



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:31 am BST

PDB ID : 2ZA2  
Title : Crystal Structure of the apo-form of orotidine-5'-monophosphate decarboxylase from *P.falciparum*  
Authors : Tokuoka, K.; Inoue, T.  
Deposited on : 2007-09-26  
Resolution : 2.70 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](mailto: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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

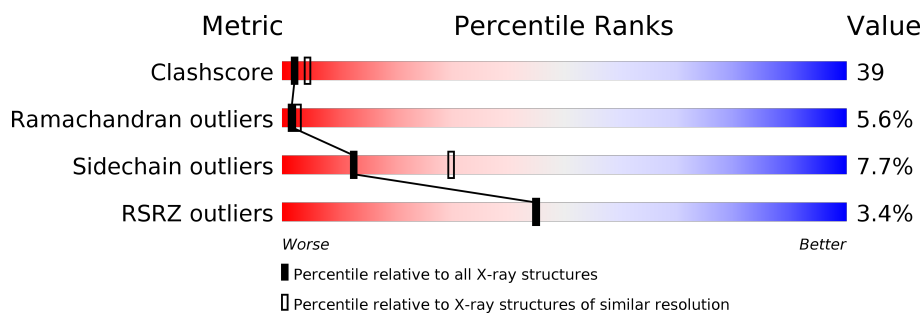
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	323	
1	B	323	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5002 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2458	1589	395	459	15			
1	B	310	Total	C	N	O	S	0	0	0
			2506	1615	404	472	15			

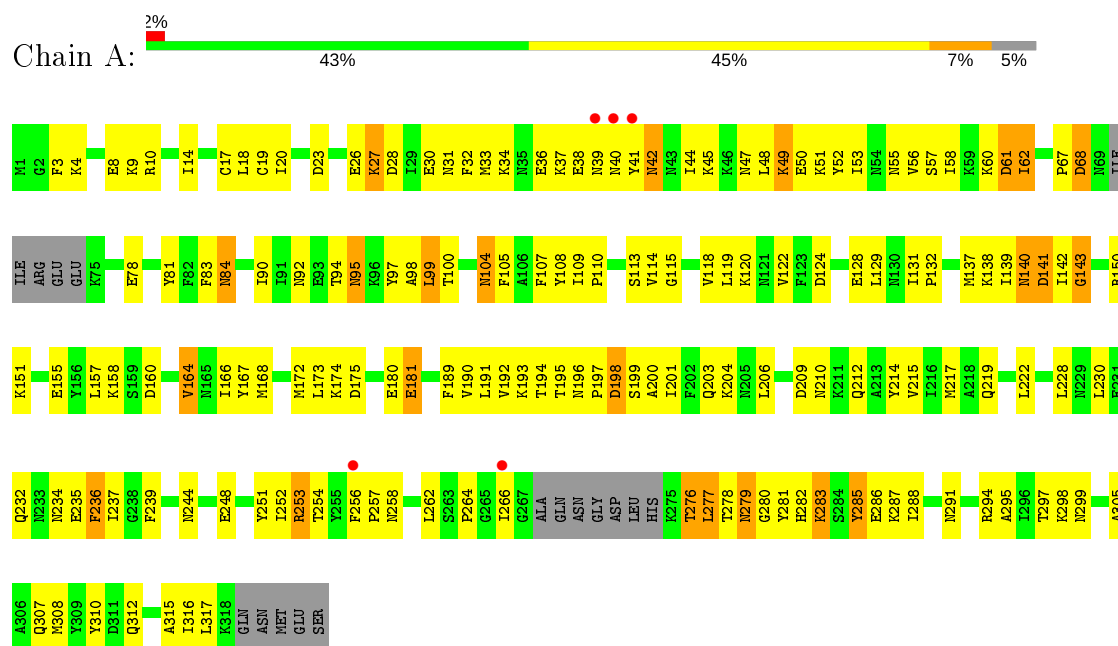
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	15	Total	O	0	0
			15	15		

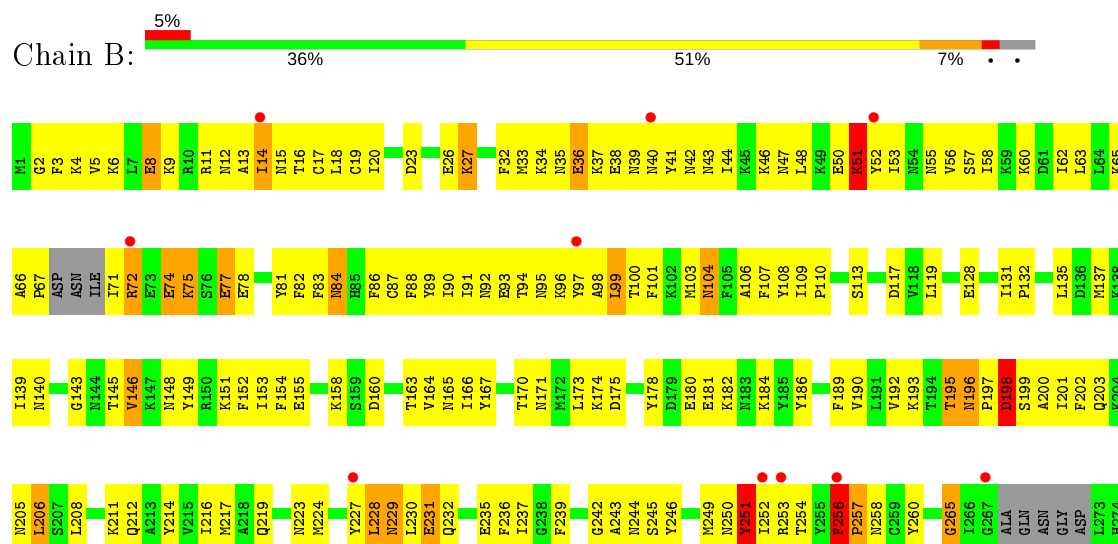
### 3 Residue-property plots

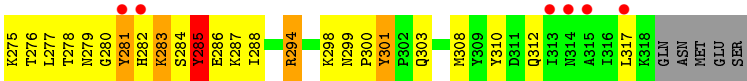
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Orotidine 5'-phosphate decarboxylase



#### • Molecule 1: Orotidine 5'-phosphate decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.80 Å   201.80 Å   44.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	39.30 – 2.70 39.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.30-2.70) 99.6 (39.30-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.69 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 ,   0.309 0.221 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 70.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.40	0/2508	0.63	0/3387
1	B	0.37	0/2557	0.67	2/3450 (0.1%)
All	All	0.38	0/5065	0.65	2/6837 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	TYR	N-CA-C	-5.90	95.07	111.00
1	B	256	PHE	C-N-CD	-5.56	108.37	120.60

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	2458	0	2387	172	0
1	B	2506	0	2427	222	0
2	A	23	0	0	2	0
2	B	15	0	0	1	0
All	All	5002	0	4814	384	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 39.

All (384) 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:A:151:LYS:HE3	1:B:110:PRO:HB2	1.27	1.08
1:B:283:LYS:HG2	1:B:284:SER:H	1.22	1.04
1:B:294:ARG:HB2	1:B:294:ARG:HH11	1.29	0.97
1:B:17:CYS:HA	1:B:99:LEU:HD12	1.45	0.96
1:B:201:ILE:HG12	1:B:202:PHE:H	1.31	0.93
1:B:202:PHE:HA	1:B:206:LEU:HD22	1.50	0.93
1:A:277:LEU:H	1:A:277:LEU:HD23	1.34	0.90
1:B:212:GLN:HE21	1:B:214:TYR:HE1	1.15	0.90
1:A:253:ARG:HG3	1:A:281:TYR:HA	1.53	0.89
1:A:17:CYS:HA	1:A:99:LEU:HD12	1.58	0.86
1:A:266:ILE:HG21	1:A:294:ARG:HB2	1.58	0.85
1:A:113:SER:HB2	1:B:113:SER:HB2	1.58	0.85
1:A:20:ILE:HD12	1:A:98:ALA:HB2	1.58	0.84
1:B:52:TYR:CD2	1:B:128:GLU:HB3	2.14	0.83
1:B:27:LYS:HB3	1:B:27:LYS:NZ	1.94	0.82
1:A:308:MET:HG2	1:A:312:GLN:HE21	1.44	0.81
1:B:294:ARG:CB	1:B:294:ARG:HH11	1.94	0.79
1:A:9:LYS:NZ	1:A:9:LYS:HB3	1.98	0.78
1:A:33:MET:O	1:A:37:LYS:HG2	1.85	0.77
1:A:253:ARG:CG	1:A:281:TYR:HA	2.16	0.76
1:B:55:ASN:CB	1:B:128:GLU:HG3	2.16	0.75
1:B:212:GLN:NE2	1:B:214:TYR:HE1	1.84	0.75
1:B:196:ASN:HB3	1:B:197:PRO:HD3	1.68	0.74
1:B:251:TYR:HD2	1:B:252:ILE:H	1.31	0.74
1:B:201:ILE:HG12	1:B:202:PHE:N	2.01	0.74
1:B:283:LYS:HG2	1:B:284:SER:N	2.00	0.74
1:B:27:LYS:HB3	1:B:27:LYS:HZ3	1.50	0.73
1:A:124:ASP:O	1:A:128:GLU:HG2	1.88	0.73
1:B:294:ARG:HB2	1:B:294:ARG:NH1	2.03	0.73
1:B:253:ARG:HH21	1:B:283:LYS:HB3	1.52	0.73
1:A:28:ASP:OD1	1:A:298:LYS:HD3	1.89	0.72
1:B:228:LEU:HD13	1:B:230:LEU:CD2	2.20	0.72
1:B:228:LEU:HD13	1:B:230:LEU:HD21	1.69	0.72
1:B:56:VAL:HG11	1:B:88:PHE:HZ	1.55	0.72
1:B:137:MET:HE2	1:B:153:ILE:HD11	1.70	0.72
1:A:104:ASN:C	1:A:104:ASN:HD22	1.94	0.72
1:A:235:GLU:O	1:A:236:PHE:HB3	1.90	0.71
1:A:4:LYS:HD2	1:A:235:GLU:O	1.90	0.70
1:B:72:ARG:HB2	1:B:72:ARG:HH21	1.57	0.70
1:B:65:LYS:HG3	1:B:66:ALA:H	1.55	0.70
1:A:49:LYS:HA	1:A:49:LYS:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HB3	1:A:9:LYS:HZ2	1.57	0.69
1:B:197:PRO:C	1:B:199:SER:H	1.93	0.69
1:B:74:GLU:OE2	1:B:78:GLU:HB2	1.92	0.69
1:B:99:LEU:HD11	1:B:286:GLU:HB3	1.72	0.69
1:A:32:PHE:O	1:A:36:GLU:HB2	1.93	0.69
1:A:49:LYS:HA	1:A:49:LYS:NZ	2.07	0.69
1:A:266:ILE:CG2	1:A:295:ALA:H	2.06	0.68
1:A:194:THR:H	1:A:203:GLN:HE22	1.42	0.68
1:A:142:ILE:HG22	1:B:197:PRO:HG3	1.77	0.67
1:B:3:PHE:CD1	1:B:160:ASP:HB3	2.30	0.66
1:B:285:TYR:H	1:B:285:TYR:HD1	1.42	0.66
1:A:140:ASN:O	1:A:141:ASP:HB2	1.94	0.66
1:A:39:ASN:HD21	1:A:42:ASN:HB2	1.61	0.66
1:A:100:THR:HG22	1:A:132:PRO:HB2	1.78	0.65
1:B:139:ILE:O	1:B:164:VAL:HG23	1.96	0.65
1:B:14:ILE:O	1:B:16:THR:HG22	1.96	0.65
1:B:17:CYS:HB3	1:B:285:TYR:HB2	1.77	0.65
1:A:266:ILE:HG22	1:A:295:ALA:H	1.63	0.64
1:B:62:ILE:HD13	1:B:77:GLU:CG	2.27	0.64
1:B:100:THR:HG22	1:B:132:PRO:HB2	1.79	0.64
1:A:151:LYS:O	1:A:155:GLU:HB3	1.98	0.64
1:B:195:THR:O	1:B:196:ASN:HB2	1.96	0.64
1:B:99:LEU:HD11	1:B:286:GLU:CB	2.28	0.64
1:B:87:CYS:O	1:B:91:ILE:HG13	1.99	0.63
1:B:164:VAL:CG1	1:B:190:VAL:HG12	2.28	0.63
1:B:282:HIS:ND1	1:B:283:LYS:N	2.47	0.63
1:B:36:GLU:HG3	1:B:41:TYR:HA	1.81	0.63
1:A:10:ARG:HD3	1:A:99:LEU:O	1.99	0.62
1:B:219:GLN:HE22	1:B:223:ASN:HD21	1.47	0.62
1:B:171:ASN:O	1:B:174:LYS:HG2	1.99	0.62
1:A:196:ASN:O	1:A:198:ASP:N	2.29	0.62
1:B:279:ASN:C	1:B:281:TYR:H	2.03	0.62
1:A:158:LYS:NZ	1:A:158:LYS:HB2	2.15	0.62
1:B:140:ASN:HB3	1:B:165:ASN:O	2.00	0.61
1:A:308:MET:HG2	1:A:312:GLN:NE2	2.15	0.61
1:A:222:LEU:HD13	1:A:239:PHE:CZ	2.35	0.61
1:B:195:THR:HB	1:B:244:ASN:ND2	2.15	0.61
1:B:53:ILE:HG13	1:B:88:PHE:CE1	2.36	0.61
1:A:38:GLU:HG2	1:A:38:GLU:O	2.01	0.60
1:A:49:LYS:HZ3	1:A:49:LYS:HA	1.65	0.60
1:B:230:LEU:HB3	1:B:235:GLU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ASN:HB2	1:B:128:GLU:HG3	1.83	0.60
1:B:251:TYR:CD2	1:B:252:ILE:N	2.70	0.60
1:A:279:ASN:C	1:A:281:TYR:H	2.04	0.60
1:B:56:VAL:HG11	1:B:88:PHE:CZ	2.37	0.60
1:A:230:LEU:CD1	1:A:237:ILE:HG13	2.31	0.60
1:B:192:VAL:CG1	1:B:214:TYR:HB2	2.32	0.60
1:A:276:THR:C	1:A:278:THR:H	2.04	0.59
1:B:27:LYS:CB	1:B:27:LYS:NZ	2.64	0.59
1:B:72:ARG:N	1:B:72:ARG:HH21	1.99	0.59
1:B:41:TYR:CD1	1:B:67:PRO:HB2	2.37	0.59
1:B:251:TYR:HD2	1:B:252:ILE:N	1.99	0.58
1:B:16:THR:HB	1:B:310:TYR:HE1	1.67	0.58
1:A:294:ARG:HH11	1:A:294:ARG:HB3	1.68	0.58
1:B:72:ARG:NH2	1:B:72:ARG:HB2	2.17	0.58
1:A:41:TYR:HD1	1:A:44:ILE:HD12	1.68	0.58
1:A:51:LYS:HE3	1:A:52:TYR:CE1	2.38	0.58
1:B:202:PHE:CA	1:B:206:LEU:HD22	2.30	0.58
1:A:288:ILE:HG13	1:A:288:ILE:O	2.03	0.58
1:B:197:PRO:C	1:B:199:SER:N	2.56	0.58
1:B:72:ARG:CB	1:B:72:ARG:HH21	2.16	0.58
1:A:254:THR:O	1:A:257:PRO:HD3	2.04	0.58
1:A:27:LYS:O	1:A:30:GLU:HG2	2.03	0.58
1:A:41:TYR:CD1	1:A:67:PRO:HB3	2.39	0.58
1:B:91:ILE:O	1:B:95:ASN:HB3	2.04	0.58
1:B:58:ILE:HG21	1:B:117:ASP:CG	2.24	0.58
1:B:65:LYS:HG3	1:B:66:ALA:N	2.18	0.58
1:A:215:VAL:O	1:A:219:GLN:HG3	2.04	0.58
1:B:284:SER:O	1:B:285:TYR:O	2.21	0.58
1:B:197:PRO:O	1:B:200:ALA:N	2.34	0.57
1:A:196:ASN:HB3	1:A:199:SER:CB	2.35	0.57
1:B:5:VAL:HA	1:B:8:GLU:CG	2.34	0.57
1:A:180:GLU:O	1:A:181:GLU:HG3	2.04	0.57
1:A:204:LYS:O	1:A:212:GLN:HG2	2.05	0.57
1:A:308:MET:CG	1:A:312:GLN:HE21	2.17	0.57
1:A:316:ILE:HG22	1:A:316:ILE:O	2.04	0.57
1:B:86:PHE:O	1:B:89:TYR:HB3	2.04	0.57
1:A:262:LEU:O	1:A:264:PRO:HD3	2.04	0.57
1:A:168:MET:HA	1:B:203:GLN:HE21	1.70	0.57
1:B:246:TYR:CD2	1:B:277:LEU:HB2	2.40	0.57
1:A:50:GLU:O	1:A:53:ILE:HG22	2.04	0.57
1:A:196:ASN:C	1:A:198:ASP:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLY:HA2	1:A:175:ASP:OD2	2.05	0.56
1:A:97:TYR:CZ	1:A:307:GLN:HB3	2.40	0.56
1:A:138:LYS:HG2	1:A:191:LEU:HD21	1.86	0.56
1:A:278:THR:C	1:A:280:GLY:H	2.08	0.56
1:B:195:THR:HB	1:B:244:ASN:HD21	1.69	0.56
1:B:288:ILE:O	1:B:288:ILE:HG13	2.04	0.56
1:B:251:TYR:O	1:B:252:ILE:HB	2.06	0.56
1:B:109:ILE:N	1:B:110:PRO:HD2	2.21	0.56
1:B:174:LYS:HA	1:B:228:LEU:HD23	1.88	0.56
1:B:91:ILE:O	1:B:95:ASN:ND2	2.36	0.56
1:B:155:GLU:OE2	1:B:182:LYS:HE3	2.05	0.55
1:B:308:MET:HG2	1:B:312:GLN:HE21	1.71	0.55
1:B:44:ILE:O	1:B:48:LEU:HG	2.07	0.55
1:A:166:ILE:HD11	1:A:217:MET:HB3	1.88	0.55
1:A:37:LYS:C	1:A:39:ASN:H	2.09	0.55
1:A:58:ILE:N	1:A:58:ILE:HD12	2.21	0.55
1:B:201:ILE:C	1:B:203:GLN:H	2.09	0.55
1:B:103:MET:O	1:B:135:LEU:HD12	2.07	0.55
1:B:201:ILE:CG1	1:B:202:PHE:H	2.12	0.55
1:B:166:ILE:HD11	1:B:217:MET:HG2	1.88	0.55
1:B:219:GLN:NE2	1:B:223:ASN:HD21	2.05	0.55
1:A:20:ILE:HD13	1:A:94:THR:HB	1.88	0.54
1:B:5:VAL:HA	1:B:8:GLU:HG3	1.90	0.54
1:A:50:GLU:OE1	1:A:50:GLU:HA	2.07	0.54
1:A:53:ILE:O	1:A:56:VAL:HG22	2.07	0.54
1:B:16:THR:HB	1:B:310:TYR:CE1	2.42	0.54
1:A:109:ILE:N	1:A:110:PRO:CD	2.70	0.54
1:A:276:THR:C	1:A:278:THR:N	2.61	0.54
1:B:137:MET:CE	1:B:153:ILE:HD11	2.37	0.54
1:A:84:ASN:HA	1:A:118:VAL:HG13	1.91	0.53
1:B:285:TYR:CD1	1:B:285:TYR:N	2.76	0.53
1:B:253:ARG:NH2	1:B:283:LYS:HB3	2.20	0.53
1:B:201:ILE:O	1:B:202:PHE:HB2	2.09	0.53
1:A:232:GLN:CD	1:A:232:GLN:H	2.12	0.53
1:B:192:VAL:HG13	1:B:214:TYR:HB2	1.90	0.53
1:B:252:ILE:O	1:B:256:PHE:HB2	2.08	0.53
1:A:100:THR:CG2	1:A:132:PRO:HB2	2.39	0.53
1:B:109:ILE:N	1:B:110:PRO:CD	2.72	0.52
1:A:279:ASN:C	1:A:281:TYR:N	2.63	0.52
1:A:294:ARG:HG3	2:A:337:HOH:O	2.09	0.52
1:B:201:ILE:CD1	1:B:205:ASN:HD22	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:HE2	1:B:72:ARG:HE	1.73	0.52
1:B:178:TYR:CE2	1:B:180:GLU:HB3	2.44	0.52
1:B:250:ASN:O	1:B:251:TYR:HB2	2.09	0.52
1:A:248:GLU:O	1:A:252:ILE:HG12	2.10	0.52
1:B:46:LYS:NZ	1:B:46:LYS:HB3	2.25	0.52
1:A:193:LYS:HA	1:A:203:GLN:NE2	2.25	0.52
1:B:14:ILE:HG13	1:B:14:ILE:O	2.10	0.52
1:B:23:ASP:HB3	1:B:107:PHE:CE2	2.45	0.52
1:A:47:ASN:O	1:A:49:LYS:N	2.43	0.52
1:A:47:ASN:C	1:A:49:LYS:H	2.14	0.52
2:A:333:HOH:O	1:B:26:GLU:HB2	2.09	0.52
1:B:2:GLY:O	1:B:6:LYS:HB2	2.09	0.52
1:B:9:LYS:C	1:B:11:ARG:H	2.13	0.52
1:B:53:ILE:HG12	1:B:53:ILE:O	2.09	0.51
1:B:86:PHE:O	1:B:90:ILE:HG12	2.10	0.51
1:B:20:ILE:HD12	1:B:98:ALA:HB2	1.91	0.51
1:A:108:TYR:O	1:A:115:GLY:HA3	2.10	0.51
1:A:193:LYS:HD3	1:A:203:GLN:NE2	2.25	0.51
1:A:266:ILE:HD13	1:A:294:ARG:HB2	1.91	0.51
1:B:253:ARG:NH2	1:B:283:LYS:HD3	2.24	0.51
1:B:56:VAL:O	1:B:60:LYS:CE	2.59	0.51
1:A:278:THR:O	1:A:280:GLY:N	2.36	0.51
1:A:204:LYS:HE3	1:A:212:GLN:HE22	1.76	0.51
1:A:285:TYR:O	1:A:286:GLU:HB3	2.10	0.51
1:B:9:LYS:C	1:B:11:ARG:N	2.64	0.51
1:B:252:ILE:HA	1:B:256:PHE:CD1	2.45	0.51
1:B:164:VAL:HG13	1:B:190:VAL:HG12	1.92	0.51
1:B:174:LYS:HG3	1:B:175:ASP:N	2.25	0.50
1:B:196:ASN:O	1:B:198:ASP:N	2.44	0.50
1:B:163:THR:HA	1:B:189:PHE:O	2.12	0.50
1:B:34:LYS:O	1:B:38:GLU:HG3	2.11	0.50
1:A:90:ILE:HD12	1:A:297:THR:HG22	1.93	0.50
1:A:57:SER:C	1:A:58:ILE:HD12	2.32	0.50
1:A:222:LEU:HD13	1:A:239:PHE:HZ	1.74	0.50
1:B:201:ILE:HG13	1:B:205:ASN:HB2	1.93	0.50
1:B:58:ILE:N	1:B:58:ILE:HD12	2.25	0.50
1:B:230:LEU:HD11	1:B:237:ILE:HG13	1.94	0.50
1:A:61:ASP:OD1	1:A:62:ILE:HG12	2.12	0.50
1:A:195:THR:HG21	1:A:244:ASN:HB2	1.94	0.49
1:A:200:ALA:HB1	1:A:204:LYS:HB2	1.94	0.49
1:B:146:VAL:CG2	1:B:175:ASP:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ALA:C	1:A:317:LEU:H	2.13	0.49
1:B:282:HIS:CG	1:B:283:LYS:N	2.80	0.49
1:B:104:ASN:HD22	1:B:106:ALA:H	1.61	0.49
1:B:18:LEU:HD12	1:B:19:CYS:H	1.76	0.49
1:B:55:ASN:CG	1:B:128:GLU:HG3	2.33	0.49
1:A:36:GLU:HG2	1:A:44:ILE:CD1	2.42	0.49
1:A:95:ASN:HB2	1:A:131:ILE:CD1	2.43	0.49
1:B:294:ARG:O	1:B:298:LYS:HB2	2.13	0.49
1:A:307:GLN:HA	1:A:310:TYR:HB3	1.93	0.49
1:A:41:TYR:CD1	1:A:44:ILE:HD12	2.48	0.49
1:A:276:THR:HG21	1:A:316:ILE:HD11	1.94	0.48
1:B:182:LYS:O	1:B:184:LYS:HG3	2.13	0.48
1:B:62:ILE:HD13	1:B:77:GLU:HG2	1.93	0.48
1:B:208:LEU:C	1:B:208:LEU:HD23	2.33	0.48
1:A:34:LYS:C	1:A:36:GLU:N	2.66	0.48
1:A:193:LYS:HE3	1:A:204:LYS:HD2	1.96	0.48
1:A:257:PRO:O	1:A:258:ASN:CB	2.60	0.48
1:A:150:ARG:HD3	1:A:175:ASP:O	2.14	0.48
1:B:36:GLU:OE1	1:B:43:ASN:HB2	2.14	0.48
1:B:75:LYS:NZ	1:B:75:LYS:HB3	2.28	0.48
1:A:97:TYR:CE2	1:A:307:GLN:HB3	2.49	0.47
1:B:166:ILE:HG21	1:B:173:LEU:HD11	1.96	0.47
1:B:109:ILE:HG13	1:B:109:ILE:O	2.15	0.47
1:B:197:PRO:O	1:B:199:SER:N	2.47	0.47
1:A:164:VAL:O	1:A:190:VAL:HA	2.14	0.47
1:A:294:ARG:NH1	1:A:294:ARG:HB3	2.30	0.47
1:B:104:ASN:ND2	1:B:106:ALA:H	2.11	0.47
1:B:104:ASN:ND2	1:B:106:ALA:HB3	2.30	0.47
1:B:230:LEU:CD1	1:B:237:ILE:HG13	2.44	0.47
1:B:173:LEU:HB2	1:B:224:MET:HG2	1.96	0.47
1:B:154:PHE:CE1	1:B:186:TYR:HB3	2.49	0.47
1:B:4:LYS:HE3	1:B:260:TYR:HE1	1.80	0.47
1:A:266:ILE:HD13	1:A:294:ARG:HG3	1.96	0.47
1:B:195:THR:OG1	1:B:242:GLY:HA3	2.14	0.47
1:B:250:ASN:O	1:B:251:TYR:CB	2.63	0.46
1:A:104:ASN:C	1:A:104:ASN:ND2	2.66	0.46
1:A:20:ILE:CD1	1:A:94:THR:HB	2.45	0.46
1:A:299:ASN:ND2	1:A:305:ALA:HB2	2.31	0.46
1:A:39:ASN:HD21	1:A:42:ASN:H	1.63	0.46
1:A:41:TYR:CG	1:A:67:PRO:HB3	2.51	0.46
1:B:32:PHE:O	1:B:36:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:THR:HG21	1:B:97:TYR:O	2.14	0.46
1:B:174:LYS:HA	1:B:228:LEU:CD2	2.45	0.46
1:B:300:PRO:HB2	1:B:301:TYR:CE1	2.50	0.46
1:B:71:ILE:N	1:B:72:ARG:NH2	2.63	0.46
1:B:4:LYS:HE3	1:B:260:TYR:CE1	2.50	0.46
1:B:47:ASN:ND2	1:B:92:ASN:HD22	2.13	0.46
1:B:288:ILE:O	1:B:288:ILE:HG23	2.16	0.46
1:A:307:GLN:O	1:A:310:TYR:HB3	2.16	0.46
1:B:71:ILE:N	1:B:72:ARG:HH22	2.14	0.46
1:A:283:LYS:HG3	1:A:287:LYS:HD2	1.98	0.46
1:A:41:TYR:CE1	1:A:67:PRO:HB3	2.51	0.46
1:B:201:ILE:HG13	1:B:205:ASN:ND2	2.31	0.46
1:B:23:ASP:HB3	1:B:107:PHE:CD2	2.51	0.46
1:A:109:ILE:N	1:A:110:PRO:HD2	2.30	0.46
1:B:146:VAL:O	1:B:149:TYR:N	2.49	0.46
1:A:167:TYR:CE2	1:B:217:MET:HE1	2.51	0.46
1:B:20:ILE:HD13	1:B:94:THR:OG1	2.16	0.46
1:A:198:ASP:HA	1:A:201:ILE:HG12	1.97	0.45
1:B:95:ASN:HB2	1:B:131:ILE:CD1	2.47	0.45
1:B:192:VAL:HG12	1:B:214:TYR:HB2	1.97	0.45
1:B:285:TYR:O	1:B:286:GLU:HG3	2.15	0.45
1:A:78:GLU:O	1:A:81:TYR:HB3	2.16	0.45
1:A:217:MET:HE1	1:B:167:TYR:CE2	2.51	0.45
1:B:300:PRO:HB2	1:B:301:TYR:CD1	2.51	0.45
1:A:257:PRO:O	1:A:258:ASN:HB3	2.16	0.45
1:A:23:ASP:HB3	1:A:107:PHE:CD2	2.51	0.45
1:A:118:VAL:O	1:A:122:VAL:HG23	2.17	0.45
1:B:219:GLN:HG3	2:B:332:HOH:O	2.16	0.45
1:B:13:ALA:O	1:B:14:ILE:C	2.54	0.45
1:A:110:PRO:HA	1:B:152:PHE:HB2	1.97	0.45
1:B:86:PHE:CE1	1:B:90:ILE:HD11	2.52	0.45
1:A:230:LEU:HD12	1:A:237:ILE:HG13	1.98	0.45
1:B:279:ASN:C	1:B:281:TYR:N	2.70	0.45
1:B:282:HIS:O	1:B:283:LYS:HB2	2.17	0.45
1:B:278:THR:C	1:B:280:GLY:H	2.20	0.45
1:B:44:ILE:HD13	1:B:81:TYR:HE2	1.82	0.45
1:B:154:PHE:O	1:B:158:LYS:HA	2.17	0.44
1:A:39:ASN:ND2	1:A:42:ASN:H	2.14	0.44
1:B:201:ILE:HG23	1:B:202:PHE:CD2	2.52	0.44
1:B:34:LYS:HD3	1:B:34:LYS:HA	1.83	0.44
1:A:23:ASP:HB3	1:A:107:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:C	1:A:236:PHE:CD1	2.90	0.44
1:A:97:TYR:HB3	1:A:310:TYR:CD1	2.52	0.44
1:A:34:LYS:C	1:A:36:GLU:H	2.20	0.44
1:B:249:MET:O	1:B:251:TYR:O	2.35	0.44
1:A:4:LYS:O	1:A:8:GLU:HB2	2.17	0.44
1:B:258:ASN:ND2	1:B:283:LYS:HZ2	2.16	0.44
1:A:266:ILE:HG23	1:A:294:ARG:N	2.33	0.44
1:A:174:LYS:HG3	1:A:228:LEU:HD21	1.99	0.44
1:B:180:GLU:HG3	1:B:180:GLU:O	2.18	0.44
1:B:201:ILE:O	1:B:203:GLN:N	2.49	0.44
1:B:260:TYR:CE1	1:B:287:LYS:HE2	2.53	0.44
1:A:157:LEU:O	1:A:158:LYS:HB2	2.18	0.43
1:B:4:LYS:HG3	1:B:260:TYR:OH	2.18	0.43
1:A:61:ASP:OD1	1:A:62:ILE:N	2.48	0.43
1:B:20:ILE:CD1	1:B:98:ALA:HB2	2.48	0.43
1:B:229:ASN:OD1	1:B:231:GLU:HB3	2.18	0.43
1:B:253:ARG:HH22	1:B:283:LYS:HD3	1.83	0.43
1:A:14:ILE:HD11	1:A:99:LEU:HA	2.00	0.43
1:A:18:LEU:HD12	1:A:19:CYS:N	2.33	0.43
1:B:243:ALA:HB3	1:B:265:GLY:HA3	2.00	0.43
1:A:41:TYR:O	1:A:45:LYS:HB2	2.18	0.43
1:A:47:ASN:C	1:A:49:LYS:N	2.72	0.43
1:B:192:VAL:CG2	1:B:239:PHE:HB3	2.47	0.43
1:B:299:ASN:HA	1:B:300:PRO:HD3	1.91	0.43
1:A:137:MET:O	1:A:138:LYS:C	2.57	0.43
1:B:57:SER:C	1:B:58:ILE:HD12	2.39	0.43
1:A:168:MET:HA	1:B:203:GLN:NE2	2.33	0.43
1:A:252:ILE:O	1:A:256:PHE:HB2	2.18	0.43
1:B:171:ASN:ND2	1:B:174:LYS:NZ	2.67	0.43
1:A:131:ILE:HA	1:A:132:PRO:HD3	1.87	0.43
1:A:209:ASP:O	1:A:210:ASN:HB2	2.18	0.43
1:A:3:PHE:CD1	1:A:160:ASP:HB3	2.54	0.43
1:B:251:TYR:N	1:B:254:THR:HG23	2.34	0.43
1:A:47:ASN:ND2	1:A:92:ASN:HD22	2.17	0.43
1:B:18:LEU:HD12	1:B:19:CYS:N	2.33	0.43
1:B:94:THR:C	1:B:96:LYS:H	2.22	0.43
1:B:63:LEU:HD21	1:B:84:ASN:CB	2.49	0.43
1:A:137:MET:HB3	1:A:139:ILE:HG23	2.01	0.42
1:A:67:PRO:O	1:A:68:ASP:C	2.57	0.42
1:B:236:PHE:C	1:B:236:PHE:CD1	2.92	0.42
1:B:58:ILE:CD1	1:B:58:ILE:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HD21	1:B:84:ASN:HB3	2.00	0.42
1:B:251:TYR:H	1:B:254:THR:HG23	1.84	0.42
1:B:285:TYR:O	1:B:286:GLU:CG	2.67	0.42
1:A:164:VAL:N	1:A:189:PHE:O	2.47	0.42
1:B:12:ASN:O	1:B:13:ALA:C	2.57	0.42
1:B:245:SER:O	1:B:249:MET:HB2	2.19	0.42
1:A:172:MET:HG3	1:A:173:LEU:N	2.34	0.42
1:A:33:MET:HG3	1:A:37:LYS:NZ	2.35	0.42
1:B:201:ILE:O	1:B:202:PHE:CB	2.67	0.42
1:B:211:LYS:HD2	1:B:216:ILE:HD11	2.02	0.42
1:A:266:ILE:HD13	1:A:294:ARG:CG	2.50	0.42
1:B:196:ASN:HB3	1:B:197:PRO:CD	2.44	0.42
1:B:193:LYS:HA	1:B:203:GLN:OE1	2.20	0.42
1:A:167:TYR:HE2	1:B:217:MET:HE1	1.85	0.42
1:A:31:ASN:C	1:A:31:ASN:OD1	2.58	0.42
1:A:315:ALA:C	1:A:317:LEU:N	2.73	0.42
1:B:151:LYS:HA	1:B:155:GLU:OE1	2.19	0.42
1:B:229:ASN:OD1	1:B:232:GLN:HG2	2.20	0.42
1:B:35:ASN:O	1:B:39:ASN:ND2	2.53	0.42
1:A:119:LEU:O	1:A:122:VAL:HB	2.19	0.42
1:A:39:ASN:CG	1:A:40:ASN:N	2.73	0.42
1:B:145:THR:O	1:B:148:ASN:ND2	2.53	0.42
1:B:201:ILE:C	1:B:203:GLN:N	2.73	0.42
1:B:251:TYR:O	1:B:252:ILE:CB	2.64	0.42
1:A:120:LYS:HD2	1:A:120:LYS:O	2.20	0.41
1:A:278:THR:C	1:A:280:GLY:N	2.73	0.41
1:A:55:ASN:O	1:A:56:VAL:C	2.57	0.41
1:A:198:ASP:CA	1:A:201:ILE:HG12	2.50	0.41
1:B:93:GLU:OE2	1:B:303:GLN:HB2	2.20	0.41
1:A:214:TYR:CE1	1:A:215:VAL:HG23	2.56	0.41
1:A:192:VAL:HG13	1:A:214:TYR:O	2.21	0.41
1:B:11:ARG:HD3	1:B:286:GLU:HG2	2.03	0.41
1:B:71:ILE:C	1:B:72:ARG:HH21	2.23	0.41
1:A:10:ARG:HH11	1:A:10:ARG:HG3	1.86	0.41
1:A:198:ASP:O	1:A:201:ILE:HG12	2.20	0.41
1:A:192:VAL:HG12	1:A:214:TYR:HB2	2.03	0.41
1:B:98:ALA:HB3	1:B:101:PHE:CE1	2.55	0.41
1:B:283:LYS:CG	1:B:284:SER:H	2.06	0.41
1:A:3:PHE:CE1	1:A:160:ASP:HB3	2.55	0.41
1:A:27:LYS:HE3	1:A:27:LYS:HA	2.02	0.41
1:A:56:VAL:O	1:A:60:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:TYR:CD2	1:B:119:LEU:HD13	2.56	0.41
1:B:166:ILE:HD11	1:B:217:MET:CG	2.51	0.41
1:B:195:THR:O	1:B:196:ASN:CB	2.65	0.41
1:A:104:ASN:HD22	1:A:105:PHE:N	2.17	0.41
1:A:109:ILE:HG13	1:A:109:ILE:O	2.21	0.41
1:A:277:LEU:N	1:A:277:LEU:HD23	2.17	0.41
1:A:33:MET:CG	1:A:37:LYS:NZ	2.84	0.40
1:A:206:LEU:HD23	1:B:206:LEU:HD23	2.02	0.40
1:B:275:LYS:O	1:B:276:THR:HG23	2.21	0.40
1:B:51:LYS:HE3	1:B:52:TYR:CD1	2.56	0.40
1:A:4:LYS:HD3	1:A:234:ASN:HA	2.01	0.40
1:A:20:ILE:CD1	1:A:98:ALA:HB2	2.41	0.40
1:B:285:TYR:C	1:B:287:LYS:N	2.74	0.40
1:A:19:CYS:O	1:A:291:ASN:HA	2.21	0.40
1:B:33:MET:HG3	1:B:82:PHE:CD2	2.56	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	300/323 (93%)	246 (82%)	40 (13%)	14 (5%)	2	4
1	B	304/323 (94%)	234 (77%)	50 (16%)	20 (7%)	1	2
All	All	604/646 (94%)	480 (80%)	90 (15%)	34 (6%)	2	3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY
1	B	181	GLU
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	231	GLU
1	B	251	TYR
1	B	283	LYS
1	B	285	TYR
1	B	317	LEU
1	A	48	LEU
1	A	68	ASP
1	A	198	ASP
1	A	279	ASN
1	B	15	ASN
1	B	42	ASN
1	B	143	GLY
1	A	141	ASP
1	A	197	PRO
1	A	236	PHE
1	A	276	THR
1	B	51	LYS
1	B	229	ASN
1	B	256	PHE
1	B	281	TYR
1	A	181	GLU
1	A	285	TYR
1	B	198	ASP
1	B	257	PRO
1	A	95	ASN
1	A	282	HIS
1	B	227	TYR
1	B	14	ILE
1	B	50	GLU
1	A	62	ILE
1	B	265	GLY

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/295 (89%)	246 (94%)	17 (6%)	17	38
1	B	269/295 (91%)	245 (91%)	24 (9%)	9	22
All	All	532/590 (90%)	491 (92%)	41 (8%)	13	30

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	27	LYS
1	A	42	ASN
1	A	49	LYS
1	A	61	ASP
1	A	83	PHE
1	A	84	ASN
1	A	99	LEU
1	A	104	ASN
1	A	114	VAL
1	A	129	LEU
1	A	140	ASN
1	A	164	VAL
1	A	251	TYR
1	A	253	ARG
1	A	277	LEU
1	A	283	LYS
1	B	8	GLU
1	B	27	LYS
1	B	36	GLU
1	B	40	ASN
1	B	51	LYS
1	B	72	ARG
1	B	74	GLU
1	B	75	LYS
1	B	77	GLU
1	B	83	PHE
1	B	84	ASN
1	B	99	LEU
1	B	104	ASN
1	B	146	VAL
1	B	170	THR

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Mol	Chain	Res	Type
1	B	195	THR
1	B	198	ASP
1	B	206	LEU
1	B	228	LEU
1	B	251	TYR
1	B	257	PRO
1	B	285	TYR
1	B	294	ARG
1	B	301	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	42	ASN
1	A	47	ASN
1	A	104	ASN
1	A	203	GLN
1	A	212	GLN
1	A	223	ASN
1	A	234	ASN
1	A	312	GLN
1	B	12	ASN
1	B	40	ASN
1	B	42	ASN
1	B	47	ASN
1	B	54	ASN
1	B	104	ASN
1	B	171	ASN
1	B	205	ASN
1	B	212	GLN
1	B	219	GLN
1	B	223	ASN
1	B	232	GLN
1	B	234	ASN
1	B	258	ASN
1	B	279	ASN
1	B	303	GLN
1	B	312	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	306/323 (94%)	-0.07	5 (1%) 72 74	18, 48, 85, 110	0
1	B	310/323 (95%)	0.19	16 (5%) 27 25	21, 58, 103, 139	0
All	All	616/646 (95%)	0.06	21 (3%) 45 45	18, 55, 95, 139	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	ILE	4.6
1	A	41	TYR	3.9
1	B	14	ILE	3.7
1	A	266	ILE	3.6
1	B	256	PHE	3.4
1	B	40	ASN	3.1
1	B	252	ILE	3.1
1	B	227	TYR	2.7
1	B	315	ALA	2.6
1	B	97	TYR	2.6
1	A	40	ASN	2.5
1	B	267	GLY	2.5
1	B	52	TYR	2.3
1	B	281	TYR	2.3
1	B	282	HIS	2.3
1	A	39	ASN	2.3
1	B	253	ARG	2.2
1	B	72	ARG	2.1
1	A	256	PHE	2.1
1	B	314	ASN	2.1
1	B	317	LEU	2.0

## 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 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.