wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 04:56 AM EST

PDB ID	:	1NJ8
Title	:	Crystal Structure of Prolyl-tRNA Synthetase from Methanocaldococcus janaschii
Authors	:	Kamtekar, S.; Kennedy, W.D.; Wang, J.; Stathopoulos, C.; Soll, D.; Steitz, T.A.
Deposited on	:	2002-12-30
Resolution	:	3.20 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:

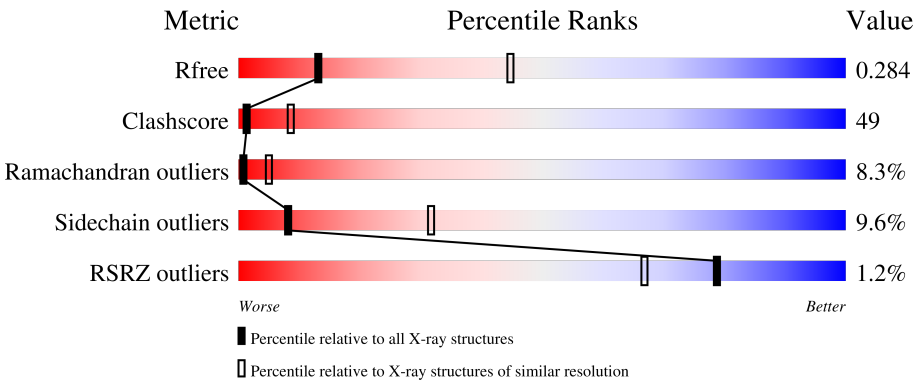
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	459	2% 31% 56% 12% ••
1	B	459	% 31% 57% 10% ••
1	C	459	% 29% 58% 12% ••
1	D	459	2% 31% 58% 10% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15182 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 Proline-tRNA Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3772	2447	614	698	13	0	0	0
1	B	456	3772	2447	614	698	13	0	0	0
1	C	456	3772	2447	614	698	13	0	0	0
1	D	456	3772	2447	614	698	13	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q58635
A	-2	SER	-	expression tag	UNP Q58635
A	-1	HIS	-	expression tag	UNP Q58635
A	0	MET	-	expression tag	UNP Q58635
A	1	LEU	MET	cloning artifact	UNP Q58635
B	-3	GLY	-	expression tag	UNP Q58635
B	-2	SER	-	expression tag	UNP Q58635
B	-1	HIS	-	expression tag	UNP Q58635
B	0	MET	-	expression tag	UNP Q58635
B	1	LEU	MET	cloning artifact	UNP Q58635
C	-3	GLY	-	expression tag	UNP Q58635
C	-2	SER	-	expression tag	UNP Q58635
C	-1	HIS	-	expression tag	UNP Q58635
C	0	MET	-	expression tag	UNP Q58635
C	1	LEU	MET	cloning artifact	UNP Q58635
D	-3	GLY	-	expression tag	UNP Q58635
D	-2	SER	-	expression tag	UNP Q58635
D	-1	HIS	-	expression tag	UNP Q58635
D	0	MET	-	expression tag	UNP Q58635
D	1	LEU	MET	cloning artifact	UNP Q58635

- Molecule 2 is water.

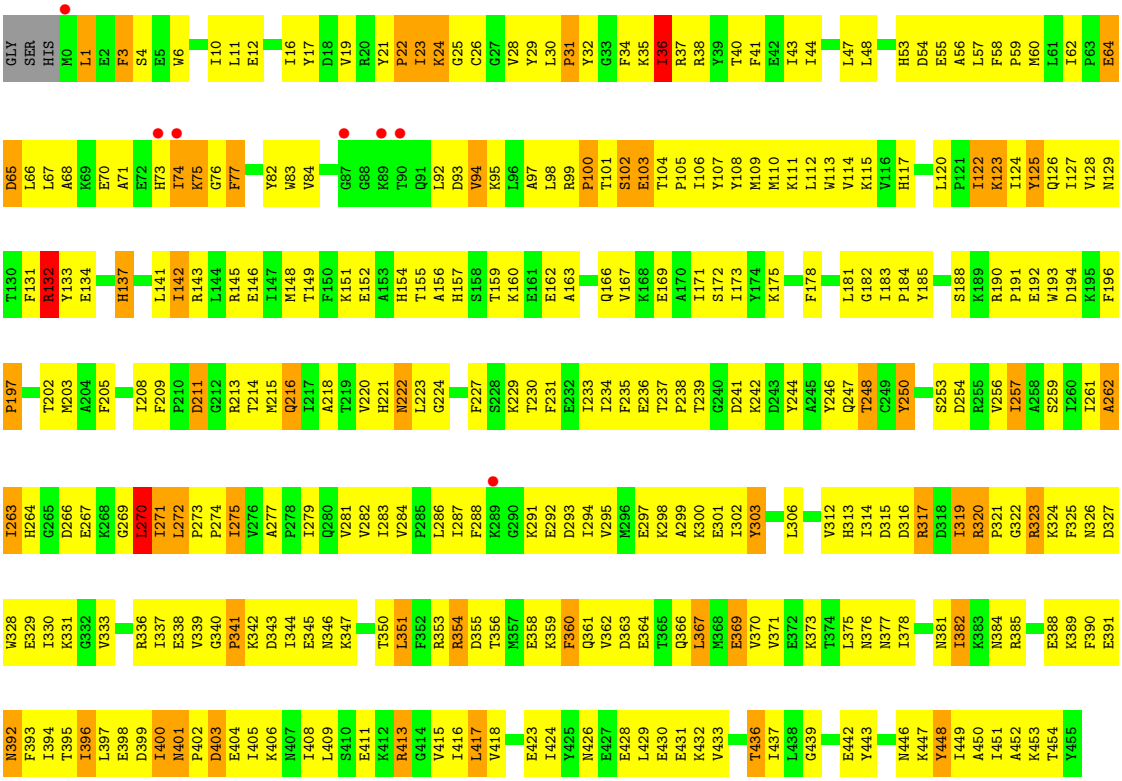
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	35	35	35	0	0
			Total	O		
2	B	16	16	16	0	0
			Total	O		
2	C	25	25	25	0	0
			Total	O		
2	D	18	18	18	0	0

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.

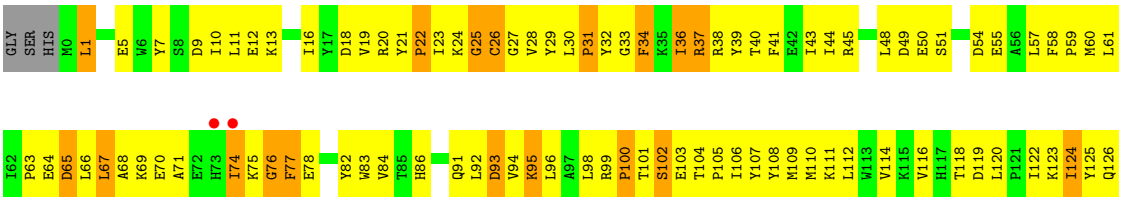
- Molecule 1: Proline-tRNA Synthetase

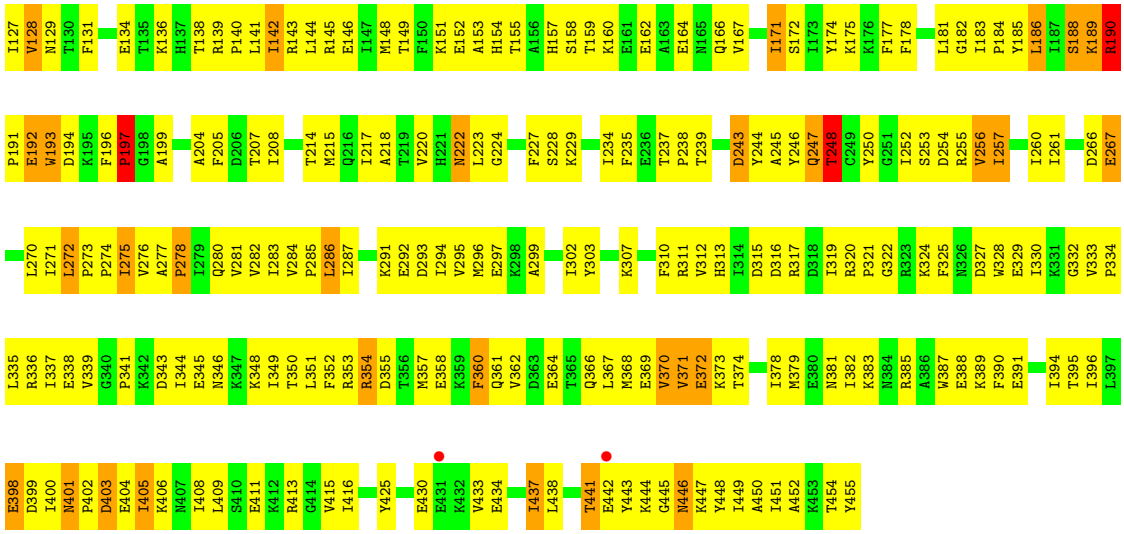
Chain A: 2% 31% 56% 12%



- Molecule 1: Proline-tRNA Synthetase

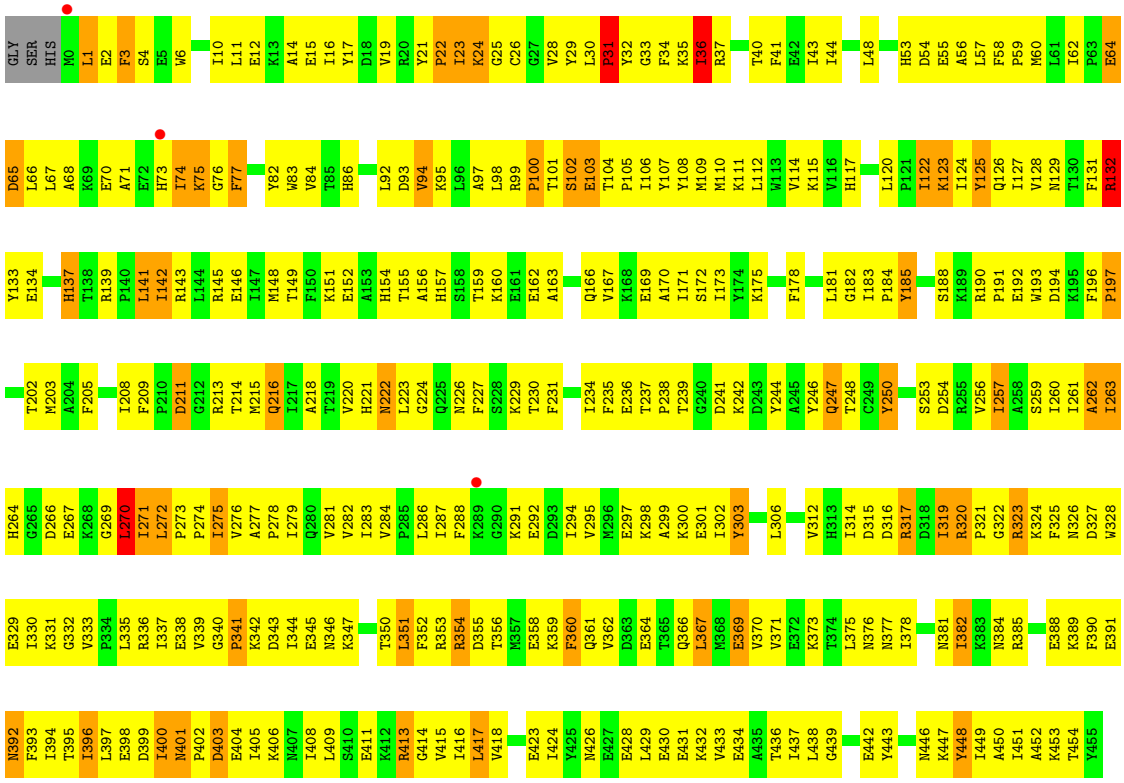
Chain B: % 31% 57% 10%





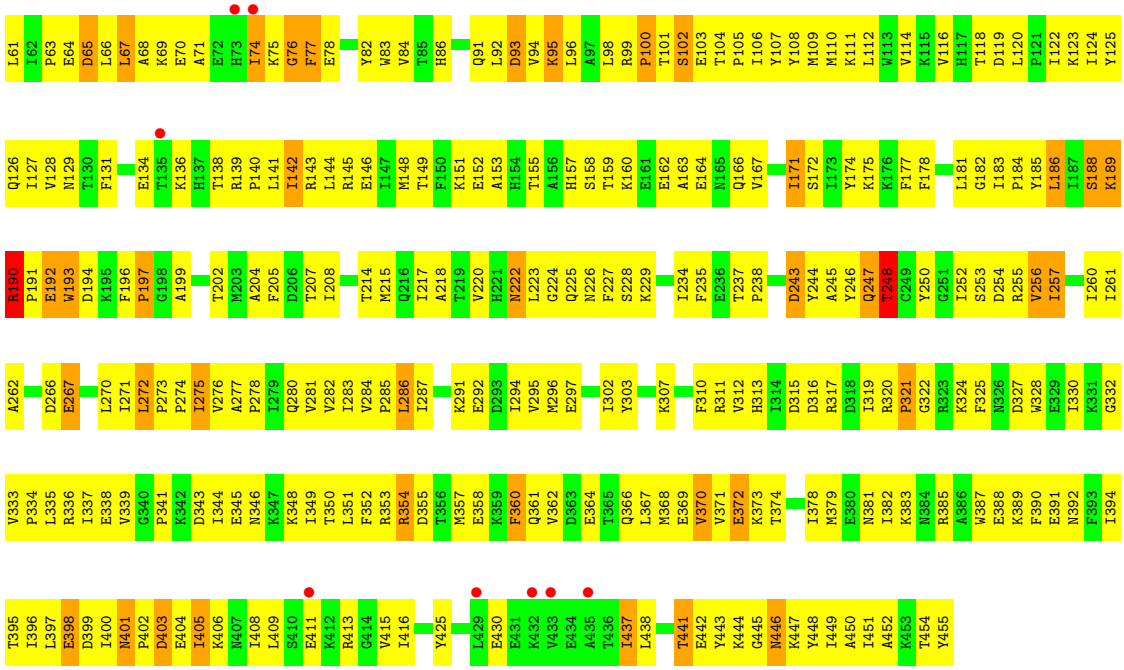
• Molecule 1: Proline-tRNA Synthetase

Chain C:



• Molecule 1: Proline-tRNA Synthetase

Chain D:


L61 I62 P63 E64 D65 L66 L67 A68 K69 E70 A71 E72 H73 I74 K75 G76 F77 E78 Y82 W83 V84 T85 H86 Q91 L92 D93 V94 K95 L96 A97 L98 R99 P100 T101 S102 E103 T104 P105 I106 Y107 Y108 M109 M110 K111 L112 W113 V114 K115 V116 H117 T118 D119 L120 P121 I122 K123 I124 Y125
Q126 I127 V128 N129 T130 F131 E134 T135 K136 H137 T138 R139 P140 L141 I142 R143 L144 R145 E146 I147 M148 T149 F150 K151 E152 A153 H154 T155 A156 H157 S158 T159 K160 E161 E162 A163 E164 M165 Q166 V167 I171 S172 I173 Y174 K175 K176 F177 F178 L181 G182 I183 P184 Y185 L186 I187 S188 K189
R190 P191 E192 W193 D194 K195 F196 P197 G198 A199 T202 M203 A204 F205 D206 T207 I208 T214 M215 Q216 I217 A218 T219 V220 H221 N222 L223 G224 Q225 N226 F227 S228 K229 I234 F235 E236 T237 P238 D243 Y244 A245 Y246 Q247 T248 C249 Y250 G251 I252 S253 D254 R255 V256 I257 I260 I261
A262 D266 E267 L270 I271 L272 P273 P274 I275 V276 A277 P278 I279 Q280 V281 V282 I283 V284 P285 L286 I287 K291 E292 D293 I294 V295 M296 E297 I302 Y303 K307 F310 R311 V312 H313 I314 D315 D316 R317 D318 I319 R320 P321 G322 R323 K324 F325 N326 D327 W328 E329 I330 K331 G332
V333 P334 L335 R336 I337 E338 V339 G340 P341 K342 D343 I344 E345 N346 K347 K348 I349 T350 L351 F352 R353 R354 D355 T356 M357 E358 K359 F360 Q361 V362 D363 E364 T365 Q366 L367 M368 E369 V370 V371 E372 K373 T374 I378 M379 E380 N381 I382 K383 N384 R385 A386 W387 E388 K389 F390 E391 N392 F393 I394
T395 I396 L397 E398 D399 I400 N401 P402 D403 E404 I405 K406 N407 I408 L409 S410 E411 K412 R413 G414 V415 I416 Y425 L429 E430 E431 K432 V433 E434 A435 T436 I437 L438 T441 E442 Y443 K444 G445 N446 K447 Y448 I449 A450 I451 A452 K453 T454 Y455

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.94Å 104.84Å 91.75Å 90.00° 93.63° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 29.81 – 3.16	Depositor EDS
% Data completeness (in resolution range)	87.0 (20.00-3.20) 84.9 (29.81-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	720.88 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.301 0.223 , 0.284	Depositor DCC
R_{free} test set	2974 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15182	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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 (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	0.44	0/3860	0.71	3/5213 (0.1%)
1	B	0.40	0/3860	0.63	0/5213
1	C	0.44	0/3860	0.70	3/5213 (0.1%)
1	D	0.39	0/3860	0.63	0/5213
All	All	0.42	0/15440	0.67	6/20852 (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	A	320	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	C	320	ARG	NE-CZ-NH1	-11.40	114.60	120.30
1	C	320	ARG	NE-CZ-NH2	11.27	125.94	120.30
1	A	320	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	C	320	ARG	CD-NE-CZ	5.36	131.10	123.60

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	3772	0	3804	386	2
1	B	3772	0	3804	353	0
1	C	3772	0	3804	409	1
1	D	3772	0	3804	363	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	35	0	0	2	0
2	B	16	0	0	1	0
2	C	25	0	0	6	0
2	D	18	0	0	3	0
All	All	15182	0	15216	1472	2

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 49.

The worst 5 of 1472 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:B:275:ILE:HD12	1:B:275:ILE:H	1.06	1.14
1:D:275:ILE:HD12	1:D:275:ILE:H	1.08	1.11
1:B:48:LEU:HD11	1:B:151:LYS:HD2	1.32	1.10
1:D:48:LEU:HD11	1:D:151:LYS:HD2	1.34	1.07
1:A:337:ILE:HG12	1:A:351:LEU:HD12	1.36	1.02

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:NH1	1:C:323:ARG:NH1[2_646]	1.95	0.25
1:A:293:ASP:OD1	1:D:392:ASN:OD1[1_554]	2.10	0.10

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
1	A	454/459 (99%)	331 (73%)	84 (18%)	39 (9%)	1 4
1	B	454/459 (99%)	313 (69%)	104 (23%)	37 (8%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	454/459 (99%)	330 (73%)	85 (19%)	39 (9%)	1 4
1	D	454/459 (99%)	312 (69%)	107 (24%)	35 (8%)	1 6
All	All	1816/1836 (99%)	1286 (71%)	380 (21%)	150 (8%)	1 5

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	74	ILE
1	A	75	LYS
1	A	76	GLY
1	A	102	SER

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
1	A	412/414 (100%)	373 (90%)	39 (10%)	8 32
1	B	412/414 (100%)	373 (90%)	39 (10%)	8 32
1	C	412/414 (100%)	370 (90%)	42 (10%)	7 29
1	D	412/414 (100%)	374 (91%)	38 (9%)	9 33
All	All	1648/1656 (100%)	1490 (90%)	158 (10%)	8 32

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	442	GLU
1	D	272	LEU
1	C	454	THR
1	D	124	ILE
1	D	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	216	GLN
1	C	384	ASN
1	D	401	ASN
1	C	222	ASN
1	C	247	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	456/459 (99%)	-0.45	7 (1%)	73	61	10, 49, 112, 140	0
1	B	456/459 (99%)	-0.30	4 (0%)	84	75	17, 69, 129, 144	0
1	C	456/459 (99%)	-0.44	3 (0%)	87	81	11, 49, 111, 140	0
1	D	456/459 (99%)	-0.25	8 (1%)	68	55	16, 69, 129, 144	0
All	All	1824/1836 (99%)	-0.36	22 (1%)	79	67	10, 58, 122, 144	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	HIS	6.3
1	B	74	ILE	4.7
1	C	73	HIS	4.5
1	D	74	ILE	4.0
1	B	73	HIS	3.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.