



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:55 am BST

PDB ID : 2BTU  
Title : Crystal structure of Phosphoribosylformylglycinamide cyclo-ligase from Bacillus Anthracis at 2.3Å resolution.  
Authors : Moroz, O.V.; Blagova, E.V.; Levnikov, V.M.; Fogg, M.J.; Lebedev, A.A.; Brannigan, J.A.; Wilkinson, A.J.; Wilson, K.S.  
Deposited on : 2005-06-07  
Resolution : 2.31 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

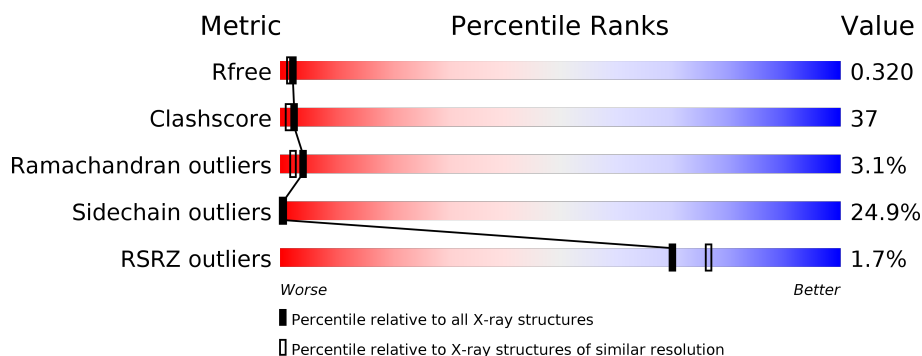
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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  $\geq 3$ , 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	346	<div> <div> <div></div> <div>42%</div> <div>38%</div> <div>12%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	346	<div> <div>2%</div> <div> <div></div> <div>36%</div> <div>41%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4584 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 PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2284	1464	369	434	17			
1	B	307	Total	C	N	O	S	0	0	0
			2134	1358	350	409	17			

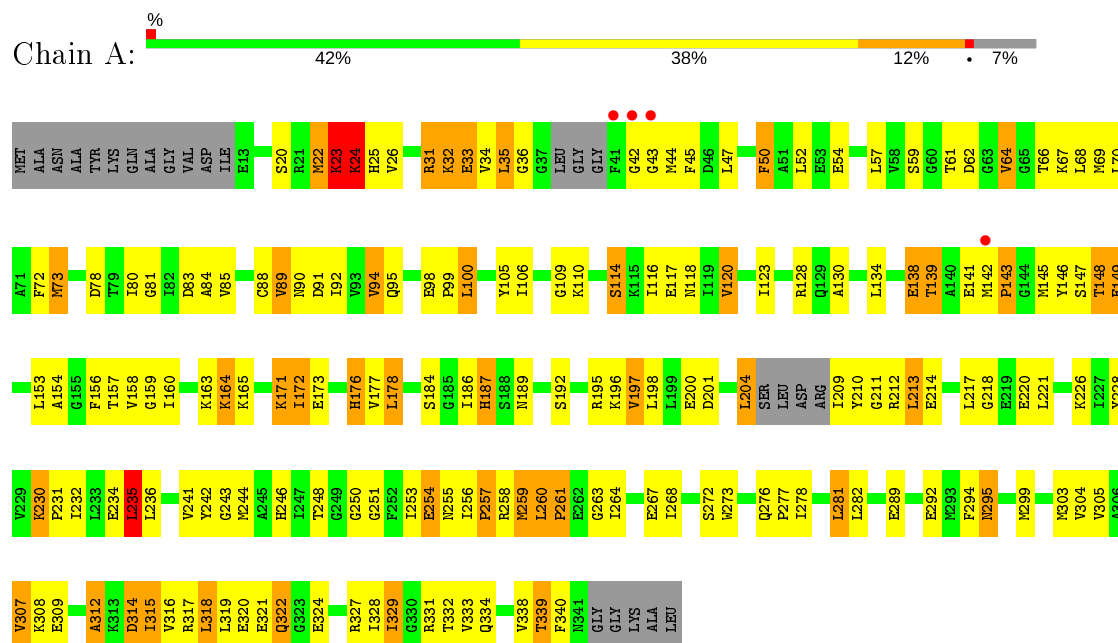
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	92	Total	O	0	0
			92	92		

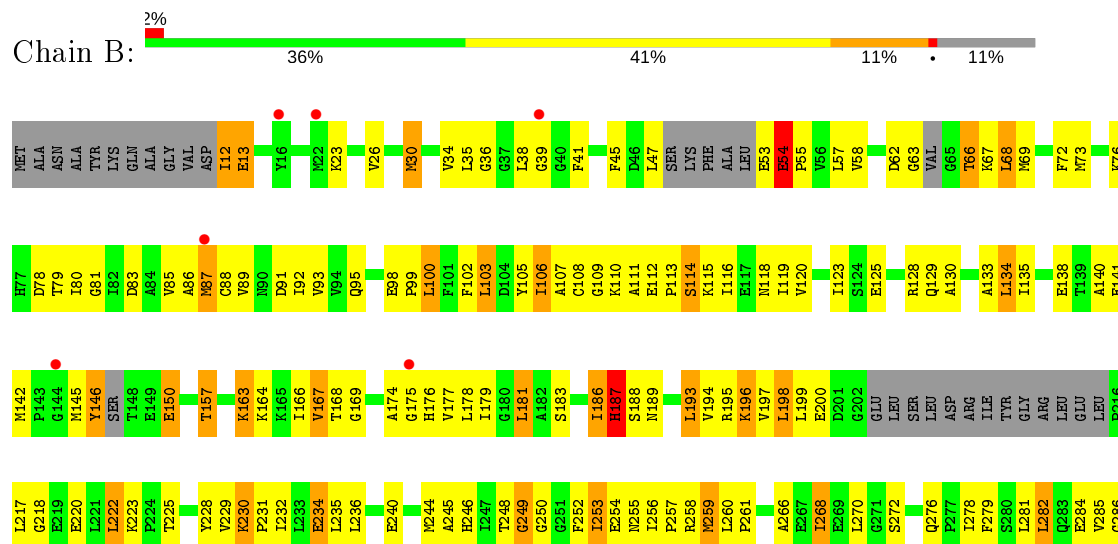
### 3 Residue-property plots

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: PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE



#### • Molecule 1: PHOSPHORIBOSYL-AMINOIMIDAZOLE SYNTHETASE



K287	L288	E289	E290	K291	E292	M293	F294	N295	I296	F297	N298	M299	G300	I301	M303	V304	V305	A306	V307	K308	E309	E310	D311	I315	V316	L319	E320	E321	Q322	G323	E324	T325	A326	K327	I328	I329	G330	R331	T332	V333	Q334	G335	A336	G337	V338	THR	PHE	ASN	GLY	GLY	LYS	ALA	LEU
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.49Å 89.49Å 88.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.31 24.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	93.3 (25.00-2.31) 90.2 (24.82-2.31)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.31Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.182 , 0.249 0.290 , 0.320	Depositor DCC
$R_{free}$ test set	1375 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 69.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.098 for -h,-l,-k 0.097 for -h,l,k 0.104 for l,-k,h 0.106 for -l,-k,-h 0.388 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [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	0.33	0/2317	0.99	4/3131 (0.1%)
1	B	0.34	0/2160	0.96	7/2909 (0.2%)
All	All	0.33	0/4477	0.98	11/6040 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	VAL	C-N-CA	16.78	163.65	121.70
1	B	168	THR	C-N-CA	7.59	138.25	122.30
1	B	39	GLY	C-N-CA	7.11	137.24	122.30
1	B	327	ARG	CD-NE-CZ	6.99	133.39	123.60
1	A	35	LEU	C-N-CA	6.73	136.43	122.30
1	B	35	LEU	C-N-CA	6.62	136.20	122.30
1	A	23	LYS	C-N-CA	6.07	136.88	121.70
1	B	327	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	198	LEU	C-N-CA	5.23	134.78	121.70
1	B	23	LYS	C-N-CA	5.21	134.72	121.70
1	A	32	LYS	C-N-CA	5.06	134.34	121.70

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	2284	0	2182	167	0
1	B	2134	0	1994	169	0
2	A	74	0	0	15	0
2	B	92	0	0	11	0
All	All	4584	0	4176	321	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 37.

All (321) 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:87:MET:HE1	1:B:248:THR:HG21	1.16	1.08
1:B:87:MET:CE	1:B:248:THR:HG21	1.92	0.99
1:A:261:PRO:HG2	1:A:264:ILE:HD12	1.42	0.98
1:A:164:LYS:HE2	1:A:164:LYS:H	1.28	0.95
1:B:87:MET:HE1	1:B:248:THR:CG2	1.96	0.95
1:A:89:VAL:HG21	1:A:130:ALA:HB1	1.51	0.90
1:A:235:LEU:HD12	1:A:319:LEU:HD21	1.56	0.86
1:B:30:MET:HE3	1:B:34:VAL:HG21	1.56	0.86
1:A:90:ASN:HD21	1:A:228:TYR:H	1.24	0.86
1:B:272:SER:O	1:B:327:ARG:HD2	1.77	0.84
1:B:87:MET:CE	1:B:246:HIS:NE2	2.40	0.84
1:A:110:LYS:HA	1:A:141:GLU:HB3	1.58	0.84
1:A:273:TRP:HB3	1:A:329:ILE:HD11	1.57	0.84
1:B:87:MET:HE3	1:B:246:HIS:NE2	1.93	0.83
1:B:66:THR:HG22	1:B:69:MET:HE1	1.60	0.83
1:B:244:MET:HG2	1:B:305:VAL:HB	1.59	0.82
1:B:257:PRO:HA	1:B:260:LEU:HG	1.60	0.81
1:B:30:MET:HB3	2:B:2021:HOH:O	1.81	0.81
1:B:87:MET:CE	1:B:248:THR:CG2	2.54	0.80
1:B:125:GLU:O	1:B:129:GLN:HG3	1.82	0.79
1:A:44:MET:HE3	1:B:58:VAL:HG22	1.65	0.78
1:A:70:LEU:HA	1:A:73:MET:HG3	1.64	0.78
1:A:312:ALA:O	1:A:316:VAL:HG23	1.85	0.77
1:B:110:LYS:HA	1:B:141:GLU:OE2	1.85	0.77
1:A:334:GLN:HG2	2:A:2072:HOH:O	1.84	0.76
1:B:255:ASN:O	1:B:258:ARG:HB2	1.85	0.75
1:B:73:MET:HA	2:B:2035:HOH:O	1.86	0.75
1:B:78:ASP:OD1	1:B:79:THR:HG23	1.87	0.75
1:A:81:GLY:O	1:A:85:VAL:HG23	1.88	0.74
1:A:31:ARG:O	1:A:34:VAL:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:O	1:B:285:VAL:HG23	1.88	0.73
1:B:253:ILE:HG12	1:B:295:ASN:ND2	2.05	0.72
1:A:228:TYR:O	1:A:232:ILE:HG12	1.90	0.72
1:B:311:ASP:O	1:B:315:ILE:HG23	1.90	0.72
1:B:83:ASP:O	1:B:86:ALA:HB3	1.91	0.71
1:B:87:MET:HA	1:B:87:MET:HE2	1.71	0.70
1:B:99:PRO:HG2	2:B:2051:HOH:O	1.90	0.70
1:B:197:VAL:HG12	1:B:198:LEU:HD23	1.73	0.70
1:B:245:ALA:O	1:B:303:MET:HG3	1.93	0.69
1:B:177:VAL:HG13	1:B:328:ILE:HG23	1.74	0.68
1:A:116:ILE:O	1:A:120:VAL:HG13	1.94	0.67
1:A:253:ILE:HG21	1:A:295:ASN:OD1	1.95	0.67
1:B:129:GLN:O	1:B:230:LYS:HD2	1.94	0.67
1:A:317:ARG:O	1:A:321:GLU:HG3	1.95	0.67
1:A:204:LEU:H	1:A:204:LEU:HD23	1.59	0.67
1:B:163:LYS:O	1:B:166:ILE:HD12	1.95	0.66
1:B:81:GLY:O	1:B:85:VAL:HG23	1.94	0.66
1:B:334:GLN:HG2	1:B:334:GLN:O	1.94	0.66
1:B:98:GLU:O	1:B:100:LEU:HD13	1.94	0.66
1:A:164:LYS:HE2	1:A:164:LYS:N	2.06	0.66
1:A:145:MET:HG2	1:B:150:GLU:OE1	1.94	0.66
1:B:196:LYS:O	1:B:200:GLU:HG2	1.96	0.66
1:A:173:GLU:O	1:A:176:HIS:HB2	1.96	0.66
1:A:31:ARG:HB2	1:A:33:GLU:HG3	1.77	0.65
1:B:54:GLU:HB2	2:B:2030:HOH:O	1.95	0.65
1:B:174:ALA:HA	1:B:332:THR:HG22	1.79	0.65
1:B:181:LEU:HD21	1:B:319:LEU:HD22	1.78	0.65
1:A:171:LYS:HD3	1:A:242:TYR:HA	1.78	0.64
1:B:116:ILE:O	1:B:120:VAL:HG13	1.98	0.64
1:B:187:HIS:CD2	1:B:225:THR:HG23	2.33	0.64
1:B:266:ALA:HB3	2:B:2092:HOH:O	1.97	0.63
1:B:92:ILE:HD12	1:B:93:VAL:N	2.14	0.63
1:B:53:GLU:O	1:B:55:PRO:HD3	1.99	0.63
1:A:230:LYS:O	1:A:234:GLU:HG2	1.97	0.63
1:A:263:GLY:O	1:A:334:GLN:HA	1.99	0.63
1:A:148:THR:HG22	1:A:149:GLU:OE1	2.00	0.62
1:A:80:ILE:O	1:A:83:ASP:HB2	1.99	0.62
1:B:231:PRO:HA	1:B:322:GLN:HG2	1.82	0.62
1:B:220:GLU:O	1:B:223:LYS:HB2	2.00	0.62
1:A:254:GLU:HG3	1:A:258:ARG:NH2	2.15	0.62
1:B:30:MET:HE2	1:B:34:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:HG3	1:A:176:HIS:CE1	2.35	0.61
1:B:289:GLU:HB3	1:B:292:GLU:HB2	1.82	0.61
1:A:90:ASN:ND2	1:A:228:TYR:H	1.97	0.61
1:B:327:ARG:HG3	1:B:327:ARG:HH11	1.66	0.61
1:B:230:LYS:O	1:B:234:GLU:HG2	2.00	0.60
1:B:106:ILE:HD13	1:B:119:ILE:HD13	1.83	0.60
1:A:44:MET:HE2	1:B:166:ILE:HG12	1.84	0.60
1:B:176:HIS:N	1:B:332:THR:HB	2.17	0.59
1:B:30:MET:HE1	1:B:133:ALA:HB1	1.83	0.59
1:B:268:ILE:HD12	1:B:329:ILE:HG23	1.84	0.59
1:B:186:ILE:O	1:B:187:HIS:HB2	2.03	0.58
1:A:105:TYR:CE1	1:B:63:GLY:HA3	2.39	0.58
1:A:187:HIS:CE1	1:A:226:LYS:H	2.21	0.57
1:A:171:LYS:HE2	1:A:242:TYR:CD2	2.39	0.57
1:A:231:PRO:HA	1:A:322:GLN:HG2	1.86	0.57
1:B:333:VAL:HG12	1:B:334:GLN:H	1.69	0.57
1:B:89:VAL:HG22	1:B:92:ILE:HD11	1.86	0.57
1:A:98:GLU:O	1:A:100:LEU:HD13	2.05	0.57
1:B:45:PHE:CE2	1:B:100:LEU:HG	2.39	0.57
1:A:230:LYS:HE3	2:A:2056:HOH:O	2.05	0.56
1:A:254:GLU:HG3	1:A:258:ARG:HH21	1.69	0.56
1:A:189:ASN:HD21	1:A:248:THR:HB	1.68	0.56
1:A:212:ARG:O	1:A:214:GLU:OE1	2.23	0.56
1:A:178:LEU:HD21	1:A:332:THR:HG23	1.88	0.56
1:B:197:VAL:HG12	1:B:198:LEU:CD2	2.34	0.56
1:B:181:LEU:HD23	1:B:324:GLU:HB3	1.87	0.56
1:A:57:LEU:HG	1:B:47:LEU:HD11	1.88	0.56
1:B:252:PHE:HB3	1:B:256:ILE:HD12	1.87	0.55
1:A:257:PRO:HD3	1:A:338:VAL:HG23	1.88	0.55
1:A:177:VAL:HG21	1:A:309:GLU:HA	1.88	0.55
1:A:276:GLN:HB3	2:A:2053:HOH:O	2.05	0.55
1:A:261:PRO:HA	2:A:2064:HOH:O	2.05	0.55
1:B:176:HIS:H	1:B:332:THR:HB	1.72	0.55
1:A:294:PHE:CD1	1:A:299:MET:HG3	2.42	0.55
1:A:289:GLU:HB2	1:A:292:GLU:OE1	2.06	0.55
1:A:61:THR:HG22	1:B:103:LEU:HD12	1.89	0.55
1:B:228:TYR:CD2	1:B:303:MET:HE3	2.42	0.55
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.72	0.54
1:B:193:LEU:O	1:B:197:VAL:HG23	2.07	0.54
1:B:193:LEU:HD11	1:B:288:LEU:HD11	1.89	0.54
1:B:89:VAL:O	1:B:92:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PRO:HD3	1:A:338:VAL:CG2	2.37	0.54
1:B:68:LEU:HD23	1:B:80:ILE:HG12	1.89	0.54
1:A:114:SER:O	1:A:117:GLU:HB3	2.07	0.54
1:B:178:LEU:HD22	1:B:304:VAL:HG11	1.88	0.54
1:A:176:HIS:HD2	1:A:308:LYS:HA	1.71	0.54
1:A:307:VAL:HG21	1:A:315:ILE:HD13	1.89	0.54
1:B:108:CYS:HB3	1:B:140:ALA:O	2.08	0.54
1:A:23:LYS:O	1:A:26:VAL:HG13	2.08	0.53
1:B:107:ALA:HB1	1:B:146:TYR:OH	2.08	0.53
1:A:89:VAL:HG22	1:A:99:PRO:HG2	1.90	0.53
1:B:12:ILE:HG23	1:B:12:ILE:O	2.09	0.53
1:B:177:VAL:HA	1:B:331:ARG:CG	2.38	0.53
1:A:23:LYS:HE3	1:A:120:VAL:HG11	1.91	0.53
1:A:44:MET:CE	1:B:166:ILE:HG12	2.38	0.53
1:A:172:ILE:HD11	1:A:264:ILE:HG21	1.90	0.53
1:A:31:ARG:HB2	1:A:33:GLU:CG	2.39	0.53
1:B:175:GLY:HA2	1:B:332:THR:O	2.09	0.52
1:A:72:PHE:HA	2:A:2011:HOH:O	2.09	0.52
1:B:186:ILE:HG22	1:B:189:ASN:O	2.09	0.52
1:B:279:PHE:HA	1:B:282:LEU:HD12	1.90	0.52
1:A:24:LYS:HG2	1:A:24:LYS:O	2.08	0.52
1:A:186:ILE:HG13	2:A:2043:HOH:O	2.10	0.52
1:A:256:ILE:O	1:A:259:MET:HG3	2.10	0.52
1:A:259:MET:HG3	1:A:260:LEU:HD13	1.90	0.52
1:A:228:TYR:CD2	1:A:303:MET:HE3	2.45	0.52
1:B:338:VAL:HG22	2:B:2092:HOH:O	2.10	0.52
1:B:89:VAL:HG21	1:B:130:ALA:HB1	1.92	0.52
1:B:72:PHE:CE1	1:B:150:GLU:HB3	2.45	0.51
1:B:88:CYS:HB3	1:B:157:THR:OG1	2.11	0.51
1:B:26:VAL:HG22	1:B:134:LEU:HD13	1.92	0.51
1:A:213:LEU:O	1:A:214:GLU:OE1	2.29	0.51
1:A:47:LEU:HB2	1:B:55:PRO:O	2.10	0.51
1:A:220:GLU:OE2	1:A:278:ILE:HB	2.11	0.51
1:B:316:VAL:O	1:B:320:GLU:HG2	2.11	0.51
1:A:187:HIS:HD2	2:A:2060:HOH:O	1.93	0.51
1:A:318:LEU:O	1:A:322:GLN:OE1	2.29	0.51
1:B:253:ILE:O	1:B:257:PRO:HG2	2.10	0.51
1:A:250:GLY:O	1:A:254:GLU:HB2	2.11	0.51
1:A:91:ASP:OD1	1:A:246:HIS:HD2	1.94	0.51
1:A:110:LYS:HA	1:A:141:GLU:CB	2.37	0.50
1:B:256:ILE:HB	1:B:257:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:O	1:A:73:MET:HG2	2.11	0.50
1:B:178:LEU:HD22	1:B:304:VAL:CG1	2.41	0.50
1:A:187:HIS:CE1	1:A:226:LYS:HB2	2.46	0.50
1:B:321:GLU:OE1	1:B:321:GLU:O	2.29	0.50
1:A:106:ILE:HG12	1:A:153:LEU:HD13	1.94	0.50
1:A:277:PRO:HD2	2:A:2053:HOH:O	2.11	0.50
1:B:177:VAL:CG1	1:B:328:ILE:HG23	2.42	0.50
1:A:50:PHE:O	1:A:52:LEU:HD12	2.13	0.49
1:B:175:GLY:H	1:B:332:THR:HG22	1.76	0.49
1:A:241:VAL:HG13	1:A:305:VAL:HG23	1.93	0.49
1:B:248:THR:O	1:B:249:GLY:O	2.30	0.49
1:B:256:ILE:HG22	2:B:2092:HOH:O	2.12	0.49
1:A:197:VAL:HG13	1:A:197:VAL:O	2.12	0.49
1:B:54:GLU:OE1	1:B:163:LYS:HB2	2.12	0.49
1:A:89:VAL:HG21	1:A:130:ALA:CB	2.33	0.49
1:B:87:MET:CE	1:B:246:HIS:CD2	2.96	0.49
1:A:32:LYS:HG3	1:A:33:GLU:N	2.26	0.49
1:B:284:GLU:O	1:B:287:LYS:HG2	2.13	0.49
1:A:243:GLY:O	1:A:305:VAL:HG23	2.13	0.48
1:A:186:ILE:O	1:A:186:ILE:HG22	2.13	0.48
1:B:253:ILE:HG12	1:B:295:ASN:HD21	1.78	0.48
1:B:89:VAL:HA	1:B:92:ILE:HG13	1.94	0.48
1:B:218:GLY:O	1:B:222:LEU:HB2	2.13	0.48
1:B:179:ILE:HD13	1:B:328:ILE:HA	1.96	0.48
1:A:232:ILE:O	1:A:236:LEU:HG	2.14	0.48
1:A:267:GLU:HA	1:A:339:THR:O	2.14	0.48
1:A:178:LEU:HD21	1:A:332:THR:CG2	2.44	0.47
1:A:69:MET:HG2	2:A:2010:HOH:O	2.14	0.47
1:B:257:PRO:HA	1:B:260:LEU:CG	2.40	0.47
1:B:186:ILE:O	1:B:298:ASN:OD1	2.30	0.47
1:B:87:MET:CE	1:B:87:MET:HA	2.42	0.47
1:A:171:LYS:HE2	1:A:242:TYR:HD2	1.77	0.47
1:A:64:VAL:HG22	1:A:84:ALA:HB2	1.96	0.47
1:A:57:LEU:CG	1:B:47:LEU:HD11	2.45	0.47
1:A:67:LYS:HD3	1:A:80:ILE:HD12	1.95	0.47
1:B:334:GLN:HE21	1:B:334:GLN:HB3	1.54	0.47
1:A:327:ARG:HB2	1:A:329:ILE:CD1	2.45	0.47
1:B:220:GLU:HA	1:B:223:LYS:HG3	1.97	0.47
1:A:23:LYS:HD3	1:A:23:LYS:HA	1.58	0.47
1:B:193:LEU:HD13	1:B:197:VAL:HG23	1.97	0.47
1:B:289:GLU:O	1:B:293:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:NZ	1:A:164:LYS:HB3	2.30	0.47
1:A:176:HIS:N	1:A:332:THR:OG1	2.48	0.47
1:B:89:VAL:HG22	1:B:229:VAL:HG21	1.95	0.47
1:B:30:MET:CE	1:B:34:VAL:HG11	2.45	0.47
1:B:333:VAL:HG12	1:B:334:GLN:N	2.29	0.46
1:A:59:SER:HB3	1:A:158:VAL:HG22	1.97	0.46
1:B:301:ILE:HG22	1:B:301:ILE:O	2.13	0.46
1:B:30:MET:CE	1:B:133:ALA:HB1	2.45	0.46
1:A:177:VAL:CG2	1:A:309:GLU:HA	2.45	0.46
1:A:154:ALA:HB2	1:B:105:TYR:CE1	2.51	0.46
1:A:88:CYS:O	1:A:92:ILE:HG12	2.14	0.46
1:B:297:PHE:HA	2:B:2086:HOH:O	2.14	0.46
1:A:204:LEU:HD13	1:A:218:GLY:HA3	1.97	0.46
1:B:89:VAL:HA	1:B:92:ILE:CG1	2.46	0.46
1:B:68:LEU:HD13	1:B:72:PHE:CZ	2.51	0.46
1:A:210:TYR:O	1:A:214:GLU:HG2	2.16	0.46
1:B:193:LEU:HD13	1:B:197:VAL:CG2	2.46	0.46
1:B:53:GLU:N	2:B:2029:HOH:O	2.49	0.46
1:B:286:GLY:O	1:B:288:LEU:HD23	2.16	0.45
1:B:91:ASP:O	1:B:95:GLN:NE2	2.49	0.45
1:B:128:ARG:HG2	1:B:128:ARG:HH11	1.82	0.45
1:B:195:ARG:O	1:B:199:LEU:N	2.50	0.45
1:A:268:ILE:O	1:A:340:PHE:HA	2.17	0.45
1:B:89:VAL:CG2	1:B:92:ILE:HD11	2.47	0.45
1:A:138:GLU:HG3	1:A:139:THR:N	2.31	0.45
1:B:89:VAL:CG2	1:B:229:VAL:HG21	2.46	0.45
1:A:197:VAL:HG23	1:A:200:GLU:HB2	1.99	0.45
1:A:187:HIS:HE1	1:A:226:LYS:HB2	1.82	0.45
1:A:251:GLY:O	1:A:255:ASN:ND2	2.50	0.45
1:B:114:SER:O	1:B:118:ASN:ND2	2.50	0.45
1:A:146:TYR:HA	2:B:2054:HOH:O	2.16	0.45
1:A:22:MET:O	1:A:25:HIS:NE2	2.50	0.45
1:B:193:LEU:HD22	1:B:193:LEU:HA	1.84	0.45
1:B:320:GLU:OE2	1:B:324:GLU:O	2.34	0.45
1:A:250:GLY:HA3	1:A:254:GLU:HG2	1.97	0.45
1:B:102:PHE:N	1:B:133:ALA:O	2.50	0.44
1:B:253:ILE:HG13	1:B:254:GLU:N	2.32	0.44
1:B:327:ARG:HG3	1:B:327:ARG:NH1	2.28	0.44
1:A:204:LEU:HD13	2:A:2052:HOH:O	2.17	0.44
1:A:235:LEU:HD22	1:A:241:VAL:HG21	1.99	0.44
1:B:108:CYS:SG	1:B:111:ALA:HA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLU:O	1:B:115:LYS:N	2.50	0.44
1:B:179:ILE:HA	1:B:179:ILE:HD13	1.79	0.44
1:B:289:GLU:OE2	1:B:290:GLU:N	2.50	0.44
1:A:128:ARG:NH1	1:A:128:ARG:HG2	2.32	0.44
1:A:209:ILE:N	2:A:2051:HOH:O	2.49	0.44
1:A:319:LEU:O	1:A:322:GLN:HB2	2.17	0.44
1:B:278:ILE:O	1:B:281:LEU:HB3	2.18	0.44
1:A:254:GLU:HB3	1:A:258:ARG:HH21	1.83	0.44
1:B:67:LYS:HG2	1:B:80:ILE:HD11	1.99	0.44
1:A:250:GLY:HA3	1:A:254:GLU:HB2	2.00	0.44
1:A:44:MET:HA	1:B:57:LEU:O	2.17	0.44
1:B:335:GLY:O	1:B:336:ALA:HB2	2.16	0.43
1:B:13:GLU:HG3	1:B:13:GLU:H	1.54	0.43
1:B:87:MET:HE1	1:B:246:HIS:CD2	2.53	0.43
1:A:57:LEU:HD12	1:B:47:LEU:HD21	2.00	0.43
1:A:256:ILE:HB	1:A:257:PRO:HD3	2.00	0.43
1:A:264:ILE:HA	1:A:333:VAL:O	2.18	0.43
1:B:189:ASN:ND2	1:B:248:THR:HA	2.34	0.43
1:B:234:GLU:H	1:B:234:GLU:HG2	1.37	0.43
1:B:270:LEU:HD21	1:B:294:PHE:CZ	2.53	0.43
1:A:235:LEU:HA	1:A:318:LEU:CD2	2.48	0.43
1:B:260:LEU:HA	1:B:261:PRO:HD3	1.89	0.43
1:A:195:ARG:O	1:A:198:LEU:HB2	2.18	0.43
1:A:88:CYS:HB3	1:A:157:THR:OG1	2.19	0.43
1:B:259:MET:HG2	1:B:260:LEU:HD23	2.00	0.43
1:B:179:ILE:O	1:B:304:VAL:HA	2.19	0.43
1:A:64:VAL:HG23	1:A:153:LEU:O	2.19	0.42
1:B:83:ASP:OD1	1:B:225:THR:N	2.50	0.42
1:A:68:LEU:HA	1:A:68:LEU:HD23	1.89	0.42
1:B:232:ILE:CG2	1:B:236:LEU:HD12	2.50	0.42
1:A:78:ASP:N	1:A:78:ASP:OD1	2.49	0.42
1:B:112:GLU:HA	1:B:113:PRO:HD2	1.79	0.42
1:B:181:LEU:HD22	1:B:324:GLU:HG3	2.01	0.42
1:B:189:ASN:ND2	2:B:2058:HOH:O	2.50	0.42
1:B:80:ILE:HD12	1:B:80:ILE:HA	1.81	0.42
1:A:212:ARG:O	1:A:213:LEU:O	2.38	0.42
1:A:320:GLU:HA	1:A:324:GLU:O	2.20	0.42
1:A:327:ARG:HB2	1:A:329:ILE:HD13	2.00	0.42
1:B:167:VAL:O	1:B:167:VAL:HG22	2.19	0.42
1:B:197:VAL:C	1:B:198:LEU:HD23	2.39	0.42
1:A:307:VAL:CG2	1:A:315:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:HG2	1:A:165:LYS:N	2.35	0.42
1:A:331:ARG:HB3	2:A:2071:HOH:O	2.18	0.42
1:B:250:GLY:O	1:B:254:GLU:HB2	2.20	0.42
1:A:148:THR:HG22	1:A:149:GLU:N	2.35	0.42
1:A:94:VAL:HG22	1:A:244:MET:HB3	2.01	0.42
1:B:106:ILE:CD1	1:B:119:ILE:HD13	2.47	0.42
1:A:156:PHE:CE2	1:B:103:LEU:HG	2.55	0.42
1:A:62:ASP:HA	1:B:138:GLU:OE1	2.20	0.42
1:B:276:GLN:OE1	1:B:300:GLY:HA2	2.20	0.42
1:A:235:LEU:HA	1:A:318:LEU:HD21	2.02	0.42
1:A:172:ILE:O	1:A:172:ILE:HG13	2.20	0.41
1:A:294:PHE:HD1	2:A:2068:HOH:O	2.03	0.41
1:A:234:GLU:HG3	1:A:322:GLN:NE2	2.35	0.41
1:A:259:MET:HE2	1:A:259:MET:HB2	1.85	0.41
1:A:281:LEU:HD23	2:A:2047:HOH:O	2.20	0.41
1:A:78:ASP:HA	1:A:118:ASN:O	2.20	0.41
1:B:98:GLU:HA	1:B:99:PRO:HD2	1.82	0.41
1:A:45:PHE:CE2	1:A:100:LEU:HG	2.55	0.41
1:A:231:PRO:HA	1:A:322:GLN:CG	2.49	0.41
1:B:45:PHE:CZ	1:B:100:LEU:HG	2.55	0.41
1:B:89:VAL:HG23	1:B:99:PRO:HB3	2.02	0.41
1:A:244:MET:HA	1:A:304:VAL:O	2.20	0.41
1:B:177:VAL:N	1:B:307:VAL:O	2.53	0.41
1:A:197:VAL:HG22	1:A:201:ASP:CB	2.51	0.41
1:A:332:THR:N	2:A:2071:HOH:O	2.49	0.41
1:A:66:THR:O	1:A:66:THR:HG22	2.20	0.41
1:B:194:VAL:O	1:B:198:LEU:HG	2.20	0.41
1:A:123:ILE:HG21	1:A:123:ILE:HD13	1.70	0.41
1:A:184:SER:H	1:A:187:HIS:CE1	2.39	0.41
1:A:272:SER:OG	1:A:329:ILE:HA	2.21	0.41
1:A:307:VAL:HG12	1:A:308:LYS:O	2.21	0.41
1:A:94:VAL:HG13	1:A:94:VAL:O	2.21	0.41
1:A:98:GLU:O	1:A:159:GLY:HA2	2.20	0.41
1:A:61:THR:CG2	1:B:103:LEU:HD12	2.49	0.41
1:B:253:ILE:O	1:B:257:PRO:HD2	2.21	0.41
1:A:314:ASP:OD1	1:A:314:ASP:N	2.52	0.40
1:A:54:GLU:HG3	1:A:164:LYS:NZ	2.35	0.40
1:A:192:SER:O	1:A:196:LYS:HG2	2.20	0.40
1:A:220:GLU:OE2	1:A:278:ILE:HD13	2.21	0.40
1:A:33:GLU:H	1:A:33:GLU:HG2	1.17	0.40
1:B:174:ALA:HA	1:B:332:THR:CG2	2.49	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	316/346 (91%)	279 (88%)	26 (8%)	11 (4%)	3	2
1	B	297/346 (86%)	263 (89%)	26 (9%)	8 (3%)	5	3
All	All	613/692 (89%)	542 (88%)	52 (8%)	19 (3%)	4	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLY
1	A	43	GLY
1	A	143	PRO
1	A	213	LEU
1	B	38	LEU
1	B	169	GLY
1	B	249	GLY
1	A	211	GLY
1	B	36	GLY
1	B	54	GLU
1	B	109	GLY
1	B	187	HIS
1	B	309	GLU
1	A	235	LEU
1	A	312	ALA
1	A	24	LYS
1	A	261	PRO
1	A	64	VAL
1	A	42	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/274 (79%)	167 (77%)	50 (23%)	1	0
1	B	192/274 (70%)	140 (73%)	52 (27%)	0	0
All	All	409/548 (75%)	307 (75%)	102 (25%)	0	0

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	22	MET
1	A	23	LYS
1	A	24	LYS
1	A	31	ARG
1	A	33	GLU
1	A	35	LEU
1	A	50	PHE
1	A	73	MET
1	A	89	VAL
1	A	94	VAL
1	A	95	GLN
1	A	100	LEU
1	A	114	SER
1	A	120	VAL
1	A	134	LEU
1	A	138	GLU
1	A	139	THR
1	A	142[A]	MET
1	A	147	SER
1	A	148	THR
1	A	149	GLU
1	A	160	ILE
1	A	163	LYS
1	A	164	LYS
1	A	171	LYS
1	A	172	ILE

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Mol	Chain	Res	Type
1	A	176	HIS
1	A	178	LEU
1	A	187	HIS
1	A	204	LEU
1	A	217	LEU
1	A	221	LEU
1	A	230	LYS
1	A	235	LEU
1	A	254	GLU
1	A	257	PRO
1	A	259	MET
1	A	260	LEU
1	A	281	LEU
1	A	282	LEU
1	A	295	ASN
1	A	307	VAL
1	A	314	ASP
1	A	315	ILE
1	A	318	LEU
1	A	322	GLN
1	A	328	ILE
1	A	329	ILE
1	A	339	THR
1	B	12	ILE
1	B	13	GLU
1	B	30	MET
1	B	41	PHE
1	B	54	GLU
1	B	62	ASP
1	B	66	THR
1	B	68	LEU
1	B	76	LYS
1	B	87	MET
1	B	100	LEU
1	B	103	LEU
1	B	106	ILE
1	B	114	SER
1	B	123	ILE
1	B	134	LEU
1	B	135	ILE
1	B	142	MET
1	B	145	MET

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Mol	Chain	Res	Type
1	B	146	TYR
1	B	150	GLU
1	B	157	THR
1	B	163	LYS
1	B	164	LYS
1	B	167	VAL
1	B	181	LEU
1	B	183	SER
1	B	186	ILE
1	B	187	HIS
1	B	188	SER
1	B	193	LEU
1	B	196	LYS
1	B	217	LEU
1	B	222	LEU
1	B	230	LYS
1	B	234	GLU
1	B	235	LEU
1	B	240	GLU
1	B	253	ILE
1	B	259	MET
1	B	268	ILE
1	B	282	LEU
1	B	288	LEU
1	B	298	ASN
1	B	305	VAL
1	B	315	ILE
1	B	321	GLU
1	B	322	GLN
1	B	325	THR
1	B	327	ARG
1	B	329	ILE
1	B	334	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	95	GLN
1	A	187	HIS
1	A	189	ASN
1	A	246	HIS

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Mol	Chain	Res	Type
1	A	322	GLN
1	B	90	ASN
1	B	95	GLN
1	B	187	HIS
1	B	189	ASN
1	B	238	ASN
1	B	334	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 [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, 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	322/346 (93%)	-0.23	4 (1%) 79 83	22, 41, 68, 107	1 (0%)
1	B	307/346 (88%)	-0.08	7 (2%) 60 67	27, 48, 70, 109	0
All	All	629/692 (90%)	-0.16	11 (1%) 70 76	22, 45, 70, 109	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	GLY	6.4
1	A	41	PHE	3.8
1	B	22	MET	3.3
1	A	43	GLY	3.2
1	B	87	MET	2.8
1	B	333	VAL	2.7
1	B	175	GLY	2.7
1	B	16	TYR	2.6
1	A	142[A]	MET	2.5
1	B	144	GLY	2.3
1	B	39	GLY	2.2

### 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.