



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 AM GMT

PDB ID : 2HSG  
Title : Structure of transcription regulator CcpA in its DNA-free state  
Authors : Loll, B.; Alings, C.; Saenger, W.; Biesiadka, J.  
Deposited on : 2006-07-21  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

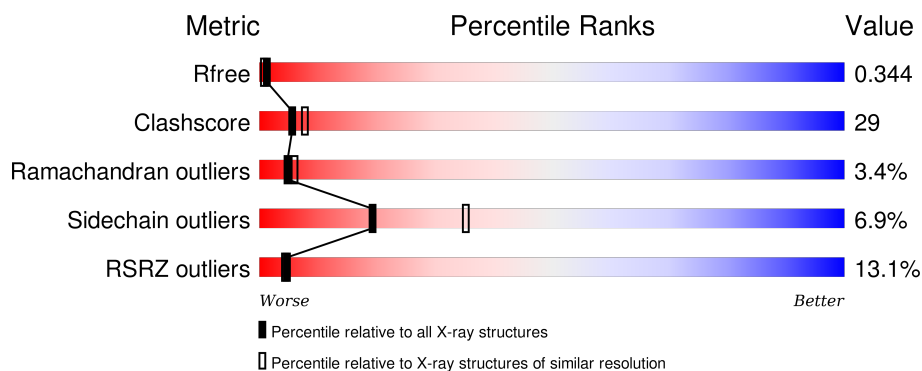
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	332	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2506 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.

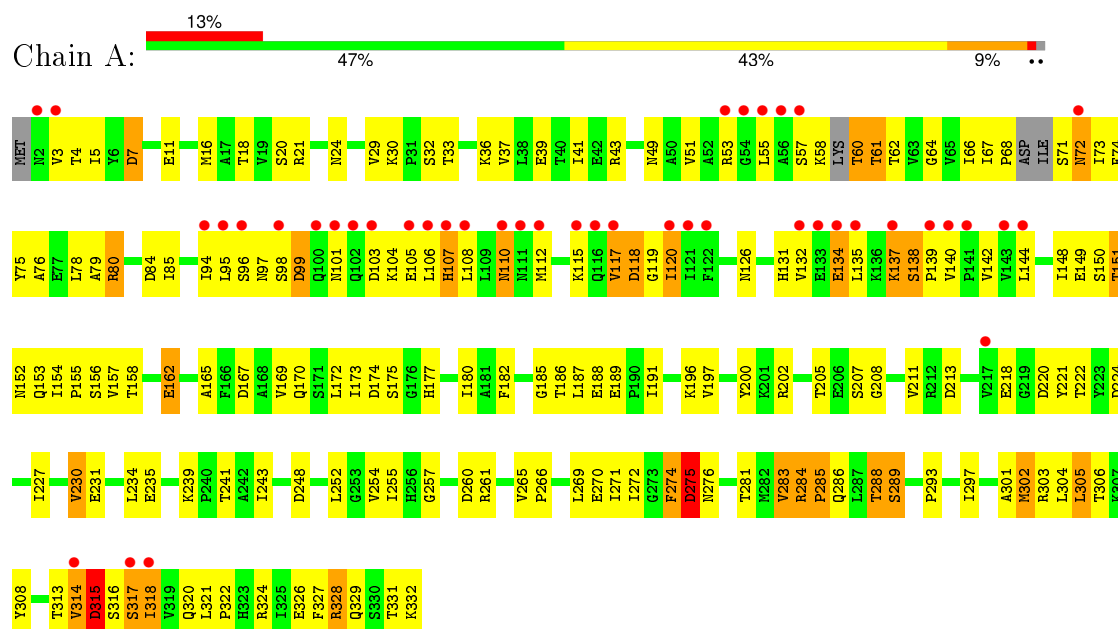
- Molecule 1 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2506	1573	430	495	8	0	0	0

### 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 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 ( $\text{RSRZ} > 2$ ). 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: Glucose-resistance amylase regulator



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.46 Å 74.46 Å 238.92 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 31.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (30.00-2.50) 98.4 (31.60-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.271 , 0.337 0.270 , 0.344	Depositor DCC
$R_{free}$ test set	710 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 14159 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.66	0/2541	0.95	14/3447 (0.4%)

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	A	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	328	ARG	NE-CZ-NH1	-13.68	113.46	120.30
1	A	328	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	A	283	VAL	CB-CA-C	-8.32	95.58	111.40
1	A	167	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	260	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	103	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	174	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	248	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	7	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	275	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	84	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	315	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	99	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	285	PRO	N-CA-C	-5.22	98.52	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	GLN	Sidechain

## 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	2506	0	2499	147	0
All	All	2506	0	2499	147	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 29.

All (147) 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:265:VAL:O	1:A:269:LEU:O	1.72	1.08
1:A:132:VAL:HG21	1:A:151:THR:HG21	1.46	0.96
1:A:149:GLU:CB	1:A:151:THR:OG1	2.17	0.93
1:A:49:ASN:OD1	1:A:51:VAL:HG12	1.76	0.85
1:A:120:ILE:HG23	1:A:142:VAL:HG22	1.59	0.84
1:A:288:THR:HG21	1:A:331:THR:OG1	1.77	0.83
1:A:108:LEU:O	1:A:112:MET:HB2	1.84	0.78
1:A:73:ILE:HG23	1:A:74:PHE:N	2.01	0.75
1:A:150:SER:O	1:A:152:ASN:ND2	2.20	0.75
1:A:318:ILE:HG22	1:A:318:ILE:O	1.86	0.73
1:A:288:THR:HB	1:A:327:PHE:HA	1.69	0.73
1:A:281:THR:HG22	1:A:286:GLN:HE21	1.53	0.73
1:A:68:PRO:O	1:A:71:SER:N	2.22	0.72
1:A:286:GLN:HB2	1:A:329:GLN:NE2	2.05	0.72
1:A:188:GLU:N	1:A:188:GLU:OE1	2.21	0.72
1:A:162:GLU:OE2	1:A:202:ARG:NH1	2.23	0.71
1:A:150:SER:C	1:A:152:ASN:HD22	1.93	0.71
1:A:132:VAL:CG2	1:A:151:THR:HG21	2.19	0.71
1:A:316:SER:O	1:A:318:ILE:N	2.24	0.70
1:A:243:ILE:HG13	1:A:269:LEU:HD11	1.75	0.69
1:A:131:HIS:O	1:A:135:LEU:HG	1.91	0.69
1:A:32:SER:O	1:A:36:LYS:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG22	1:A:16:MET:HG2	1.75	0.69
1:A:154:ILE:HG23	1:A:154:ILE:O	1.94	0.68
1:A:68:PRO:HA	1:A:98:SER:O	1.94	0.68
1:A:101:ASN:O	1:A:105:GLU:HG2	1.94	0.67
1:A:58:LYS:CB	1:A:60:THR:HG23	2.25	0.67
1:A:220:ASP:O	1:A:221:TYR:HB2	1.94	0.67
1:A:284:ARG:O	1:A:286:GLN:N	2.28	0.66
1:A:288:THR:HG22	1:A:328:ARG:H	1.61	0.65
1:A:51:VAL:O	1:A:55:LEU:HG	1.96	0.64
1:A:150:SER:C	1:A:152:ASN:ND2	2.51	0.64
1:A:67:ILE:HD11	1:A:75:TYR:HB3	1.79	0.64
1:A:106:LEU:O	1:A:110:ASN:N	2.31	0.63
1:A:107:HIS:HA	1:A:110:ASN:HB3	1.81	0.63
1:A:61:THR:HG23	1:A:117:VAL:HG11	1.81	0.62
1:A:4:THR:N	1:A:7:ASP:OD2	2.31	0.62
1:A:112:MET:CE	1:A:139:PRO:HD2	2.29	0.62
1:A:281:THR:HG22	1:A:286:GLN:NE2	2.15	0.61
1:A:265:VAL:O	1:A:269:LEU:C	2.39	0.61
1:A:308:TYR:OH	1:A:316:SER:HB3	2.00	0.61
1:A:61:THR:HA	1:A:117:VAL:HB	1.81	0.61
1:A:151:THR:O	1:A:154:ILE:HG22	2.01	0.60
1:A:205:THR:O	1:A:208:GLY:N	2.30	0.60
1:A:220:ASP:OD1	1:A:222:THR:HG23	2.00	0.60
1:A:308:TYR:OH	1:A:316:SER:CB	2.50	0.60
1:A:275:ASP:O	1:A:289:SER:OG	2.19	0.60
1:A:177:HIS:HB2	1:A:180:ILE:HD11	1.84	0.60
1:A:73:ILE:CG2	1:A:74:PHE:N	2.64	0.60
1:A:321:LEU:HB3	1:A:322:PRO:HD2	1.84	0.58
1:A:37:VAL:O	1:A:41:ILE:HG13	2.02	0.58
1:A:118:ASP:HB3	1:A:140:VAL:HG11	1.85	0.58
1:A:274:PHE:C	1:A:275:ASP:O	2.40	0.58
1:A:186:THR:HA	1:A:218:GLU:OE1	2.03	0.57
1:A:57:SER:O	1:A:58:LYS:CB	2.53	0.57
1:A:112:MET:HE3	1:A:112:MET:O	2.06	0.56
1:A:67:ILE:O	1:A:97:ASN:HA	2.05	0.56
1:A:257:GLY:O	1:A:261:ARG:HG2	2.06	0.55
1:A:288:THR:CG2	1:A:328:ARG:H	2.19	0.55
1:A:254:VAL:HG12	1:A:271:ILE:CD1	2.36	0.55
1:A:112:MET:HE1	1:A:139:PRO:HD2	1.86	0.55
1:A:230:VAL:HG13	1:A:254:VAL:HG13	1.88	0.55
1:A:73:ILE:HG23	1:A:74:PHE:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:O	1:A:306:THR:HB	2.07	0.55
1:A:108:LEU:HD21	1:A:134:GLU:HB3	1.89	0.54
1:A:255:ILE:HG23	1:A:265:VAL:HG21	1.89	0.54
1:A:230:VAL:HG22	1:A:254:VAL:HA	1.89	0.54
1:A:254:VAL:HG12	1:A:271:ILE:HD13	1.89	0.53
1:A:211:VAL:O	1:A:211:VAL:HG12	2.09	0.53
1:A:314:VAL:HG12	1:A:315:ASP:N	2.23	0.53
1:A:18:THR:OG1	1:A:21:ARG:NH1	2.43	0.52
1:A:144:LEU:HG	1:A:154:ILE:CG1	2.40	0.52
1:A:177:HIS:HD2	1:A:241:THR:OG1	1.94	0.51
1:A:126:ASN:ND2	1:A:189:GLU:OE2	2.43	0.51
1:A:20:SER:O	1:A:24:ASN:ND2	2.43	0.51
1:A:272:ILE:HD11	1:A:331:THR:HG21	1.91	0.50
1:A:3:VAL:O	1:A:53:ARG:HD2	2.11	0.50
1:A:108:LEU:CD2	1:A:134:GLU:HB3	2.41	0.50
1:A:73:ILE:CG2	1:A:74:PHE:H	2.23	0.50
1:A:284:ARG:O	1:A:285:PRO:C	2.47	0.50
1:A:29:VAL:O	1:A:30:LYS:C	2.50	0.50
1:A:107:HIS:CA	1:A:110:ASN:HB3	2.41	0.50
1:A:230:VAL:CG2	1:A:254:VAL:HA	2.41	0.50
1:A:154:ILE:CG2	1:A:154:ILE:O	2.59	0.49
1:A:234:LEU:O	1:A:239:LYS:HE2	2.12	0.49
1:A:144:LEU:HG	1:A:154:ILE:HG13	1.94	0.49
1:A:112:MET:SD	1:A:138:SER:HB3	2.52	0.49
1:A:149:GLU:C	1:A:151:THR:H	2.16	0.49
1:A:150:SER:HA	1:A:152:ASN:HD21	1.77	0.49
1:A:286:GLN:HB2	1:A:329:GLN:HE21	1.77	0.48
1:A:71:SER:N	1:A:97:ASN:OD1	2.47	0.47
1:A:95:LEU:HD23	1:A:96:SER:N	2.29	0.47
1:A:148:ILE:HD11	1:A:191:ILE:N	2.29	0.47
1:A:157:VAL:HG21	1:A:301:ALA:HA	1.96	0.47
1:A:324:ARG:NH2	1:A:326:GLU:OE1	2.42	0.47
1:A:39:GLU:O	1:A:43:ARG:HB2	2.14	0.47
1:A:293:PRO:O	1:A:297:ILE:HG13	2.15	0.47
1:A:265:VAL:O	1:A:266:PRO:C	2.49	0.47
1:A:304:LEU:O	1:A:305:LEU:C	2.52	0.47
1:A:149:GLU:C	1:A:151:THR:N	2.69	0.46
1:A:119:GLY:HA2	1:A:140:VAL:HB	1.97	0.46
1:A:252:LEU:HG	1:A:283:VAL:HG22	1.96	0.46
1:A:60:THR:O	1:A:61:THR:HB	2.15	0.46
1:A:156:SER:H	1:A:317:SER:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HB2	1:A:196:LYS:HA	1.98	0.46
1:A:11:GLU:OE1	1:A:43:ARG:NH2	2.48	0.46
1:A:85:ILE:HB	1:A:302:MET:HG2	1.98	0.46
1:A:169:VAL:HG21	1:A:200:TYR:HD2	1.80	0.46
1:A:108:LEU:O	1:A:112:MET:CB	2.59	0.46
1:A:60:THR:O	1:A:61:THR:CB	2.63	0.45
1:A:286:GLN:HB2	1:A:329:GLN:HE22	1.80	0.45
1:A:182:PHE:HE1	1:A:197:VAL:HG23	1.82	0.45
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.78	0.45
1:A:265:VAL:HG12	1:A:266:PRO:N	2.31	0.45
1:A:231:GLU:HG2	1:A:235:GLU:OE2	2.16	0.45
1:A:99:ASP:O	1:A:104:LYS:HE2	2.17	0.45
1:A:117:VAL:HG12	1:A:118:ASP:N	2.31	0.45
1:A:284:ARG:HD3	1:A:284:ARG:HA	1.49	0.44
1:A:220:ASP:O	1:A:221:TYR:CB	2.65	0.44
1:A:224:ASP:O	1:A:227:ILE:N	2.51	0.44
1:A:154:ILE:HD12	1:A:155:PRO:HD2	1.99	0.44
1:A:187:LEU:N	1:A:218:GLU:OE1	2.45	0.44
1:A:144:LEU:CD1	1:A:154:ILE:HG21	2.48	0.44
1:A:173:ILE:C	1:A:175:SER:H	2.20	0.43
1:A:144:LEU:HD11	1:A:154:ILE:HG21	1.99	0.43
1:A:76:ALA:O	1:A:79:ALA:HB3	2.19	0.43
1:A:265:VAL:C	1:A:269:LEU:O	2.52	0.43
1:A:137:LYS:O	1:A:138:SER:C	2.57	0.43
1:A:270:GLU:OE2	1:A:332:LYS:HB2	2.18	0.42
1:A:173:ILE:O	1:A:175:SER:N	2.52	0.42
1:A:144:LEU:HG	1:A:154:ILE:HG12	2.03	0.41
1:A:67:ILE:HG13	1:A:68:PRO:HD2	2.02	0.41
1:A:66:ILE:HD12	1:A:107:HIS:HB3	2.03	0.41
1:A:62:THR:O	1:A:118:ASP:HA	2.20	0.41
1:A:30:LYS:O	1:A:33:THR:HB	2.20	0.41
1:A:252:LEU:CG	1:A:283:VAL:HG22	2.49	0.41
1:A:276:ASN:OD1	1:A:328:ARG:NH2	2.51	0.41
1:A:72:ASN:ND2	1:A:73:ILE:HG22	2.36	0.41
1:A:115:LYS:O	1:A:118:ASP:HB2	2.21	0.40
1:A:158:THR:O	1:A:320:GLN:HA	2.21	0.40
1:A:80:ARG:HA	1:A:80:ARG:HD3	1.91	0.40
1:A:101:ASN:HA	1:A:104:LYS:HB2	2.03	0.40
1:A:230:VAL:O	1:A:234:LEU:HD12	2.22	0.40
1:A:49:ASN:OD1	1:A:51:VAL:CG1	2.60	0.40
1:A:64:GLY:HA2	1:A:94:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:C	1:A:78:LEU:HD23	2.42	0.40
1:A:185:GLY:HA3	1:A:221:TYR:CZ	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	322/332 (97%)	275 (85%)	36 (11%)	11 (3%)	<b>5</b> <b>6</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	275	ASP
1	A	314	VAL
1	A	110	ASN
1	A	117	VAL
1	A	151	THR
1	A	317	SER
1	A	61	THR
1	A	305	LEU
1	A	313	THR
1	A	318	ILE

### 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	275/289 (95%)	256 (93%)	19 (7%)	19	35

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	80	ARG
1	A	107	HIS
1	A	118	ASP
1	A	120	ILE
1	A	134	GLU
1	A	137	LYS
1	A	138	SER
1	A	153	GLN
1	A	162	GLU
1	A	207	SER
1	A	213	ASP
1	A	230	VAL
1	A	274	PHE
1	A	284	ARG
1	A	288	THR
1	A	289	SER
1	A	302	MET
1	A	315	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	72	ASN
1	A	126	ASN
1	A	152	ASN
1	A	177	HIS
1	A	286	GLN
1	A	329	GLN

### 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, 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	328/332 (98%)	0.74	43 (13%) 5 4	33, 54, 101, 110	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ARG	5.7
1	A	56	ALA	5.4
1	A	102	GLN	5.1
1	A	140	VAL	5.0
1	A	116	GLN	4.8
1	A	57	SER	4.7
1	A	107	HIS	4.5
1	A	95	LEU	4.4
1	A	318	ILE	4.4
1	A	108	LEU	4.3
1	A	101	ASN	4.3
1	A	54	GLY	4.2
1	A	117	VAL	4.1
1	A	133	GLU	4.0
1	A	135	LEU	3.9
1	A	3	VAL	3.9
1	A	103	ASP	3.9
1	A	115	LYS	3.9
1	A	98	SER	3.7
1	A	111	ASN	3.7
1	A	137	LYS	3.7
1	A	122	PHE	3.6
1	A	112	MET	3.3
1	A	134	GLU	3.2
1	A	139	PRO	3.2
1	A	106	LEU	3.2
1	A	2	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	141	PRO	3.0
1	A	55	LEU	2.9
1	A	314	VAL	2.6
1	A	110	ASN	2.6
1	A	105	GLU	2.5
1	A	132	VAL	2.5
1	A	72	ASN	2.4
1	A	144	LEU	2.4
1	A	120	ILE	2.4
1	A	143	VAL	2.3
1	A	121	ILE	2.2
1	A	96	SER	2.2
1	A	100	GLN	2.2
1	A	94	ILE	2.1
1	A	217	VAL	2.0
1	A	317	SER	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.