



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 04:10 PM EST

PDB ID : 5Z7H
Title : Crystal structure of CcpE regulatory domain in citrate-bound form from *Staphylococcus aureus*
Authors : Chen, J.; Wang, L.; Shang, F.; Xu, Y.
Deposited on : 2018-01-28
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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

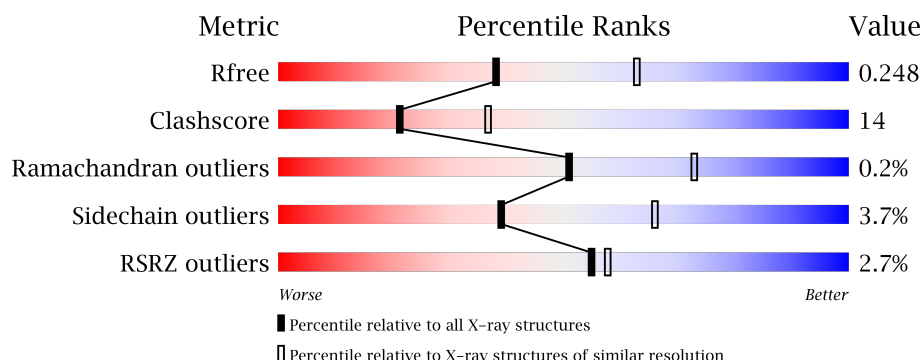
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 ≥ 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	288	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>13%</div> <div>•</div> <div>33%</div> </div> </div>
1	B	288	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>16%</div> <div>•</div> <div>32%</div> </div> </div>
1	C	288	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>11%</div> <div>•</div> <div>33%</div> </div> </div>
1	D	288	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>12%</div> <div>•</div> <div>32%</div> </div> </div>
1	E	288	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>8%</div> <div>•</div> <div>33%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	288	<div> <div>%</div> <div> <div>58%</div> <div>9%</div> <div>33%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	A	301	-	-	X	X
2	FLC	D	301	-	-	X	X

2 Entry composition [i](#)

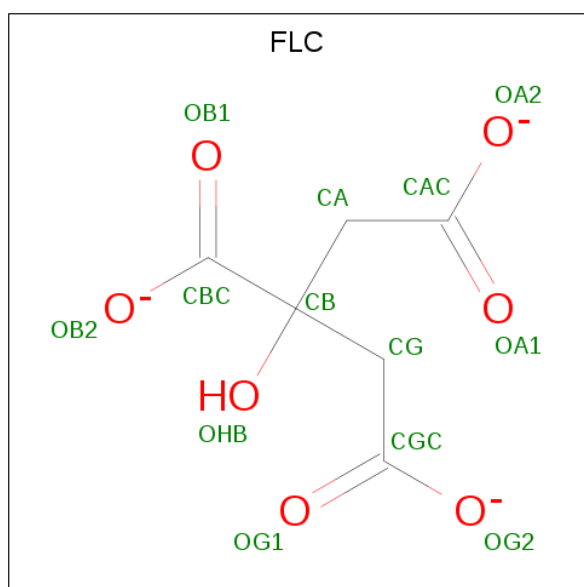
There are 3 unique types of molecules in this entry. The entry contains 19674 atoms, of which 9070 are hydrogens and 0 are deuteriums.

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 LysR family transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	193	Total	C	H	N	O	S	0	0	0
			3037	988	1498	246	295	10			
1	B	196	Total	C	H	N	O	S	0	0	0
			3078	1001	1516	254	297	10			
1	C	193	Total	C	H	N	O	S	0	0	0
			3038	989	1496	245	298	10			
1	D	197	Total	C	H	N	O	S	0	0	0
			3116	1010	1538	257	301	10			
1	E	194	Total	C	H	N	O	S	0	0	0
			3031	988	1492	246	295	10			
1	F	194	Total	C	H	N	O	S	0	0	0
			3047	992	1500	246	299	10			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 18	C 6	H 5	O 7	0	0
2	B	1	Total 18	C 6	H 5	O 7	0	0
2	C	1	Total 18	C 6	H 5	O 7	0	0
2	D	1	Total 18	C 6	H 5	O 7	0	0
2	E	1	Total 18	C 6	H 5	O 7	0	0
2	F	1	Total 18	C 6	H 5	O 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	206	Total 206	O 206	0	0
3	B	207	Total 207	O 207	0	0
3	C	230	Total 230	O 230	0	0
3	D	182	Total 182	O 182	0	0
3	E	190	Total 190	O 190	0	0
3	F	204	Total 204	O 204	0	0

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.

- Chain B:
-
- 2% 50% 16% 32%
- | Label | Color |
|-------|--------|
| GLY | Grey |
| THR | Grey |
| MET | Grey |
| LYS | Grey |
| ILE | Grey |
| ASP | Grey |
| GLU | Grey |
| HIS | Grey |
| ARG | Grey |
| ALA | Grey |
| ASP | Grey |
| MET | Grey |
| LEU | Grey |
| LYS | Grey |
| THR | Grey |
| GLU | Grey |
| ASP | Grey |
| ARG | Grey |
| ALA | Grey |
| GLN | Grey |
| ALA | Grey |
| HIS | Grey |
| ILE | Grey |
| THR | Grey |
| GLY | Grey |
| E88 | Orange |
| I93 | Yellow |
| S94 | Green |
| I95 | Yellow |
| G96 | Yellow |
| S99 | Yellow |
| L100 | Orange |
| Q103 | Yellow |
| Q116 | Yellow |
| V124 | Yellow |
| Q125 | Yellow |
| S128 | Yellow |
| T129 | Yellow |
| F130 | Green |
| Q131 | Yellow |
| I132 | Yellow |
| K133 | Yellow |
| V141 | Yellow |
| M142 | Yellow |
| R145 | Orange |
| G146 | Green |
| N147 | Yellow |
| M151 | Yellow |
| D160 | Orange |
| K168 | Red |
| ASN | Grey |
| ARG | Grey |
| R171 | Red |
| D172 | Red |
| D173 | Red |
| V174 | Green |
| T175 | Yellow |
| Y188 | Yellow |
| I192 | Yellow |
| K193 | Green |
| Q194 | Yellow |
| N199 | Yellow |
| L200 | Grey |
| Q202 | Yellow |
| E205 | Yellow |
| Q212 | Yellow |
| G225 | Yellow |
| I228 | Yellow |
| E231 | Yellow |
| K235 | Yellow |
| E240 | Red |
| E243 | Yellow |
| I249 | Yellow |
| D250 | Red |
| N251 | Red |
| E252 | Red |
| I255 | Yellow |
| R256 | Yellow |
| L267 | Yellow |
| V272 | Yellow |
| D273 | Yellow |
| M279 | Yellow |
| A280 | Yellow |
| S281 | Yellow |
| Q285 | Yellow |
| P286 | Yellow |
| LYS | Grey |
| ALA | Grey |

- Chain C: 

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.79 Å 111.66 Å 152.97 Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	31.89 – 2.50 33.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (31.89-2.50) 92.1 (33.05-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.95 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.196 , 0.247 0.196 , 0.248	Depositor DCC
R_{free} test set	962 reflections (1.70%)	DCC
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19674	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.45 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3624e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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](#)

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	0.66	1/1572 (0.1%)	0.75	3/2137 (0.1%)
1	B	0.64	0/1594	0.73	1/2164 (0.0%)
1	C	0.69	0/1575	0.70	0/2141
1	D	0.74	3/1611 (0.2%)	0.71	0/2187
1	E	0.65	0/1572	0.70	1/2138 (0.0%)
1	F	0.65	0/1580	0.68	0/2148
All	All	0.67	4/9504 (0.0%)	0.71	5/12915 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	GLU	CD-OE2	6.67	1.32	1.25
1	D	252	GLU	CD-OE1	6.64	1.32	1.25
1	D	240	GLU	CD-OE2	5.38	1.31	1.25
1	A	211	ASP	CB-CG	-5.05	1.41	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	145	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	211	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	145	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	211	ASP	CB-CA-C	-5.05	100.30	110.40

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	1539	1498	1503	48	0
1	B	1562	1516	1524	57	0
1	C	1542	1496	1503	44	1
1	D	1578	1538	1546	39	0
1	E	1539	1492	1497	30	0
1	F	1547	1500	1505	33	0
2	A	13	5	5	5	0
2	B	13	5	5	3	0
2	C	13	5	5	0	0
2	D	13	5	5	6	0
2	E	13	5	5	1	0
2	F	13	5	5	3	0
3	A	206	0	0	39	4
3	B	207	0	0	36	8
3	C	230	0	0	31	7
3	D	182	0	0	25	1
3	E	190	0	0	23	3
3	F	204	0	0	25	6
All	All	10604	9070	9108	252	16

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 14.

All (252) 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:116:GLN:NE2	3:B:401:HOH:O	1.69	1.19
1:A:209:THR:O	3:A:401:HOH:O	1.66	1.12
1:E:116:GLN:NE2	3:E:401:HOH:O	1.96	0.98
1:F:129:THR:O	3:F:401:HOH:O	1.82	0.97
1:B:251:ASN:CA	1:B:252:GLU:HB2	1.97	0.94
1:A:283:VAL:HG12	3:A:538:HOH:O	1.68	0.94
1:F:116:GLN:NE2	3:F:402:HOH:O	2.00	0.93
1:A:192:ILE:HD11	3:A:467:HOH:O	1.67	0.92
1:B:251:ASN:N	1:B:252:GLU:HB2	1.83	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:GLU:N	3:F:403:HOH:O	2.02	0.91
1:A:211:ASP:OD2	1:B:125:GLN:NE2	2.07	0.88
1:E:100:LEU:HD22	3:E:576:HOH:O	1.73	0.87
1:C:122:ILE:O	3:C:401:HOH:O	1.92	0.86
1:E:211:ASP:OD2	1:F:125:GLN:NE2	2.09	0.85
1:C:129:THR:HG22	3:C:432:HOH:O	1.77	0.84
1:A:94:SER:HB3	3:A:415:HOH:O	1.77	0.83
1:A:132:ILE:HG23	3:A:535:HOH:O	1.77	0.82
1:D:100:LEU:HD22	3:D:575:HOH:O	1.79	0.81
1:D:215:THR:OG1	3:D:401:HOH:O	1.99	0.80
2:B:301:FLC:OA2	3:B:402:HOH:O	1.98	0.80
1:E:284:GLU:O	3:E:402:HOH:O	2.00	0.80
1:D:219:MET:SD	3:D:579:HOH:O	2.39	0.79
1:A:140:HIS:CG	3:A:415:HOH:O	2.35	0.79
1:A:132:ILE:HD12	3:A:535:HOH:O	1.82	0.78
1:B:128:SER:O	3:B:403:HOH:O	2.01	0.78
1:C:211:ASP:O	3:C:402:HOH:O	2.02	0.78
1:B:279:MET:HE2	3:B:543:HOH:O	1.85	0.77
1:A:129:THR:OG1	3:A:402:HOH:O	2.02	0.77
1:A:210:VAL:HA	3:A:401:HOH:O	1.84	0.76
1:A:279:MET:SD	3:A:570:HOH:O	2.42	0.76
1:E:183:GLN:NE2	3:E:407:HOH:O	2.19	0.75
1:C:126:VAL:HG21	3:D:401:HOH:O	1.87	0.74
1:B:103:GLN:NE2	3:B:405:HOH:O	2.18	0.73
1:C:129:THR:OG1	3:C:403:HOH:O	2.05	0.73
1:C:138:ASP:OD1	3:C:404:HOH:O	2.07	0.73
1:C:88:GLU:N	3:C:408:HOH:O	2.22	0.72
1:D:129:THR:OG1	3:D:402:HOH:O	2.06	0.71
1:C:100:LEU:HD22	3:C:612:HOH:O	1.90	0.71
1:F:129:THR:OG1	3:F:404:HOH:O	2.09	0.71
1:A:284:GLU:O	3:A:403:HOH:O	2.08	0.70
1:B:131:GLN:HB2	3:B:403:HOH:O	1.90	0.70
1:A:133:LYS:NZ	3:A:412:HOH:O	2.24	0.70
1:E:88:GLU:OE1	3:E:403:HOH:O	2.10	0.68
2:F:301:FLC:OG1	2:F:301:FLC:OHB	2.12	0.68
1:A:152:LEU:O	3:A:404:HOH:O	2.12	0.68
1:C:285:GLN:HA	3:C:412:HOH:O	1.94	0.67
1:D:100:LEU:HD21	1:D:145:ARG:NE	2.10	0.67
1:B:192:ILE:HD12	3:B:555:HOH:O	1.92	0.67
1:E:145:ARG:NH2	1:E:160:ASP:OD2	2.28	0.67
1:D:160:ASP:OD1	3:D:403:HOH:O	2.12	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLU:OE2	3:B:404:HOH:O	2.14	0.66
1:B:279:MET:HB2	3:B:543:HOH:O	1.96	0.66
1:A:140:HIS:ND1	3:A:415:HOH:O	2.29	0.66
1:A:99:SER:HB2	3:A:460:HOH:O	1.94	0.66
1:E:129:THR:OG1	3:E:404:HOH:O	2.13	0.66
1:F:192:ILE:HD12	3:F:566:HOH:O	1.95	0.66
1:D:231:GLU:OE1	3:D:404:HOH:O	2.14	0.65
1:A:185:ASP:HB2	3:A:466:HOH:O	1.98	0.64
1:A:261:SER:OG	3:A:405:HOH:O	2.14	0.64
1:E:125:GLN:NE2	1:F:211:ASP:OD2	2.31	0.63
2:A:301:FLC:OG1	3:A:406:HOH:O	2.15	0.63
1:D:129:THR:HG22	1:D:133:LYS:HE2	1.80	0.63
1:B:251:ASN:CA	1:B:252:GLU:CB	2.70	0.63
1:A:279:MET:HB3	3:A:570:HOH:O	1.99	0.62
1:F:202:GLN:HB2	3:F:417:HOH:O	1.99	0.62
1:B:145:ARG:NH2	1:B:160:ASP:OD2	2.33	0.61
1:C:108:GLU:OE2	3:C:405:HOH:O	2.16	0.61
1:C:233:MET:HG3	3:C:612:HOH:O	1.99	0.61
1:A:132:ILE:HG22	1:A:142:MET:HE3	1.81	0.60
1:A:282:PHE:HD2	3:A:538:HOH:O	1.84	0.60
1:E:141:VAL:HB	3:E:574:HOH:O	2.01	0.60
1:F:268:GLN:OE1	3:F:405:HOH:O	2.17	0.60
1:A:231:GLU:OE1	3:A:407:HOH:O	2.16	0.59
1:F:133:LYS:HE2	3:F:401:HOH:O	2.03	0.59
1:C:129:THR:HG23	1:C:144:THR:HB	1.85	0.59
1:F:131:GLN:OE1	3:F:406:HOH:O	2.17	0.58
1:D:218:GLU:OE1	3:D:405:HOH:O	2.17	0.58
1:B:151:ASN:ND2	3:B:417:HOH:O	2.35	0.58
1:A:140:HIS:N	3:A:415:HOH:O	2.37	0.58
2:A:301:FLC:OHB	2:A:301:FLC:OA2	2.16	0.58
1:B:251:ASN:HA	1:B:252:GLU:HB2	1.85	0.58
1:D:246:LYS:HE2	1:D:253:PRO:HB3	1.83	0.58
1:B:267:LEU:HD23	3:B:422:HOH:O	2.03	0.58
1:B:267:LEU:HA	3:B:422:HOH:O	2.03	0.58
1:B:251:ASN:HA	1:B:252:GLU:CB	2.34	0.58
1:E:212:GLN:OE1	3:E:405:HOH:O	2.17	0.57
1:D:233:MET:HG3	3:D:575:HOH:O	2.04	0.57
1:C:285:GLN:NE2	3:C:412:HOH:O	2.24	0.57
1:C:211:ASP:C	3:C:402:HOH:O	2.41	0.56
1:D:122:ILE:CG1	3:D:485:HOH:O	2.53	0.56
1:B:205:HIS:O	3:B:406:HOH:O	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HB	3:D:484:HOH:O	2.05	0.56
1:B:128:SER:N	3:B:403:HOH:O	2.39	0.56
1:B:141:VAL:HB	3:B:585:HOH:O	2.04	0.56
1:D:129:THR:OG1	2:D:301:FLC:OG2	2.22	0.56
1:B:273:ASP:N	3:B:422:HOH:O	2.38	0.55
2:A:301:FLC:CGC	3:A:406:HOH:O	2.53	0.55
1:A:212:GLN:HE22	1:B:212:GLN:HE22	1.54	0.55
1:B:285:GLN:HA	3:B:558:HOH:O	2.07	0.55
1:E:129:THR:HG22	1:E:133:LYS:HE2	1.88	0.55
1:F:183:GLN:O	3:F:407:HOH:O	2.18	0.55
1:B:280:ALA:HB3	3:B:428:HOH:O	2.07	0.54
1:B:235:LYS:NZ	3:B:424:HOH:O	2.40	0.54
1:E:205:HIS:O	3:E:406:HOH:O	2.18	0.54
1:E:212:GLN:HE22	1:F:212:GLN:HE22	1.55	0.54
1:D:122:ILE:HG13	3:D:485:HOH:O	2.08	0.53
1:E:112:LEU:HD22	3:E:430:HOH:O	2.08	0.53
2:B:301:FLC:OHB	2:B:301:FLC:OA2	2.24	0.53
1:F:286:PRO:C	3:F:415:HOH:O	2.46	0.53
1:A:139:TYR:CE2	3:A:535:HOH:O	2.54	0.53
1:C:130:GLU:HA	3:C:432:HOH:O	2.09	0.52
1:D:132:ILE:HG22	1:D:142:MET:SD	2.49	0.52
1:D:100:LEU:HD23	2:D:301:FLC:HA1	1.90	0.52
1:F:202:GLN:CB	3:F:417:HOH:O	2.57	0.52
1:A:157:LEU:HD22	1:A:283:VAL:HG11	1.91	0.52
1:B:286:PRO:HD2	3:B:558:HOH:O	2.10	0.52
1:E:103:GLN:HE22	1:F:103:GLN:HE22	1.57	0.52
1:A:274:SER:O	3:A:408:HOH:O	2.19	0.52
1:B:281:SER:N	3:B:428:HOH:O	2.42	0.52
1:C:133:LYS:HE2	3:C:432:HOH:O	2.09	0.52
1:E:100:LEU:HD13	3:E:576:HOH:O	2.10	0.52
3:A:401:HOH:O	1:B:124:VAL:N	2.04	0.51
1:C:129:THR:C	3:C:432:HOH:O	2.49	0.51
1:D:129:THR:HG1	2:D:301:FLC:CGC	2.23	0.51
1:B:225:GLY:O	3:B:408:HOH:O	2.19	0.51
1:F:211:ASP:OD1	3:F:408:HOH:O	2.19	0.51
1:E:235:LYS:NZ	3:E:422:HOH:O	2.39	0.51
1:F:129:THR:C	3:F:401:HOH:O	2.41	0.51
1:B:99:SER:HB3	3:B:509:HOH:O	2.10	0.51
1:B:272:VAL:HG12	3:B:422:HOH:O	2.10	0.51
1:D:209:THR:HG21	3:D:519:HOH:O	2.10	0.50
1:A:192:ILE:HG23	1:A:228:ILE:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:THR:HG22	1:B:133:LYS:HE2	1.93	0.50
1:A:266:MET:HE3	3:A:478:HOH:O	2.11	0.50
1:B:124:VAL:O	3:B:407:HOH:O	2.19	0.50
1:A:256:ARG:NH1	3:A:422:HOH:O	2.40	0.50
1:C:236:ASN:ND2	3:C:416:HOH:O	2.28	0.50
1:A:100:LEU:C	1:A:100:LEU:HD23	2.33	0.49
1:A:275:PHE:HA	3:A:408:HOH:O	2.12	0.49
3:A:413:HOH:O	1:B:103:GLN:HG3	2.12	0.49
1:C:212:GLN:HE22	1:D:212:GLN:HE22	1.58	0.49
1:F:133:LYS:HB2	3:F:401:HOH:O	2.12	0.49
1:A:211:ASP:HB2	3:B:483:HOH:O	2.13	0.49
1:D:192:ILE:HG23	1:D:228:ILE:HD12	1.93	0.49
1:B:99:SER:CB	3:B:509:HOH:O	2.61	0.49
1:C:100:LEU:HD21	1:C:145:ARG:NE	2.27	0.49
1:D:236:ASN:ND2	3:D:425:HOH:O	2.45	0.48
1:D:252:GLU:HG3	3:D:429:HOH:O	2.13	0.48
2:E:301:FLC:CAC	3:E:488:HOH:O	2.62	0.48
1:C:100:LEU:HB2	3:C:612:HOH:O	2.14	0.48
1:C:210:VAL:HG12	1:D:124:VAL:HB	1.95	0.48
1:F:116:GLN:OE1	3:F:409:HOH:O	2.20	0.48
1:F:133:LYS:HD3	1:F:149:VAL:HG22	1.96	0.48
1:A:174:VAL:HA	1:A:177:LEU:HD22	1.95	0.48
1:B:147:ASN:ND2	3:B:432:HOH:O	2.47	0.47
1:D:199:ASN:O	1:D:200:LEU:HD23	2.14	0.47
1:E:192:ILE:HG23	1:E:228:ILE:HD12	1.97	0.47
1:D:268:GLN:OE1	3:D:408:HOH:O	2.20	0.47
1:F:118:PRO:O	3:F:410:HOH:O	2.20	0.47
1:D:129:THR:CB	2:D:301:FLC:OG2	2.63	0.47
1:D:253:PRO:HG2	3:D:570:HOH:O	2.13	0.47
1:A:279:MET:CG	3:A:570:HOH:O	2.62	0.47
1:D:188:TYR:CE2	1:D:256:ARG:CD	2.98	0.47
1:C:133:LYS:CE	3:C:432:HOH:O	2.63	0.46
1:C:209:THR:HG21	3:C:517:HOH:O	2.14	0.46
1:F:127:GLY:N	3:F:429:HOH:O	2.48	0.46
1:C:281:SER:HB2	3:C:482:HOH:O	2.14	0.46
1:B:132:ILE:HG22	1:B:142:MET:SD	2.56	0.46
1:C:100:LEU:CB	3:C:612:HOH:O	2.64	0.46
1:E:141:VAL:CB	3:E:574:HOH:O	2.62	0.46
1:E:92:THR:HG22	3:E:562:HOH:O	2.16	0.46
1:A:150:MET:HA	3:A:508:HOH:O	2.15	0.46
1:B:250:ASP:N	1:B:251:ASN:CB	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:VAL:C	3:B:422:HOH:O	2.55	0.46
1:D:160:ASP:O	1:D:255:ILE:HA	2.16	0.46
1:E:141:VAL:CG1	3:E:574:HOH:O	2.64	0.45
1:F:214:ALA:HB3	3:F:413:HOH:O	2.16	0.45
1:A:205:HIS:O	3:A:409:HOH:O	2.21	0.45
1:C:132:ILE:HG22	1:C:142:MET:SD	2.56	0.45
1:F:205:HIS:O	3:F:411:HOH:O	2.21	0.45
1:B:192:ILE:HG23	1:B:228:ILE:HD12	1.97	0.45
2:F:301:FLC:HG1	3:F:492:HOH:O	2.16	0.45
1:B:88:GLU:HG3	3:B:552:HOH:O	2.16	0.45
1:B:95:ILE:HG12	3:B:585:HOH:O	2.15	0.45
1:B:273:ASP:CA	3:B:422:HOH:O	2.64	0.45
1:A:96:GLY:O	1:A:142:MET:HA	2.17	0.45
1:F:100:LEU:C	1:F:100:LEU:HD23	2.37	0.45
1:C:261:SER:OG	3:C:406:HOH:O	2.21	0.45
1:B:267:LEU:CD2	3:B:422:HOH:O	2.63	0.45
1:C:182:PHE:HB2	3:C:402:HOH:O	2.17	0.45
1:C:233:MET:CG	3:C:612:HOH:O	2.60	0.45
1:B:273:ASP:HA	3:B:422:HOH:O	2.16	0.44
1:C:128:SER:OG	1:C:131:GLN:HB2	2.16	0.44
1:D:129:THR:N	2:D:301:FLC:OG2	2.39	0.44
1:D:205:HIS:O	3:D:407:HOH:O	2.20	0.44
1:D:100:LEU:HD21	1:D:145:ARG:CZ	2.47	0.44
1:D:208:ILE:HG21	3:D:579:HOH:O	2.16	0.44
1:F:129:THR:H	2:F:301:FLC:CGC	2.30	0.44
1:B:160:ASP:O	1:B:255:ILE:HA	2.17	0.44
1:B:93:ILE:HD11	3:B:585:HOH:O	2.17	0.44
1:C:142:MET:HE2	3:C:555:HOH:O	2.18	0.44
1:B:249:ILE:O	1:B:252:GLU:HB3	2.17	0.43
1:E:116:GLN:NE2	3:E:430:HOH:O	2.51	0.43
1:B:96:GLY:O	1:B:142:MET:HA	2.18	0.43
1:F:126:VAL:HG23	3:F:429:HOH:O	2.17	0.43
1:D:114:ASN:ND2	3:D:417:HOH:O	2.29	0.43
1:D:175:THR:HB	1:D:202:GLN:HG3	1.99	0.43
1:D:252:GLU:OE2	3:D:409:HOH:O	2.21	0.43
2:B:301:FLC:HA1	3:B:461:HOH:O	2.18	0.43
1:C:284:GLU:O	3:C:407:HOH:O	2.21	0.43
1:F:130:GLU:N	1:F:130:GLU:OE1	2.43	0.43
1:E:209:THR:HG21	3:E:530:HOH:O	2.18	0.42
1:D:213:VAL:HG11	3:D:575:HOH:O	2.18	0.42
1:A:213:VAL:HG23	2:A:301:FLC:CG	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD23	1:B:100:LEU:C	2.39	0.42
1:C:99:SER:HA	1:C:126:VAL:HG13	2.00	0.42
1:E:268:GLN:OE1	3:E:408:HOH:O	2.20	0.42
1:E:129:THR:HA	3:E:404:HOH:O	2.19	0.42
1:E:217:LYS:NZ	3:E:434:HOH:O	2.52	0.42
1:A:188:TYR:CZ	1:A:256:ARG:HD3	2.55	0.42
1:A:283:VAL:CG1	3:A:538:HOH:O	2.44	0.42
1:A:99:SER:CB	3:A:460:HOH:O	2.60	0.42
1:B:199:ASN:O	1:B:200:LEU:HD23	2.20	0.42
1:A:140:HIS:CE1	3:A:415:HOH:O	2.69	0.42
1:C:182:PHE:HB2	3:C:495:HOH:O	2.19	0.42
1:F:133:LYS:CG	3:F:401:HOH:O	2.68	0.42
1:C:281:SER:HB2	3:C:413:HOH:O	2.20	0.41
1:D:194:GLN:HB3	3:D:511:HOH:O	2.20	0.41
1:B:188:TYR:CE2	1:B:256:ARG:HD3	2.56	0.41
1:C:133:LYS:HD2	1:C:149:VAL:HG13	2.01	0.41
1:F:130:GLU:HA	3:F:401:HOH:O	2.20	0.41
1:A:249:ILE:HD13	3:A:523:HOH:O	2.20	0.41
1:C:188:TYR:CZ	1:C:256:ARG:HD3	2.56	0.41
1:B:188:TYR:CZ	1:B:256:ARG:HD3	2.55	0.41
1:B:168:LYS:HA	1:B:243:GLU:HG3	2.02	0.41
1:C:188:TYR:CE2	1:C:256:ARG:CD	3.03	0.41
1:A:210:VAL:HG12	1:B:124:VAL:HB	2.03	0.41
1:B:188:TYR:CE2	1:B:256:ARG:CD	3.03	0.41
1:C:213:VAL:CG2	3:C:480:HOH:O	2.69	0.41
1:E:100:LEU:HD21	1:E:145:ARG:HD2	2.03	0.41
1:E:92:THR:CG2	3:E:562:HOH:O	2.69	0.41
1:F:100:LEU:HD23	1:F:101:ILE:N	2.36	0.41
1:A:278:LEU:HB2	3:A:408:HOH:O	2.20	0.40
1:C:127:GLY:HA2	3:C:443:HOH:O	2.21	0.40
2:D:301:FLC:HG2	3:D:549:HOH:O	2.21	0.40
1:A:279:MET:CB	3:A:570:HOH:O	2.66	0.40
1:E:213:VAL:HG23	3:E:447:HOH:O	2.20	0.40
1:F:133:LYS:HG3	3:F:401:HOH:O	2.20	0.40
1:A:213:VAL:HG23	2:A:301:FLC:HG1	2.04	0.40
1:C:211:ASP:HB2	3:C:510:HOH:O	2.21	0.40
1:C:96:GLY:O	1:C:142:MET:HA	2.21	0.40
1:D:233:MET:CG	3:D:575:HOH:O	2.67	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:582:HOH:O	3:E:573:HOH:O[2_755]	1.88	0.32
3:B:580:HOH:O	3:C:590:HOH:O[1_655]	1.90	0.30
3:B:445:HOH:O	3:C:497:HOH:O[1_655]	1.93	0.27
3:B:605:HOH:O	3:B:607:HOH:O[2_856]	1.94	0.26
3:B:510:HOH:O	3:F:530:HOH:O[4_755]	1.97	0.23
1:C:277:ASN:O	3:E:401:HOH:O[2_755]	2.03	0.17
3:B:520:HOH:O	3:F:519:HOH:O[4_755]	2.05	0.15
3:A:602:HOH:O	3:C:629:HOH:O[3_555]	2.08	0.12
3:D:552:HOH:O	3:E:542:HOH:O[4_655]	2.08	0.12
3:A:561:HOH:O	3:C:615:HOH:O[1_655]	2.09	0.11
3:A:587:HOH:O	3:F:527:HOH:O[2_755]	2.09	0.11
3:B:401:HOH:O	3:B:428:HOH:O[2_856]	2.09	0.11
3:B:589:HOH:O	3:C:438:HOH:O[1_655]	2.10	0.10
3:B:520:HOH:O	3:F:530:HOH:O[4_755]	2.11	0.09
3:C:597:HOH:O	3:F:583:HOH:O[4_655]	2.15	0.05
3:A:587:HOH:O	3:F:563:HOH:O[2_755]	2.18	0.02

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	189/288 (66%)	184 (97%)	5 (3%)	0	100	100
1	B	190/288 (66%)	183 (96%)	6 (3%)	1 (0%)	32	53
1	C	189/288 (66%)	183 (97%)	5 (3%)	1 (0%)	32	53
1	D	193/288 (67%)	188 (97%)	5 (3%)	0	100	100
1	E	190/288 (66%)	183 (96%)	7 (4%)	0	100	100
1	F	190/288 (66%)	187 (98%)	3 (2%)	0	100	100
All	All	1141/1728 (66%)	1108 (97%)	31 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	GLN
1	B	252	GLU

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	176/263 (67%)	168 (96%)	8 (4%)	32	56
1	B	177/263 (67%)	168 (95%)	9 (5%)	28	50
1	C	177/263 (67%)	171 (97%)	6 (3%)	42	69
1	D	180/263 (68%)	172 (96%)	8 (4%)	33	57
1	E	175/263 (66%)	174 (99%)	1 (1%)	89	97
1	F	177/263 (67%)	170 (96%)	7 (4%)	36	62
All	All	1062/1578 (67%)	1023 (96%)	39 (4%)	39	66

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	99	SER
1	A	100	LEU
1	A	177	LEU
1	A	235	LYS
1	A	265	SER
1	A	279	MET
1	A	281	SER
1	B	88	GLU
1	B	100	LEU
1	B	160	ASP
1	B	168	LYS
1	B	175	THR
1	B	194	GLN
1	B	202	GLN
1	B	240	GLU
1	B	252	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	88	GLU
1	C	126	VAL
1	C	160	ASP
1	C	175	THR
1	C	211	ASP
1	C	281	SER
1	D	88	GLU
1	D	100	LEU
1	D	160	ASP
1	D	172	ASP
1	D	175	THR
1	D	211	ASP
1	D	240	GLU
1	D	252	GLU
1	E	160	ASP
1	F	88	GLU
1	F	98	SER
1	F	100	LEU
1	F	108	GLU
1	F	160	ASP
1	F	176	LYS
1	F	240	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	212	GLN
1	B	125	GLN
1	C	125	GLN
1	C	212	GLN
1	D	125	GLN
1	D	205	HIS
1	E	103	GLN
1	E	125	GLN
1	F	125	GLN
1	F	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](#)

6 ligands are 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	$\# Z > 2$
2	FLC	A	301	-	3,12,12	2.00	2 (66%)	3,17,17	2.47	1 (33%)
2	FLC	B	301	-	3,12,12	1.52	1 (33%)	3,17,17	1.74	1 (33%)
2	FLC	C	301	-	3,12,12	1.15	0	3,17,17	1.79	1 (33%)
2	FLC	D	301	-	3,12,12	1.71	1 (33%)	3,17,17	0.80	0
2	FLC	E	301	-	3,12,12	1.51	0	3,17,17	1.39	0
2	FLC	F	301	-	3,12,12	1.35	0	3,17,17	1.70	1 (33%)

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
2	FLC	A	301	-	-	0/6/16/16	0/0/0/0
2	FLC	B	301	-	-	0/6/16/16	0/0/0/0
2	FLC	C	301	-	-	0/6/16/16	0/0/0/0
2	FLC	D	301	-	-	0/6/16/16	0/0/0/0
2	FLC	E	301	-	-	0/6/16/16	0/0/0/0
2	FLC	F	301	-	-	0/6/16/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	FLC	CG-CB	-2.56	1.50	1.54
2	A	301	FLC	CA-CB	-2.13	1.51	1.54
2	A	301	FLC	CG-CB	-2.09	1.51	1.54
2	B	301	FLC	CA-CB	-2.09	1.51	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FLC	CB-CA-CAC	-3.85	108.94	114.95
2	C	301	FLC	CB-CA-CAC	-2.77	110.62	114.95
2	B	301	FLC	CB-CA-CAC	-2.69	110.74	114.95
2	F	301	FLC	CB-CG-CGC	-2.46	111.11	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FLC	5	0
2	B	301	FLC	3	0
2	D	301	FLC	6	0
2	E	301	FLC	1	0
2	F	301	FLC	3	0

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	193/288 (67%)	-0.51	4 (2%) 64 66	15, 34, 68, 97	0
1	B	196/288 (68%)	-0.47	7 (3%) 43 45	16, 34, 67, 121	1 (0%)
1	C	193/288 (67%)	-0.51	3 (1%) 72 73	15, 34, 68, 94	0
1	D	197/288 (68%)	-0.45	7 (3%) 43 45	16, 34, 69, 126	1 (0%)
1	E	194/288 (67%)	-0.50	7 (3%) 43 45	17, 33, 70, 100	0
1	F	194/288 (67%)	-0.50	3 (1%) 74 75	16, 34, 72, 111	0
All	All	1167/1728 (67%)	-0.49	31 (2%) 55 58	15, 34, 69, 126	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	ASP	6.5
1	D	201	GLU	4.4
1	D	172	ASP	4.2
1	F	201	GLU	3.8
1	F	250	ASP	3.7
1	E	201	GLU	3.7
1	B	252	GLU	3.4
1	E	250	ASP	3.3
1	E	173	ASP	3.0
1	B	168	LYS	3.0
1	A	201	GLU	3.0
1	D	251	ASN	2.9
1	D	173	ASP	2.9
1	A	175	THR	2.9
1	D	168	LYS	2.8
1	A	250	ASP	2.7
1	C	240	GLU	2.7
1	B	250	ASP	2.7
1	A	240	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	250	ASP	2.6
1	F	240	GLU	2.5
1	C	201	GLU	2.3
1	B	171	ARG	2.2
1	D	240	GLU	2.2
1	E	252	GLU	2.2
1	E	240	GLU	2.2
1	E	202	GLN	2.1
1	D	176	LYS	2.1
1	B	251	ASN	2.1
1	B	240	GLU	2.1
1	E	251	ASN	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	FLC	A	301	13/13	0.78	0.26	4.55	44,68,93,93	0
2	FLC	D	301	13/13	0.78	0.23	2.30	48,65,82,86	0
2	FLC	B	301	13/13	0.78	0.21	1.79	52,68,77,82	0
2	FLC	F	301	13/13	0.83	0.17	1.17	32,54,67,71	0
2	FLC	E	301	13/13	0.92	0.14	0.31	38,50,60,62	0
2	FLC	C	301	13/13	0.89	0.14	0.30	39,48,56,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.