



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:23 pm GMT

PDB ID : 2FH2
Title : C-terminal half of gelsolin soaked in EGTA at pH 4.5
Authors : Chumnarnsilpa, S.; Loonchanta, A.; Xue, B.; Choe, H.; Urosev, D.; Wang, H.;
Burtnick, L.D.; Robinson, R.C.
Deposited on : 2005-12-23
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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

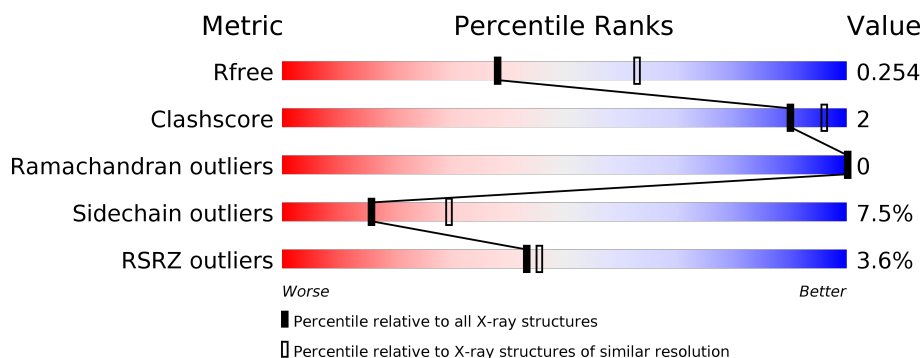
1 Overall quality at a glance

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	344	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>
1	B	344	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	C	344	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7835 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 Gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2485	1571	425	482	7			
1	B	324	Total	C	N	O	S	0	0	0
			2515	1587	433	489	6			
1	C	322	Total	C	N	O	S	0	0	0
			2495	1576	427	486	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		
2	C	2	Total	Ca	0	0
			2	2		

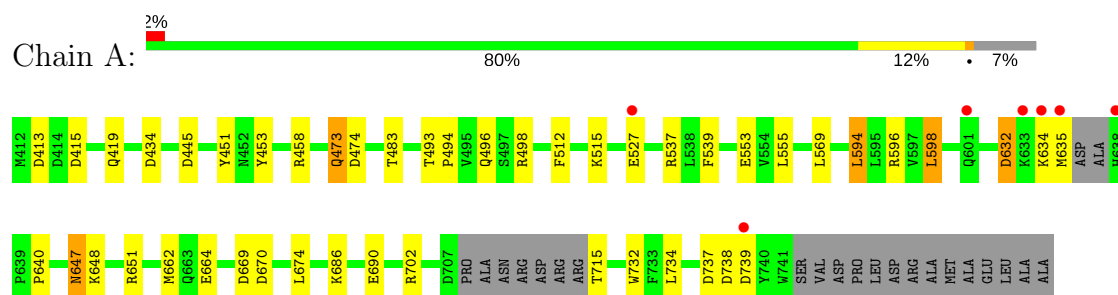
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	125	Total	O	0	0
			125	125		
3	C	73	Total	O	0	0
			73	73		

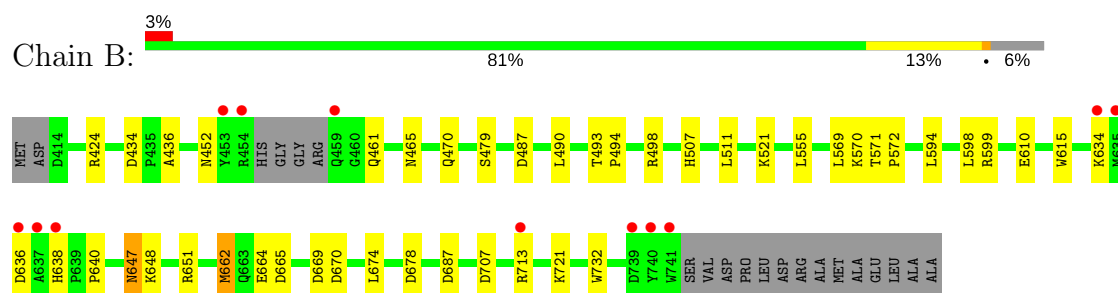
3 Residue-property plots [i](#)

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.

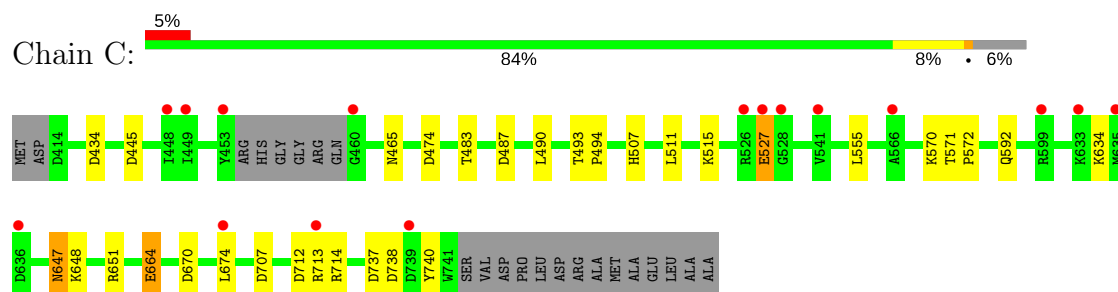
• Molecule 1: Gelsolin



• Molecule 1: Gelsolin



• Molecule 1: Gelsolin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.29Å 90.93Å 157.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.50 19.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.92-2.50) 99.5 (19.91-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.255 0.209 , 0.254	Depositor DCC
R_{free} test set	2165 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7835	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

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	0.57	0/2542	0.80	10/3447 (0.3%)
1	B	0.56	0/2573	0.81	9/3493 (0.3%)
1	C	0.51	0/2553	0.79	9/3467 (0.3%)
All	All	0.55	0/7668	0.80	28/10407 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	670	ASP	CB-CG-OD2	7.26	124.83	118.30
1	B	434	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	487	ASP	CB-CG-OD2	6.84	124.45	118.30
1	C	434	ASP	CB-CG-OD2	6.68	124.31	118.30
1	B	670	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	687	ASP	CB-CG-OD2	6.58	124.23	118.30
1	A	445	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	434	ASP	CB-CG-OD2	6.42	124.07	118.30
1	A	738	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	707	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	487	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	737	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	474	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	737	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	707	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	670	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	474	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	445	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	712	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	678	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	636	ASP	CB-CG-OD2	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	669	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	415	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	632	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	738	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	739	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	665	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2485	0	2405	12	0
1	B	2515	0	2437	12	0
1	C	2495	0	2416	8	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
3	A	134	0	0	2	0
3	B	125	0	0	2	0
3	C	73	0	0	0	0
All	All	7835	0	7258	31	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 2.

All (31) 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:647:ASN:HD22	1:B:647:ASN:C	1.98	0.67
1:B:465:ASN:ND2	1:B:479:SER:OG	2.32	0.63
1:A:715:THR:N	3:A:234:HOH:O	2.32	0.61
1:B:647:ASN:ND2	3:B:5072:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:MET:CE	1:A:734:LEU:HB3	2.37	0.55
1:A:647:ASN:C	1:A:647:ASN:HD22	2.12	0.52
1:B:493:THR:N	1:B:494:PRO:CD	2.72	0.52
1:A:483:THR:HG22	1:A:496:GLN:HE22	1.76	0.50
1:B:662:MET:HB3	1:B:664:GLU:OE1	2.12	0.50
1:B:507:HIS:HA	3:B:108:HOH:O	2.13	0.49
1:B:610:GLU:HG3	1:B:615:TRP:CZ2	2.48	0.48
1:C:571:THR:HG23	1:C:572:PRO:HD2	1.96	0.48
1:A:640:PRO:HG2	1:A:732:TRP:CZ3	2.51	0.46
1:C:571:THR:CG2	1:C:572:PRO:HD2	2.45	0.46
1:A:539:PHE:CE2	1:A:553:GLU:HB2	2.51	0.45
1:A:493:THR:N	1:A:494:PRO:CD	2.79	0.45
1:B:571:THR:HB	1:B:572:PRO:CD	2.46	0.45
1:B:436:ALA:HB2	1:C:527:GLU:HB3	1.99	0.45
1:C:664:GLU:HG2	1:C:740:TYR:OH	2.17	0.44
1:C:647:ASN:C	1:C:647:ASN:HD22	2.20	0.43
1:C:507:HIS:O	1:C:511:LEU:HD13	2.19	0.43
1:B:640:PRO:HG3	1:B:732:TRP:CE3	2.54	0.42
1:A:473:GLN:HB3	3:A:140:HOH:O	2.19	0.42
1:A:451:TYR:CE2	1:A:453:TYR:HB3	2.53	0.42
1:C:465:ASN:ND2	1:C:483:THR:OG1	2.37	0.42
1:A:512:PHE:O	1:A:515:LYS:HB2	2.20	0.41
1:C:493:THR:N	1:C:494:PRO:CD	2.82	0.41
1:B:647:ASN:ND2	1:B:647:ASN:C	2.68	0.41
1:A:640:PRO:HG2	1:A:732:TRP:CE3	2.56	0.41
1:B:452:ASN:ND2	1:B:461:GLN:HG2	2.36	0.40
1:A:594:LEU:HD22	1:A:598:LEU:HD22	2.03	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	315/344 (92%)	310 (98%)	5 (2%)	0	100	100
1	B	320/344 (93%)	313 (98%)	7 (2%)	0	100	100
1	C	318/344 (92%)	307 (96%)	11 (4%)	0	100	100
All	All	953/1032 (92%)	930 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	257/274 (94%)	234 (91%)	23 (9%)	11	22
1	B	260/274 (95%)	239 (92%)	21 (8%)	14	26
1	C	258/274 (94%)	244 (95%)	14 (5%)	26	47
All	All	775/822 (94%)	717 (92%)	58 (8%)	16	29

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	413	ASP
1	A	419	GLN
1	A	458	ARG
1	A	473	GLN
1	A	498	ARG
1	A	527	GLU
1	A	537	ARG
1	A	555	LEU
1	A	569	LEU
1	A	594	LEU
1	A	596	ARG
1	A	598	LEU
1	A	632	ASP
1	A	634	LYS
1	A	635	MET

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Mol	Chain	Res	Type
1	A	647	ASN
1	A	648	LYS
1	A	651	ARG
1	A	664	GLU
1	A	674	LEU
1	A	686	LYS
1	A	690	GLU
1	A	702	ARG
1	B	424	ARG
1	B	470	GLN
1	B	490	LEU
1	B	498	ARG
1	B	511	LEU
1	B	521	LYS
1	B	555	LEU
1	B	569	LEU
1	B	570	LYS
1	B	594	LEU
1	B	598	LEU
1	B	599	ARG
1	B	634	LYS
1	B	638	HIS
1	B	647	ASN
1	B	648	LYS
1	B	651	ARG
1	B	662	MET
1	B	674	LEU
1	B	713	ARG
1	B	721	LYS
1	C	490	LEU
1	C	515	LYS
1	C	527	GLU
1	C	555	LEU
1	C	570	LYS
1	C	592	GLN
1	C	634	LYS
1	C	647	ASN
1	C	648	LYS
1	C	651	ARG
1	C	664	GLU
1	C	674	LEU
1	C	713	ARG

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Mol	Chain	Res	Type
1	C	714	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	452	ASN
1	A	461	GLN
1	A	647	ASN
1	B	452	ASN
1	B	461	GLN
1	B	465	ASN
1	B	470	GLN
1	B	592	GLN
1	B	604	GLN
1	B	647	ASN
1	C	421	GLN
1	C	452	ASN
1	C	461	GLN
1	C	507	HIS
1	C	647	ASN
1	C	679	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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

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	321/344 (93%)	-0.17	7 (2%) 62 64	26, 35, 52, 81	0
1	B	324/344 (94%)	-0.09	12 (3%) 42 44	25, 36, 57, 76	0
1	C	322/344 (93%)	0.09	16 (4%) 30 31	31, 43, 58, 73	0
All	All	967/1032 (93%)	-0.06	35 (3%) 43 45	25, 39, 57, 81	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	635	MET	5.6
1	B	636	ASP	5.2
1	B	459	GLN	4.6
1	B	454	ARG	4.2
1	A	635	MET	4.2
1	C	453	TYR	4.2
1	B	741	TRP	3.9
1	B	739	ASP	3.8
1	A	638	HIS	3.7
1	B	637	ALA	3.6
1	C	713	ARG	3.4
1	A	633	LYS	3.4
1	C	636	ASP	3.2
1	C	599	ARG	3.1
1	B	638	HIS	3.0
1	A	634	LYS	2.9
1	C	527	GLU	2.8
1	B	713	ARG	2.8
1	B	634	LYS	2.7
1	A	739	ASP	2.7
1	B	453	TYR	2.6
1	C	449	ILE	2.5
1	B	635	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	528	GLY	2.5
1	C	448	ILE	2.5
1	A	601	GLN	2.4
1	C	526	ARG	2.3
1	B	740	TYR	2.3
1	C	674	LEU	2.2
1	C	633	LYS	2.1
1	C	739	ASP	2.1
1	A	527	GLU	2.1
1	C	541	VAL	2.1
1	C	460	GLY	2.0
1	C	566	ALA	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	CA	B	2002	1/1	0.98	0.05	-1.45	25,25,25,25	0
2	CA	B	2003	1/1	0.99	0.07	-2.09	35,35,35,35	0
2	CA	A	1001	1/1	0.99	0.04	-2.32	27,27,27,27	0
2	CA	B	2001	1/1	0.99	0.04	-3.32	27,27,27,27	0
2	CA	C	3002	1/1	0.99	0.05	-3.32	30,30,30,30	0
2	CA	A	1003	1/1	0.99	0.03	-4.79	26,26,26,26	0
2	CA	C	3001	1/1	0.99	0.02	-5.08	31,31,31,31	0
2	CA	A	1002	1/1	1.00	0.03	-5.33	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.