



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 PM UTC

PDB ID : 2XMH / pdb_00002xmh
Title : The X-ray structure of CTP:inositol-1-phosphate cytidylyltransferase from *Archaeoglobus fulgidus*
Authors : Brito, J.A.; Borges, N.; Vornrhein, C.; Santos, H.; Archer, M.
Deposited on : 2010-07-27
Resolution : 2.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

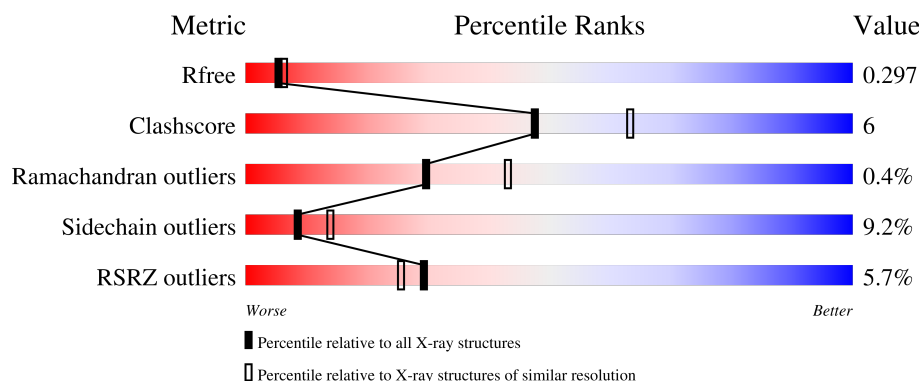
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	232	9% 67% 15% • 16%
1	B	232	11% 66% 15% • 16%
1	C	232	• 65% 19% • 13%
1	D	232	3% 69% 17% • 12%
1	E	232	5% 69% 16% • 12%

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Mol	Chain	Length	Quality of chain
1	F	232	% 71% 12% 14%

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	D	501	-	X	-	-
2	FLC	E	501	-	X	-	-

2 Entry composition [i](#)

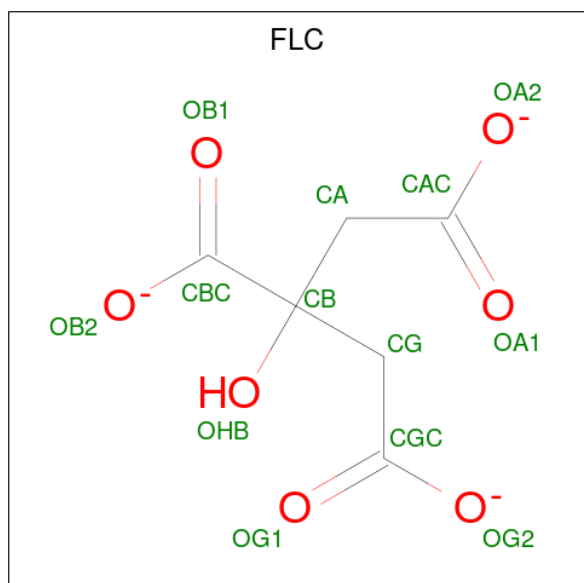
There are 3 unique types of molecules in this entry. The entry contains 9857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	1	0
			1581	1015	272	288	6			
1	B	196	Total	C	N	O	S	0	0	0
			1571	1005	272	288	6			
1	C	201	Total	C	N	O	S	0	0	0
			1600	1022	279	293	6			
1	D	205	Total	C	N	O	S	0	0	0
			1628	1040	284	298	6			
1	E	205	Total	C	N	O	S	0	0	0
			1628	1040	284	298	6			
1	F	200	Total	C	N	O	S	0	1	0
			1606	1030	277	293	6			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		

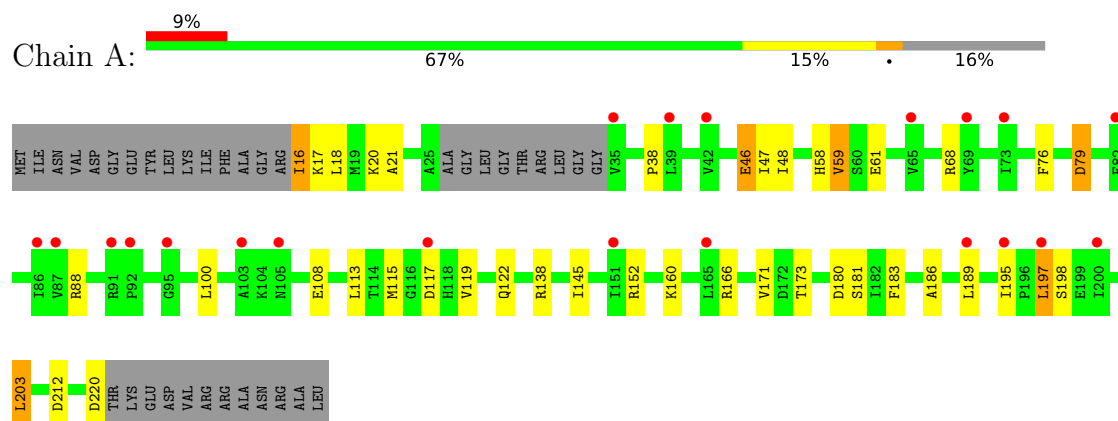
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	26	Total	O	0	0
			26	26		
3	C	51	Total	O	0	0
			51	51		
3	D	31	Total	O	0	0
			31	31		
3	E	22	Total	O	0	0
			22	22		
3	F	42	Total	O	0	0
			42	42		

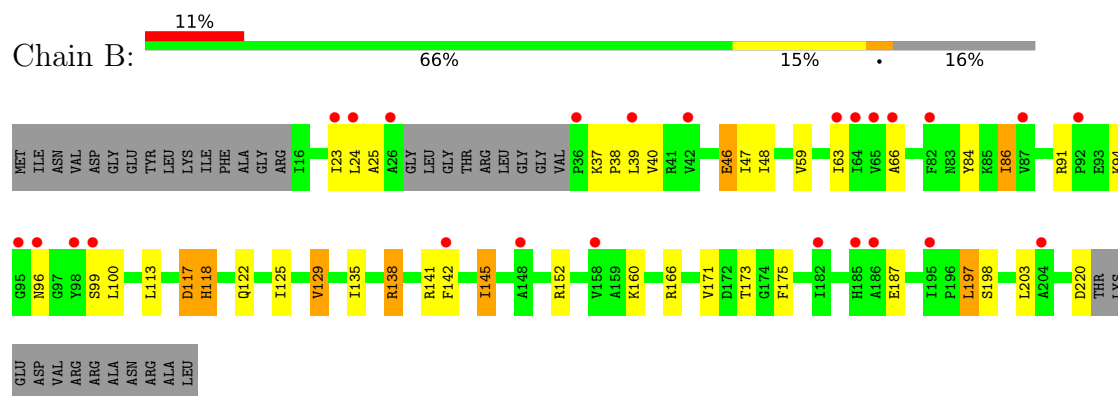
3 Residue-property plots

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.

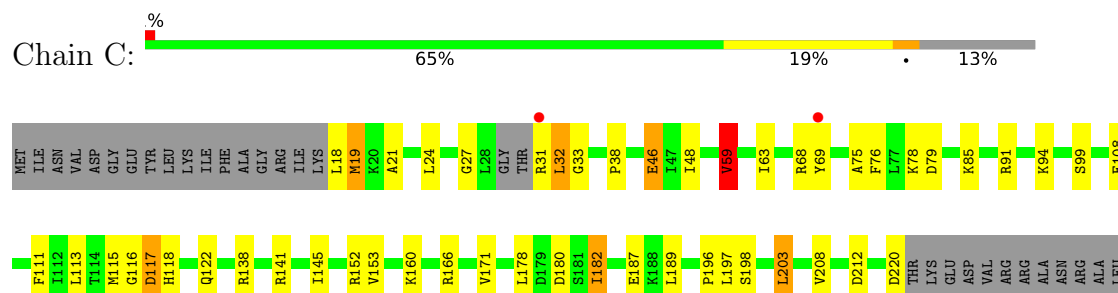
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



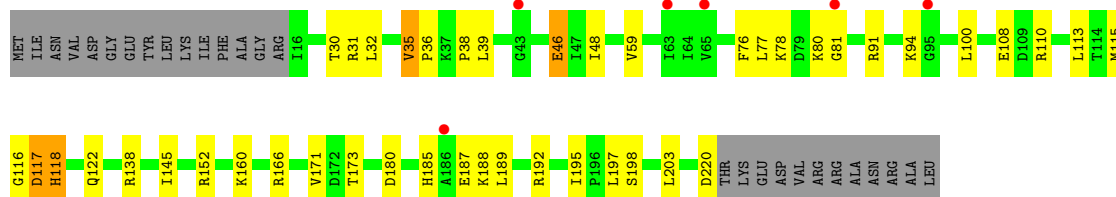
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



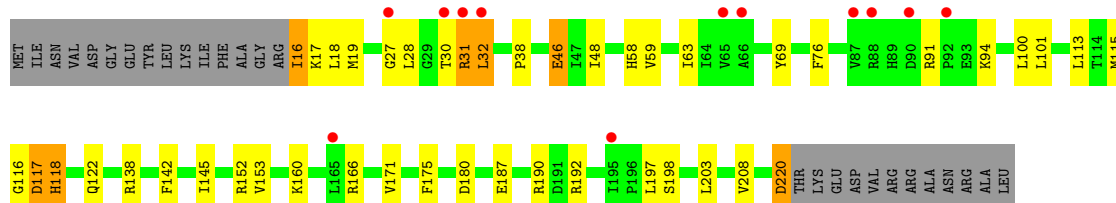
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



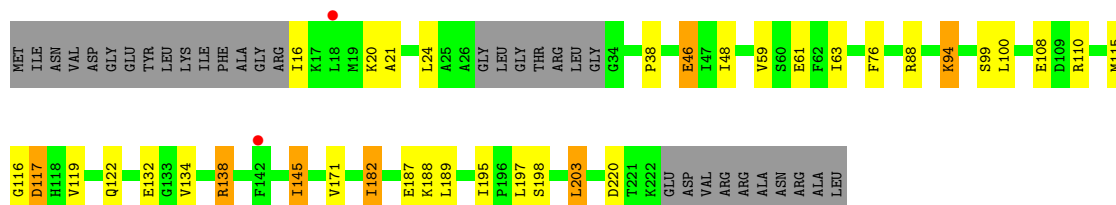
• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



• Molecule 1: CTP-INOSITOL-1-PHOSPHATE CYTIDYLYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.68Å 83.85Å 127.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.14 – 2.40 35.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (35.14-2.40) 69.8 (35.14-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.233 , 0.275 (Not available) , 0.297	Depositor DCC
R_{free} test set	3285 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9857	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.333 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	0.84	0/1612	1.36	6/2170 (0.3%)
1	B	0.87	1/1598 (0.1%)	1.43	10/2150 (0.5%)
1	C	0.89	0/1627	1.36	8/2190 (0.4%)
1	D	0.86	0/1656	1.42	12/2230 (0.5%)
1	E	0.83	0/1656	1.39	10/2230 (0.4%)
1	F	0.93	1/1637 (0.1%)	1.36	6/2203 (0.3%)
All	All	0.87	2/9786 (0.0%)	1.39	52/13173 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	61	GLU	CA-C	-5.16	1.46	1.52
1	B	25	ALA	CA-C	5.02	1.59	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASP	CA-CB-CG	9.39	121.99	112.60
1	D	116	GLY	CA-C-N	8.22	131.96	120.29
1	D	116	GLY	C-N-CA	8.22	131.96	120.29
1	B	117	ASP	CA-C-N	8.17	132.47	120.87
1	B	117	ASP	C-N-CA	8.17	132.47	120.87
1	A	173	THR	N-CA-C	-7.62	97.16	109.96
1	E	116	GLY	CA-C-N	7.56	133.53	120.68
1	E	116	GLY	C-N-CA	7.56	133.53	120.68
1	B	173	THR	N-CA-C	-7.26	99.78	110.52
1	B	118	HIS	N-CA-C	7.21	120.95	110.28
1	E	118	HIS	N-CA-C	7.07	121.35	109.76
1	C	116	GLY	CA-C-N	6.88	136.28	121.64
1	C	116	GLY	C-N-CA	6.88	136.28	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	ARG	N-CA-C	-6.87	104.53	113.12
1	F	122	GLN	CA-C-N	6.83	129.44	120.28
1	F	122	GLN	C-N-CA	6.83	129.44	120.28
1	D	59	VAL	N-CA-C	6.54	117.33	108.17
1	A	59	VAL	N-CA-C	6.48	117.18	108.11
1	C	122	GLN	CA-C-N	6.47	128.96	120.28
1	C	122	GLN	C-N-CA	6.47	128.96	120.28
1	D	77	LEU	N-CA-C	6.45	120.98	113.18
1	B	46	GLU	N-CA-C	6.33	119.85	110.48
1	B	122	GLN	CA-C-N	6.29	128.71	120.28
1	B	122	GLN	C-N-CA	6.29	128.71	120.28
1	D	118	HIS	N-CA-C	6.27	120.29	110.32
1	A	122	GLN	CA-C-N	6.11	128.46	120.28
1	A	122	GLN	C-N-CA	6.11	128.46	120.28
1	A	79	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	122	GLN	CA-C-N	5.79	128.04	120.28
1	D	122	GLN	C-N-CA	5.79	128.04	120.28
1	F	116	GLY	CA-C-N	5.75	132.10	121.52
1	F	116	GLY	C-N-CA	5.75	132.10	121.52
1	E	117	ASP	CA-CB-CG	5.74	118.33	112.60
1	E	122	GLN	CA-C-N	5.62	127.81	120.28
1	E	122	GLN	C-N-CA	5.62	127.81	120.28
1	D	173	THR	N-CA-C	-5.57	101.72	110.36
1	E	27	GLY	CA-C-N	5.57	127.68	120.44
1	E	27	GLY	C-N-CA	5.57	127.68	120.44
1	C	59	VAL	N-CA-CB	-5.56	102.32	111.44
1	E	175	PHE	N-CA-C	5.54	118.12	108.76
1	D	35	VAL	N-CA-C	5.42	114.06	107.61
1	B	86	ILE	N-CA-CB	5.39	117.14	111.00
1	B	59	VAL	N-CA-C	5.32	115.56	108.11
1	D	30	THR	N-CA-C	5.30	117.44	109.23
1	D	35	VAL	CB-CA-C	5.28	115.25	110.13
1	C	63	ILE	CB-CA-C	5.27	118.99	112.45
1	C	19	MET	N-CA-C	5.25	116.81	108.79
1	F	134	VAL	N-CA-CB	5.24	116.24	110.53
1	C	212	ASP	N-CA-C	5.21	118.10	109.46
1	F	117	ASP	N-CA-CB	-5.12	102.65	110.33
1	A	212	ASP	N-CA-C	5.11	117.95	109.46
1	E	59	VAL	N-CA-C	5.08	115.23	108.11

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	1581	0	1610	21	0
1	B	1571	0	1598	27	0
1	C	1600	0	1626	22	0
1	D	1628	0	1661	14	0
1	E	1628	0	1661	23	0
1	F	1606	0	1638	13	0
2	A	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	1	0
3	A	32	0	0	2	0
3	B	26	0	0	4	0
3	C	51	0	0	4	0
3	D	31	0	0	0	0
3	E	22	0	0	0	0
3	F	42	0	0	0	0
All	All	9857	0	9809	109	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 (109) 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:C:21:ALA:HB2	1:C:59:VAL:HG21	1.64	0.77
1:A:189:LEU:HB3	1:A:195:ILE:HD12	1.68	0.76
1:F:20:LYS:HD3	1:F:63:ILE:HD11	1.68	0.75
1:A:189:LEU:HD11	1:A:203:LEU:HD13	1.69	0.73
1:F:189:LEU:HD11	1:F:203:LEU:HD13	1.73	0.71
1:D:46:GLU:HG3	1:D:76:PHE:CZ	2.26	0.71
1:E:46:GLU:HG3	1:E:76:PHE:CZ	2.26	0.70
1:F:46:GLU:HG3	1:F:76:PHE:CZ	2.26	0.70
1:E:117:ASP:HB3	1:E:118:HIS:HD2	1.56	0.70
1:C:46:GLU:HG3	1:C:76:PHE:CZ	2.26	0.69
1:B:24:LEU:HD22	1:B:99:SER:HB3	1.74	0.68
1:A:46:GLU:HG3	1:A:76:PHE:CZ	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:195:ILE:HD11	1.94	0.68
1:A:189:LEU:O	1:A:195:ILE:CD1	2.42	0.67
1:C:117:ASP:HB3	1:C:118:HIS:HD2	1.57	0.67
1:B:197:LEU:HB2	3:B:2013:HOH:O	1.95	0.66
1:E:117:ASP:HB3	1:E:118:HIS:CD2	2.32	0.65
1:D:117:ASP:HB3	1:D:118:HIS:CD2	2.31	0.65
1:F:24:LEU:HD22	1:F:99:SER:HB3	1.81	0.62
1:C:189:LEU:HD21	1:C:203:LEU:HD13	1.82	0.62
1:C:79:ASP:HB3	3:C:2011:HOH:O	2.00	0.61
1:C:31:ARG:HB3	1:C:69:TYR:CE2	2.37	0.59
1:D:36:PRO:HG2	1:D:39:LEU:HD12	1.85	0.59
1:A:20:LYS:NZ	1:A:61:GLU:OE2	2.36	0.59
1:B:138:ARG:CG	1:E:17:LYS:HG2	2.32	0.59
1:E:16:ILE:HD11	1:E:58:HIS:HB3	1.85	0.58
1:B:40:VAL:O	1:B:47:ILE:HG13	2.02	0.58
1:B:100:LEU:HD13	1:B:113:LEU:HD22	1.87	0.57
1:D:117:ASP:HB3	1:D:118:HIS:HD2	1.69	0.56
1:A:115:MET:HE1	1:A:197:LEU:CD1	2.36	0.56
1:B:138:ARG:HG3	1:E:17:LYS:HG2	1.89	0.55
1:C:115:MET:C	1:C:117:ASP:H	2.15	0.55
1:C:178:LEU:HD22	1:C:182:ILE:HD13	1.89	0.54
1:E:31:ARG:HD2	1:E:220:ASP:O	2.07	0.54
1:A:115:MET:HB3	1:A:117:ASP:OD1	2.08	0.52
1:F:21:ALA:HB2	1:F:59:VAL:HG11	1.92	0.52
1:D:38:PRO:HB3	1:D:48:ILE:HB	1.92	0.51
1:B:96:ASN:HB2	3:B:2013:HOH:O	2.10	0.51
1:A:16:ILE:HD11	1:A:58:HIS:HB3	1.93	0.50
1:B:145:ILE:HD11	1:E:18:LEU:HD11	1.92	0.50
1:C:32:LEU:HD23	1:D:32:LEU:HD21	1.94	0.50
1:C:196:PRO:HA	3:C:2042:HOH:O	2.11	0.50
1:A:17:LYS:HG2	1:F:138:ARG:HG3	1.93	0.50
1:E:16:ILE:HD13	1:E:19:MET:HE2	1.93	0.50
1:A:38:PRO:HB3	1:A:48:ILE:HB	1.94	0.49
1:A:119:VAL:HG11	1:B:142:PHE:HZ	1.77	0.49
1:B:117:ASP:CB	1:B:118:HIS:HD2	2.24	0.49
1:E:16:ILE:HD13	1:E:19:MET:CE	2.42	0.49
1:A:189:LEU:O	1:A:195:ILE:HD12	2.11	0.49
1:E:115:MET:HB2	1:E:118:HIS:CD2	2.47	0.49
1:D:78:LYS:C	1:D:80:LYS:H	2.21	0.48
1:C:38:PRO:HB3	1:C:48:ILE:HB	1.96	0.48
1:B:117:ASP:HB2	1:B:118:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:PRO:HB3	1:E:48:ILE:HB	1.96	0.48
1:E:100:LEU:HD13	1:E:113:LEU:HD22	1.96	0.48
1:B:23:ILE:HG21	1:B:48:ILE:HD12	1.94	0.48
1:C:31:ARG:HH11	1:C:69:TYR:HE2	1.62	0.48
1:D:115:MET:HB2	1:D:118:HIS:CD2	2.48	0.47
1:A:47:ILE:HG22	3:A:2003:HOH:O	2.14	0.47
1:C:19:MET:HB2	1:C:111:PHE:HA	1.96	0.47
1:B:135:ILE:HB	1:B:175:PHE:HB3	1.96	0.47
1:B:117:ASP:HB2	1:B:118:HIS:HD2	1.80	0.47
1:A:100:LEU:HD13	1:A:113:LEU:HD22	1.97	0.47
1:C:24:LEU:HD22	1:C:99:SER:HB3	1.96	0.47
1:B:66:ALA:HB1	3:B:2007:HOH:O	2.15	0.46
1:E:28:LEU:HD22	1:E:117:ASP:HB2	1.97	0.46
1:B:138:ARG:HG2	1:E:17:LYS:HG2	1.97	0.46
1:D:100:LEU:HD13	1:D:113:LEU:HD22	1.98	0.46
1:F:38:PRO:HB3	1:F:48:ILE:HB	1.98	0.46
1:B:24:LEU:HD13	1:B:96:ASN:HB3	1.96	0.46
1:E:31:ARG:O	1:E:32:LEU:HB2	2.14	0.45
1:A:181:SER:HB2	3:A:2021:HOH:O	2.17	0.45
1:F:110:ARG:HH22	1:F:132:GLU:HG3	1.80	0.45
1:C:33:GLY:HA3	3:C:2004:HOH:O	2.17	0.44
1:B:84:TYR:HE1	1:B:86:ILE:HD11	1.83	0.44
1:A:152:ARG:HB3	1:A:160:LYS:HB2	1.98	0.44
1:C:31:ARG:HB3	1:C:69:TYR:HE2	1.80	0.44
1:B:152:ARG:HB3	1:B:160:LYS:HB2	1.99	0.44
1:E:152:ARG:HB3	1:E:160:LYS:HB2	2.01	0.43
1:F:115:MET:C	1:F:117:ASP:H	2.26	0.43
1:B:125:ILE:O	1:B:129:VAL:HB	2.19	0.43
1:F:94:LYS:HG2	1:F:195:ILE:HD12	2.01	0.43
1:E:69:TYR:CE2	2:E:501:FLC:HG1	2.54	0.43
1:F:100:LEU:HD21	1:F:182:ILE:HG12	1.99	0.43
1:D:189:LEU:O	1:D:195:ILE:HG12	2.18	0.43
1:B:23:ILE:HG21	1:B:48:ILE:CD1	2.49	0.42
1:A:119:VAL:CG1	1:B:142:PHE:HZ	2.33	0.42
1:D:152:ARG:HB3	1:D:160:LYS:HB2	2.01	0.42
1:A:183:PHE:HA	1:A:186:ALA:HB3	2.02	0.42
1:B:37:LYS:HB2	1:B:38:PRO:HD3	2.02	0.42
1:D:185:HIS:HA	1:D:188:LYS:HE3	2.01	0.42
1:B:47:ILE:HG21	1:B:117:ASP:O	2.20	0.42
1:C:91:ARG:HB3	1:C:94:LYS:HG3	2.02	0.41
1:A:18:LEU:HD11	1:F:145:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HB3	1:B:94:LYS:HG3	2.02	0.41
1:C:21:ALA:HB2	1:C:59:VAL:CG2	2.43	0.41
1:E:153:VAL:HG22	1:E:208:VAL:HG21	2.03	0.41
1:C:75:ALA:O	1:C:78:LYS:HG2	2.21	0.41
1:D:118:HIS:CD2	1:D:118:HIS:N	2.88	0.41
1:D:91:ARG:HB3	1:D:94:LYS:HG3	2.03	0.41
1:E:31:ARG:NH1	1:E:220:ASP:O	2.54	0.41
1:C:152:ARG:HB3	1:C:160:LYS:HB2	2.01	0.41
1:B:39:LEU:HB3	3:B:2005:HOH:O	2.21	0.41
1:C:85:LYS:NZ	3:C:2017:HOH:O	2.54	0.41
1:E:142:PHE:HZ	1:F:119:VAL:HG11	1.85	0.41
1:C:153:VAL:HG22	1:C:208:VAL:HG21	2.03	0.40
1:E:91:ARG:HB3	1:E:94:LYS:HG3	2.03	0.40
1:A:21:ALA:HB2	1:A:59:VAL:HG21	2.03	0.40
1:B:145:ILE:HD11	1:E:18:LEU:CD1	2.51	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	193/232 (83%)	181 (94%)	12 (6%)	0	100	100
1	B	192/232 (83%)	182 (95%)	10 (5%)	0	100	100
1	C	197/232 (85%)	183 (93%)	13 (7%)	1 (0%)	24	37
1	D	203/232 (88%)	190 (94%)	12 (6%)	1 (0%)	24	37
1	E	203/232 (88%)	186 (92%)	14 (7%)	3 (2%)	8	12
1	F	197/232 (85%)	187 (95%)	10 (5%)	0	100	100
All	All	1185/1392 (85%)	1109 (94%)	71 (6%)	5 (0%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	180	ASP
1	C	27	GLY
1	E	190	ARG
1	E	32	LEU
1	D	81	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	172/197 (87%)	157 (91%)	15 (9%)	9	16
1	B	170/197 (86%)	157 (92%)	13 (8%)	12	21
1	C	172/197 (87%)	152 (88%)	20 (12%)	5	8
1	D	175/197 (89%)	159 (91%)	16 (9%)	9	14
1	E	175/197 (89%)	159 (91%)	16 (9%)	9	14
1	F	174/197 (88%)	159 (91%)	15 (9%)	10	16
All	All	1038/1182 (88%)	943 (91%)	95 (9%)	8	14

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	46	GLU
1	A	68	ARG
1	A	79	ASP
1	A	88	ARG
1	A	108	GLU
1	A	138	ARG
1	A	145	ILE
1	A	166	ARG
1	A	171	VAL
1	A	180	ASP
1	A	197	LEU
1	A	198	SER
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	220	ASP
1	B	46	GLU
1	B	63	ILE
1	B	129	VAL
1	B	138	ARG
1	B	141	ARG
1	B	145	ILE
1	B	166	ARG
1	B	171	VAL
1	B	187	GLU
1	B	197	LEU
1	B	198	SER
1	B	203	LEU
1	B	220	ASP
1	C	18	LEU
1	C	32	LEU
1	C	46	GLU
1	C	59	VAL
1	C	68	ARG
1	C	108	GLU
1	C	113	LEU
1	C	117	ASP
1	C	138	ARG
1	C	141	ARG
1	C	145	ILE
1	C	166	ARG
1	C	171	VAL
1	C	180	ASP
1	C	182	ILE
1	C	187	GLU
1	C	197	LEU
1	C	198	SER
1	C	203	LEU
1	C	220	ASP
1	D	35	VAL
1	D	46	GLU
1	D	108	GLU
1	D	110	ARG
1	D	117	ASP
1	D	138	ARG
1	D	145	ILE
1	D	166	ARG

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Mol	Chain	Res	Type
1	D	171	VAL
1	D	180	ASP
1	D	187	GLU
1	D	192	ARG
1	D	197	LEU
1	D	198	SER
1	D	203	LEU
1	D	220	ASP
1	E	16	ILE
1	E	30	THR
1	E	31	ARG
1	E	46	GLU
1	E	63	ILE
1	E	101	LEU
1	E	138	ARG
1	E	145	ILE
1	E	166	ARG
1	E	171	VAL
1	E	187	GLU
1	E	192	ARG
1	E	197	LEU
1	E	198	SER
1	E	203	LEU
1	E	220	ASP
1	F	16	ILE
1	F	46	GLU
1	F	88	ARG
1	F	94	LYS
1	F	108	GLU
1	F	138	ARG
1	F	145	ILE
1	F	171	VAL
1	F	182	ILE
1	F	187	GLU
1	F	188	LYS
1	F	197	LEU
1	F	198	SER
1	F	203	LEU
1	F	220	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	96	ASN
1	C	106	HIS
1	D	118	HIS
1	E	83	ASN
1	E	118	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	E	501	-	12,12,12	2.20	6 (50%)	17,17,17	1.83	7 (41%)
2	FLC	A	501	-	12,12,12	3.09	8 (66%)	17,17,17	1.91	4 (23%)
2	FLC	D	501	-	12,12,12	2.06	5 (41%)	17,17,17	2.08	5 (29%)

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	E	501	-	-	7/16/16/16	-
2	FLC	A	501	-	-	3/16/16/16	-
2	FLC	D	501	-	-	9/16/16/16	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FLC	CG-CB	6.68	1.62	1.54
2	A	501	FLC	CB-CBC	5.10	1.58	1.53
2	E	501	FLC	CB-CBC	4.33	1.58	1.53
2	D	501	FLC	CB-CBC	4.02	1.57	1.53
2	A	501	FLC	OB1-CBC	3.30	1.32	1.22
2	D	501	FLC	OA2-CAC	-3.23	1.20	1.30
2	A	501	FLC	CA-CB	2.95	1.57	1.54
2	E	501	FLC	CA-CB	2.93	1.57	1.54
2	A	501	FLC	OHB-CB	2.88	1.48	1.43
2	E	501	FLC	OB1-CBC	2.83	1.31	1.22
2	D	501	FLC	OB1-CBC	2.57	1.30	1.22
2	D	501	FLC	CA-CB	2.48	1.57	1.54
2	E	501	FLC	OG2-CGC	-2.45	1.22	1.30
2	D	501	FLC	OG2-CGC	-2.34	1.23	1.30
2	E	501	FLC	CG-CB	2.23	1.56	1.54
2	A	501	FLC	OA2-CAC	-2.18	1.23	1.30
2	A	501	FLC	CG-CGC	2.16	1.57	1.50
2	A	501	FLC	OG2-CGC	-2.15	1.23	1.30
2	E	501	FLC	OA2-CAC	-2.06	1.24	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FLC	CB-CG-CGC	4.48	126.17	113.92
2	D	501	FLC	OB2-CBC-CB	4.37	121.53	113.14
2	D	501	FLC	OHB-CB-CG	-3.91	100.47	109.38
2	A	501	FLC	OB2-CBC-CB	3.67	120.17	113.14
2	D	501	FLC	OHB-CB-CBC	3.61	114.08	108.96
2	A	501	FLC	OG2-CGC-OG1	-3.46	114.44	123.33
2	E	501	FLC	OHB-CB-CG	-3.16	102.16	109.38
2	E	501	FLC	CG-CB-CBC	2.82	116.27	110.03
2	E	501	FLC	OB2-CBC-OB1	-2.61	115.51	123.86
2	E	501	FLC	OB1-CBC-CB	2.49	126.92	122.09
2	E	501	FLC	OG2-CGC-OG1	-2.38	117.20	123.33
2	D	501	FLC	OB2-CBC-OB1	-2.34	116.36	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FLC	OG2-CGC-CG	2.32	121.69	114.35
2	E	501	FLC	OB2-CBC-CB	2.30	117.56	113.14
2	E	501	FLC	OG2-CGC-CG	2.21	121.34	114.35
2	A	501	FLC	OG2-CGC-CG	2.02	120.74	114.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	FLC	CG-CB-CBC-OB1
2	D	501	FLC	CG-CB-CBC-OB2
2	D	501	FLC	OHB-CB-CBC-OB1
2	D	501	FLC	OHB-CB-CBC-OB2
2	E	501	FLC	CG-CB-CBC-OB1
2	E	501	FLC	CG-CB-CBC-OB2
2	E	501	FLC	OHB-CB-CBC-OB1
2	E	501	FLC	OHB-CB-CBC-OB2
2	A	501	FLC	CA-CB-CG-CGC
2	D	501	FLC	CAC-CA-CB-CBC
2	E	501	FLC	CAC-CA-CB-CBC
2	A	501	FLC	CBC-CB-CG-CGC
2	E	501	FLC	CAC-CA-CB-CG
2	E	501	FLC	CAC-CA-CB-OHB
2	D	501	FLC	CAC-CA-CB-CG
2	A	501	FLC	OHB-CB-CG-CGC
2	D	501	FLC	CAC-CA-CB-OHB
2	D	501	FLC	CA-CB-CG-CGC
2	D	501	FLC	CBC-CB-CG-CGC

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	FLC	1	0

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, 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	196/232 (84%)	0.89	21 (10%) 11 8	43, 80, 109, 127	1 (0%)
1	B	196/232 (84%)	1.01	25 (12%) 7 6	55, 79, 109, 130	0
1	C	201/232 (86%)	0.28	2 (0%) 79 76	34, 60, 90, 124	0
1	D	205/232 (88%)	0.48	6 (2%) 53 50	46, 72, 106, 138	0
1	E	205/232 (88%)	0.52	12 (5%) 28 24	43, 68, 100, 128	0
1	F	200/232 (86%)	0.18	2 (1%) 79 76	31, 57, 92, 104	1 (0%)
All	All	1203/1392 (86%)	0.56	68 (5%) 29 25	31, 70, 104, 138	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ALA	3.9
1	B	195	ILE	3.8
1	B	98	TYR	3.8
1	B	87	VAL	3.8
1	B	66	ALA	3.8
1	E	32	LEU	3.5
1	A	87	VAL	3.4
1	C	31	ARG	3.4
1	A	195	ILE	3.1
1	A	189	LEU	3.1
1	B	23	ILE	3.1
1	E	66	ALA	3.0
1	F	142[A]	PHE	3.0
1	B	158	VAL	2.9
1	B	148	ALA	2.9
1	B	96	ASN	2.9
1	A	197	LEU	2.9
1	F	18	LEU	2.8
1	A	39	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	2.8
1	B	63	ILE	2.7
1	B	36	PRO	2.7
1	A	151	ILE	2.7
1	A	200	ILE	2.7
1	B	42	VAL	2.6
1	B	185	HIS	2.6
1	D	186	ALA	2.6
1	B	26	ALA	2.5
1	E	31	ARG	2.5
1	D	81	GLY	2.5
1	E	87	VAL	2.5
1	B	64	ILE	2.4
1	A	65	VAL	2.4
1	D	95	GLY	2.4
1	B	92	PRO	2.4
1	A	35	VAL	2.4
1	B	99	SER	2.4
1	E	27	GLY	2.4
1	A	165	LEU	2.3
1	A	103	ALA	2.3
1	D	63	ILE	2.3
1	B	82	PHE	2.3
1	E	88	ARG	2.3
1	B	95	GLY	2.3
1	B	24	LEU	2.3
1	D	65	VAL	2.3
1	B	142	PHE	2.2
1	A	92	PRO	2.2
1	B	39	LEU	2.2
1	D	43	GLY	2.2
1	A	86	ILE	2.2
1	E	195	ILE	2.2
1	A	42	VAL	2.1
1	E	165	LEU	2.1
1	A	69	TYR	2.1
1	A	95	GLY	2.1
1	E	90	ASP	2.1
1	A	82	PHE	2.1
1	E	65	VAL	2.1
1	C	69	TYR	2.1
1	E	92	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	ILE	2.1
1	A	117	ASP	2.1
1	A	91	ARG	2.0
1	B	186	ALA	2.0
1	A	105	ASN	2.0
1	B	182	ILE	2.0
1	E	30	THR	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	FLC	A	501	13/13	0.73	0.14	101,102,103,104	0
2	FLC	E	501	13/13	0.81	0.11	85,86,86,87	0
2	FLC	D	501	13/13	0.86	0.12	89,89,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.