



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:33 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 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

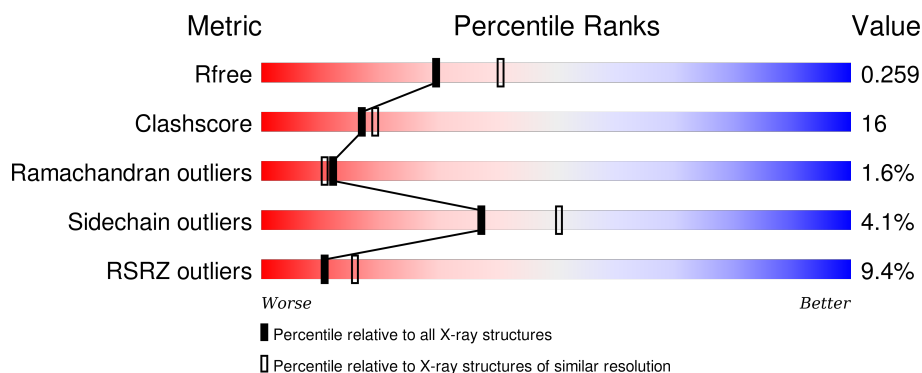
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 ≥ 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	230	<div> <div>3%</div> <div>62%</div> <div>27%</div> <div>•</div> <div>10%</div> </div>
1	B	230	<div> <div>6%</div> <div>66%</div> <div>23%</div> <div>•</div> <div>10%</div> </div>
1	C	230	<div> <div>16%</div> <div>54%</div> <div>30%</div> <div>5%</div> <div>10%</div> </div>
1	D	230	<div> <div>9%</div> <div>57%</div> <div>32%</div> <div>•</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6817 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 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			

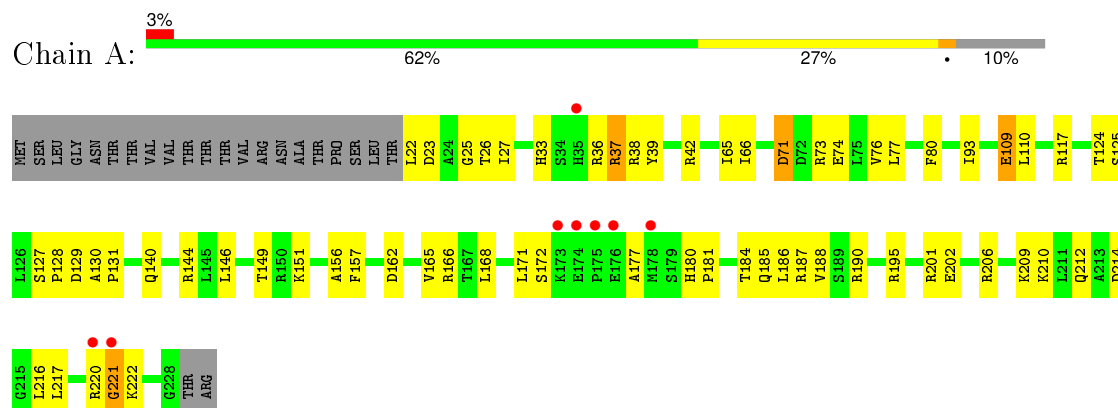
- Molecule 2 is water.

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		

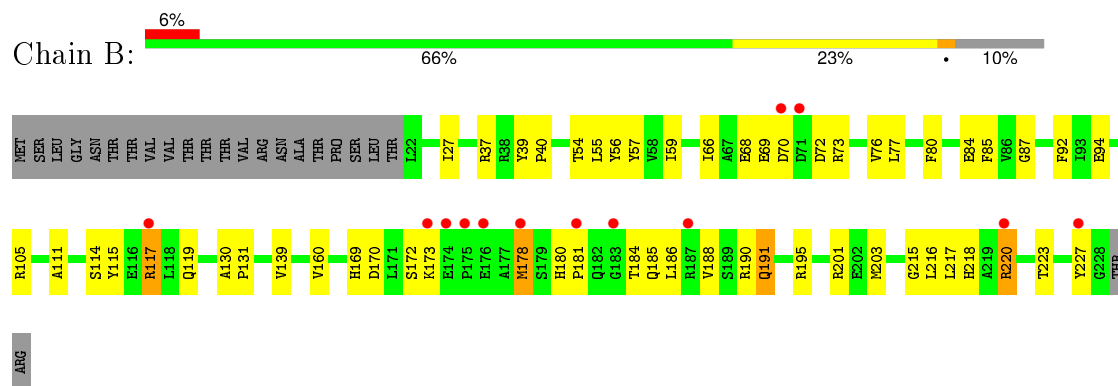
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

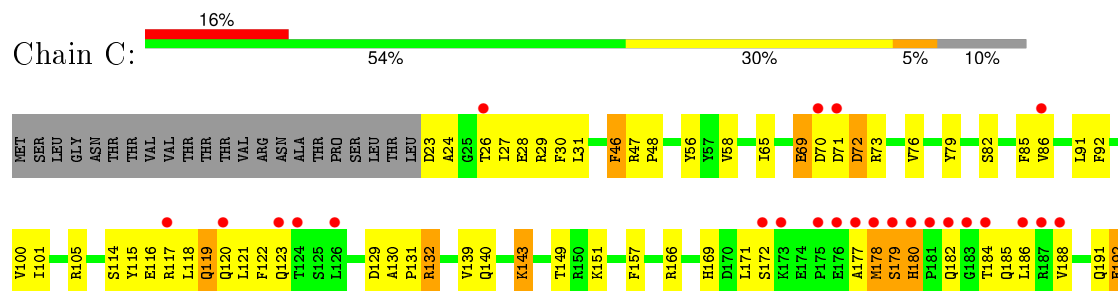
• Molecule 1: Catabolite activation-like protein

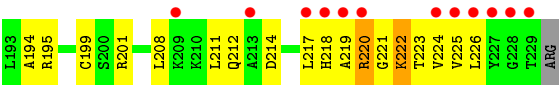


• Molecule 1: Catabolite activation-like protein

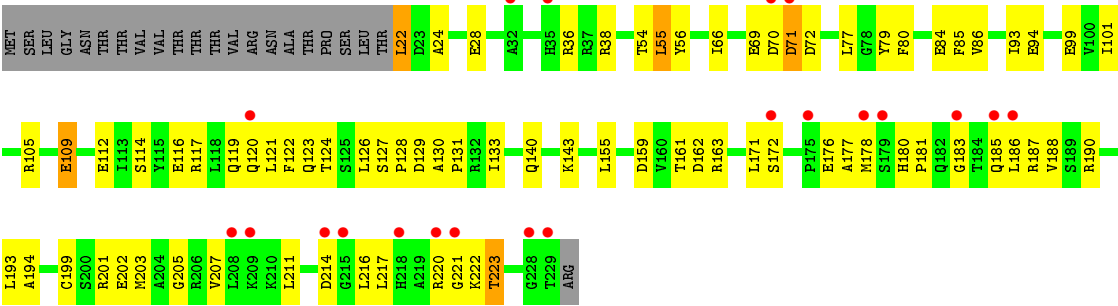


• Molecule 1: Catabolite activation-like protein





● Molecule 1: Catabolite activation-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.69 Å 67.69 Å 110.37 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.244 , 0.305 0.257 , 0.259	Depositor DCC
R_{free} test set	2113 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	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 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	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

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 16.

All (214) 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: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
1:B:160:VAL:HG21	1:B:203:MET:SD	2.39	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LEU:O	1:D:217:LEU:HD12	2.14	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	34	41
1	B	205/230 (89%)	198 (97%)	6 (3%)	1 (0%)	34	41
1	C	205/230 (89%)	185 (90%)	14 (7%)	6 (3%)	6	3
1	D	206/230 (90%)	191 (93%)	10 (5%)	5 (2%)	7	5
All	All	821/920 (89%)	772 (94%)	36 (4%)	13 (2%)	12	11

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	72	ASP
1	C	180	HIS
1	C	222	LYS
1	D	216	LEU
1	D	214	ASP
1	B	178	MET
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%)	38	52
1	B	177/198 (89%)	171 (97%)	6 (3%)	44	59
1	C	174/198 (88%)	167 (96%)	7 (4%)	38	52
1	D	175/198 (88%)	166 (95%)	9 (5%)	29	39
All	All	703/792 (89%)	674 (96%)	29 (4%)	37	50

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/230 (90%)	0.26	8 (3%) 43 52	21, 39, 59, 63	0
1	B	207/230 (90%)	0.54	13 (6%) 23 31	22, 40, 63, 68	0
1	C	207/230 (90%)	1.10	36 (17%) 2 3	22, 49, 68, 72	0
1	D	208/230 (90%)	0.77	21 (10%) 9 13	22, 49, 65, 69	0
All	All	829/920 (90%)	0.67	78 (9%) 11 16	21, 43, 65, 72	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	THR	9.8
1	D	229	THR	8.6
1	D	183	GLY	8.2
1	C	183	GLY	7.7
1	C	226	LEU	7.1
1	C	219	ALA	6.4
1	C	228	GLY	6.2
1	C	181	PRO	5.5
1	C	186	LEU	5.5
1	C	217	LEU	5.3
1	B	178	MET	5.3
1	C	178	MET	5.2
1	B	220	ARG	5.2
1	C	180	HIS	4.8
1	D	178	MET	4.7
1	C	175	PRO	4.6
1	C	177	ALA	4.6
1	D	228	GLY	4.5
1	B	175	PRO	4.5
1	B	174	GLU	4.5
1	C	179	SER	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	184	THR	4.0
1	C	220	ARG	3.9
1	B	183	GLY	3.9
1	D	70	ASP	3.8
1	D	186	LEU	3.8
1	C	218	HIS	3.7
1	C	187	ARG	3.6
1	B	187	ARG	3.6
1	D	179	SER	3.5
1	C	227	TYR	3.4
1	D	220	ARG	3.2
1	D	120	GLN	3.2
1	C	188	VAL	3.2
1	D	208	LEU	3.1
1	B	227	TYR	3.1
1	D	218	HIS	3.1
1	D	221	GLY	3.0
1	C	225	VAL	3.0
1	C	123	GLN	2.9
1	D	35	HIS	2.9
1	A	173	LYS	2.9
1	D	185	GLN	2.9
1	C	124	THR	2.8
1	A	221	GLY	2.8
1	C	182	GLN	2.8
1	D	209	LYS	2.7
1	B	70	ASP	2.7
1	A	174	GLU	2.7
1	D	32	ALA	2.7
1	C	126	LEU	2.6
1	C	213	ALA	2.6
1	D	172	SER	2.6
1	C	70	ASP	2.6
1	D	71	ASP	2.6
1	C	173	LYS	2.6
1	C	71	ASP	2.6
1	C	117	ARG	2.4
1	C	176	GLU	2.4
1	D	214	ASP	2.4
1	B	173	LYS	2.4
1	D	175	PRO	2.4
1	C	209	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	215	GLY	2.3
1	B	71	ASP	2.3
1	C	120	GLN	2.3
1	C	172	SER	2.2
1	A	178	MET	2.2
1	C	224	VAL	2.2
1	A	175	PRO	2.2
1	B	176	GLU	2.2
1	C	86	VAL	2.1
1	C	26	THR	2.1
1	A	220	ARG	2.1
1	B	181	PRO	2.1
1	B	117	ARG	2.0
1	A	35	HIS	2.0
1	A	176	GLU	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.