



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:46 AM GMT

PDB ID : 3IWZ  
Title : The c-di-GMP Responsive Global Regulator CLP Links Cell-Cell Signaling to Virulence Gene Expression in *Xanthomonas campestris*  
Authors : Chin, K.H.; Tu, Z.L.; Tseng, Y.H.; Dow, J.M.; Wang, A.H.J.; Chou, S.H.  
Deposited on : 2009-09-03  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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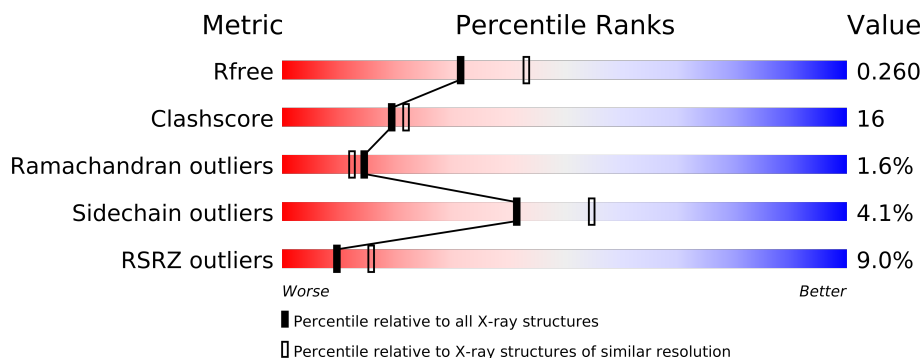
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	230	
1	B	230	
1	C	230	
1	D	230	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6817 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Catabolite activation-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1639	1025	301	308	5			
1	B	207	Total	C	N	O	S	0	0	0
			1639	1025	301	308	5			
1	C	207	Total	C	N	O	S	0	0	0
			1626	1016	300	305	5			
1	D	208	Total	C	N	O	S	0	0	0
			1634	1022	301	306	5			

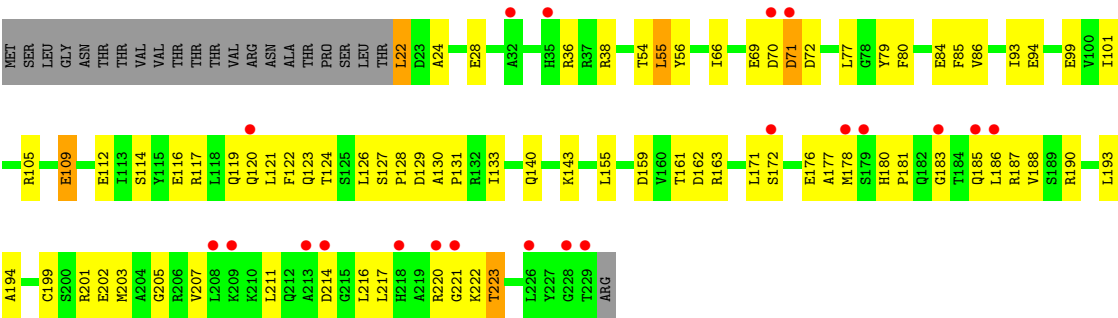
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total	O	0	0
			96	96		
2	B	71	Total	O	0	0
			71	71		
2	C	64	Total	O	0	0
			64	64		
2	D	48	Total	O	0	0
			48	48		



● Molecule 1: Catabolite activation-like protein

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.69Å 67.69Å 110.37Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	29.85 – 2.30 29.84 – 2.28	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.85-2.30) 96.9 (29.84-2.28)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.244 , 0.305 0.258 , 0.260	Depositor DCC
$R_{free}$ test set	2113 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 42901 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.38	0/1664	0.62	0/2244
1	B	0.37	0/1664	0.60	0/2244
1	C	0.35	0/1651	0.59	0/2229
1	D	0.33	0/1659	0.59	0/2240
All	All	0.36	0/6638	0.60	0/8957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1639	0	1661	51	0
1	B	1639	0	1661	45	0
1	C	1626	0	1638	73	0
1	D	1634	0	1649	58	0
2	A	96	0	0	1	0
2	B	71	0	0	4	0
2	C	64	0	0	2	0
2	D	48	0	0	0	0
All	All	6817	0	6609	214	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (214) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:85:PHE:H	1:D:140:GLN:HE22	1.01	0.99
1:C:85:PHE:H	1:C:140:GLN:HE22	1.05	0.98
1:C:218:HIS:HB3	1:C:225:VAL:HG13	1.49	0.93
1:B:178:MET:HB2	1:B:185:GLN:HB3	1.49	0.93
1:B:185:GLN:HE22	1:B:223:THR:HB	1.34	0.91
1:C:180:HIS:NE2	1:C:182:GLN:HB3	1.92	0.84
1:C:212:GLN:HE22	1:C:218:HIS:HA	1.41	0.84
1:C:222:LYS:HA	1:C:222:LYS:HE2	1.61	0.82
1:D:171:LEU:HD13	1:D:188:VAL:HG21	1.60	0.81
1:C:85:PHE:H	1:C:140:GLN:NE2	1.80	0.79
1:A:76:VAL:HG23	1:A:195:ARG:HB3	1.68	0.75
1:A:37:ARG:NH1	1:A:37:ARG:HB3	2.02	0.74
1:C:130:ALA:HB3	1:C:131:PRO:HD3	1.68	0.74
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.69	0.73
1:A:117:ARG:HH11	1:A:117:ARG:HG2	1.54	0.72
1:C:116:GLU:O	1:C:120:GLN:HG3	1.90	0.72
1:B:55:LEU:HD23	1:B:56:TYR:N	2.06	0.71
1:D:185:GLN:NE2	1:D:223:THR:HB	2.05	0.71
1:D:121:LEU:HB3	1:D:126:LEU:HD22	1.72	0.70
1:D:129:ASP:O	1:D:133:ILE:HG12	1.90	0.70
1:B:185:GLN:NE2	1:B:223:THR:HB	2.06	0.69
1:D:172:SER:HA	1:D:186:LEU:HD21	1.72	0.69
1:B:130:ALA:HB3	1:B:131:PRO:HD3	1.74	0.69
1:A:71:ASP:OD1	1:A:73:ARG:HB2	1.93	0.68
1:C:30:PHE:HD2	1:C:31:LEU:HD22	1.56	0.68
1:C:85:PHE:N	1:C:140:GLN:HE22	1.87	0.67
1:B:190:ARG:HD3	1:B:201:ARG:HH21	1.59	0.66
1:C:117:ARG:HH22	1:C:121:LEU:HD21	1.61	0.66
1:C:180:HIS:CD2	1:C:182:GLN:HB3	2.30	0.66
1:D:185:GLN:HE22	1:D:223:THR:HB	1.61	0.66
1:C:171:LEU:HD13	1:C:188:VAL:HG11	1.78	0.65
1:B:55:LEU:HD21	1:B:85:PHE:HD1	1.61	0.65
1:D:180:HIS:ND1	1:D:181:PRO:HD2	2.12	0.65
1:D:24:ALA:O	1:D:28:GLU:HG2	1.98	0.64
1:D:70:ASP:C	1:D:72:ASP:H	1.99	0.63
1:A:217:LEU:HD12	1:A:217:LEU:C	2.18	0.63
1:C:218:HIS:HB3	1:C:225:VAL:CG1	2.26	0.63
1:D:85:PHE:H	1:D:140:GLN:NE2	1.84	0.62
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:160:VAL:HG21	1:B:203:MET:SD	2.39	0.62
1:C:114:SER:HB3	1:C:117:ARG:HB2	1.81	0.62
1:A:190:ARG:HD2	1:A:201:ARG:NH2	2.15	0.61
1:B:172:SER:OG	1:B:186:LEU:HD21	2.00	0.61
1:A:131:PRO:HG3	1:D:131:PRO:HG3	1.82	0.61
1:A:80:PHE:CE1	1:A:144:ARG:HD2	2.35	0.61
1:A:146:LEU:HD11	1:D:99:GLU:HG2	1.81	0.61
1:A:149:THR:HG23	1:D:77:LEU:HD11	1.83	0.61
1:D:116:GLU:O	1:D:120:GLN:HG3	2.01	0.61
1:D:194:ALA:HB1	1:D:199:CYS:O	2.01	0.61
1:B:80:PHE:HB3	1:B:84:GLU:HG3	1.83	0.60
1:C:191:GLN:HE22	1:C:201:ARG:HD2	1.66	0.60
1:A:171:LEU:HD13	1:A:188:VAL:HG21	1.84	0.59
1:D:119:GLN:HA	1:D:122:PHE:HB2	1.82	0.59
1:D:80:PHE:HB3	1:D:84:GLU:HG3	1.84	0.59
1:A:127:SER:HB3	1:A:128:PRO:HD3	1.84	0.59
1:B:115:TYR:O	1:B:119:GLN:HG2	2.03	0.59
1:D:187:ARG:HA	1:D:223:THR:HG22	1.85	0.58
1:C:220:ARG:HG2	1:C:220:ARG:HH11	1.69	0.58
1:A:117:ARG:HG2	1:A:117:ARG:NH1	2.19	0.58
1:C:191:GLN:NE2	1:C:201:ARG:HD2	2.19	0.57
1:B:69:GLU:OE1	1:B:69:GLU:HA	2.03	0.57
1:B:114:SER:OG	1:B:117:ARG:HB2	2.04	0.57
1:A:212:GLN:HA	1:A:217:LEU:O	2.04	0.57
1:C:218:HIS:HD2	1:C:225:VAL:HG11	1.69	0.57
1:A:80:PHE:HE1	1:A:144:ARG:HD2	1.70	0.57
1:D:190:ARG:HH11	1:D:205:GLY:HA3	1.69	0.56
1:B:178:MET:CB	1:B:185:GLN:HB3	2.29	0.56
1:D:172:SER:OG	1:D:186:LEU:HD11	2.05	0.56
1:C:91:LEU:HD11	1:C:118:LEU:HD23	1.88	0.56
1:B:105:ARG:HD3	2:B:258:HOH:O	2.05	0.56
1:D:207:VAL:O	1:D:211:LEU:HG	2.05	0.56
1:C:24:ALA:O	1:C:28:GLU:HG3	2.06	0.55
1:C:47:ARG:HB3	1:C:47:ARG:NH1	2.21	0.55
1:C:79:TYR:CD1	1:C:105:ARG:HD2	2.41	0.55
1:D:217:LEU:C	1:D:217:LEU:HD12	2.26	0.55
1:D:85:PHE:N	1:D:140:GLN:HE22	1.86	0.54
1:D:161:THR:HG22	1:D:207:VAL:HG22	1.88	0.54
1:A:172:SER:HB3	1:A:186:LEU:HD11	1.88	0.54
1:C:132:ARG:HG3	2:C:241:HOH:O	2.05	0.54
1:C:23:ASP:O	1:C:27:ILE:HG12	2.08	0.54
1:D:79:TYR:CD1	1:D:105:ARG:HD2	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:221:GLY:C	1:C:223:THR:H	2.12	0.53
1:A:220:ARG:HH22	1:C:166:ARG:HH22	1.54	0.53
1:B:218:HIS:CD2	1:B:220:ARG:HB2	2.43	0.53
1:A:26:THR:HG23	1:A:129:ASP:HB3	1.91	0.53
1:B:92:PHE:HB3	1:C:139:VAL:HA	1.91	0.53
1:C:30:PHE:CD2	1:C:31:LEU:HD22	2.41	0.53
1:C:169:HIS:ND1	1:C:226:LEU:HD21	2.24	0.53
1:A:210:LYS:HE3	1:A:214:ASP:OD1	2.10	0.52
1:A:93:ILE:HD11	1:D:143:LYS:HG3	1.91	0.52
1:B:59:ILE:HD11	1:B:111:ALA:HB2	1.92	0.52
1:A:37:ARG:CZ	1:A:37:ARG:HB3	2.39	0.52
1:A:220:ARG:NH2	1:C:166:ARG:HH22	2.08	0.52
1:C:194:ALA:HB1	1:C:199:CYS:O	2.09	0.52
1:C:69:GLU:CD	1:C:70:ASP:H	2.14	0.52
1:C:172:SER:OG	1:C:186:LEU:HD21	2.10	0.51
1:B:172:SER:HA	1:B:186:LEU:HD21	1.92	0.51
1:D:70:ASP:C	1:D:72:ASP:N	2.64	0.51
1:C:201:ARG:HH22	1:C:222:LYS:HZ1	1.57	0.51
1:C:132:ARG:HE	1:C:132:ARG:HA	1.76	0.51
1:B:188:VAL:HG12	2:B:275:HOH:O	2.09	0.51
1:B:172:SER:OG	1:B:186:LEU:HD11	2.11	0.51
1:C:65:ILE:HG23	1:C:100:VAL:HG21	1.93	0.51
1:A:157:PHE:HB2	1:D:69:GLU:HG3	1.93	0.51
1:D:56:TYR:HB2	1:D:86:VAL:HG23	1.93	0.50
1:A:39:TYR:CE2	1:A:110:LEU:HD12	2.46	0.50
1:D:22:LEU:O	1:D:22:LEU:HD23	2.12	0.50
1:C:218:HIS:CD2	1:C:225:VAL:HG11	2.47	0.50
1:C:186:LEU:HB2	1:C:224:VAL:HB	1.93	0.50
1:C:212:GLN:HB2	1:C:217:LEU:HD11	1.93	0.50
1:D:127:SER:HB3	1:D:128:PRO:HD3	1.93	0.50
1:A:140:GLN:O	1:A:144:ARG:HD3	2.12	0.49
1:B:68:GLU:HG2	1:B:69:GLU:N	2.27	0.49
1:B:191:GLN:NE2	1:B:201:ARG:HD2	2.27	0.49
1:A:156:ALA:HB2	1:D:155:LEU:HD13	1.94	0.49
1:D:171:LEU:CD1	1:D:188:VAL:HG21	2.38	0.49
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.77	0.49
1:D:70:ASP:O	1:D:72:ASP:N	2.45	0.49
1:D:201:ARG:HG3	1:D:201:ARG:HH11	1.77	0.49
1:C:178:MET:O	1:C:179:SER:HB2	2.13	0.49
1:A:221:GLY:HA3	1:B:70:ASP:O	2.13	0.48
1:A:214:ASP:HB3	1:A:216:LEU:HD13	1.94	0.48
1:D:217:LEU:O	1:D:217:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:217:LEU:C	1:B:217:LEU:HD12	2.35	0.48
1:C:27:ILE:O	1:C:31:LEU:HD23	2.14	0.48
1:C:192:GLU:OE1	1:C:192:GLU:HA	2.14	0.48
1:C:29:ARG:CZ	1:C:29:ARG:HB2	2.44	0.48
1:C:71:ASP:O	1:C:72:ASP:CB	2.61	0.47
1:A:180:HIS:HB2	1:A:185:GLN:HB2	1.96	0.47
1:D:123:GLN:HA	1:D:123:GLN:OE1	2.14	0.47
1:A:165:VAL:HG23	1:A:166:ARG:N	2.30	0.47
1:D:220:ARG:O	1:D:222:LYS:N	2.47	0.47
1:C:91:LEU:HG	1:C:115:TYR:CD1	2.50	0.47
1:C:119:GLN:O	1:C:123:GLN:HG3	2.14	0.47
1:A:37:ARG:HB3	1:A:37:ARG:HH11	1.77	0.47
1:A:38:ARG:NH1	2:A:296:HOH:O	2.47	0.47
1:A:177:ALA:HB1	1:A:184:THR:CG2	2.45	0.47
1:A:168:LEU:O	1:A:186:LEU:HD21	2.14	0.47
1:A:210:LYS:O	1:A:210:LYS:HD3	2.15	0.46
1:C:71:ASP:HB3	1:C:73:ARG:HG2	1.97	0.46
1:A:187:ARG:HD3	1:A:222:LYS:O	2.16	0.46
1:A:65:ILE:HG22	1:A:77:LEU:HD12	1.98	0.46
1:D:71:ASP:N	1:D:71:ASP:OD2	2.49	0.46
1:A:124:THR:OG1	1:A:125:SER:N	2.47	0.46
1:D:114:SER:OG	1:D:117:ARG:HB2	2.16	0.45
1:C:58:VAL:HG12	1:C:82:SER:HA	1.98	0.45
1:C:212:GLN:NE2	1:C:219:ALA:H	2.14	0.45
1:A:76:VAL:O	1:A:151:LYS:HE3	2.16	0.45
1:A:190:ARG:HD2	1:A:201:ARG:HH21	1.81	0.45
1:C:184:THR:OG1	1:C:226:LEU:HB3	2.16	0.45
1:B:139:VAL:HA	1:C:92:PHE:HB3	1.99	0.45
1:B:55:LEU:C	1:B:55:LEU:HD23	2.36	0.45
1:C:220:ARG:HH11	1:C:220:ARG:CG	2.28	0.45
1:C:47:ARG:CB	1:C:47:ARG:HH11	2.29	0.45
1:D:187:ARG:CA	1:D:223:THR:HG22	2.46	0.45
1:D:121:LEU:O	1:D:126:LEU:HB2	2.17	0.45
1:B:227:TYR:CD2	1:B:227:TYR:N	2.84	0.44
1:C:48:PRO:HD3	1:C:101:ILE:HG12	1.98	0.44
1:B:169:HIS:O	1:B:173:LYS:HG2	2.17	0.44
1:B:77:LEU:HD11	1:C:149:THR:HG23	2.00	0.44
1:B:87:GLY:HA2	2:B:240:HOH:O	2.17	0.44
1:B:172:SER:CA	1:B:186:LEU:HD21	2.48	0.44
1:D:159:ASP:O	1:D:162:ASP:HB3	2.18	0.44
1:D:117:ARG:O	1:D:121:LEU:HG	2.18	0.44
1:B:76:VAL:HG23	1:B:195:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:66:ILE:HG12	1:B:76:VAL:HG22	1.99	0.44
1:B:180:HIS:ND1	1:B:181:PRO:HD2	2.33	0.43
1:C:71:ASP:O	1:C:72:ASP:HB3	2.18	0.43
1:B:215:GLY:O	1:B:216:LEU:HD23	2.18	0.43
1:C:211:LEU:O	1:C:214:ASP:HB2	2.18	0.43
1:D:121:LEU:HD13	1:D:126:LEU:HD22	2.00	0.43
1:B:220:ARG:HH11	1:B:220:ARG:HG2	1.83	0.43
1:A:210:LYS:HD3	1:A:210:LYS:C	2.38	0.43
1:A:33:HIS:HD2	1:A:117:ARG:NH2	2.17	0.43
1:A:171:LEU:HD13	1:A:188:VAL:CG2	2.48	0.43
1:B:94:GLU:HA	2:B:267:HOH:O	2.18	0.43
1:A:162:ASP:HA	1:A:165:VAL:HG22	2.00	0.43
1:D:159:ASP:O	1:D:163:ARG:HG3	2.19	0.43
1:D:117:ARG:NH2	1:D:121:LEU:HD21	2.34	0.43
1:D:190:ARG:HD2	1:D:205:GLY:CA	2.49	0.43
1:B:27:ILE:HD13	1:B:57:TYR:OH	2.19	0.43
1:C:26:THR:HG23	1:C:129:ASP:HB3	1.99	0.43
1:C:46:PHE:C	1:C:46:PHE:CD1	2.92	0.43
1:C:76:VAL:HG23	1:C:195:ARG:HB3	2.00	0.42
1:D:55:LEU:HD22	1:D:56:TYR:N	2.34	0.42
1:A:22:LEU:HG	1:A:27:ILE:HG13	2.01	0.42
1:A:190:ARG:HE	1:A:201:ARG:HE	1.67	0.42
1:A:66:ILE:CG2	1:A:74:GLU:HB3	2.49	0.42
1:C:201:ARG:NH2	1:C:222:LYS:NZ	2.67	0.42
1:C:114:SER:HB3	1:C:117:ARG:CB	2.48	0.42
1:A:36:ARG:HB3	1:A:109:GLU:OE2	2.20	0.42
1:D:117:ARG:HA	1:D:117:ARG:HD2	1.84	0.41
1:B:54:THR:HA	1:B:114:SER:HA	2.02	0.41
1:C:119:GLN:HA	1:C:122:PHE:HB2	2.02	0.41
1:C:132:ARG:CA	1:C:132:ARG:HE	2.33	0.41
1:C:76:VAL:O	1:C:151:LYS:HE2	2.20	0.41
1:C:56:TYR:HB2	1:C:86:VAL:HG23	2.03	0.41
1:D:66:ILE:HB	1:D:101:ILE:HB	2.03	0.41
1:C:208:LEU:O	1:C:212:GLN:HB2	2.20	0.41
1:C:178:MET:HB2	1:C:185:GLN:H	1.86	0.41
1:B:57:TYR:HB3	1:B:111:ALA:HB3	2.02	0.41
1:B:39:TYR:HA	1:B:40:PRO:HD3	1.92	0.41
1:D:193:LEU:HD12	1:D:193:LEU:HA	1.95	0.41
1:A:23:ASP:OD1	1:A:25:GLY:N	2.53	0.41
1:D:54:THR:HG21	1:D:112:GLU:OE2	2.21	0.41
1:C:222:LYS:CE	1:C:222:LYS:HA	2.42	0.41
1:C:201:ARG:HH22	1:C:222:LYS:NZ	2.19	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:180:HIS:ND1	1:A:181:PRO:N	2.69	0.40
1:D:93:ILE:O	1:D:94:GLU:C	2.59	0.40
1:D:38:ARG:CD	1:D:109:GLU:HG3	2.51	0.40
1:C:143:LYS:HD3	2:C:284:HOH:O	2.20	0.40
1:B:73:ARG:CZ	1:C:157:PHE:HB3	2.51	0.40
1:B:191:GLN:HB2	1:B:191:GLN:HE21	1.57	0.40
1:D:176:GLU:O	1:D:177:ALA:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	205/230 (89%)	198 (97%)	6 (3%)	1 (0%)	38	45
1	B	205/230 (89%)	198 (97%)	6 (3%)	1 (0%)	38	45
1	C	205/230 (89%)	185 (90%)	14 (7%)	6 (3%)	7	4
1	D	206/230 (90%)	191 (93%)	10 (5%)	5 (2%)	9	6
All	All	821/920 (89%)	772 (94%)	36 (4%)	13 (2%)	14	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	179	SER
1	D	221	GLY
1	D	71	ASP
1	A	221	GLY
1	C	178	MET
1	C	72	ASP
1	C	180	HIS
1	C	222	LYS
1	D	216	LEU
1	D	214	ASP
1	B	178	MET

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Mol	Chain	Res	Type
1	C	177	ALA
1	D	183	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	177/198 (89%)	170 (96%)	7 (4%)	42	56
1	B	177/198 (89%)	171 (97%)	6 (3%)	49	64
1	C	174/198 (88%)	167 (96%)	7 (4%)	42	56
1	D	175/198 (88%)	166 (95%)	9 (5%)	33	43
All	All	703/792 (89%)	674 (96%)	29 (4%)	41	55

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	42	ARG
1	A	71	ASP
1	A	109	GLU
1	A	202	GLU
1	A	206	ARG
1	A	209	LYS
1	B	72	ASP
1	B	117	ARG
1	B	170	ASP
1	B	184	THR
1	B	191	GLN
1	B	220	ARG
1	C	46	PHE
1	C	69	GLU
1	C	119	GLN
1	C	132	ARG
1	C	143	LYS
1	C	192	GLU
1	C	220	ARG

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Mol	Chain	Res	Type
1	D	22	LEU
1	D	36	ARG
1	D	55	LEU
1	D	109	GLU
1	D	124	THR
1	D	178	MET
1	D	202	GLU
1	D	203	MET
1	D	223	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	107	GLN
1	A	169	HIS
1	B	120	GLN
1	B	123	GLN
1	B	185	GLN
1	B	191	GLN
1	C	33	HIS
1	C	120	GLN
1	C	140	GLN
1	C	191	GLN
1	C	212	GLN
1	C	218	HIS
1	D	120	GLN
1	D	140	GLN
1	D	185	GLN
1	D	212	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	207/230 (90%)	0.26	7 (3%) 43 53	21, 39, 59, 63	0
1	B	207/230 (90%)	0.47	12 (5%) 22 31	22, 40, 63, 68	0
1	C	207/230 (90%)	1.04	35 (16%) 2 4	22, 49, 68, 72	0
1	D	208/230 (90%)	0.73	21 (10%) 7 12	22, 49, 65, 69	0
All	All	829/920 (90%)	0.62	75 (9%) 10 16	21, 43, 65, 72	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	THR	9.4
1	D	229	THR	8.3
1	D	183	GLY	8.1
1	C	183	GLY	7.9
1	C	226	LEU	6.1
1	C	219	ALA	5.7
1	C	217	LEU	5.6
1	C	228	GLY	5.6
1	C	181	PRO	5.6
1	B	178	MET	5.1
1	C	180	HIS	4.9
1	C	177	ALA	4.9
1	C	175	PRO	4.7
1	C	178	MET	4.6
1	D	186	LEU	4.6
1	B	174	GLU	4.4
1	B	220	ARG	4.4
1	C	186	LEU	4.4
1	D	228	GLY	4.1
1	B	175	PRO	4.0
1	D	178	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	120	GLN	3.8
1	C	227	TYR	3.8
1	C	184	THR	3.7
1	C	179	SER	3.7
1	C	187	ARG	3.7
1	D	70	ASP	3.6
1	C	220	ARG	3.6
1	D	185	GLN	3.6
1	D	179	SER	3.3
1	C	225	VAL	3.3
1	D	220	ARG	3.3
1	D	218	HIS	3.2
1	D	71	ASP	3.2
1	B	187	ARG	3.2
1	C	188	VAL	3.2
1	D	172	SER	3.0
1	B	183	GLY	3.0
1	A	173	LYS	2.9
1	C	218	HIS	2.9
1	B	176	GLU	2.9
1	B	173	LYS	2.9
1	C	123	GLN	2.8
1	C	126	LEU	2.8
1	B	70	ASP	2.6
1	C	182	GLN	2.6
1	A	220	ARG	2.5
1	C	176	GLU	2.5
1	A	174	GLU	2.5
1	C	117	ARG	2.5
1	D	209	LYS	2.5
1	D	214	ASP	2.5
1	C	71	ASP	2.4
1	D	208	LEU	2.4
1	C	124	THR	2.3
1	D	35	HIS	2.3
1	A	176	GLU	2.3
1	C	70	ASP	2.3
1	C	209	LYS	2.3
1	C	120	GLN	2.3
1	B	71	ASP	2.3
1	B	227	TYR	2.2
1	C	213	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	226	LEU	2.2
1	C	173	LYS	2.2
1	C	172	SER	2.1
1	D	213	ALA	2.1
1	C	222	LYS	2.1
1	D	32	ALA	2.1
1	A	178	MET	2.1
1	C	26	THR	2.0
1	B	222	LYS	2.0
1	D	221	GLY	2.0
1	A	219	ALA	2.0
1	A	175	PRO	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.