wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 06:32 AM EDT

PDB ID	:	5DVA
Title	:	Fragments bound to the OXA-48 beta-lactamase: Compound 1
Authors	:	Lund, B.A.; Christopeit, T.; Leiros, H.-K.S.
Deposited on	:	2015-09-21
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

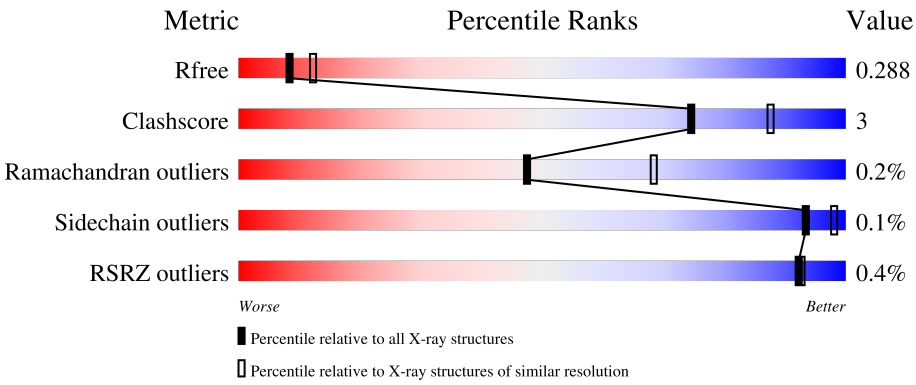
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	244	% 94% 5% •
1	B	244	92% 7% •
1	C	244	93% 7% •
1	D	244	93% 6% •

2 Entry composition (i)

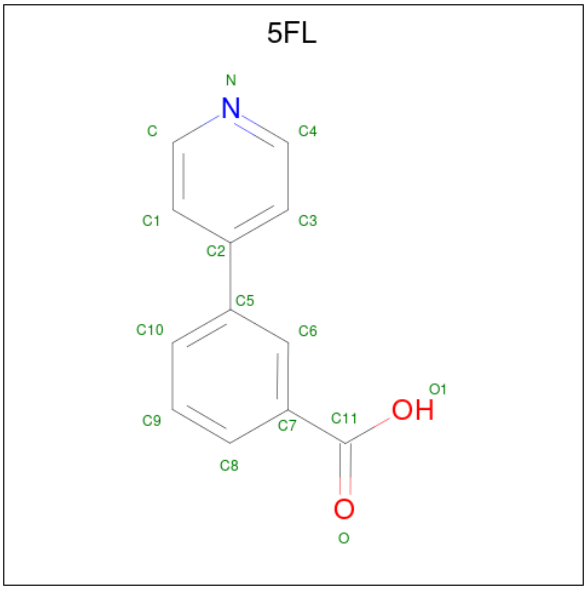
There are 4 unique types of molecules in this entry. The entry contains 16381 atoms, of which 7714 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	242	3889	1259	1910	348	365	7	0	0	0
1	B	242	3908	1267	1917	350	366	8	0	1	0
1	C	242	3904	1262	1921	349	365	7	0	0	0
1	D	242	3901	1262	1918	349	365	7	0	0	0

- Molecule 2 is 3-(pyridin-4-yl)benzoic acid (three-letter code: 5FL) (formula: $C_{12}H_9NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	23	12	8	1	2	0	0
2	B	1	23	12	8	1	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	C	1	46	24	16	2	4	0	1
			Total	C	H	N	O		
2	D	1	46	24	16	2	4	0	1

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	B	1	1	1	0	0
			Total	Cl		
3	C	1	1	1	0	0

- Molecule 4 is water.

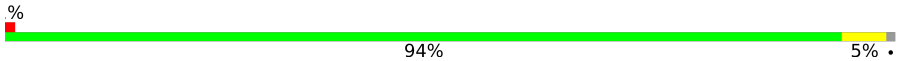
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	172	172	172	0	0
			Total	O		
4	B	143	143	143	0	0
			Total	O		
4	C	164	164	164	0	0
			Total	O		
4	D	160	160	160	0	0

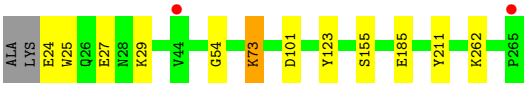
3 Residue-property plots (i)

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: Beta-lactamase

Chain A:



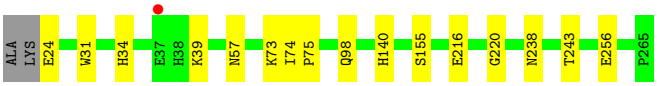


- Molecule 1: Beta-lactamase

Chain B:

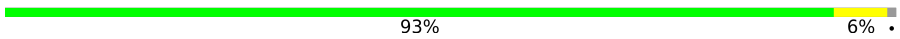
- Molecule 1: Beta-lactamase

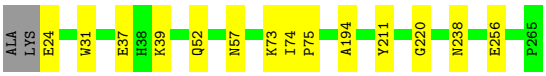
Chain C:



- Molecule 1: Beta-lactamase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.04Å 109.66Å 124.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.95-2.50) 83.8 (19.95-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.50Å)	Xtriage
Refinement program	PHENIX dev_2328	Depositor
R, R_{free}	0.232 , 0.287 0.233 , 0.288	Depositor DCC
R_{free} test set	2101 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	1.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16381	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 50.33 % 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 6.5723e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, 5FL, CL

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	0.24	0/2015	0.42	0/2726
1	B	0.24	0/2027	0.42	0/2740
1	C	0.24	0/2019	0.41	0/2730
1	D	0.23	0/2019	0.42	0/2730
All	All	0.24	0/8080	0.42	0/10926

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	37	GLU	Peptide

5.2 Too-close contacts (i)

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	1979	1910	1921	9	0
1	B	1991	1917	1940	18	0
1	C	1983	1921	1932	14	0
1	D	1983	1918	1932	12	0
2	A	15	8	0	0	0
2	B	15	8	0	0	0
2	C	30	16	0	0	0
2	D	30	16	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
4	A	172	0	0	5	0
4	B	143	0	0	7	3
4	C	164	0	0	6	0
4	D	160	0	0	8	3
All	All	8667	7714	7725	50	3

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 3.

The worst 5 of 50 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:24:GLU:HG2	1:C:24:GLU:HB3	1.47	0.97
1:A:101:ASP:OD2	4:A:401:HOH:O	1.88	0.90
1:D:194:ALA:O	4:D:401:HOH:O	2.01	0.78
1:A:211:TYR:OH	4:A:402:HOH:O	2.05	0.74
1:C:256:GLU:O	4:C:401:HOH:O	2.09	0.71

All (3) 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)
4:B:459:HOH:O	4:D:519:HOH:O[2_794]	2.06	0.14
4:B:453:HOH:O	4:D:520:HOH:O[4_495]	2.13	0.07
4:B:526:HOH:O	4:D:508:HOH:O[4_495]	2.19	0.01

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	239/244 (98%)	231 (97%)	7 (3%)	1 (0%)	34	54
1	B	240/244 (98%)	232 (97%)	8 (3%)	0	100	100
1	C	239/244 (98%)	232 (97%)	6 (2%)	1 (0%)	34	54
1	D	239/244 (98%)	232 (97%)	7 (3%)	0	100	100
All	All	957/976 (98%)	927 (97%)	28 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	SER
1	C	155	SER

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	209/211 (99%)	209 (100%)	0	100	100
1	B	211/211 (100%)	210 (100%)	1 (0%)	88	96
1	C	210/211 (100%)	210 (100%)	0	100	100
1	D	210/211 (100%)	210 (100%)	0	100	100
All	All	840/844 (100%)	839 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KCX	B	73	1	9,11,12	0.88	0	5,12,14	1.48	1 (20%)
1	KCX	D	73	1	9,11,12	0.87	0	5,12,14	1.56	1 (20%)
1	KCX	A	73	1	9,11,12	0.84	0	5,12,14	1.49	1 (20%)
1	KCX	C	73	1	9,11,12	0.88	0	5,12,14	1.56	1 (20%)

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
1	KCX	B	73	1	-	0/9/10/12	-
1	KCX	D	73	1	-	0/9/10/12	-
1	KCX	A	73	1	-	0/9/10/12	-
1	KCX	C	73	1	-	0/9/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	73	KCX	OQ1-CX-NZ	-3.43	119.63	124.96
1	D	73	KCX	OQ1-CX-NZ	-3.35	119.77	124.96
1	B	73	KCX	OQ1-CX-NZ	-3.15	120.08	124.96
1	A	73	KCX	OQ1-CX-NZ	-3.10	120.15	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	5FL	C	301[B]	-	16,16,16	0.09	0	21,21,21	0.13	0
2	5FL	B	301	-	16,16,16	0.92	2 (12%)	21,21,21	0.82	2 (9%)
2	5FL	C	301[A]	-	16,16,16	0.08	0	21,21,21	0.13	0
2	5FL	D	301[B]	-	16,16,16	0.93	2 (12%)	21,21,21	0.81	2 (9%)
2	5FL	D	301[A]	-	16,16,16	0.92	2 (12%)	21,21,21	0.81	2 (9%)
2	5FL	A	301	-	16,16,16	0.93	2 (12%)	21,21,21	0.81	2 (9%)

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	5FL	C	301[B]	-	-	0/8/8/8	0/2/2/2
2	5FL	B	301	-	-	0/8/8/8	0/2/2/2
2	5FL	C	301[A]	-	-	0/8/8/8	0/2/2/2
2	5FL	D	301[B]	-	-	4/8/8/8	0/2/2/2
2	5FL	D	301[A]	-	-	4/8/8/8	0/2/2/2
2	5FL	A	301	-	-	0/8/8/8	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	5FL	O-C11	2.72	1.30	1.22
2	B	301	5FL	O-C11	2.72	1.30	1.22
2	D	301[B]	5FL	O-C11	2.71	1.30	1.22
2	D	301[A]	5FL	O-C11	2.69	1.30	1.22
2	D	301[B]	5FL	O1-C11	-2.53	1.22	1.30

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	5FL	O1-C11-C7	2.70	121.86	114.85
2	D	301[A]	5FL	O1-C11-C7	2.67	121.78	114.85
2	A	301	5FL	O1-C11-C7	2.66	121.76	114.85
2	D	301[B]	5FL	O1-C11-C7	2.66	121.76	114.85
2	B	301	5FL	O-C11-C7	-2.51	114.76	121.45

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301[B]	5FL	C3-C2-C5-C6
2	D	301[B]	5FL	C1-C2-C5-C6
2	D	301[B]	5FL	C1-C2-C5-C10
2	D	301[B]	5FL	C3-C2-C5-C10
2	D	301[A]	5FL	C1-C2-C5-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301[B]	5FL	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	241/244 (98%)	0.16	2 (0%)	86	87	24, 37, 57, 79	0
1	B	241/244 (98%)	0.22	1 (0%)	92	93	30, 39, 60, 85	0
1	C	241/244 (98%)	0.14	1 (0%)	92	93	25, 39, 62, 91	0
1	D	241/244 (98%)	0.18	0	100	100	29, 41, 65, 96	0
All	All	964/976 (98%)	0.17	4 (0%)	92	93	24, 39, 61, 96	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	ALA	2.4
1	A	265	PRO	2.3
1	A	44	VAL	2.1
1	C	37	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	KCX	C	73	12/13	0.90	0.17	25,31,38,40	0
1	KCX	B	73	12/13	0.91	0.18	30,35,42,43	0
1	KCX	A	73	12/13	0.92	0.20	25,35,43,45	0
1	KCX	D	73	12/13	0.94	0.16	29,32,37,38	0

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, 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	5FL	D	301[A]	15/15	0.76	0.38	69,72,87,89	23
2	5FL	D	301[B]	15/15	0.76	0.38	69,79,95,97	23
2	5FL	A	301	15/15	0.79	0.26	34,36,44,44	23
2	5FL	B	301	15/15	0.81	0.23	42,50,60,61	0
2	5FL	C	301[A]	15/15	0.89	0.22	34,34,41,42	23
2	5FL	C	301[B]	15/15	0.89	0.22	34,36,43,44	23
3	CL	C	302	1/1	0.90	0.09	39,39,39,39	0
3	CL	B	302	1/1	0.94	0.17	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.