Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 01:06 PM EDT

PDB ID	:	7JV7
Title	:	Crystal Structure of the yeast RNA Pol II CTD kinase CTDK-1 complex
Authors	:	Xie, Y.; Ren, Y.
Deposited on	:	2020-08-20
Resolution	:	1.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

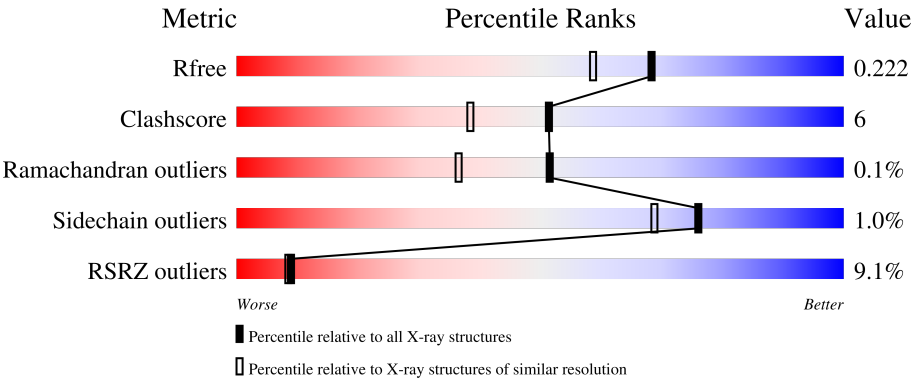
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	355	7% 75% 10% • 14%
2	B	325	2% 86% 9% 5%
3	C	296	16% 69% 16% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7813 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 CTD kinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	11	0
			2514	1623	409	465	17			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	-	expression tag	UNP Q03957
A	155	ALA	-	expression tag	UNP Q03957
A	156	MET	-	expression tag	UNP Q03957
A	157	GLY	-	expression tag	UNP Q03957
A	158	SER	-	expression tag	UNP Q03957

- Molecule 2 is a protein called CTD kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	310	Total	C	N	O	S	0	5	0
			2601	1678	434	479	10			

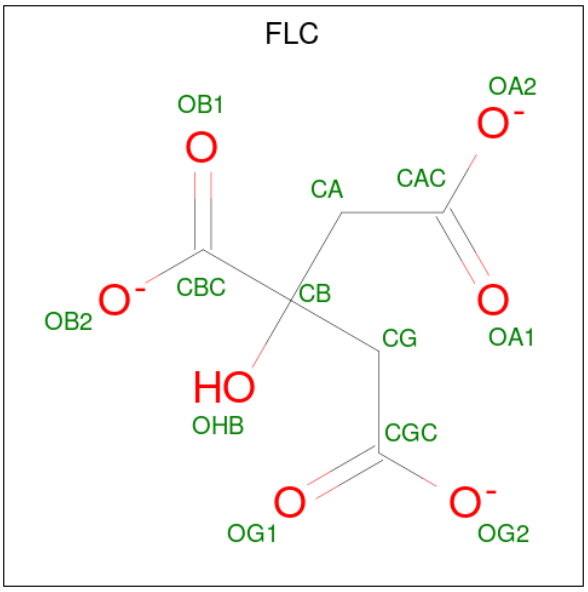
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P46962
B	0	SER	-	expression tag	UNP P46962

- Molecule 3 is a protein called CTD kinase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	7	0
			2136	1366	355	407	8			

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

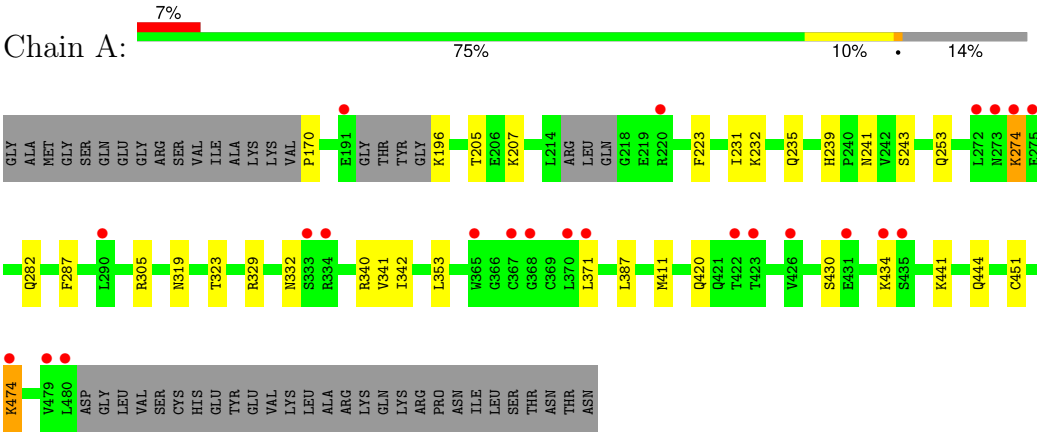
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	173	Total O 173 173	0	0
5	B	259	Total O 259 259	0	0
5	C	117	Total O 117 117	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

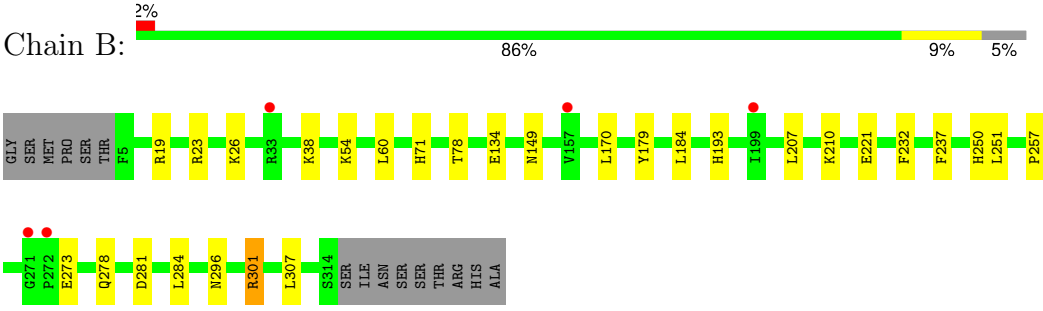
• Molecule 1: CTD kinase subunit alpha

Chain A:



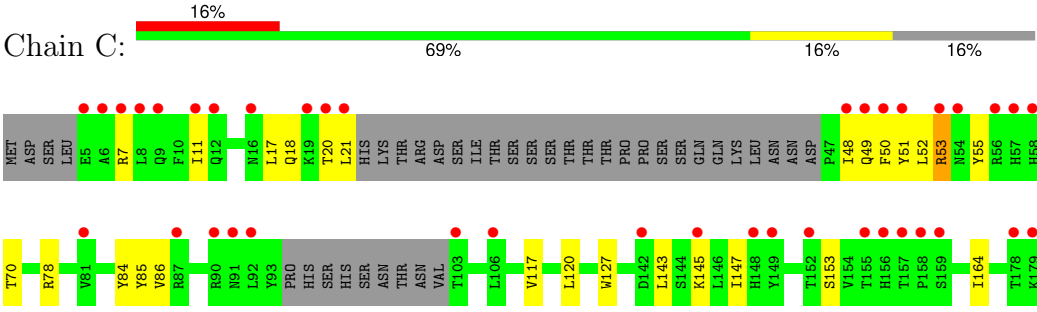
• Molecule 2: CTD kinase subunit beta

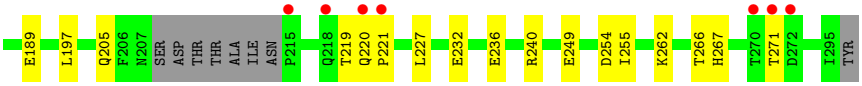
Chain B:



• Molecule 3: CTD kinase subunit gamma

Chain C:




E189
L197
Q205
F206
N207
SER
ASP
THR
THR
ALA
ILE
ASN
P215
Q218
T219
Q220
P221
L227
E232
E236
R240
E249
D254
I255
K262
T266
H267
T270
T271
D272
I295
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.17Å 71.09Å 84.80Å 79.08° 86.22° 72.69°	Depositor
Resolution (Å)	29.24 – 1.85 29.24 – 1.85	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.24-1.85) 89.2 (29.24-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.184 , 0.222 0.185 , 0.222	Depositor DCC
R_{free} test set	1999 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7813	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC

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	0.35	0/2596	0.55	0/3504
2	B	0.44	0/2669	0.57	0/3609
3	C	0.35	0/2200	0.52	0/2974
All	All	0.39	0/7465	0.55	0/10087

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	2514	0	2585	25	0
2	B	2601	0	2625	24	0
3	C	2136	0	2125	44	0
4	A	13	0	5	0	0
5	A	173	0	0	2	0
5	B	259	0	0	1	0
5	C	117	0	0	1	0
All	All	7813	0	7340	82	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 6.

All (82) 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)
3:C:49:GLN:HG2	3:C:53:ARG:HH11	1.06	1.14
3:C:49:GLN:HG2	3:C:53:ARG:NH1	1.65	1.11
3:C:49:GLN:CG	3:C:53:ARG:NH1	2.38	0.87
3:C:49:GLN:CG	3:C:53:ARG:HH11	1.91	0.83
3:C:50:PHE:HA	3:C:53:ARG:HG2	1.65	0.78
3:C:117:VAL:HA	3:C:120:LEU:HD12	1.70	0.72
3:C:267:HIS:O	3:C:271[A]:THR:HG22	1.93	0.69
3:C:50:PHE:HA	3:C:53:ARG:CG	2.22	0.68
1:A:420[B]:GLN:HE22	3:C:227:LEU:HD11	1.64	0.62
3:C:52:LEU:HA	3:C:55:TYR:HD2	1.64	0.62
3:C:205[B]:GLN:NE2	5:C:302:HOH:O	2.33	0.62
1:A:196:LYS:N	5:A:707:HOH:O	2.35	0.60
1:A:205:THR:HB	1:A:207:LYS:HE3	1.84	0.60
1:A:170:PRO:HB3	2:B:307:LEU:HD21	1.83	0.60
3:C:50:PHE:O	3:C:53:ARG:HB2	2.02	0.59
3:C:49:GLN:O	3:C:53:ARG:HG2	2.01	0.59
1:A:279:SER:H	1:A:282:GLN:HE21	1.53	0.57
2:B:54:LYS:HE3	3:C:249:GLU:OE1	2.05	0.57
2:B:19:ARG:HD2	2:B:278:GLN:HG2	1.86	0.57
2:B:179:TYR:HE1	3:C:255:ILE:HD13	1.70	0.56
1:A:441:LYS:HD2	1:A:467:ASP:HB2	1.88	0.55
3:C:11:ILE:HG12	3:C:69:THR:HG21	1.88	0.55
3:C:52:LEU:HA	3:C:55:TYR:CD2	2.41	0.54
2:B:179:TYR:CE1	3:C:255:ILE:HD13	2.43	0.53
2:B:193:HIS:HE1	2:B:221:GLU:O	1.91	0.53
2:B:296:ASN:O	2:B:301:ARG:NH1	2.41	0.53
1:A:274:LYS:HE2	1:A:274:LYS:HA	1.91	0.53
2:B:19:ARG:NH2	2:B:281:ASP:OD1	2.42	0.52
1:A:223:PHE:N	2:B:134[B]:GLU:OE2	2.29	0.52
3:C:50:PHE:CA	3:C:53:ARG:HG2	2.37	0.52
2:B:23:ARG:HD2	2:B:26:LYS:HD3	1.91	0.51
3:C:70:THR:HG22	3:C:78:ARG:HD3	1.93	0.50
2:B:19:ARG:HB3	2:B:284:LEU:HD11	1.95	0.49
3:C:85:TYR:CE2	3:C:117:VAL:HG21	2.47	0.49
3:C:127:TRP:HB2	3:C:219:THR:HG21	1.94	0.49
2:B:170:LEU:HD13	2:B:207:LEU:HD12	1.95	0.49
1:A:430:SER:O	1:A:434:LYS:HB3	2.13	0.48
2:B:38:LYS:HE2	2:B:78:THR:HG23	1.94	0.48
3:C:262:LYS:O	3:C:266:THR:HG23	2.14	0.48
1:A:287:PHE:CE1	1:A:371:LEU:HB2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:LEU:HA	3:C:20:THR:HG22	1.95	0.47
2:B:261:GLU:CD	2:B:261:GLU:H	2.18	0.47
2:B:250:HIS:HE1	3:C:254[B]:ASP:OD2	1.99	0.46
1:A:253:GLN:OE1	2:B:296:ASN:ND2	2.48	0.46
1:A:329:ARG:NH2	1:A:332:ASN:OD1	2.48	0.46
3:C:153:SER:OG	3:C:189:GLU:OE1	2.33	0.46
2:B:71:HIS:HE1	5:B:550:HOH:O	1.99	0.46
1:A:353[B]:LEU:HB3	1:A:411:MET:HB3	1.98	0.45
2:B:261:GLU:HA	2:B:264:MET:CE	2.47	0.45
1:A:319:ASN:HB3	5:A:753:HOH:O	2.15	0.45
1:A:474:LYS:HE2	1:A:474:LYS:HB2	1.68	0.45
3:C:18:GLN:H	3:C:18:GLN:HG2	1.51	0.45
3:C:220[B]:GLN:H	3:C:220[B]:GLN:HG3	1.45	0.44
3:C:236:GLU:O	3:C:240:ARG:HG3	2.17	0.44
2:B:184:LEU:HD21	2:B:237:PHE:CG	2.52	0.44
1:A:279:SER:H	1:A:282:GLN:NE2	2.15	0.44
3:C:145:LYS:N	3:C:145:LYS:HD3	2.32	0.43
3:C:86:VAL:HG13	3:C:143:LEU:HD22	2.01	0.43
3:C:220[A]:GLN:HG3	3:C:221:PRO:HD2	2.00	0.43
1:A:243:SER:HB2	1:A:323[B]:THR:HG22	2.00	0.43
3:C:17:LEU:HD11	3:C:84:TYR:CD2	2.52	0.43
3:C:51:TYR:O	3:C:55:TYR:HB3	2.17	0.43
1:A:239:HIS:HE1	1:A:241:ASN:HD22	1.66	0.43
3:C:48:ILE:O	3:C:52:LEU:HD12	2.19	0.43
2:B:251:LEU:HD11	2:B:257:PRO:HA	2.01	0.43
3:C:164[B]:ILE:HD13	3:C:197:LEU:HD22	2.00	0.43
1:A:340:ARG:NH1	3:C:232:GLU:OE1	2.52	0.42
2:B:232:PHE:CD1	2:B:273:GLU:HG2	2.54	0.42
2:B:261:GLU:HA	2:B:264:MET:HE3	2.02	0.42
3:C:21:LEU:HD12	3:C:21:LEU:HA	1.81	0.42
1:A:441:LYS:NZ	1:A:444:GLN:OE1	2.45	0.42
1:A:387:LEU:H	1:A:387:LEU:HG	1.74	0.42
1:A:353[A]:LEU:HB3	1:A:411:MET:HB3	2.01	0.41
3:C:182:LYS:O	3:C:186:GLN:HG3	2.20	0.41
1:A:232:LYS:HD3	2:B:149:ASN:ND2	2.35	0.41
1:A:231:ILE:O	1:A:235:GLN:HG3	2.19	0.41
2:B:60:LEU:HD22	3:C:255:ILE:HD11	2.02	0.41
3:C:49:GLN:HG3	3:C:53:ARG:NH1	2.32	0.41
3:C:55:TYR:O	3:C:59:TYR:HB3	2.21	0.40
3:C:143:LEU:O	3:C:147:ILE:HG13	2.21	0.40
1:A:305:ARG:HD2	1:A:341:VAL:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:ARG:HH11	3:C:240:ARG:HG2	1.87	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	309/355 (87%)	299 (97%)	9 (3%)	1 (0%)	41 26
2	B	313/325 (96%)	311 (99%)	2 (1%)	0	100 100
3	C	249/296 (84%)	241 (97%)	8 (3%)	0	100 100
All	All	871/976 (89%)	851 (98%)	19 (2%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	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	292/323 (90%)	287 (98%)	5 (2%)	60 47
2	B	295/303 (97%)	293 (99%)	2 (1%)	84 79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	246/284 (87%)	244 (99%)	2 (1%)	81 76
All	All	833/910 (92%)	824 (99%)	9 (1%)	76 65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	A	277	GLN
1	A	451[A]	CYS
1	A	451[B]	CYS
1	A	474	LYS
2	B	210	LYS
2	B	301	ARG
3	C	7	ARG
3	C	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	282	GLN
1	A	316	ASN
1	A	382	GLN
1	A	454	GLN
1	A	465	GLN
2	B	37	GLN
2	B	71	HIS
2	B	125	ASN
2	B	193	HIS
2	B	250	HIS
3	C	57	HIS
3	C	186	GLN
3	C	223	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FLC	A	601	-	12,12,12	1.12	0	17,17,17	1.26	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLC	A	601	-	-	0/16/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	FLC	OB2-CBC-CB	2.97	118.84	113.14
4	A	601	FLC	OG2-CGC-OG1	-2.06	118.03	123.33
4	A	601	FLC	OG2-CGC-CG	2.03	120.77	114.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	304/355 (85%)	0.23	26 (8%) 10 10	16, 32, 58, 77	0
2	B	310/325 (95%)	-0.08	5 (1%) 72 72	13, 22, 38, 56	0
3	C	250/296 (84%)	0.68	48 (19%) 1 1	16, 41, 80, 93	0
All	All	864/976 (88%)	0.25	79 (9%) 9 8	13, 29, 68, 93	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	270	THR	5.9
1	A	276	VAL	5.1
3	C	53	ARG	5.1
3	C	148	HIS	4.7
3	C	6	ALA	4.7
3	C	57	HIS	4.6
3	C	56	ARG	4.5
3	C	8	LEU	4.3
1	A	334	ARG	4.2
3	C	152	THR	4.1
3	C	272	ASP	3.9
1	A	479	VAL	3.9
3	C	156	HIS	3.8
3	C	5	GLU	3.7
1	A	333	SER	3.7
1	A	422	THR	3.6
3	C	9	GLN	3.6
1	A	191	GLU	3.6
1	A	275	GLU	3.5
3	C	220[A]	GLN	3.5
3	C	221	PRO	3.3
3	C	19	LYS	3.2
1	A	273	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	21	LEU	3.2
1	A	277	GLN	3.2
3	C	157	THR	3.1
3	C	58	HIS	3.1
3	C	49	GLN	3.1
1	A	367	CYS	3.1
3	C	11	ILE	3.0
1	A	274	LYS	3.0
1	A	474	LYS	3.0
1	A	431[A]	GLU	3.0
3	C	54	ASN	2.9
3	C	7	ARG	2.9
3	C	179	LYS	2.9
3	C	87	ARG	2.9
3	C	149	TYR	2.8
3	C	145	LYS	2.8
3	C	158	PRO	2.7
1	A	434	LYS	2.7
3	C	155	THR	2.7
1	A	272	LEU	2.6
3	C	12	GLN	2.6
3	C	103	THR	2.6
3	C	50	PHE	2.6
1	A	368	GLY	2.6
2	B	272	PRO	2.6
3	C	218	GLN	2.6
3	C	271[A]	THR	2.5
1	A	370	LEU	2.5
1	A	426	VAL	2.5
1	A	423	THR	2.4
1	A	365	TRP	2.4
2	B	33	ARG	2.4
3	C	106	LEU	2.3
3	C	51	TYR	2.3
1	A	435	SER	2.3
3	C	159	SER	2.3
3	C	20	THR	2.3
3	C	215	PRO	2.2
1	A	290	LEU	2.2
1	A	470	LYS	2.2
3	C	142	ASP	2.2
2	B	271	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	480	LEU	2.2
3	C	48	ILE	2.2
1	A	371	LEU	2.2
2	B	199	ILE	2.1
3	C	68	ASP	2.1
2	B	157	VAL	2.1
1	A	220	ARG	2.1
3	C	81	VAL	2.1
3	C	92	LEU	2.1
3	C	178	THR	2.0
3	C	91	ASN	2.0
3	C	16	ASN	2.0
3	C	59	TYR	2.0
3	C	90	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FLC	A	601	13/13	0.92	0.15	21,33,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.