Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 05:40 pm BST

PDB ID	:	6QE7
Title	:	anti-sigma factor domain-containing protein
Authors	:	Voronov, M.; Livnah, O.; Bayer, E.A.
Deposited on	:	2019-01-07
Resolution	:	2.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

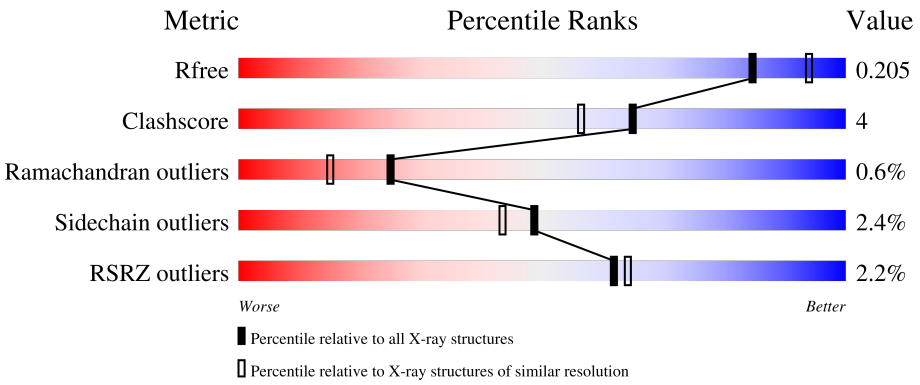
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	291	.% 86% 14%
1	B	291	2% 81% 17% •
1	C	291	3% 87% 10% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7586 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 Anti-sigma-I factor RsgI3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	291	2391	1523	403	459	6	0	0	0
1	B	287	2366	1507	399	454	6	0	0	0
1	C	286	2360	1506	397	451	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP A3DC75
A	19	SER	-	expression tag	UNP A3DC75
A	20	HIS	-	expression tag	UNP A3DC75
A	21	MET	-	expression tag	UNP A3DC75
B	18	GLY	-	expression tag	UNP A3DC75
B	19	SER	-	expression tag	UNP A3DC75
B	20	HIS	-	expression tag	UNP A3DC75
B	21	MET	-	expression tag	UNP A3DC75
C	18	GLY	-	expression tag	UNP A3DC75
C	19	SER	-	expression tag	UNP A3DC75
C	20	HIS	-	expression tag	UNP A3DC75
C	21	MET	-	expression tag	UNP A3DC75

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0

- Molecule 3 is water.

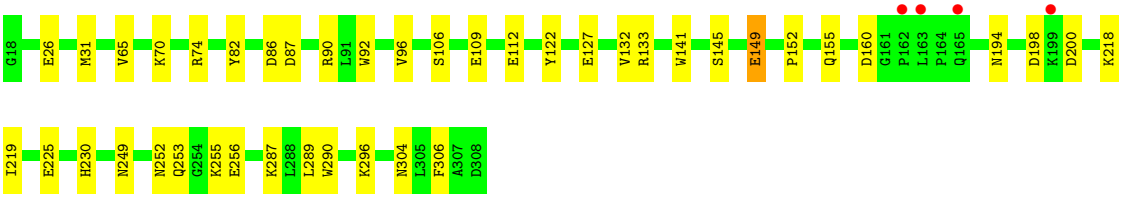
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	174	174	174	0	0
			Total	O		
3	B	141	141	141	0	0
			Total	O		
3	C	148	148	148	0	0

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.

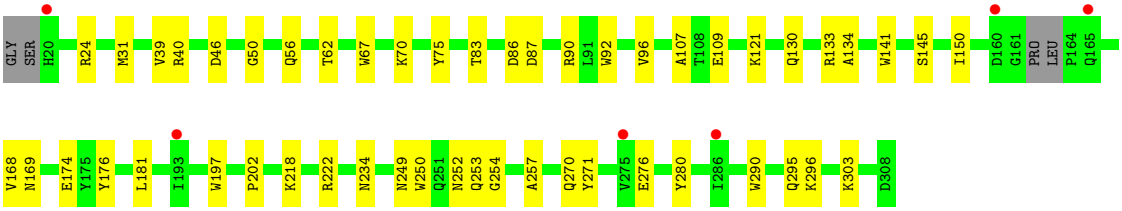
• Molecule 1: Anti-sigma-I factor RsgI3

Chain A:



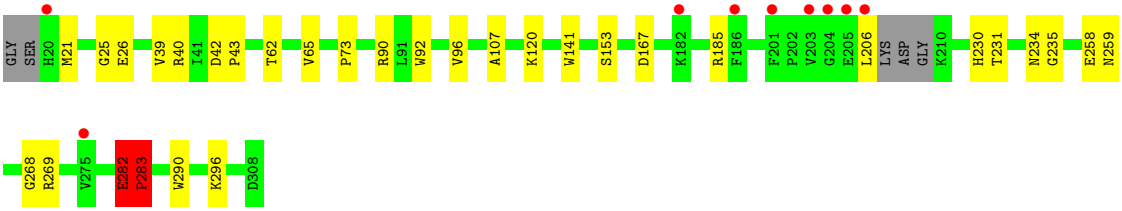
• Molecule 1: Anti-sigma-I factor RsgI3

Chain B:



• Molecule 1: Anti-sigma-I factor RsgI3

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.34Å 121.67Å 65.94Å 90.00° 106.39° 90.00°	Depositor
Resolution (Å)	28.42 – 2.06 28.40 – 2.06	Depositor EDS
% Data completeness (in resolution range)	95.7 (28.42-2.06) 95.8 (28.40-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.255 0.198 , 0.205	Depositor DCC
R_{free} test set	479 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.92	3/2454 (0.1%)	1.08	2/3317 (0.1%)
1	B	0.84	0/2427	1.08	3/3277 (0.1%)
1	C	0.86	1/2422 (0.0%)	1.12	6/3274 (0.2%)
All	All	0.87	4/7303 (0.1%)	1.09	11/9868 (0.1%)

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	A	0	1
1	C	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	GLU	CD-OE1	5.37	1.31	1.25
1	A	127	GLU	CD-OE1	-5.19	1.20	1.25
1	A	109	GLU	CD-OE1	-5.13	1.20	1.25
1	C	235	GLY	C-O	5.10	1.31	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	C	282	GLU	C-N-CD	-9.78	99.09	120.60
1	C	283	PRO	CA-N-CD	-9.34	98.42	111.50
1	B	133	ARG	NE-CZ-NH2	-7.67	116.47	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	269	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	167	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	90	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	31	MET	CB-CG-SD	-5.77	95.10	112.40
1	B	133	ARG	CG-CD-NE	-5.42	100.42	111.80
1	B	90	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	296	LYS	CB-CA-C	5.04	120.49	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLU	Peptide
1	C	282	GLU	Mainchain,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	2391	0	2286	15	0
1	B	2366	0	2260	31	0
1	C	2360	0	2257	11	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	174	0	0	0	0
3	B	141	0	0	7	0
3	C	148	0	0	0	0
All	All	7586	0	6803	57	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 4.

All (57) 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:270:GLN:NE2	3:B:502:HOH:O	2.20	0.73
1:B:222:ARG:NH1	1:B:295:GLN:OE1	2.21	0.72
1:C:21:MET:HE3	1:C:153:SER:O	2.01	0.60
1:A:249:ASN:ND2	1:A:252:ASN:HB2	2.18	0.59
1:B:276:GLU:OE2	3:B:501:HOH:O	2.17	0.58
1:C:234:ASN:HB3	1:C:283:PRO:O	2.05	0.57
1:B:234:ASN:HA	1:B:254:GLY:O	2.05	0.56
1:B:222:ARG:HH21	1:B:303:LYS:NZ	2.03	0.56
1:B:24:ARG:O	1:B:67:TRP:HA	2.08	0.54
1:C:92:TRP:HA	1:C:96:VAL:O	2.08	0.54
1:B:92:TRP:HA	1:B:96:VAL:O	2.07	0.53
1:B:107:ALA:HB2	3:B:569:HOH:O	2.09	0.52
1:B:31:MET:HG2	1:B:62:THR:HA	1.91	0.52
1:A:249:ASN:HD21	1:A:252:ASN:HB2	1.73	0.52
1:A:26:GLU:O	1:A:65:VAL:HA	2.11	0.50
1:A:70:LYS:HA	1:A:122:TYR:O	2.13	0.49
1:B:197:TRP:CE2	1:B:202:PRO:HG3	2.48	0.49
1:A:132:VAL:HG23	1:A:133:ARG:HG3	1.95	0.49
1:A:253:GLN:HA	1:A:253:GLN:OE1	2.13	0.48
1:B:168:VAL:HG12	1:B:169:ASN:O	2.13	0.48
1:C:40:ARG:HG3	1:C:42:ASP:OD1	2.14	0.48
1:B:70:LYS:HD3	1:B:121:LYS:HB3	1.95	0.47
1:A:74:ARG:NH1	1:A:149:GLU:OE2	2.44	0.47
1:B:222:ARG:HH21	1:B:303:LYS:HZ1	1.62	0.47
1:A:230:HIS:HB2	1:A:289:LEU:HB2	1.94	0.47
1:B:176:TYR:CG	1:B:181:LEU:HA	2.51	0.46
1:B:46:ASP:OD2	1:B:150:ILE:HD13	2.15	0.46
1:B:168:VAL:CG1	3:B:504:HOH:O	2.63	0.46
1:B:75:TYR:CD2	1:B:145:SER:HB2	2.52	0.44
1:A:218:LYS:HB2	1:A:306:PHE:HB2	1.99	0.44
1:B:253:GLN:HB2	1:B:257:ALA:CB	2.47	0.44
1:A:86:ASP:HA	1:A:87:ASP:HA	1.83	0.44
1:B:24:ARG:HG3	1:B:39:VAL:HG13	1.99	0.44
1:B:46:ASP:CG	1:B:150:ILE:HD13	2.38	0.44
1:B:250:TRP:O	1:B:280:TYR:OH	2.24	0.44
1:B:249:ASN:HB3	1:B:253:GLN:NE2	2.32	0.44
1:C:73:PRO:HD2	1:C:120:LYS:O	2.18	0.44
1:B:174:GLU:HG3	3:B:536:HOH:O	2.17	0.43
1:C:26:GLU:O	1:C:65:VAL:HA	2.18	0.43
1:A:92:TRP:HA	1:A:96:VAL:O	2.19	0.43
1:B:86:ASP:HA	1:B:87:ASP:HA	1.74	0.43
1:A:219:ILE:HA	1:A:304:ASN:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PRO:O	1:C:153:SER:HB3	2.20	0.42
1:A:152:PRO:HG2	1:A:155:GLN:HG2	2.02	0.42
1:B:39:VAL:CG1	1:B:40:ARG:N	2.82	0.42
1:B:83:THR:O	1:B:109:GLU:HA	2.20	0.42
1:B:50:GLY:O	1:B:134:ALA:HA	2.20	0.41
1:B:218:LYS:HA	1:B:271:TYR:O	2.20	0.41
1:A:194:ASN:OD1	1:A:287:LYS:HG2	2.21	0.41
1:B:168:VAL:HG13	3:B:504:HOH:O	2.18	0.41
1:A:255:LYS:O	1:A:256:GLU:C	2.59	0.41
1:C:231:THR:O	1:C:258:GLU:HA	2.21	0.41
1:B:249:ASN:HB3	1:B:253:GLN:HE21	1.86	0.41
1:C:25:GLY:O	1:C:39:VAL:HA	2.21	0.41
1:B:252:ASN:N	3:B:505:HOH:O	2.34	0.41
1:C:62:THR:HB	1:C:268:GLY:HA3	2.02	0.41
1:C:230:HIS:HA	1:C:259:ASN:O	2.22	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	289/291 (99%)	267 (92%)	20 (7%)	2 (1%)	22 11
1	B	283/291 (97%)	260 (92%)	23 (8%)	0	100 100
1	C	282/291 (97%)	259 (92%)	20 (7%)	3 (1%)	14 5
All	All	854/873 (98%)	786 (92%)	63 (7%)	5 (1%)	25 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	282	GLU
1	C	283	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	SER
1	A	225	GLU
1	C	107	ALA

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	256/256 (100%)	248 (97%)	8 (3%)	40	34
1	B	253/256 (99%)	248 (98%)	5 (2%)	55	51
1	C	253/256 (99%)	248 (98%)	5 (2%)	55	51
All	All	762/768 (99%)	744 (98%)	18 (2%)	49	43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	141	TRP
1	A	145	SER
1	A	160	ASP
1	A	198	ASP
1	A	200	ASP
1	A	290	TRP
1	A	296	LYS
1	B	56	GLN
1	B	130	GLN
1	B	141	TRP
1	B	290	TRP
1	B	296	LYS
1	C	141	TRP
1	C	185	ARG
1	C	206	LEU
1	C	282	GLU
1	C	290	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	GLN
1	B	259	ASN
1	C	113	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	291/291 (100%)	-0.25	4 (1%)	75	76	24, 37, 60, 95	0
1	B	287/291 (98%)	0.01	6 (2%)	63	65	29, 43, 67, 105	0
1	C	286/291 (98%)	-0.02	9 (3%)	49	52	28, 42, 66, 98	0
All	All	864/873 (98%)	-0.09	19 (2%)	62	64	24, 41, 65, 105	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	LEU	6.3
1	B	20	HIS	5.2
1	B	286	ILE	3.4
1	B	165	GLN	3.2
1	C	275	VAL	3.0
1	A	162	PRO	3.0
1	C	204	GLY	2.9
1	B	275	VAL	2.8
1	A	199	LYS	2.5
1	C	182	LYS	2.5
1	A	163	LEU	2.3
1	C	205	GLU	2.3
1	B	160	ASP	2.3
1	C	203	VAL	2.2
1	B	193	ILE	2.2
1	C	186	PHE	2.1
1	C	201	PHE	2.1
1	C	20	HIS	2.1
1	A	165	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	CA	C	401	1/1	0.98	0.07	37,37,37,37	0
2	CA	C	402	1/1	0.98	0.05	37,37,37,37	0
2	CA	B	402	1/1	0.99	0.04	40,40,40,40	0
2	CA	A	401	1/1	0.99	0.09	30,30,30,30	0
2	CA	B	401	1/1	0.99	0.06	34,34,34,34	0
2	CA	A	402	1/1	1.00	0.09	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.