



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2016 – 07:57 PM EDT

PDB ID : 5EUC
Title : The role of the C-terminal region on the oligomeric state and enzymatic activity of Trypanosoma cruzi hypoxanthine phosphoribosyl transferase
Authors : Valsecchi, W.M.; Cousido-Siah, A.; Mitschler, A.; Podjarny, A.; Delfino, J.M.; Santos, J.
Deposited on : 2015-11-18
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

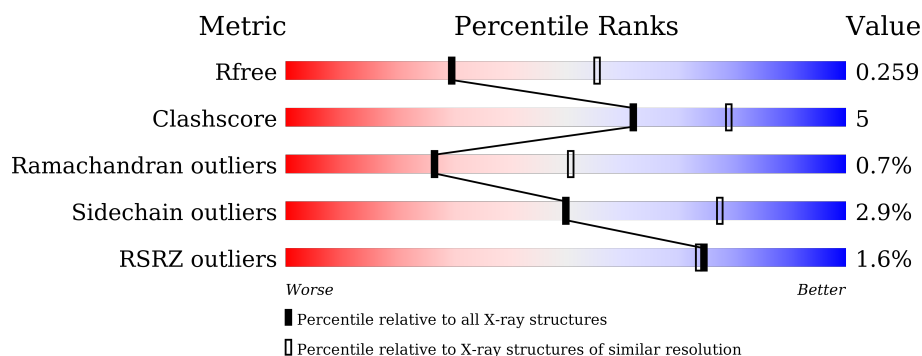
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 $\leq 5\%$. 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	229	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	229	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>15%</div> </div> </div>
1	C	229	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>16%</div> </div> </div>
1	D	229	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6389 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 Hypoxanthine-guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1601	1024	277	293	7			
1	B	195	Total	C	N	O	S	0	0	0
			1581	1013	271	290	7			
1	C	193	Total	C	N	O	S	0	0	0
			1563	1002	266	288	7			
1	D	189	Total	C	N	O	S	0	0	0
			1533	985	259	282	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LEU	-	expression tag	UNP Q4DRC4
A	223	GLU	-	expression tag	UNP Q4DRC4
A	224	HIS	-	expression tag	UNP Q4DRC4
A	225	HIS	-	expression tag	UNP Q4DRC4
A	226	HIS	-	expression tag	UNP Q4DRC4
A	227	HIS	-	expression tag	UNP Q4DRC4
A	228	HIS	-	expression tag	UNP Q4DRC4
A	229	HIS	-	expression tag	UNP Q4DRC4
B	222	LEU	-	expression tag	UNP Q4DRC4
B	223	GLU	-	expression tag	UNP Q4DRC4
B	224	HIS	-	expression tag	UNP Q4DRC4
B	225	HIS	-	expression tag	UNP Q4DRC4
B	226	HIS	-	expression tag	UNP Q4DRC4
B	227	HIS	-	expression tag	UNP Q4DRC4
B	228	HIS	-	expression tag	UNP Q4DRC4
B	229	HIS	-	expression tag	UNP Q4DRC4
C	222	LEU	-	expression tag	UNP Q4DRC4
C	223	GLU	-	expression tag	UNP Q4DRC4
C	224	HIS	-	expression tag	UNP Q4DRC4
C	225	HIS	-	expression tag	UNP Q4DRC4
C	226	HIS	-	expression tag	UNP Q4DRC4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	227	HIS	-	expression tag	UNP Q4DRC4
C	228	HIS	-	expression tag	UNP Q4DRC4
C	229	HIS	-	expression tag	UNP Q4DRC4
D	222	LEU	-	expression tag	UNP Q4DRC4
D	223	GLU	-	expression tag	UNP Q4DRC4
D	224	HIS	-	expression tag	UNP Q4DRC4
D	225	HIS	-	expression tag	UNP Q4DRC4
D	226	HIS	-	expression tag	UNP Q4DRC4
D	227	HIS	-	expression tag	UNP Q4DRC4
D	228	HIS	-	expression tag	UNP Q4DRC4
D	229	HIS	-	expression tag	UNP Q4DRC4

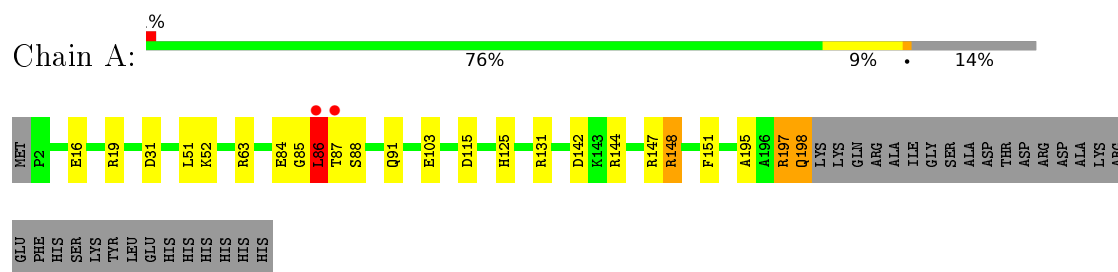
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	40	Total	O	0	0
			40	40		
2	C	19	Total	O	0	0
			19	19		
2	D	23	Total	O	0	0
			23	23		

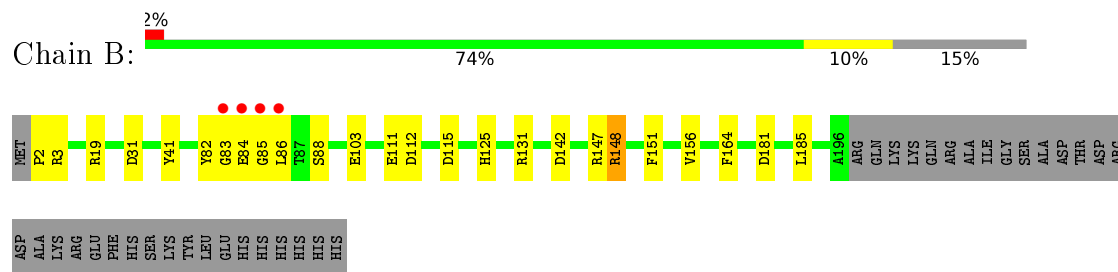
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

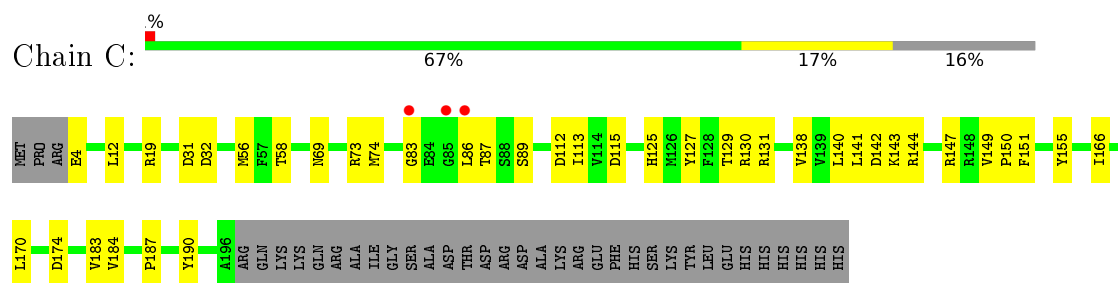
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



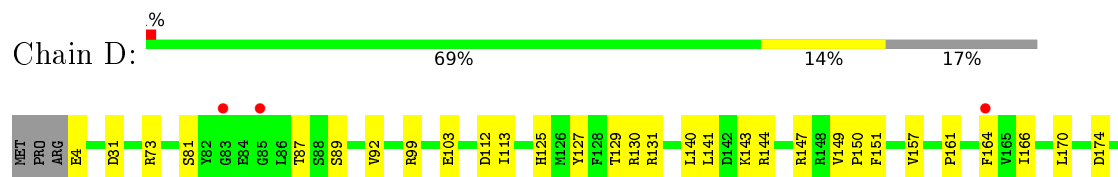
- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



Y183	E192
	ARG
	GLU
	ALA
	ALA
	ARG
	GLN
	LYS
	LYS
	GLN
	ARG
	ALA
	ILE
	GLY
	SER
	ALA
	ASP
	THR
	ASP
	ARG
	ASP
	ALA
	LYS
	ARG
	GLU
	PHE
	HIS
	SER
	SER
	LYS
	TYR
	LEU
	GLU
	HIS
	HIS
	HIS
	HIS
	HIS
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	95.67Å 95.67Å 75.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.34 – 2.65 36.34 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.34-2.65) 99.9 (36.34-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.264 0.193 , 0.259	Depositor DCC
R_{free} test set	1150 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.1	EDS
Estimated twinning fraction	0.032 for -h,-k,l 0.470 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22501 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.64	0/1633	0.80	1/2209 (0.0%)
1	B	0.63	0/1613	0.81	1/2183 (0.0%)
1	C	0.60	0/1594	0.79	0/2158
1	D	0.60	0/1564	0.80	0/2118
All	All	0.62	0/6404	0.80	2/8668 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	19	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	86	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	LEU	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	1601	0	1611	19	0
1	B	1581	0	1590	17	0
1	C	1563	0	1569	25	0
1	D	1533	0	1540	18	0
2	A	29	0	0	3	0
2	B	40	0	0	4	0
2	C	19	0	0	1	0
2	D	23	0	0	1	0
All	All	6389	0	6310	68	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 5.

All (68) 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:147:ARG:NH1	1:B:151:PHE:O	2.14	0.79
1:A:16:GLU:OE1	1:A:19:ARG:NH1	2.17	0.77
1:A:147:ARG:NH1	1:A:151:PHE:O	2.22	0.72
1:A:85:GLY:C	1:A:86:LEU:HD22	2.12	0.68
1:A:87:THR:HB	1:D:103:GLU:OE1	1.95	0.67
1:D:149:VAL:HG22	1:D:150:PRO:HD2	1.75	0.66
1:C:149:VAL:HG22	1:C:150:PRO:HD2	1.77	0.65
1:A:195:ALA:O	1:A:198:GLN:HB2	1.98	0.64
1:B:88:SER:OG	1:C:131:ARG:NH1	2.34	0.60
1:B:82:TYR:O	1:B:84:GLU:N	2.36	0.58
1:A:85:GLY:O	1:A:86:LEU:HD13	2.03	0.58
1:C:125:HIS:O	1:C:129:THR:HG23	2.05	0.57
1:A:84:GLU:O	1:A:85:GLY:C	2.41	0.57
1:A:148:ARG:NH2	2:A:302:HOH:O	2.37	0.56
1:D:140:LEU:O	1:D:157:VAL:HB	2.07	0.55
1:C:112:ASP:HB2	1:C:170:LEU:HD21	1.89	0.54
1:D:73:ARG:HG3	1:D:73:ARG:HH11	1.72	0.54
1:A:88:SER:OG	1:D:131:ARG:NH1	2.41	0.53
1:B:148:ARG:NH2	2:B:303:HOH:O	2.42	0.53
1:B:156:VAL:HG22	2:B:301:HOH:O	2.08	0.53
1:D:147:ARG:NH1	1:D:151:PHE:O	2.42	0.53
1:A:63:ARG:HD3	1:C:56:MET:SD	2.49	0.52
1:D:125:HIS:O	1:D:129:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:CG2	2:B:301:HOH:O	2.59	0.50
1:D:112:ASP:O	1:D:140:LEU:HB3	2.12	0.50
1:A:103:GLU:OE1	1:D:87:THR:OG1	2.30	0.49
1:A:197:ARG:O	1:A:198:GLN:NE2	2.45	0.49
1:C:73:ARG:HH11	1:C:73:ARG:HG3	1.78	0.49
1:A:125:HIS:CD2	1:D:129:THR:HG21	2.47	0.48
1:A:142:ASP:OD1	1:A:147:ARG:NH2	2.46	0.48
1:B:164:PHE:HB2	1:B:185:LEU:HB3	1.95	0.48
1:B:125:HIS:CD2	1:C:129:THR:HG21	2.49	0.48
1:B:142:ASP:OD1	1:B:147:ARG:NH2	2.46	0.48
1:D:166:ILE:HG13	1:D:183:VAL:HG22	1.96	0.48
1:C:32:ASP:OD2	1:C:155:TYR:OH	2.18	0.47
1:A:131:ARG:HD2	1:D:89:SER:HB3	1.96	0.47
1:B:85:GLY:C	2:B:316:HOH:O	2.53	0.47
1:C:69:ASN:CG	2:C:302:HOH:O	2.54	0.46
1:C:127:TYR:O	1:C:130:ARG:HB2	2.15	0.46
1:D:127:TYR:O	1:D:130:ARG:HB2	2.15	0.46
1:C:142:ASP:OD1	1:C:144:ARG:HG3	2.16	0.46
1:B:131:ARG:HD2	1:C:89:SER:HB3	1.98	0.46
1:D:112:ASP:HB2	1:D:170:LEU:HD21	1.97	0.46
1:C:112:ASP:HB2	1:C:170:LEU:CD2	2.46	0.46
1:C:166:ILE:HG13	1:C:183:VAL:HG22	1.98	0.45
1:B:3:ARG:HD2	1:B:181:ASP:OD2	2.16	0.45
1:C:147:ARG:NH1	1:C:151:PHE:O	2.49	0.45
1:C:112:ASP:O	1:C:140:LEU:HB3	2.18	0.44
1:D:113:ILE:HD11	1:D:143:LYS:HE3	2.00	0.44
1:A:51:LEU:HB3	1:A:52:LYS:HA	1.99	0.43
1:B:148:ARG:HA	1:B:148:ARG:HD2	1.95	0.43
1:D:144:ARG:HD3	2:D:301:HOH:O	2.18	0.43
1:D:140:LEU:HG	1:D:141:LEU:HG	2.01	0.42
1:A:144:ARG:HB2	1:A:144:ARG:HE	1.60	0.42
1:B:164:PHE:CB	1:B:185:LEU:HB3	2.49	0.42
1:C:113:ILE:HD11	1:C:143:LYS:HE3	2.02	0.42
1:C:12:LEU:HG	1:C:184:VAL:HG23	2.02	0.42
1:A:91:GLN:O	2:A:301:HOH:O	2.22	0.42
1:B:103:GLU:OE1	1:C:87:THR:OG1	2.34	0.42
1:C:58:THR:HG22	1:C:74:MET:HE1	2.02	0.41
1:C:138:VAL:HG23	1:C:155:TYR:HB2	2.03	0.41
1:B:125:HIS:HD2	1:C:129:THR:HG21	1.86	0.41
1:B:111:GLU:HG3	1:B:112:ASP:N	2.36	0.41
1:C:19:ARG:HH11	1:C:19:ARG:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:O	1:C:141:LEU:HD23	2.22	0.40
1:A:197:ARG:H	1:A:197:ARG:HG2	1.69	0.40
1:C:187:PRO:O	1:C:190:TYR:HB3	2.22	0.40
2:A:315:HOH:O	1:D:99:ARG:HB2	2.20	0.40

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	
1	A	195/229 (85%)	188 (96%)	7 (4%)	0	100	100
1	B	193/229 (84%)	184 (95%)	7 (4%)	2 (1%)	19	41
1	C	191/229 (83%)	183 (96%)	7 (4%)	1 (0%)	34	59
1	D	187/229 (82%)	180 (96%)	5 (3%)	2 (1%)	17	38
All	All	766/916 (84%)	735 (96%)	26 (3%)	5 (1%)	26	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	GLY
1	C	83	GLY
1	D	164	PHE
1	B	41	TYR
1	D	161	PRO

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	174/202 (86%)	168 (97%)	6 (3%)	44	72
1	B	172/202 (85%)	168 (98%)	4 (2%)	58	83
1	C	170/202 (84%)	165 (97%)	5 (3%)	50	77
1	D	168/202 (83%)	163 (97%)	5 (3%)	48	77
All	All	684/808 (85%)	664 (97%)	20 (3%)	50	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	86	LEU
1	A	115	ASP
1	A	148	ARG
1	A	197	ARG
1	A	198	GLN
1	B	2	PRO
1	B	31	ASP
1	B	115	ASP
1	B	148	ARG
1	C	4	GLU
1	C	31	ASP
1	C	86	LEU
1	C	115	ASP
1	C	174	ASP
1	D	4	GLU
1	D	31	ASP
1	D	81	SER
1	D	92	VAL
1	D	174	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 carbohydrates 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	A	197/229 (86%)	-0.62	2 (1%) 84 84	24, 37, 72, 115	0
1	B	195/229 (85%)	-0.58	4 (2%) 67 66	23, 37, 61, 118	0
1	C	193/229 (84%)	-0.42	3 (1%) 74 74	23, 42, 107, 135	0
1	D	189/229 (82%)	-0.44	3 (1%) 74 74	24, 43, 92, 124	0
All	All	774/916 (84%)	-0.52	12 (1%) 74 74	23, 39, 85, 135	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLU	5.2
1	B	83	GLY	4.7
1	B	85	GLY	4.3
1	A	87	THR	2.8
1	D	85	GLY	2.7
1	C	85	GLY	2.6
1	B	86	LEU	2.5
1	C	83	GLY	2.3
1	D	83	GLY	2.3
1	D	164	PHE	2.1
1	A	86	LEU	2.1
1	C	86	LEU	2.0

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.