



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2016 – 04:40 PM EDT

PDB ID : 5FL0
Title : Structure of a hydrolase with an inhibitor
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Deposited on : 2015-10-20
Resolution : 1.95 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

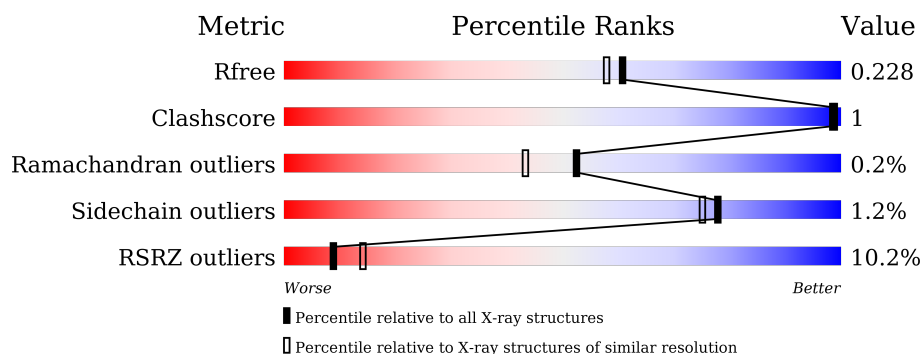
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	716	<div> <div>9%</div> <div>90%</div> <div>7%</div> </div>
1	B	716	<div> <div>10%</div> <div>92%</div> <div>5%</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	EDO	A	1717	-	-	-	X

2 Entry composition [i](#)

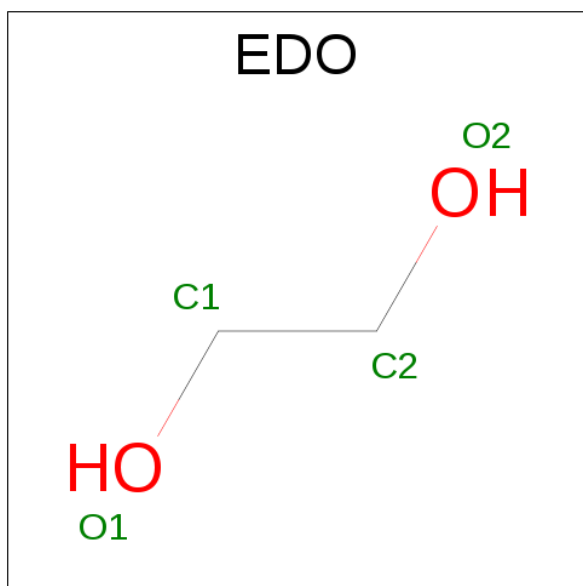
There are 5 unique types of molecules in this entry. The entry contains 22515 atoms, of which 10909 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE BT_4395.

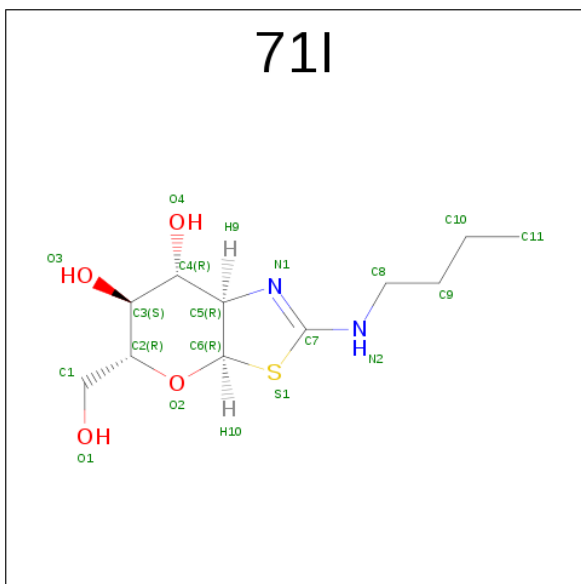
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	668	Total	C	H	N	O	S	0	6	0
			10816	3487	5368	918	1023	20			
1	B	682	Total	C	H	N	O	S	0	3	0
			11025	3546	5477	942	1041	19			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is (3 {A} {R},5 {R},6 {S},7 {R},7 {A} {R})-2-(BUTYLAMINO)-5-(HYDROXYMETHYL)-5,6,7,7 {A}-TETRAHYDRO-3 {A} {H}-PYRANO[3,2-D][1,3]THIAZOLE-6,7-DIOL (three-letter code: 71I) (formula: C₁₁H₂₀N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			38	11	20	2	4	1		
3	B	1	Total	C	H	N	O	S	0	0
			38	11	20	2	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total	O	0	0
			294	294		
5	B	263	Total	O	0	0
			263	263		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	51.53Å 162.13Å 223.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.96 – 1.95 44.96 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.96-1.95) 99.9 (44.96-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.200 , 0.227 0.198 , 0.228	Depositor DCC
R_{free} test set	6874 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22515	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.63% 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: CA, EDO, 7II

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	0.39	0/5597	0.53	0/7580
1	B	0.39	0/5698	0.52	0/7720
All	All	0.39	0/11295	0.52	0/15300

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	5448	5368	5348	11	0
1	B	5548	5477	5466	7	0
2	A	8	12	12	0	0
2	B	8	12	12	0	0
3	A	18	20	0	1	0
3	B	18	20	0	0	0
4	B	1	0	0	0	0
5	A	294	0	0	1	0
5	B	263	0	0	0	0
All	All	11606	10909	10838	18	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 1.

All (18) 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:A:4:SER:N	5:A:2001:HOH:O	2.38	0.57
1:B:673:LEU:HD23	1:B:682:ALA:HB2	1.91	0.52
1:A:444:GLN:HG3	1:A:445:PRO:HD3	1.92	0.52
1:B:70:TYR:OH	1:B:89:GLU:OE2	2.24	0.51
1:A:238:ALA:HA	1:A:276:VAL:O	2.15	0.46
1:A:282:TYR:HB2	3:A:1718:7II:C11	2.47	0.45
1:B:238:ALA:HA	1:B:276:VAL:O	2.18	0.43
1:A:164:GLY:N	1:A:165:PRO:HD3	2.34	0.42
1:A:37:ALA:HB1	1:A:104:LEU:HD12	2.01	0.41
1:A:355:VAL:O	1:A:399:THR:HG23	2.20	0.41
1:B:278[B]:CYS:SG	1:B:308:MET:SD	3.18	0.41
1:A:37:ALA:O	1:A:104:LEU:HD13	2.21	0.41
1:B:209:GLY:HA3	1:B:244:ILE:HD13	2.03	0.41
1:A:262:ASP:HA	1:A:266:ALA:HB3	2.03	0.41
1:B:131:GLY:HA3	1:B:160:THR:O	2.21	0.41
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.55	0.40
1:B:662:SER:OG	1:B:664:ASP:O	2.23	0.40
1:A:308:MET:HA	1:A:335:TYR:O	2.21	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	662/716 (92%)	645 (97%)	16 (2%)	1 (0%)	52	43
1	B	677/716 (95%)	651 (96%)	25 (4%)	1 (0%)	56	48
All	All	1339/1432 (94%)	1296 (97%)	41 (3%)	2 (0%)	52	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	GLY
1	B	518	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	594/630 (94%)	589 (99%)	5 (1%)	86	85
1	B	605/630 (96%)	595 (98%)	10 (2%)	68	63
All	All	1199/1260 (95%)	1184 (99%)	15 (1%)	78	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	TRP
1	A	371	THR
1	A	444	GLN
1	A	519	ARG
1	A	647	ASN
1	B	278[A]	CYS
1	B	278[B]	CYS
1	B	337	TRP
1	B	371	THR
1	B	598	ASN
1	B	642	GLU
1	B	658	ARG
1	B	661	ILE
1	B	666	LYS
1	B	676	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	B	372	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is 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	EDO	A	1716	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	A	1717	-	3,3,3	0.58	0	2,2,2	0.19	0
3	71I	A	1718	-	16,19,19	2.02	1 (6%)	15,26,26	1.56	2 (13%)
2	EDO	B	1717	-	3,3,3	0.42	0	2,2,2	0.23	0
2	EDO	B	1718	-	3,3,3	0.44	0	2,2,2	0.46	0
3	71I	B	1719	-	16,19,19	2.20	1 (6%)	15,26,26	0.96	0

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	EDO	A	1716	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1717	-	-	0/1/1/1	0/0/0/0
3	7II	A	1718	-	-	0/7/35/35	0/2/2/2
2	EDO	B	1717	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1718	-	-	0/1/1/1	0/0/0/0
3	7II	B	1719	-	-	0/7/35/35	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1719	7II	C7-S1	-8.47	1.67	1.76
3	A	1718	7II	C7-S1	-7.68	1.68	1.76

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1718	7II	N2-C7-N1	-4.28	120.19	124.38
3	A	1718	7II	C9-C8-N2	-2.34	105.67	112.29

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
3	A	1718	7II	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 ⓘ

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	668/716 (93%)	0.64	65 (9%) 10 16	30, 46, 94, 136	0
1	B	682/716 (95%)	0.66	73 (10%) 8 12	27, 45, 99, 131	0
All	All	1350/1432 (94%)	0.65	138 (10%) 9 14	27, 46, 96, 136	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	706	LEU	7.4
1	A	646	ILE	7.1
1	B	290	ASN	6.7
1	B	673	LEU	6.5
1	B	661	ILE	6.2
1	A	673	LEU	5.9
1	A	680	LEU	5.8
1	A	661	ILE	5.7
1	A	709	PHE	5.7
1	B	601	GLN	5.4
1	A	671	VAL	5.3
1	A	14	VAL	5.3
1	B	48	LYS	5.3
1	A	47	GLY	4.8
1	B	688	PRO	4.8
1	A	659	LEU	4.7
1	B	602	ILE	4.7
1	A	616	ILE	4.6
1	B	674	LYS	4.5
1	A	644	ILE	4.5
1	B	679	ARG	4.4
1	A	604	ASN	4.3
1	B	599	VAL	4.3
1	A	88	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	51	SER	4.1
1	A	115	LYS	4.1
1	B	687	ALA	4.1
1	B	666	LYS	4.0
1	A	21	LEU	4.0
1	B	47	GLY	3.9
1	A	53	LYS	3.9
1	B	685	GLN	3.8
1	A	16	ASN	3.8
1	A	52	LYS	3.7
1	A	19	ILE	3.6
1	A	668	TRP	3.6
1	B	631	VAL	3.6
1	B	291	GLY	3.6
1	B	583	HIS	3.6
1	B	680	LEU	3.6
1	A	666	LYS	3.5
1	A	65	LYS	3.5
1	B	715	LYS	3.5
1	A	24	VAL	3.5
1	A	669	LYS	3.3
1	B	16	ASN	3.3
1	A	667	GLU	3.3
1	A	85	VAL	3.3
1	B	659	LEU	3.3
1	A	116	LEU	3.3
1	B	604	ASN	3.1
1	A	596	ILE	3.1
1	B	18	THR	3.1
1	B	52	LYS	3.1
1	B	707	ARG	3.0
1	B	695	THR	3.0
1	B	689	VAL	3.0
1	B	452	LYS	3.0
1	B	696	ASN	3.0
1	A	672	ASP	3.0
1	B	19	ILE	2.9
1	A	694	PHE	2.9
1	A	113	ASP	2.9
1	B	600	GLU	2.9
1	A	684	LEU	2.9
1	A	119	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	18	THR	2.8
1	B	53	LYS	2.8
1	A	597	SER	2.8
1	B	580	PHE	2.8
1	B	671	VAL	2.8
1	B	114	GLY	2.7
1	A	49	GLN	2.7
1	B	676	LYS	2.7
1	A	607	LEU	2.7
1	B	658	ARG	2.7
1	B	668	TRP	2.6
1	A	388	ALA	2.6
1	A	72	ARG	2.6
1	B	288	ASN	2.6
1	B	453	ALA	2.6
1	B	46	SER	2.6
1	B	644	ILE	2.6
1	A	129	TYR	2.5
1	A	711	LEU	2.5
1	B	456	GLU	2.5
1	B	667	GLU	2.5
1	B	603	LYS	2.5
1	B	692	VAL	2.5
1	A	693	ARG	2.5
1	A	22	PRO	2.5
1	A	687	ALA	2.5
1	B	519	ARG	2.5
1	A	15	GLN	2.5
1	A	27	LEU	2.5
1	B	450	PHE	2.5
1	B	582	ALA	2.4
1	A	46	SER	2.4
1	A	631	VAL	2.4
1	A	13	ILE	2.3
1	A	682	ALA	2.3
1	A	470	TYR	2.3
1	B	384	ILE	2.3
1	B	598	ASN	2.3
1	B	677	GLU	2.3
1	A	620	ASN	2.3
1	B	113	ASP	2.3
1	B	567	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	641	GLY	2.3
1	B	581	ASN	2.3
1	B	385	TYR	2.2
1	A	57	ILE	2.2
1	B	51	SER	2.2
1	B	513	LEU	2.2
1	B	684	LEU	2.2
1	B	286	TRP	2.2
1	A	681	SER	2.2
1	A	685	GLN	2.2
1	B	576	PHE	2.2
1	A	132	VAL	2.2
1	A	371	THR	2.2
1	A	290	ASN	2.2
1	A	665	GLY	2.1
1	B	454	PHE	2.1
1	B	638	ILE	2.1
1	B	3	VAL	2.1
1	B	646	ILE	2.1
1	B	675	GLN	2.1
1	A	692	VAL	2.1
1	B	387	VAL	2.1
1	A	660	GLU	2.1
1	B	7	PRO	2.1
1	A	17	LYS	2.1
1	A	25	TYR	2.0
1	B	669	LYS	2.0
1	B	657	GLY	2.0
1	B	712	THR	2.0
1	A	645	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	EDO	A	1717	4/4	0.92	0.15	2.40	36,43,49,49	0
2	EDO	B	1718	4/4	0.86	0.15	1.87	63,76,77,78	0
2	EDO	B	1717	4/4	0.90	0.14	0.78	50,60,65,65	0
3	71I	B	1719	18/18	0.96	0.10	-0.55	32,41,52,55	0
3	71I	A	1718	18/18	0.96	0.12	-0.61	31,42,61,61	0
4	CA	B	1716	1/1	0.99	0.08	-0.91	40,40,40,40	0
2	EDO	A	1716	4/4	0.96	0.11	-1.14	41,49,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.