-C-N	-11.35	109.19	120.31
3	B	224	ALA	C-N-CA	-11.35	109.19	120.31
2	A	246	GLY	CA-C-N	11.30	133.96	119.84

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	19	G	Sidechain
1	C	30	G	Sidechain
1	C	48	C	Sidechain
1	C	57	G	Sidechain
1	C	60	U	Sidechain

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	C	1623	0	822	133	0
2	A	2735	0	2725	249	0
3	B	6127	0	6180	435	0
All	All	10485	0	9727	777	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 38.

The worst 5 of 777 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)
3:B:239:MET:CE	3:B:239:MET:SD	2.12	1.38
1:C:58:A:H4'	1:C:59:U:OP1	1.41	1.17
3:B:706:PRO:HG2	3:B:709:GLU:HB2	1.29	1.08
1:C:39:U:C2'	1:C:40:C:H5'	1.83	1.07
1:C:39:U:H2'	1:C:40:C:H5'	1.38	1.02

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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
2	A	343/350 (98%)	286 (83%)	42 (12%)	15 (4%)	2 13
3	B	783/785 (100%)	647 (83%)	97 (12%)	39 (5%)	1 11
All	All	1126/1135 (99%)	933 (83%)	139 (12%)	54 (5%)	2 12

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	48	ARG
2	A	130	GLU
2	A	135	ASP
3	B	16	GLU
3	B	39	PHE

5.3.2 Protein sidechains (i)

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
2	A	272/277 (98%)	223 (82%)	49 (18%)	2 8
3	B	630/630 (100%)	505 (80%)	125 (20%)	1 6
All	All	902/907 (99%)	728 (81%)	174 (19%)	1 6

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	394	GLU

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Mol	Chain	Res	Type
3	B	544	LEU
3	B	409	GLU
3	B	476	LEU
3	B	576	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	350	HIS
3	B	381	GLN
3	B	373	GLN
3	B	467	GLN
2	A	143	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	75/76 (98%)	33 (44%)	8 (10%)

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	C
1	C	7	G
1	C	8	U
1	C	10	G
1	C	11	C

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	58	A
1	C	57	G
1	C	47	U
1	C	20	U
1	C	56	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	C	76/76 (100%)	3.43	67 (88%) 0 0	34, 49, 56, 58	76 (100%)
2	A	345/350 (98%)	0.64	49 (14%) 6 5	17, 55, 95, 138	71 (20%)
3	B	785/785 (100%)	0.26	19 (2%) 59 40	9, 62, 98, 140	0
All	All	1206/1211 (99%)	0.57	135 (11%) 10 9	9, 58, 98, 140	147 (12%)

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	76	A	8.2
2	A	8	ALA	6.4
1	C	63	G	6.4
2	A	26	LEU	6.0
2	A	39	LEU	5.9

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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.