



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:33 AM UTC

PDB ID : 2FH1 / pdb_00002fh1
Title : C-terminal half of gelsolin soaked in low calcium 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 : 1.55 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
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

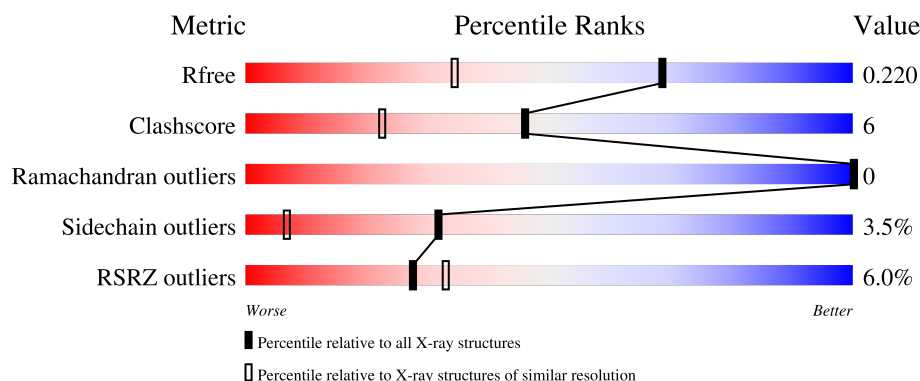
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	344	5% 82% 10% 7%
1	B	344	6% 84% 10% 6%
1	C	344	6% 86% 7% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8675 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
			2486	1571	425	483	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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total	O	0	0
			437	437		
3	B	416	Total	O	0	0
			416	416		
3	C	317	Total	O	0	0
			317	317		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.82Å 90.32Å 156.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.69 – 1.55 19.69 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.69-1.55) 99.7 (19.69-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.214 0.202 , 0.220	Depositor DCC
R_{free} test set	8728 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8675	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.98	3/2543 (0.1%)	0.88	0/3449
1	B	0.90	3/2573 (0.1%)	0.88	1/3493 (0.0%)
1	C	0.80	1/2553 (0.0%)	0.83	0/3467
All	All	0.90	7/7669 (0.1%)	0.86	1/10409 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	MET	SD-CE	-11.33	1.51	1.79
1	B	517	MET	SD-CE	-9.61	1.55	1.79
1	A	691	GLU	CD-OE2	8.41	1.41	1.25
1	B	662	MET	CG-SD	-5.85	1.66	1.80
1	C	517	MET	SD-CE	-5.42	1.66	1.79
1	A	644	ALA	CA-CB	-5.07	1.46	1.53
1	B	639	PRO	CA-C	5.02	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	610	GLU	CA-CB-CG	5.20	124.51	114.10

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	2486	0	2405	37	1
1	B	2515	0	2437	30	0
1	C	2495	0	2416	18	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	437	0	0	24	1
3	B	416	0	0	27	1
3	C	317	0	0	11	0
All	All	8675	0	7258	85	2

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 (85) 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:581:THR:HB	3:A:2423:HOH:O	1.06	1.20
1:B:648:LYS:HB3	3:B:3410:HOH:O	1.43	1.16
1:C:490:LEU:O	3:C:4314:HOH:O	1.62	1.14
1:B:720:VAL:HB	3:B:3417:HOH:O	1.48	1.11
1:C:490:LEU:C	3:C:4314:HOH:O	2.01	1.03
1:C:479:SER:HB2	3:C:4313:HOH:O	1.62	0.98
1:B:706:THR:HB	3:B:3414:HOH:O	1.68	0.92
1:B:658:PRO:C	3:B:3411:HOH:O	2.13	0.89
1:B:464:TYR:N	3:B:3402:HOH:O	2.06	0.88
1:A:609:SER:HB3	3:A:2425:HOH:O	1.75	0.87
1:A:465:ASN:OD1	1:A:483:THR:HG21	1.76	0.84
1:B:618:LEU:N	3:B:3408:HOH:O	2.09	0.83
1:A:609:SER:CB	3:A:2425:HOH:O	2.27	0.81
1:C:465:ASN:OD1	3:C:4313:HOH:O	2.00	0.80
1:B:446:SER:HB3	3:B:3400:HOH:O	1.83	0.79
1:A:568:VAL:O	3:A:2421:HOH:O	2.03	0.77
1:B:459:GLN:N	3:B:3219:HOH:O	2.17	0.77
1:A:461:GLN:NE2	3:A:2204:HOH:O	2.18	0.76
1:B:639:PRO:HD3	3:B:3409:HOH:O	1.87	0.75
1:B:562:ASN:ND2	3:B:3407:HOH:O	2.19	0.74
1:C:414:ASP:N	3:C:4310:HOH:O	2.21	0.71
1:A:609:SER:OG	3:A:2425:HOH:O	2.07	0.71
1:A:568:VAL:N	3:A:2421:HOH:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:GLY:O	3:B:3411:HOH:O	2.11	0.68
1:C:521:LYS:NZ	3:C:4315:HOH:O	2.18	0.67
1:A:472:THR:OG1	1:A:474:ASP:OD2	2.09	0.66
1:A:465:ASN:ND2	3:A:2100:HOH:O	2.27	0.66
1:B:616:GLU:C	3:B:3408:HOH:O	2.37	0.66
1:A:462:ILE:HG21	3:A:2416:HOH:O	1.96	0.65
1:B:463:ILE:C	3:B:3402:HOH:O	2.39	0.64
1:B:465:ASN:OD1	3:B:3403:HOH:O	2.14	0.64
1:A:462:ILE:CG2	3:A:2416:HOH:O	2.49	0.60
1:A:538:LEU:HD12	3:A:2421:HOH:O	2.02	0.59
1:B:647:ASN:HD22	1:B:647:ASN:C	2.09	0.59
1:A:581:THR:CB	3:A:2423:HOH:O	1.89	0.59
1:A:539:PHE:O	3:A:2421:HOH:O	2.16	0.58
1:A:678:ASP:CG	3:A:2201:HOH:O	2.46	0.58
1:A:465:ASN:CG	1:A:483:THR:HG21	2.31	0.56
1:A:647:ASN:C	1:A:647:ASN:HD22	2.12	0.56
1:A:638:HIS:N	3:A:2410:HOH:O	2.37	0.56
1:C:645:CYS:HB3	1:C:652:PHE:CZ	2.40	0.56
1:B:493:THR:HA	3:B:3404:HOH:O	2.06	0.55
1:C:647:ASN:C	1:C:647:ASN:HD22	2.15	0.54
1:B:562:ASN:CG	3:B:3407:HOH:O	2.50	0.53
1:B:446:SER:CB	3:B:3400:HOH:O	2.50	0.52
1:C:664:GLU:HG2	1:C:740:TYR:OH	2.10	0.52
1:B:526:ARG:HB3	3:B:3406:HOH:O	2.09	0.51
1:B:462:ILE:HG12	3:B:3402:HOH:O	2.10	0.51
1:A:720:VAL:HG12	3:B:3234:HOH:O	2.11	0.50
1:A:665:ASP:HB2	3:A:2432:HOH:O	2.13	0.49
1:A:479:SER:O	1:A:483:THR:HG23	2.12	0.48
1:B:564:ASN:HD21	1:B:635:MET:HE1	1.80	0.47
1:B:713:ARG:HD3	3:B:3416:HOH:O	2.14	0.46
1:A:539:PHE:CG	1:A:594:LEU:HD11	2.50	0.46
1:A:665:ASP:CB	3:A:2432:HOH:O	2.64	0.46
1:B:470:GLN:NE2	3:B:3341:HOH:O	2.48	0.46
1:A:504:GLU:HG2	1:A:517:MET:HE1	1.98	0.46
1:C:479:SER:CB	3:C:4313:HOH:O	2.40	0.46
1:C:718:THR:OG1	3:C:4319:HOH:O	2.21	0.46
1:A:461:GLN:HB2	3:A:2204:HOH:O	2.15	0.46
1:A:493:THR:N	1:A:494:PRO:CD	2.78	0.46
1:A:640:PRO:HG2	1:A:732:TRP:CE3	2.52	0.45
1:B:647:ASN:C	1:B:647:ASN:ND2	2.75	0.45
1:B:702:ARG:HB2	3:B:3412:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:ASP:N	3:B:3419:HOH:O	2.51	0.44
1:C:491:GLY:CA	3:C:4314:HOH:O	2.66	0.43
1:B:659:GLY:N	3:B:3411:HOH:O	2.44	0.43
1:C:572:PRO:HD3	3:C:4317:HOH:O	2.17	0.43
1:A:635:MET:HE3	3:A:2407:HOH:O	2.18	0.43
1:C:465:ASN:HD21	1:C:483:THR:CG2	2.32	0.43
1:A:488:GLU:HG3	3:A:2233:HOH:O	2.18	0.43
1:C:610:GLU:HG3	1:C:615:TRP:CZ2	2.54	0.43
1:A:465:ASN:ND2	1:A:483:THR:HG21	2.33	0.42
1:C:414:ASP:OD2	1:C:507:HIS:HE1	2.01	0.42
1:C:711:ARG:HB2	3:C:4252:HOH:O	2.19	0.42
1:C:464:TYR:OH	1:C:507:HIS:HD2	2.03	0.42
1:A:494:PRO:CG	3:A:2417:HOH:O	2.67	0.42
1:B:617:ALA:N	3:B:3408:HOH:O	2.53	0.41
1:B:485:GLN:CD	3:B:3178:HOH:O	2.63	0.41
1:B:610:GLU:CG	1:B:615:TRP:CZ2	3.03	0.41
1:A:451:TYR:CE2	1:A:453:TYR:HB3	2.55	0.41
1:A:648:LYS:HE3	3:A:2136:HOH:O	2.20	0.41
1:A:470:GLN:NE2	3:A:2206:HOH:O	2.53	0.40
1:A:589:THR:HA	1:A:592:GLN:HE21	1.87	0.40
1:A:494:PRO:HG2	3:A:2417:HOH:O	2.21	0.40

All (2) 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)
1:A:498:ARG:NH2	3:B:3110:HOH:O[1_455]	1.67	0.53
3:A:2413:HOH:O	3:A:2436:HOH:O[3_445]	1.77	0.43

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	315/344 (92%)	312 (99%)	3 (1%)	0	100	100
1	B	320/344 (93%)	317 (99%)	3 (1%)	0	100	100
1	C	318/344 (92%)	314 (99%)	4 (1%)	0	100	100
All	All	953/1032 (92%)	943 (99%)	10 (1%)	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%)	248 (96%)	9 (4%)	32	7
1	B	260/274 (95%)	252 (97%)	8 (3%)	35	8
1	C	258/274 (94%)	248 (96%)	10 (4%)	28	5
All	All	775/822 (94%)	748 (96%)	27 (4%)	32	7

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	465	ASN
1	A	511	LEU
1	A	527	GLU
1	A	569	LEU
1	A	594	LEU
1	A	598	LEU
1	A	647	ASN
1	A	678	ASP
1	B	454	ARG
1	B	474	ASP
1	B	515	LYS
1	B	555	LEU
1	B	557	LYS
1	B	610	GLU

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Mol	Chain	Res	Type
1	B	647	ASN
1	B	673	LEU
1	C	419	GLN
1	C	473	GLN
1	C	490	LEU
1	C	498	ARG
1	C	511	LEU
1	C	599	ARG
1	C	601	GLN
1	C	610	GLU
1	C	647	ASN
1	C	713	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	A	470	GLN
1	A	592	GLN
1	A	604	GLN
1	A	647	ASN
1	B	452	ASN
1	B	465	ASN
1	B	470	GLN
1	B	473	GLN
1	B	592	GLN
1	B	604	GLN
1	B	638	HIS
1	B	647	ASN
1	B	710	ASN
1	C	452	ASN
1	C	465	ASN
1	C	470	GLN
1	C	473	GLN
1	C	507	HIS
1	C	601	GLN
1	C	638	HIS
1	C	647	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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%)	0.30	18 (5%) 30 36	15, 21, 35, 50	0
1	B	324/344 (94%)	0.38	21 (6%) 25 29	14, 22, 35, 51	0
1	C	322/344 (93%)	0.61	19 (5%) 28 34	19, 27, 38, 48	0
All	All	967/1032 (93%)	0.43	58 (5%) 27 33	14, 23, 37, 51	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	635	MET	7.6
1	B	636	ASP	6.3
1	A	703	TYR	5.8
1	B	454	ARG	5.3
1	C	635	MET	5.1
1	B	635	MET	4.7
1	B	453	TYR	4.4
1	B	634	LYS	4.1
1	C	713	ARG	3.9
1	C	453	TYR	3.9
1	B	459	GLN	3.9
1	A	638	HIS	3.8
1	C	599	ARG	3.8
1	B	741	TRP	3.7
1	A	633	LYS	3.7
1	A	706	THR	3.5
1	C	528	GLY	3.4
1	A	412	MET	3.4
1	A	527	GLU	3.4
1	B	638	HIS	3.3
1	B	637	ALA	3.3
1	C	601	GLN	3.2
1	A	702	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	709	ALA	3.1
1	C	712	ASP	3.1
1	B	639	PRO	3.1
1	A	413	ASP	3.0
1	B	677	TRP	3.0
1	B	740	TYR	2.8
1	A	639	PRO	2.8
1	C	527	GLU	2.7
1	B	485	GLN	2.7
1	C	636	ASP	2.7
1	C	634	LYS	2.6
1	C	714	ARG	2.6
1	B	703	TYR	2.6
1	A	596	ARG	2.6
1	B	739	ASP	2.6
1	A	458	ARG	2.5
1	A	707	ASP	2.5
1	C	739	ASP	2.4
1	A	677	TRP	2.3
1	A	649	ILE	2.3
1	C	490	LEU	2.3
1	A	678	ASP	2.3
1	A	601	GLN	2.3
1	C	419	GLN	2.3
1	C	633	LYS	2.3
1	B	664	GLU	2.3
1	B	633	LYS	2.3
1	B	737	ASP	2.2
1	A	664	GLU	2.2
1	C	592	GLN	2.2
1	C	677	TRP	2.2
1	B	713	ARG	2.1
1	C	608	GLY	2.1
1	C	615	TRP	2.1
1	B	678	ASP	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 [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($\text{\AA}^2$)	Q<0.9
2	CA	C	4001	1/1	0.93	0.09	25,25,25,25	0
2	CA	C	4003	1/1	0.98	0.16	25,25,25,25	0
2	CA	B	3001	1/1	0.99	0.03	18,18,18,18	0
2	CA	B	3003	1/1	0.99	0.03	22,22,22,22	0
2	CA	A	2001	1/1	0.99	0.03	19,19,19,19	0
2	CA	C	4002	1/1	0.99	0.05	21,21,21,21	0
2	CA	A	2003	1/1	0.99	0.02	17,17,17,17	0
2	CA	A	2002	1/1	1.00	0.03	17,17,17,17	0
2	CA	B	3002	1/1	1.00	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.